

Liquid-state dynamic nuclear polarization (DNP) on small molecules

Small molecules play an important role in many biological systems. DNP can be used to enhance the NMR sensitivity of these molecules by increasing their initial degree of nuclear polarization. This is achieved resonating the electronic spins from unpaired electrons (usually a nitroxide radical) and through a process called the Overhauser Effect, polarization is transferred from unpaired electron spins to the nuclear spins in a target molecule. These experiments will be conducted on a specially build DNP spectrometer, which combines a standard 400 MHz NMR Bruker spectrometer, with a custom-made microwave bridge and double resonator operating at 400 MHz /260 GHz.

Building on a preliminary study on small metabolites, DNP experiments will be performed on a variety of small molecules in combination with different nitroxide radicals (for example, TEMPOL or Fremy's Salt). DNP transfer will be investigated on both exchangeable protons and non-exchangeable protons. Additionally a study will be made of the selectivity of the DNP process on different functional groups.