NIR spectroscopy (NIRS) combined with advanced computer aided multivariate analysis is a new, non-invasive analytical technique with high potential for investigation of biological systems\(^1\,^2\). Recently, multivariate analysis and artificial intelligence, together with, very rapidly developing computer technique have contributed to the worldwide spread of NIR technology.

The near-infrared part of the spectrum, 600-2500 nm, has been widely used to measure chemical composition and, recently, for non-destructive, real-time monitoring of biological systems at molecule level. It has the advantage that water absorption becomes relatively weak and overtones of various hydrogen bonds in the solute can be observed simultaneously. Moreover, the wavelength range used is of low energy and thus has little effect on the studied object.

Water absorbance patterns (WAPs) of a biological system, in the Visible and MR ranges, are proposed to be used as "Extended Water Mirror" that reflects details about the structure and composition of bio-molecules in aqueous solution, Fig. 1,2 Difference in WAPs has been found for different physiological conditions of biological objects.

Biological systems are complex, multidimensional, with numerous changes in time. Substantial evidences have been presented to demonstrate that NIR spectroscopy is a convenient, noninvasive method for health monitoring, for inflammation and stress diagnosis, and for analyzing the interrelations between respective body fluids\(^3\,^4\), as well as, the tissue of a living object\(^5\).
Near infrared spectra of dairy cow’s biological fluids provide information for the animal’s physiological condition and give valuable information for functional studies. Links between bioprocesses in the rumen, blood composition and quantity and quality of the produced milk have been studied by NIRS.

This work also shows that NIRS is a valuable technique for examining protein structure and dynamics in a way that does not damage the protein and requires only physiological concentrations. We present new approach for biomolecules study where water species interacting with protein and surrounding it are analyzed and used as a common platform for comparison of proteins.

New methods for NIR spectral data analysis, such as chemometrics, two dimensional correlation spectroscopy (2DCOS), wavelets, neural networks etc., have been discussed as valuable tools for dynamic biological studies based on individual spectra acquired in time series.

References