TITLE: **Semi-automatic NMR analysis of body fluids / tissue extracts as applied to metabolomics studies**

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Auxillary supervisior (*optional*):

DOCTORAL SCHOOL (*delete as appropriate*):

1. Doctoral School of Information and Biomedical Technologies Polish Academy of Science (TIB PAN)
2. ~~DOCTORAL SCHOOL OF TRANSLATION MEDICINE „Bench to Bedside – B 2 B 4 PhD"~~

AFFILIATION: Instytut Biocybernetyki i Inżynierii Biomedycznej im. Macieja Nałęcza Polskiej Akademii Nauk, ul. Ks. Trojdena 4, 02-109 Warszawa (IBIB PAN)

SCIENTIFIC DISCIPLINE: biomedical engineering

PROJECT DESCRIPTION (max. 2500 characters; *containing general information on the scientific purpose of the project and research hypotheses, the current state of art, a short research plan and research methodology*)

The thesis concerns the preparation of an application that allows for semi-automatic analysis of NMR spectra. Currently there are several programs to analyze spectra, including body fluids, but they do not identify metabolites correctly. This is due to the shift of the signals in the spectrum as the pH changes, with each compound behaving differently. All these programs work in an automatic mode, identifying compounds that cannot be in the samples (pollutants or toxins), and they omit important compounds due to their signal position change in the spectrum. Hence the need to create a semi-automatic application that allows the operator to make corrections resulting from the change of pH. Application should also support in searching databases of standard spectra. The spectra of different body fluids (serum, cerebrospinal fluid, lipid extracts) can be measured with different NMR spectrometers (different data formats) under different measuring conditions (different sequences) depending on the fluid being tested. The aim of the PhD thesis is to prepare an application that: reads raw data (FID) saved in the spectrometer format, performs Fourier transform of data, phase and baseline corrections, normalization of the spectrum in accordance with the signal of the reference substance with a known concentration. Based on the existing databases of spectra of standard substances (HMDB) - metabolites present in the sample, the application should allow for their identification in a mixture, which is a body fluid, and for the determination of their concentrations using a reference substance which is measured together with the sample. The thesis should also include an analysis of selected spectra owned by the Laboratory. Due to the software available in the Laboratory, the application should be written in Pascal (Delphi) or C ++.

REQUIRMENTS FOR CANDIDATES

1. Master's degree in computer science / biomedical engineering / physics / biophysics or related;
2. Basic knowledge of NMR spectroscopy;
3. Basic knowledge of programming in Pascal / C ++ / Matlab /.