Studies on the structure of the compounds with accuracy up to the mutual distribution of the atoms are among the fundamental tasks of science in general and chemical analysis in particular. The task is not easy, however, as evidenced by a number of spectacular mistakes made in the past. Nobel Prize winners have not avoided them either. Adolf Windaus, who won the Nobel Prize in 1928 for his research on the structure of sterols and their relation to vitamins, in the 1930s corrected the previously proposed erroneous structure of cholesterol.

Despite the improvement of the equipment and measurement methodology, such mistakes still happen very often. Dozens of publications are published every year, verifying the previously proposed structures of chemical molecules, especially substances of natural origin.

Nuclear magnetic resonance spectroscopy (NMR) is one of the most important modern tools for analysing molecular structures. It is based on the phenomenon of the interaction of magnetic momentum, shown by some atomic nuclei (also endowed with spin, 'internal angular momentum"), with the magnetic field generated in the NMR spectrometer. This phenomenon can be utilised to generate a radio frequency signal which contains information about the energy of this interaction. What is essential from the point of view of a chemist, is that the magnetic field "felt" by a given atomic nucleus is slightly (at the level of parts per million) modified by the local structure of the molecule. This is reflected in the frequencies of the mentioned radio signal, i.e. the NMR spectrum. Such a spectrum is a kind of "fingerprint"' of a molecule from which one can read how its atoms are mutually located.

Unfortunately, even such precise tools as NMR have their limitations. The most important of these is the small scale of the mentioned "chemical" contribution to the energy of the interaction of the nucleus with the magnetic field of the spectrometer. As a result, resonant frequencies can have very similar values. A number of techniques have been proposed to overcome this problem, such as correlation spectroscopy, diffusion spectroscopy, "pure-shift" spectroscopy and many others. It still happens, however, that it is impossible to unequivocally determine the structure of the chemical compound under study.

This project proposes to use a source of information present in NMR spectra which has not been systematically exploited so far, namely solvent and temperature influence. The results of the last work from the team of the author of the project [1] indicate that these effects can be explained by classical molecular dynamics and therefore worth considering for measurement in a standard set of techniques for analysing the structure of molecules. A new approach is proposed in the following areas:

1. Analysis of the structures of small molecules, especially of natural origin and organic synthesis products (pharmacy, chemical industry)

2. Identification of components of mixtures, especially natural metabolites such as urine and blood.

3. Analysis of intrinsically disordered protein spectra, especially difficult cases with a high degree of disorder.

The experience of the project's author, as a head of NMR Spectroscopy Laboratory, shows that improving the methodology in the above areas will not only contribute to the development of basic research, but also strengthen the support for the innovation departments of domestic chemical companies requesting NMR measurements in academia.

[1] Rytel, M.; Kasprzak, P.; Setny, P.; Kazimierczuk, K. Quick Temperature-Sweep Pure-Shift Pure-Shift NMR: The Case of Solvent Effects in Atorvastatin. Phys. Chem. Chem. Phys. 2019, 21 (35), 19209-19215.