Contribution ID: **28** Type: **not specified**

Spectroscopic markers of biological molecules and cells

Tuesday, 17 March 2026 14:54 (12 minutes)

arious spectral methods-optical and vibrational spectroscopy, mass spectroscopy, luminescence, NMR, X-ray etc.- play a key role in analytical and prognostic research in various fields of science, industry, and medicine.In this report, we will focus on vibrational spectroscopy, its linear (IR, Raman) and nonlinear (CARS, SFG) methods, and a new method - surface-enhanced spectroscopy (SES).

In vibrational spectroscopy, spectroscopic markers are the intensity, half-width, frequency, polarization of bands, and their combinations, which are sensitive to changes in the structure of molecules or crystals under the influence of external factors. The establishment of spectral markers is an important direction in modern biophysics, because, thanks to the high specificity of vibrational spectra and their conformational sensitivity, it is possible to detect differences in the structure of DNA, proteins, lipids el without the additional labels, to determine the conformational states of biomolecules, structural rearrangements in the cell membrane, changes in the molecular composition of tissues, o to distinguish the normal state from the pathological, with an accuracy not available to other methods. Experimental and computational data obtained at the Institute of Physics of the NASU on markers of metastatic cells, lipids from resistant cells, cells interacting with the antiviral drug will be discussed. New data on CARS spectroscopy es will be presented here. Now and in the future, the main emphasis will be on mathematical processing of spectral information, correlations in spectra, machine learning and prediction.

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