

NMR-based quantitative metabolomics of biological tissues

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A metabolome – a complete set of small-molecular-weight compounds in a tissue – reflects an actual state of the tissue and may significantly vary depending on the age, diet and health status. Quantitative metabolomics is probably the most promising and sought-after branch of metabolomics, which is actively developing and integrating into novel applications in biology and medicine. Unlike qualitative (where only the presence of certain metabolites is detected) and semi-quantitative (the ratio of metabolite levels in the “case” and “control” samples is estimated) metabolomics, the quantitative measurements imply the determination of absolute values of metabolite concentrations in a biological tissue (typically, in moles per gram of tissue).

High-field NMR spectroscopy is one of the most suitable tools for quantitative metabolomics, allowing to determine the concentrations of 50-80 metabolites in a tissue from a single NMR spectrum. In this report, we discuss an optimal workflow of metabolomic studies, including sample collection, sample preparation, analytical measurements, and post-analytical data treatment. During last few years, we successfully applied the metabolomic approach to the solution of a wide range of medical and biological tasks: 1) mechanisms of development of ophthalmological diseases in humans (cataract, keratoconus); 2) study of pathogenesis of metabolic diseases in model animals (mice, rats); 3) influence of water temperature, salinity, level of dissolved oxygen, and anthropogenic pollution on fish metabolome; 4) determination of post-mortem interval for forensic science; 5) mechanism of animal adaptation for survival under extreme conditions (low temperature, hypoxia); 6) mechanism of extremely acute eyesight of birds of prey.

This work was supported by RSF (Project 22-23-00021).