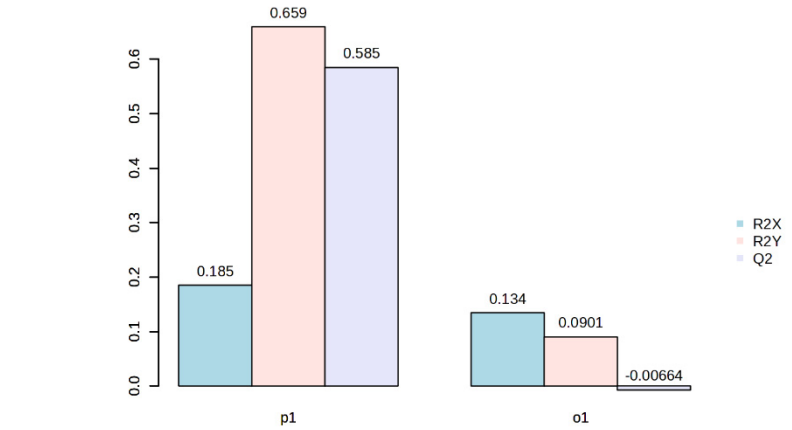
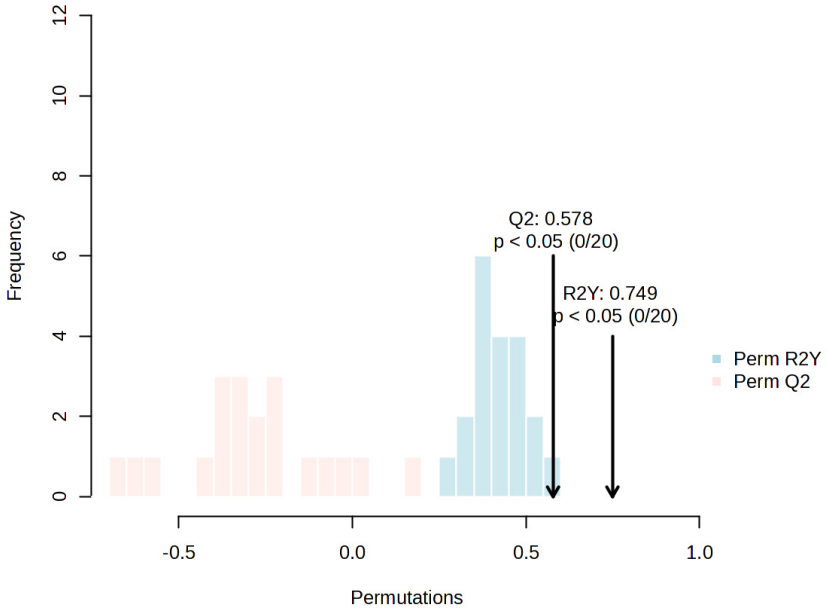
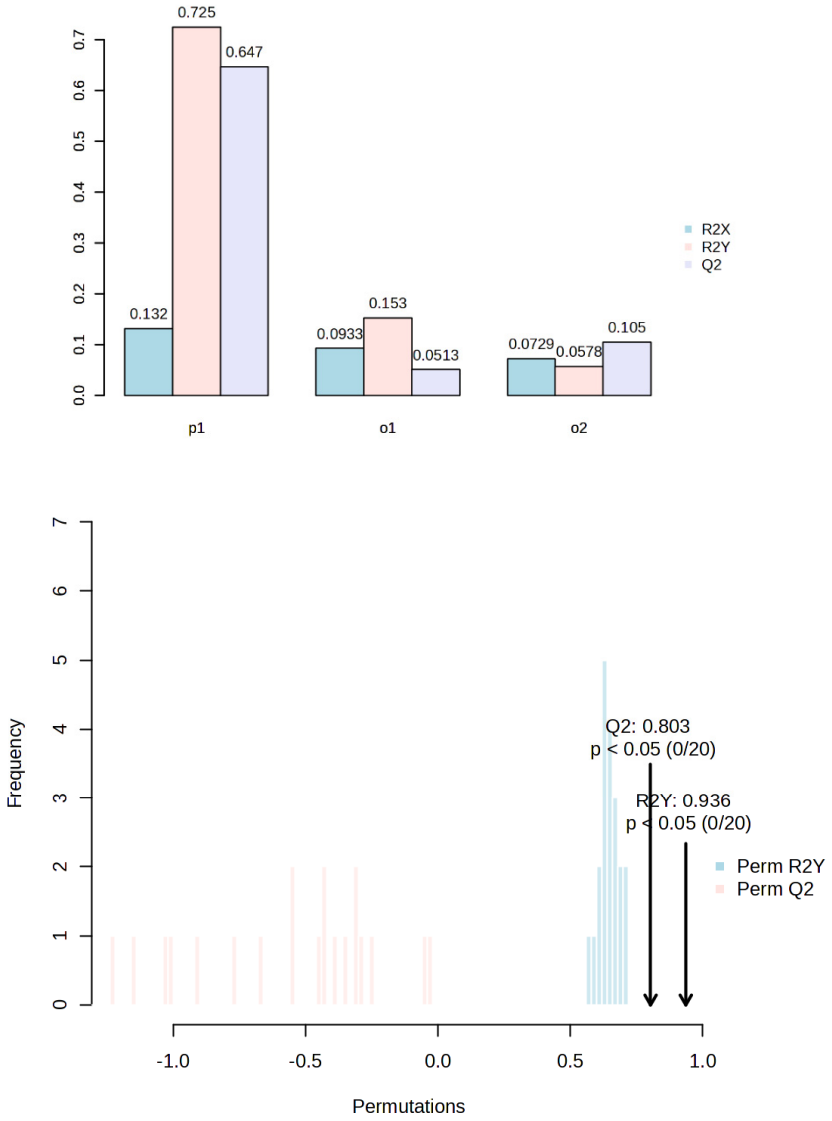
(A)


0.659
0.585
0.185
0.134
0.0901
-0.00664
0.0
0.1
0.2
0.3
0.4
0.5
0.6
p1
o1
R2X
R2Y
Q2


Frequency
0
2
4
6
8
10
12
Q2: 0.578
p < 0.05 (0/20)
R2Y: 0.749
p < 0.05 (0/20)
Perm R2Y
Perm Q2
-0.5
0.0
0.5
1.0
Permutations

(B)



Supplementary Figure S1. Validation of orthogonal partial least-squares discriminant analysis (o-PLS-DA) models used for discrimination between non-MASLD and MASLD patients. **(A)** Positive-ion mode o-PLS-DA model. Model-fit statistics (R^2X, R^2Y, and Q^2) and permutation-test results are shown. $R^2X = 0.195$, $R^2Y = 0.650$, and $Q^2 = 0.585$. Permutation testing yielded $R^2Y = 0.749$ ($p < 0.05$) and $Q^2 = 0.578$ ($p < 0.05$). **(B)** Negative-ion mode o-PLS-DA model. Model-fit statistics (R^2X, R^2Y, and Q^2) and permutation-test results are shown. $R^2X = 0.182$, $R^2Y = 0.729$, and $Q^2 = 0.647$. Permutation testing yielded $R^2Y = 0.936$ ($p < 0.05$) and $Q^2 = 0.803$ ($p < 0.05$).