Electronic Supplementary Material (ESI) for Molecular BioSystems.

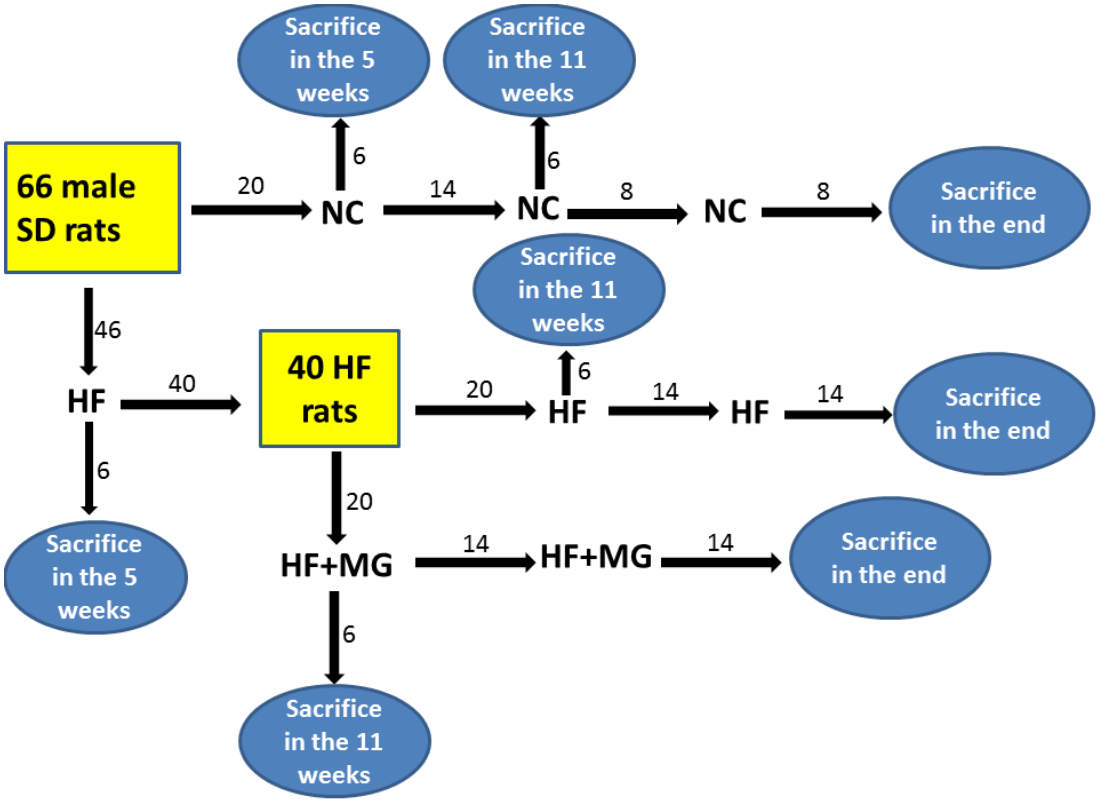


Fig. S1. Study design.

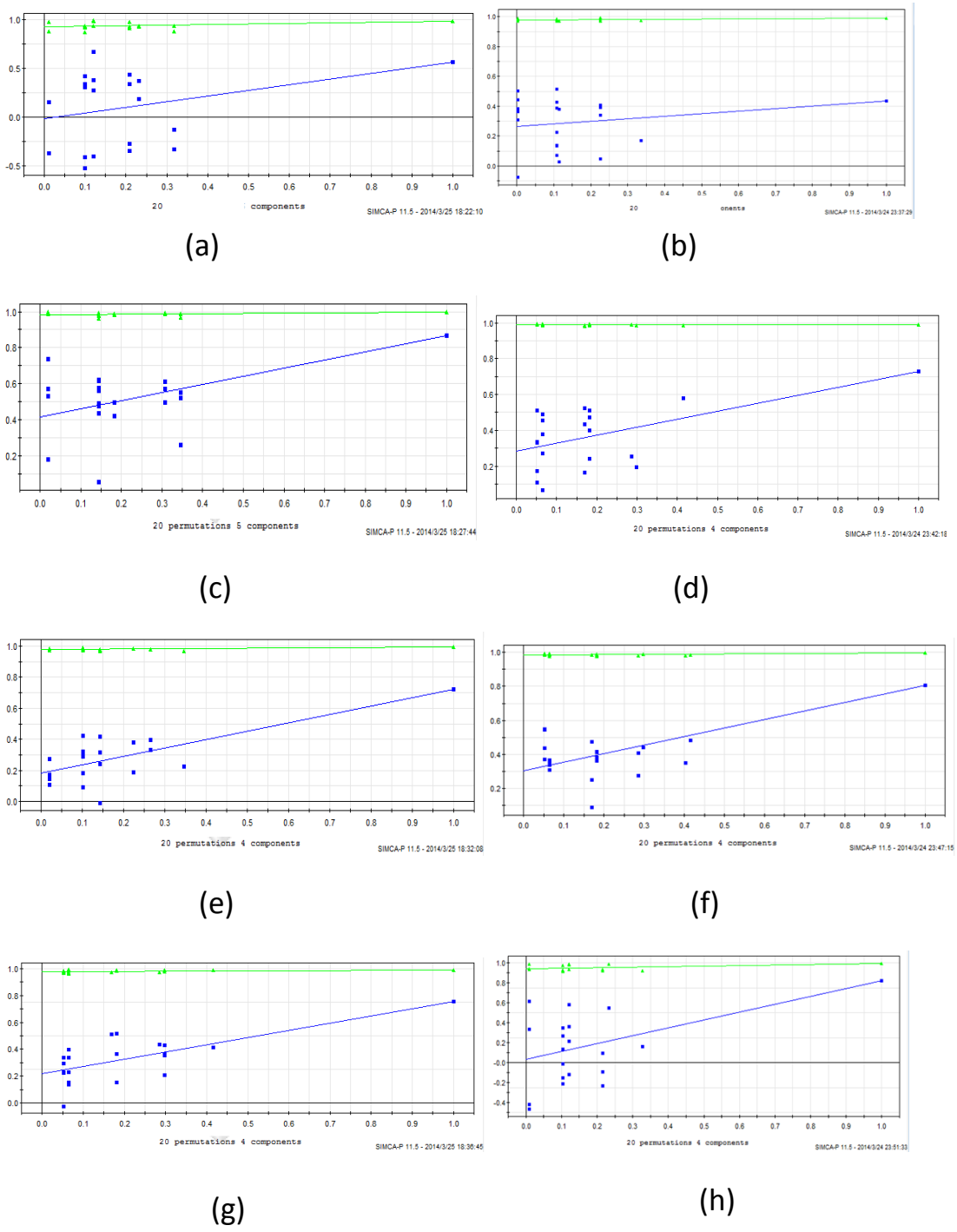
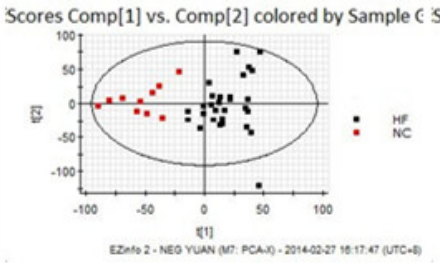
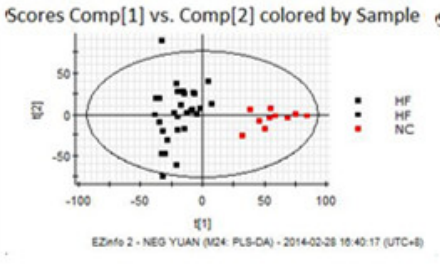


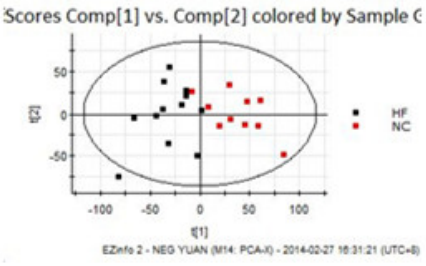
Fig S2. Permutation test result of PLS-DA model in the ESI^+ and ESI^-.(a)At the 5 weeks in the ESI^+,R^2(0.98, 0.93),Q^2(0.56, -0.01); (b) in the ESI^- , R^2(0.98, 0.97),Q^2(0.43, 0.26). (c) At the 10 weeks in the ESI^+,R^2(0.99, 0.98), Q^2(0.86, 0.41); (d) in the ESI^-, R^2(0.98, 0.98), Q^2(0.73, 0.28). (e) At the 14 weeks in the ESI^+,R^2(0.99, 0.97). Q^2(0.72, 0.18); (f) in the ESI^-, R^2(0.99, 0.98), Q^2(0.8, 0.3). (g) At the 18 weeks in the ESI^+,R^2(0.98, 0.97), Q^2(0.75, 0.21); (h) in the ESI^-, R^2(0.99, 0.94). Q^2(0.82, 0.03).


Scores Comp[1] vs. Comp[2] colored by Sample
HF
NC
t[1]
t[2]

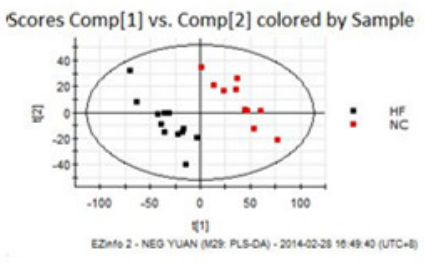
(a)


Scores Comp[1] vs. Comp[2] colored by Sample
HF
HF
NC
t[1]
t[2]

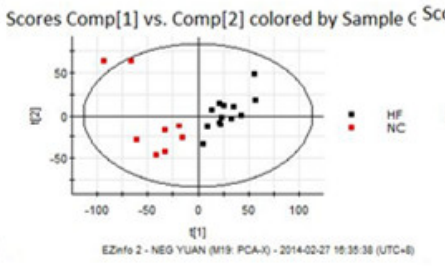
(b)


Scores Comp[1] vs. Comp[2] colored by Sample
HF
NC
t[1]
t[2]

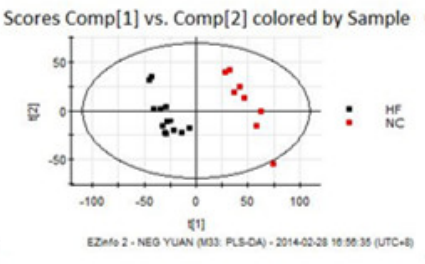
(c)


Scores Comp[1] vs. Comp[2] colored by Sample
HF
NC
t[1]
t[2]

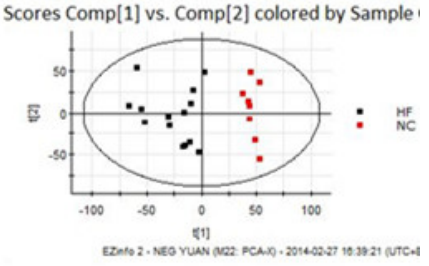
(d)


Scores Comp[1] vs. Comp[2] colored by Sample
HF
NC
t[1]
t[2]

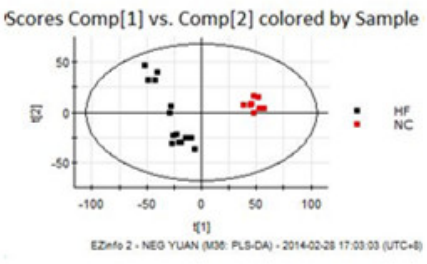
(e)


Scores Comp[1] vs. Comp[2] colored by Sample
HF
NC
t[1]
t[2]

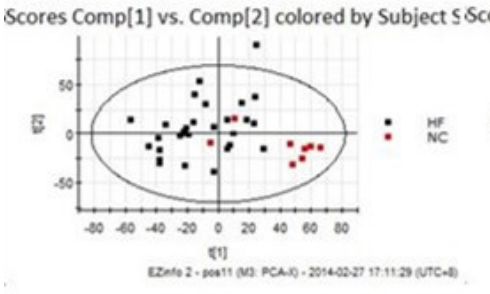
(f)


Scores Comp[1] vs. Comp[2] colored by Sample
HF
NC
t[1]
t[2]

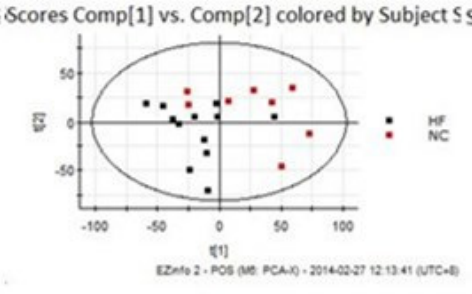
(g)


Scores Comp[1] vs. Comp[2] colored by Sample
HF
NC
t[1]
t[2]

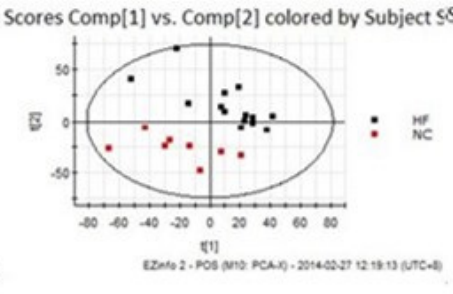
(h)


Scores Comp[1] vs. Comp[2] colored by Subject S
t[2]
t[1]
HF
NC

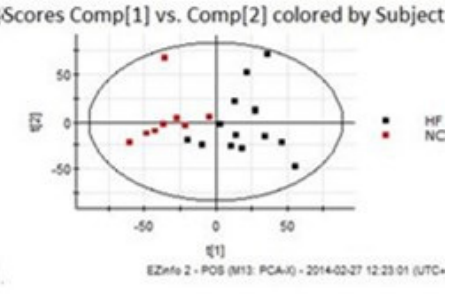
(i)


Scores Comp[1] vs. Comp[2] colored by Subject S
t[2]
t[1]
HF
NC

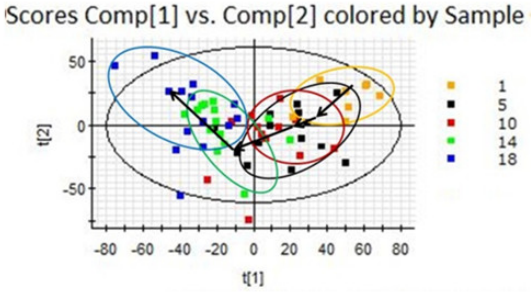
(j)


Scores Comp[1] vs. Comp[2] colored by Subject S
t[2]
t[1]
HF
NC

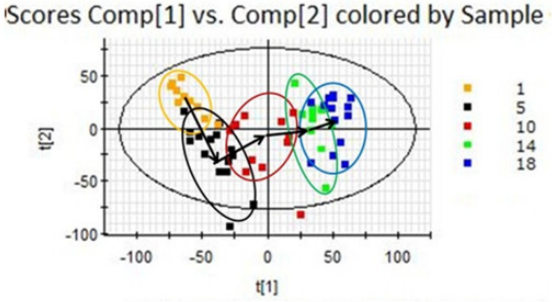
(k)


Scores Comp[1] vs. Comp[2] colored by Subject
t[2]
t[1]
HF
NC

(l)

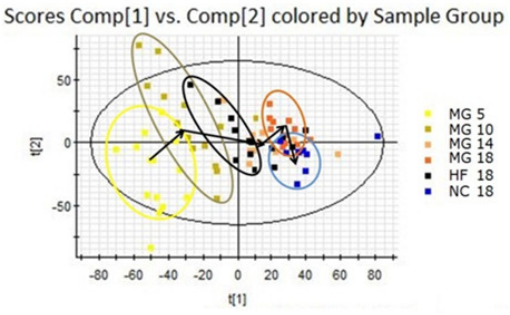

Scores Comp[1] vs. Comp[2] colored by Sample
t[2]
t[1]
1
5
10
14
18

(m)

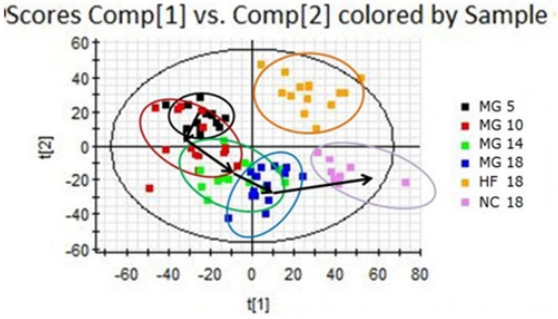

Scores Comp[1] vs. Comp[2] colored by Sample
t[2]
t[1]
1
5
10
14
18

(n)

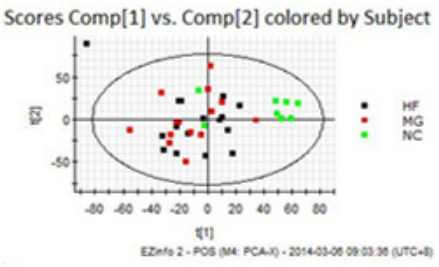
Fig.S3. (a-d)Principal component analysis (PCA) score plots and(e-f) partial least-squares discriminant analysis (PLS-DA) score plots of rats in the ESI^- in the NC group and HF group; (i-l) Principal component analysis (PCA) score plotsa **o**f rats in the ESI^+ in the NC group and HF group. (a,e) Week 5, n =8(NC),28(HF) (for two components, R^2Y = 0.3061, Q^2 = 0.0800; for one components, R^2Y = 0.8896, Q^2 =0.7898); (b,f)week 10, n = 8(NC),14(HF) (for two components R^2Y = 0.3053, Q^2 = 0.0586; for two components R^2Y = 0.9540, Q^2 = 0.5752);and(c,g) week 14,n = 8(NC),14(HF) (for two components R^2Y =0.3090, Q^2 =0.0351;for one components R^2Y =0.8987, Q^2 =0.8181); (d,h) week 18,n = 8(NC),14(HF) (for two components R^2Y = 0.3057, Q^2 =0.0747; for two components R^2Y = 0.9127, Q^2 = 0.7974).NC rats are indicated by black squares and HF rats by red triangles. (i) Week 5, n =8(NC),28(HF) (for four components, R^2Y = 0.4873, Q^2 = 0.1251); (j)week 10, n = 8(NC),14(HF) (for four components R^2Y = 0.5249, Q^2 = 0.1338);and(k) week 14,n = 8(NC),14(HF) (for two components R^2Y =0.2883, Q^2 =0.0572); (l) week 18,n = 8(NC),14(HF) (for three components R^2Y = 0.4181, Q^2 =0.1217). (m-n) Metabolic trajectory scores plots by principal component analysis (PCA) in the (m) ESI^+ and (n) ESI^- derived from the urine of rats on high fat diet. Samples were collected during weeks 1 to 18. Yellow star(1): weeks 1 to5; Black star(5): weeks 6 to 10; red star(10): weeks 11 to 14;Green star(14): weeks 15 to 18.


Scores Comp[1] vs. Comp[2] colored by Sample Group
t[2]
t[1]
MG 5
MG 10
MG 14
MG 18
HF 18
NC 18

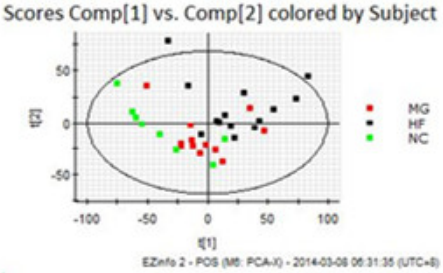
(a)


Scores Comp[1] vs. Comp[2] colored by Sample
t[2]
t[1]
MG 5
MG 10
MG 14
MG 18
HF 18
NC 18

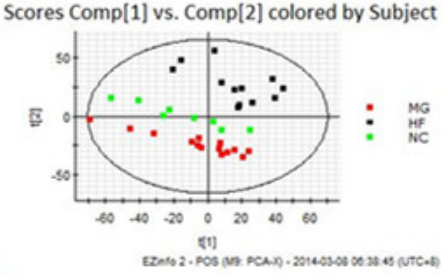
(b)


Scores Comp[1] vs. Comp[2] colored by Subject
t[2]
t[1]
HF
MG
NC

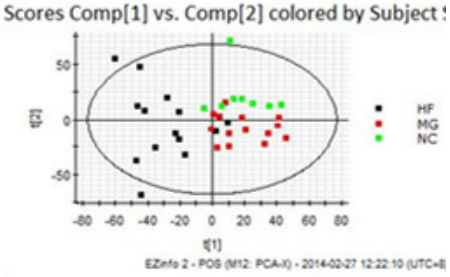
(c)


Scores Comp[1] vs. Comp[2] colored by Subject
t[2]
t[1]
MG
HF
NC

(d)


Scores Comp[1] vs. Comp[2] colored by Subject
t[2]
t[1]
MG
HF
NC

(e)


Scores Comp[1] vs. Comp[2] colored by Subject
t[2]
t[1]
HF
MG
NC

(f)

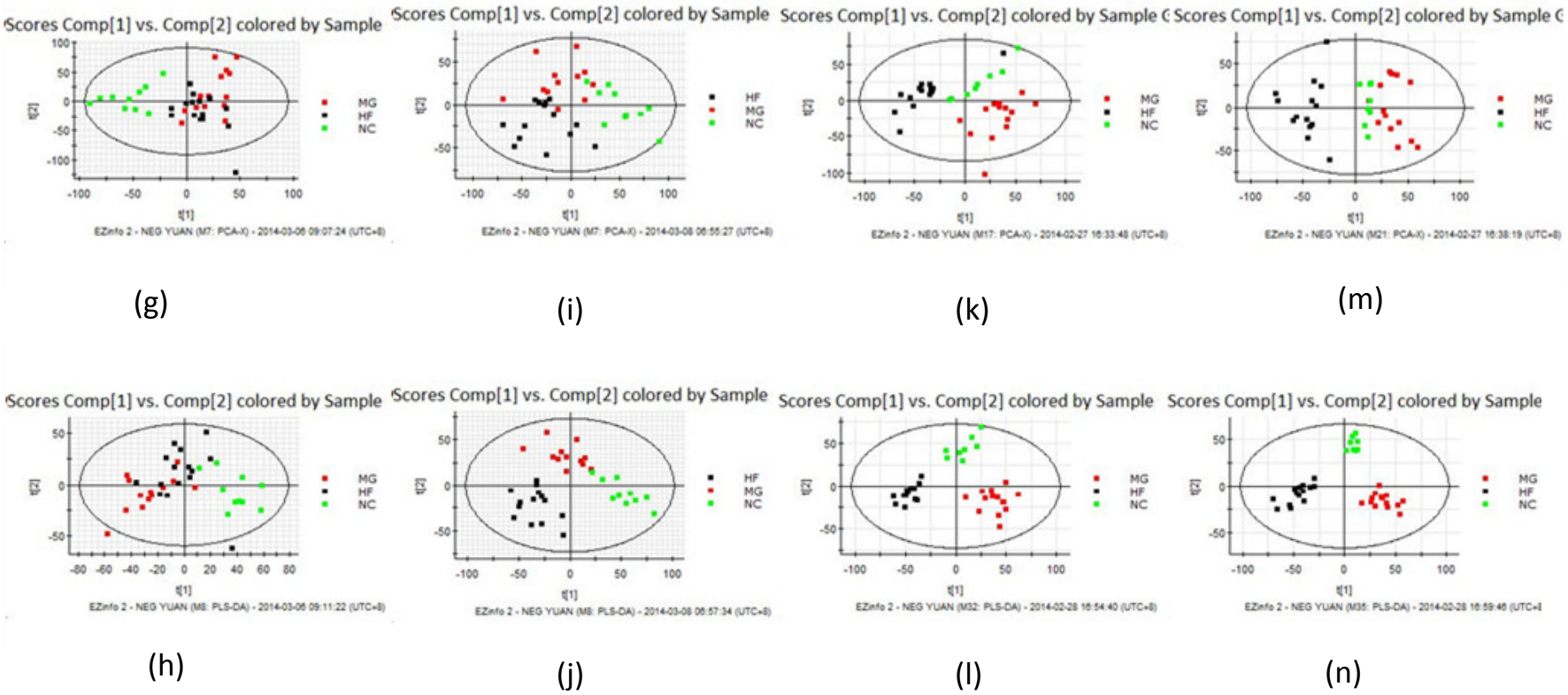


Fig S4. (a-b)Metabolic trajectory scores plots by principal component analysis (PCA) in the (a)ESI$^+$ and (b)ESI$^-$derived from the urine of rats on high fat diet after MG supplementation.Samples were collected during 0-13 weeks after MG supplementation. MG 5: weeks 0; MG10: weeks 5; MG14: weeks 9;MG 18: weeks 13; HF 18: weeks 18:NC 18:18weeks. (c-f) Principal component analysis (PCA) score plots a in the ESI$^+$ in

the NC group , HF group and MG group.(c) Week 5（before MG supplementation）, n =8(NC),14(HF),14(MG) (for five components, R^2Y = 0.4614, Q^2 = 0.1787); (d) week 10(after MG supplementation for 5 week), n = 8(NC),14(HF),14(MG) (for five components R^2Y = 0.5029, Q^2 = 0.1721); (e) week 14(after MG supplementation for 9 weeks),n = 8(NC),14(HF),14(MG) (for six components R^2Y =0.4634, Q^2 =0.0261); (f) week 18(after MG supplementation for 13 weeks),n = 8(NC),14(HF),14(MG) (for five components R^2Y = 0.4412, Q^2 =0.1244). (g,I,k,m) Principal component analysis (PCA) score plots and (h,j l,n) partial least-squares discriminant analysis (PLS-DA) score plots of rats in the ESI^- in the NC group , HF group and MG group.(g,h) Week 5（before MG supplementation）, n =8(NC),14(HF),14(MG) (for two components, R^2Y = 0.2503, Q^2 = 0.0283; for two components, R^2Y =0.6592, Q^2 = 0.4601);(i,j)week 10(after MG supplementation for 5 week), n = 8(NC),14(HF),14(MG) (for three components R^2Y = 0.3286, Q^2 = 0.1000; for two components R^2Y =0.7704, Q^2 =0.6152); (k,l) week 14(after MG supplementation for 9 weeks),n = 8(NC),14(HF),14(MG) (for two components R^2Y =0.2760, Q^2 =0.1052;for two components R^2Y =0.8742, Q^2 = 0.7662);(m,n) week 18(after MG supplementation for 13 weeks),n = 8(NC),14(HF),14(MG) (for two components R^2Y = 0.2756, Q^2 = 0.1159; for two components R^2Y =0.9143, Q^2 = 0.8358).

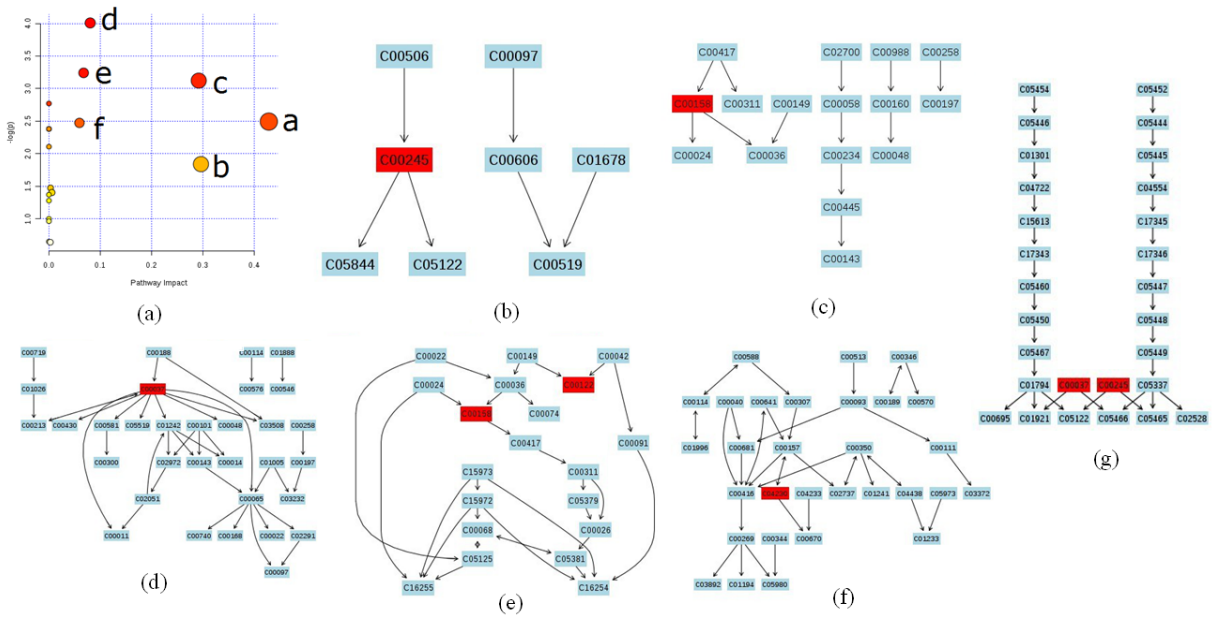


Fig.S5. Summary of pathway analysis and identifying network pathway by MetPA software in rats. (a) a,Taurine and hypotaurine metabolism; b, Glyoxylate and dicarboxylate metabolism; c, Glycine, serine and threonine metabolism; d, Citrate cycle (TCA cycle); e, Glycerophospholipid metabolism; f, Primary bile acid biosynthesis (b), Taurine and hypotaurine metabolism; (c), Glyoxylate and dicarboxylate metabolism; (d), Glycine, serine and threonine metabolism; (e), Citrate cycle (TCA cycle); (f), Glycerophospholipid metabolism; (g), Primary bile acid biosynthesis. Metabolism were inferred in the hyperlipemia rats from changes in the urine levels of intermediates during substance metabolism. Red denotes affected metabolites related to the pathway. The map was generated using the reference map by KEGG (http://www.genome.jp/kegg/).