# SUPPORTING INFORMATION

# NMR Metabolomics and Chemometrics of Commercial Varieties of *Phaseolus vulgaris* L. Seeds from Italy and In Vitro Antioxidant and Antifungal Activity

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† These authors contributed equally to this work.

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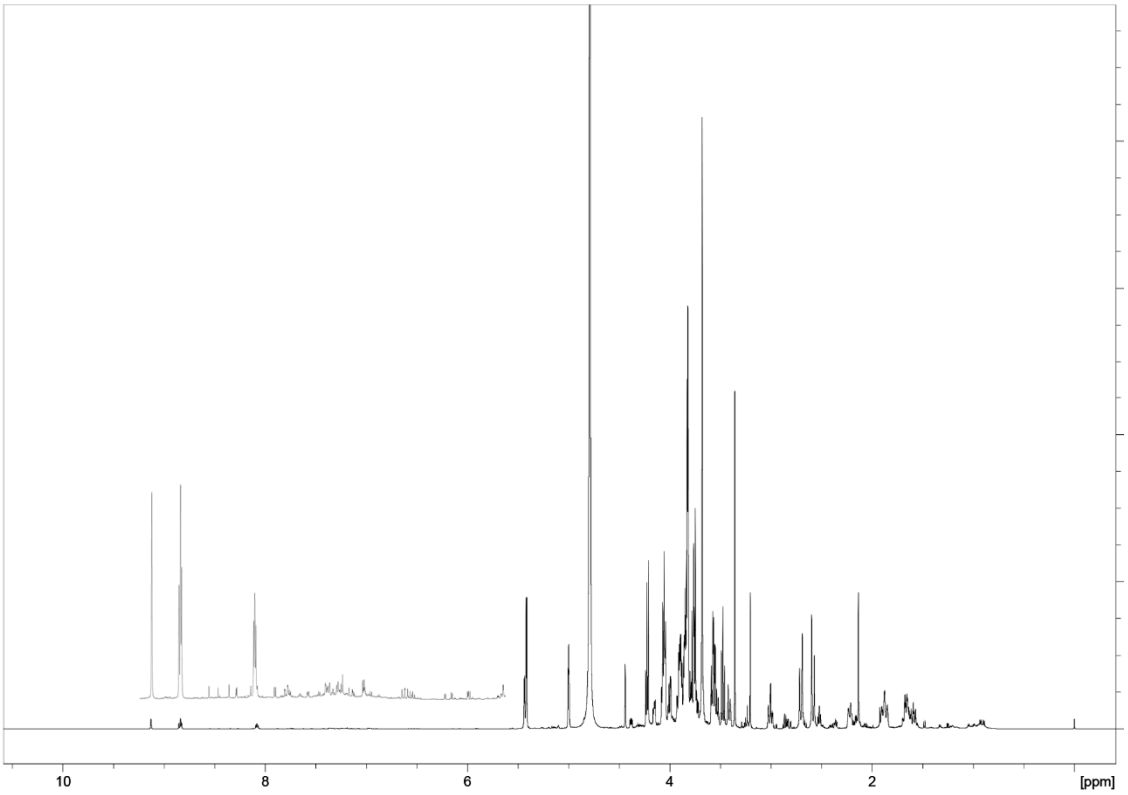


**Figure S1.** $^{1}$H-NMR spectrum in $D_2O$ of polar extract of *Phaseolus* Cannellino (PCANN) at 600 MHz.

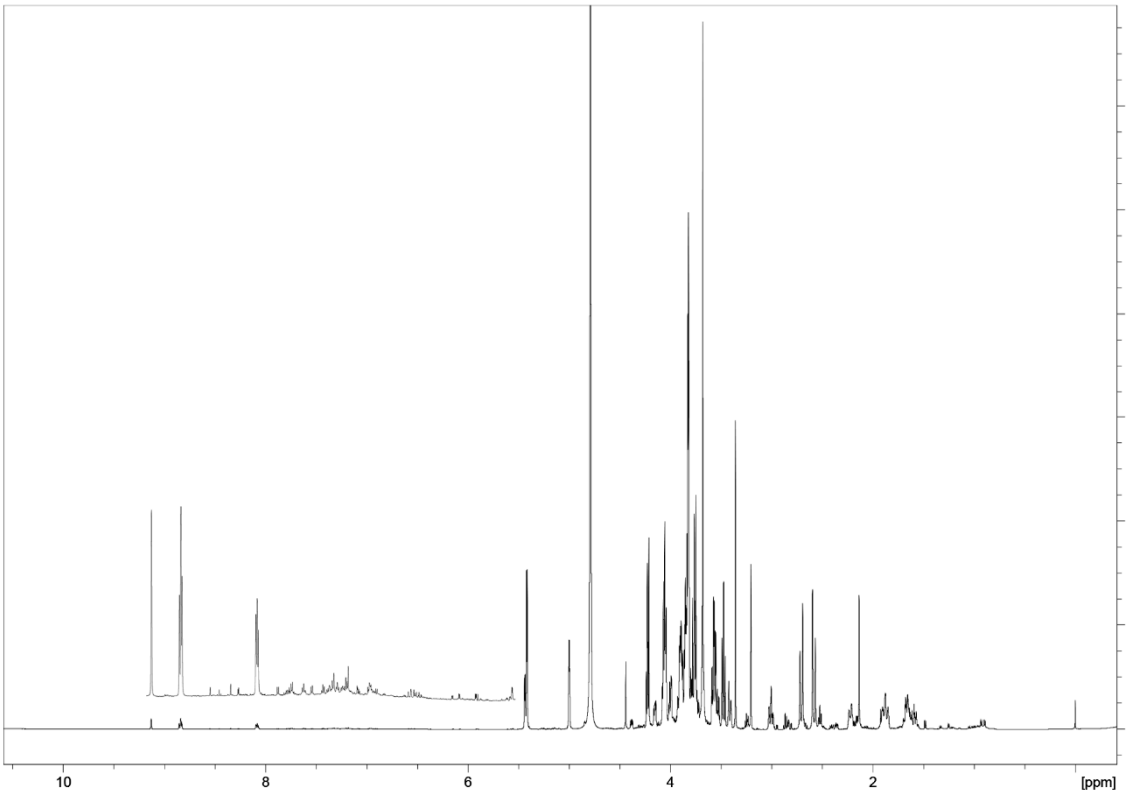


**Figure S2.** $^{1}$H-NMR spectrum in $D_2O$ of polar extract of *Phaseolus* Controne (PCON) at 600 MHz.

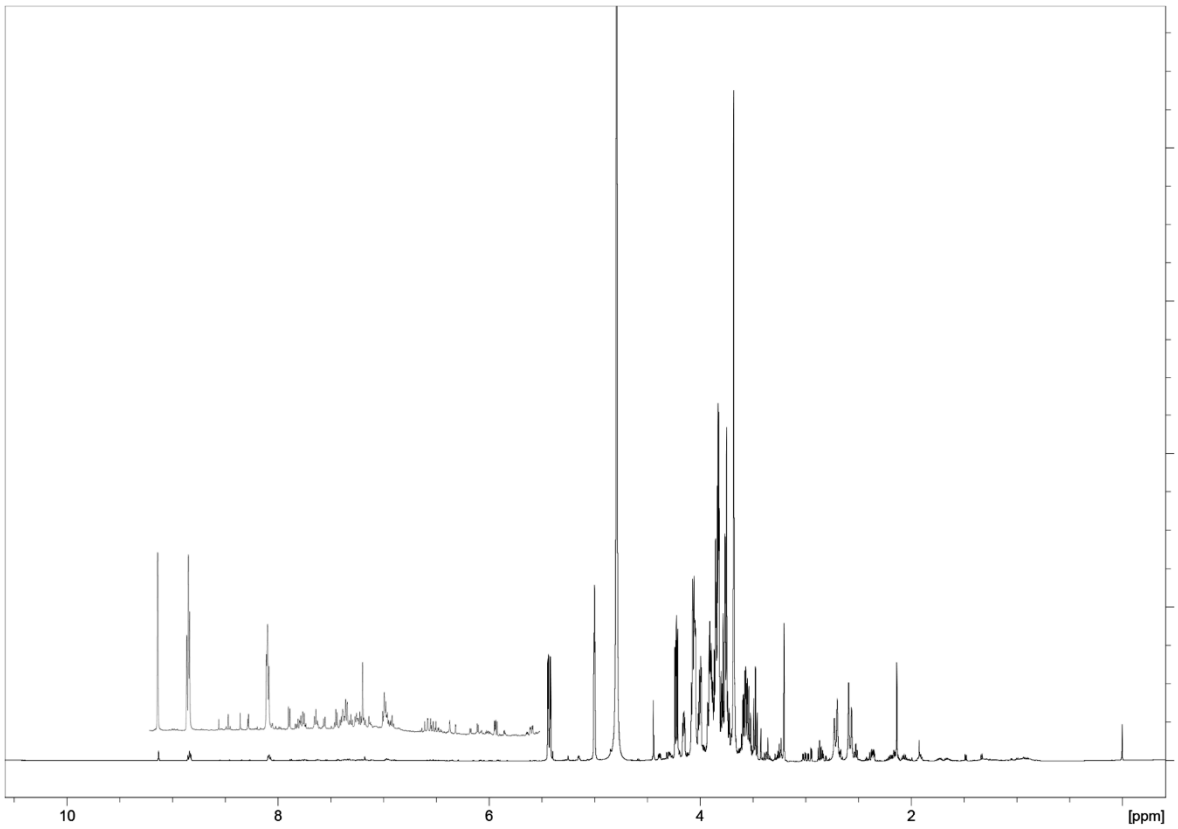


**Figure S3.** $^{1}$H-NMR spectrum in $D_2O$ of polar extract of *Phaseolus* Occhio Nero (PON) at 600 MHz.

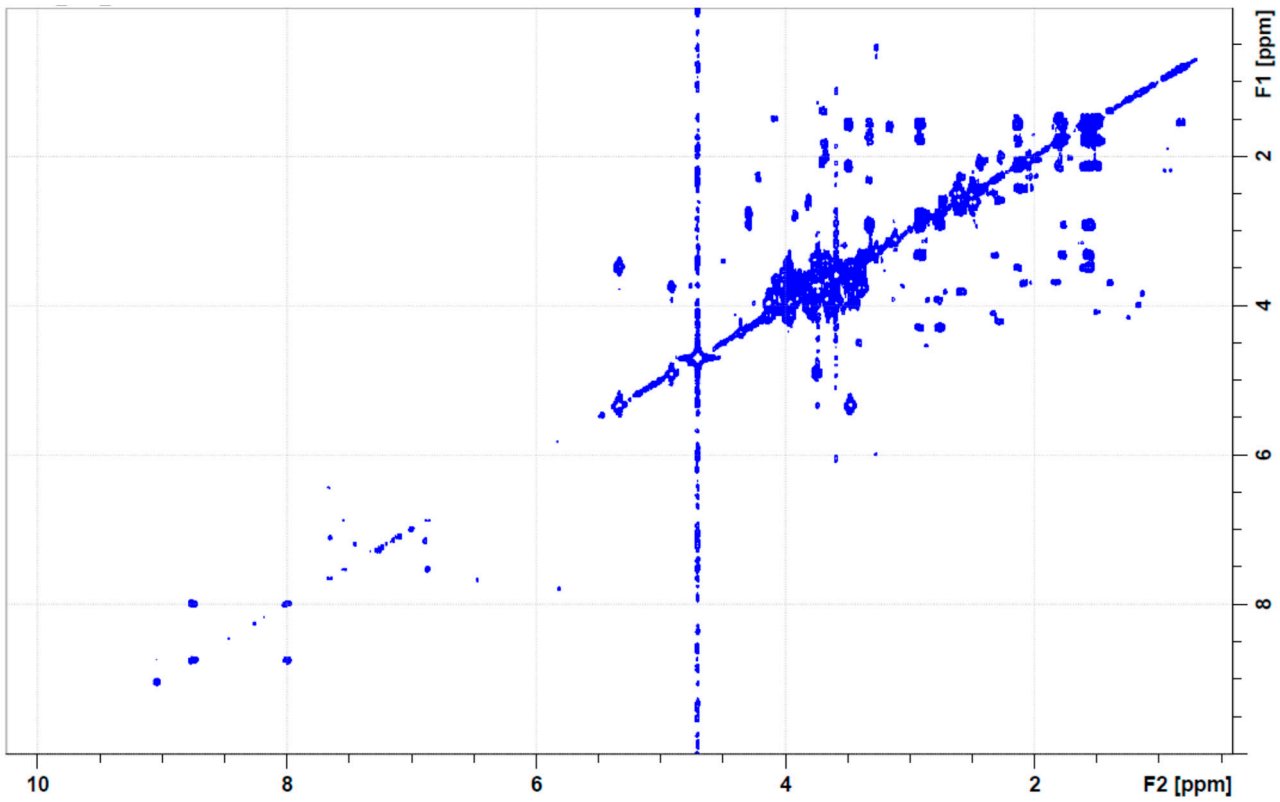


**Figure S4.** $^{1}$H-$^{1}$H-COSY NMR spectrum in $D_2O$ of polar extract of *Phaseolus* Vellutina (PVEL) at 600 MHz.

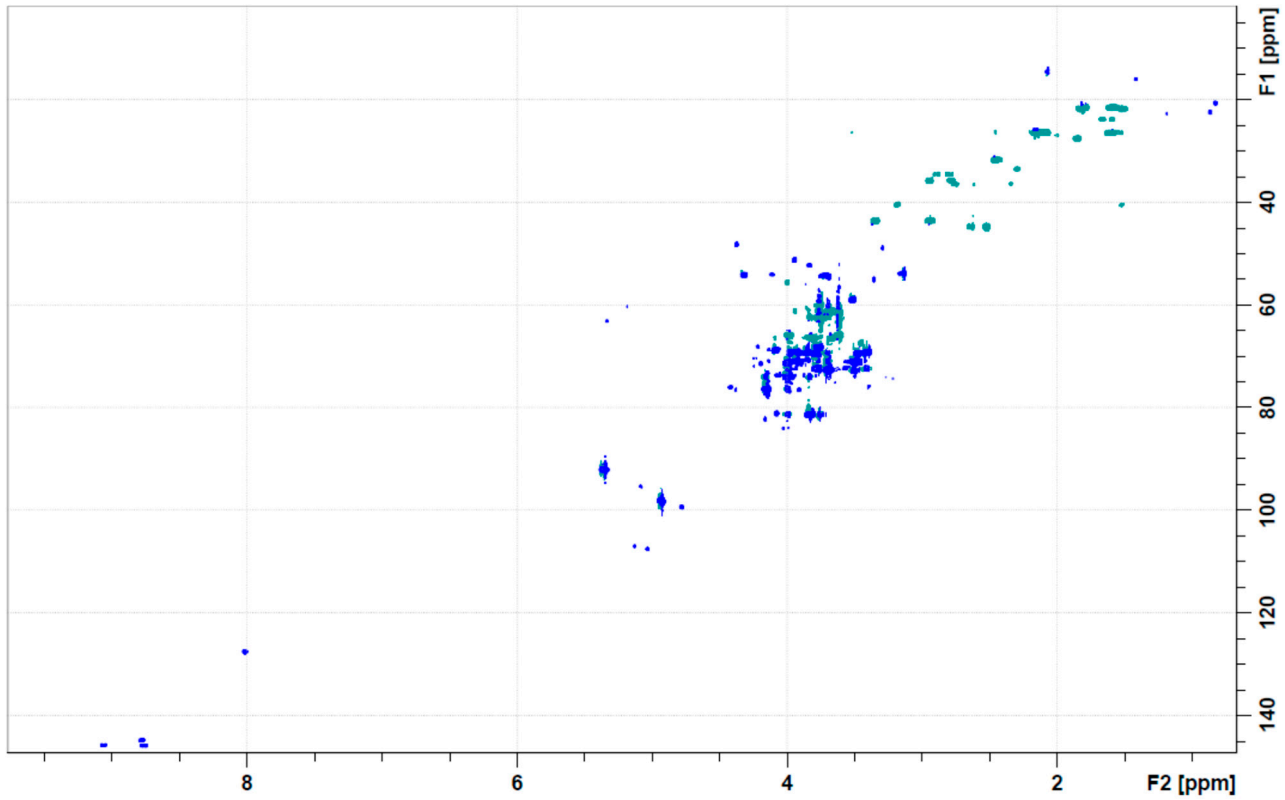


**Figure S5.** HSQC spectrum in $D_2O$ of polar extract of *Phaseolus* Vellutina (PVEL) at 600 MHz.

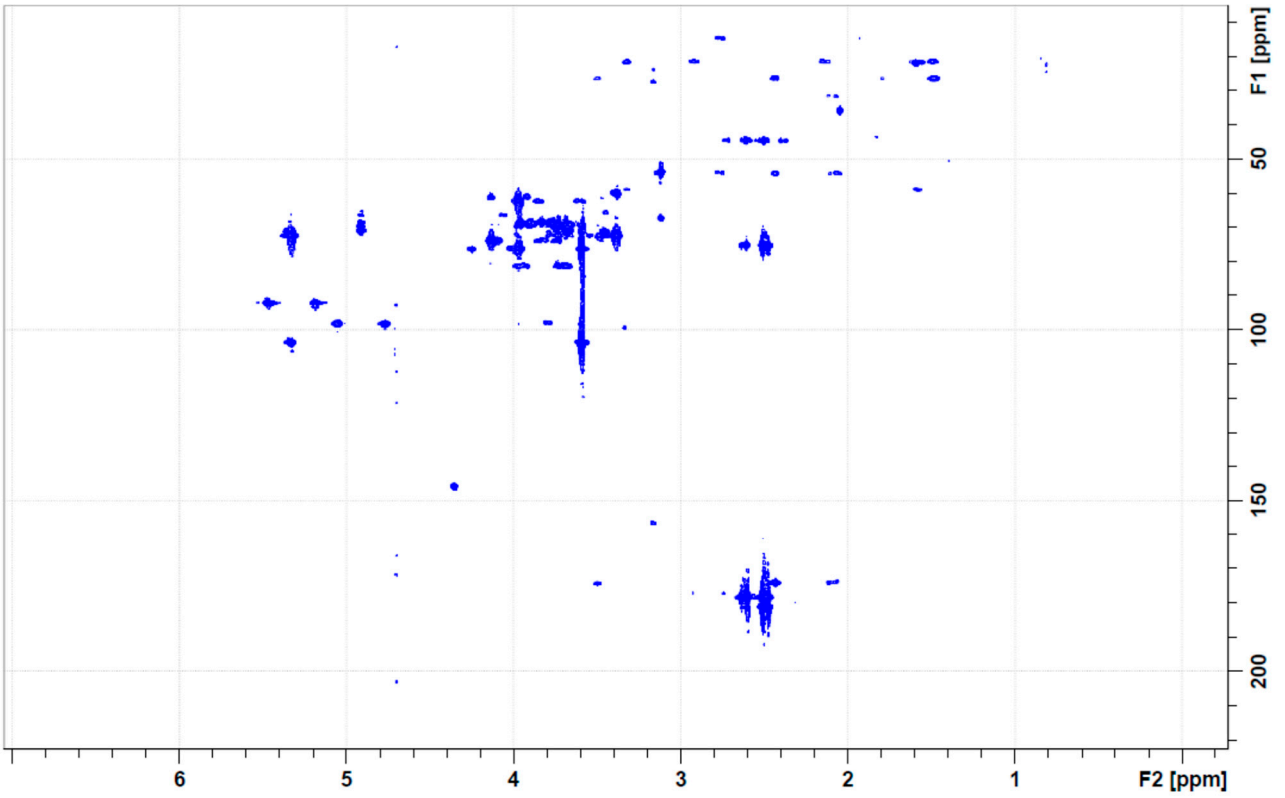


**Figure S6.** HMBC spectrum in $D_2O$ of polar extract of *Phaseolus* Vellutina (PVEL) at 600 MHz.

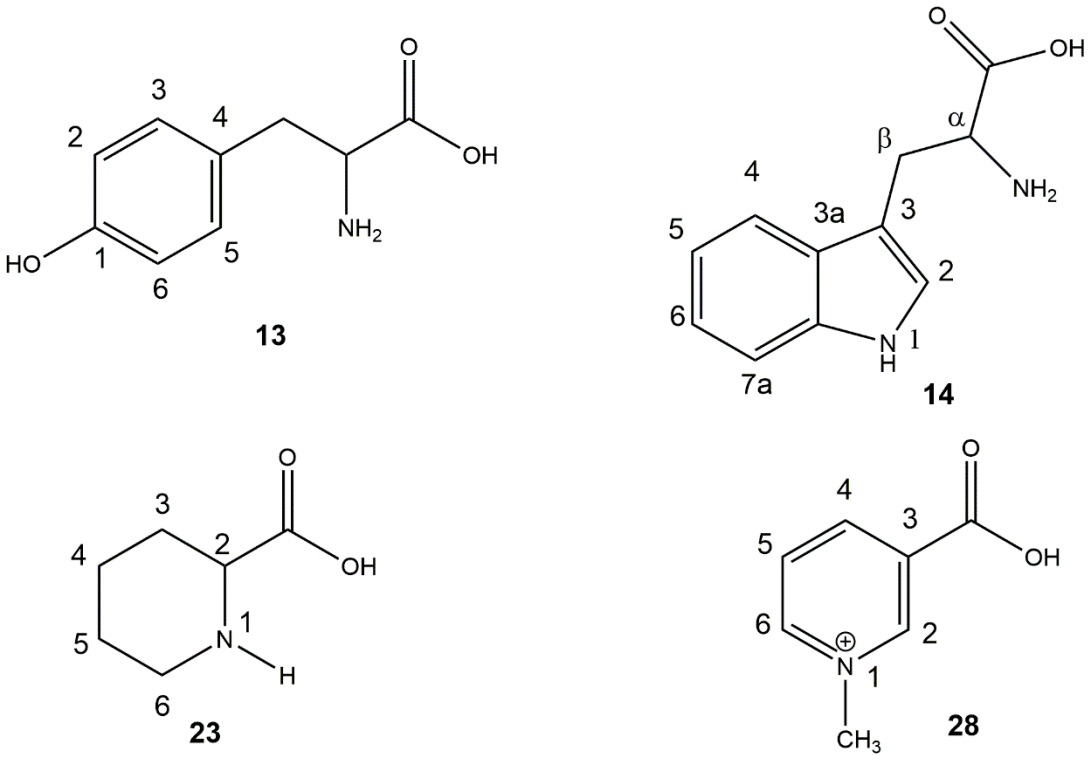


**Figure S7.** Chemical structure of selected metabolites of both polar and apolar extract of *Phaseolus* seeds, namely Tyrosine (**13**, Tyr), Tryptophan (**14**, Trp), Pipecolic acid (**23**, Pip) and Trigonelline (**28**, Tri).

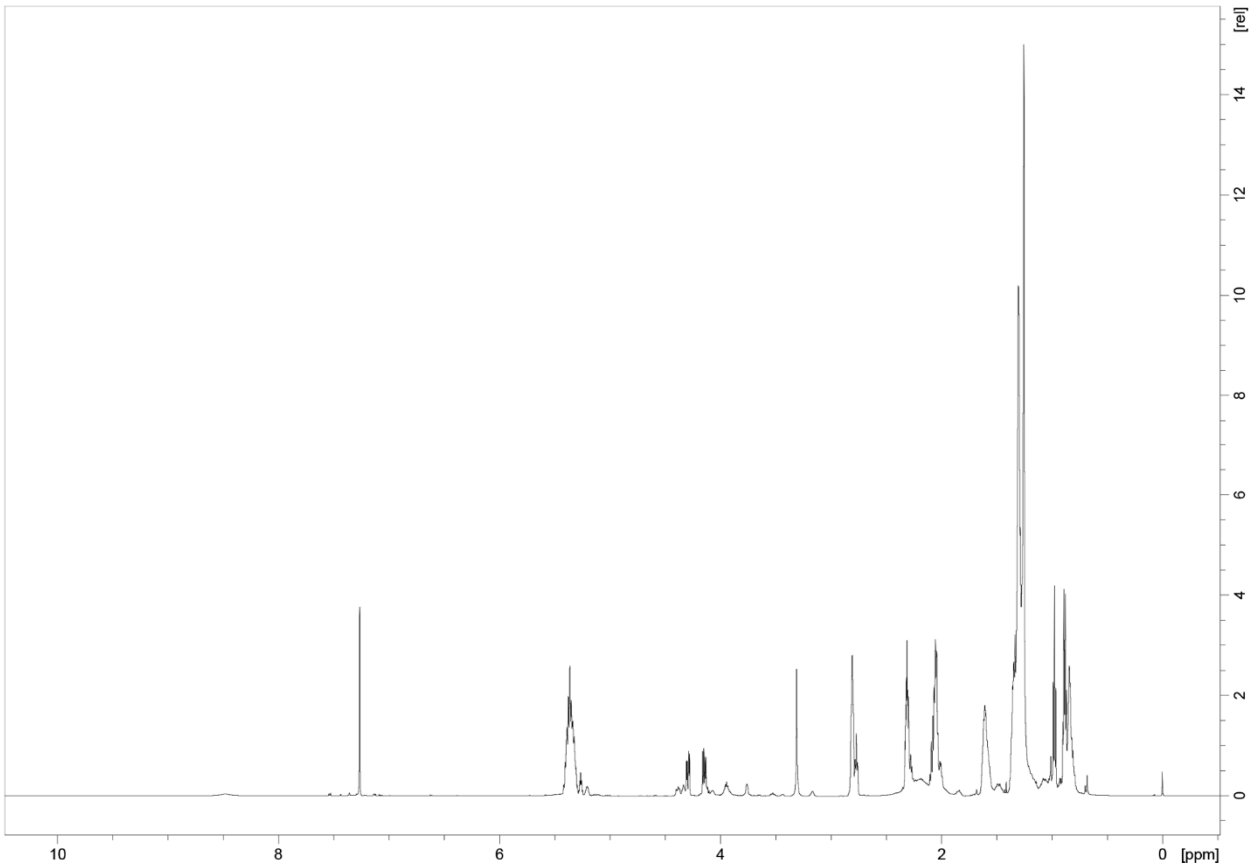


**Figure S8.** $^{1}$H-NMR spectrum in $CDCl_3$ of apolar extract of *Phaseolus* Cannellino (PCANN) at 600 MHz.

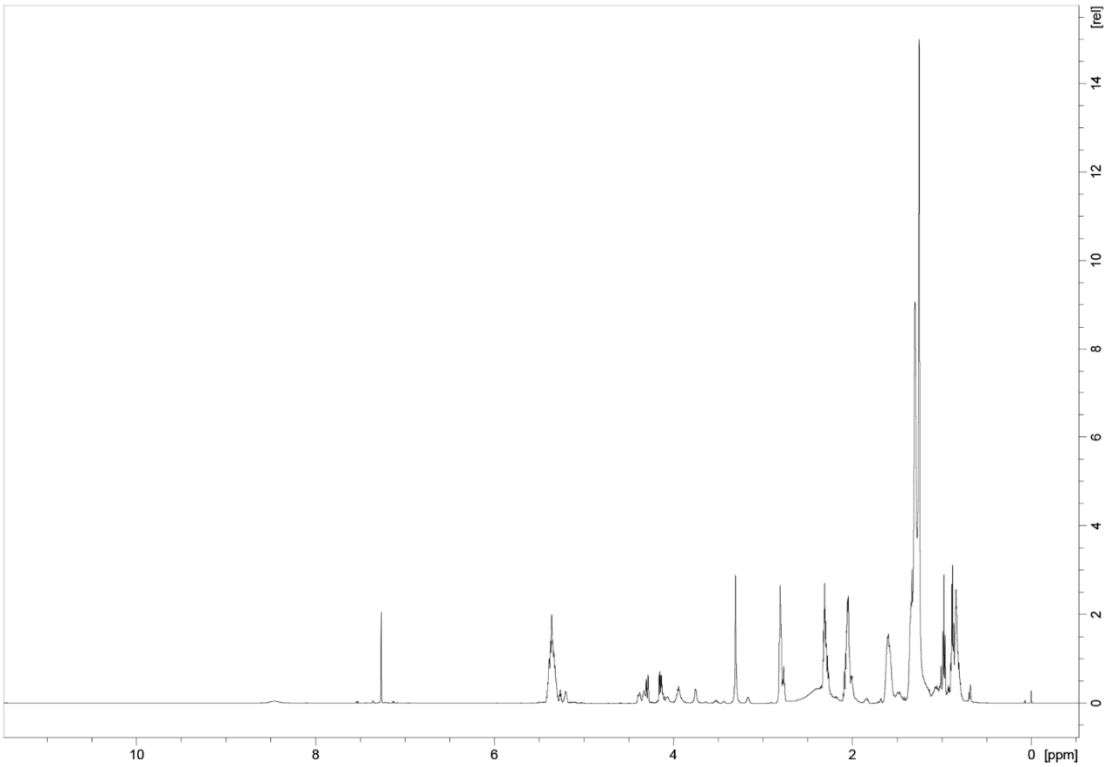


**Figure S9.** $^{1}$H-NMR spectrum in $CDCl_3$ of apolar extract of *Phaseolus* Controne (PCON) at 600 MHz.

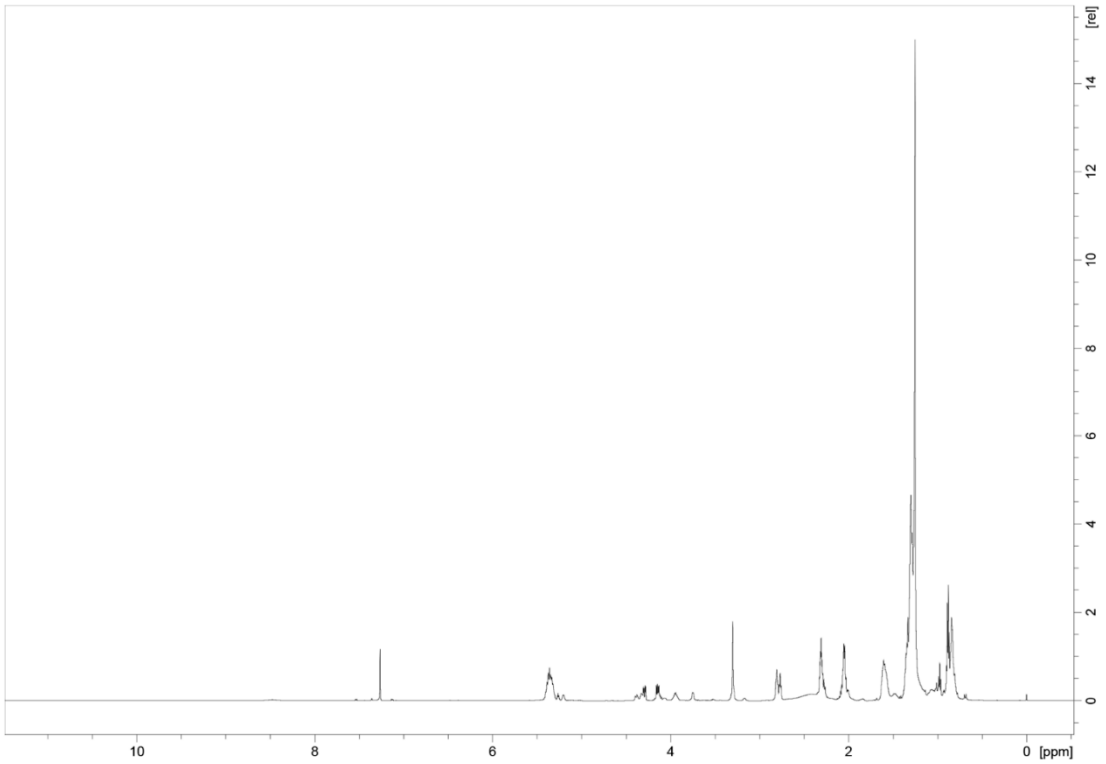


**Figure S10.** $^{1}$H-NMR spectrum in $CDCl_3$ of apolar extract of *Phaseolus* Occhio Nero (PON) at 600 MHz.

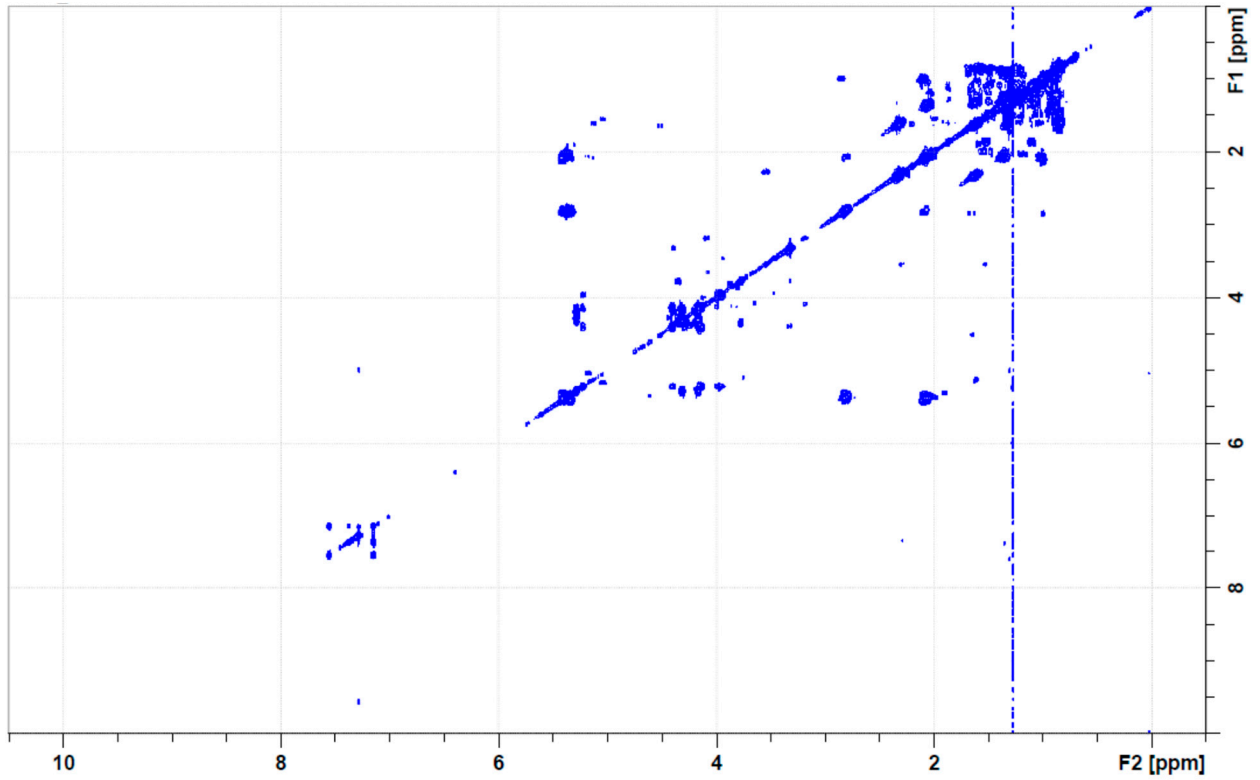


**Figure S11.** $^{1}H$-$^{1}H$-COSY NMR spectrum in $CDCl_3$ of apolar extract of *Phaseolus* Vellutina (PVEL) at 600 MHz.

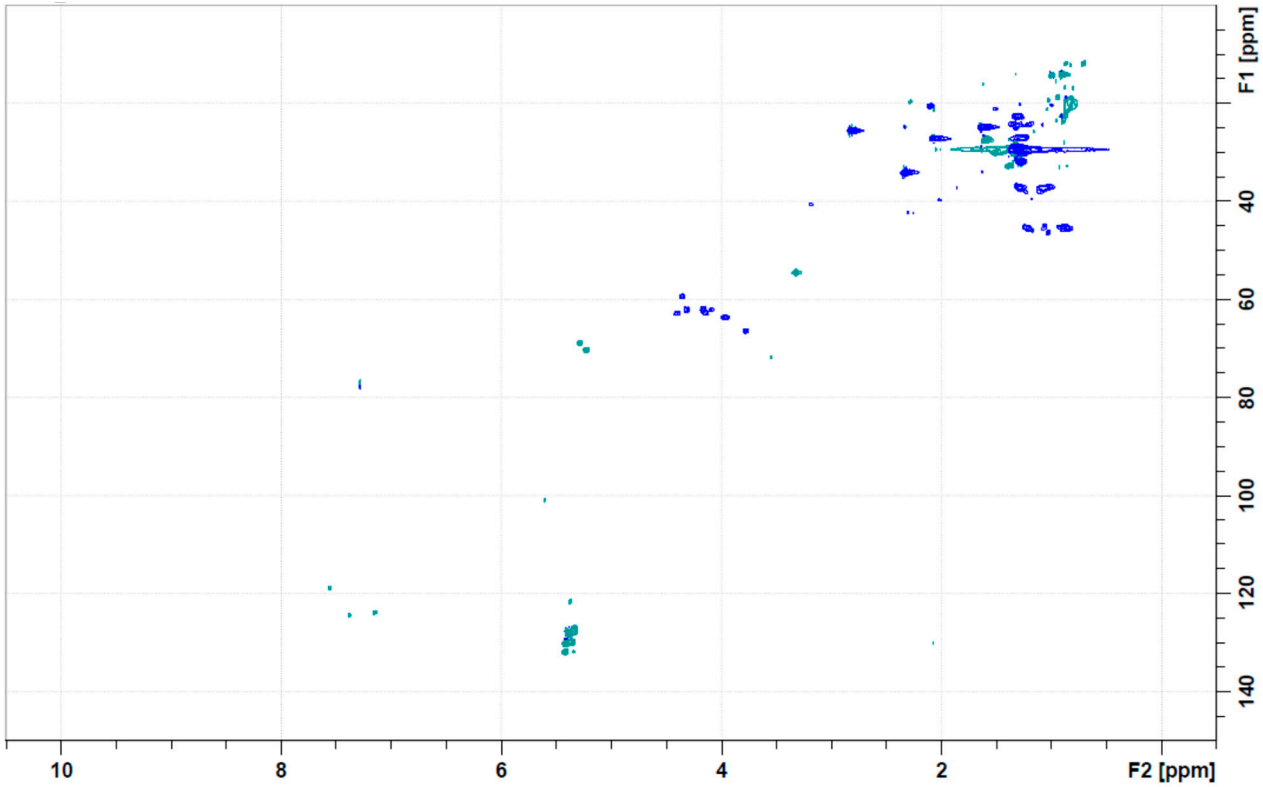


**Figure S12.** HSQC spectrum in $CDCl_3$ of apolar extract of *Phaseolus* Vellutina (PVEL) at 600 MHz

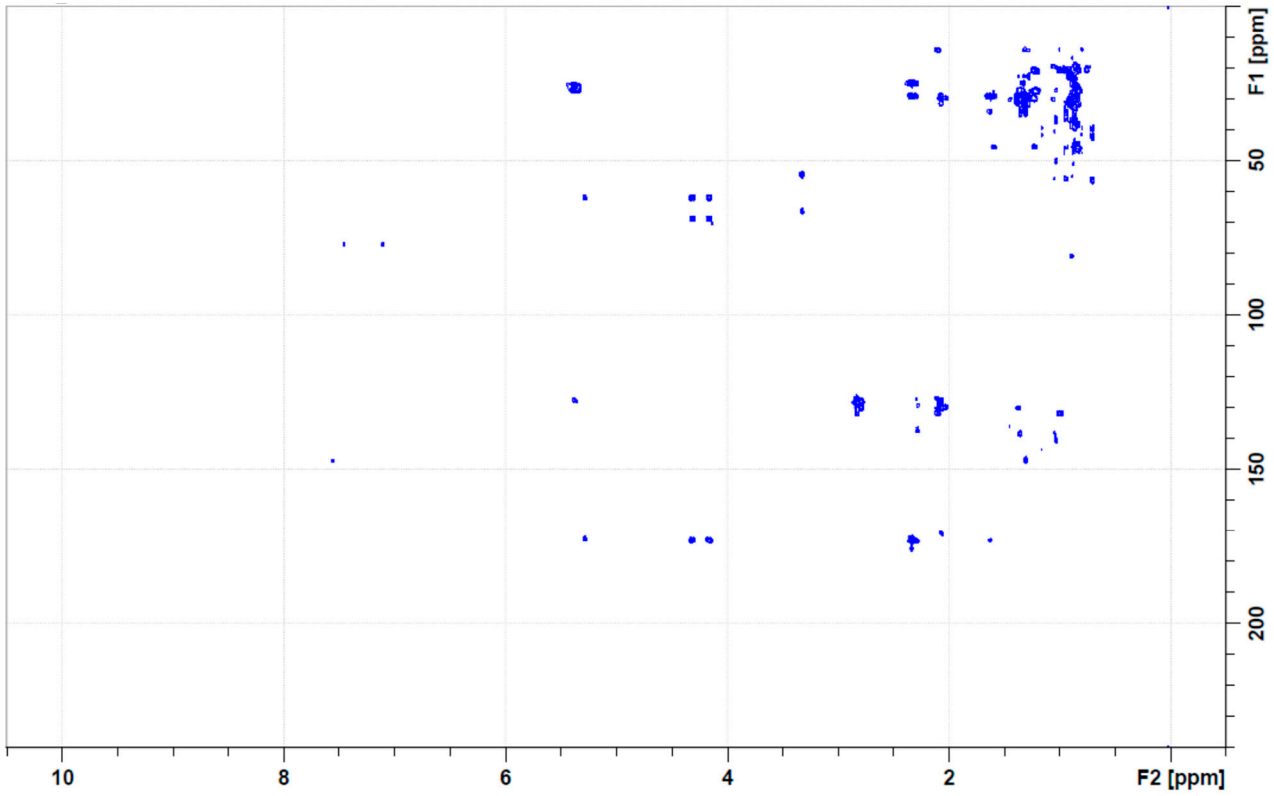


**Figure S13.** HMBC spectrum in $CDCl_3$ of apolar extract of *Phaseolus* Vellutina (PVEL) at 600 MHz.

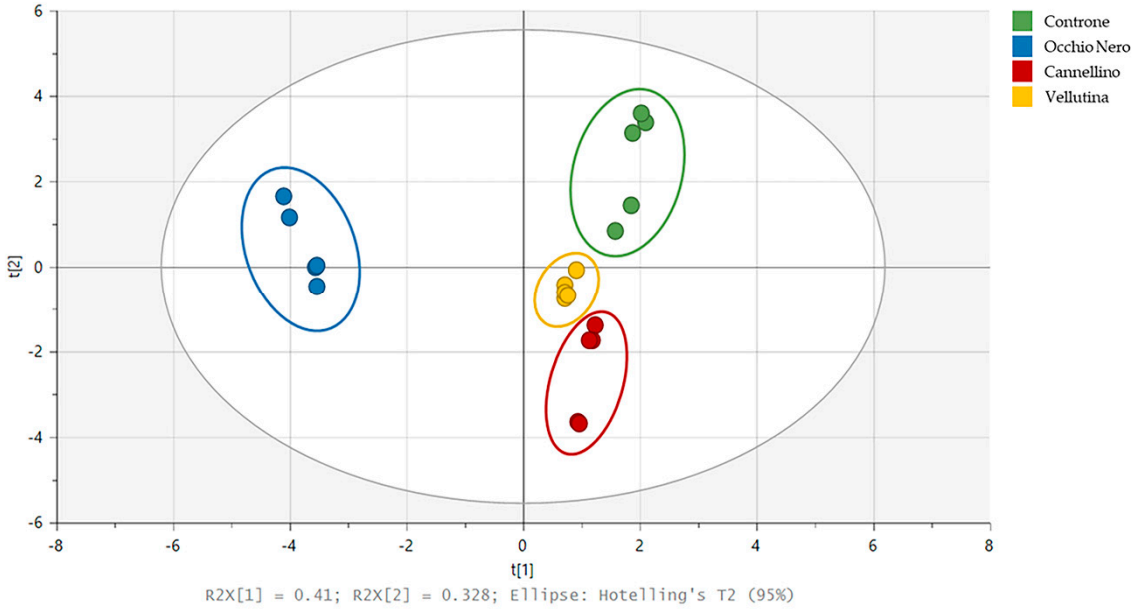


**Figure S14.** 2D representation of Principal Component Analysis (PCA) of polar extracts of bean varieties. PCANN (red), PCON (green), PVEL (yellow) and PON (blue) are separated in the score plot.

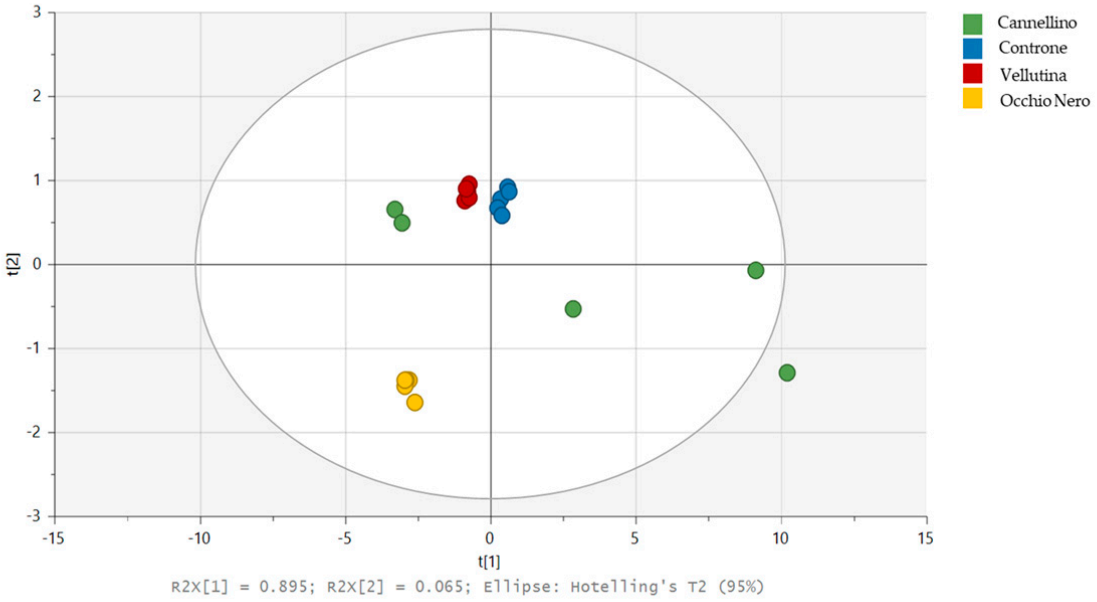


**Figure S15.** Partial Least Square – Discriminant Analysis (PLS-DA) of the selected metabolites of polar extracts.

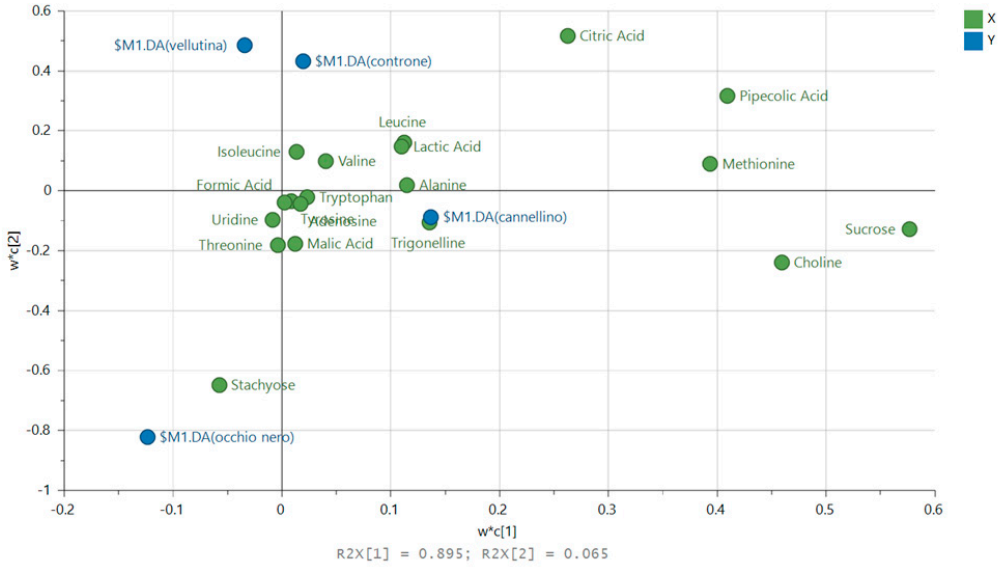


**Figure S16.** Loading Plot of PLS-DA.

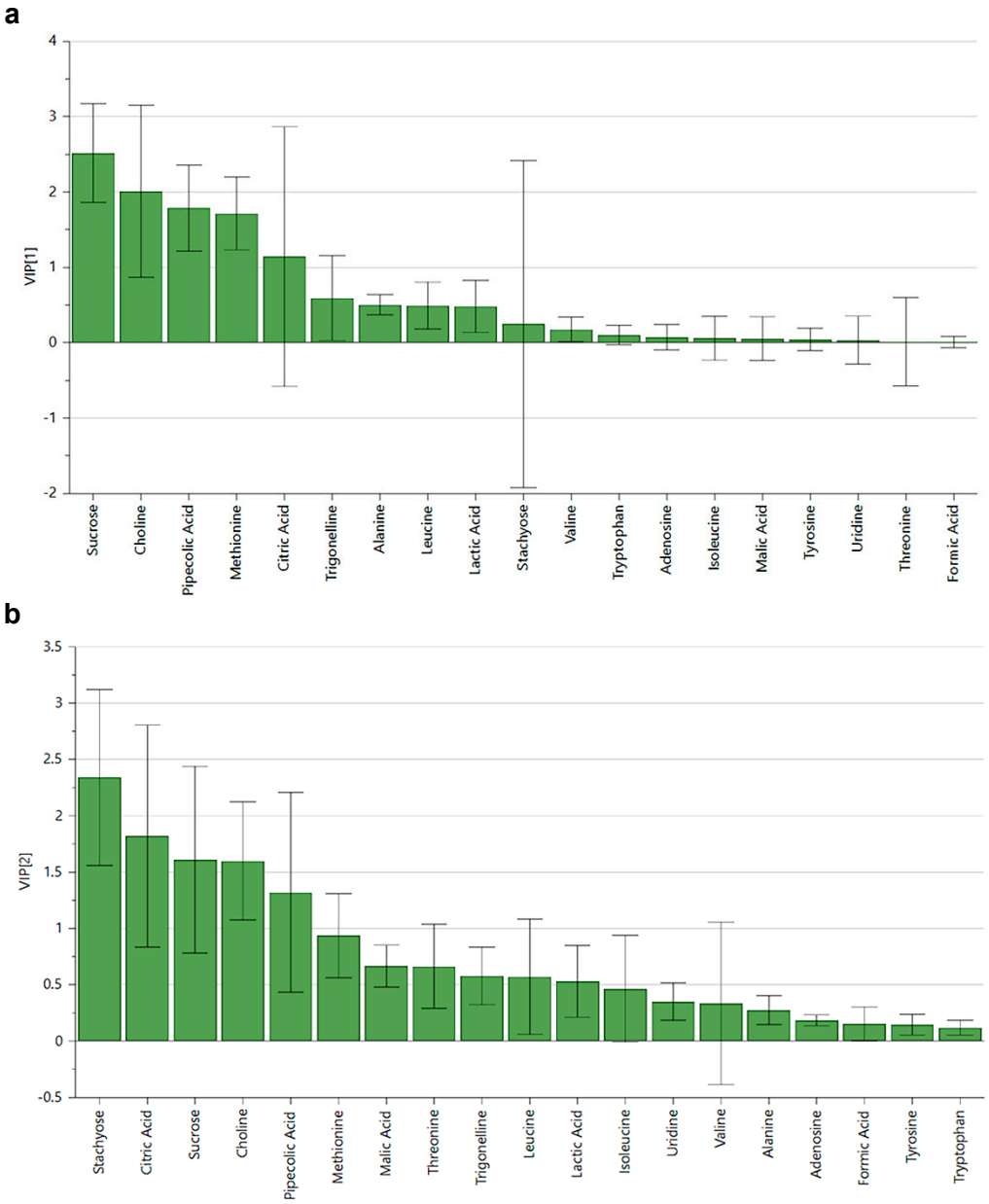


**Figure S17.** a) Variable Importance in Projection on component 1. b) Variable Importance in Projection on component 2.