Polyphenols Identification and Characterization of Palatinate German Wines Using NMR Spectroscopy and Multivariate Data Analysis

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ABSTRACT

^{1}H NMR has been used for metabolic profiling of five different German wines from the Palatinate region. Samples from the different vintages of Riesling wine were also analyzed to understand its effects. For metabolites identification, especially the phenolics in wine, two-dimensional NMR techniques were employed. Principal component analysis (PCA) was also performed to emphasize differences among different wines and vintages. Different compounds were found dictating in different wines like succinate and citrate in Moriomuskat, alanine and lactic acid in Mullerthurgau, and GABA and Proline in Riesling. Rivaner and Kerner were characterized by higher levels of threonine and fumarate, and glucose and malate, respectively. Among the phenolics, Kerner and Riesling showed high contents of coumarate and benzoate while quercetin and gallic acid were found discriminating for Mullerthurgau and Moriomuskat, correspondingly. Rivaner was found with higher levels of compounds like kaempferol and sinapic acid. The PCA analysis showed clear differences among the vintages of Riesling. The vintage of 2005 showed more phenolic contents with higher proline levels suggesting longer sun expose time and shorter rainfall periods during that year. Based on these findings, identification of wine metabolites along with the metabolic characterization of different wines and vintages has been discussed.

Keywords: Metabolic Fingerprinting, NMR, PCA, Phenolics, Wine.

INTRODUCTION

Most liquid foods have a complex chemical profile and similarly wine, the most important beverage in the world, contains a mixture of compounds at diverse concentrations. NMR has been already demonstrated as a robust method and unaffected by a number of instrumental and experimental factors (Tabago et al, 2021).

OBJECTIVE

Our study was targeted to analyze different wines using ^{1}H NMR spectroscopy with an emphasis on identifying phenolics in wines. Based on these analyses, characterization of different wines and vintages has been done.

MATERIALS AND METHOD

Five different German wines from Palatinate region were used in this study which includes Riesling, Moriomuskat, Mullerthurgau, Kerner, and Rivaner. Samples from three vintages of 2005, 2006, and 2007 were also analyzed but only for Riesling. Samples were subjected to NMR spectroscopy and multivariate data analysis (Emwas et al., 2019).

RESULTS AND DISCUSSION

Around fifty metabolites have been identified in different wine samples using ^{1}H NMR with the help of different 2D techniques like *J*-resolved with COSY, HMBC, and HSQC spectra (Mao et al., 2023). The

metabolites identified cover a wide range of diversity. The ^{1}H NMR data were further subjected to principal component analysis using SIMCA-P+ (ver. 12.0) software. This is a method useful in grouping or differentiating samples according to their spectral characteristics which can be seen in a graphical form known as "score plot". The loadings are the coefficients multiplied with original variables to obtain principal components (Debik et al., 2022 and Kim et al., 2023). The replicates showed tight clustering and it can easily observed from the score plot that wines like Riesling, Mullerthurgau, and Moriomuskat were well separated from each other and also from Rivaner and Kerner. This explained that these three wines are quite different with each other in their metabolic profile. It has been shown that hot and dry climate result in the higher proline and phenolic contents in wine. In our case the 2005 vintage for Riesling wine showed higher phenolic and proline contents which might be due to longer sun-exposed time with shorter rainfall periods.

CONCLUSION

In conclusion, ^{1}H NMR based metabolic profiling was proved to be effective in terms of identifying diverse metabolites. In combination with ^{1}H NMR, PCA was found very effective in highlighting the varietal differences among the wine. The effect of vintages on metabolic profiles of wine has also been studied effectively.

REFERENCES

1. Tabago, M. K. A. G., Calingacion, M. N., & Garcia, J. (2021). Recent advances in NMR-based metabolomics of alcoholic beverages. Food Chemistry: Molecular Sciences, 2, 100009.
2. Emwas AH, Roy R, McKay RT, Tenori L, Saccenti E, Gowda GN, Raftery D, Alahmari F, Jaremko L, Jaremko M, Wishart DS. (2019). NMR spectroscopy for metabolomics research. Metabolites, 9(7), 123.
3. Le Mao, I., Da Costa, G., Bautista, C., de Revel, G., & Richard, T. (2023). Application of 1H NMR metabolomics to French sparkling wines. Food Control, 145, 109423.
4. Debik, J., Sangermani, M., Wang, F., Madssen, T. S., & Giskeødegård, G. F. (2022). Multivariate analysis of NMR-based metabolomic data. NMR in Biomedicine, 35(2), e4638.
5. Kim YM, Lubinska-Szczygeł M, Park YS, Deutsch J, Ezra A, Luksrikul P, Beema Shafreen RM, Gorinstein S. (2023). Characterization of bioactivity of selective molecules in fruit wines by FTIR and NMR spectroscopies, fluorescence and docking calculations. Molecules, 28(16), 6036.