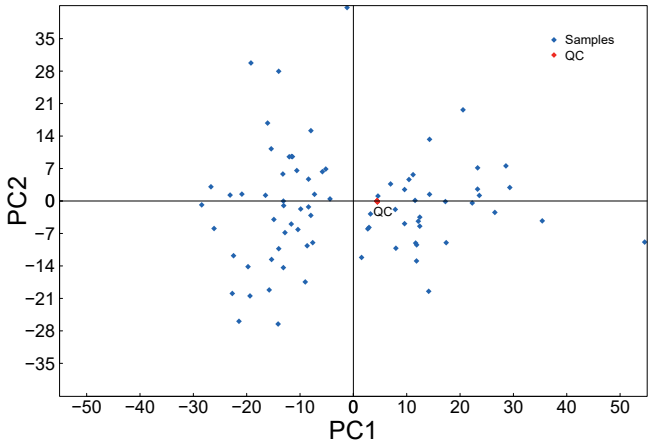
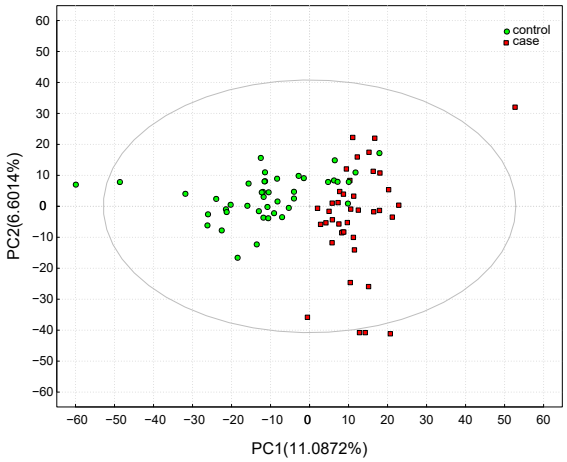
Supplementary materials

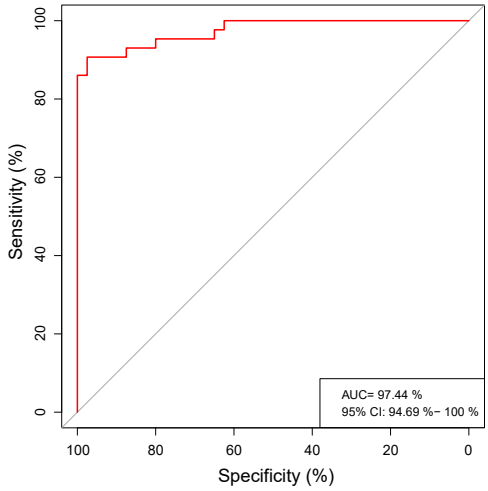
1.1 Supplementary graphics



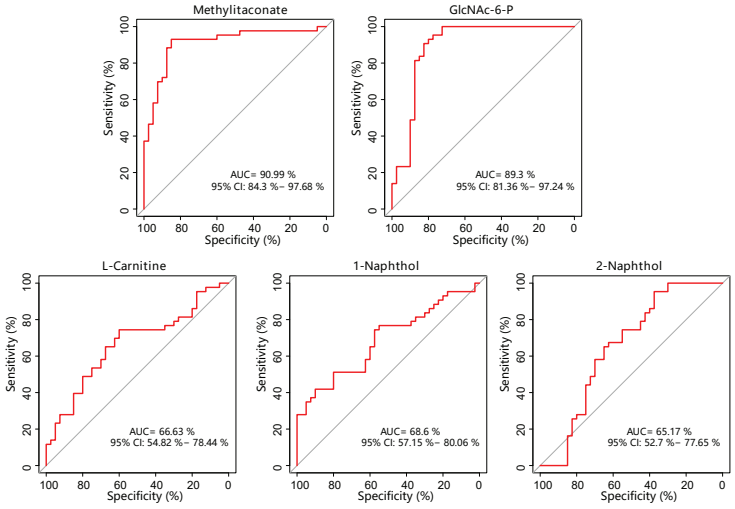
Supplementary figure 1 Two dimensions principal component analysis (PCA) score plot among QC samples and tested samples. Each point on the plot represents a sample. Blue points are CHD samples, red points are QC samples.



Supplementary figure 2 PCA score plot between 40 CHD patients and 43 controls. Each point on the plot represents a sample. Green points are control samples and red points are CHD patients.



(a)



(b)

Supplementary figure 3 (a).Receiver operating characteristic analysis (ROC) for combining 5 metabolites biomarkers by random forest classifier in training dataset. (b).ROC for 5 individual metabolites biomarkers in training dataset.

1.2 Supplementary tables

Supplementary table 1 List of 37 potential metabolites annotated in KEGG or HMDB database.

m/z	NAME	RT	FC	q-value	VIP	Formula	ppm	Adduct Ion	KEGG ID
496.3058791	20,26-Dihydroxyecdysone	744.104	42.22277725	0.016537466	5.860576254	C27H44O8	4.555162899	NAN	C16500
386.2897576	Cortol	662.962	0.177256317	1.17965E-08	1.127039967	C21H36O5	0.922283659	NH4+	C05482
372.0845309	10-Hydroxydihydrosanguinarine	684.837	677.6923435	9.06094E-12	1.152524356	C20H15NO5	0.831736433	Na+	C05247
337.215992	Progesterone	774.709	0.116855535	8.39054E-05	1.394324614	C21H30O2	6.981522154	Na+	C00410
330.2635353	(9Z,11E)-(13S)-13-Hydroperoxyoctadeca-9,11-dienoic acid	653.076	0.066128794	1.18451E-08	1.125637479	C18H32O4	1.112000483	NH4+	C04717
324.0458651	N-Acetyl-D-glucosamine 6-phosphate	541.3545	16.58021966	2.85283E-10	1.13430565	C8H16NO9P	1.260022221	Na+	C00357
318.2999289	Phytosphingosine	656.764	0.125893793	2.88908E-06	1.364406697	C18H39NO3	1.075521125	H+	C12144
315.1211881	p-Coumaroylagmatine	145.31	0.055570756	0.002488346	11.72764284	C14H20N4O2	2.157612793	K+	C04498
315.096019	N6-(L-1,3-Dicarboxypropyl)-L-lysine	142.1965	1.592761031	0.036647449	1.83995082	C11H20N2O6	2.624066784	K+	C00449
311.0511119	Dihydrokaempferol	611.26	374.5030074	2.3627E-10	1.1413235	C15H12O6	5.18705781	Na+	C00974
310.0474631	Indoleglycerol phosphate	611.2495	6672.904368	2.5567E-12	1.144547978	C11H14NO6P	8.26088368	Na+	C03506
309.0542143	Medicarpin	611.434	112.101097	5.01144E-12	1.139040566	C16H14O4	6.83977517	K+	C10503
274.9929078	2-Carboxy-2-hydroxy-8-carboxychromene	91.3841	0.093092459	0.002158523	1.639179892	C11H8O6	9.906101971	K+	C14094
274.2736949	Hexadecanoic acid	656.679	0.587371243	0.013559472	7.944786552	C16H32O2	1.398491469	NH4+	C00249
268.1909849	Xanthoxin	571.68	136.591287	4.25694E-05	1.028619144	C15H22O3	1.068740737	NH4+	C13453
255.0378919	5-(3'-Carboxy-3'-oxopropyl)-4,6-dihydroxypicolinate	117.92	2.380334491	0.000212966	1.1251526	C10H9NO7	0.038231114	NAN	C05656
249.1082592	N-Acetyl-L-2-amino-6-oxopimelate	117.643	2.34300363	7.79908E-08	1.034450246	C9H13NO6	0.645151037	NH4+	C05539
247.0927331	4-(L-Alanin-3-yl)-2-hydroxy-cis,cis-muconate 6-semialdehyde	146.379	2.089020606	4.15404E-06	1.166956456	C9H11NO6	1.192087644	NH4+	C04796
223.0935157	4-[(Hydroxymethyl)nitrosoamino]-1-(3-pyridinyl)-1-butanone	644.408	0.218596446	0.01310796	1.19187159	C10H13N3O3	9.751791312	NAN	C19563
203.1391048	Ecgonine	119.338	9.451089096	0.001669027	4.571128188	C9H15NO3	0.478055409	NH4+	C10858
170.0328456	Creatine	202.182	60.10103849	0.000899912	4.38910166	C4H9N3O2	1.610273281	K+	C00300
167.0564801	7-Methylxanthine	502.8765	0.574176323	0.00610874	1.356281558	C6H6N4O2	0.774809813	H+	C16353
167.0315121	Methylitaconate	104.76	1.379822769	3.14059E-11	1.413895688	C6H8O4	0.245625265	Na+	C02295
166.0956757	Cyromazine	485.317	0.263651446	0.000927962	1.331115204	C6H10N6	6.132959094	NAN	C14147
165.0548439	Phenylpyruvate	183.8775	0.061360622	0.019795195	1.6426491	C9H8O3	1.364400522	H+	C00166
162.1122492	L-Carnitine	114.494	0.060141963	0.007928564	4.09199533	C7H15NO3	1.366267104	H+	C00318
146.0600839	3-Fluorocatechol	531.627	0.033234667	0.004338839	3.362862486	C6FH5O2	8.566078644	NH4+	C16472
145.0649552	1-Naphthol	531.467	0.268318622	0.003501529	2.16639535	C10H8O	1.140369054	H+	C11714
145.0496085	2,3-Dimethylmaleate	1156.85	4.237658146	3.88395E-09	1.595234889	C6H8O4	0.511934162	H+	C00922
144.0761483	Thymine	532.091	11.14033766	0.0190977	2.509501537	C5H6N2O2	4.776910845	NH4+	C00178
144.0571958	2-Naphthol	531.9175	17.60713144	0.013559472	2.711841051	C10H8O	2.215229197	NAN	C11713
123.9826417	Sulfoacetaldehyde	769.939	6.838080583	0.002103838	1.268763864	C2H4O4S	3.128414471	NAN	C00593
103.0389661	2-Oxobutanoate	114.685	14.94987497	0.035362506	1.20782616	C4H6O3	0.038724242	H+	C00109
103.0500104	N-Formiminoglycine	485.3545	1.58903394	0.028471865	1.381467531	C3H6N2O2	1.891764033	H+	C02718
141.0908185	2,4-Diene-VPA	634.193	7.166516022	0.049497492	1.078658653	C8H12O2	1.335800813	H+	C16656
206.0948611	3-Dimethylallyl-4-hydroxybenzoate	531.681	0.751336614	2.13009E-05	1.031782125	C12H14O3	2.75016027	NAN	C12458
356.2792855	Aphidicolin	666.068	0.249898458	3.64113E-10	1.019572906	C20H34O4	0.730441253	NH4+	C06088

Supplementary table 2 Pathways related to the 7 signifiantly changed metabolites.

Pathway	Total[1]	Hits[2]	p-value[3]	Impact[4]
Nicotinate and nicotinamide metabolism	44	2	0.0064714	0.05538
Metabolism of xenobiotics by cytochrome P450	65	2	0.013818	0
Phenylalanine, tyrosine and tryptophan biosynthesis	27	1	0.076019	0
Phenylalanine metabolism	45	1	0.1239	0.04875
Amino sugar and nucleotide sugar metabolism	88	1	0.22976	0.01426

[1] Total metabolites in the pathway;
[2] Number of matched metabolites from the uploaded data to the metabolite's in the pathway;
[3] Significance of the uploaded metabolites enrich in the pathway by Fisher's exact test;
[4] Impact of the uploaded metabolites in the pathway;

Supplementary table 3 Information of 102 participants in testing dataset.

	CHD case	Healthy control	p-value	No. of participents (CHD/Control)
Gender(M/F)	45/10	16/26	NA	59/43
AGE	60.97(35-79)	58.63(50-70)	0.0536E-02	59/43
BMI	0	24.78(16.02-65.75)	NA	0/36
TRIG	1.80(0.67-4.83)	1.79(0.37-5.09)	0.956	59/43
LDLC	2.88(0.87-4.99)	3.32(1.79-5.64)	0.011	59/43
HDLC	1.03(0.66-1.59)	1.32(0.90-2.21)	3.17E-07	59/43
LPA	245.85(23.93-1386.11)	240.68(18.00-678.00)	0.908	59/43