Table S1. ^{1}H NMR chemical shifts for metabolites assigned in liver extracts and serum.

key	metabolites	moieties	δ ^{1}H (ppm) and multiplicity[a]	Samples[b]
1	Lipid	CH_3, $(CH_2)_n$, CH_2-C=C, CH_2-C=O,C-CH_2-C=,-CH=CH-	0.89(m), 1.27(m), 2.0(m), 2.3(m), 2.78(m), 5.3(m)	L, S
2	Isoleucine	αCH, βCH, γCH_3, δCH_3	3.65(d), 1.95(m), 0.99(t), 1.02(d)	L, S
3	Leucine	αCH, βCH_2, γCH_3, δCH_3	0.94(d), 3.72(t), 1.96(m), 0.91(d)	L, S
4	Valine	αCH, βCH, γCH_3	3.6(d), 2.26(m), 0.98(d), 1.04(d)	L, S
5	D-3-hydroxybutyrate	CH, CH_2, γCH_3, CH_2	4.16(dt),2.41(dd),1.20(d),2.31(dd)	L, S
6	Lactate	αCH, βCH_3	4.11(q), 1.32(d)	L, S
7	Alanine	αCH, βCH_3	3.77(q), 1.48(d)	L, S
8	Acetate	CH_3	1.91(s)	L, S
9	HDL	CH_3	0.82(m)	S
10	LDL	CH_3	0.85(m)	S
11	VLDL	CH_3	0.88(m)	S
12	Glutamate	αCH, βCH_2, γCH_2	2.08(m), 2.34(m), 3.75(m)	L, S
13	Glutamine	αCH, βCH_2, γCH_2	2.15(m), 2.44(m), 3.77(m)	L, S
14	Glutathione	CH_2, CH_2, S-CH_2, N-CH, CH	2.16(m), 2.55(m), 2.95(dd), 3.78(m), 4.56(q)	L
15	*N*-acetyl-glycoproteins	CH_3	2.04(S)	S
16	*O*-acetyl-glycoproteins	CH_3	2.14(S)	S
17	Acetoacetate	CH_3	2.26(S)	S
18	Choline	$N(CH_3)_3$, OCH_2, NCH_2	3.2(s), 4.05(t), 3.51(t)	L, S
19	Phosphocholine(PC)	$N(CH_3)_3$, OCH_2, NCH_2	3.22(s), 4.21(t), 3.61(t)	L, S
20	Glycerophosphocholine	$N(CH_3)_3$, OCH_2, NCH_2	3.22(s), 4.32(t), 3.68(t)	L, S
21	β-Glucose	1-CH	4.66(d)	L, S
22	α-Glucose	1-CH	5.23(d)	L, S

23	Unsaturated fatty acid	CH=CH	5.3(m)	L, S
24	TMAO	CH_3	3.27(s)	L
25	Tyrosine	CH, CH	6.89(dd), 7.18(dd)	L, S
26	Histidine	2-CH, 4-CH, CH_2	7.75(t), 7.08(d), 6.05(d)	L, S
27	Phenylalanine	Ring-CH	7.40(m), 7.33(m), 7.35(m)	L, S
28	Formate	CH	8.45(s)	L, S
29	Betaine	CH_2, CH_3	3.27(s), 3.93(s)	L
30	Glycogen	1-CH	5.38-5.45(m)	L
31	Bile acid	CH_3	0.73(m)	L
32	Lysine	αCH, βCH_2, γCH_2, δCH_2	3.76(t), 1.89(m), 1.72(m), 3.01(t)	L, S
33	N-acetyl aspartate	CH_3	2.01(s)	L
34	PUFA	CH_3	2.73(m)	S
35	Succinate	CH_3	2.41(s)	L, S
36	Taurine	S-CH_2, N-CH_2	3.26(t), 3.40(t)	L
37	Glycine	CH_2	3.57(s)	L, S
38	Inosine	14-CH, 1-CH, 8-CH, 4'-CH, 5'-CH, CH_2(1/2), CH_2(1/2)	8.34(s), 6.09(d), 8.22(s), 4.76(t), 4.47(m)	L
39	Uridine	11-CH, 7-CH, 12-CH, 6-CH, 5-CH, 4-CH, CH_2, CH_2	7.88(d), 5.92(d), 5.9(d), 4.36(m), 4.24(t)	L
40	Fumarate	CH	6.53(s)	L, S
41	Nicotinurate	2-CH, 6-CH, 4-CH, 5-CH	8.93(s),8.62(d), 8.25(d),7.60(dd),	L
42	Adenosine	14-CH	8.32(s)	L, C
43	Uracil	1-CH, 2-CH	5.81(d), 7.54(d)	L
44	Citrate	CH_2(1/2), CH_2(1/2)	2.55(d), 2.65(d)	S
45	Creatine	CH_2, CH_3	3.03(s), 3.92(s)	S
46	Glucose & amino acids	αCH resonances	3.3-3.9	L, S

47	Pyruvate	CH_3	2.38(s)	S
48	Triglycerides	CH	4.08(m), 4.21(m), 5.18(m)	S

[a] Key: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doublet of doublet.
[b] Liver aqueous extracts (L) and serum (S).