

An integrated analytical approach based on NMR and HPLC-UV-ESI-MS/MS to characterize Calabrian apple juices and its Nanofiltration (NF) extracts.

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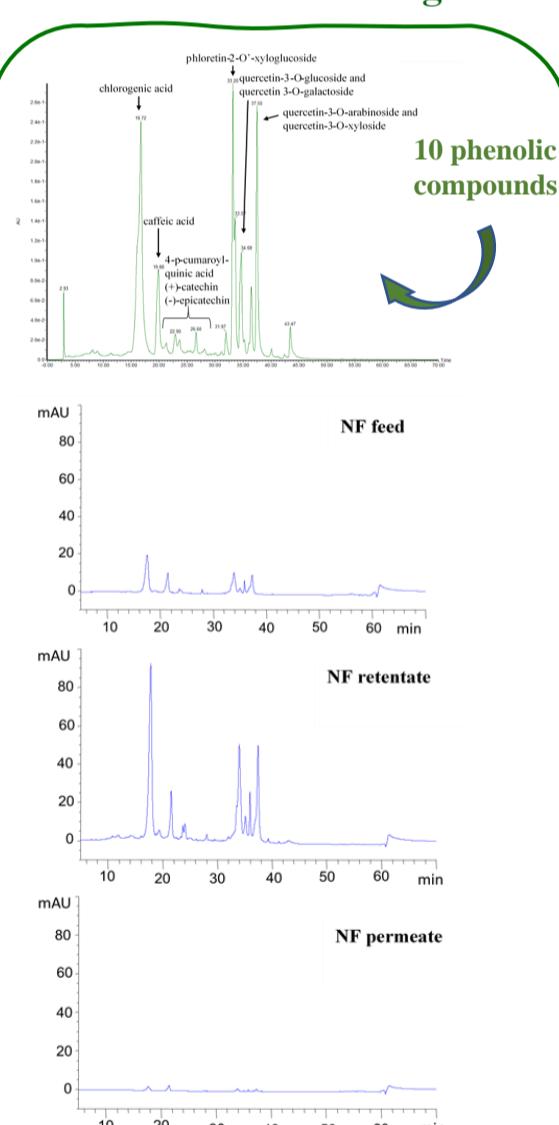
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Background

- Apple juice quality properties such as its nutritional value, aroma, firmness, and health-promoting effects are based on the metabolic composition (primary and secondary metabolites) of the juice [1].
- Nuclear Magnetic Resonance (NMR) is an ideal tool for metabolomic studies, especially for the untargeted analyses [2,3].
- Mass Spectrometry (MS) hyphenated to Liquid Chromatography is preferred for the targeted analysis of compounds present in minor quantity on the food matrix [4].
- Ultrafiltration (UF) process and Nanofiltration (NF) process are today well-established technologies for the recovery of bioactive compounds [5,6].

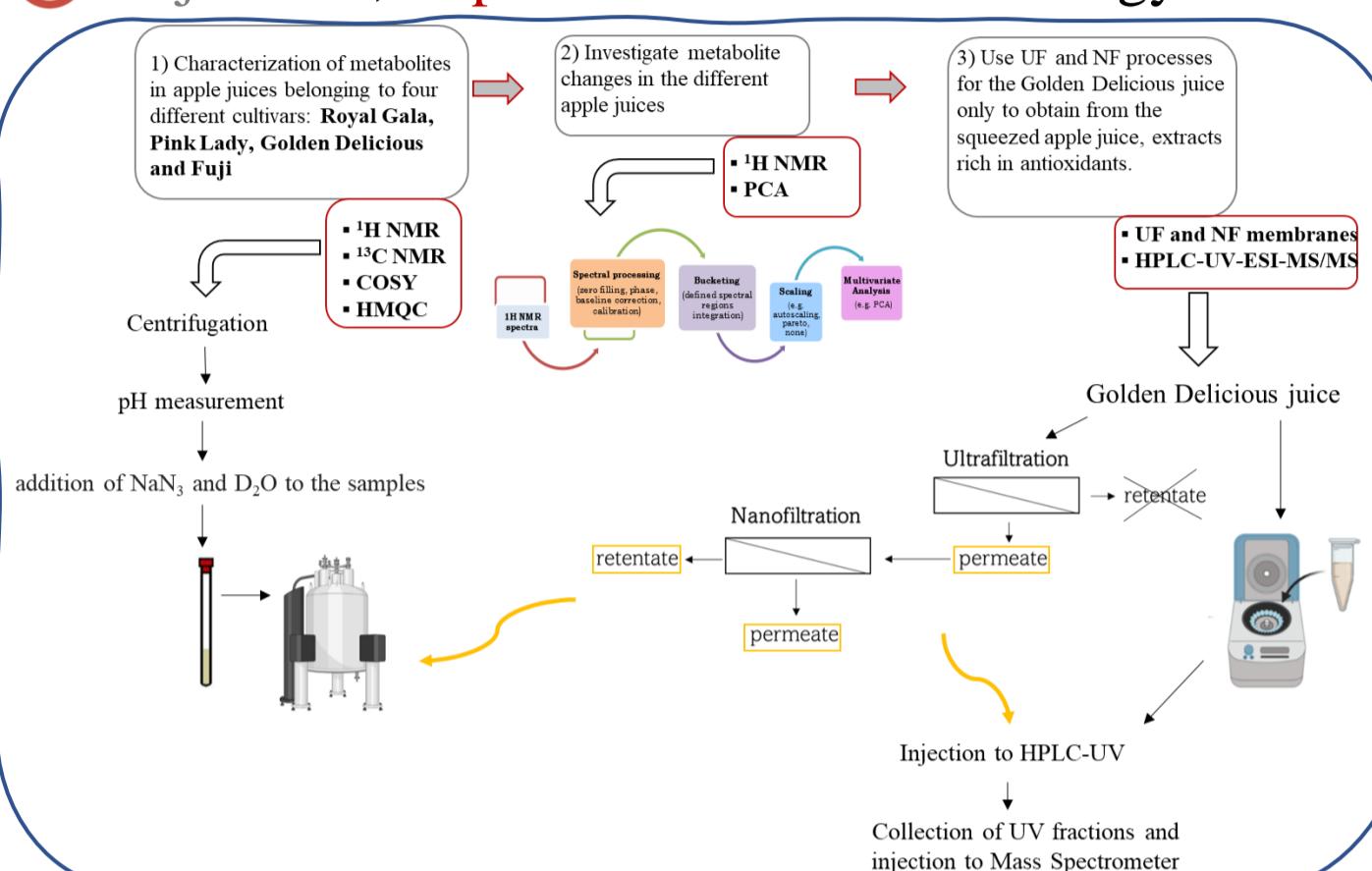
HPLC-UV chromatograms



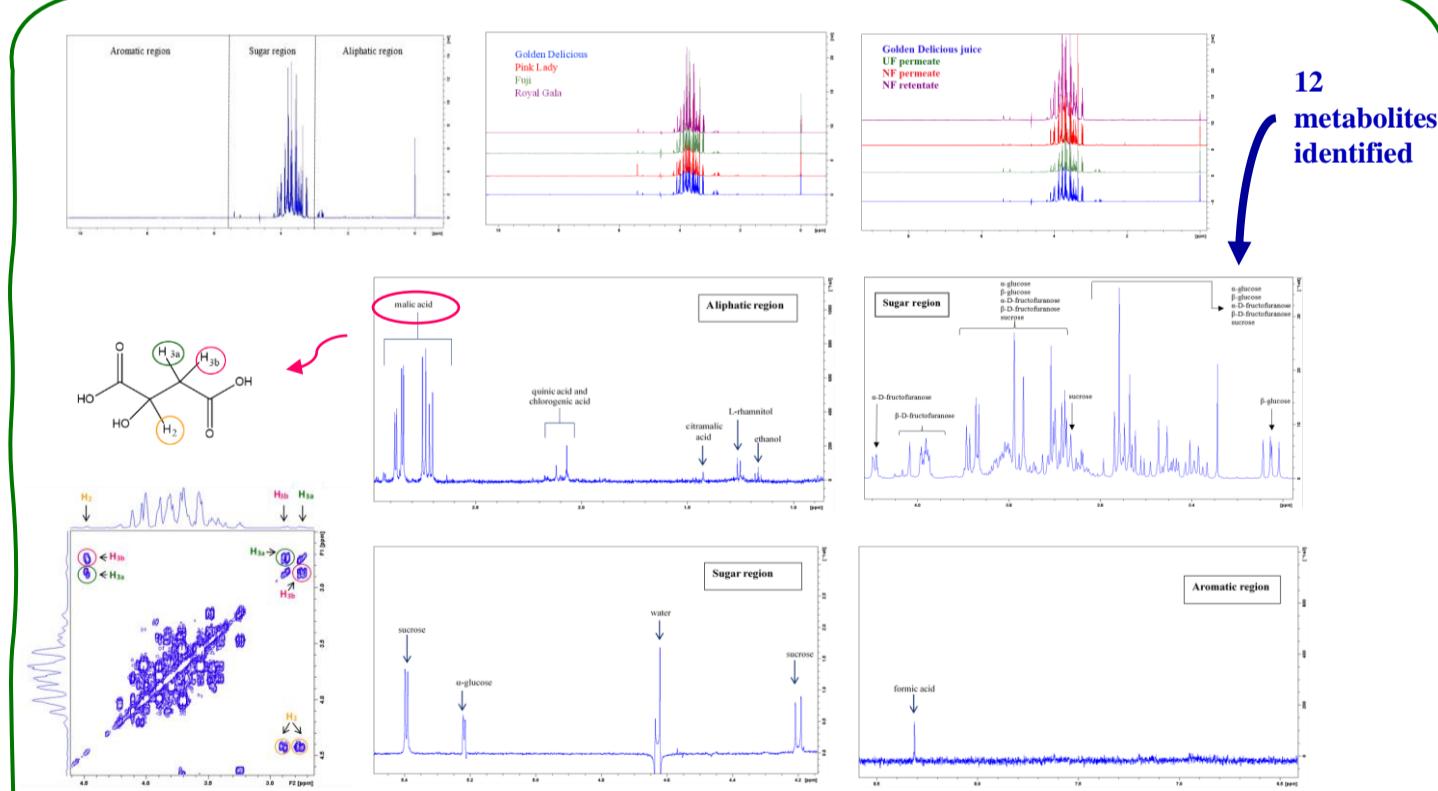
Conclusions

- 12 metabolites identified using 1D and 2D NMR spectra
- NMR and PCA combination allowed to separate samples belonging to the four apple varieties
- 10 phenolic compounds identified in the Golden Delicious juice using HPLC-UV-ESI-MS/MS
- NF process concentrate phenolic compounds of Golden Delicious juice.

Objectives, Experiments and Methodology

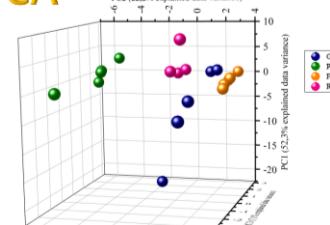


Results

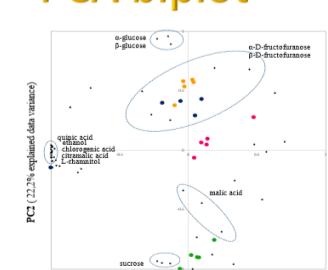


Chemometric Analysis

PCA



PCA biplot



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[4] R. M. Gathungu, R. Kautz, B. S. Kristal, S. S. Bird, and P. Vourous *Mass Spectrom. Rev.*, **39**, 35-54 (2018)

[5] R. Castro-Muñoz, J. Yáñez-Fernández, and V. Fila *Food Chem.*, **213**, 753-762 (2016)

[6] A. Figoli, A. Tagarelli, A. Mecchia, A. Trotta, B. Cavaliere, R. Lavecchia, G. Sindona, and E. Drioli *Desalination*, **199**, 111-112 (2006)