Abstract

Comparative study of near infrared and ATR-MIR for quantification of quality-determining compounds in medicinal plants

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Introduction

NIR reflectance and ATR-MIR methods were developed to predict the content of verbascoside and verbenalin in Verbena officinalis. For reference quantification, high-performance liquid chromatography (HPLC) was used. To correlate the reference and spectral data, a PLS calibration model was established. Contrary to the time- consuming HPLC-procedure, fast infrared measurement can be carried out within few minutes. Both methods can be used as fast tools for quality control in the phytopharmaceutical industry.

Materials and Methods

Samples (n = 73) of Verbena herb were milled on a Retsch ZM 200 Mill (Retsch, Haan, Germany). For HPLC-measurements, a Shimadzu LC-10AD (Shimadzu, Kyoto, Japan) was used. Spectra were recorded on a Büchi Nirvis FT-NIR spectrometer (Büchi, Flawil, Switzerland) and a Perkin Elmer Spectrum 100 ATR-IR spectrometer (Perkin Elmer, Waltham, USA). In NIR, the samples were measured in reflectance mode. Multivariate data analysis was executed using The Unscrambler X (Camo, Oslo, Norway) software. Different wavelength regions and pre-treatments were compared. Due to the sample quantity available, a test set validation was used.

Results and Discussion

For ATR-MIR-calibrations, good quality parameters were achieved with high correlation coefficients and low standard errors of prediction (SEPs). NIR calibrations showed disadvantages for verbenalin and verbascoside prediction.

Conclusion

The potential of NIR and ATR-MIR spectroscopy for prediction of verbenalin and verbascoside as fast tools for quality control was shown.