



Comparison of NMR and LC-HRMS Platforms in the Metabolic Profiling of Greek Table Olives

Stavros Beteinakis¹, Anastasia Papachristodoulou¹, Emmanuel Mikros², Maria Halabalaki¹

¹Division of Pharmacognosy and Natural Products Chemistry, Faculty of Pharmacy, NKUA, Panepistimiopolis, Zografou, 15771 Athens, Greece,

²Division of Pharmaceutical Chemistry, Faculty of Pharmacy, NKUA, Panepistimiopolis, Zografou, 15771 Athens, Greece



9th Virtual Panhellenic Conference of Greek Lipid Forum



HELLENIC REPUBLIC
National and Kapodistrian University of Athens

Introduction



- Food commodities: intricate, highly variable matrices of unexpected nature
- “Food Quality” **historically** linked with absence of adulteration, fraud or defect in a product
- **Now:** expectancy over certain desirable characteristics such as organoleptic and nutritional – can justify the added value paid by the customer



Features contributing to the characterization of “Food Quality” as defined by the European Commission

Foodomics Era

- ❖ A new approach in food science and nutrition that provides information about the **food metabolome**
- ❖ Employment of high-end instrumentation (NMR & HRMS platforms)
- ❖ Implementation in food profiling, biomarker detection, authenticity control and food quality or safety evaluation

Acknowledgements

This research was co-financed by Greek national funds through the Public Investments Program (PIP) of General Secretariat for Research & Technology (GSRT), under the Emblematic Action “The Olive Road” (project code: 2018ΣΕ01300000) & the European Union (ERDF) and Greek national funds through the Operational Program “Competitiveness, Entrepreneurship and Innovation”, (PlantUp, MIS 5002803 & FoodOmicsGR Comprehensive Characterisation of Foods, MIS 5029057). The authors would also like to thank the European Olive-Net project (Horizon2020-MSCA-RISE-2016-734899).

References

S. Beteinakis *et al.* NMR-based metabolic profiling of edible olives-determination of quality parameters. *Molecules*. 2020;25(15). doi:10.3390/molecules25153339

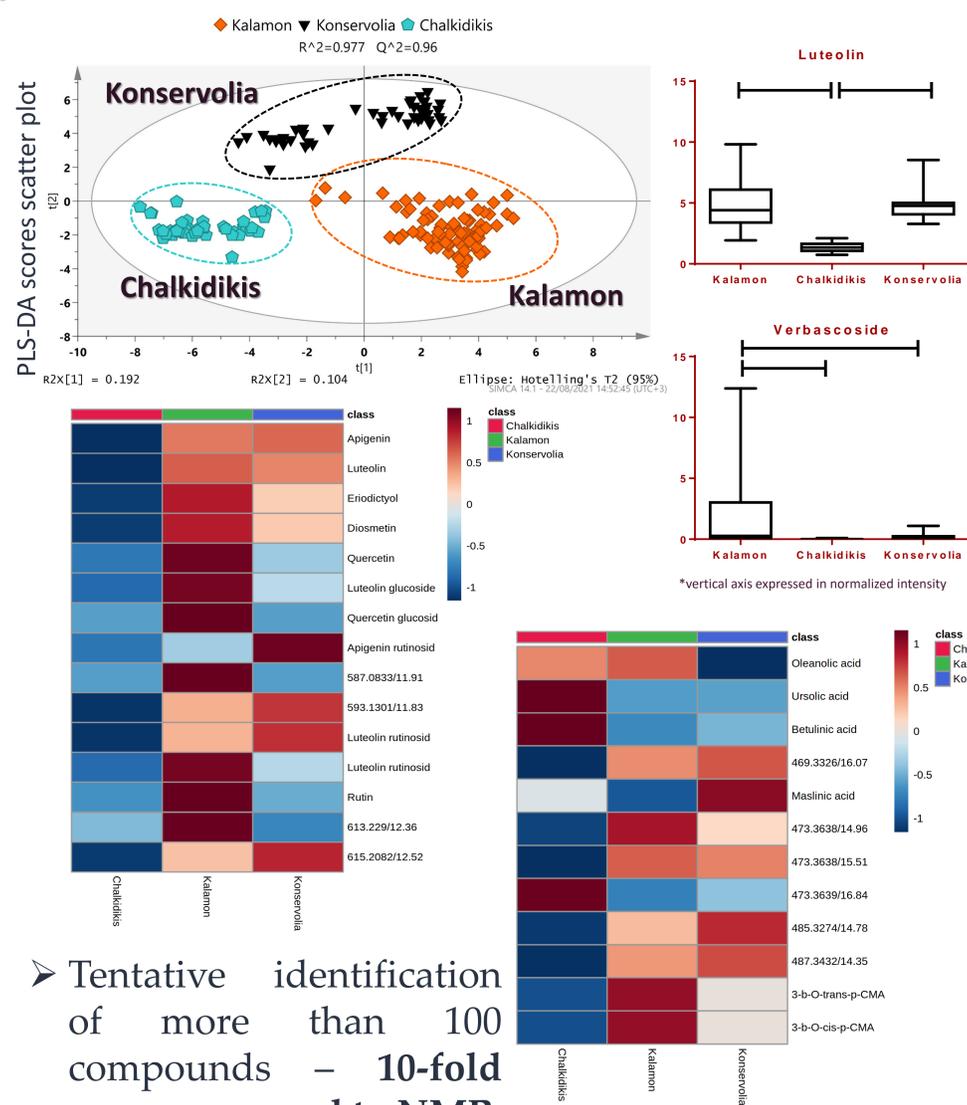
Aim

Juxtaposition of LC-HRMS & NMR metabolomics platforms in table olives’ metabolic profiling, exploring different cultivars, geographical origin and debittering methods.

The Choice of a Metabolic Profiling Platform: HRMS or NMR...?

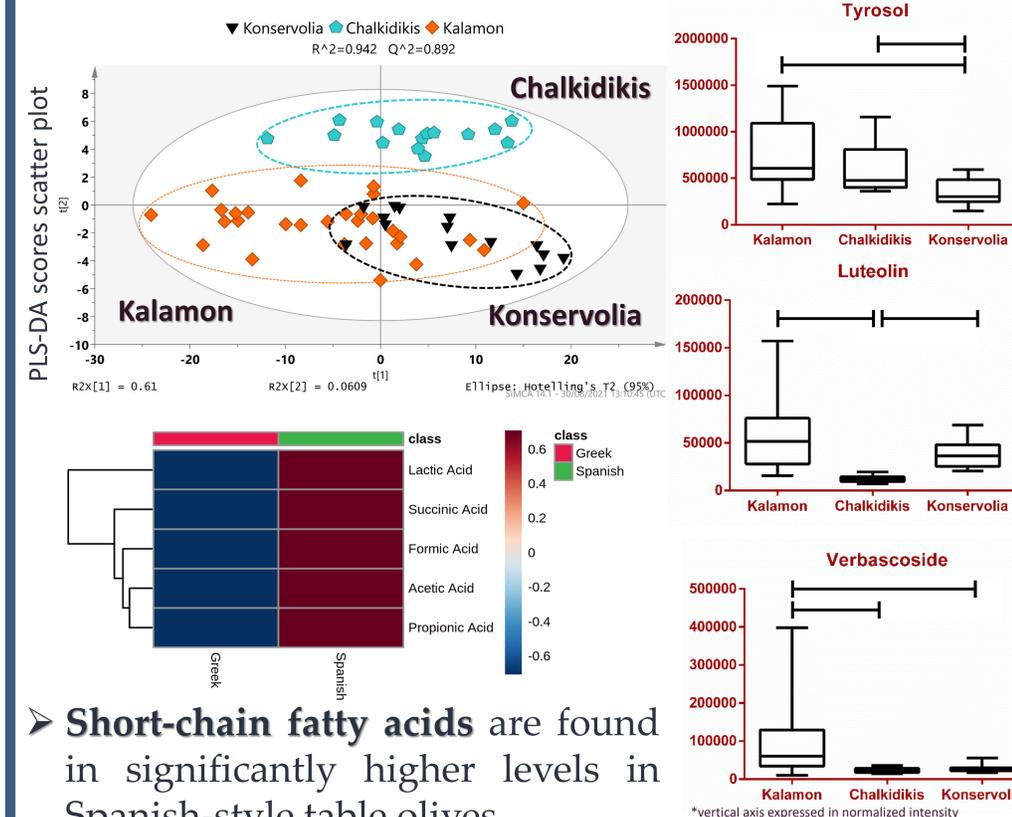
- Steps prior to analysis (collection/extraction) were **identical** to ensure reliability of inter-platform comparison
- Data processing: different software for each platform (NMR: Topspin & MATLAB / HRMS: Xcalibur & MZmine)

✓ HRMS – Hybrid LTQ-Orbitrap XL



- Tentative identification of more than 100 compounds – **10-fold more compared to NMR**
- Detection of numerous compounds along with their isomers in the classes of **flavonoids** and **triterpenoids** – strong effect of Spanish-style processing evident in the respective heatmaps

✓ NMR platform – 600MHz Avance III



- **Short-chain fatty acids** are found in significantly higher levels in Spanish-style table olives
- **Tyrosol**, the second most abundant compound in table olives, is not well-ionized → detected only with NMR

Conclusions

- ❖ Statistics with **HRMS** showed less dispersion, higher robustness, and improved classification parameters
- ❖ **High similarity** in the fluctuation of the concentration levels of tentative markers
- ❖ The two platforms are **complementary** with each one bringing something else to the table