

Quantitative Determination of Polyphenols and Flavonoids in *Cistus × incanus* on the Basis of IR, NIR and Raman Spectra

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Streszczenie

Cistus is a plant that has been used in natural medicine for hundreds of years; it works primarily as an antioxidant and cleansing agent. *Cistus × incanus* leaves or herb can be an attractive source of polyphenols and flavonoids. The official protocols of active compound analysis relies on the extraction of compounds of interest from plant matter, which makes their determination long and costly. An analysis of plant material in its native state can be performed using vibrational spectroscopy. This paper presents a comparison of Raman spectroscopy, attenuated total reflection in mid-infrared and diffuse reflectance technique in the near-infrared region for the simultaneous quantification of total polyphenols (TPC) and flavonoids (TF) content, as well as the determination of FRAP antioxidant activity of *C. incanus* material. Utilizing vibrational spectra and using partial least squares algorithm, TPC and TF were quantified with the $RSEP_{VAL}$ errors in the 2.7–5.4% range, while FRAP antioxidant activity for validation sets was determined with relative errors ranged from 5.2 to 9.3%. For the analyzed parameters, the lowest errors of predictions were computed for models constructed using Raman data. The developed models allow for fast and precise quantification of the studied active compounds in *C. incanus* material without any chemical sample treatment.

Słowa kluczowe

Cistus, polyphenols, flavonoids, FRAP, vibrational spectroscopy, multivariate analysis, principal component analysis, partial least squares regression

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