Measuring methods available and examples of their applications

2D ROESY (Rotating frame nuclear Overhauser Effect Spectroscopy)

ROESY method is useful for certain molecules whose rotational correlation time falls in a range where the Nuclear Overhauser effect is too weak to be detectable, usually molecules with a molecular weight around 1000. ROESY has a different dependence between the correlation time and the cross-relaxation rate constant. In NOESY the cross-relaxation rate constant goes from positive to negative as the correlation time increases, giving a range where it is near zero, whereas in ROESY the cross-relaxation rate constant is always positive.
Measurements are carried out under spinlock conditions. Experiment provides essentially the same information as NOESY. Red peaks in the figure are negative and black signals are positive. Spectrum is symmetrical about the diagonal and cross peaks means spatial proximity (within 5 Å). For large molecules, ROESY allows distinguishing between true NOE signals and exchange peaks as they have oposite signs. In NOESY, both types of peaks have the same sign.

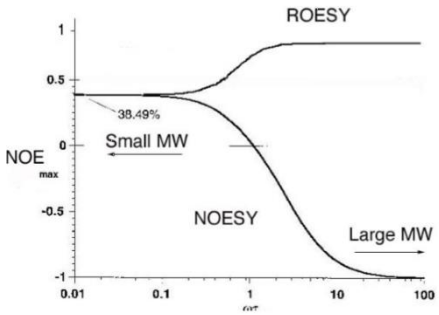

Fig. 1. *NOE dependence on molecular weight*

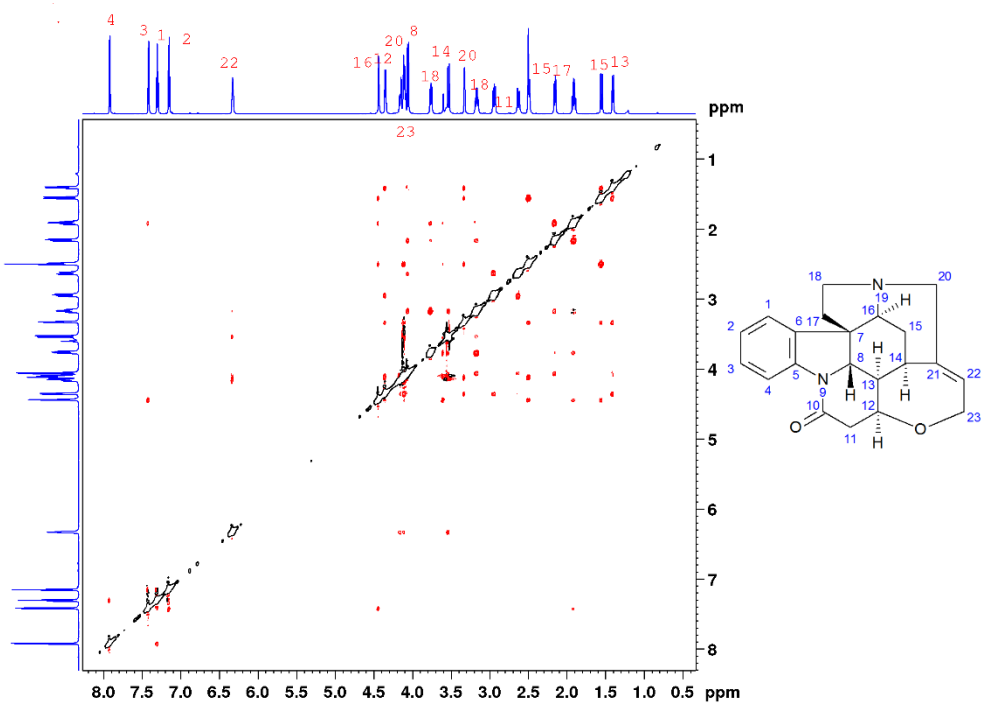

Fig. 2. Strychnine in DMSO-d6, 2D–ROESY, mixing time?, Spectrometer: AVANCE III HD 700, Probehead: 5 mm CPTXO 13C/15N-1H/D with z gradients, Experiment time: 72 min

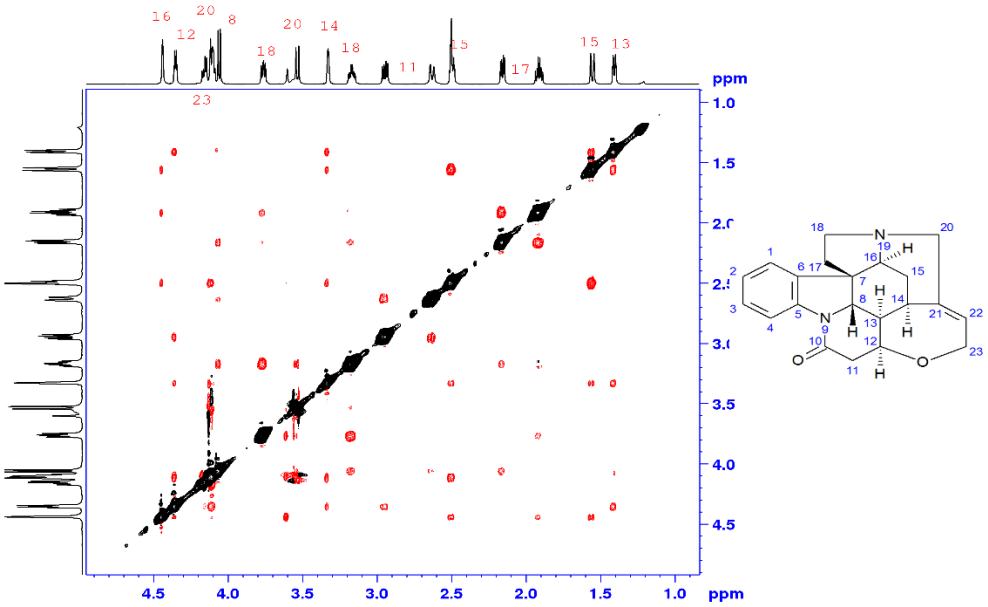

Fig. 3. Strychnine in DMSO-d6, 2D–ROESY, the aliphatic area expanded