

P20: ESTIMATION OF *SIDERITIS* SPECIES GEOGRAPHICAL ORIGIN USING DIFFUSE REFLECTANCE FOURIER TRANSFORM INFRARED SPECTROSCOPY (DRIFTS) AND CHEMOMETRICS

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Abstract – The aim of this paper is the estimation of *Sideritis* samples geographical origin using Diffuse Reflectance Fourier Transform Infrared Spectroscopy (DRIFTS) and chemometrics. The infrared spectra of 46 samples from eight greek regions were recorded in triplicate. The spectral region 1800-1530 cm⁻¹ of each average spectrum was correlated with the corresponding geographical region using TQ Analyst software. The samples were placed in the correct class at 91.3 %. The results show that the infrared spectroscopy can estimate the geographical origin of *Sideritis* samples.

Keywords: *Sideritis*, DRIFTS, geographical origin, chemometrics, FTIR

1. INTRODUCTION

Sideritis species thrive mainly in the Mediterranean countries and they are known for the anti-inflammatory, anti-ulcerogenic, digestive, antimicrobial, and antioxidant properties [1].

Over the last few years, the consumers have increasingly wanted to know the geographical origin of the foods they consume.

In the last years Fourier Transform Infrared (FTIR) spectroscopy has been used for discrimination of

geographical origin in combination with chemometrics [2, 3].

In this work the estimation of *Sideritis* samples geographical origin was studied using the Fourier transform infrared (FTIR) spectroscopy combined with chemometrics. The proposed method is simple, rapid, accurate and economical.

2. EXPERIMENTAL

Forty six *Sideritis* samples were collected from eight greek geographical regions (Table 1).

The flowers were separated from the plant, milled in a common blender and pulverized in a ball mill (Retsch MM 2000) for 15 min and sieved with a 90 µm diameter holes sieve. The portion of sample size ≤90 µm was collected for spectroscopic study.

Triplicate FTIR spectra of each sample were recorded in diffuse reflectance mode (DRIFTS) using a Thermo Nicolet 6700 spectrophotometer equipped with a deuterated triglycine sulfate (DTGS) detector, resolution 4 cm⁻¹ and 100 scans per sample. The collected spectra were smoothed and the baselines were corrected using the software accompanying the spectrophotometer (OMNIC 7.3, Thermo Fisher Scientific Inc.). Then the average spectrum of each sample was measured

and its absorbance axis was normalized from a value 0 to 1.

The average spectra were input into TQ Analyst (ver. 8.0.0.245, Thermo Fisher Scientific Inc.). Eight classes, one of each geographical region, were determined using the TQ Analyst (actual classes). The spectra were linked to the actual class of each sample. The 1800-1530 cm^{-1} spectral region in 1st derivative form and the actual class of sample were correlated and the chemometric model was developed. Then the chemometric model repositioned the samples in one of the eight classes.

Table 1. Geographical origin of *Sideritis* samples.

Region	Number of samples
Central Greece	8
Crete	3
Epirus	5
Euboea	4
Lesvos	3
Macedonia	6
Poloponnese	11
Thessaly	6

3. RESULTS AND DISCUSSION

Fig. 1 shows a typical FTIR spectrum of *Sideritis* sample.

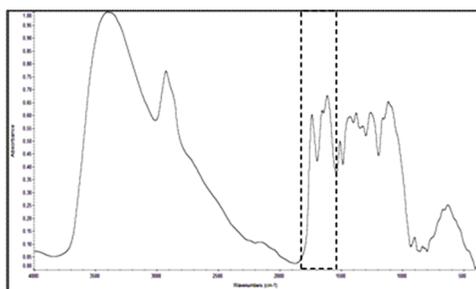


Figure 1. A typical FTIR spectrum of *Sideritis* sample. (The rectangle encloses the spectral range 1800-1530 cm^{-1}).

The FTIR spectra are very similar. The largest differences, as they were determined by the OMNIC software, were found in the 1800-1530 cm^{-1} spectral region. This spectral region has been correlated with the stretching of $>\text{C}=\text{O}$ and $>\text{C}=\text{C}$. The water and the proteins absorb as well [4]. The first derivative was chosen to maximize the differences between the spectra.

The chemometric model was developed as described in experimental section. The TQ Analyst software measured a mean spectrum, one for each geographical region. Subsequently, the Mahalanobis distances of the 46 spectra from each mean spectrum were calculated and the sample was placed in the class having the shortest distance. Forty two samples (91.3 %) were placed in the correct class (Fig.2). Twenty principal components were used, according to cumulative eigenvalues diagnostic plot, with a 99.97 % cumulative value.

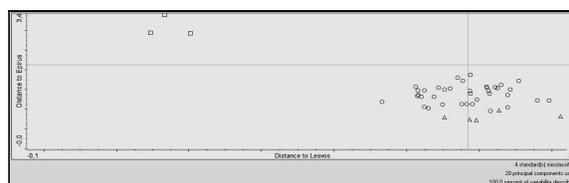


Figure 2. The Mahalanobis distances of the samples from the Epirus and Lesvos classes.

4. CONCLUSIONS

The estimation of *Sideritis* geographical origin was studied using FTIR spectroscopy and chemometrics, in this work. The results showed that the 91.3 % of the samples were recognized correctly. Therefore the FTIR spectroscopy can be used for *Sideritis* geographical origin. Furthermore the proposed method is simple, rapid and economical.

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