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# Application of FT-MIR Spectroscopy for Fingerprinting Bioactive Molecules of Plant Ingredients and a New Formula with Antimicrobial Effect

**Florina BUNGHEZ [1)], Carmen SOCACIU [1,2)], Florina ZĂGREAN [1,2)], Florinela FETEA[1)]**

[1)] University of Agricultural Sciences and Veterinary Medicine, Faculty of Agriculture, 3-5 Mănăştur street, Cluj-Napoca, România
[2)] Center for Applied Biotechnology CCD-BIODIATEC, Proplanta Cluj-Napoca, Romania
florinabunghez@gmail.com

**Abstract.** The present study aims to fingerprint 7 aromatic herbs (basil, thyme, oregano, rosemary, sage, clove, cinnamon) and an original derived formula (EPC), in order to find specific biomarkers by Fourier Transform Middle Infrared Spectroscopy (FT-MIR) spectroscopy. The studied aromatic herbs are well known for their antioxidant, antimicrobial and anticarcinogenic effect. After comparison of each plant FT-MIR fingerprint region (1400-1760 $cm^{-1}$), divided in three areas. One can see similar peaks for thyme, sage and clove, as well similar spectra of oregano and rosemary. Basil and cinnamon had different fingerprints and the spectra of product EPC resembled more to clove spectra. FTIR peaks are attributed for stretching and bending vibrations that characterize the functional groups, this kind of spectroscopy being recommended as a reliable tool to evaluate the quality and authenticity of plant formulas.

**Keywords**: EPC, FT-MIR, polyphenols, antimicrobial activity, authenticity

**Introduction** Aromatic plants and herbs have traditionally been considered rich sources of essential phytochemicals (vitamins, polyphenols and pigments such as carotenoids, chlorophylls, flavonoids, secondary metabolites). Naturally occurring compounds such as phytochemicals, which possess anticarcinogenic, antiparasitic, antimicrobial, anti-inflammatory properties, are referred to as chemopreventers.

**Aims and objectives.** The aim of the present study was the identification of the main biomarkers of plant ingredients (basil, thyme, oregano, rosemary, sage, clove, cinnamon), and for the final formula (EPC) in order to establish the authenticity and the quality of the studied herbs. The objectives of the study are as following: characterization of the methanolic extracts of the selected plant ingredients and of the final product EPC using advanced methods like FT-MIR.

**Materials and methods.** Methanolic extracts (15% MeOH, 1%HCl) were prepared from 7 plants (basil, thyme, oregano, rosemary, sage, clove, cinnamon). The new plant based formula (EPC) was obtained by mixing the plant powders according to a default recipe (20% basil, 10% thyme, 10% clove, 15% oregano, 15% rosemary, 15% sage, 15% cinnamon), the purified fractions were analyzed using a Shimatsu FTIR spectrometer using the Horizontal Attenuated Total Reflection (HATR). The Fourier Transform Infrared spectrum was recorded in the MIR region (FTMIR) of each extract, from 4000 to 900 $cm^{-1}$, and then the fingerprint region (1400-1760 $cm^{-1}$) was selected for data analysis.

**Results and Discussion.** The FTIR spectra of all individual extracts are presented in Figs.1-5. Fig.1 represents the comparative fingerprint of thyme and sage extracts, Fig.2 the fingerprints of oregano and rosemary extract, Fig. 3 the fingerprint of clove and EPC extracts. One can see similar peaks for thyme, sage and clove, as well similar spectra of oregano and rosemary. Basil (Fig.4) and cinnamon (Fig.5) had different fingerprints and the spectra of product EPC resembles more to clove spectra. FTIR peaks are attributed for stretching and bending vibrations that characterize the functional groups. The FTIR spectra was divided in eight regions, the most significant differences being observed between 1400-1760 $cm^{-1}$ named fingerprint region. This region included three areas: **Area 1** (1400-1500 $cm^{-1}$)

corresponding to C-O and C-C stretching vibrations specific to phenyl groups, **Area 2** (1500-1600 $cm^{-1}$) coresponding to aromatic domain and N-H bending and **Area 3** (1600-1760 $cm^{-1}$), corresponding to bending N-H, C=O stretchings (aldehydes, ketones, esters) as well to free fatty acids (1710 $cm^{-1}$) and glycerides (1740 $cm^{-1}$) (Socaciu *et al*., 2009a,b). In cinnamon extract there were identified specific peaks at 1727, 1679 and 1626 $cm^{-1}$, corresponding to stretching vibrations of cinnamaldehyde, while at 1573 $cm^{-1}$ a peak assigned to an aromatic ring. The peak at 1450 $cm^{-1}$ is characteristic to a C-OH bending (Li *et al*., 2013).

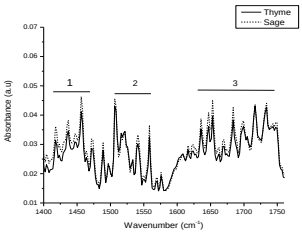


Fig. 1. Comparative FTIR spectra of thyme and sage

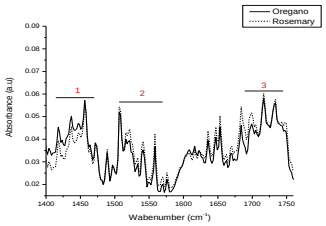


Fig. 2. Comparative FTIR spectra of oregano and rosemary

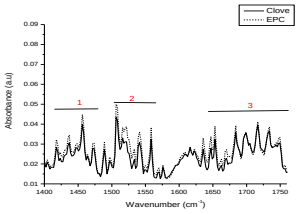


Fig. 3. Comparative FTIR spectra of clove and EPC

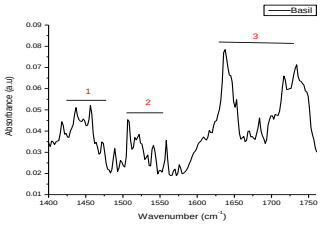


Fig. 4. FTIR spectra of basil

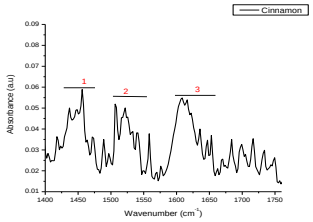


Fig. 5. FTIR spectra of cinnamon

**Conclusion.** According to the experimental data we conclude that FTMIR area 3 is the most relevant for the discrimination between plants, product EPC having a fingerprint similar to clove. FT-MIR spectroscopy is a rapid, efficient and non-destructive method, offers fast data acquisition, is simple to operate, cheaper comparing with chromatographic analysis, gives accurate information about the main biomarkers of authenticity but needs careful chemometric analysis and validation. Further studies will compare the intensity of specific peaks and also the comparison of first and second derivative of spectra in order to find the most relevant biomarkers of each plant.

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