

Application of FT-IR Spectroscopy for Fingerprinting Bioactive Molecules in a Nutraceutical PROMEN, comparatively with Plantingredients

Florina CSERNATONI^{1,2)}, Carmen SOCACIU¹⁾, Raluca Maria POP^{2,3)}, Florinela FETEA¹⁾, Florina BUNGHEZ¹⁾

¹⁾University of Agricultural Sciences and Veterinary Medicine, Faculty of Agriculture, 3-5 Mănăştur Street, Cluj-Napoca, Romania; florina.csernaton@gmail.com

²⁾Center for Applied Biotechnology CCD-BIODIATEC, Proplanta Cluj-Napoca, Romania

³⁾University of Medicine and Pharmacy Iuliu Hatieganu Cluj-Napoca, Victor Babes, 8, Cluj-Napoca, Romania

Abstract. The aim of this study is to characterize and identify the main biomarkers of food supplement PROMEN by analysis of plant ingredients comparatively with the final product. Alcoholic extracts of plants were prepared at 15% plant content and purified fractions were analyzed by FTIR screening. The fingerprint region (1000 to 1500 cm^{-1}) indicated the presence of specific functional groups to identify and monitor the phenolic derivatives.

Keywords: PROMEN, nutraceutical, yeast, plants, prostate protection, FTIR spectroscopy

Introduction. In recent years, an increasing interest of population towards food supplements was observed, mainly because of their prophylactic effect on various diseases (Chen *et al.*, 2013). For this reason quality control of medicinal plants and new dietary formulas are becoming of major importance. For this purpose, Fourier transform infrared spectroscopy (FTIR) is an advanced, rapid and non-destructive technique frequently used to authenticate raw materials and final products using their specific fingerprints (Neha *et al.*, 2013) and to determine plant extracts biomarkers based on their functional groups (Socaciu *et al.*, 2009).

Aims and objectives. To characterize and identify the main biomarkers of nutraceutical PROMEN comparatively with plant and fruit ingredients.

Materials and methods. Seven plant and fruit sources, namely nettle (*Urtica dioica*), green tea (*Camellia sinensis*), fluff with small flowers (*Epilobium parviflorum*), tomato (*Solanum lycopersicum*), sea buckthorn (*Hippophae rhamnoides*), pumpkin (*Cucurbita maxima*) sunflower (*Helianthus annuus*) and lyophilized beer yeast (*Saccharomyces cerevisiae*), were investigated. Alcoholic extracts were prepared at 15% plant concentration and the purified fractions were analyzed using FT-IR spectroscopy. Samples were analyzed using a Shimadzu FTIR spectrometer using the Horizontal Attenuated Total Reflection (HATR). The Fourier Transform Infrared spectrum (FTIR) of each extract was recorded in the MIR region, from 1500 to 1000 cm^{-1} , and then the fingerprint region was selected for data analysis (Gorinstein *et al.*, 2013).

Results and Discussion. Fig. 1 represents the comparative FTIR fingerprints of the nutraceutical product Promen and yeast, its major ingredient. The fingerprint region (1000 and 1500 cm^{-1}) analysis yielded the presence of specific functional groups, included in three areas as follows: (1) 1000 - 1130 cm^{-1} characterized by stretching vibrations C-O of mono-, oligo- and carbohydrates, with signals at 1030, 1054, 1104, and 1130 cm^{-1} ; (2): 1150-1270 cm^{-1} corresponding to stretching vibrations of carbonyl C-O or O-H bendings and (3): 1300-1450 cm^{-1} specific for stretching vibrations of C-O (amide) and C-C stretching from phenyl groups.

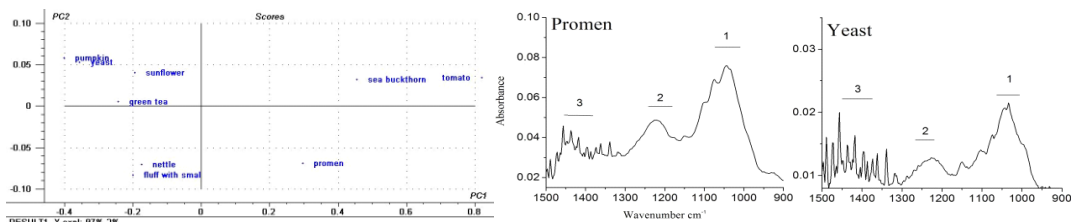


Fig. 1. Principal Component Analysis (A), explaining 99% of total variance and comparative FT-IR fingerprints of methanol sample extracts for PROMEN and its major ingredient, yeast (B)

Thus, most of the plant extracts were rich in phenolic derivatives mostly flavonoid glucosides, while yeast was rich in aminoacids, peptides and B vitamins. To illustrate the variability between raw materials and final products obtained thereof, the intensities of the identified peaks in the fingerprint region was done comparatively for both plants and final product. Tab. 1 presents the comparison of FT-IR absorption bands and the vibration assignments for plant extracts and literature data (Saymanska-Chargot *et al.*, 2013).

Tab. 1. Comparison of FT-IR absorption bands and the vibration assignments for plant extracts

Frequency of measured peaks/literature data	Assignment	Frequency of measured peaks/literature data	Assignment
1436/1426	CH ₂ symmetric bending	1167/1160	O–C–O asymmetric stretching
1398/1400	COO- symmetric stretching of Carboxylate	1115/1115	C–O and C–C stretching
1362/1370	CH ₂ bending of Xyloglucan	1076/1075	C–O and C–C stretching
1315/1317	CH ₂ symmetric bending	1048/1042	C–O and C–C stretching
1237/1243	C–O stretching	1033/1030	C–O and C–C stretching

Conclusion. The FTIR fingerprint region (1000 to 1500 cm⁻¹) allowed easy discriminations between PROMEN product and its ingredients. According to PCA analysis of FTIR spectra, the samples clustering were mainly related to the bands in the 1300-1489 cm⁻¹ zone, which had the main contribution to spectra grouping. Bands in the zone 1000-1082 cm⁻¹ were also important in sample classification. The data presented in this study showed that FTIR spectroscopy is an adequate technique to fingerprint comparatively and to evaluate the extraction yield of medicinal herbs and food supplements.

REFERENCES

- Gorinstein, S. *et al.* (2013). Application of Analytical Methods for the Determination of Bioactive Compounds in some Berries. *Food Anal. Methods* 6:432-444.
- Neha, R. *et al.*, (2013). To investigate and assess why some food/ dietary supplements are health hazardous. *Journal of Drugs Delivery & Therapeutics* 3(1):65-69.
- Saymanska-Chargot, M. and A. Zdunek (2013). Use of FT-IR Spectra and PCA to the Bulk Characterization of Cell Wall Residues of Fruits and Vegetables Along a Fraction Process. *Food Biophysics* 8:29–42.
- Socaciu, C. *et al.* (2009). IR and Raman spectroscopy-advanced and versatile techniques for Agrifood quality and authenticity assessment. *Bull. of USAMV Cluj-Napoca. Agriculture*, 66: 459-465.
- Song, C.J.Y. and L. Zhang (2013). Lycopene/Tomato Consumption and the Risk of Prostate Cancer: A Systematic Review and Meta-Analysis of Prospective Studies. *J Nutr Sci Vitaminol* 59:213-223.