Electronic Supplementary Material (ESI) for Molecular BioSystems.

Figure S1 Permutation test plots (200 permutations) for all the biological matrices: a) Plasma (3rd week); b) urine (b1 (2nd week) b2 (3rd week)).

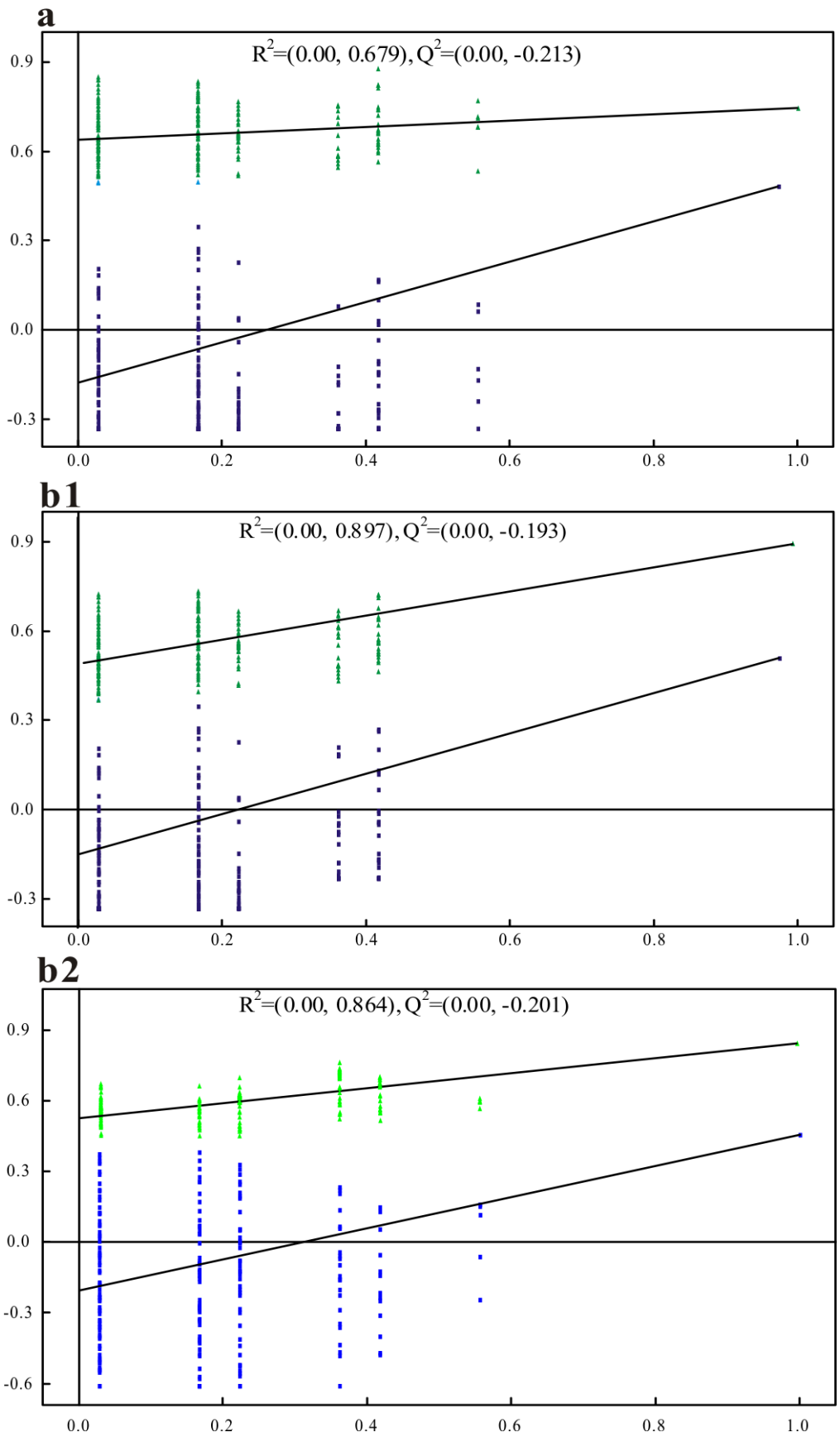

Table S1

^{1}H NMR data and assignments of the metabolites in plasma.

key	metabolites	δ^{1}H (ppm) and multiplicity
1,2	HDL, LDL	0.84(t), 1.25(m)
3	VLDL	0.87(t), 1.57(m)
4	isoleucine	0.94(t)
5	leucine	0.97(d)
6	valine	1.05(d)
7	lactate	1.33(d), 4.20(q)
8	alanine	1.48(d)
9	acetate	1.92(s)
10	N-acetylglyprotein	2.04(s)
11	O-acetylglyprotein	2.14(s)
12	acetate	2.23(s)
13	acetoacetate	2.27(s), 3.49(s)
14	pyruvate	2.38(s)
15	glutamine	2.44(m), 3.76(m)
16,17	creatine,creatinine	3.04(s)
18	choline	3.19(s)
19,20	GPC,PC	3.23(s)
21	taurine	3.25(t),3.41(t)
22,23	TMAO,betaine	3.26(s)
24	glycine	3.54(s)
25	glycerol	3.64(t), 3.87(m)
26,27	α-glucose, β-glucose	3.3-3.9, 5.20(d), 5.25(d)
28	unsaturated lipid	5.32(s)
29	tyrosine	6.88(d), 7.18(d)
30	1-methylhistidine	7.05(s), 7.75(s)
31	phenylalanine	7.34(m), 7.38(m),7.44(m)
32	formate	8.45(s)

[a] Key: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doublet of doublet.

Table S2 ^{1}H NMR data and assignments of the metabolites in urine.

key	metabolites	δ^{1}H (ppm) and multiplicity
1	2-hydroxyisovalerate	0.84(m), 0.97(s)
2	2-hydroxybutyrate	0.88(s)
3	2-hydroxyvalerate	0.89(t)
4	2-oxoisocaproate	0.94(t)
5	valine	0.99(t), 1.05(d)
6	3-hydroxybutyrate	1.20(d)
7	lactate	1.33(d), 4.11(q)
8	alanine	1.48(d)
9	acetate	1.92(s)
10	N-acetylglycine	2.05(s)
11	acetone	2.23(s)
12	acetoacetate	2.27(s)
13	pyruvate	2.35(s)
14	succinate	2.39(s)
15	2-oxoglutarate	2.45(t), 3.01(t)
16	citrate	2.58(d), 2.69(d)
17	N,N-dimethylglycine	2.93(s)
18	creatinine	3.05(s), 4.06(s)
19	cis-aconitate	3.11(s)
20	O-acetylcarnitine	3.14(s)
21	choline	3.19(s)
22	carnitine	3.21(s)
23	taurine	3.25(t), 3.41(t)
24,25	TMAO, betaine	3.26(s)
26	glycine	3.56(s)
27	glycerol	3.66(dd), 3.87(m)
28	hippurate	3.94(s), 7.56(t), 7.66(t), 7.84(d)
29	phenylalanine	3.97(dd), 7.36(t), 7.39(t)
30,31	α-glucose, β-glucose	3.3-3.9, 5.20(d), 5.25(d)
32	tryptophan	4.07(dd)
33	uridine	4.30(t), 7.84(d)
34	inosine	4.44(s)
35	N-methylnicotinamide	4.46(t), 8.19(t)
36	fumarate	6.53(s)
37	trans-aconitate	6.59(s)
38	4-hydroxyphenylpyruvate	6.88(d)
39	tyrosine	6.89(d), 7.05(d)
40	formate	8.46(s)

[a] Key: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doublet of doublet.