Table S1 The information of indicated metabolites related to hypertension.

Metabolite	Mode	RT	MS_level	Precursor m/z	Detected m/z	HMDB_ID	Metlin _ID	VIP	p_value
Bile acid	P	7.1389	1	353.2467	408.2876	—	—	1.417619272	0.013464496
Ursodeoxycholic acid	N	9.457	2-search-DB	783.5778	392.2927	HMDB0000946	—	1.448699841	1.7234E-06
Glycocholic acid	P	6.79	2-search-DB	488.2975	465.309	HMDB0000138	202	1.32279313	0.026729034
Glycoursodeoxycholic acid	N	8.061	2-search-DB	448.307	449.3141	HMDB0000708	—	1.458432002	1.37428E-09
Taurodeoxycholic acid	N	6.7814	1	498.2893	499.2968	HMDB00896	—	1.343580894	0.000607975
12-ketochenodeoxycholic acid	N	7.1719	1	377.27	406.2719	HMDB0000400	—	1.438701692	1.76264E-08
TG(a-21:0/i-16:0/10:0)	P	12.041	1	133.0134	280.043	HMDB0065752	—	1.570660972	0.004855736
TG(a-21:0/18:0/15:0)	P	13.046	1	207.0323	536.153	HMDB0067196	—	1.60075907	0.005968879
TG(i-21:0/14:0/10:0)	P	12.71	1	298.0836	594.1373	HMDB0065754	—	1.190016327	0.035620744
LysoPC(18:0)	P	10.03	2-search-DB	568.3393	523.3638	HMDB0010384	—	1.583611266	0.004464442
LysoPS(18:1(9Z)/0:0)	N	7.953	2-search-DB	522.2488	523.291	HMDB0240603	40829	1.301962058	0.000310767
Glycerophosphorylcholine	P	2.446	2-MetDNA	276.1417	258.1101	HMDB0000086	—	1.392978691	0.01639914
PC(22:5(7Z,10Z,13Z,16Z,19Z)/14:1(9Z))	P	9.939	1	297.0826	314.0837	HMDB0008690	—	1.51171364	0.005071407
PC（O-16:0/2:0）	P	11.16	2-search-DB	546.3634	523.3638	HMDB0062195	—	1.108178927	0.043883643
SM(d18:1/24:1(15Z))	P	12.564	1	813.6841	812.6771	HMDB0012107	—	1.208825937	0.043291199
Methionine sulfoxide	P	3.566	2-search-DB	166.0498	154.1358	HMDB0002005	—	1.454308473	0.018208084
L-Tryptophan	P	5.319	2-search-DB	251.1028	204.0899	HMDB0000929	33	1.903783776	1.36004E-10
N-(Linolenoyl) Tyrosine	N	7.953	1	476.2631	441.2879	—	64731	1.460899334	1.86661E-08
Hippuric acid	P	5.028	2-search-DB	180.0654	179.0582	HMDB0000714	—	1.829399938	8.57128E-05
Adenosine	P	1.431	2-search-DB	268.099	267.0968	HMDB0000050	86	1.499987744	0.009864331
Pantothenic acid	P	3.458	1	129.5362	219.1107	HMDB0000210	241	1.521979018	0.00718797

Table S1 (*Cont*.)

Metabolite	Mode	RT	MS_level	Precursor m/z	Detected m/z	HMDB_ID	Metlin_ID	VIP	p_value
S-Citramalic acid	P	12.0409	2-search-DB	149.0448	148.0372	—	—	1.581312923	0.007993563
Propiolic acid	N	1.464	2-search-DB	68.9956	70.0055	HMDB0006804	4117	1.466785576	2.54623E-10
Succinic acid semialdehyde	N	1.913	2-search-DB	101.0242	102.0317	HMDB0001259	—	1.316338661	0.000230399
4-Hydroxyacid	P	2.727	2-search-DB	72.0046	104.0473	HMDB0000710	—	1.711207519	0.000264891

Note: RT, retention time. P, positive mode in LC–MS/MS analysis. N, negative mode in LC–MS/MS analysis.

Figure captions

Fig.S1The representative total ion current chromatograms (TIC) in ESI positive (a) and negative (b) modes.

Fig.S2 2D PCA plots from the serum samples of NCW/SHR group, SHR group rats and the QC sample in ESI positive (a) and negative (b) modes. SHR group (red circle, n = 6); NCW/SHR group (green triangle, n = 6); QC (quality control samples, black square, n = 3).

Fig.S3 OPLS-DA plots from the serum samples of NCW/SHR group and SHR group rats in ESI positive (a) and negative (b) modes. SHR group (green square, n = 6); NCW/SHR group (orange circle, n = 6).

Fig.S4 OPLS-DA permutation test results from the serum samples of NCW/SHR group and SHR group rats in ESI positive (a) and negative (b) modes.

Fig.S1

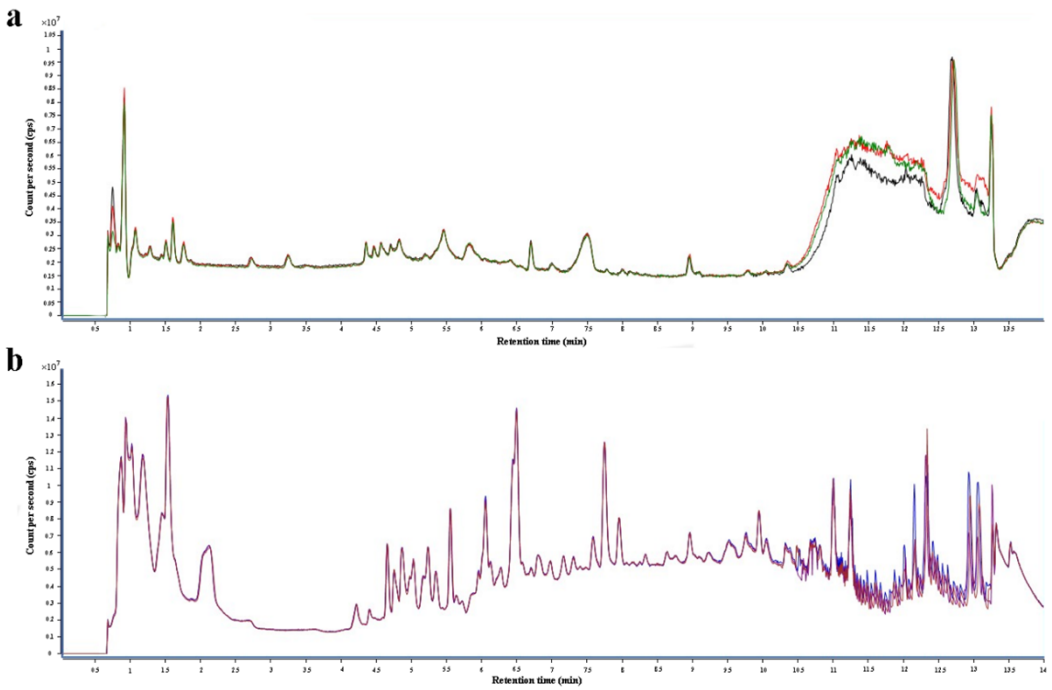

a
×10^7
Count per second (cps)
Retention time (min)
b
×10^7
Count per second (cps)
Retention time (min)

Fig.S2

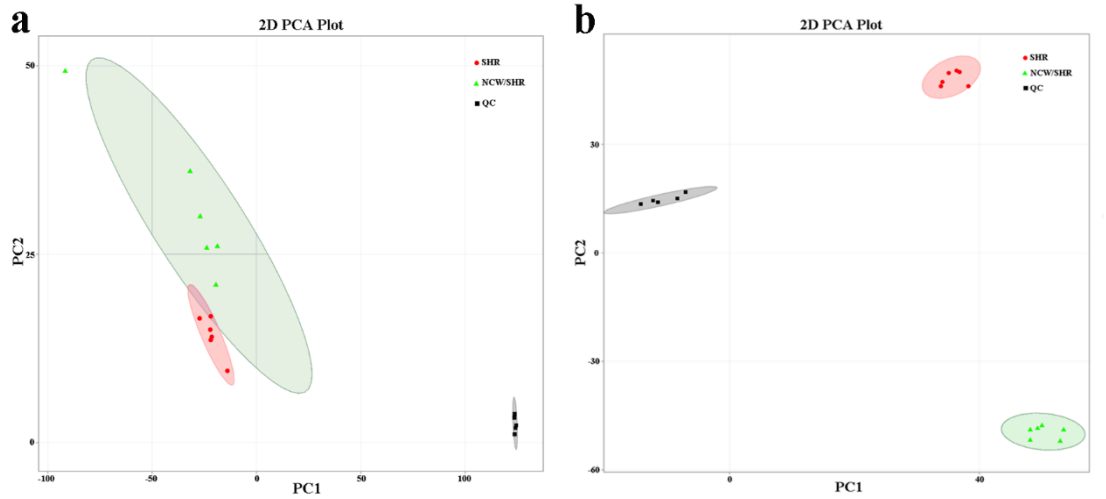

a
2D PCA Plot
SHR
NCW/SHR
QC
PC2
PC1
50
25
0
-100
-50
0
50
100
b
2D PCA Plot
SHR
NCW/SHR
QC
PC2
PC1
30
0
-30
-60
0
40

Fig.S3

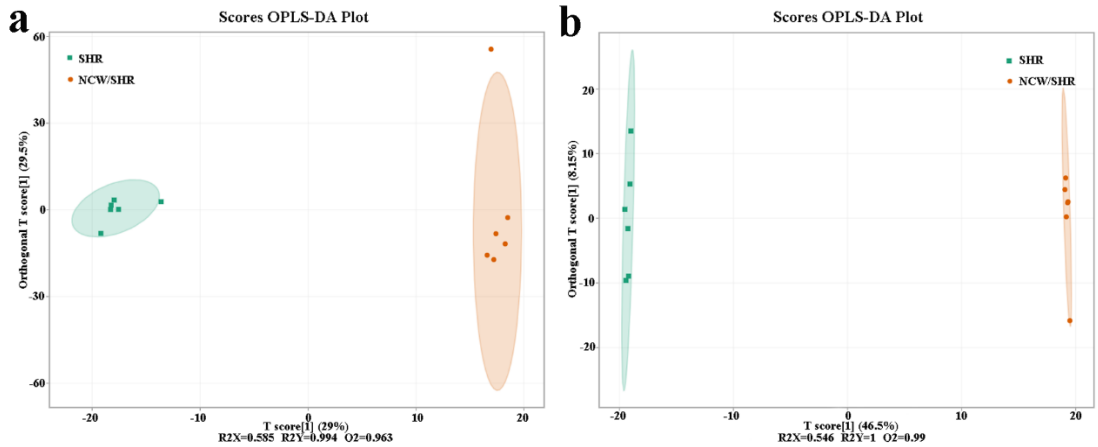
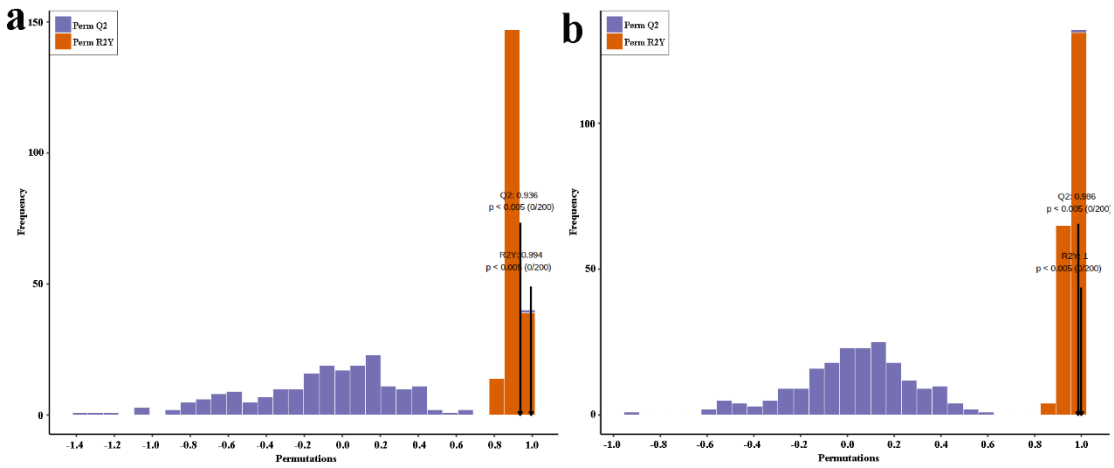

a
Scores OPLS-DA Plot
SHR
NCW/SHR
Orthogonal T score[1] (29.5%)
T score[1] (29%)
R2X=0.585 R2Y=0.994 O2=0.963
b
Scores OPLS-DA Plot
SHR
NCW/SHR
Orthogonal T score[1] (8.15%)
T score[1] (46.5%)
R2X=0.546 R2Y=1 O2=0.99

Fig.S4


a
Perm Q2
Perm R2Y
Frequency
Permutations
Q2: 0.936
p < 0.005 (0/200)
R2Y: 0.994
p < 0.005 (0/200)
b
Perm Q2
Perm R2Y
Frequency
Permutations
Q2: 0.986
p < 0.005 (0/200)
R2Y: 1
p < 0.005 (0/200)