

ID	Annotation	KEGG ID	'Mode	m/z	^RelArea ± std (×1000)														
					Liver			Aorta			Cardiac muscle			Plasma			Brain		
					HC	DL	DLS	HC	DL	DLS	HC	DL	DLS	HC	DL	DLS	HC	DL	DLS
<i>Amino acid</i>																			
AN_001	Gly	C00037	C	76.04	3079.1 ± 423.9	2758.8 ± 212.6	2383.9 ± 563.7	524.7 ± 22.9	1127.1 ± 63.1	1127.4 ± 197.2	487.5 ± 38.3	446.6 ± 81.5	395.9 ± 27.2	1730.5 ± 393.2	2046.3 ± 377.6	1523.0 ± 78.4	1052.7 ± 183.7	1150.8 ± 193.9	1218.7 ± 64.2
AN_002	Ala	C00041	C	90.05	902.5 ± 409.7	795.3 ± 220.9	1075.8 ± 691.0	447.8 ± 49.5	661.0 ± 73.9	590.8 ± 79.3	4129.6 ± 374.9	4367.7 ± 277.8	3856.0 ± 123.5	965.2 ± 158.5	970.3 ± 158.8	863.3 ± 37.5	1661.6 ± 204.4	1601.2 ± 406.7	1573.2 ± 94.9
AN_003	Ser	C00065	C	106.05	287.1 ± 54.0	440.7 ± 161.4	661.6 ± 304.3	233.6 ± 27.0	509.4 ± 73.5	424.2 ± 40.9	406.0 ± 79.0	431.5 ± 23.1	458.1 ± 59.2	857.3 ± 109.5	900.1 ± 150.3	714.2 ± 64.9	1342.3 ± 11.5	1330.2 ± 197.7	1329.2 ± 158.0
AN_004	Pro	C00017	C	116.07	968.0 ± 273.7	547.4 ± 141.9	441.0 ± 194.4	215.2 ± 19.5	474.2 ± 30.4	400.2 ± 31.0	414.4 ± 89.4	334.1 ± 48.4	348.3 ± 44.7	1509.8 ± 320.2	1306.5 ± 259.7	926.4 ± 78.1	276.8 ± 35.8	310.8 ± 26.7	268.7 ± 9.2
AN_005	Val	C00183	C	118.09	595.9 ± 159.9	530.8 ± 58.0	538.8 ± 188.9	274.7 ± 28.9	557.7 ± 53.6	494.1 ± 33.5	270.9 ± 62.1	246.1 ± 32.1	249.6 ± 50.9	2142.2 ± 271.5	2101.6 ± 83.3	1807.3 ± 233.1	370.4 ± 56.2	383.9 ± 63.5	339.4 ± 37.4
AN_006	Thr	C00188	C	120.05	503.7 ± 65.6	460.7 ± 63.3	479.8 ± 202.2	146.5 ± 21.8	349.7 ± 21.9	289.1 ± 18.8	235.9 ± 15.0	209.1 ± 17.1	196.8 ± 4.4	676.1 ± 189.3	680.8 ± 92.0	469.8 ± 28.6	475.1 ± 97.8	487.8 ± 86.9	425.7 ± 39.4
AN_007	Cys	C00097	C	122.03	37.9 ± 15.9	9.7 ± 15.2	19.5 ± 16.1				8.0 ± 2.9	4.1 ± 1.4	4.4 ± 0.1	0.5 ± 0.3	0.5 ± 0.2	0.7 ± 0.1	140.2 ± 45.3	112.0 ± 49.4	79.4 ± 14.7
AN_008	Ile	C00407	C	132.10	397.2 ± 125.7	338.0 ± 44.3	349.4 ± 130.8	169.5 ± 21.7	367.3 ± 42.6	330.1 ± 3.5	160.2 ± 42.7	129.8 ± 23.2	146.1 ± 34.1	994.1 ± 144.7	981.0 ± 68.6	901.2 ± 138.5	205.5 ± 30.5	204.8 ± 40.9	190.1 ± 17.3
AN_009	Leu	C00123	C	132.10	765.1 ± 201.4	664.6 ± 81.1	695.3 ± 250.1	476.0 ± 72.0	789.2 ± 156.9	659.3 ± 25.1	367.3 ± 76.8	330.2 ± 55.8	355.1 ± 66.4	1852.6 ± 298.1	1800.7 ± 153.1	1715.4 ± 262.9	482.8 ± 67.4	466.2 ± 112.5	430.4 ± 40.8
AN_010	Asn	C00152	C	133.06	215.4 ± 17.8	177.1 ± 35.3	210.5 ± 48.3	64.3 ± 13.2	167.4 ± 13.4	166.1 ± 17.2	330.0 ± 23.4	298.8 ± 41.1	362.5 ± 33.9	170.6 ± 46.0	186.2 ± 17.2	149.5 ± 4.5	103.1 ± 28.7	135.4 ± 15.9	134.2 ± 2.1
AN_011	Asp	C00049	C	134.04	841.7 ± 338.1	624.5 ± 36.0	906.8 ± 307.1	334.6 ± 90.4	471.0 ± 48.2	556.3 ± 72.4	367.2 ± 54.6	375.1 ± 79.4	317.7 ± 44.7	31.0 ± 1.9	29.5 ± 9.0	23.0 ± 1.4	3270.2 ± 462.9	3401.2 ± 667.3	3352.0 ± 394.0
AN_012	Gln	C00064	C	147.08	2795.2 ± 688.9	2464.1 ± 210.9	2223.7 ± 624.7	487.7 ± 57.9	689.0 ± 161.3	647.9 ± 94.8	>5000 <sup>3</sup>	>5000 <sup>3</sup>	>5000 <sup>3</sup>	2249.8 ± 262.8	2354.4 ± 53.0	2027.8 ± 105.5	>5000 <sup>3</sup>	>5000 <sup>3</sup>	>5000 <sup>3</sup>
AN_013	Lys	C00047	C	147.11	558.8 ± 149.4	400.3 ± 41.2	423.5 ± 113.6	163.4 ± 13.2	423.2 ± 40.6	401.6 ± 64.4	268.9 ± 13.0	286.3 ± 41.6	92.96 ± 308.2	876.2 ± 29.2	626.6 ± 58.5	288.5 ± 17.5	292.6 ± 8.8	273.9 ± 11.6	
AN_014	Glu	C00025	C	148.06	3762.9 ± 204.2	4199.0 ± 326.7	4269.8 ± 950.7	1261.1 ± 164.9	2239.2 ± 51.5	2467.1 ± 377.1	2516.4 ± 793.7	3454.5 ± 477.7	2603.2 ± 358.9	156.9 ± 3.4	150.5 ± 20.8	87.1 ± 6.6	>5000 <sup>3</sup>	>5000 <sup>3</sup>	>5000 <sup>3</sup>
AN_015	Met	C00073	C	150.06	38.7 ± 7.2	37.8 ± 9.3	46.1 ± 20.5	116.9 ± 12.3	154.6 ± 29.0	106.6 ± 4.1	57.4 ± 6.3	71.3 ± 10.2	62.5 ± 12.3	257.9 ± 51.4	287.5 ± 89.3	211.8 ± 60.3	86.7 ± 24.0	77.1 ± 68.2	85.1 ± 17.7
AN_016	His	C00135	C	156.08	991.8 ± 277.4	830.5 ± 56.8	802.2 ± 217.7	100.2 ± 16.1	232.7 ± 21.2	231.3 ± 46.6	959.5 ± 80.7	933.7 ± 45.2	957.6 ± 50.3	691.4 ± 89.6	689.5 ± 86.3	641.0 ± 52.9	369.9 ± 54.3	360.0 ± 72.6	369.9 ± 38.3
AN_017	Phe	C00079	C	166.09	172.6 ± 23.9	164.1 ± 18.7	156.2 ± 43.2	126.1 ± 13.1	234.4 ± 40.9	192.9 ± 8.8	183.7 ± 13.3	174.1 ± 18.0	164.4 ± 19.4	520.4 ± 45.5	517.1 ± 41.4	465.4 ± 29.6	209.6 ± 26.6	205.7 ± 40.3	192.3 ± 17.0
AN_018	Arg	C00062	C	175.12	18.4 ± 10.6	9.9 ± 2.9	14.3 ± 3.1	197.7 ± 18.7	424.1 ± 31.5	348.1 ± 28.7	537.4 ± 77.3	583.4 ± 47.8	461.5 ± 41.1	1043.9 ± 189.0	955.5 ± 131.6	662.3 ± 48.1	318.2 ± 64.5	381.1 ± 27.6	320.8 ± 36.0
AN_019	Tyr	C00082	C	182.08	156.4 ± 55.9	130.0 ± 21.2	131.1 ± 58.1	121.7 ± 11.1	206.8 ± 32.0	168.5 ± 9.0	116.2 ± 8.3	104.3 ± 9.6	87.1 ± 11.6	396.9 ± 125.0	383.5 ± 37.9	280.5 ± 20.2	144.4 ± 17.2	151.7 ± 10.7	119.4 ± 12.3
AN_020	Trp	C00078	C	205.10	32.5 ± 3.7	31.9 ± 2.0	25.2 ± 3.4	24.1 ± 2.0	45.6 ± 2.2	41.0 ± 1.0	42.0 ± 2.2	31.9 ± 7.1	33.8 ± 2.9	330.7 ± 54.5	314.3 ± 22.2	262.1 ± 26.9	34.3 ± 4.2	34.6 ± 4.6	30.6 ± 3.0
AN_021	β-Ala	C00099	C	90.05	107.7 ± 38.3	118.1 ± 17.8	74.6 ± 29.8	15.2 ± 3.6	37.1 ± 9.5	44.9 ± 12.0	11.7 ± 0.7	13.6 ± 3.0	13.1 ± 1.2	10.0 ± 0.7	10.3 ± 1.7	10.3 ± 0.3	73.9 ± 10.2	83.7 ± 12.1	82.7 ± 10.0
AN_022	α-Aminobutyric acid	C02356	C	104.07	17.8 ± 3.0	23.4 ± 3.9	16.8 ± 5.2	3.7 ± 0.2	14.9 ± 2.8	10.4 ± 1.2	5.1 ± 1.3	6.5 ± 0.1	4.5 ± 1.0	31.1 ± 4.9	30.9 ± 6.6	20.0 ± 2.9	10.2 ± 4.2	13.8 ± 2.5	10.3 ± 1.6
AN_023	2,3-Diaminopropionic acid	C03401	C	105.06	0.9 ± 0.2	1.0 ± 0.2	0.8 ± 0.2												
AN_024	2-Methylserine	C02115	C	120.07	1.3 ± 0.6	1.0 ± 0.2	0.9 ± 0.3										5.8 ± 0.4	5.5 ± 0.6	5.5 ± 0.4
AN_025	Homoserine	C00263	C	120.07</td															

**Supplementary Material (ESI) for Molecular BioSystems**  
**This journal is (c) The Royal Society of Chemistry, 2011**

AN_083	Choline	C00114	C	104.11	1337.1 ± 244.5	1217.5 ± 146.4	1350.9 ± 370.8	997.1 ± 141.6	1590.4 ± 54.7	1592.1 ± 197.5	414.2 ± 120.6	348.0 ± 32.8	506.1 ± 189.7	205.1 ± 12.2	204.5 ± 12.1	178.0 ± 23.9	1972.8 ± 320.4	1979.3 ± 437.0	1740.1 ± 173.4	
AN_084	Betaine aldehyde	C00576	C	102.09	8.9 ± 6.1	6.3 ± 2.6	11.9 ± 1.6										333.6 ± 120.7	317.7 ± 88.5		
AN_085	Glycine betaine	C00719	C	118.09	259.2 ± 73.6	958.2 ± 237.1	466.7 ± 171.7	115.1 ± 10.2	446.3 ± 154.5	226.5 ± 21.5	994.9 ± 665.1	2785.6 ± 884.3	1975.9 ± 258.1	1916.2 ± 1079.0	1874.2 ± 1026.9	1189.5 ± 357.5	319.6 ± 26.8			
AN_086	N,N-Dimethylglycine	C01026	C	104.07	11.9 ± 1.6	60.6 ± 14.8	29.3 ± 12.3				1.7 ± 0.3	5.5 ± 0.7	3.0 ± 0.9	16.2 ± 13.1	23.8 ± 16.4	14.6 ± 4.6				
AN_087	Sarcosine	C00213	C	90.05	44.6 ± 1.9	81.9 ± 20.4	55.0 ± 30.9	4.3 ± 1.4	11.2 ± 1.8	8.7 ± 0.9	4.8 ± 1.7	6.0 ± 0.2	4.0 ± 1.3	26.2 ± 1.9	24.4 ± 7.3	18.0 ± 5.1	1.3 ± 0.3	1.6 ± 0.1	1.4 ± 0.5	
AN_088	S-Adenosylhomocysteine	C00021	C	385.13	33.8 ± 5.6	28.3 ± 0.6	31.3 ± 11.7	3.9 ± 0.4	5.0 ± 0.3	4.4 ± 0.5	2.6 ± 0.4	2.3 ± 0.4	1.9 ± 0.2				5.0 ± 0.6	5.6 ± 0.3	4.4 ± 0.7	
AN_089	S-adenosylmethionine	C00019	C	399.14	10.9 ± 7.0	10.2 ± 3.9	6.9 ± 2.3				26.3 ± 1.9	29.7 ± 1.3	24.6 ± 4.3	0.3 ± 0.1	0.3 ± 0.1	0.3 ± 0.0	15.6 ± 2.3	19.8 ± 0.3	18.4 ± 0.9	
AN_090	Glyceric acid	C00258	A	105.02	6.7 ± 4.7	5.7 ± 1.2	5.1 ± 1.2	3.0 ± 1.3	4.1 ± 1.8	2.1 ± 0.3	5.0 ± 1.5	4.0 ± 0.6	4.0 ± 0.6	16.6 ± 3.1	15.8 ± 2.9	4.0 ± 0.7	3.4 ± 0.9	4.2 ± 1.8		
AN_091	Glycerol 3-phosphate	C00093	A	171.01	1486.9 ± 552.1	1501.4 ± 211.0	1077.7 ± 418.1	109.4 ± 51.3	114.8 ± 62.7	188.7 ± 62.7	718.9 ± 66.1	913.0 ± 249.8	749.9 ± 142.7	14.3 ± 2.4	12.8 ± 1.5	12.6 ± 1.6	67.6 ± 6.9	82.4 ± 31.6	106.1 ± 92.9	
AN_092	Triethanolamine	C06771	C	150.11						3.6 ± 0.8	4.4 ± 1.4	3.8 ± 0.7								
AN_093	Diethanolamine	C06772	C	106.09	6.8 ± 2.4	6.0 ± 2.8	4.6 ± 0.4	1.9 ± 0.0	2.2 ± 0.6	2.1 ± 0.2						2.4 ± 0.4	2.9 ± 0.3	3.0 ± 0.7		
AN_094	Ethanolamine phosphate	C00346	A	140.01	123.2 ± 35.2	121.4 ± 31.5	153.8 ± 43.7	164.3 ± 37.6	166.7 ± 10.0	186.1 ± 40.6	166.8 ± 17.3	189.5 ± 17.4	161.1 ± 12.4	10.5 ± 1.7	11.1 ± 3.6	9.6 ± 1.6	952.5 ± 132.6	972.1 ± 167.6	1053.4 ± 158.5	
AN_095	Adipic acid	C06104	A	145.05	2.3 ± 0.1	3.0 ± 1.1	2.1 ± 0.6	0.4 ± 0.0	0.4 ± 0.0	0.8 ± 0.1	0.6 ± 0.1	0.7 ± 0.1								
AN_096	Prostaglandin F2 $\alpha$	C00639	A	353.23													3.6 ± 1.0	3.5 ± 1.4	4.1 ± 0.5	
AN_097	O-Acetyl carnitine	C02571	C	204.12	103.9 ± 61.5	140.8 ± 100.1	134.5 ± 75.9	108.2 ± 37.2	152.0 ± 20.5	148.5 ± 22.2	1149.0 ± 799.2	2077.1 ± 355.1	2040.2 ± 522.6	198.0 ± 44.4	184.3 ± 27.7	155.9 ± 30.1	47.8 ± 15.3	67.8 ± 21.8	53.7 ± 8.6	
AN_098	Propionic acid	C00163	A	73.03	8.2 ± 1.2	7.8 ± 3.7	5.6 ± 1.4				2.1 ± 0.6	2.1 ± 0.2	2.5 ± 0.4	7.8 ± 3.2	7.7 ± 2.1	8.4 ± 1.9	3.6 ± 0.2	3.9 ± 0.2	3.8 ± 0.9	
AN_099	Butanoic acid	C00246	A	87.05	2.6 ± 0.9	4.2 ± 3.4	2.2 ± 0.6	0.3 ± 0.0	0.4 ± 0.1	0.4 ± 0.0			33.7 ± 19.3	30.9 ± 19.2	23.2 ± 4.5					
AN_100	Pentanoic acid	C00803	A	101.06	4.1 ± 0.7	6.6 ± 2.2	3.1 ± 0.9						20.0 ± 8.3	22.6 ± 4.4	23.7 ± 3.8					
AN_101	Hexanoic acid	C01585	A	115.08	4.7 ± 1.1	4.4 ± 1.7	3.8 ± 1.2	0.7 ± 0.2	0.9 ± 0.2	1.2 ± 0.2	4.6 ± 1.8	2.2 ± 0.2	3.6 ± 0.4	18.3 ± 5.2	20.5 ± 2.8	28.0 ± 1.9	2.5 ± 0.3	2.8 ± 0.5	3.0 ± 0.5	
AN_102	Heptanoic acid	C00002	A	129.09						0.3 ± 0.1	0.4 ± 0.1			12.6 ± 3.0	13.3 ± 1.2	15.5 ± 0.3				
AN_103	Octanoic acid	C06423	A	143.11						0.7 ± 0.2	0.7 ± 0.3	1.1 ± 0.3	3.2 ± 0.8	2.6	2.8 ± 0.5	11.1 ± 0.7	11.0 ± 0.5	11.8 ± 0.5		
AN_104	Pelargonic acid	C01601	A	157.12	4.6 ± 0.3	4.2 ± 0.2	3.7 ± 0.5				2.3 ± 0.2	1.8 ± 0.4	2.6 ± 0.5	19.2 ± 3.5	20.4 ± 2.9	21.0 ± 0.4	5.7 ± 0.8	6.0 ± 1.7	6.2 ± 1.8	
AN_105	Undecanoic acid	C00004	A	185.15									3.3 ± 0.2	3.4 ± 0.8	3.8 ± 0.4					
AN_106	10-Hydroxydecanoic acid	C02774	A	187.13						0.4 ± 0.1	0.5 ± 0.0	0.4 ± 0.0	2.1 ± 1.5	1.2 ± 0.2	1.5 ± 0.1					
AN_107	Lauric acid	C02679	A	199.17	9.1 ± 1.8	9.9 ± 1.6	11.0 ± 3.1								25.8 ± 2.2	27.9 ± 4.8	23.9 ± 0.5	13.4 ± 0.5	16.2 ± 2.1	14.5 ± 1.9
<i>Nucleotide metabolism</i>																				
AN_108	Adenine	C00147	C	136.06	19.4 ± 2.4	12.9 ± 1.1	15.0 ± 7.5	1.9 ± 1.5	1.4 ± 0.1	2.2 ± 0.7	47.0 ± 2.2	49.0 ± 5.7	58.9 ± 14.7				11.6 ± 4.4	10.8 ± 3.5	12.7 ± 0.7	
AN_109	Adenosine	C00212	C	268.10	19.6 ± 2.9	10.7 ± 1.9	15.7 ± 2.6	3.5 ± 1.6	7.8 ± 4.0	69.5 ± 53.8	314.1 ± 462.7	276.9 ± 314.0	504.1 ± 421.7				30.0 ± 21.4	60.1 ± 10.5	175.2 ± 132.3	
AN_110	AMP	C00020	A	346.06	10.7 ± 3.5	8.1 ± 2.9	10.4 ± 3.4	1.3 ± 0.4	3.3 ± 4.4	3.5 ± 1.8	1470.8 ± 90.1	1635.7 ± 153.1	1172.1 ± 541.7	1.1 ± 0.4	1.1 ± 0.4	0.8 ± 0.1	11.4 ± 2.9	14.4 ± 1.3	20.7 ± 7.8	
AN_111	ADP	C00008	A	426.02	103.9 ± 22.3	82.1 ± 28.6	103.6 ± 32.2	90.2 ± 78.1	34.3 ± 8.4	33.6 ± 13.4	296.3 ± 52.6	292.9 ± 30.9	253.7 ± 20.3				176.8 ± 62.8	183.5 ± 24.8	239.5 ± 92.5	
AN_112	ATP	C00002	A	505.99	9.8 ± 2.6	7.6 ± 5.0	11.8 ± 5.0	4.4 ± 0.6	2.6 ± 1.2	2.0 ± 0.3	68.1 ± 57.9	27.1 ± 9.8	21.2 ± 1.8				39.2 ± 26.3	39.7 ± 7.9	73.7 ± 51.3	
AN_113	cAMP	C00575	A	328.05	3.2	2.9	2.8 ± 0.8				7.0 ± 0.8	5.9 ± 0.7	5.3 ± 0.7							
AN_114	Adenylosuccinic acid	C03794	A	462.07	53.9 ± 27.7	28.2 ± 7.1	25.5 ± 11.6				33.5 ± 8.5	65.1 ± 6.8	42.4 ± 13.3				53.8 ± 7.9	49.9 ± 17.9	53.6 ± 4.2	
AN_115	Guanine	C00242	C	152.06	1.7 ± 0.2	1.7 ± 0.5	2.0 ± 0.7				4.6 ± 1.1	6.2 ± 1.2	6.0 ± 0.8	2.3 ± 1.1	2.9 ± 1.2					

<sup>1</sup> Peaks were detected in CE-TOF MS measurement for cation mode (C) or anion mode (A).

<sup>2</sup> Raw area values of each sample were normalized (see Experimental Procedures) and standard deviations (SDs) were calculated ( $n=3$ ).

<sup>3</sup> Peaks could not be quantified because of saturated values in detection.

DL: untreated Watanabe heritable hyperlipidemic rabbits; DLS: simvastatin-treated Watanabe heritable hyperlipidemic rabbits; HC: Japanese white healthy control rabbits