

## **Distinguishing skin neoplasms using the multivariate curve resolution analysis of Raman spectra**

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Despite the development of technical means for recording Raman scattering, the analysis of the Raman spectra is still a difficult task. It is topical to search for new methods for the analysis of Raman spectra.

In this paper, we use the multivariate curve resolution alternating least squares (MCR-ALS) method for the analysis of skin Raman spectra. This method allows one to optimally divide the matrix of Raman spectra into two smaller matrices: the matrix of the concentrations of the components of the skin sample and the matrix of the spectra of these components.

We used 1000 in vivo Raman spectra including 540 spectra of healthy skin and 460 spectra of different neoplasms. The spectra were recorded using a portable spectroscopic setup (radiation source 785 nm) in the range 1114-1874  $\text{cm}^{-1}$ . Then the spectra were subjected to pre-processing with baseline removal and smoothing.

As a result of the MCR-ALS analysis, the spectra of skin components and their contribution (that is relative concentrations) to the Raman spectra were obtained. The results demonstrate the possibility of distinguishing several components and obtaining the relative contribution of the components to the overall spectrum using the MCR-ALS analysis. Further, several machine learning methods were applied for two cases: malignant neoplasms versus benign neoplasms, malignant melanoma versus pigmented neoplasms. The results give us the courage to talk about the possible effective use of the MCR-ALS analysis in portable devices for data dimensionality reduction.