



Training Future Food Scientists in PAT through ATR-FTIR spectroscopy & chemometrics: a fruit winemaking project

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KEY FINDING

A research-based learning project for integrated master (EQF level 7) students to monitor peach wine fermentation in real-time using ATR-FTIR spectroscopy & chemometrics

01 Introduction & Aim of the study

Transition to Food Industry 5.0 and Future Work requires reskilling food scientists to move from single-parameter testing to high-level interpretation of process-analytical signals for decision-making [1].

Incorporating these modules into the educational programme of integrated master's (EQF level 7) students is challenging.

Over the last decade, **non-destructive spectroscopic sensing combined with non-targeted, multivariate analysis** has been increasingly used for real-time process control and quality assurance in wineries and breweries, along with other Process Analytical Technologies (PAT). Nowadays, special attention is given to integrating high-precision signals from **Attenuated Total Reflectance (ATR)-mid-IR sensors** [2].

This work aims to introduce a research-based learning project for master's students using **ATR-FTIR spectroscopy & chemometrics** to monitor and control alcoholic fermentation at-line

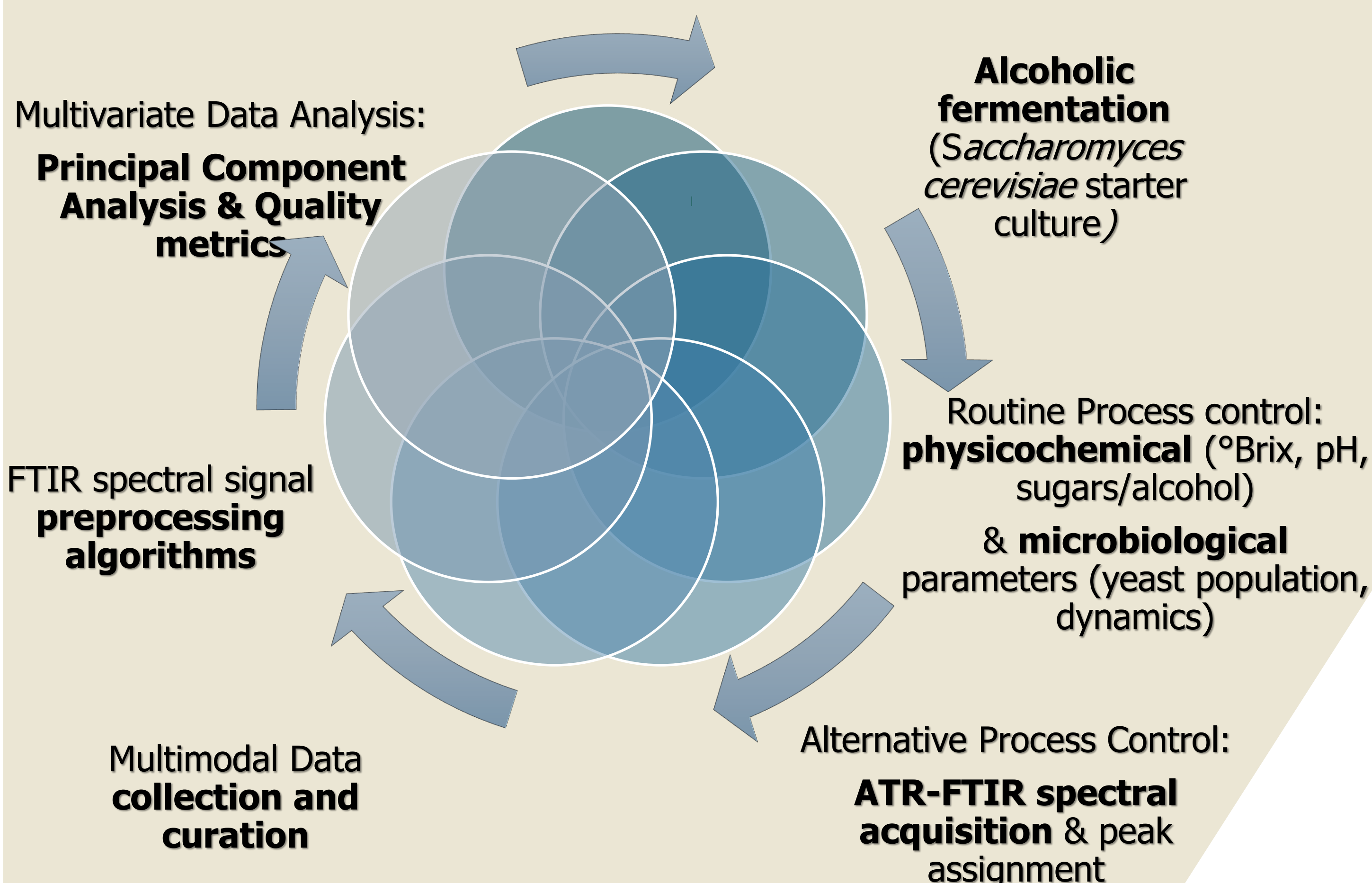
Two undergraduates and one MSc student of Food Science & Technology were engaged in a structured project using **fermenting peach puree** as a model system.

The results obtained from guiding students through the entire process, as well as the feasibility of executing such a project at the integrated master-educational level, are discussed

02 Methodology

Fruit winemaking: Project workflow description & training topics

Peach puree processing & must preparation:
Enzymatic maceration & water-dilution effects



03 Results

A tutorial for hands-on laboratory training & feedback reports:



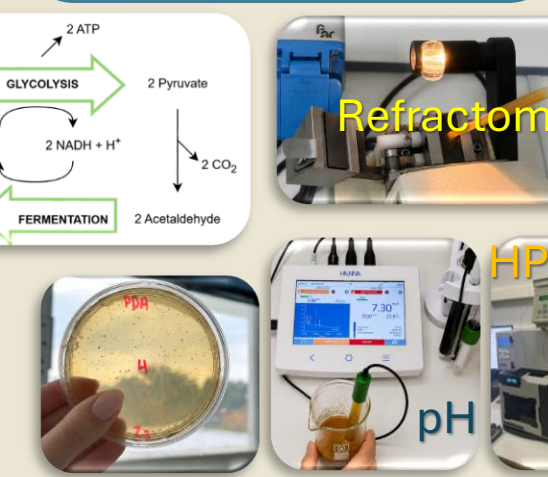
Sample selection & pretreatment

- Food Chemistry & Technology:** Peach chemistry. Understanding the challenges & advantages of using puree instead of fresh fruits
- Hands-on training:** sample handling & treatment, dilutions
- RQ1:** Any green technologies for fruit pre-processing and bioactives extraction?



Bioprocess & Routine Control

- Biochemistry:** Yeast metabolism & Alcoholic fermentation (AF)
- Hands-on training:** yeast culture inoculation, microbial counts; critical steps
- RQ2:** How is AF usually monitored or controlled (chemical/microbiological analyses)?



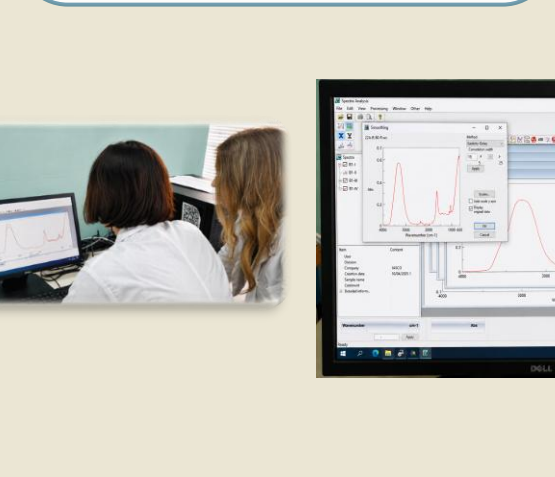
Advanced spectroscopic sensing & PAT

- Vibrational (infrared) spectroscopy principles**
- Hands-on training:** FTIR spectra acquisition with a 3-bounce diamond ATR cell
- RQ3:** Peak assignment & visual observations?



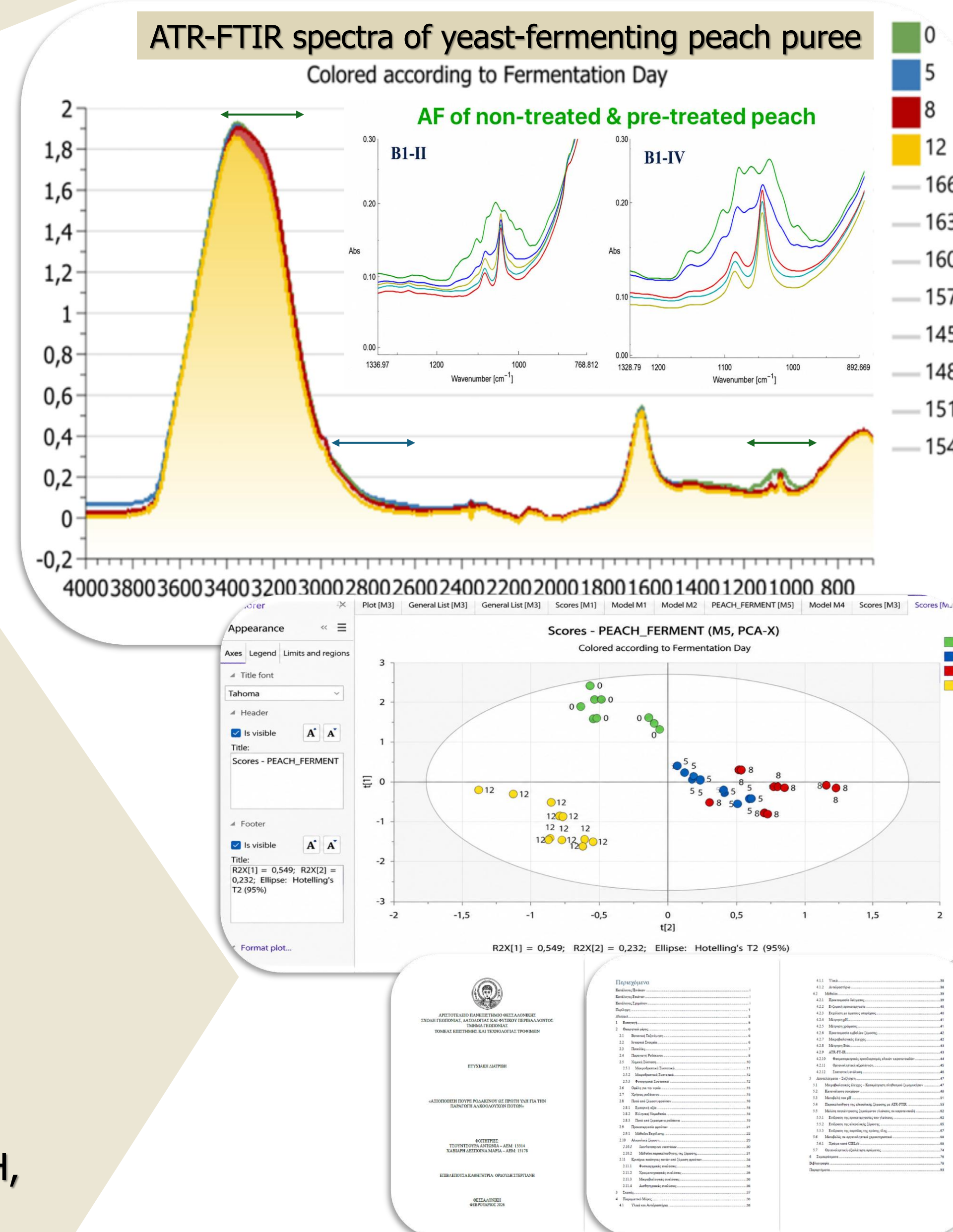
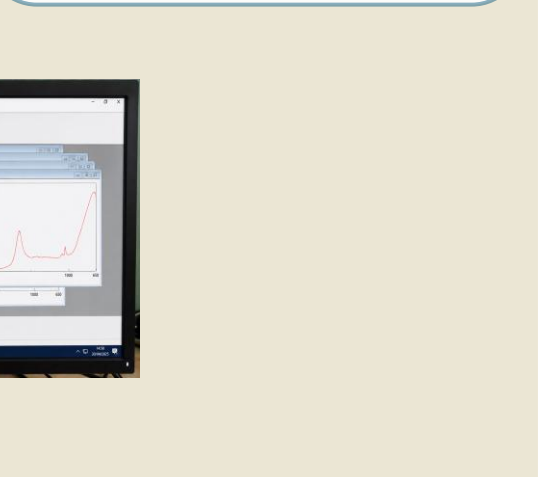
Chemometrics & Reporting

- Basic chemometrics**
- Hands-on training:** signal preprocessing (smoothing, normalization), extraction, curation of spectral data
- RQ4:** Any time-related Patterns recognized with Principal Component Analysis (PCA)?



Decision making

- Final Report** Evaluation of scores, loadings, data-of-variance explained, T2 Hotelling and Distance-to-the-model parameters
- RQ5:** Next steps for the validation of the methodology?



04 Discussion

RQ1: Students were familiarized with enzymic pretreatment & ultrasound-assisted extraction

RQ2: HPLC-RI analysis of sugars and organic acids, accompanied by external standard calibration curves, allowed the determination of residual sugars and ethanol (% vol)

RQ3: Visually recognised changes in the overlapped spectra
940-1160 cm⁻¹: sugar conversion to alcohol || 3160-3400 cm⁻¹: H-bonds/water-ethanol complex formation || 2600-3000 cm⁻¹: ethanol & wine-system interactions

RQ4: >8 Different spectral datasets were generated: raw or normalized spectra || pretreated or no pretreated peach || 2 dilution levels || PCA was performed on mean-centred scaled data. Model quality was evaluated by: Number of PCs explaining >95% variance, %Variance explained by 2 PCs, Cross-validation Q2, Outliers by Hotelling's T2 & Distance-to-the Model → Recognition of time-related patterns

RQ5: Feedback reports, public presentation and final project evaluation demonstrated satisfactory understanding and competence in multivariate data interpretation

05 Conclusions

- Students were able to describe how sample pretreatment influenced the spectral profile
- PCA-based exploratory analysis enabled them to recognize temporal spectral patterns and comprehend the fingerprinting process
- ATR-FTIR spectroscopy provided an accessible laboratory tool for introducing modern process-monitoring concepts in Food Industry 5.0
- Students' final report demonstrated their research-based learning, system-thinking and scientific communication skills

06 References

[1] Leon, R. D. (2023). Employees' reskilling and upskilling for industry 5.0: Selecting the best professional development programmes *Technology in Society*, 102393, <https://doi.org/10.1016/j.techsoc.2023.102393>; [2] Ordoudi, S. A. (2026). *MIR/FTIR spectroscopy for precision winemaking in smart wineries: state of the art, challenges, and prospects*. *Applied Spectroscopy Reviews*, 1-27. <https://doi.org/10.1080/05704928.2026.2629006>