

1           **Analysis of Serum metabolites to Diagnose Bicuspid Aortic Valve**

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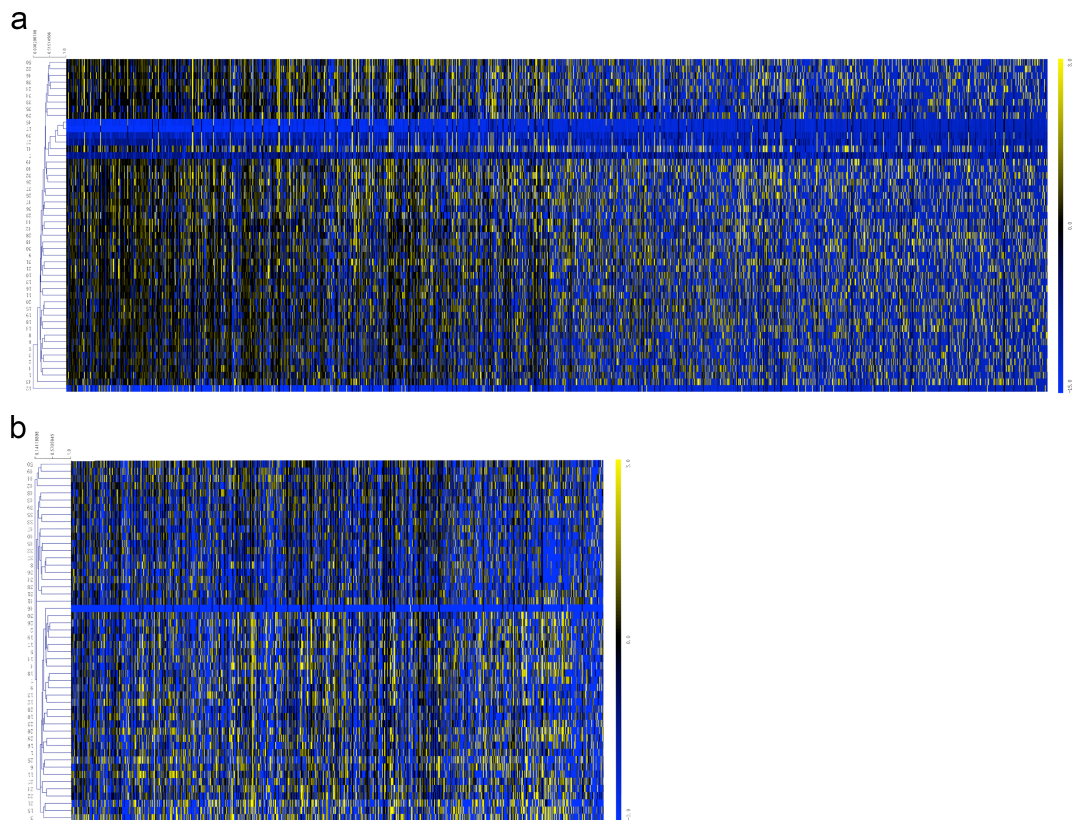
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43 **Supplementary Material**



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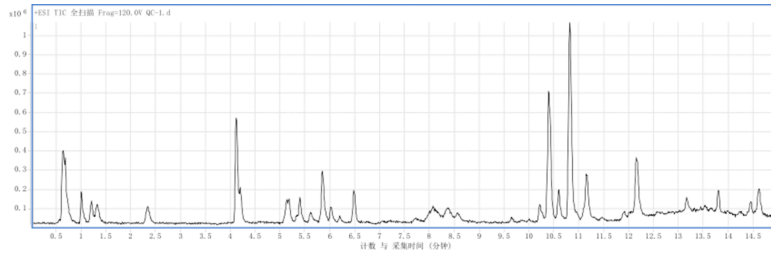
45 **Figure 1.** The metabolic profiles of BAV patients versus healthy participants.

46 Heat maps of metabolite features identified from members of the

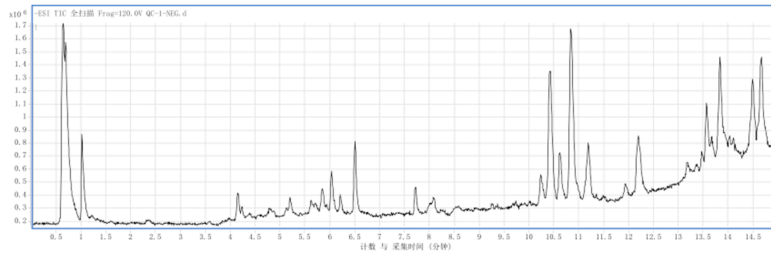
47 patient group and control group under negative-ion mode (a) and

48 positive-ion mode (b) were shown. The data were displayed on a

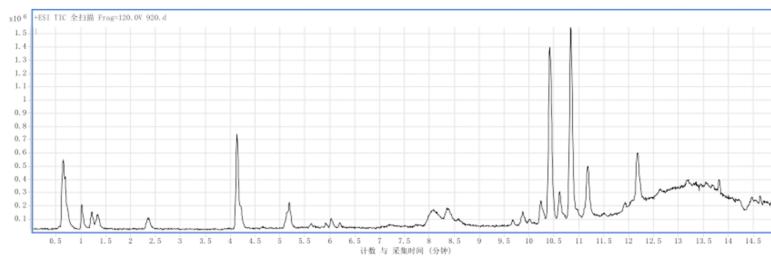
49 log<sub>2</sub> scale and clustered based on Spearman distance.



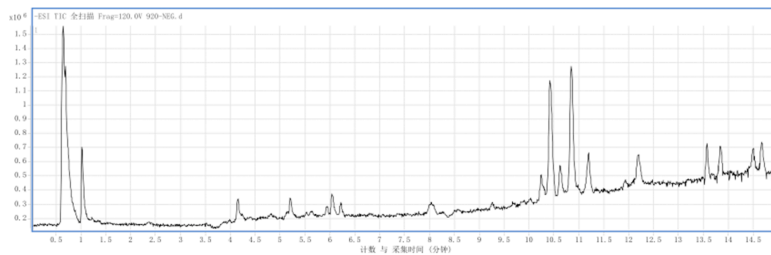
Total Ions Chromatograph  
of QC in positive mode



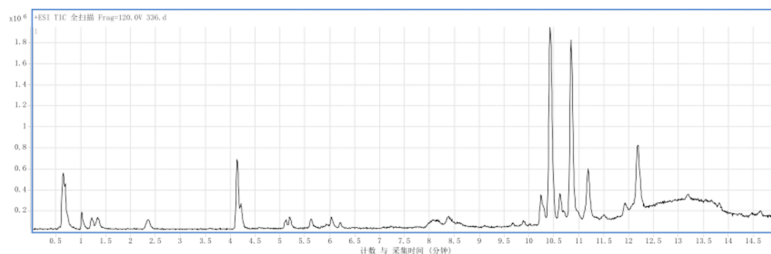
Total Ions Chromatograph  
of QC in negative mode



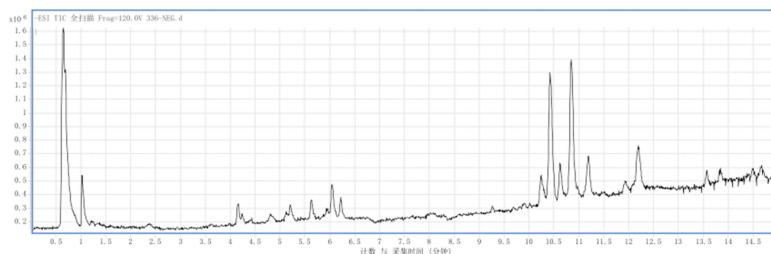
Total Ions Chromatograph of  
patients with BAV in positive mode



Total Ions Chromatograph of  
patients with BAV in negative mode



Total Ions Chromatograph  
of control in positive mode



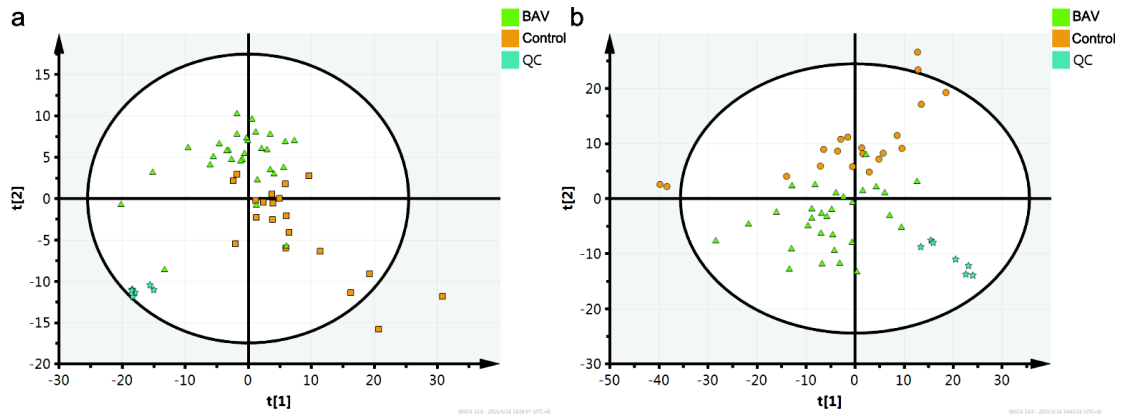
Total Ions Chromatograph  
of control in negative mode

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51 **Figure 2.** The TIC of all groups in positive- and negative-ion modes. TIC =

52 total ions chromatography

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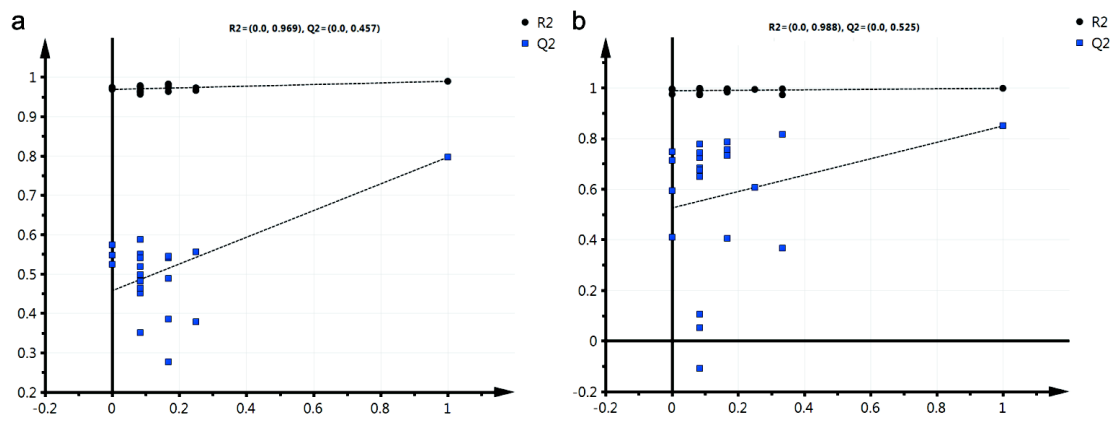
55 **Figure 3.** The PCA scores of patients with BAV and controls in positive- (a)

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and negative-ion (b) modes. PCA = Principle Component Analysis.

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BAV = bicuspid aortic valve. QC = Quality Control.



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59 **Figure 4.** The validation of PLS-DA models in positive (a) and negative (b)

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mode. PLS-DA = Partial Least Squares Discriminant Analysis.

Metabolites	R	P-value
Gluconic acid	0.2813	0.0478
Inosine	0.2805	0.0485
HETE	0.2884	0.0422
HpOTrE	0.3542	0.0116
Purine	0.3762	0.0071
HOME	0.3379	0.0164
Clupanodonic acid	0.3331	0.0181
palmitoleic acid	0.3154	0.0257
Oleic Acid	0.3855	0.0057
Linoleic acid	0.4484	0.0006
Glycerophospho-N-Palmitoyl Ethanolamine	0.2828	0.0466
MG(18:4)	0.3566	0.0110
Uridine	0.3811	0.0063
Clupanodonic acid	0.3513	0.0124
LysoPE(22:5)	0.3000	0.0343
Isoleucine/Leucine	-0.3263	0.0207
Tryptophan	-0.3797	0.0065
Ketoleucine	-0.4126	0.0029
Uridine	-0.3152	0.0258
DL-2-hydroxy valeric acid	-0.3203	0.0233
5-S-Cysteinyldopamine	-0.4024	0.0038
Deoxyuridine monophosphate (dUMP)	-0.2984	0.0353
Palmitic acid	-0.3217	0.0227
PE(20:1)	-0.4385	0.0014
D-myo-Inositol-tetraphosphate	-0.3656	0.0090
Adenosine	0.3522	0.0121
Se-Methylselenomethionine	0.4308	0.0018
MG(18:2)	0.4637	0.0007
Acetylcarnitine	0.3079	0.0296
Linolenic Acid	0.4093	0.0032
N-palmitoyl alanine	0.4042	0.0036
Bilirubin	0.3513	0.0124
Glycerophospho-N-Oleoyl Ethanolamine	0.4711	0.0006
Glycerophospho-N-Arachidonoyl Ethanolamine	0.3668	0.0088
PE(18:2)	0.4537	0.0009
PC(16:0)	-0.3496	0.0128
Hypoxanthine	-0.2861	0.0440
Choline	-0.3183	0.0243
Dodecanoylcarnitine	-0.4446	0.0012
PC(20:4)	-0.3795	0.0066
N-palmitoyl threonine	-0.3251	0.0212

62 **Table 1.** The correlation of metabolites with BAV. BAV = bicuspid aortic  
63 valve