

## **Doctoral School of Information and Biomedical Technologies Polish Academy of Sciences**

### **Title**

Semi-automatic NMR spectra analysis of biofluids and tissue extracts for metabolomics.

### **Supervisors, contact, place of research**

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### **Project description**

The thesis concerns the preparation of an application that allows semi-automatic NMR spectra analysis. The spectra of various body fluids (serum, cerebrospinal fluid, lipid extracts) are measured with different spectrometers (different data formats) under different conditions depending on the fluid being tested. The goal of the PhD thesis is to write an application that: reads FID data saved in the spectrometer format, performs Fourier transform data, phase and baseline correction, spectrum normalization (according to reference standard). Based on the existing databases of reference substance spectra (HMDB), it supports the identification of compounds in a mixture, which is a body fluid, and allows concentration determination using a standard substance of known concentration. The work should include error analysis.