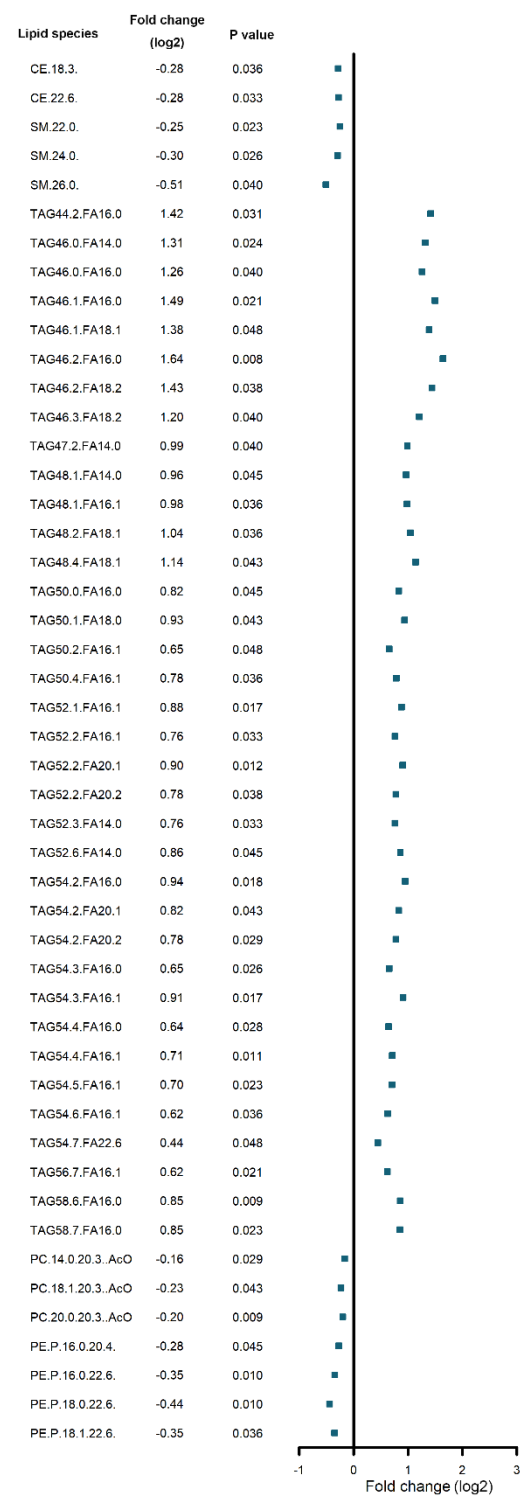


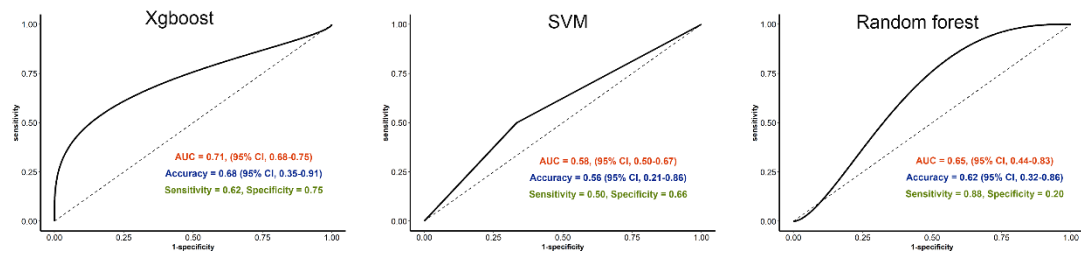
Supplemental Figure 1. Fold change of altered lipid species in CMD



Fold change and statistical significance of lipid species significantly altered in CMD patients are displayed. P values were corrected using the Benjamini-Hochberg method.

CE, cholesterol ester; CMD, coronary microvascular dysfunction; DAG, diacylglycerol; PC, phosphatidylcholine; PE(P), alkenylphosphatidylethanolamine; SM, sphingomyelin; TAG, triacylglycerol.

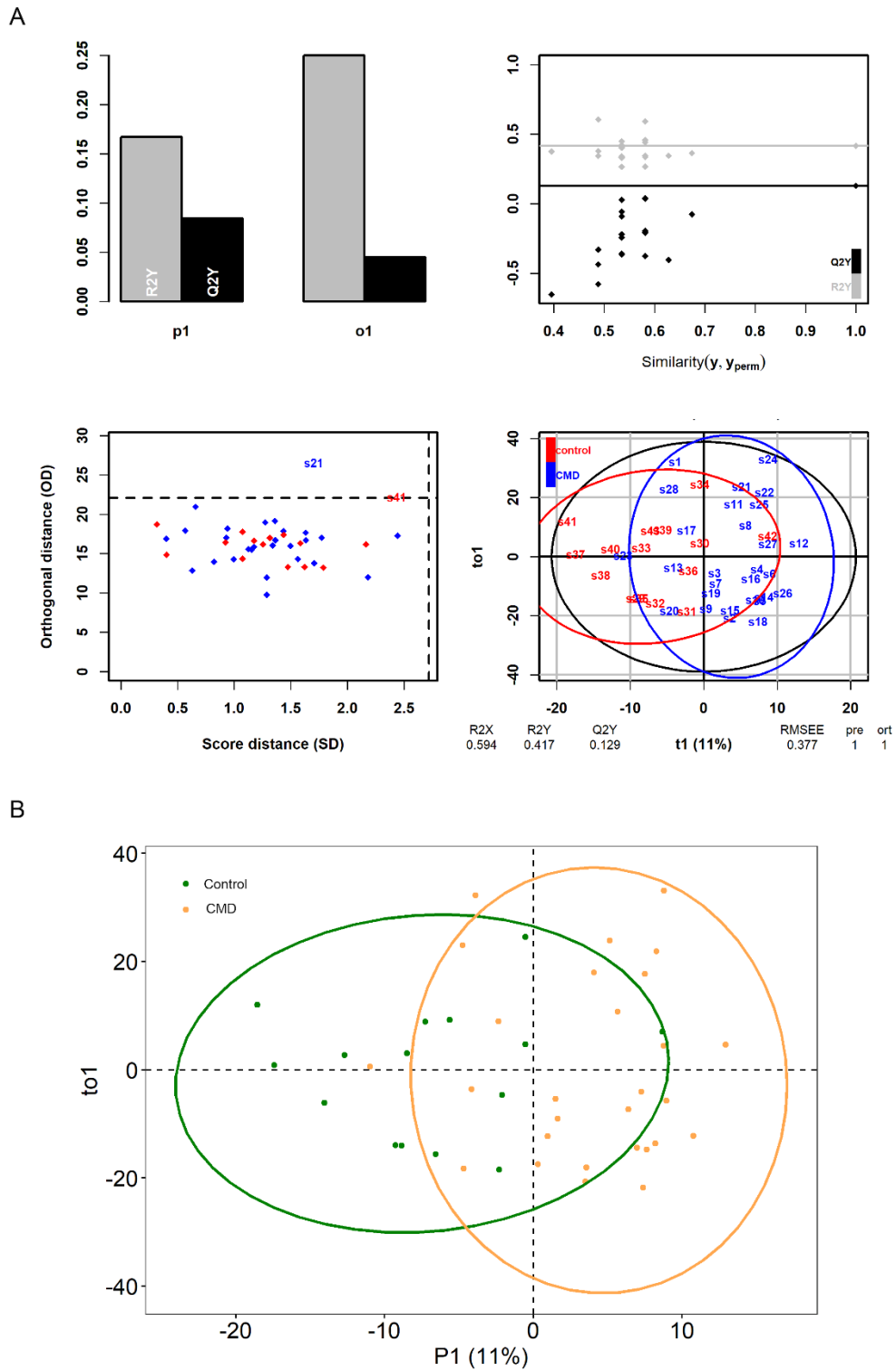
Supplemental Figure 2. Comparison of machine learning models



The diagnostic performance of three machine learning models is shown.

AUC, are under the receiver operating characteristic curve.

Supplemental Figure 3. Details of OPLS-DA.



(A) Overview of OPLS-DA model. (B) Sample distribution.

CMD, coronary microvascular dysfunction; OPLS-DA, orthogonal partial least squares discriminant analysis.

Supplemental table 1. Frequency of lipid species in lasso regression repeated 200 times

Lipid species	Frequency
CE(18:3)	200
PE(P-18:0/22:6)	200
TAG47:2-FA14:0	200
TAG48:4-FA18:1	200
TAG57:10-FA22:6	200
DAG(16:1/20:0)	199
PE(16:0/22:6)	199
PC(18:1/20:3)	197
PE(16:0/18:3)	197
DAG(14:0/18:1)	184
DAG(18:2/22:4)	180
PE(14:0/18:2)	175
DAG(18:2/20:3)	159
PC(16:0/22:4)	158
PE(18:0/22:6)	151

CE, cholesterol ester; DAG, diacylglycerol; PC, phosphatidylcholine; PE, phosphatidylethanolamine; PE(P), alkenylphosphatidylethanolamine; TAG, triacylglycerol.

Supplemental Table 2. VIP scores from OPLS-DA

Lipid species with VIP score >1 derived from OPLS-DA are displayed.

VIP, variable importance in projection; OPLS-DA, orthogonal partial least squares discriminant analysis.

Lipids	Vip score
CE(16:1)	1.116291
CE(18:0)	1.447354
CE(18:1)	1.491676
CE(18:2)	1.355203
CE(18:3)	1.8472
CE(22:4)	1.029348
CE(22:5)	1.172887
CE(22:6)	1.57623
CER(16:0)	1.185579
DAG(16:1/20:0)	1.25869
DAG(18:1/20:5)	1.004893
DAG(18:2/20:3)	1.01429
DAG(18:2/22:4)	1.404031
DAG(18:2/22:5)	1.047785
LPC(18:0)	1.20934
LPC(18:3)	1.534306
LPC(22:4)	1.014665
LPC(22:5)	1.395954
LPC(22:6)	1.548172
PC(14:0/20:3)	1.818895
PC(16:0/18:0)	1.151586
PC(16:0/18:2)	1.076216
PC(16:0/18:3)	1.69967
PC(16:0/20:2)	1.578032
PC(16:0/20:3)	1.533138
PC(16:0/20:4)	1.309817
PC(16:0/22:4)	1.490328
PC(16:0/22:5)	1.007853
PC(16:0/22:6)	1.723875
PC(18:0/18:0)	1.049104
PC(18:0/18:1)	1.030024
PC(18:0/18:2)	1.207888
PC(18:0/18:3)	1.509237
PC(18:0/20:1)	1.551263
PC(18:0/20:2)	1.540059
PC(18:0/20:3)	1.538251
PC(18:0/20:4)	1.273282

PC(18:0/22:4)	1.443958
PC(18:0/22:5)	1.288023
PC(18:0/22:6)	1.636261
PC(18:1/18:3)	1.681265
PC(18:1/20:3)	1.618261
PC(18:1/20:4)	1.056448
PC(18:1/22:4)	1.234061
PC(18:1/22:5)	1.515966
PC(18:1/22:6)	1.588763
PC(18:2/18:2)	1.368939
PC(18:2/18:3)	1.566716
PC(18:2/20:3)	1.378426
PC(18:2/20:4)	1.637465
PC(18:2/20:5)	1.303222
PC(18:2/22:4)	1.365597
PC(18:2/22:5)	1.482077
PC(18:2/22:6)	1.902144
PC(20:0/20:3)	1.900538
PE(16:0/18:1)	1.069966
PE(16:0/18:2)	1.322309
PE(16:0/18:3)	1.819459
PE(16:0/20:3)	1.02413
PE(16:0/20:4)	1.627401
PE(16:0/20:5)	1.167134
PE(16:0/22:5)	1.311899
PE(16:0/22:6)	1.994862
PE(18:0/18:0)	1.654023
PE(18:0/18:1)	1.030183
PE(18:0/18:2)	1.237553
PE(18:0/18:3)	1.696015
PE(18:0/20:4)	1.511027
PE(18:0/20:5)	1.245616
PE(18:0/22:4)	1.26016
PE(18:0/22:5)	1.461303
PE(18:0/22:6)	1.923882
PE(18:1/18:2)	1.018346
PE(18:1/18:3)	1.382237
PE(18:1/20:4)	1.152718
PE(18:1/22:5)	1.428766
PE(18:1/22:6)	1.769823
PE(18:2/16:1)	1.246538
PE(18:2/18:2)	1.1087
PE(18:2/18:3)	1.482722

PE(18:2/20:4)	1.354401
PE(18:2/22:6)	1.003547
PE(O-16:0/20:5)	1.41694
PE(O-16:0/22:6)	1.498323
PE(O-18:0/18:2)	1.317148
PE(O-18:0/20:4)	1.095727
PE(O-18:0/20:5)	1.332935
PE(O-18:0/22:6)	1.259472
PE(P-16:0/16:1)	1.046873
PE(P-16:0/18:2)	1.121973
PE(P-16:0/18:3)	1.379465
PE(P-16:0/20:4)	1.483697
PE(P-16:0/22:6)	2.094759
PE(P-18:0/16:1)	1.395008
PE(P-18:0/18:1)	1.231048
PE(P-18:0/18:2)	1.29373
PE(P-18:0/18:3)	1.73655
PE(P-18:0/20:4)	1.400711
PE(P-18:0/22:6)	2.005375
PE(P-18:1/18:2)	1.106089
PE(P-18:1/18:3)	1.468052
PE(P-18:1/20:4)	1.167479
PE(P-18:1/22:6)	1.932927
PE(P-18:2/18:2)	1.134129
PE(P-18:2/20:4)	1.436795
PE(P-18:2/22:6)	1.811824
SM(16:0)	1.176378
SM(22:0)	1.63562
SM(22:1)	1.279354
SM(24:0)	1.729084
SM(24:1)	1.276203
SM(26:0)	1.552432
SM(26:1)	1.026565
TAG42:1-FA18:1	1.026102
TAG44:1-FA16:0	1.190405
TAG44:1-FA18:1	1.097572
TAG44:2-FA16:0	1.074586
TAG44:2-FA18:2	1.007734
TAG46:0-FA14:0	1.155292
TAG46:0-FA16:0	1.010243
TAG46:1-FA14:0	1.009062
TAG46:1-FA16:0	1.176778
TAG46:1-FA16:1	1.148024

TAG46:1-FA18:0	1.013428
TAG46:1-FA18:1	1.121919
TAG46:2-FA16:0	1.383833
TAG46:2-FA16:1	1.141183
TAG46:2-FA18:1	1.156257
TAG46:2-FA18:2	1.157663
TAG46:3-FA16:0	1.067209
TAG46:3-FA18:2	1.050339
TAG47:1-FA18:1	1.089596
TAG47:2-FA14:0	1.854857
TAG48:0-FA14:0	1.007294
TAG48:1-FA14:0	1.040366
TAG48:1-FA16:1	1.022625
TAG48:1-FA18:0	1.205359
TAG48:2-FA14:0	1.031524
TAG48:2-FA18:0	1.115046
TAG48:2-FA18:1	1.162275
TAG48:3-FA16:1	1.043231
TAG48:3-FA18:1	1.056153
TAG48:3-FA18:2	1.090151
TAG48:4-FA18:1	1.399062
TAG48:4-FA18:2	1.018304
TAG49:1-FA17:0	1.144249
TAG49:3-FA16:0	1.010678
TAG50:0-FA14:0	1.007731
TAG50:1-FA14:0	1.073506
TAG50:1-FA18:0	1.018679
TAG50:2-FA14:0	1.022019
TAG50:2-FA18:0	1.049045
TAG50:2-FA18:1	1.005103
TAG50:3-FA16:0	1.004402
TAG50:3-FA16:1	1.03006
TAG50:3-FA18:0	1.188033
TAG50:3-FA18:1	1.005287
TAG50:3-FA18:3	1.040993
TAG50:4-FA16:1	1.029597
TAG50:4-FA18:1	1.004925
TAG51:5-FA18:2	1.064298
TAG51:5-FA18:3	1.25499
TAG52:1-FA16:1	1.094546
TAG52:2-FA14:0	1.324525
TAG52:2-FA16:1	1.065101
TAG52:2-FA20:1	1.184823

TAG52:2-FA20:2	1.044172
TAG52:3-FA14:0	1.054134
TAG52:3-FA16:1	1.046477
TAG52:3-FA18:3	1.081829
TAG52:3-FA20:0	1.072746
TAG52:4-FA14:0	1.027042
TAG52:4-FA16:1	1.017613
TAG52:4-FA18:3	1.076514
TAG52:5-FA16:0	1.052906
TAG52:5-FA18:3	1.147191
TAG52:6-FA16:0	1.293089
TAG52:6-FA18:3	1.069345
TAG52:6-FA20:4	1.020763
TAG52:8-FA16:1	1.005731
TAG52:8-FA18:2	1.066924
TAG53:2-FA18:2	1.096579
TAG53:4-FA17:0	1.00132
TAG53:4-FA18:3	1.219239
TAG53:5-FA20:4	1.005718
TAG53:6-FA20:4	1.189624
TAG54:2-FA16:0	1.123311
TAG54:2-FA20:1	1.059783
TAG54:2-FA20:2	1.040519
TAG54:3-FA16:0	1.104645
TAG54:3-FA16:1	1.18891
TAG54:4-FA16:0	1.096388
TAG54:4-FA16:1	1.162487
TAG54:4-FA18:3	1.054364
TAG54:5-FA16:1	1.202027
TAG54:5-FA18:0	1.000165
TAG54:5-FA18:3	1.024773
TAG54:5-FA20:4	1.04362
TAG54:6-FA16:1	1.053753
TAG54:6-FA18:1	1.03986
TAG54:6-FA18:3	1.160592
TAG54:6-FA20:4	1.203627
TAG54:7-FA18:1	1.266555
TAG54:7-FA18:2	1.133481
TAG54:7-FA18:3	1.116039
TAG54:7-FA20:4	1.164546
TAG54:8-FA18:2	1.334869
TAG54:8-FA18:3	1.264319
TAG54:8-FA20:4	1.0283

TAG55:2-FA18:2	1.228308
TAG55:3-FA18:2	1.062188
TAG55:5-FA20:4	1.294616
TAG56:10-FA18:2	1.040662
TAG56:3-FA16:0	1.076763
TAG56:4-FA16:0	1.014828
TAG56:5-FA20:4	1.046223
TAG56:6-FA20:4	1.137213
TAG56:6-FA20:5	1.036437
TAG56:7-FA16:1	1.195384
TAG56:7-FA18:0	1.028487
TAG56:7-FA18:3	1.308546
TAG56:7-FA20:4	1.274943
TAG56:7-FA22:5	1.03305
TAG56:8-FA18:2	1.206067
TAG56:8-FA18:3	1.38056
TAG56:8-FA20:4	1.241944
TAG56:8-FA20:5	1.028289
TAG56:9-FA18:3	1.59914
TAG56:9-FA20:4	1.355804
TAG56:9-FA20:5	1.109648
TAG57:10-FA22:6	1.47316
TAG58:10-FA20:4	1.170275
TAG58:10-FA22:5	1.174842
TAG58:6-FA16:0	1.256378
TAG58:7-FA16:0	1.166
TAG58:8-FA20:4	1.004486
TAG58:9-FA22:5	1.127259
TAG60:11-FA22:5	1.151594