

Introduction

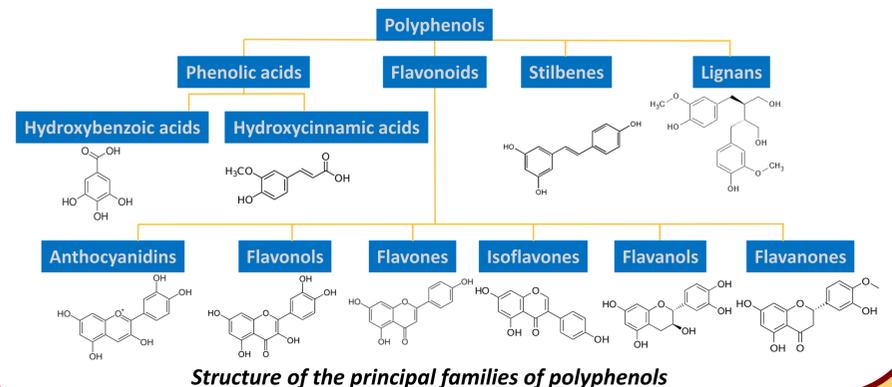
Polyphenols are ubiquitously present in plants as a large family of secondary metabolites. Depending on their structures, they can be classified in phenolic acids, flavonoids, stilbenes, lignans and tannins. Polyphenols display several healthy attributes, such as antioxidant, anti-inflammatory, antimicrobial and antineoplastic properties, so that they are commonly included as basic ingredients in several pharmaceutical and nutraceutical products.

In this research, the total content of polyphenols and the antioxidant capacity of various food supplements and nutraceuticals have been estimated, including cranberry, raspberry, artichoke, grapevine, green tea, coffee, turmeric and other medicinal plant extracts. Samples have been analyzed by using different methods, such as high-performance liquid chromatography (HPLC) and two antioxidant assays —ferric reducing antioxidant power (FRAP) and Folin-Ciocalteu (FC)—.

A preliminary data exploration by PCA has revealed that HPLC fingerprints are suitable chemical descriptors to classify the analyzed samples according to their nature and origin. Besides, chromatographic fingerprints have been correlated with antioxidant data using partial least squares (PLS). Regression models have shown a good prediction capacity to estimate the antioxidant activity from chromatographic data, with determination coefficients (R^2) of 0.903 and 0.939 for FRAP and FC assays, respectively.

Objectives

- To analyze several agri-food products, food supplements and nutraceutical products by HPLC and antioxidant indexes to calculate their antioxidant capacity expressed.
- To characterize the analyzed samples by principal component analysis (PCA) using the HPLC fingerprints depending on the polyphenolic composition as the data.
- To study the correlation by partial least square (PLS) regression between HPLC fingerprints and antioxidant capacity data.
- To try to correlate the compositional profiles of polyphenols with the antioxidant activities.

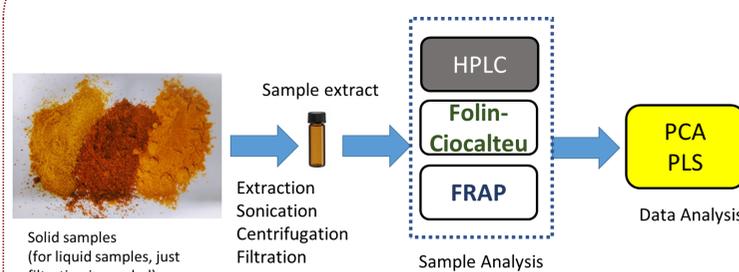


Experimental section

Samples



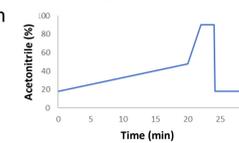
Working flowchart



Methods

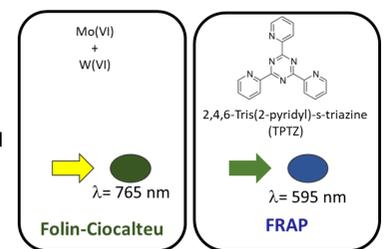
HPLC-UV:

- Separation column Kinetex C18 (100 x 4.6 mm I.D., 2.6 μ m particle size)
- Mobile phase: 0.1% aqueous formic acid solution and acetonitrile (see gradient profile below)
- Flow rate: 0.4 mL min⁻¹
- Detection wavelengths: 280, 325, 370, and 425 nm

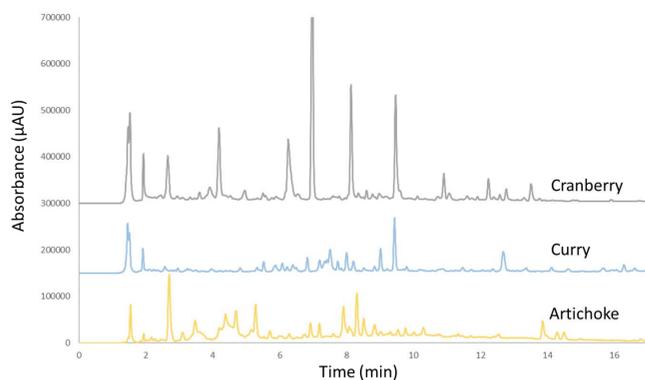


Antioxidant indexes:

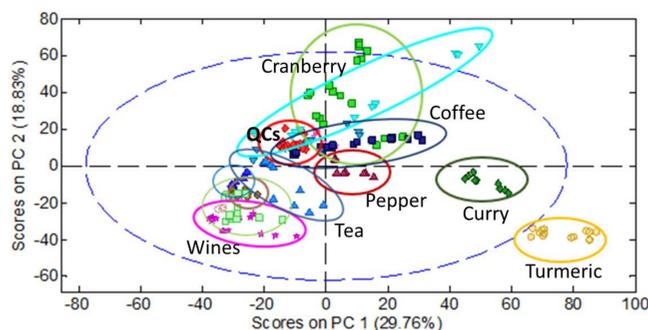
- Spectrophotometric detection



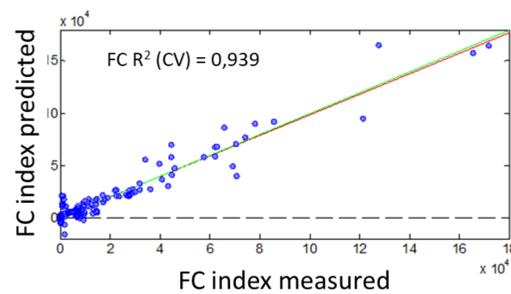
Results and discussion



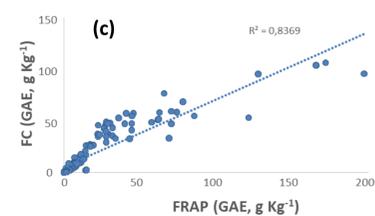
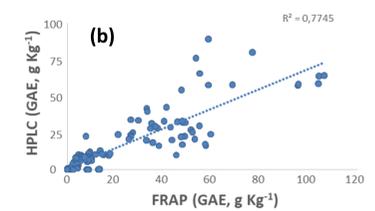
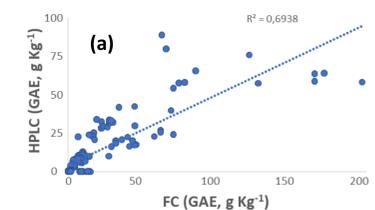
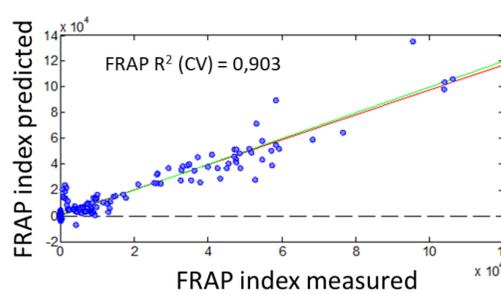
HPLC-UV chromatograms recorded at 280 nm of various sample extracts.



Characterization of nutraceutical and functional food samples by PCA using the polyphenolic fingerprints as the data.



Prediction of the antioxidant capacity (FC and FRAP indexes) using the chromatographic fingerprints by multivariate calibration by PLS



Correlation studies among the total polyphenolic concentration estimated by HPLC and the spectroscopic antioxidant indexes (Folin-Ciocalteu —FC— and Ferric Reducing Antioxidant Power —FRAP—). (a) HPLC vs FC; (b) HPLC vs FRAP; (c) FC vs FRAP.

Conclusions

- ✓ The PCA study confirms that HPLC fingerprints are suitable sample chemical descriptors to classify the analyzed samples according to their typology.
- ✓ Despite the differences between the HPLC and the antioxidant assay measurements, data was reasonably correlated, meaning that those samples richer in polyphenols exhibited higher antioxidant activities.
- ✓ PLS models built were able to predict antioxidant capacity values by employing the HPLC fingerprints, thus showing the relationship among phenolic composition and antioxidant power of the samples.

References

- Alcalde, B., Granados, M., Saurina, J. Exploring the antioxidant features of polyphenols by spectroscopic and electrochemical methods. *Antioxidants*, 2019, 8, 523.
- Montenegro-Landívar, M.F. et al. Polyphenols and their potential role to fight viral diseases: An overview. *Science of the Total Environment*, 2021, 801, 149719.
- Vidal-Casanella, O.; Nuñez, O.; Granados, M.; Saurina, J.; Sentellas, S. Analytical Methods for Exploring Nutraceuticals Based on Phenolic Acids and Polyphenols. *Appl. Sci.* 2021, 11, 8276.

Acknowledgements

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