biology and life sciences forum

MDPI

*Proceeding Paper*

# FTIR Spectroscopy in Combination with Chemometrics for the Estimation of Grape Pomace Geographical Origin †

**Marinos Xagoraris [1], Panagiota-Kyriaki Revelou [1,2], Efstathia Skotti [3], Christos Pappas [1] and Petros A. Tarantilis [1]**

[1] Laboratory of Chemistry, Department of Food Science & Human Nutrition, Agricultural University of Athens
[2] Department of Food Science and Technology, University of West Attica, Ag. Spyridonos Str., Egaleo, 12243 Athens, Greece
[3] Department of Food Science and Technology, Ionian University, Terma Leoforou Vergoti, GR28100 Argostoli, Cephalonia, Greece
* Correspondence: ptara@aua.gr
† Presented at the 3rd International Electronic Conference on Foods: Food, Microbiome, and Health—A Celebration of the 10th Anniversary of Foods' Impact on Our Wellbeing; Available online: https://foods2022.sciforum.net.

**Abstract:** A single paragraph of about 100 words to give a brief introduction to your work.

**Keywords:** keyword 1; keyword 2; keyword 3 (List three to ten pertinent keywords specific to the article yet reasonably common within the subject discipline.)

## 1. Introduction

Grape is one of the world's largest fruit crops and grape pomace is one of wastes generated by wine-making processes. According to Greek Ministry of Rural Development and Food in 2017, Greek Ionian islands produced 1179.25 tons of grapes for wine making and 175.12 tons of them were grape pomace. Protected Designation of Origin of Cephalonia Robola wine and other traditional grape varieties are of particular interest. Fourier-transformed infrared spectroscopy (FTIR) in combination with chemometric analysis is among one promising analytical method for determining the approach geographical origin of them. In this study, FTIR spectra of 31 grape pomace samples from three geographical regions, Cephalonia ($n$ = 13), Zakynthos ($n$ = 9) and Corfu ($n$ = 9), were obtained in triplicates, using a Nicolet 6700 FTIR in the Diffuse Reflectance (DRIFTS) mode with DTGS detector. Collection and processing of spectral data was carried out using OMNIC ver. 7.3. Stepwise discriminant analysis was performed using the spectral region 1900-600 $cm^{-1}$ in SPSS software ver. 25.0. The equivalence between the groups was checked with Box's M test ($p > 0.001$). Results showed that five steps were formed. The percentage of samples that were classified correctly was 90.3% while with the method of cross-validation was 87.1%. The Wilks $\lambda$ values for the two discriminant functions had $p < 0.05$, indicating a good discriminant power of the model. Eigenvalues suggest that the first discriminant function was more discriminating with high canonical correlation (0.846) which explained 84.6% of the total variance. Results showed that FTIR spectroscopy combined with chemometrics techniques can be used for the differentiation of grape pomace geographical origin.

## Reference

References must be numbered in order of appearance in the text (including citations in tables and legends) and listed individually at the end of the manuscript. We recommend preparing the references with a bibliography software package, such as EndNote, ReferenceManager or Zotero to avoid typing mistakes and duplicated references. Include the digital object identifier (DOI) for all references where available.

**Citation:** Xagoraris, M.; Revelou, P.K.; Skotti, E.; Pappas, C.; Tarantilis, P.A. FTIR Spectroscopy in Combination with Chemometrics for the Estimation of Grape Pomace Geographical Origin. *Biol. Life Sci. Forum* **2022**, 2, x. https://doi.org/10.3390/xxxxx
Published: 1 October 2022

Citations and references in the Supplementary Materials are permitted provided that they also appear in the reference list here.

In the text, reference numbers should be placed in square brackets [ ] and placed before the punctuation; for example [1], [1–3] or [1,3]. For embedded citations in the text with pagination, use both parentheses and brackets to indicate the reference number and page numbers; for example [5] (p. 10), or [6] (pp. 101–105).

1. Author 1, A.B.; Author 2, C.D. Title of the article. *Abbreviated Journal Name* **Year**, *Volume*, page range.
2. Author 1, A.; Author 2, B. Title of the chapter. In *Book Title*, 2nd ed.; Editor 1, A., Editor 2, B., Eds.; Publisher: Publisher Location, Country, 2007; Volume 3, pp. 154–196.
3. Author 1, A.; Author 2, B. *Book Title*, 3rd ed.; Publisher: Publisher Location, Country, 2008; pp. 154–196.
4. Author 1, A.B.; Author 2, C. Title of Unpublished Work. *Abbreviated Journal Name* year, *phrase indicating stage of publication (submitted; accepted; in press)*.
5. Author 1, A.B. (University, City, State, Country); Author 2, C. (Institute, City, State, Country). Personal communication, 2012.
6. Author 1, A.B.; Author 2, C.D.; Author 3, E.F. Title of Presentation. In Proceedings of the Name of the Conference, Location of Conference, Country, Date of Conference (Day Month Year).
7. Author 1, A.B. Title of Thesis. Level of Thesis, Degree-Granting University, Location of University, Date of Completion.
8. Title of Site. Available online: URL (accessed on Day Month Year).