Time (min)	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Capillary (v)	2800	3000	3200	3400	3500	3400						3400				3400		3400
Sampling Cone（v）	20					15	20	25	30	35	40	30				30		30
Extraction Cone（v）	1.0											1.0	2.0	3.0	4.0	3.0		3.0
Desolvation (℃)	200															250	300	300
Desolvation (l/h)	500																	600
Source (℃)	110																	

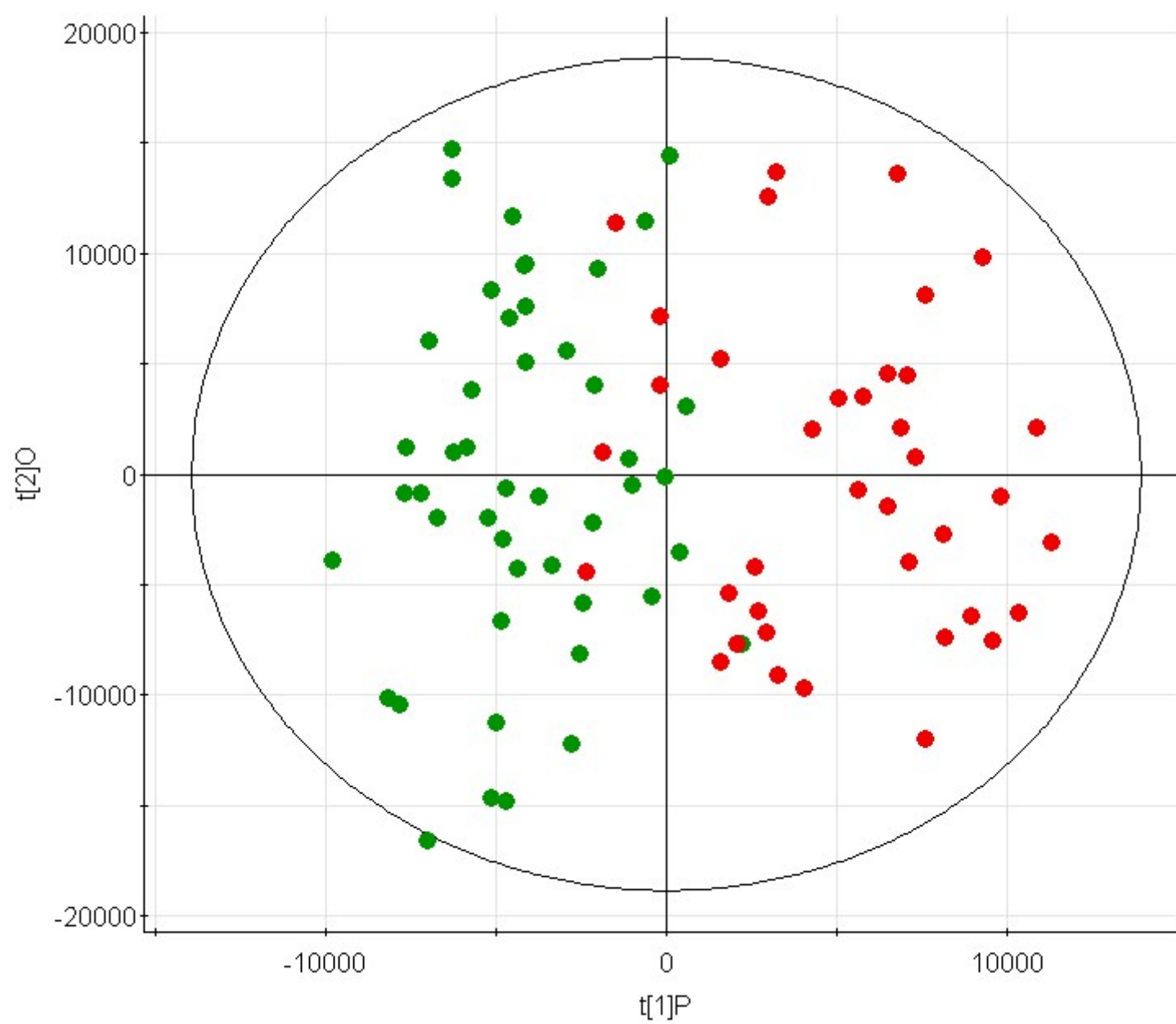**Fig S1**. Chromatogram (A) and MS (B) optimization in positive ion mode.

Fig.S2. Score plots of lipidomic profiles obtained for controls (red) and CHD (green) using ultra high-performance liquid chromatography coupled with quadrupole time-of-flight mass spectrometry at negative ESI mode.

Table S1. Biochemistry results in CHD group.

Group	SOD(U/ml)	MDA(nmol/ml)	cAMP(pmol/ml)	cGMP(pmol/ml)	ANF(ng/ml)	cTn-I（ng/ml)
Control	1.46±0.12	4.44±0.70	14.24±2.47	13.04±2.45	0.41±0.07	6.20±0.67
CHD	1.18±0.07**	5.85±0.69**	20.25±6.07*	16.93±4.02*	0.42±0.07	6.69±0.41

*Significant difference from control group at p < 0.05

Table S2. Identification of serum lipid in CHD cases.

No	Retention time (min)	m/z	Compound ID	Adducts	Formula	Mass Error (ppm)	VIP	Compound	Anova (p)	Trend
1	3.27	452.28	LMGP02050010	M+H	C21H42NO7P	1.99	16.43	PE(16:1(9Z)/0:0)	0.0079	Up
2	0.44	361.20	LMST02030026	M+H	C21H28O5	1.48	16.39	Aldosterone	0.0034	Up
3	7.56	285.10	LMGP0105AA00	M+H	C9H19NO7P	3.37	15.11	2-acyl-sn-glycero-3-phosphocholine	0.0024	Up
4	4.47	297.17	LMPR02020062	M+H	C16H24O5	-4.72	14.7	alhpa-tocopheronic acid	0.0028	Up

Table S3. Result from ingenuity pathway analysis with MetPA.

Pathway	Total	Expected	Hits	Raw p	Holm adjust	Impact
Glycerophospholipid metabolism	39	0.048608	2	0.00075984	0.060787	0.10746
Glycerolipid metabolism	32	0.039884	1	0.039372	1	0.01247
Steroid hormone biosynthesis	99	0.12339	1	0.11843	1	0.01235

Note: Total is the total number of compounds in the pathway; the Hits is the actually matched number from the user uploaded data; the Impact is the pathway impact value calculated from pathway topology analysis.