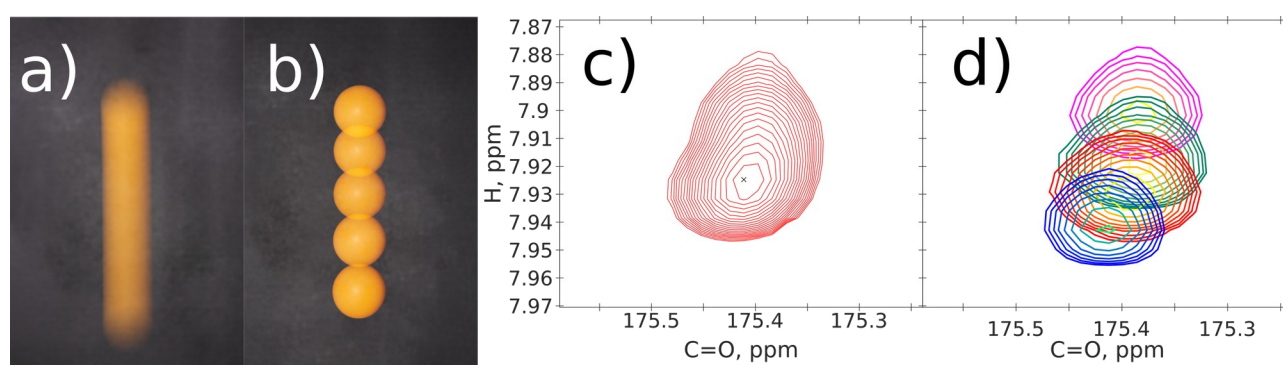


Living beings use a variety of senses to explore the world around them, from sight to magnetic field detectors. Humans are using more and more advanced artificial tools for this purpose - microscopes are used to obtain images, various chemical tests and scanners are used to check our health condition and even parking a car is made easier by squeaky ultrasonic sensors. All these devices are based on recording a signal indirectly connected with the quantity we want to measure. Importantly, when we want to study rapid processes, the signal must be recorded and processed quickly. This is a major problem limiting the applicability of many precise, though time-consuming, techniques. These include nuclear magnetic resonance (NMR) spectroscopy.

NMR takes advantage of the magnetic properties of certain atomic nuclei, e.g. the nucleus of a hydrogen atom, and the ability to excite these nuclei with electromagnetic radiation when they are in a strong magnetic field. NMR signals are the radio waves emitted by the sample as it returns to equilibrium after excitation. The resonance frequencies encoded in the signal are related to the structure of the molecules and can be their 'fingerprint'. Unfortunately, NMR signal is relatively weak and often needs to be measured for many hours to get the sufficient signal-to-noise ratio. It's just like in photography, where we have to capture an image for longer in low light. As in photography, the problem of sensitivity limits the method's use in monitoring fast processes where "snapshots" need to be short - long exposures cause "smearing" of the image in photography and a corresponding deformation of the NMR spectra.



*Images and spectral peaks in non-stationary and stationary (serial) contexts: a) photograph of a falling ball made with a long exposure time; b) series of fast stroboscopic images of the same ball; c) A66N-H-L65C peak in 3D HNCO spectrum of human osteopontin acquired with the temperature of the sample increasing during acquisition; and d) the same peak in a series of quick 3D HNCO spectra.*

Multidimensional NMR spectroscopy, in which the recorded signal is a function of several time variables, is a particularly valuable source of information. Unfortunately, it is even more time-consuming due to the lengthy process of sampling the 'extra' dimensions. Although multidimensional NMR allows for studying the structure and dynamics of very large molecules, such as proteins or nucleic acids, its use to record 'snapshots' in process monitoring is very difficult. An attempt to register such an NMR signal for a sample in which e.g. a chemical reaction or dynamic changes of a macromolecule are taking place will give unsatisfactory result - the image of the changes will be "smeared" (as shown in the picture above).

It is worth noting, however, that the blurred image contains complete information about the movement of the photographed object. In recent years, thanks to machine learning methods, more and more spectacular examples of "decoding" a film from blurred images with relatively long exposure times have been demonstrated. The application of similar techniques to NMR spectroscopy would allow it to be used in novel studies of fast processes - for example, protein dynamics, chemical reactions or processes occurring in batteries. This project proposes the development of methods for such "non-stationary NMR", based on modern neural networks and unconventional methods of signal registration. Its success would allow even wider use of NMR in the study of chemical and physical processes.