



Herbal Characterization and Discrimination Perspectives Using Fourier Transform Infrared Photoacoustic Spectroscopy (FTIR PAS) and Diffuse Reflectance Infrared Spectroscopy (DRIFT)

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INTRODUCTION

Herbal medicine (HM) has been used worldwide for more than hundreds of years as one of the most traditional forms of health care [1]. The chemical composition of herbs may vary depending on the species, a location of growth, age, harvesting season, drying conditions, and other conditions. [2]. In the field of HMs, the FTIR fingerprint spectra have been used since early 1987 and are used less frequently than chromatography methods [3]. Until now, the introduction of FTIR methods was limited by the complexity of spectra and its interpretation. FTIR spectroscopy, in conjunction with multidimensional statistical analysis (chemometrics), offers a very wide scope for HM studies [4]. This study demonstrates the significant potential of using innovative cantilever-enhanced Fourier transform infrared photoacoustic spectroscopy (PAS) principles and diffuse reflective infrared spectroscopy (DRIFT).

AIMS OF WORK

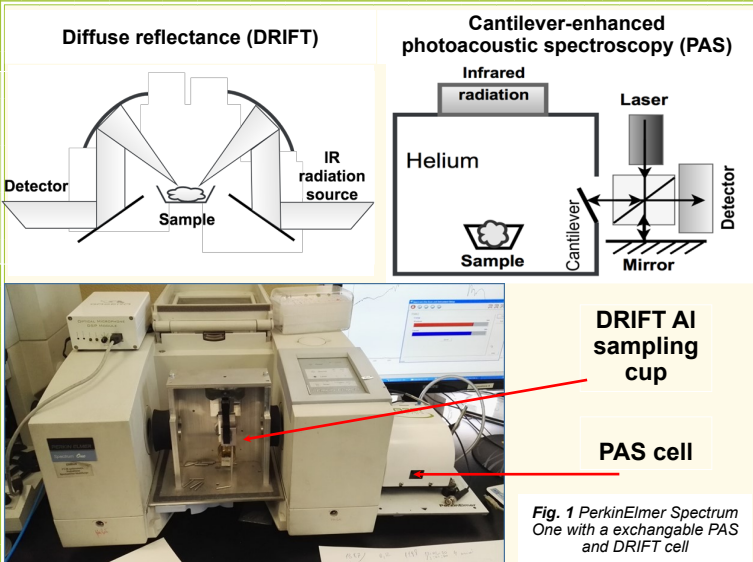
- To test non-destructive FTIR spectroscopy techniques: photoacoustic spectroscopy (PAS), diffuse reflectance (DRIFT) for herbals.
- To design and test HMs sample preparation methods for non-destructive spectroscopy techniques PAS and DRIFT.
- To design a model for unsupervised statistical data analyses (PCA, HCA).

MATERIALS

In the present work, we evaluated dried herbals and herbal extracts in ethanol. Evaluated herbals: Chamomile (*Chamomilla recutita*), cowslip (*Primula veris*), small-leaved lime (*Tilia cordata*), dwarf everlast (*Helichrysum arenarium*), marigold (*Calendula officinalis*), yarrow (*Achillea millefolium*), red clover (*Trifolium pratense*).

METHODS

PAS and DRIFT (PerkinElmer Spectrum One) spectra were taken at 450–4000 cm^{-1} , at a resolution of 4 cm^{-1} , and an average made from 10 scans. For PAS, the homogenized samples were placed in the PAS cell filled with helium gas (flow 0.5 l/min). For DRIFT homogenized samples were placed on the diamond sampling stick, but extracts in the aluminum sampling cup and evaporated.



Spectral pre-processing. *SpectraGryph 1.2.* (viewed, smoothed, baseline correction, normalization).

Statistical Analysis. The Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA) were performed using *SIMCA 14* software.

REFERENCES

- [1] P. Wang, et al., Species authentication and geographical origin discrimination of herbal medicines by near infrared spectroscopy: A review, *J. Pharm. Anal.*, vol. 5, no. 5, pp. 277–284, 2015. [2] H.A. Gad, et al., Application of chemometrics in authentication of herbal medicines: a review, *Phytochem. Anal.* 24, 1–24, 2013. [3] D. Riolo, et al., Raman spectroscopy as a PAT for pharmaceutical blending: advantages and disadvantages, *J. Pharm. Biomed. Anal.*, 5;149:329–334, 2018. [4] A. Bansal, et al., Chemometrics: A new scenario in herbal drug standardization, *J. Pharm. Anal.*, vol. 4, no. 4, pp. 223–233, 2014.

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RESULTS

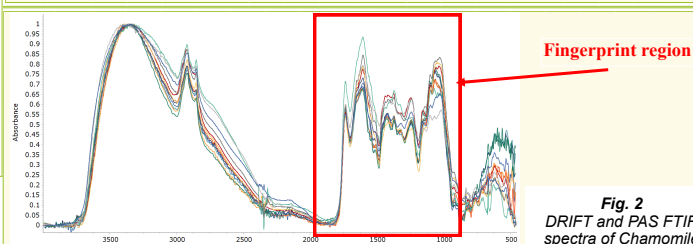


Fig. 2
DRIFT and PAS FTIR
spectra of Chamomile

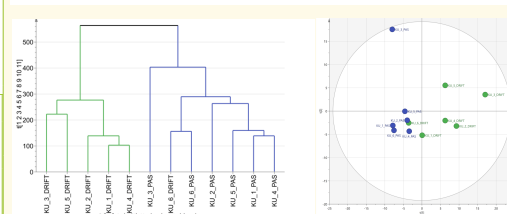


Fig. 3
PCA and HCA
diagram .DRIFT vs PAS
of homogenized
Chamomile flowers

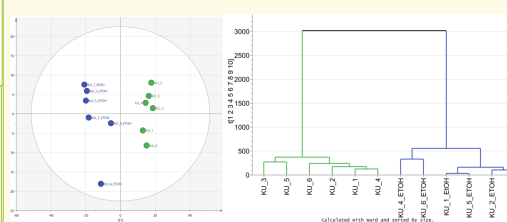


Fig. 4
PCA and HCA diagram
DRIFT Powder vs EtOH
extract of homogenized
Chamomile flowers

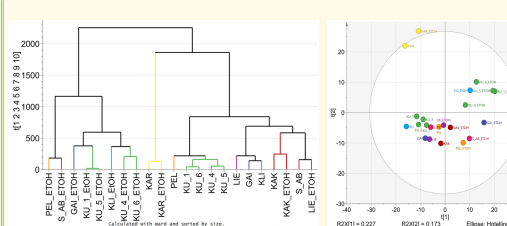


Fig. 5
PCA and HCA diagram
DRIFT Powder vs EtOH
extract of homogenized
herbal flowers: chamomile, cowslip, small-leaved lime, dwarf everlast, marigold, yarrow, red clover

CONCLUSIONS

Comparison between spectra recorded by PAS and DRIFT showed high sensitivity and good resolution. It has been demonstrated that PAS and DRIFT can be a useful experimental tool for the characterization and discrimination of herbals.

The results obtained provide information about the spectral behavior of homogenized herbal powder can be useful for establishing identification and discrimination criteria

FTIR spectroscopy, in conjunction with multidimensional statistical analysis (Chemometrics), offers an extensive scope for herbal medicine studies

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