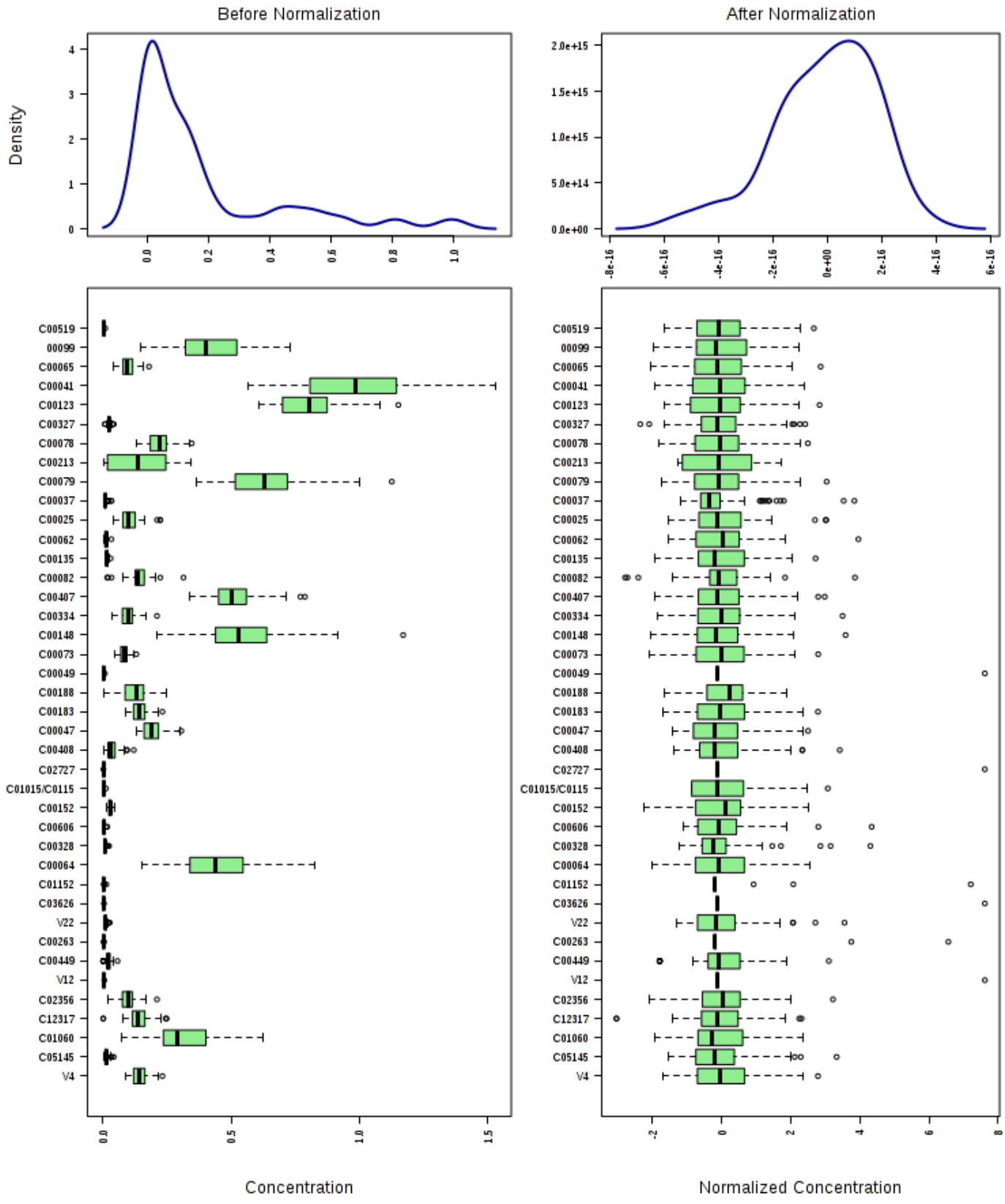
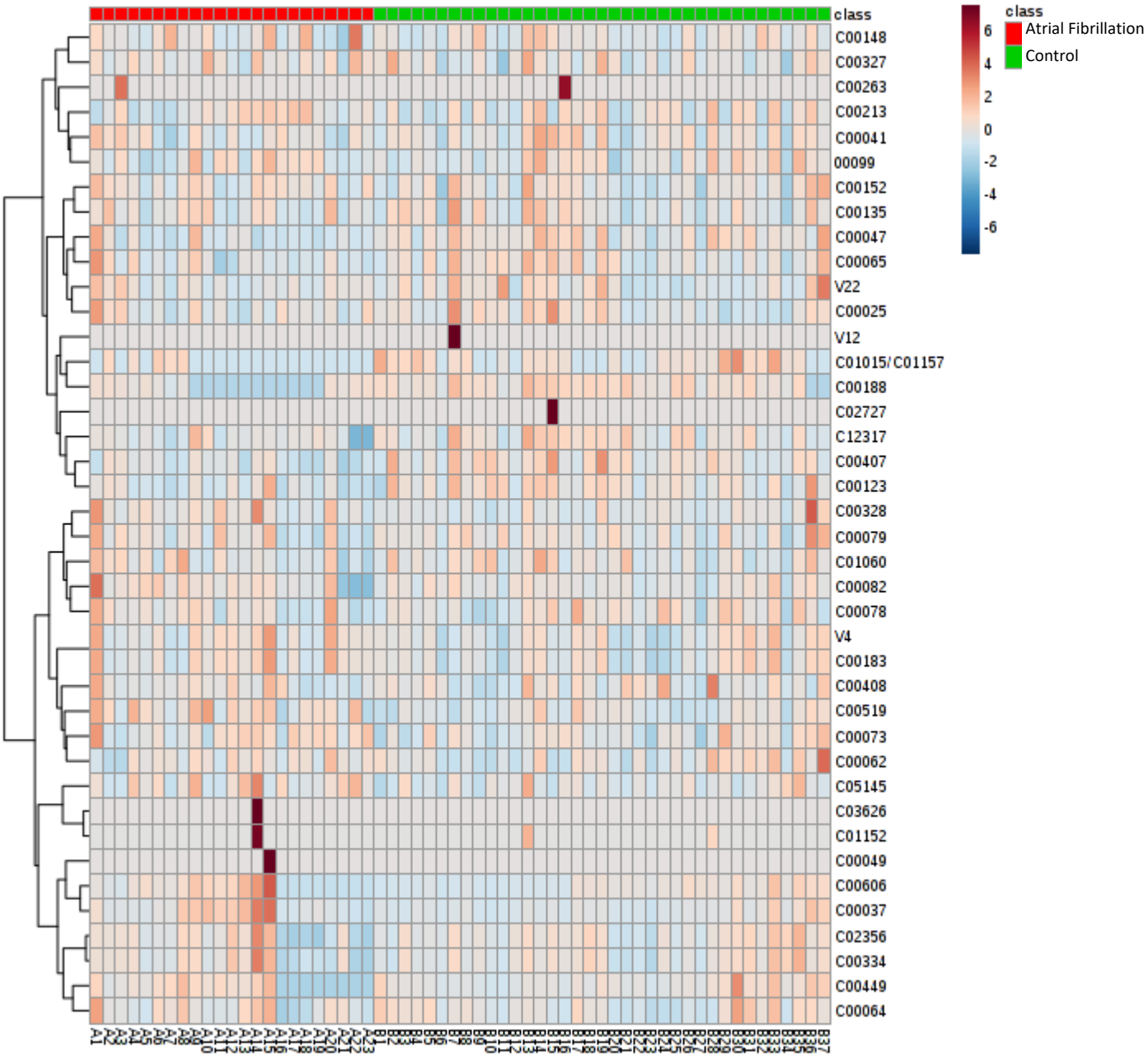
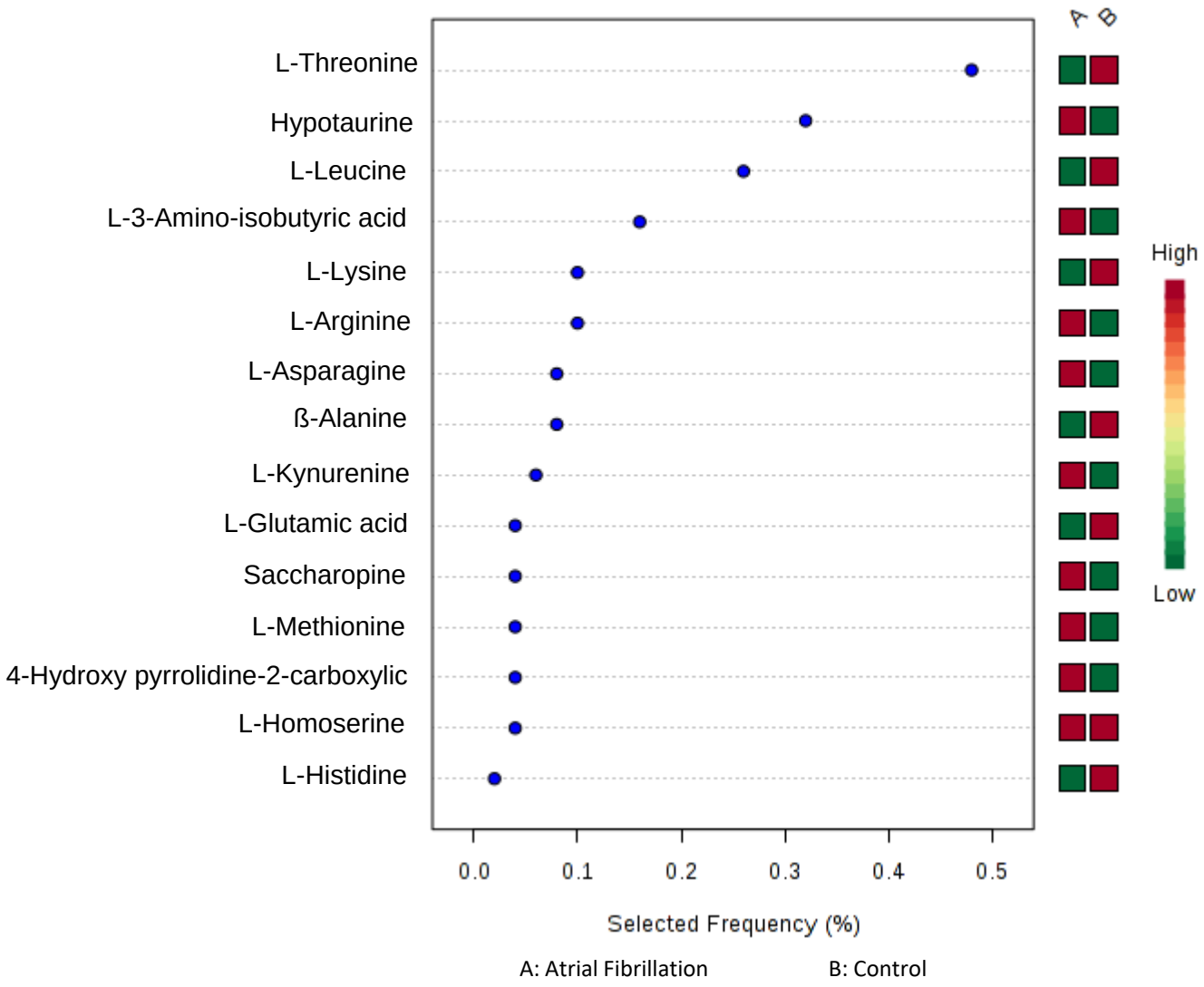
Supplementary Figure1 Data normalization



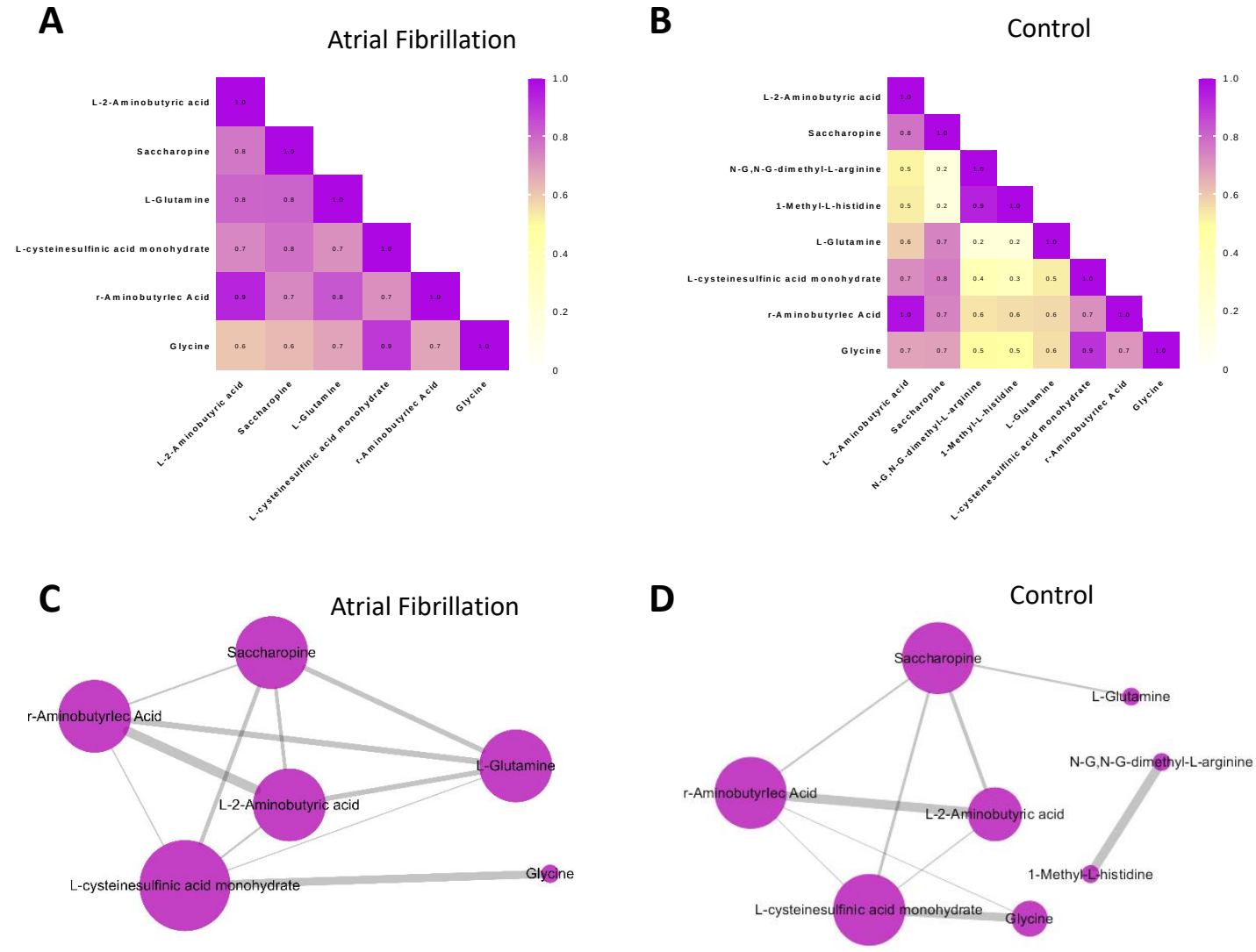
Supplementary Figure2 Heatmap of the overall amino acid



Supplementary Figure3 Multivariate Exploratory ROC Analysis



Supplementary Figure4 Correlation network of plasma amino acids between AF and Control



Supplementary Table1 List of plasma amino acids being tested

Number	Name	Molecular Formula	Molecular weight
1	L-Selenocystine	C6H12N2O4Se2	335.9122
2	5-Aminovaleric acid hydrochloride	C5H11NO2	117.079
3	h-Homoarginine	C7H16N4O2	188.1273
4	L-3-Amino-isobutyric acid	C4H9NO2	103.0633
5	3,5-Diiodo-L-tyrosine	C9H9I2NO3	432.8672
6	D-alloThreonine	C4H9NO3	119.0582
7	Seleno-L-methionine	C5H11NO2Se	196.995
8	L-2-Aminobutyric acid	C4H9NO2	103.0633
9	DL-Homocysteine	C4H9NO2S	135.0354
10	DL-Methionine sulfoxide	C5H11NO3S	165.046
11	Saccharopine	C11H20N2O6	276.1321
12	3-Hydroxyanthranilic acid	C7H7NO3	153.0426
13	Iodotyrosine	C9H10INO3	306.9706
14	L-leucyl-L-proline	C11H20N2O3	228.1474
15	DL-3,4-dihydroxyphenylalanine	C9H11NO4	197.0688
16	Glycyl-L-leucine	C8H16N2O3	188.1161
17	α-Phenylglycine	C8H9NO2	151.0633
18	L-Homoserine	C4H9NO3	119.0582
19	O-Acetyl-L-serine	C5H9NO4	147.0532
20	Iminodiacetic acid	C4H7NO4	133.0375
21	N-G,N-G-dimethyl-L-arginine	C8H18N4O2	202.143
22	1-Methyl-L-histidine	C7H11N3O2	169.0851
23	L-Glutamine	C5H10N2O3	146.0691
24	L-Kynurenine	C10H12N2O3	208.0848
25	gamma-Glu-epsilon-lys	C11H21N3O5	275.1481
26	5-Hydroxy-L-tryptophan	C11H12N2O3	220.0848
27	L-cysteinesulfinic acid monohydrate	C3H7NO4S	153.0096
28	Carnosine	C9H14N4O3	226.1066
29	L-Asparagine	C4H8N2O3	132.0535
30	4-Hydroxy pyrrolidine-2-carboxylic	C5H9NO3	131.0582
31	N-epsilon-Acetyl-L-lysine	C8H16N2O3	188.1161
32	Pipecolic acid	C6H11NO2	129.079
33	4-Aminobenzoic acid	C7H7NO2	137.0477
34	L-Cysteine-S-sulfate	C3H7NO5S2	200.9766
35	L-Lysine	C6H14N2O2	146.1055
36	L-Valine	C5H11NO2	117.079
37	L-Threonine	C4H9NO3	119.0582
38	L-Aspartic acid	C4H7NO4	133.0375
39	L-Methionine	C5H11NO2S	149.0511
40	L-Proline	C5H9NO2	115.0633
41	r-AminobutyrIec Acid	C4H9NO2	103.0633
42	L-Isoleucine	C6H13NO2	131.0946
43	L-Tyrosine	C9H11NO3	181.0739
44	L-Histidine	C6H9N3O2	155.0695
45	Taurine	C2H7NO3S	125.0147
46	L-Arginine	C6H14N4O2	174.1117
47	L-Glutamic acid	C5H9NO4	147.0532
48	Glycine	C2H5NO2	75.03203
49	L-Homocystine	C8H16N2O4S2	268.0552
50	L-Phenylalanine	C9H11NO2	165.079
51	Sarcosine	C3H7NO2	89.04768
52	L-Tryptophan	C11H12N2O2	204.0899
53	L-Citrulline	C6H13N3O3	175.0957
54	L-Leucine	C6H13NO2	131.0946
55	L-Alanine	C3H7NO2	89.04768
56	L-Serine	C3H7NO3	105.0426
57	ß-Alanine	C3H7NO2	89.04768
58	L-Cystathionine	C7H14N2O4S	222.0674
59	Hypotaurine	C2H7NO2S	109.0198
60	L-Cysteine	C3H7NO2S	121.0198
61	L-Norvaline	C5H11NO2	117.08

Supplementary Table2 Enrichment Analysis of metabolite sets associated with pathways

Metabolite Set	Total	Hits	Statistic	Expected	P value	Holm P	FDR
Threonine and 2-Oxobutanoate Degradation	20	1	31.193	1.6949	3.5316E-06	0.00015186	0.00015186
Carnitine Synthesis	22	2	12.119	1.6949	0.00037787	0.01587	0.0079718
Glycine and Serine Metabolism	59	7	7.5315	1.6949	0.00055617	0.022803	0.0079718
Valine, Leucine and Isoleucine Degradation	60	4	9.9358	1.6949	0.0011726	0.046905	0.012606
Biotin Metabolism	8	1	13.902	1.6949	0.003347	0.13053	0.028784
Taurine and Hypotaurine Metabolism	12	2	9.1238	1.6949	0.006621	0.2516	0.04745
Bile Acid Biosynthesis	65	1	10.337	1.6949	0.012249	0.45321	0.065838
Porphyrin Metabolism	40	1	10.337	1.6949	0.012249	0.45321	0.065838
Lysine Degradation	30	3	5.6139	1.6949	0.022918	0.80212	0.1095
Methionine Metabolism	43	5	4.2539	1.6949	0.029322	0.99694	0.12608
Alanine Metabolism	17	2	5.2955	1.6949	0.041662	1	0.14929
Glutathione Metabolism	21	2	5.2955	1.6949	0.041662	1	0.14929

Supplementary Table3 Enrichment Analysis of metabolite sets associated with disease

Metabolite Set	Total	Hits	Statistic	Expected	P value	Holm P	FDR
EARLY MARKERS OF MYOCARDIAL INJURY	14	5	13.955	1.6949	1.5159E-05	0.0010612	0.00098217
PYRIDOXAMINE 5-PRIME-PHOSPHATE OXIDASE DEFICIENCY	3	2	20.765	1.6949	2.8062E-05	0.0019363	0.00098217
HEART FAILURE	10	5	13.284	1.6949	4.6901E-05	、	0.0010944
REFRACTORY LOCALIZATION-RELATED EPILEPSY	10	10	9.1562	1.6949	0.00010351	0.0069351	0.0018114
PYRUVATE DEHYDROGENASE DEFICIENCY (E3)	7	3	13.163	1.6949	0.00024116	0.015916	0.0033762
NEONATAL INTRAHEPATIC CHOLESTASIS	12	5	8.1042	1.6949	0.0009638	0.062647	0.011244
METABOLITES AFFECTED BY GENDER	9	3	9.0053	1.6949	0.0014982	0.095885	0.014982

Supplementary Figure1 Data normalization.

Supplementary Figure2 Heatmap of the overall amino acid.

Supplementary Figure3 Multivariate Exploratory ROC Analysis.

Supplementary Figure4 Correlation network of amino acids between AF and Control. A. Heatmap of the strongly correlated amino acids in AF patients. B. Heatmap of the strongly correlated amino acids in control patients. The figures within each crossover represented the correlation efficiency between the respective amino acids. Purple color indicated enhanced co-expression and yellow color indicated decreased co-expression. Correlation threshold was set as 0.7. C. and D. The respective correlation network for AF and control patients.

Supplementary Table1 List of plasma amino acids being tested.

Supplementary Table2 Enrichment Analysis of metabolite sets associated with pathways.

Supplementary Table3 Enrichment Analysis of metabolite sets associated with disease.