

## **Multi-platform metabolomics: enhancing the severity risk prognosis of SARS-CoV-2 infection**

*Vinicius S. Lima,<sup>1†</sup> Sinara T. B. Morais,<sup>2†</sup> Vinicius G. Ferreira,<sup>2,3†</sup> Mariana B. Almeida,<sup>2,3†</sup>, Manuel Pedro Barros Silva<sup>1†</sup>, Thais de A. Lopes,<sup>4</sup> Juliana M. de Oliveira,<sup>4</sup> Joyce R. S. Raimundo,<sup>5</sup> Danielle Z. S. Furtado,<sup>1</sup> Fernando L. A. Fonseca,<sup>5,6</sup> Regina V. Oliveira,<sup>4</sup> Daniel R. Cardoso,<sup>2\*</sup> Emanuel Carrilho,<sup>2,3\*</sup> Nilson A. Assunção,<sup>1,6\*</sup>*

<sup>1</sup> Programa de Pós-Graduação em Medicina Translacional, Departamento de Medicina, Escola Paulista de Medicina, Universidade Federal de São Paulo, São Paulo, SP, Brazil.

<sup>2</sup> Instituto de Química de São Carlos, Universidade de São Paulo, São Carlos, SP, Brazil.

<sup>3</sup> Instituto Nacional de Ciência e Tecnologia de Bioanalítica, INCTBio, Campinas, SP, Brazil.

<sup>4</sup> Departamento de Química, Universidade Federal de São Carlos, São Carlos, SP, Brazil.

<sup>5</sup> Faculdade de Medicina do ABC, Santo André, SP, Brazil.

<sup>6</sup> Departamento de Química, Universidade Federal de São Paulo, São Paulo, SP, Brazil.

<sup>†</sup> These authors contributed equally to this work.

\*Corresponding authors:

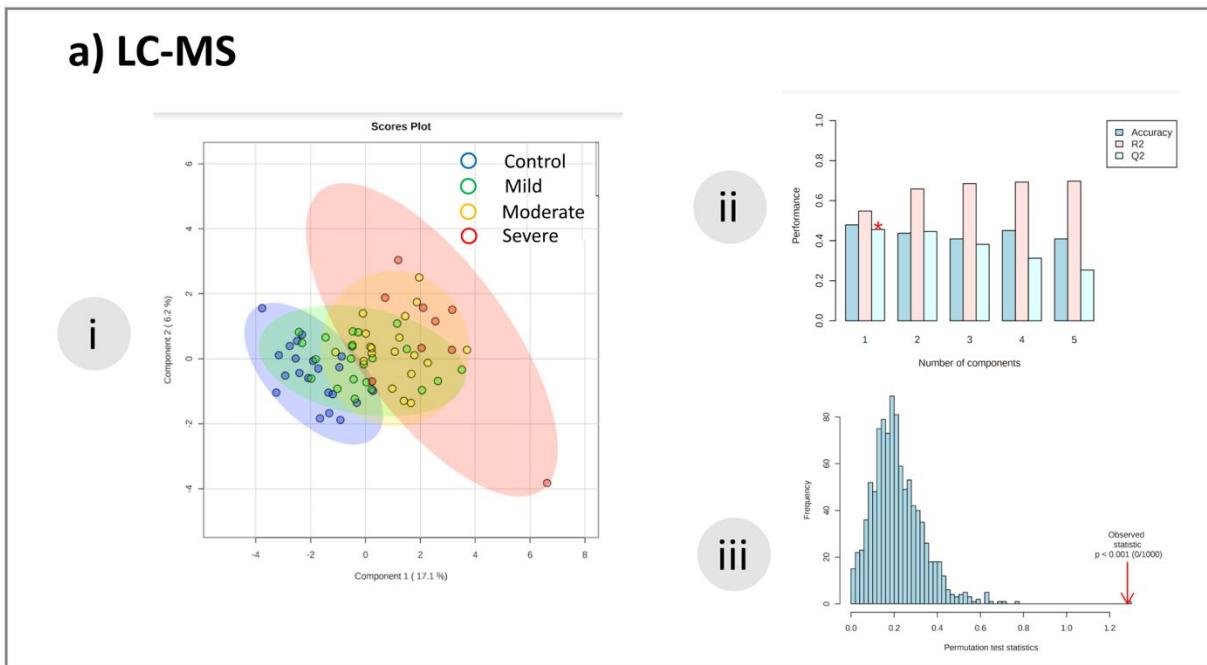
Nilson A. Assunção - [nilson.assuncao@unifesp.br](mailto:nilson.assuncao@unifesp.br)

Emanuel Carrilho - [emanuel@iqsc.usp.br](mailto:emanuel@iqsc.usp.br)

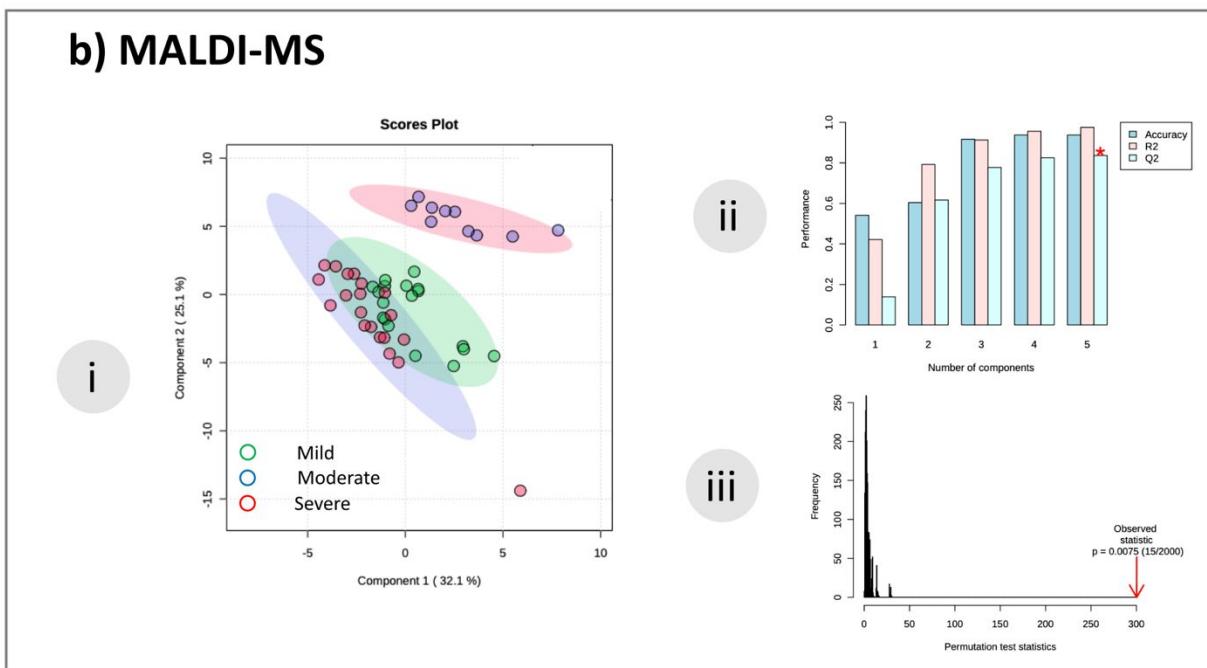
Daniel R. Cardoso - [drcardoso@usp.br](mailto:drcardoso@usp.br)

## 1. Supporting Information

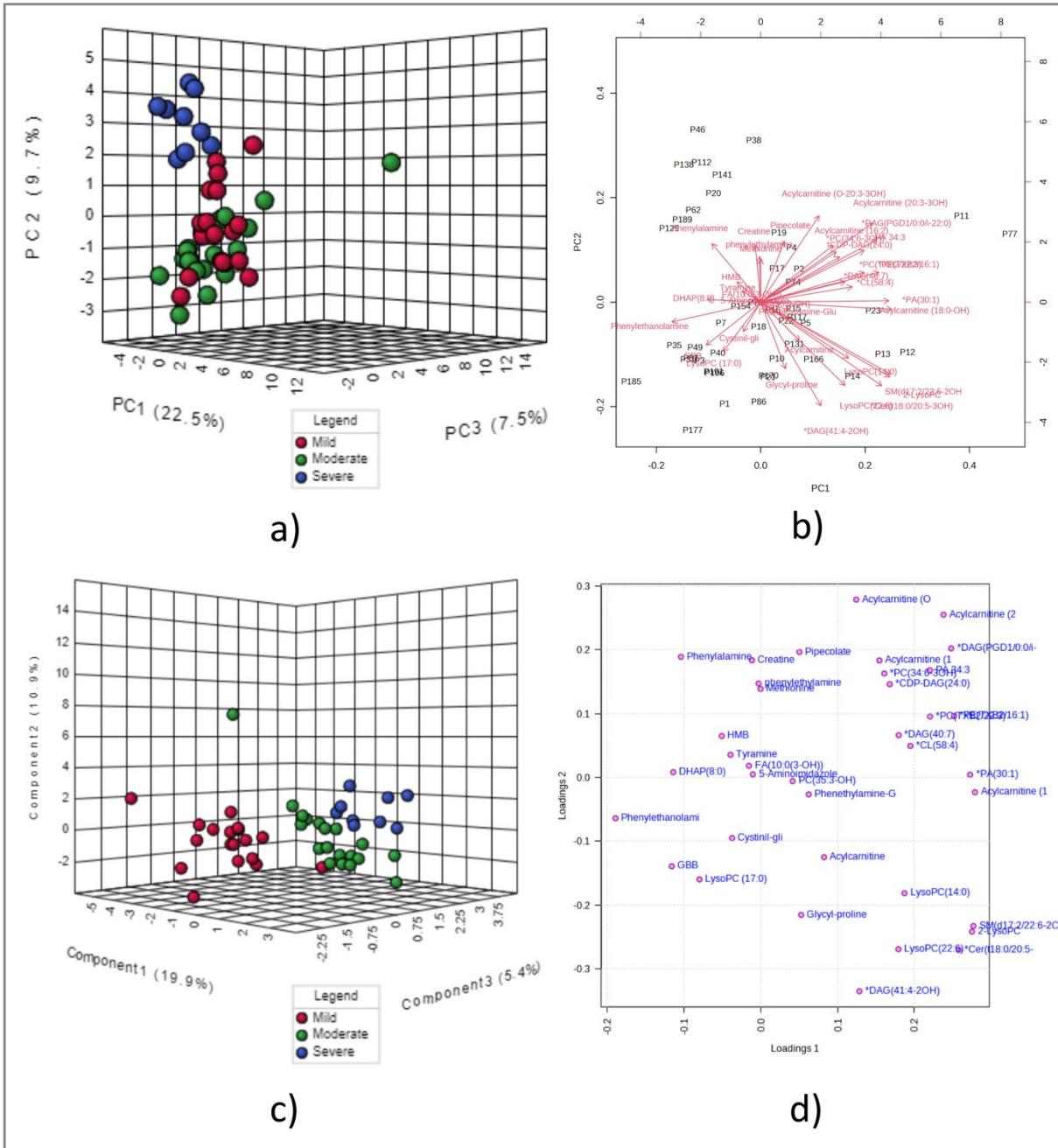
### a) LC-MS



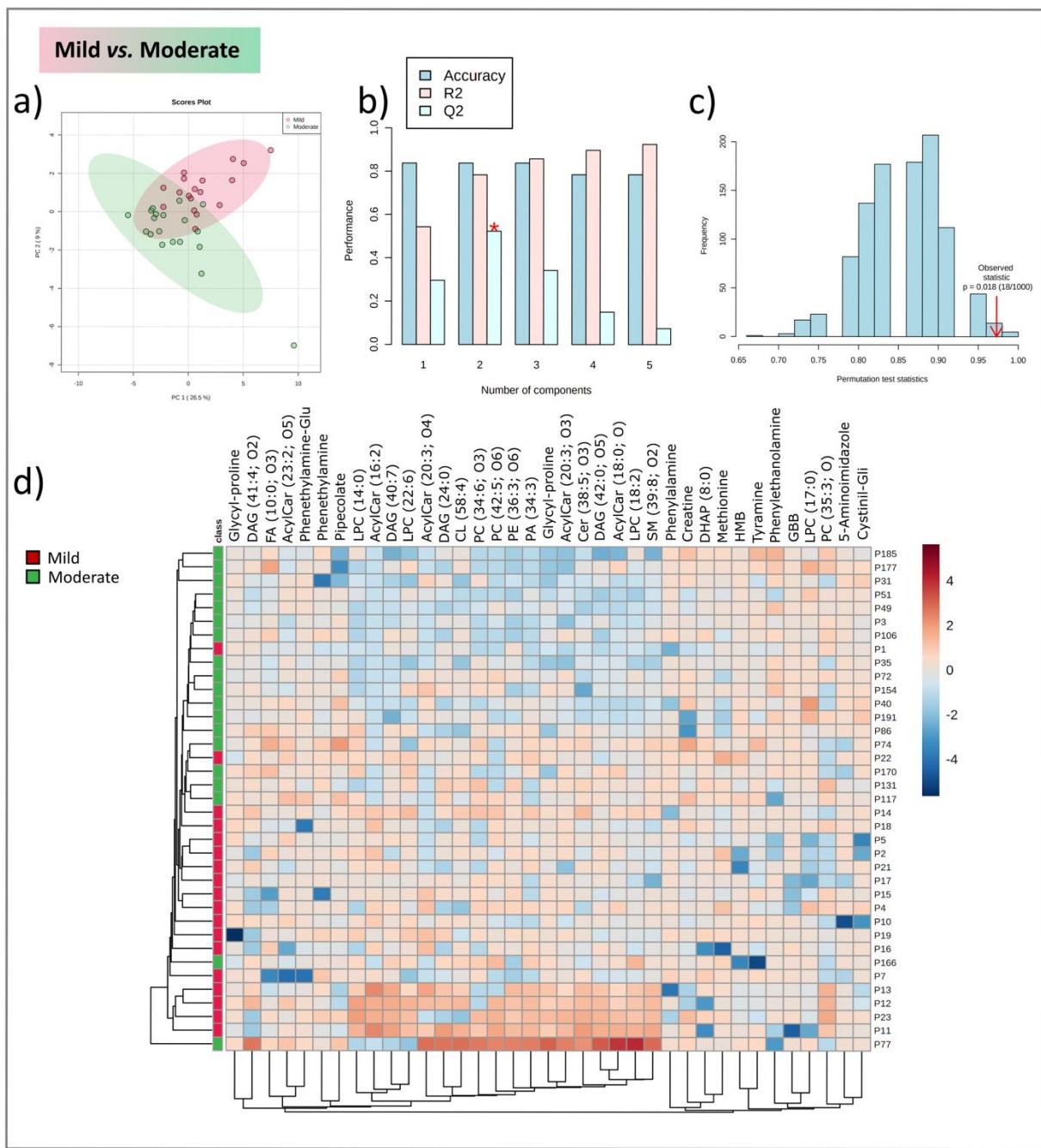
### b) MALDI-MS



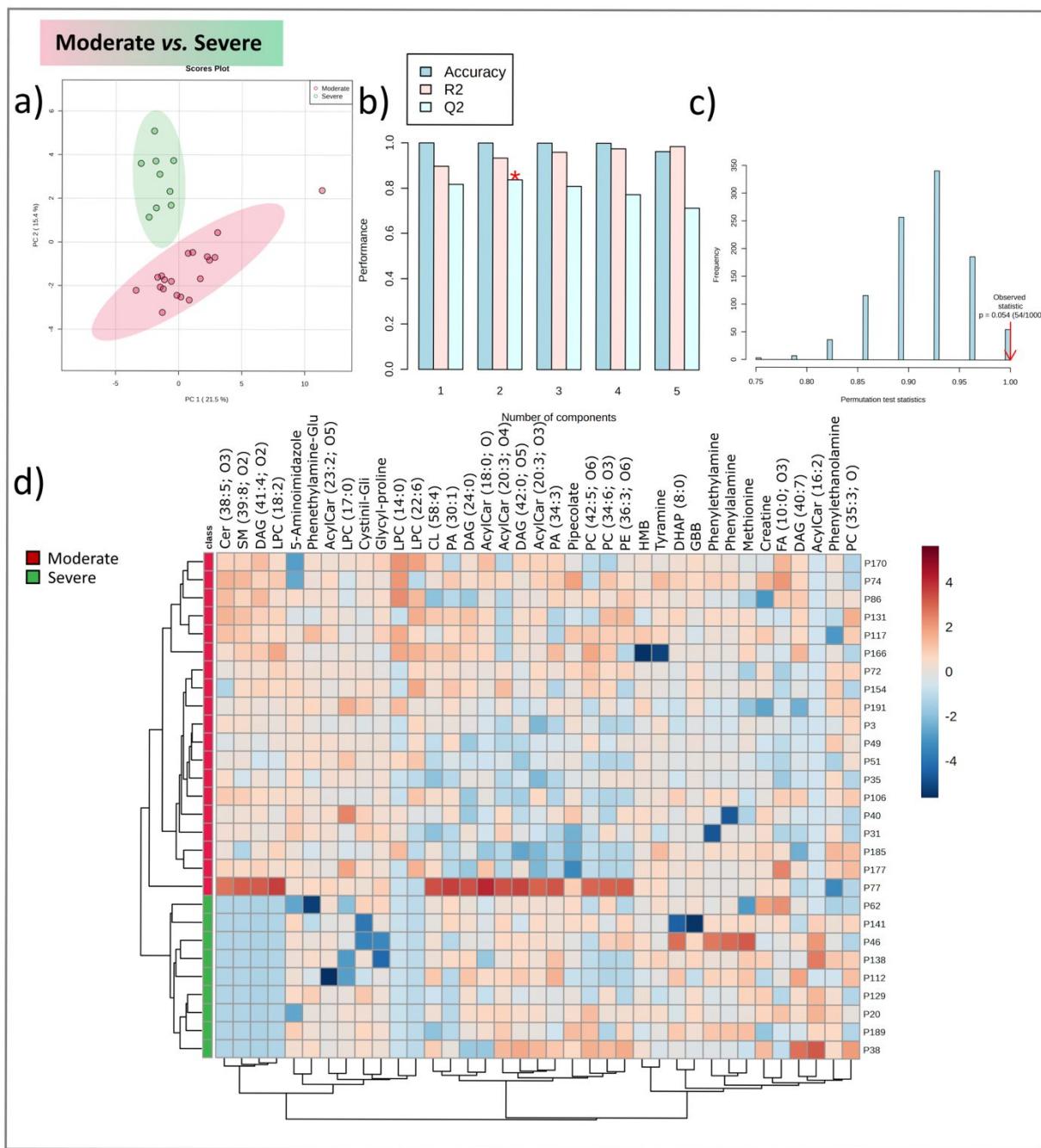
**Figure S1.** Statistical analysis for a) LC-MS and b) MALDI-MS datasets. The figure displays the plots of PLS-DA (i), cross-validation (ii), and permutation test (iii).



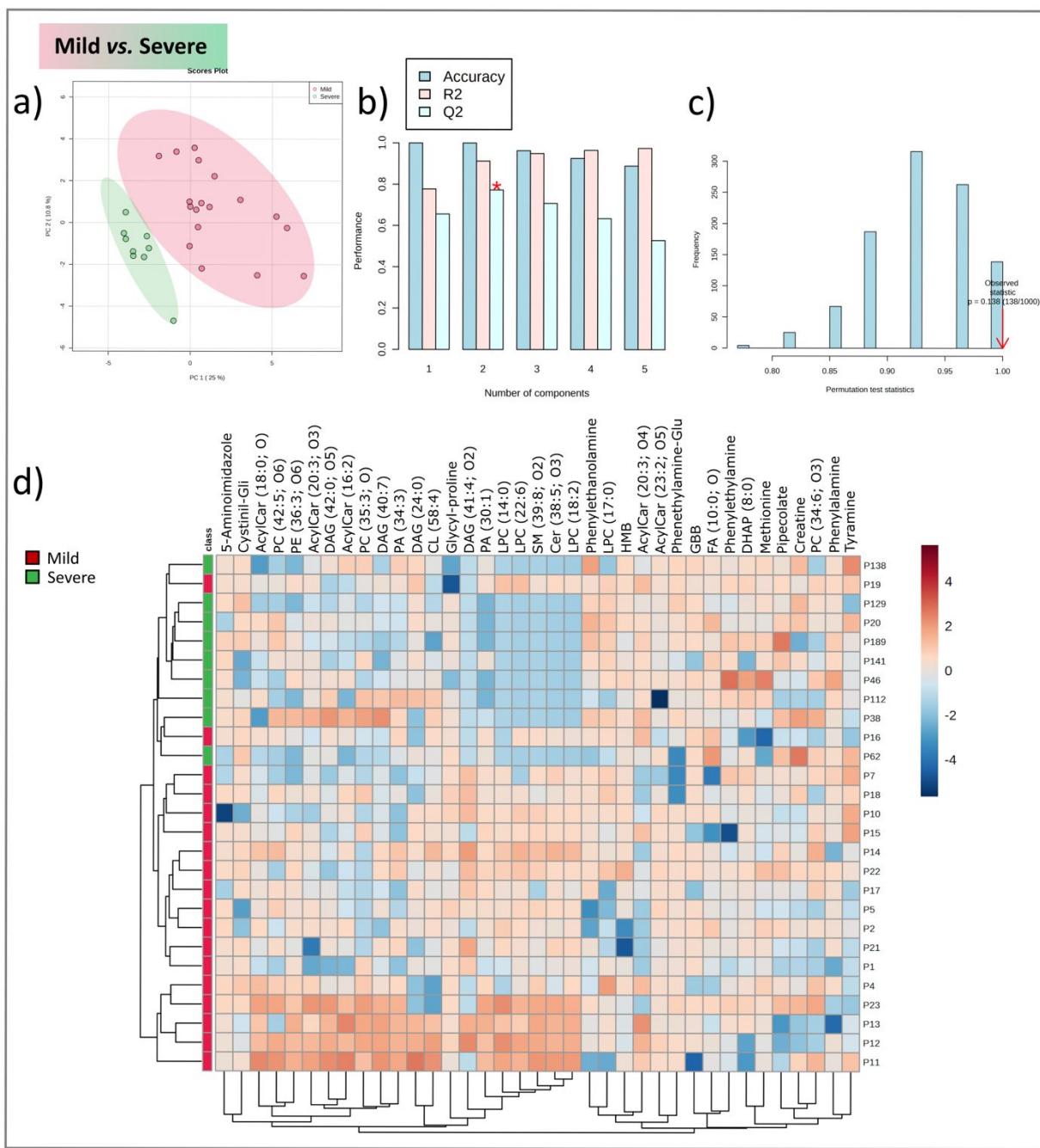
**Figure S2.** Multi-platform statistical analysis: 3D PCA (a) and biplot (b); 3D PLS-DA (c) and loadings plot (d).



**Figure S3.** Mild vs. Moderate PCA and PLS-DA validation metrics: a) PCA, b) cross-validation, c) permutation test, and d) heatmap.

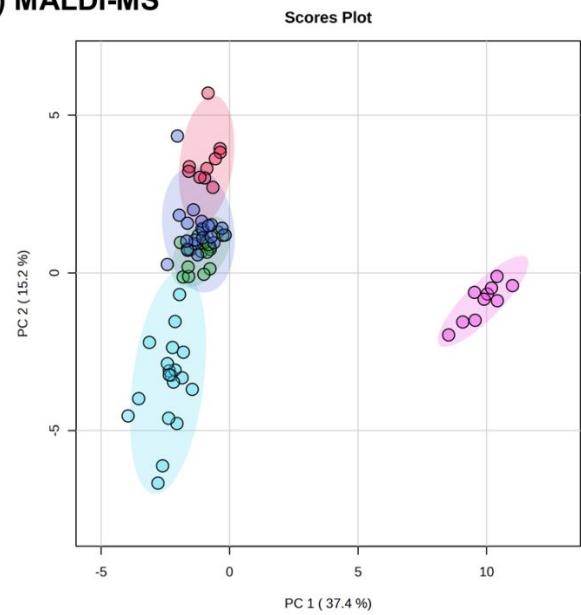


**Figure S4.** Moderate vs. Severe PCA and PLS-DA validation metrics: a) PCA, b) cross-validation, c) permutation test, and d) heatmap.

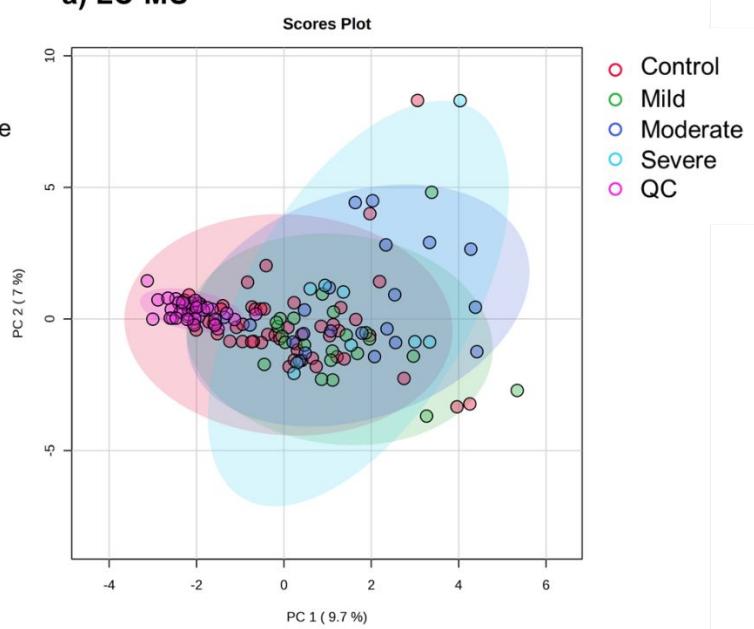


**Figure S5.** Mild vs. Severe PCA and PLS-DA validation metrics: a) PCA, b) cross-validation, c) permutation test, and d) heatmap.

**a) MALDI-MS**



**a) LC-MS**



**Figure S6.** PCA Scores Plot analysis of LC-MS and MALDI-TOF data separately.