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

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| key | metabolites | moieties | δ 1H (ppm) and multiplicitya | Samplesb |
| 1 | Lipid | CH3, (CH2)n, CH2-C=C, CH2-C=O,C-CH2-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, γCH3, δCH3 | 3.65(d), 1.95(m), 0.99(t), 1.02(d) | L, S |
| 3 | Leucine | αCH, βCH2, γCH3, δCH3 | 0.94(d), 3.72(t), 1.96(m), 0.91(d) | L, S |
| 4 | Valine | αCH, βCH, γCH3 | 3.6(d), 2.26(m), 0.98(d), 1.04(d) | L, S |
| 5 | D-3-hydroxybutyrate | CH, CH2, γCH3, CH2 | 4.16(dt),2.41(dd),1.20(d),2.31(dd) | L, S |
| 6 | Lactate | αCH, βCH3 | 4.11(q), 1.32(d) | L, S |
| 7 | Alanine | αCH, βCH3 | 3.77(q), 1.48(d) | L, S |
| 8  9  10  11 | Acetate  HDL  LDL  VLDL | CH3  CH3  CH3  CH3 | 1.91(s)  0.82(m)  0.85(m)  0.88(m) | L, S  S  S  S |
| 12 | Glutamate | αCH, βCH2, γCH2 | 2.08(m), 2.34(m), 3.75(m) | L, S |
| 13 | Glutamine | αCH, βCH2, γCH2 | 2.15(m), 2.44(m), 3.77(m) | L, S |
| 14 | Glutathione | CH2, CH2, S-CH2, N-CH, CH | 2.16(m), 2.55(m), 2.95(dd), 3.78(m), 4.56(q) | L |
| 15  16  17 | *N*-acetyl-glycoproteins *O*-acetyl-glycoproteins  Acetoacetate | CH3  CH3  CH3 | 2.04(S)  2.14(S)  2.26(S) | S  S  S |
| 18 | Choline | N(CH3)3, OCH2, NCH2 | 3.2(s), 4.05(t), 3.51(t) | L, S |
| 19 | Phosphocholine(PC) | N(CH3)3, OCH2, NCH2 | 3.22(s), 4.21(t), 3.61(t) | L, S |
| 20 | Glycerophosphocholine | N(CH3)3, OCH2, NCH2 | 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 | CH3 | 3.27(s) | L |
| 25 | Tyrosine | CH, CH | 6.89(dd), 7.18(dd) | L, S |
| 26 | Histidine | 2-CH, 4-CH, CH2 | 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 | CH2, CH3 | 3.27(s), 3.93(s) | L |
| 30 | Glycogen | 1-CH | 5.38-5.45(m) | L |
| 31 | Bile acid | CH3 | 0.73(m) | L |
| 32 | Lysine | αCH, βCH2, γCH2, δCH2 | 3.76(t), 1.89(m), 1.72(m), 3.01(t) | L, S |
| 33 | N-acetyl aspartate | CH3 | 2.01(s) | L |
| 34 | PUFA | CH3 | 2.73(m) | S |
| 35 | Succinate | CH3 | 2.41(s) | L, S |
| 36 | Taurine | S-CH2, N-CH2 | 3.26(t), 3.40(t) | L |
| 37 | Glycine | CH2 | 3.57(s) | L, S |
| 38 | Inosine | 14-CH, 1-CH, 8-CH, 4’-CH,  5’-CH, CH2(1/2), CH2(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, CH2, CH2 | 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  44  45 | Uracil  Citrate  Creatine | 1-CH, 2-CH  CH2(1/2), CH2(1/2)  CH2, CH3 | 5.81(d), 7.54(d)  2.55(d), 2.65(d)  3.03(s), 3.92(s) | L  S  S |
| 46 | Glucose & amino acids | αCH resonances | 3.3-3.9 | L, S |
| 47 | Pyruvate | CH3 | 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).