

C8953  
NMR strukturní analýza  
seminář  
TOCSY & ROESY

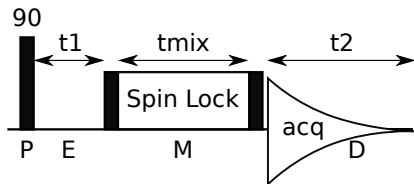
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# TOCSY (Total Correlation SpectroscopY)

spin lock - isotropic mixing

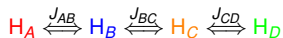
- ▶ series of short  $180^\circ$  pulses
- ▶ "lock-in" of spins in transversal plane
- ▶ higher power in case of TOCSY, offset set into the middle (on resonance)
- ▶ smaller power in case of ROESY, offset set into the edge (off resonance)
- ▶ crosstalk (ROE transfer in TOCSY,  $J$ -coupling in ROESY)



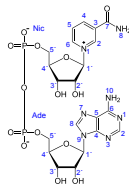
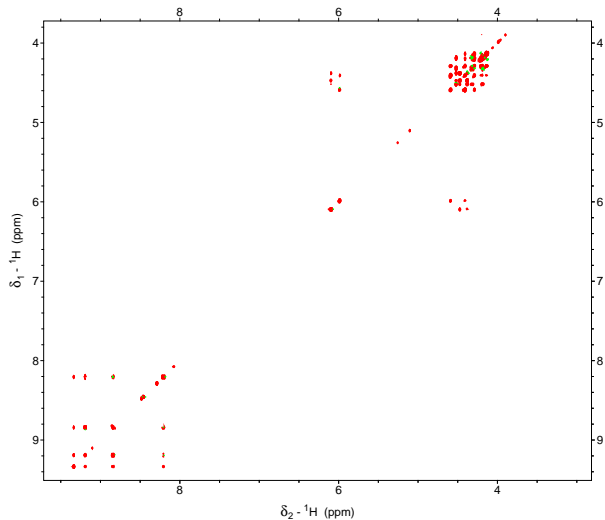
# TOCSY (Total Correlation Spectroscopy)

correlation based on  $J$

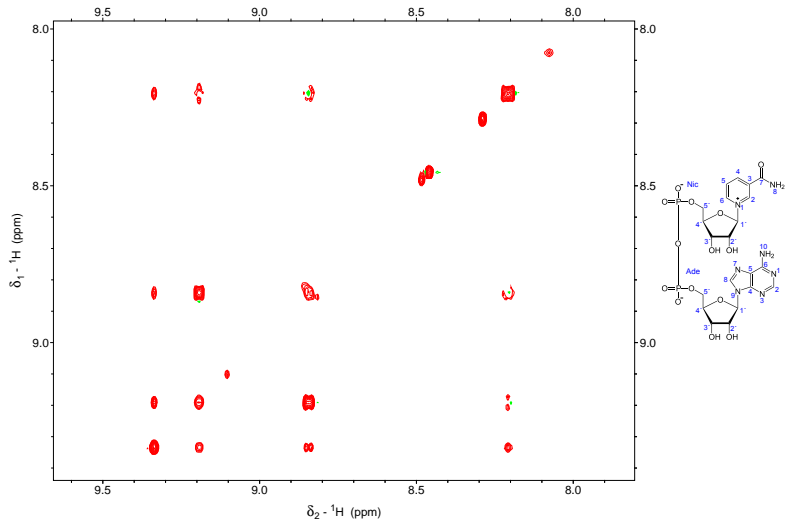
- ▶ mutual correlation of all protons in one spin system
- ▶  $\tau_{mix} \approx 20 - 120\text{ms}$
- ▶ crosspeak intensity depends on  $\tau_{mix}$  a  $J$  value



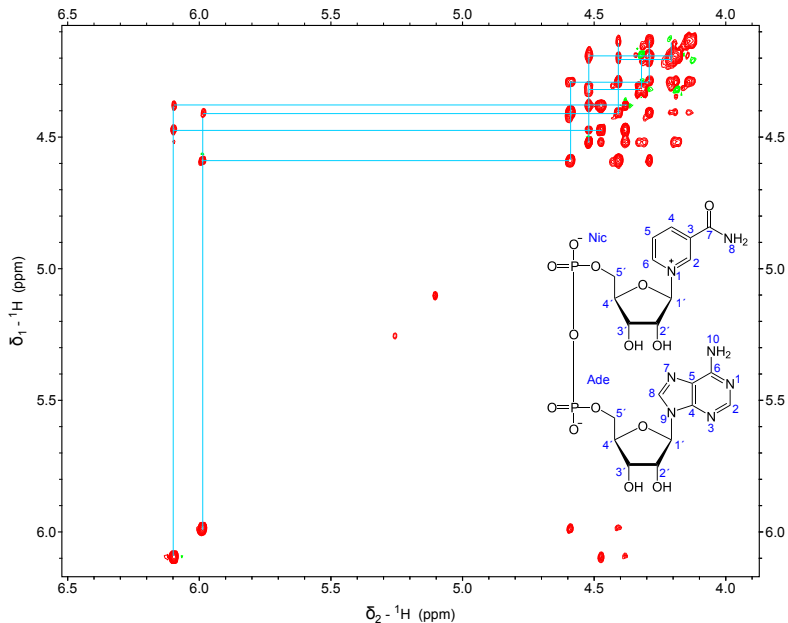
# NAD<sup>+</sup>: TOCSY (40ms)



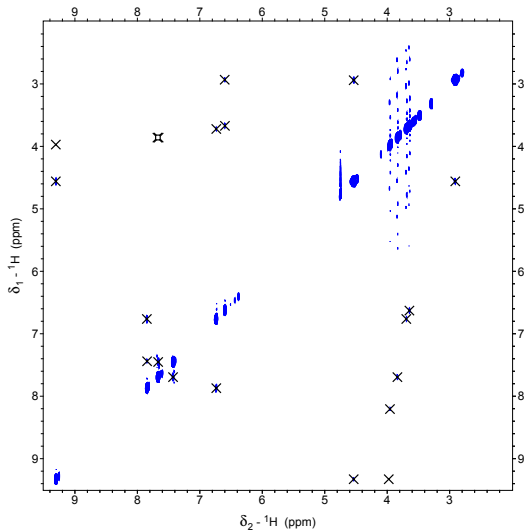
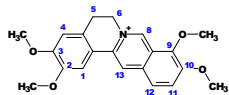
# NAD<sup>+</sup>: TOCSY (40ms), detail of aromatics



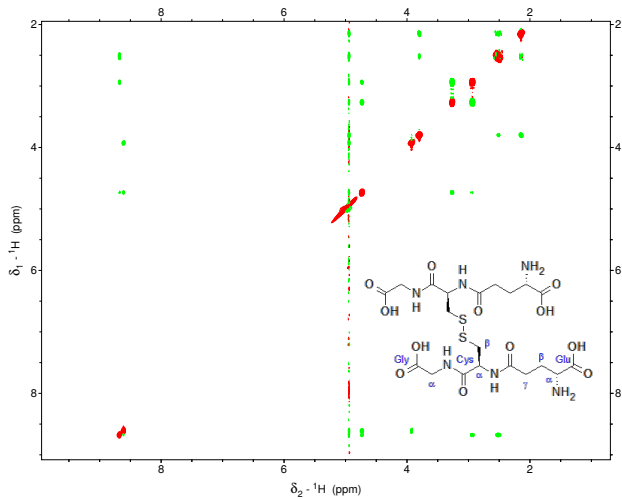
# NAD<sup>+</sup>: TOCSY (40ms), detail of aliphatics



# NOESY - Palmatine



# ROESY - Glutathione





Next session:

Heteronuclear correlations