How Does LC/MS Compare to UV in Coffee Authentication and Determination of Antioxidant Effects? Brazilian and Middle Eastern Coffee as Case Studies

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❑Introduction

Coffee is a popular beverage owing to its unique flavor and diverse health benefits.

Though there are more than 120 species of **Coffee, coffee** are brewed mainly from the seeds of Coffea arabica L. and C. canephora L.(robusta)

Besides caffeine (1–4%), **coffee** seeds are rich in other secondary metabolites with several health benefits. Major secondary metabolites in coffee include phenolic acids, i.e., chlorogenic acids, which have various pharmacological properties, such as anti-inflammatory, hepatoprotective, anti-cancer, and anti-diabetic effects.

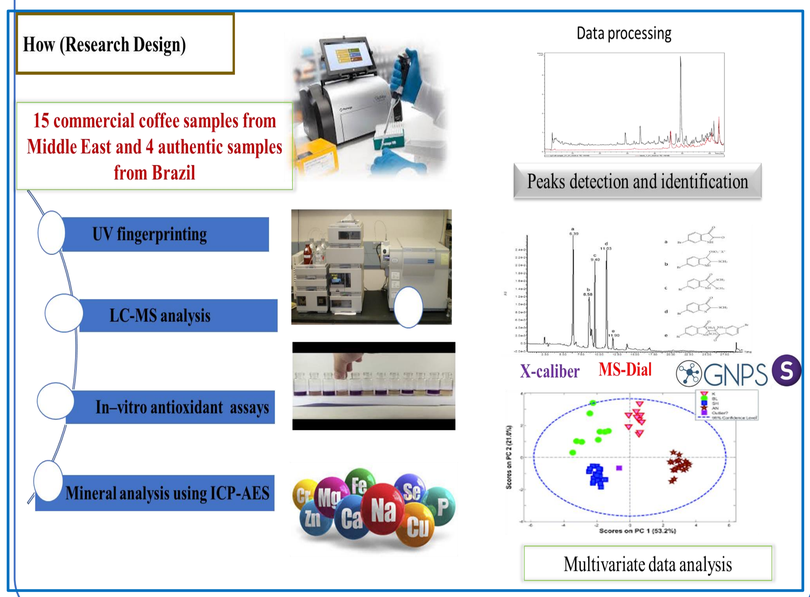
The phytochemical analyses of bioactive metabolites using advanced analytical techniques, i.e., metabolomics, are promising to identify active agents in such rich chemical matrixes.

❑Aim

The current study aimed at investigating the phytochemical composition of authenticated Brazilian green and roasted Coffee arabica and C. robusta, along with 15 commercial specimens collected from the Middle East using metabolomics

Investigating the antioxidant activity in relation to different roasting degree.

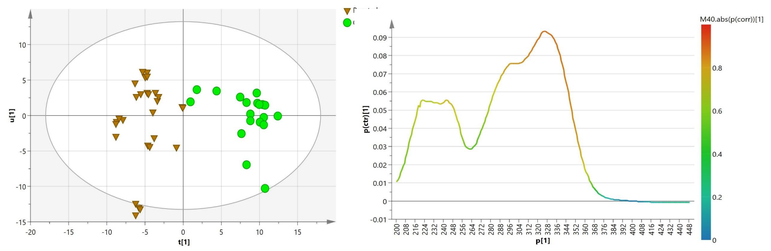
❑Methodology



❑Results (UV Fingerprinting)

The UV spectral bands provide information about metabolites absorption bands (e.g., phenolic compounds λ max 220,325nm)

Model 1 : Roasted versus Green Samples



Model 2 : Roasted versus Instant Samples

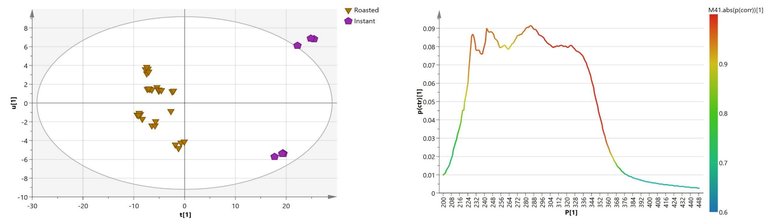


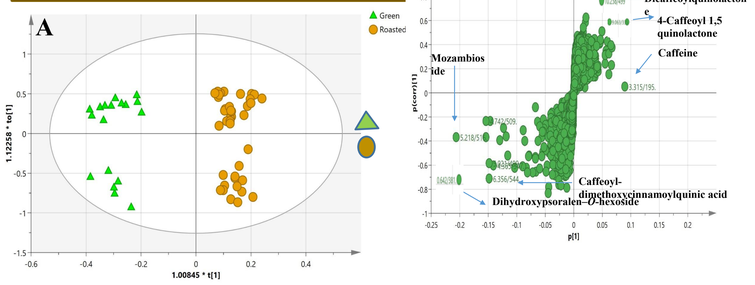
Figure 1. (**1**) OPLS-DA model for coffee samples (green versus roasted) based on UV–Vis analysis.
(**2**) S-line based on roasting effect. (**C**) OPLS-DA for roasted versus instant samples.

❑Results(LCMS)

91 peaks annotated belonging to different metabolites classes 23 hydroxycinnamates, 5 hydroxycinnamic amides, 17 diterpenes , 15 fatty acids , 7 sphingolipids, 6 nitrogenous compounds , 2 alkaloids, 2 sugars, 1 coumarin, and 1fatty acid amides

Model 1 : Roasted versus Green Coffee Samples

OPLS Score Plot (A) and S-plot (B)



Model 2 : Roasted versus Instant Coffee Samples

OPLS Score Plot (A) and S-plot (B)

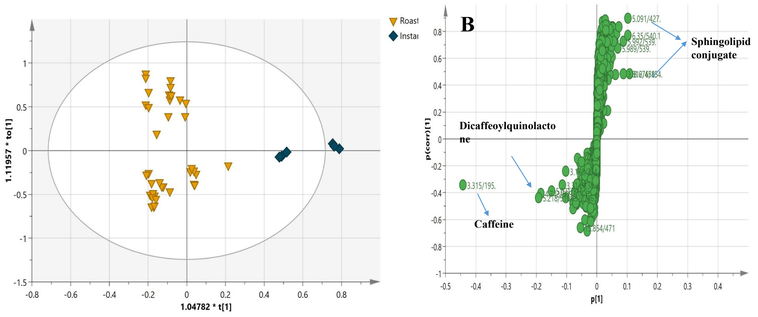


Figure 2. (**1**) OPLS-DA score plot based UPLC–MS analysis exploring green versus roasted coffee seeds. (**2**) OPLS-DA S-plot showing potential markers for green versus roasted coffee seeds..

❑Results(Antioxidant Assays)

- Highest values for light roasted and green samples

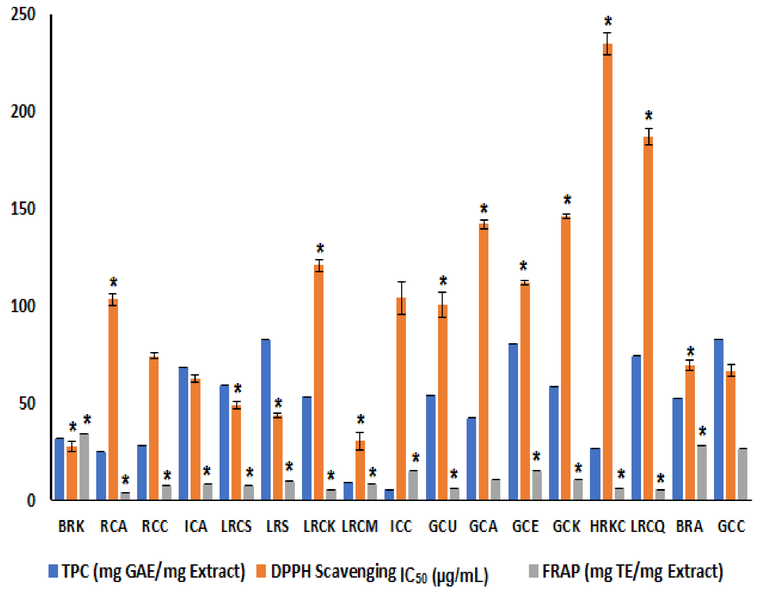


Figure3: Total phenolic content, DPPH, and FRAP test for the investigated coffee samples.

❑ Conclusion

The study represented a multiplex metabolomics approach using two different platforms—UHPLC and UV fingerprinting techniques—for the tentative identification of secondary metabolites in different coffee products resulting in the tentative identification of several novel phenolics and diterpenes in coffee seeds.

Specimens differed with respect to several variables, such as genotype, roasting process, supplier, and additives.

Both UHPLC–HRMS and UV spectroscopy coupled to multivariate data analysis revealed differences among authenticated Brazilian and commercial samples consumed in the Middle East.

❑ References

All the figures retrieved from https://doi.org/10.3390/antiox11010131

❑ Acknowledgment

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