Supporting Information

An integrating strategy for serum metabolomics and microarray analysis to expand the understanding of diet-induced obesity

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Abbreviations

LDL: low density lipoprotein

NAG: N-Acetylglutamate

PAG: Phenylacetyglycine

PUFA: polyunsaturated fatty acid

VLDL: very low density lipoprotein

28 **Table S1.** Identified metabolites from the NMR spectra of rat serum

No.	Metabolites	^{1}H chemical shift, ppm (multiplivity)	No.	Metabolites	^{1}H chemical shift, ppm (multiplivity)
1	LDL	0.88(br),1.27(br)	19	Citrate	2.54(d),2.69(d)
2	Leucine	0.95(t)	20	Ketoleucine	2.65(d)
3	Isoleucine	0.98(t),1.02(d)	21	Aspartate	2.68(m)
4	Valine	1.04(d)	22	Sarcosine	2.74(s), 3.60(s)
5	Ethanol	1.18(t)	23	Creatine	3.03(s), 3.93(s)
6	Lactate	1.33(d),4.12(q)	24	Histidine	3.25(m)
7	L-Alanine	1.48(d)	25	α-glucose	3.42(t),3.54(dd),3.72(t),
8	VLDL	1.31(br),1.58(br)			3.74(mm),5.24(d)
9	Lipid	1.78(br),2.75(br)	26	Tryptophan	3.21(dd), 3.49(dd)
10	Acetate	1.91(s)	27	Methylxanthine	3.51(s)
11	NAG	2.04(s)	28	Glycine	3.56(s)
12	Methionine	2.13(s),2.650(t)	29	PAG	3.69(s),3.76(d)
13	Acetone	2.22(s)	30	β-glucose	3.25(dd),3.46(t),3.9(dd), 4.65(dd)
14	p-Cresol	2.25(s)	31	Glycolic acid	3.93 (s)
15	Acetoacetate	2.30(s)	32	PUFA	5.30(br)
16	Pyruvate	2.36(s)	33	Tyrosine	6.89(d);7.05(d)
17	Succinic acid	2.390(s)	34	Methyhlhistidine	7.05(s),7.82(s)
18	Glutamine	2.14(m),2.44(m)	35	Formate	8.45(s)

29 Multiplicity: s, singlet; d, doublet; t, triplet; q, quartet; dd, doublets; m, multiplet, br, broad peaks

Table S2. Identified potential biomarkers from the NMR spectra of rat serum and their related parameters

Metabolites	δ(^{1}H, multiplicity, assignments)	Correlation coefficient	VIP	p-value	KEGG ID
LDL	0.88 (br, -CH_3), 1.22-1.30 (br)	0.688	5.037	0.004	C01595
Lactate	1.33 (d, -CH_3),4.12(q, -CH)	0.538	6.339	0.048	C00186
Alanine	1.48 (d, β-CH_3)	0.694	3.919	0.015	C00041
Pyruvate	2.37 (s, -CH_3)	-0.569	1.021	0.036	C00022
Acetoacetate	2.30 (s, -CH_3)	-0.667	1.473	0.016	C00383
Citrate	2.54 (d, -CH_2)	-0.597	1.335	0.026	C00300
Aspartate	2.68 (dd, β-CH_3)	-0.567	1.426	0.029	C00245
Sarcosine	2.74 (s, -CH_3)	-0.863	3.522	0.00021	C00037
Histidine	3.17-3.29(m, β-CH)	-0.661	3.395	0.016	C01026

s: singlet; d: doublet; q: quartet; dd: doublets; m: multiplet, br: broad peaks

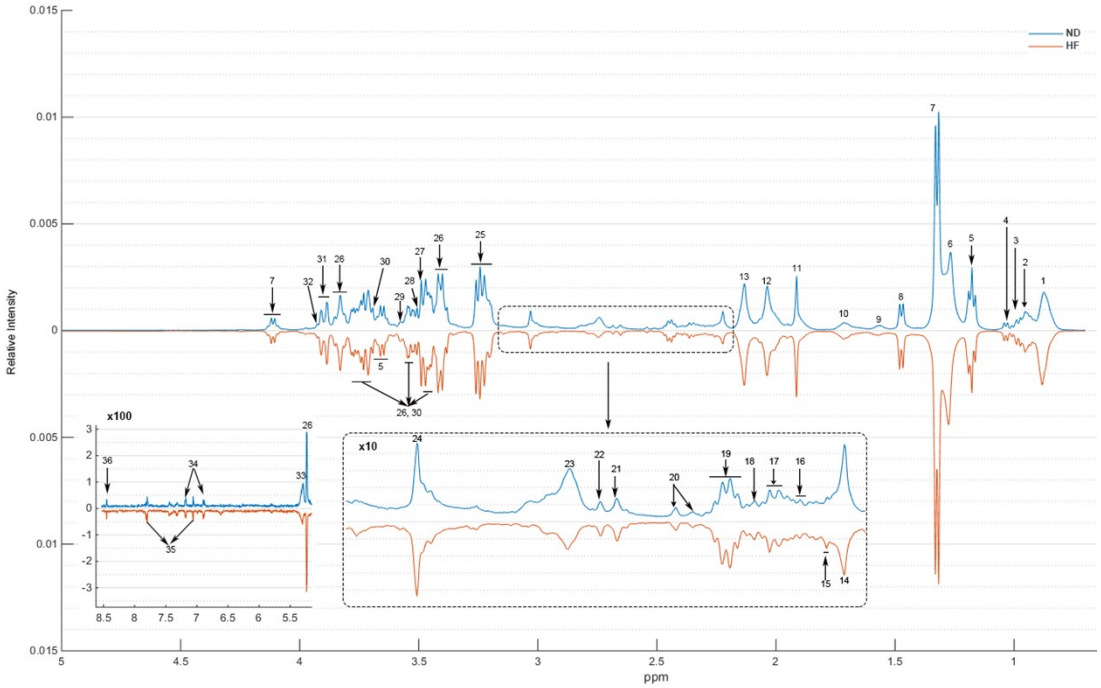

Fig. S1. Mean ^{1}H NMR serum spectra of ND and HF groups. (the spectral regions of 2.2-3.2 ppm (the dashed box) and 5.0-8.6 ppm (the lower left corner) were vertically expanded 10 and 100 times compared to the remaining spectral region for the purpose of clarity. The keys for the numbers of assigned metabolites are given in Table S1.)

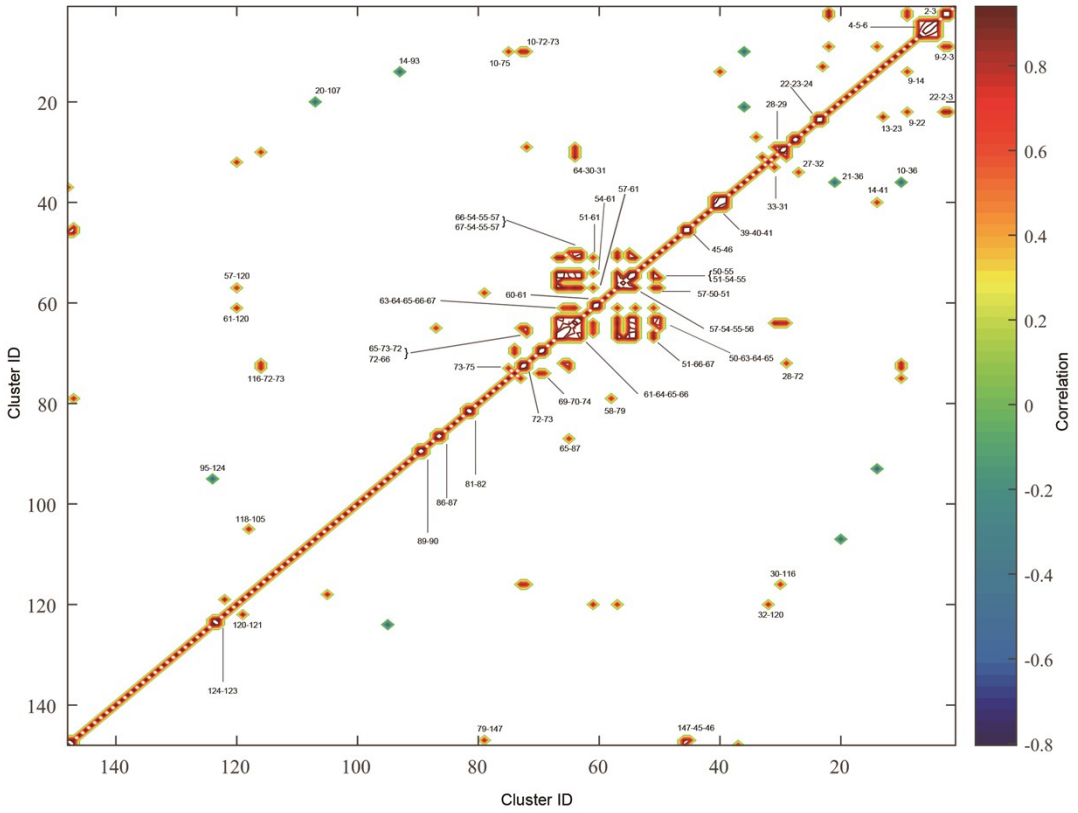

Fig. S2. 2D representation of an RSTOCSY pseudospectrum based on the clusters obtained by statistical recoupling of variables on the serum dataset. Fifty-six correlation areas are identified for a correlation threshold of 0.8 representing spin and metabolic connectivities between 2 or more clusters (these data show in https://github.com/liuwuping/RSTOCSY). The degree of correlations between clusters has been color-coded (positive correlations in red and negative correlations in blue).