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Optimization of NaDES extraction parameters of polyphenolic compounds from white grape pomace

Silviu MĂNTĂILĂ[1], Nicoleta BALAN[1], Gabriela RÂPEANU[1], Nicoleta STĂNCIUC[1]
[1]Dunarea de Jos University of Galati, Faculty of Food Science and Engineering, Department of Food Science, Food Engineering, Biotechnology and Aquaculture

1 ABSTRACT

Current trends in the food industry merge towards a circular economy, including valorization of the related food processing by-products by extraction of bioactive compounds with nutraceutical and food applications. A modern alternative method used for extracting these compounds with health-promoting properties is the use of a natural deep eutectic solvent (NaDES). The increased interest in this type of solvent is due to its low cost, ease of preparation, extraction yield and protection of compounds from plant material, but especially due to its eco-friendly on the environment.

White grape pomace (WGP) is one of the most abundant by-products generated from vinification, having a rich composition in bioactive compounds, such as phenolic acids, flavon-3-ols, flavonols, and many others. The main aim of this study was to test the efficiency and efficacy of a NaDES, consisting of a 1:2:1 molar ratio of choline chloride, lactic acid and water, respectively the application of a Central Composite Design with 3 independent variables (temperature, extraction time and NaDES volume) in order to optimize the extraction of total phenolic compounds (TFC) and total polyphenolic compounds (TPC) from WGP.

According to the regression equation generated for the TFC shows that the volume of NaDES used for ultrasonic extraction has the greatest positive impact on the extraction of phenols from WGP, with the TFC value ranging from 1.62 to 14.94 mg quercetin equivalent/100 g SU.

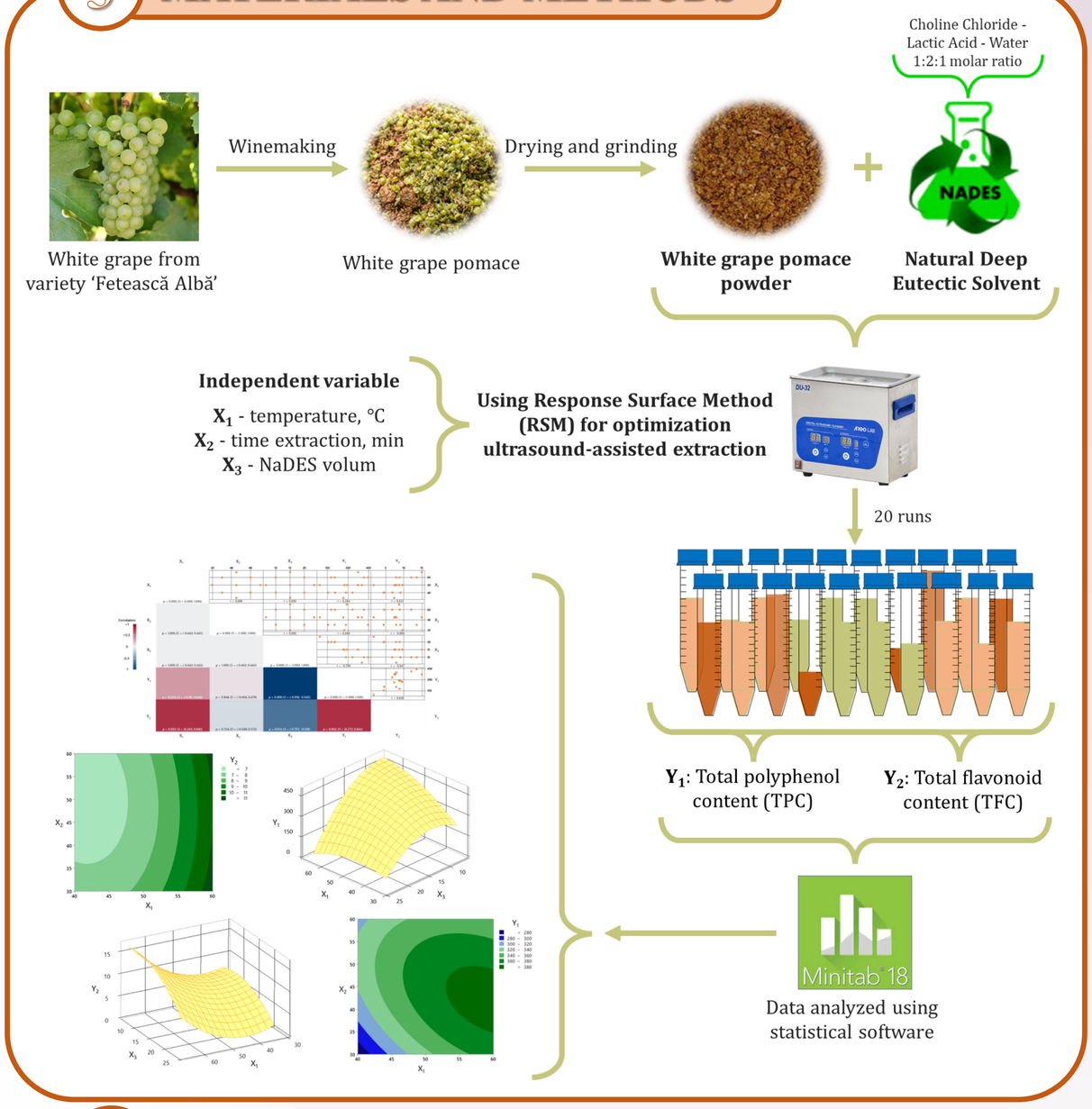
The use of NaDES extraction to obtain compounds with bioactive properties from WGP represents one of the optimal alternatives to replace traditional organic solvents such as methanol, contributing to the development of sustainable extraction methods and the future use of the optimized extract to obtain high-value products.

2 INTRODUCTION

The valorization of white grape pomace (**WGP**) through the extraction of polyphenolic compounds represents both a challenge and an opportunity. Introducing these extracts in food matrices can lead to the development of sustainable, economical, high value-added products and provide health [1].

This study aims to identify the optimal conditions: temperature ($\mathbf{X_1}$), time extraction ($\mathbf{X_2}$) and NaDES volume ($\mathbf{X_3}$) and to evaluate the efficiency of NaDES in developing a green ultrasound-assisted extraction method for polyphenolic compounds ($\mathbf{Y_1}$ and $\mathbf{Y_2}$) from the plant matrix, by applying a Central Composite Design (CCD), using a natural deep eutectic solvent (**NaDES**) composed of choline chloride, lactic acid and water, with conventional ethanol extraction serving as the reference method.

3 MATERIALS AND METHODS



4 RESULTS AND DISCUSSION

- In the 3D surface graph (**Fig. 1**), the impact of the interaction between the independent variables temperature ($\mathbf{X_1}$) and solvent volume ($\mathbf{X_3}$) on the dependent variables TPC ($\mathbf{Y_1}$) and TFC ($\mathbf{Y_2}$) can be observed. An increasing in the temperature combined with decrease in the solvent volume during ultrasound-assisted solid-liquid extraction resulted in a higher yield in polyphenolic compounds.

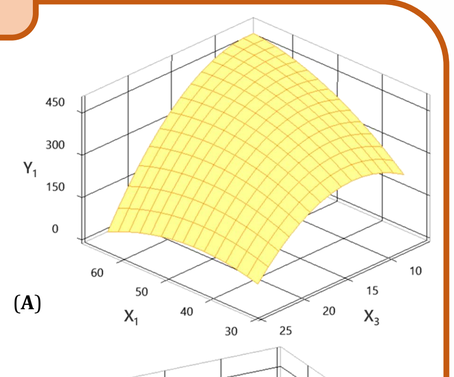


Figure 1. 3D response surface for the NaDES extract, analyzing the interaction effect between temperature ($\mathbf{X_1}$) and NaDES volume ($\mathbf{X_3}$) on the TPC (**A**) and on the TFC (**B**)

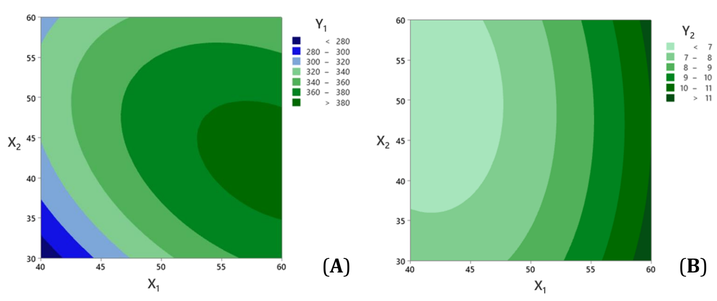


Figure 2. 2D contour plots for the NaDES extract, analyzing the interaction effect between temperature ($\mathbf{X_1}$) and time ($\mathbf{X_2}$) on the TPC (**A**) and on the TFC (**B**)

- In the 2D (**A**) contour graphs (**Fig. 2**), shows that the maximum TPC value (**443.43 mg GAE/ 100 g DW**) was achieved at temperature ($\mathbf{X_1}$) of 60°C and an extraction time ($\mathbf{X_2}$) of 30 min. Prolonging the extraction time ($\mathbf{X_2}$) while maintaining a constant $\mathbf{X_1}$ (60°C) led to a decrease in both TPC and TFC values, due to the thermal degradation of these compounds.
- According to **Fig. 3**, there is a strong positive linear correlation (**r = 0.633**) between the response TFC ($\mathbf{Y_1}$) and temperature ($\mathbf{X_1}$), with high statistical significance (***p* = 0.002**), showing that an increase in $\mathbf{X_1}$ enhances the extraction of flavonoids from WGP. Conversely, there is a strong negative Pearson correlation (**r = -0.796**) between the response $\mathbf{Y_1}$ (TPC) and the factor $\mathbf{X_3}$ (NaDES volume), with high statistical significance (***p* < 0.001**).

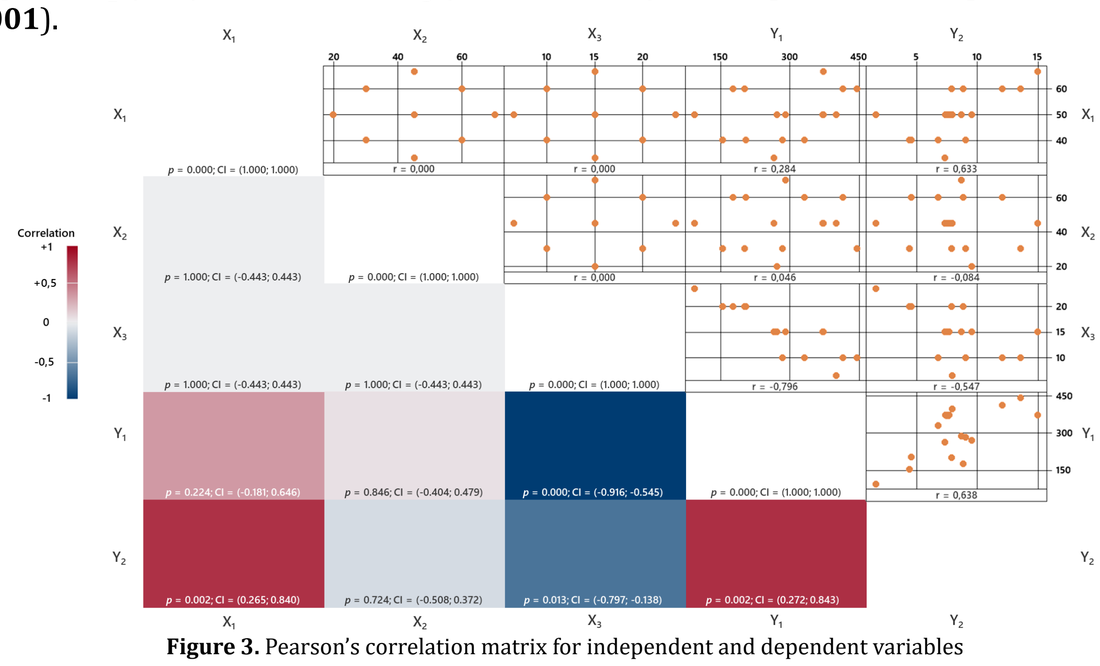


Figure 3. Pearson's correlation matrix for independent and dependent variables

5 CONCLUSION

The present study supports the feasibility of using natural deep eutectic solvents (**NaDES**) as a sustainable, eco-friendly, and efficient alternative for the extraction of polyphenolic compounds from white grape pomace (**WGP**), thereby contributing to the development of circular economy within the food industry. By applying the Central Composite Design (**CCD**), the optimal extraction conditions: temperature ($\mathbf{X_1}$), extraction time ($\mathbf{X_2}$) and solid-liquid ratio ($\mathbf{X_3}$) were determined to maximize the recovery of the target response variables **TPC** and **TFC.** The NaDES composed of choline chloride, lactic acid and water led not only yielded high amount of polyphenols ($\mathbf{Y_1}$) and flavonoids ($\mathbf{Y_2}$) from **WGP** but also aligned with the green extraction principles, due to its environmental friendliness and the application of ultrasound-assisted extraction.

6 ACKNOWLEDGEMENT

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7 REFERENCES

Dheyab, A. S., Abu Bakar, M. F., AlOmar, M., Sabran, S. F., Muhamad Hanafi, A. F., & Mohamad, A. (**2021**). Deep Eutectic Solvents (DESs) as Green Extraction Media of Beneficial Bioactive Phytochemicals. *Separations*, 8(10), 176. https://doi.org/10.3390/separations8100176