

Contract no. 651PED/2022
Project code: PN-III-P2-2.1-PED-2021-1095

Wine fingerprint recognition based on spectroscopic methods and Artificial Intelligence (WineRec – AI)

Phase 2 summary: Development and optimization of wine recognition models based on ^1H -NMR and Raman spectroscopic methods in conjunction with Artificial Intelligence.
Web application development and validation

Implementation period: 01.01.2023 – 31.12.2023

1. Summary of the activities completed during the implementation period

In this stage, the final wine recognition models based on the Raman experimental data were implemented, using an expanded dataset illustrating a greater diversity in terms of production year and cultivar. Additionally, the potential of $^1\text{H-NMR}$ spectroscopy in conjunction with various machine learning techniques (e.g. Support Vector Machines, Logistic Regression, k-Nearest Neighbors), was investigated for developing prediction models in regard to the production year, geographical origin, and grape variety, using a set of 50 wine samples from Romania. In this context, various data preprocessing techniques were tested and compared, among which applying variance scaling followed by a variable selection based on Partial Least Squares led to the most accurate results, with accuracy scores exceeding 94% in 10-fold cross-validation.

Based on these results, a new web application for wine authenticity control was developed, optimized, and validated. The software solution proposed in this execution stage represents a useful and secure tool for managing the database and applying optimized recognition models based on machine learning techniques in order to predict the origin of unknown wine samples. Moreover, the developed web application allows authenticated users to create new differentiation models based on $^1\text{H-NMR}$ or Raman experimental data, depending on their preferences, without technical expertise barriers, but through an intuitive and user-friendly interface.

The results obtained in this stage of the project were disseminated as follows:

1. **2 ISI articles** published in journals in the first quartile (Q1) according to Web of Science
2. **6 presentations** at international conferences

2. Progress summary

	Planned Deliverables/Indicators	No.	Achieved Deliverables/Indicators	No.
1.	Published ISI article	1	Published ISI articles	2
2.	Presentations at international conferences	3	Presentations at international conferences	6
3.	Optimized prediction models based on Raman data	3	Optimized prediction models based on Raman data	5
4.	Recognition models based on $^1\text{H-NMR}$ data	3	Recognition models based on $^1\text{H-NMR}$ data	3
5.	Optimized prediction models based on $^1\text{H-NMR}$ data	3	Optimized prediction models based on $^1\text{H-NMR}$ data	3
6.	Project webpage updated	1	Project webpage updated	1
7.	Database	1	Database	1
8.	Optimized and validated web application	1	Optimized and validated web application	1

The dissemination of results is presented in detail as follows:

I. Publication of two articles in first quartile journals (Q1 – Web of Science)

1. Pirnau, A., Feher, I., Sârbu, C., Hategan, A. R., Guyon, F., Magdas, D. A. (2022). Application of Fuzzy algorithms in conjunction with ^1H -NMR spectroscopy for alcoholic beverages differentiation. *Journal of the Science of Food and Agriculture*. 103(4), 1727–1735. <https://doi.org/10.1002/jsfa.12402>
2. Hategan, A. R., David, M., Berghian-Grosan, C., Magdas, D. A. (2023) Geographical and Varietal Origin Differentiation of Alcoholic Beverages through the Association between FT-Raman Spectroscopy and Advanced Data Processing Strategies, *Food Chemistry: X*, 100902. <https://doi.org/10.1016/j.fochx.2023.100902>

II. Participations at international conferences

1. Hategan, A. R., Pirnau, A., Cozar, B., Cinta-Pinzaru, S., Guyon, F., Magdas, D. A. Fusing ^1H -NMR and Raman experimental data for a new wine recognition strategy. 3rd Food Chemistry Conference, 10-12 October 2023, Dresden, Germany.
2. Hategan, A. R., Pirnau, A., Magdas, D. A. Applications of Artificial Intelligence in recognizing the origin of wine based on ^1H -NMR spectroscopy. 14th International Conference PIM – Processes in Isotopes and Molecules, 19-22 September 2023, Cluj-Napoca, Romania.
3. Hategan, A. R., Pirnau, A., Magdas, D. A. Application of Machine Learning techniques for assessing the origin of wine based on ^1H -NMR spectroscopy. 25th International Conference Materials, Methods & Technologies, 17-20 August 2023, Burgas, Bulgaria.
4. Magdas, D. A., Hategan, A. R. Raman spectroscopy – an effective tool for wine differentiation. 44th World Congress of Vine and Wine, 5-9 June 2023, Jerez de la Frontera, Cadiz, Spain.

III. Invited lectures

1. Magdas, D. A., Hategan, A. R., David, M., Berghian-Grosan, C. Application of Raman spectroscopy as a rapid tool for beverages and food authentication. International Bio-Inspiration N.I.C.E. Summer Event, 21-23 June 2023, Nice, France. The conference is endorsed by CNRS and IUPAC.
2. Magdas, D. A. Applications of Raman spectroscopy in wine differentiation, European Reference Centre for Control in the Wine Sector MSDL meeting, JRC-Geel, 7-8 February 2023, Geel, Belgium.

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