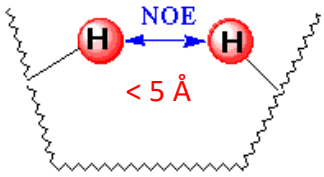
Measuring methods available and examples of their applications

2D NOESY (Nuclear Overhauser Effect Spectroscopy)

NOESY experiments are an important tool to identify stereochemistry of a molecule in solvent.



Two-dimensional NOE option allows to measure in a single experiment NOEs between all the hydrogen atoms in molecule. Instead of scalar interactions (through bonds), dipolar interactions through space are indicated. NOESY is particularly suitable for large molecules (biopolymers) to solve their 3D structure. One application of NOESY is in the study of large biomolecules such as in protein NMR, which can often be assigned using a sequential walk. For smaller molecules, the method is used to assign spatially near protons and to solve stereochemistry. The disadvantage is that for molecules with the molecular weight of approximately 700-800, the NOE effect is close to zero resulting in weak ar absent signals. Care must be taken, however, as many other processes lead to reduced NOEs including spin-lattice relaxation, temperature, increased solvent viscosity, increased molecular weight, and dissolved paramagnetic impurities including oxygen. Also important is the value used for the mixing time. The intensity of the NOE is in first approximation propotional to $1/r^6$, with r being the distance between the protons: The correlation between two protons depends on the distance between them, but normally a signal is only observed if their distance is smaller than 5 Å.
The spectrum obtained is similar to COSY, with diagonal peaks and cross peaks. For small molecules, diagonal peaks (black) have opposite phase than cross peaks (red) in the NOESY spectrum.

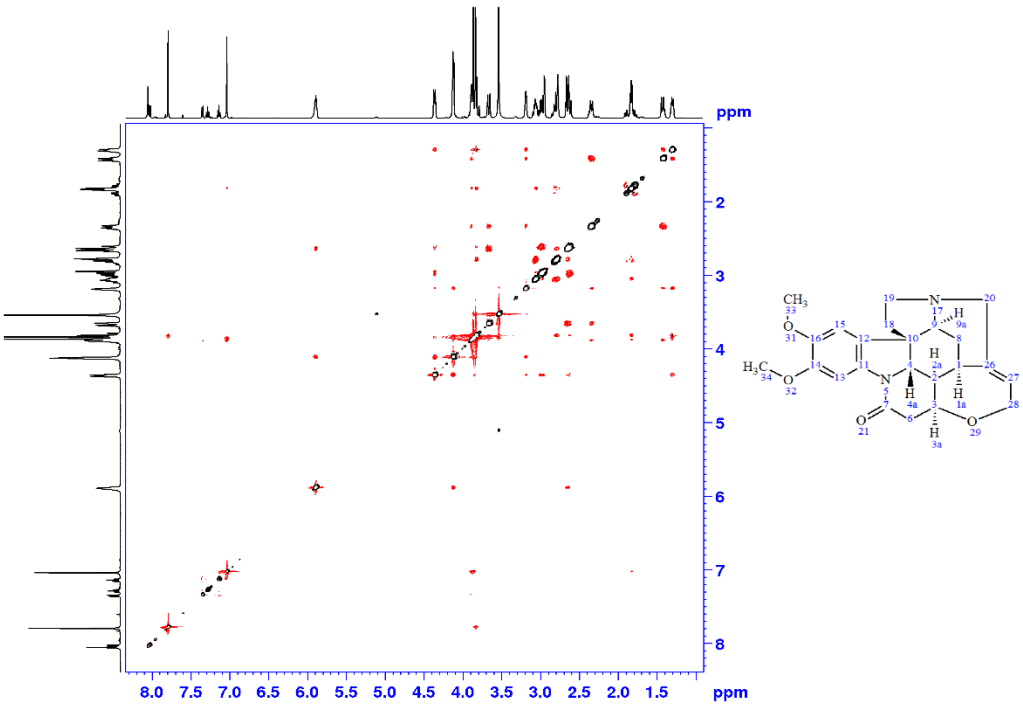


Fig. 1. Brucine in DMF-d7, 2D – NOESY, mixing time 800 ms, Spectrometer: AVANCE III 500, Probehead: 5 mm CPPBBO (Prodigy) with z gradients, Experiment time: 70 min.