Software Package for the Analysis of Spectra of Substances for Low-field Low-resolution NMR Spectrometers

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The project presents a software package and some necessary algorithms developed for the processing and analysis of spectra obtained with a low-field NMR spectrometer. Unlike the widely used high-field NMR spectroscopy, the low-field approach has only recently been theoretically developed and is currently neither technically worked up nor present on the market. The main drawback of the high-field approach is the incredibly high cost of such instruments, reaching up to tens of millions of dollars. This makes it impossible to be used by small and medium-sized companies, forcing them to turn to third-party laboratories. Nonetheless, the development of commercial low-field spectrometers has recently begun. The development of the low-field spectroscopy approach will complement the market with a much more affordable instrument, even though with lower resolution (but still enough for the majority of business cases). Nowadays, due to the lack of low-field NMR spectrometers on the market and their consequent uncommon usage, the presented software is unique and has no counterparts. The developed algorithms were successfully tested on the molecule recognition task. The calculated parameters (such as J-Coupling) were also compared with the open database, having an average deviation of 1.5-1.7%.

Awards Won: