P-019: Herbal characterization and discrimination perspectives using Fourier transform infrared photoacoustic spectroscopy (FTIR PAS) and diffuse reflectance infrared spectroscopy (DRIFT)

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This study demonstrates the significant potential of cantilever-enhanced Fourier transform infrared photoacoustic spectroscopy (FTIR PAS) principles and diffuse reflective infrared spectroscopy (DRIFT) with a diamond stick. The improved sensitivity and reproducibility of both methods present an absolute tool in the study of herbals and plants.

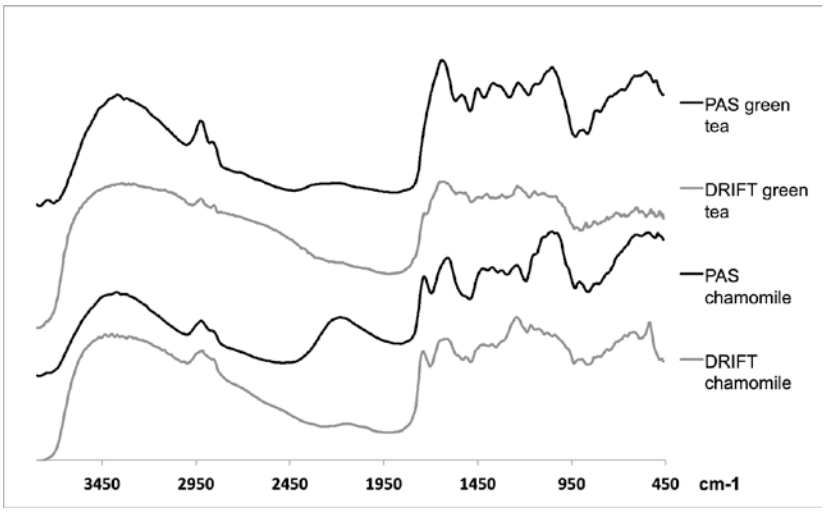

Figure 1. FTIR PAS and FTIR DRIFT spectra of green tea and chamomile

For many centuries, herbal medicine (HMs) has been used worldwide in traditional health care [1]. FTIR methods have been widely used since the 1960s [2] and can be used for both qualitative and quantitative analysis [3]. In the field of HMs, the FTIR fingerprint spectra have been used since early 1987 and are used less frequently than chromatography methods (CM) [4,5,6]. Until now, the introduction of FTIR methods was limited by the complexity of spectra and its interpretation. This problem can be resolved by using chemometrics and machine learning. The major advantages of FTIR methods are the following: it is sensitive and non-destructive or only slightly damages the sample; it requires minimal sample preparation at most; small sample quantities are necessary for measuring [2,3]. One of the important features of FTIR is the possibility to simultaneously determine different components in the same sample from a single instrumental measurement [7]. In previous studies, the FTIR spectroscopy's sampling methods transmission and ATR was most widely used as DRIFT and cantilever-enhanced photoacoustic spectroscopy (FTIR PAS). FTIR PAS is based on the photoacoustic effect. If the substance is irradiated with a pulsating light, the substance emits acoustic waves that have the same frequency as the pulsating light.

In this study, we evaluated dried herbals and green, and black tee (Figure 1). PAS and DRIFT 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), but for DRIFT homogenized samples were placed on the diamond stick.

Comparison between spectra recorded by PAS and DRIFT showed high sensitivity and good resolution. The results obtained provide information about the spectral behavior of homogenized herbal and tee powder can be a useful for establishing identification and discrimination criteria. It has been demonstrated that PAS and DRIFT can be useful experimental tool for the characterization and discrimination of herbals.

References

[1] WANG, P., et al., 2015: J. Pharm. Anal., **5**, 277–284.

[2] SMITH, B.C., 2011: CRC Press, 20–65.

[3] STUART, B.H., 2005: Infrared spectroscopy: Fundamentals and Applications. In: Analytical Techniques in the Sciences.

[4] RIOLO, D., et al., 2018: J. Pharm. Biomed. Anal., **5**, 329-334.

[5] YUAN, J.R., et al., 1987: J. of Shandong University of Traditional Chinese Medicine, **11**, 58–63.

[6] SCOPUS keywords: Herbal and Medicine and Analysis; No. of papers: 13 511; Refinement: FTIR (126 papers; only in last 10 years 12-18 papers per year) – [retrieved 16/09/2018]

[7] BANSAL, A., et al., 2014: J. Pharm. Anal., **4**, 223–233.