AN ALGORITHM FOR ANALYZING RAMAN SPECTRA OF DENTAL TISSUES FOR USE IN EXPERIMENTAL MEDICINE AND DENTISTRY

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Despite the advantages of Raman spectroscopy, there is no single universal approach to determining the baseline of fluorescence, as well as to the problem of decomposition of Raman spectra. For example, for the study of biomaterials, the method of iterative approximation of the Improved Modified Multi-Polynomial Fitting (I-ModPoly) polynomial is widely used. The disadvantage of the method is the insufficient degree of approximation of the polynomial for some forms of fluorescence spectra, which is expressed in the presence of negative intensities in the final spectrum.

Existing methods for decomposition of Raman spectra, as a rule, are positioned as algorithms for the spectra of inorganic substances without complex overlapping of many lines, which determine the line composition from only one measured spectrum. Moreover, the created model has rigidly fixed parameters for the position of the maxima and the width of the lines.

The aim of the work was to develop a new algorithm for evaluating the Raman spectra of dental tissues for use in experimental medicine and dentistry.

The developed modified method of baseline correction for Raman spectra of biomaterials is presented.

The modified polynomial approximation algorithm for baseline correction allows calculating the corrected Raman spectrum, more precisely, the polynomial approximation methods IModPoly (by 2.998%), Goldindec (by 0.136%), Penalized Poly (by 5.344%).

The developed two-stage method of decomposition of the spectral contour with a high degree of overlapping of the Raman lines, which is characteristic of biomaterials, is also presented.

The error in determining the parameters of the Raman lines from the Raman spectra at a noise level of 1% of the standard deviation corresponding to the real smoothed Raman spectra was: 0.3% for the amplitude, 0.29% for the half-width dx, and 0.11 cm^{-1} for the position of the line maxima x_0.

The proposed algorithm was tested to identify the main spectral changes in tooth enamel that appear in periodontitis.

Diagnosis of spectral changes in tooth enamel, as well as the developed algorithm for verifying enamel with a diagnosis of periodontitis, will allow identifying patients at risk and correcting their treatment with hydroxyapatite. The accuracy of the developed algorithm was 89 ± 9%.

The results obtained are a prerequisite for the creation of an express device for non-invasive (*in vivo*) assessment of tooth enamel in periodontitis.