

Discrimination of Rheumatoid and Psoriatic Arthritis Based on Raman and NIR Spectra Using Machine-Learning Algorithms

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Streszczenie

Rheumatoid arthritis (RA) and psoriatic arthritis (PsA) are chronic autoimmune diseases. They share similar symptoms. The lack of specific markers can lead to misdiagnosis. Using spectroscopic information on the chemical composition of body fluids can effectively differentiate these diseases. The discriminant analysis results are presented based on Raman and near-infrared (NIR) spectra of freeze-dried blood sera. The performance of partial least squares discriminant analysis (PLS-DA) and counter-propagation artificial neural network (CP-ANN) techniques in differentiation between RA ($n = 30$) and PsA ($n = 24$) patients and healthy controls (HC, $n = 15$) were compared. Samples were divided into calibration and validation sets using a Kennard–Stone algorithm; approximately 1/3 of the samples were selected for external validation. The PLS-DA and CP-ANN models built based on spectral features selected using the interval partial least squares (iPLS) algorithm resulted in an overall accuracy (OA) for test samples prediction in the 81.3–93.8% range. Hybrid models elaborated using a combination of selected biochemical parameters of blood serum and spectral variables were characterized by OA values from 87.5 to 93.8%. The obtained results confirm that vibrational spectroscopy and chemometric modeling enable discrimination of these two difficult-to-diagnose diseases on the basis of spectral data of the dried blood serum.

Słowa kluczowe

rheumatoid arthritis, psoriatic arthritis, Raman spectroscopy, NIR spectroscopy, machine learning, discriminant analysis

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