

Critical evaluation of NIR and ATR-IR spectroscopic quantifications of rosmarinic acid in Rosmarini folium supported by quantum chemical calculations.

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Streszczenie

The present study evaluates the analytical performance of near infrared as well as attenuated total reflection infrared spectroscopy for the determination of the rosmarinic acid content in Rosmarini folium. Therefore, the recorded near infrared and attenuated total reflection infrared spectra of 42 milled Rosmarini folium samples were correlated with reference data (range: 1.138–2.199 rosmarinic acid %) obtained by HPLC analysis. Partial least squares regression models were established as a quantitative multivariate data analysis tool. Evaluation via full cross-validation and test set validation resulted in comparable performances for both techniques: near infrared [coefficient of determination: 0.90 (test set validation); standard error of cross-validation: 0.060 rosmarinic acid %; standard error of prediction: 0.058 rosmarinic acid %] and attenuated total reflection infrared [coefficient of determination: 0.91 (test set validation); standard error of cross-validation: 0.063 rosmarinic acid %; standard error of prediction: 0.060 rosmarinic acid %]. Furthermore, quantum chemical calculations were applied to obtain a theoretical infrared spectrum of rosmarinic acid. Good agreement to the spectrum of pure rosmarinic acid was achieved in the lower wavenumber region, whereas the higher wavenumber region showed less compliance. The knowledge of the vibrational modes of rosmarinic acid was used for the association with the high values of the regression coefficient plots of the established partial least squares regression models.

Słowa kluczowe

NIR, ATR-IR, quantum calculation, PLSR, rosmarinic acid, Rosmarinus officinalis L., Lamiaceae

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