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Raman spectroscopy coupled to chemometrics to discriminate provenance and geological age of amber.

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Streszczenie

Raman spectroscopy coupled to partial least squares (PLS) was used for the classification of amber samples according to their provenance and geological age. Spectral data were from samples from Czech Republic, Baltic region, and objects dated back from Upper Cretaceous and Cenozoic ages. Intensity ratio of two wavenumbers has been used as indicator of both geological age and provenance amber so far.

In this work, an alternative chemometric approach was proposed to select additional intervals of the spectra where discrimination relies. Several metrics (number of misclassifications and permutation test) evaluated the capability of the alternative PLS models to predict future measurements.

Results achieved indicated the possibility to assess the geological age and provenance of amber considering an interval of wavenumbers instead of single wavenumbers that could be disturbed by physical effects. Furthermore, differences in the Raman spectra were highlighted by using Variable Importance Projection methodology over PLS model. The proposed methodology clearly distinguished Baltic from Czech Republic amber and resins from Cenozoic period and Upper Cretaceous. This research could represent a breakthrough for amber cultural heritage studies.

Słowa kluczowe

amber, chemometrics, cultural heritage, PLS, Raman spectroscopy

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