Abstract „Spectroscopy meets AI“

In the field of Nuclear Magnetic Resonance (NMR) spectroscopy it is a common challenge to map a chemical question to a set of appropriate NMR experiments to answer this question efficiently and with high confidence – this requires expert knowledge and experience. The most abundant of these chemical questions is addressing the task of structure verification relating to the control of a chemical synthesis. So the basic question is “Did the chemical synthesis of this compound work out well?” which can be translated into “Does this molecular structure fit to these spectroscopic data?”

We at Bruker BioSpin, the major manufacturer of NMR instrumentation, developed software that 1. can answers this question and that 2. determines which type of NMR data is the most beneficial for the given structure verification job steering the NMR instrument accordingly. For both tasks we mimic the decision making process of an NMR expert. In this talk the challenges along with our approaches to overcome them are presented.