

SUPPLEMENTARY FIGURE 4

Theoretical and Experimental Plant Physiology (Thematic Collection: Metabolomics and plant metabolism regulation and integration)

NON-TARGETED METABOLOMIC ANALYSIS OF FIELD-GROWN *Coffea arabica* CULTIVARS REVEALS DISTINCT LEAF METABOLIC SIGNATURES

Authors: Jéfyne Campos Carréra¹, Leonor Guerra-Guimarães^{2,3}, John Charles D'Auria⁴, Luana de Jesus Sartori¹, Carla Pinheiro^{5,6}, Vânia Aparecida Silva⁷, Margarete Lordelo Volpato⁷, Gladyston Rodrigues Carvalho⁷, Fabio Akira Mori¹

¹UFLA - Universidade Federal de Lavras, 37200-000 Lavras, Minas Gerais, Brasil.

²CIFC - Centro de Investigação das Ferrugens do Cafeeiro, Jardim Botânico da Ajuda, Instituto Superior de Agronomia, Universidade de Lisboa, Calçada da Ajuda, 1300-011 Lisboa, Portugal.

³LEAF - Linking Landscape, Environment, Agriculture and Food Research Centre and TERRA Associated Laboratory, Instituto Superior de Agronomia, Universidade de Lisboa, Tapada da Ajuda, 1349-017, Lisboa, Portugal.

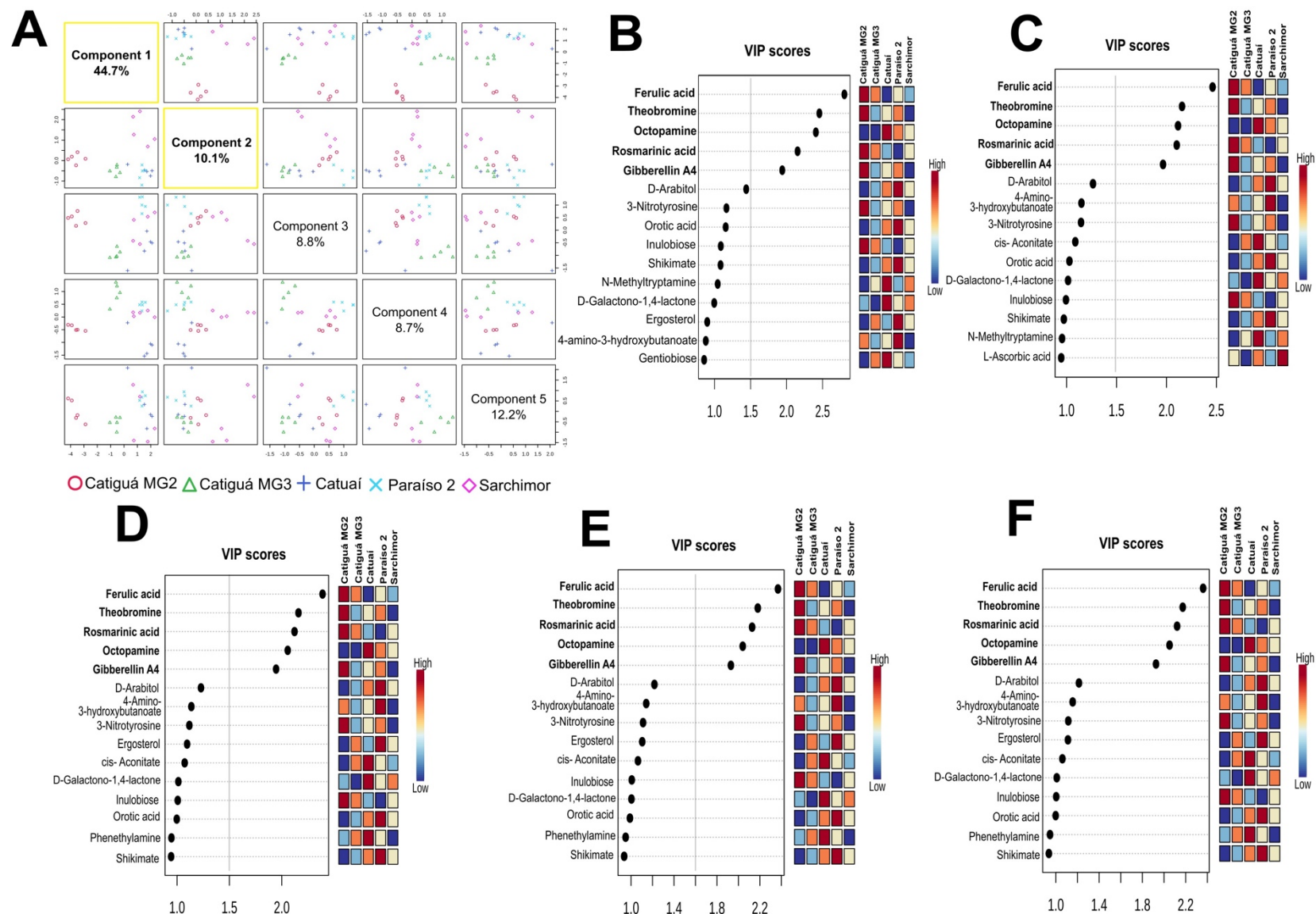
⁴Research Group Metabolic Diversity, Department of Molecular Genetics, Leibniz Institute of Plant Genetics and Crop Plant Research (IPK Gatersleben), OT Gatersleben, Corrensstraße 3, 06466 Seeland, Germany

⁵UCIBIO Applied Molecular Biosciences Unit, Department of Life Sciences, NOVA School of Science and Technology, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal.

⁶Associate Laboratory i4HB Institute for Health and Bioeconomy, NOVA School of Science and Technology, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal.

⁷EPAMIG – Empresa de Pesquisa Agropecuária de Minas Gerais, 37200-000 Lavras, Minas Gerais, Brasil.

Correspondence author: Leonor Guerra-Guimarães, CIFC - Centro de Investigação das Ferrugens do Cafeeiro, Jardim Botânico da Ajuda, Instituto Superior de Agronomia, Universidade de Lisboa, Calçada da Ajuda, 1300-011 Lisboa, Portugal. E-mail: leonorguimaraes@isa.ulisboa.pt. <https://orcid.org/0000-0002-9676-1036>.



Supplementary Figure 4 PLS-DA Model analysis. A: Percentual values of variance explanation of the five components. B: Variable Importance Plot of Component 1. C: Variable Importance Plot of Component 2. D: Variable Importance Plot of Component 3. E: Variable Importance Plot of Component 4. F: Variable Importance Plot of Component 5. (*) Indication of the highest value of accuracy. R2: Coefficient of determination. Q2: Predictive relevance, based on sum of squared errors (Szymańska et al. 2012). Metabolic features highlighted in bold were identified as key discriminants for distinguishing between cultivars based on the PLS-DA model.

Reference: Szymańska E, Saccenti E, Smilde AK, Westerhuis JA (2012) Double-check: validation of diagnostic statistics for PLS-DA models in metabolomics studies. *Metabolomics* 8(1):3-16. doi: 10.1007/s11306-011-0330-3.