





# Use of innovative FTIR spectroscopy sampling methods and chemometrics for authentication and differentiation of herbals

Agnese Brangule<sup>1</sup>, Renāte Šukele<sup>2</sup>, Dace Bandere<sup>2</sup>, Pēteris Tretjakovs<sup>1</sup>,

<sup>1</sup>Dept. of Human Physiology and Biochemistry, Riga Stradiņš University, Dzirciema 16, LV-1007, Riga, Latvia <sup>2</sup>Dept. of of Pharmaceutical Chemistry, Riga Stradiņš University, Dzirciema 16, LV-1007, Riga, Latvia E-mail: agnese.brangule@rsu.lv

#### 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 vast scope for HM studies [4].

#### **AIMS OF WORK**

This study demonstrates the significant potential of using innovative cantilever-enhanced Fourier transform infrared photoacoustic spectroscopy (PAS) principles and diffuse reflective infrared spectroscopy (DRIFT) with a diamond sampling stick and aluminum sampling cup in combination with a multivariate data processing methods.

#### **METHODS**

FTIR PAS and DRIFT (PerkinElmer Spectrum One) 450–4000cm<sup>-1</sup>, resolution of 4cm<sup>-1</sup>, average made from 10 scans.

Spectral pre-processing. Using SpectraGryph 1.2.— spectra viewing, smoothing, baseline correction, and normalization.

Chemometrics. Using SIMCA 14 software — the Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA) was performed by using Savitzky-Golay and 2nd derivative filter. For the HCA, Ward's algorithm was used.

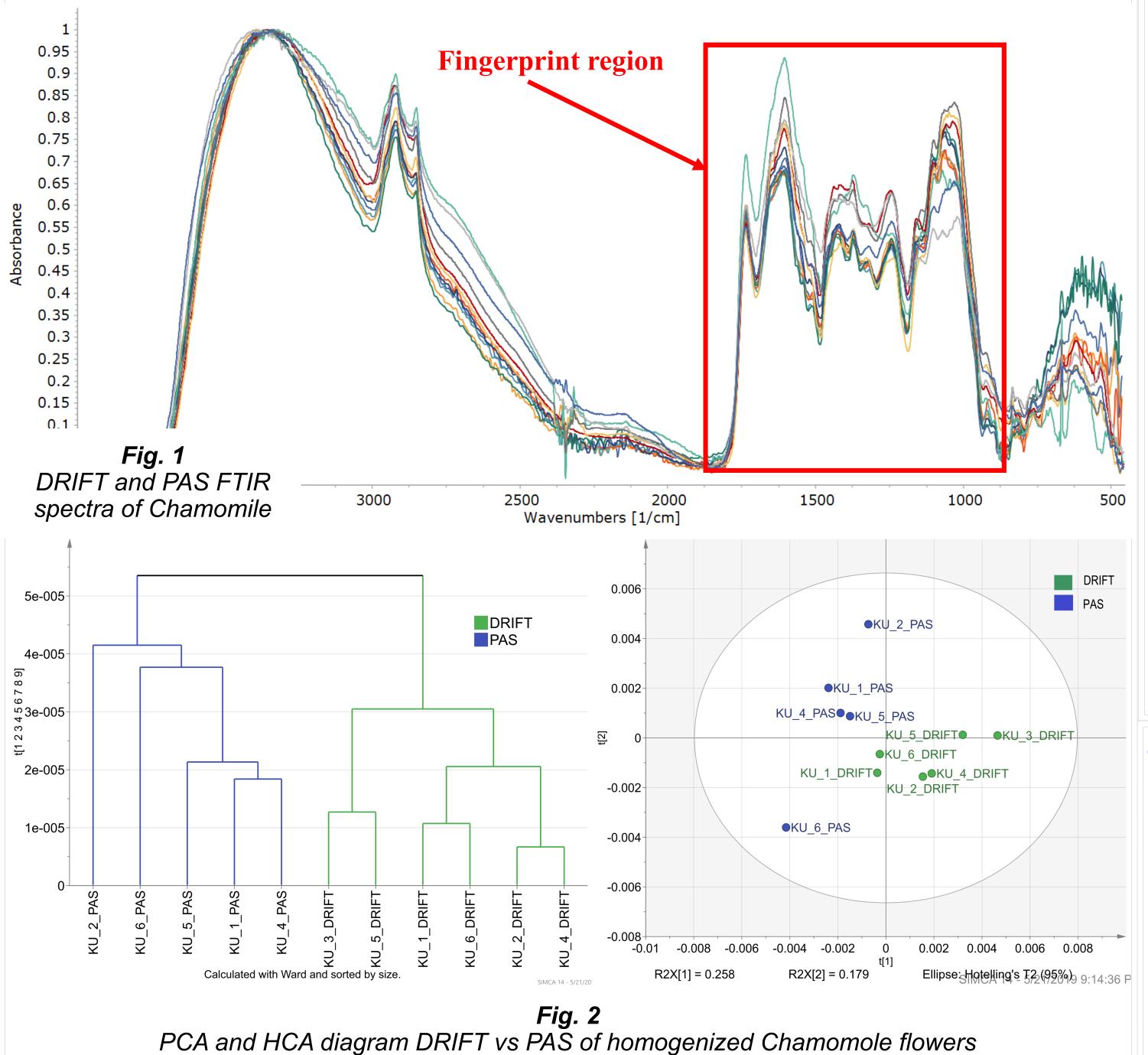
#### PLANT MATERIALS

10 medicinal plant species as dried herbals and herbal extracts in ethanol and acetone were analyzed.

Such as: 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), tansy (Tanacetum vulgare), mugwort (artemisia vulgaris), wormwood (Artemisia absinthium), heather (Calluna vulgaris)

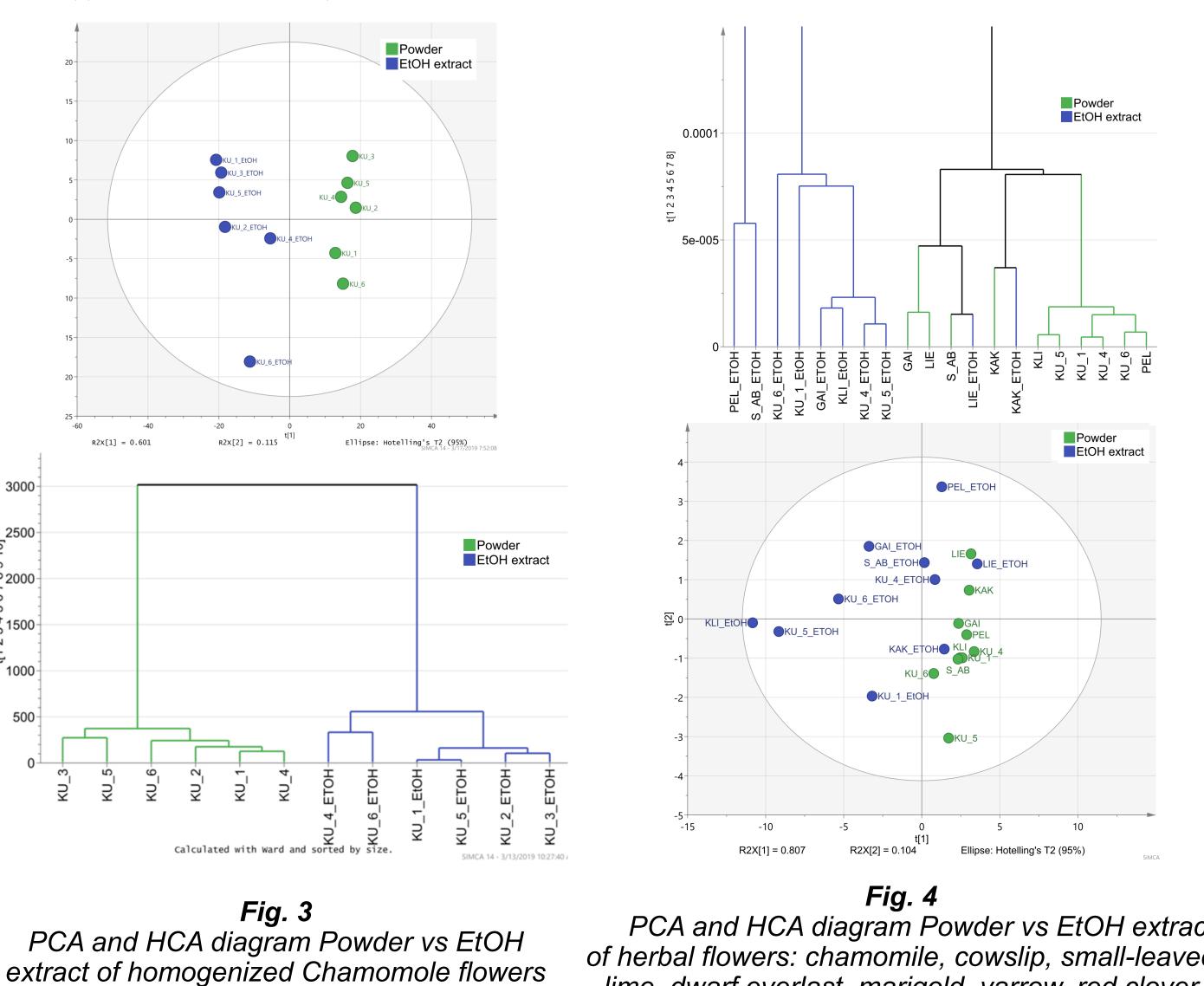
## RESULTS

### 1. Differentiation of FTIR PAS and DRIFT spectra



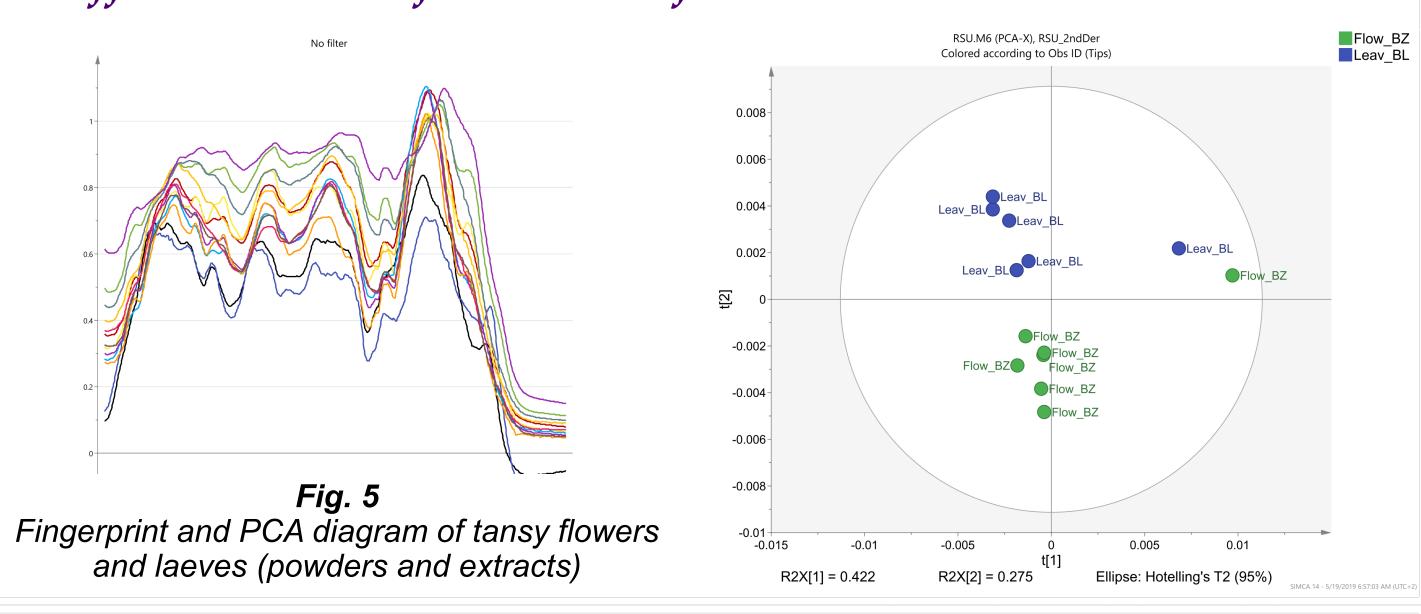
#### RESULTS

#### 2. Differentiation of dried herbals vs. extracts in ethanol and acetone



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

## 3. Differentiation of leaves vs. flowers



## **CONCLUSIONS**

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 herbal extracts can be useful for establishing identification and discrimination criteria. It has been demonstrated that PAS and DRIFT in combination with chemometrics can be a useful experimental tool for the characterization and discrimination of herbals.

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