Differentiation of six herbal extracts using principal component analysis

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Natural extracts have shown potential as biopreservatives. The objective of this work was to assess the contribution of plant type, extraction method, and solvent to the discrimination of six herbal extracts using principal component analysis (PCA). For this, rosemary, lemon balm, basil, tarragon, sage, and spearmint dry aerial parts were mechanically ground. The extractions were performed using ethanol 70% (v/v) (Et70) and distilled water as solvents, in a shaking water bath (solid-liquid extraction); or using a Soxhlet apparatus. Assays were carried to evaluate the extraction yield, chemical characteristics and antioxidant activity of the extracts. PCA was performed in R software, using the *prcomp* function from the *factoextra* package, to evaluate the contribution of factors (plant, extraction method, solvent) and variables (assays) to the discrimination of extracts.

The influence of extraction yield, chemical characteristics, and antioxidant activity on the differentiation of extracts is shown in Figure 1. PC1 and PC2 accounted for 51.4% and 20.4% of the variance observed, respectively. The variables with greatest contribution to extracts differentiation were those associated with antioxidant activity (ABTS: 13.42%; DPPH: 12.95%; FRAP: 12.86%), total flavonoid content (TFC: 12.20%), total phenolic content (TPC: 11.98%), and photosynthetic pigments (chlorophyll-a and -b, 13.09% and 9.90%, respectively). Oppositely, those with least contribution were extraction yield, total protein content, and carbohydrate content (6.36%, 4.14% and 3.10%, respectively). Figure 1 also shows that TPC and TFC are positively correlated with antioxidant activity (ABTS, DPPH and FRAP), an expected result due to the redox properties of phenolic compounds.

Figure 2 displays the grouping of plant extracts by extraction method, solvent, and plant type. These plots show a greater discrimination between extracts obtained from different solvents (B) and plants (C) than between extraction methods (A). This arises from the larger difference in chemical characteristics and antioxidant properties among extracts obtained using different solvents or feedstocks, than different extraction methods. Analysing Figure 2C, the ellipses of spearmint, rosemary, and sage overlap, indicating similar chemical characteristics and antioxidant activities. Nevertheless, they differentiate from the other plants, lemon balm, basil, and tarragon. Figure 2C also suggests that lemon balm extracts contain the highest phenolic and flavonoid contents and antioxidant activity, as the extracts are in the same direction of the arrows of TPC, TFC, DPPH, ABTS and FRAP (Figure 1), while tarragon extracts contain the lowest quantity of phenolic compounds and most reduced antioxidant potential.

Overall, these outcomes provide insight on the phytochemical profile and antioxidant activity of herbal extracts and the value of PCA in assessing similarities and differences between extracts produced using distinct plants, solvents and extraction methods and the reasons for such differences.

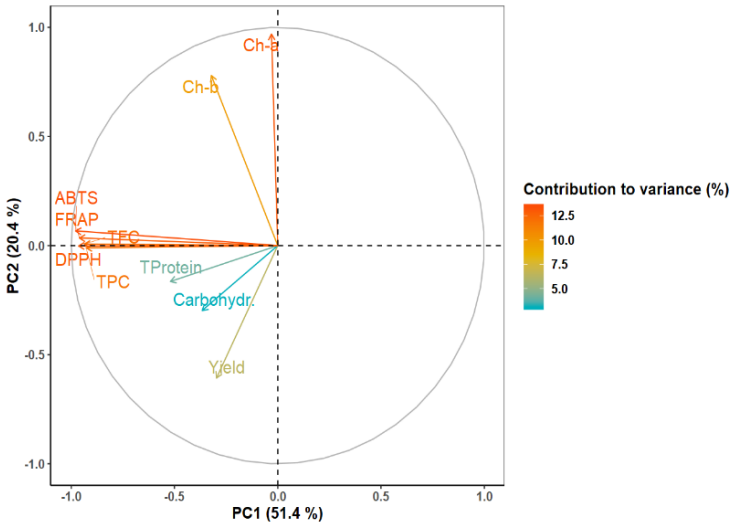

Figure 1. Loading plot of the first two components of the principal component analysis (PCA).

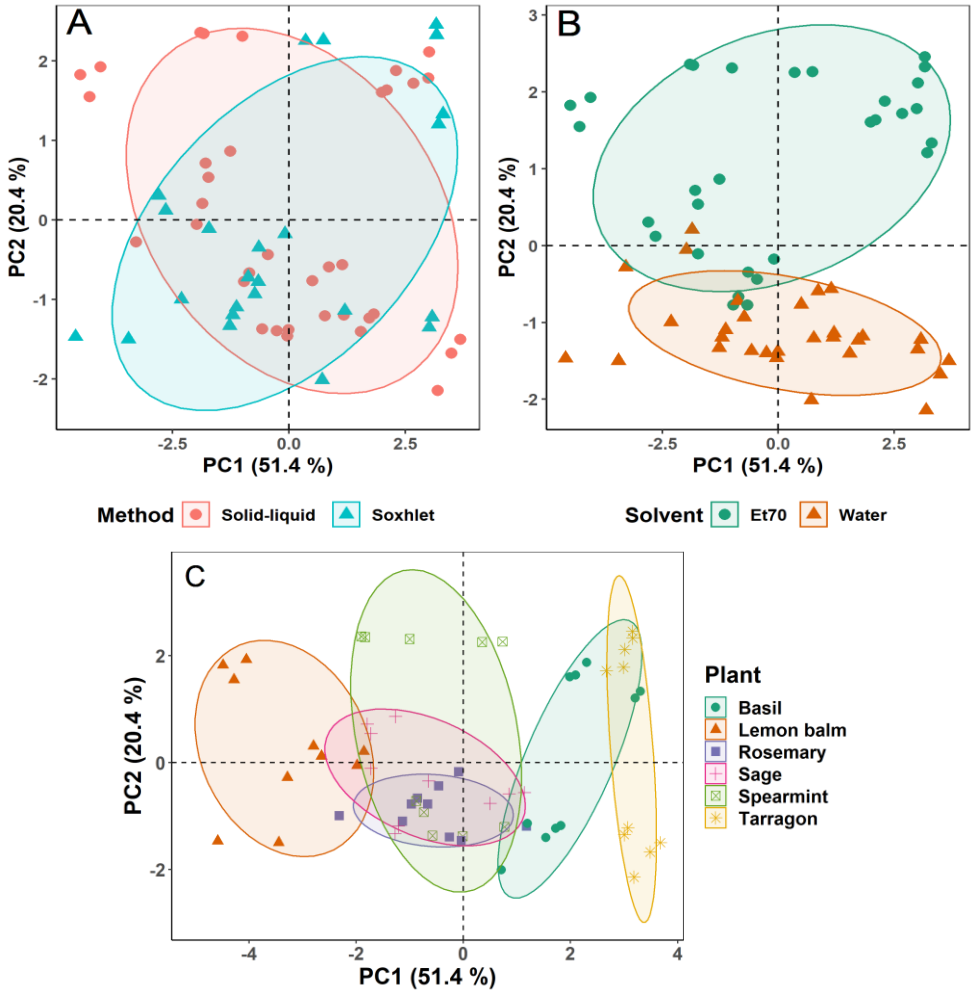

Figure 2. Score plots of the first two components of the PCA grouped by extraction method (A), solvent (B), and plant type (C).