

***Application of molecular spectroscopy in mid-infrared region to the determination of the serum and saliva biochemical parameters***

S. A. Khaustova, E. V. Trushkin, I. I. Davydov, M. U. Shkurnikov,  
R. Mueller\*, J. Backhaus\*, A. G. Tonevitsky

Russian research institute of sport and physical education, Moscow,  
svetakhaustova@gmail.com

\*Institute for Instrumental Analysis and Bioanalysis, Mannheim University of Applied  
Sciences, Mannheim, Germany

Fourier-infrared (FTIR) spectrometry has proved to be a useful tool for determining a series of serum and saliva molecular concentrations. Validated, reproducible and easy-to-use biological tool based on FTIR spectrometry in mid infrared region for analyzing several concentrations within the same small biological sample is a major challenge for the future. We compared two techniques for measuring bio-fluids concentrations of biomarkers. One of them is standard laboratory biochemical analysis. The other is experimental: FTIR spectroscopy.

Constituents of serum and saliva were analyzed without any sample preparation, sample volumes as small as 2  $\mu$ L can be used. FTIR spectrometry allows to determinate concentration of a wide range of biological molecules in a single microsample with high accuracy. Mathematical models, including partial least-squares regression (PLS), were used to contrast a prediction model which can calculate the concentration of biochemical parameters. It was obtained calibration models for the determination concentrations of albumin, cholesterol, glucose, total protein, urea, heat shock protein, malondialdehyde and others in serum, and total protein, glucose, sIgA, urea, inorganic phosphate, C-reactive protein in saliva. The absolute precision and reproductivity of the precision reached is sufficient for routine clinical analysis and is only limited by the precision of the reference analysis used for calibration.

In comparison with other bio-fluids such as whole blood, plasma, serum, or cerebrospinal fluid, saliva can easily be collected and analyzed [1]. In other hand saliva is a "mirror of disease" and indicates physiological state of organism [2, 3]. Determination major components, real time monitoring and molecular analysis of saliva can be done by FTIR spectroscopy. It can be useful as method of non-invasive diagnostic. This global analytical technique provides a great advantage in comparison with the classical clinical ones.

Key words: mid infrared spectroscopy (MIR), partial least-squares (PLS) algorithm, serum, saliva, noninvasive diagnostic

**Acknowledgements:** This work was supported financially by the project DLR number RUS 08/A13. The authors would like to thank scientific group of Institute for Instrumental Analysis and Bioanalysis, Mannheim University of Applied Sciences (Mannheim, Germany).

**References:**

- [1] Koh D. S.-Q., Koh G. C.-H., The use of salivary biomarkers in occupational and environmental medicine, *Occup. and Envir. Med.* **64**, 202-210 (2007).
- [2] Lewis J. G., Steroid Analysis in Saliva: An overview, *Clin. Biochem. Rev.* **27**(3), 139-46 (2006).
- [3] Turner R. J., Sugiya H., Understanding salivary fluid and protein secretion, *Oral Dis.* **8**(1), 3-11 (2002).