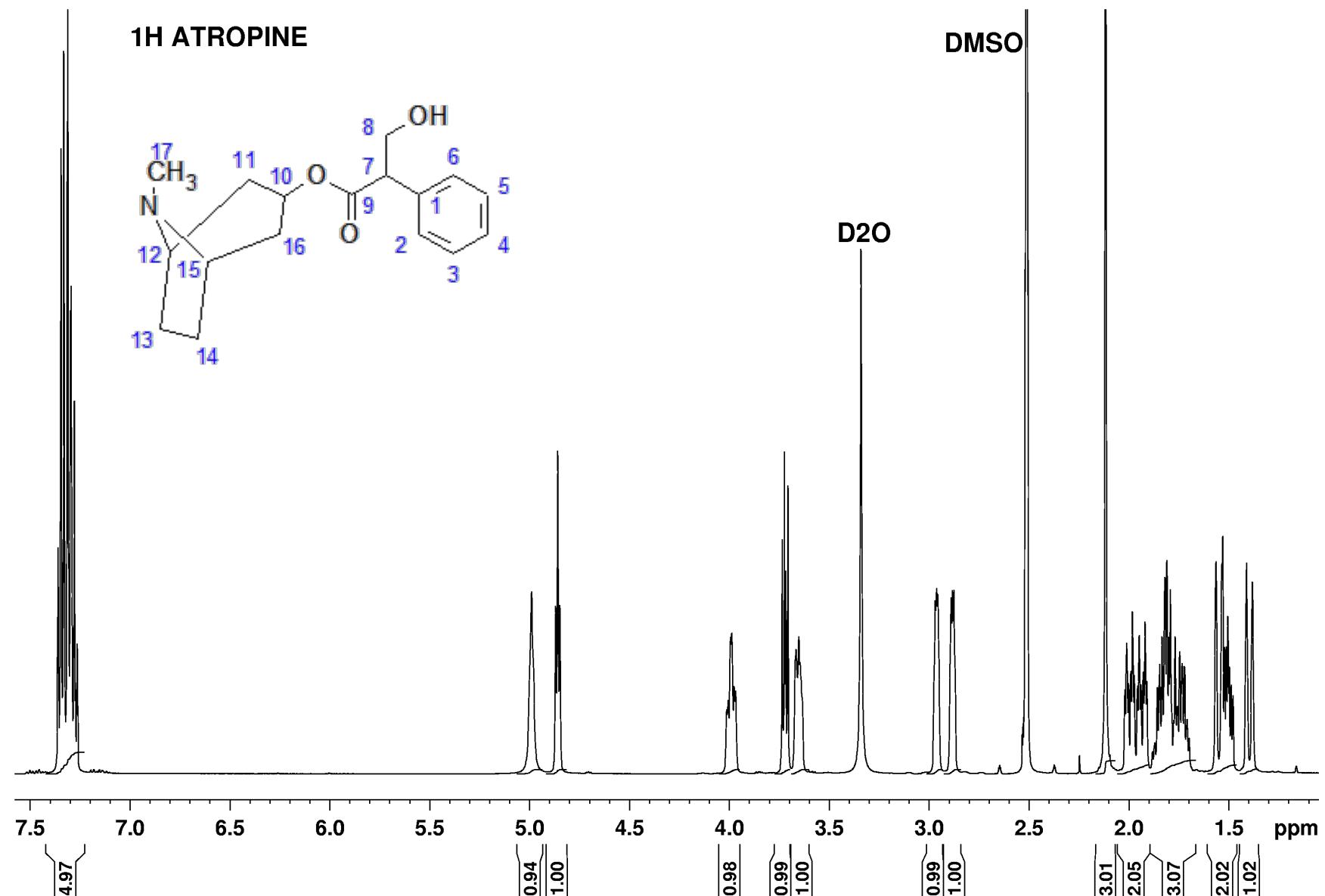


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seminář  
COSY & NOESY

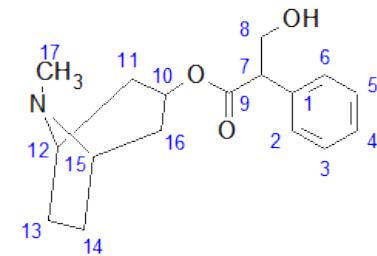
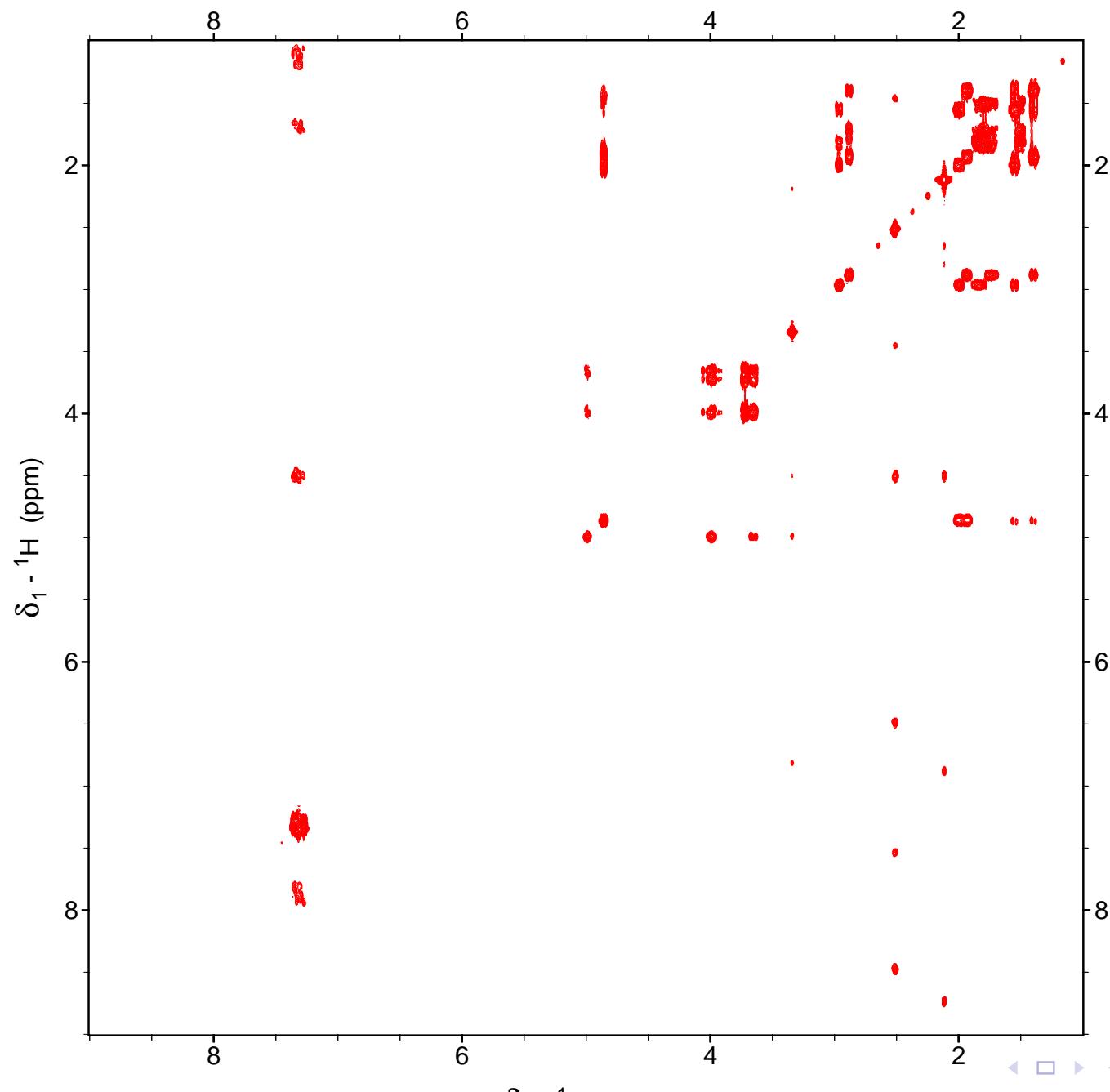
Jan Novotný, Kateřina Peterková  
176003@is.muni.cz

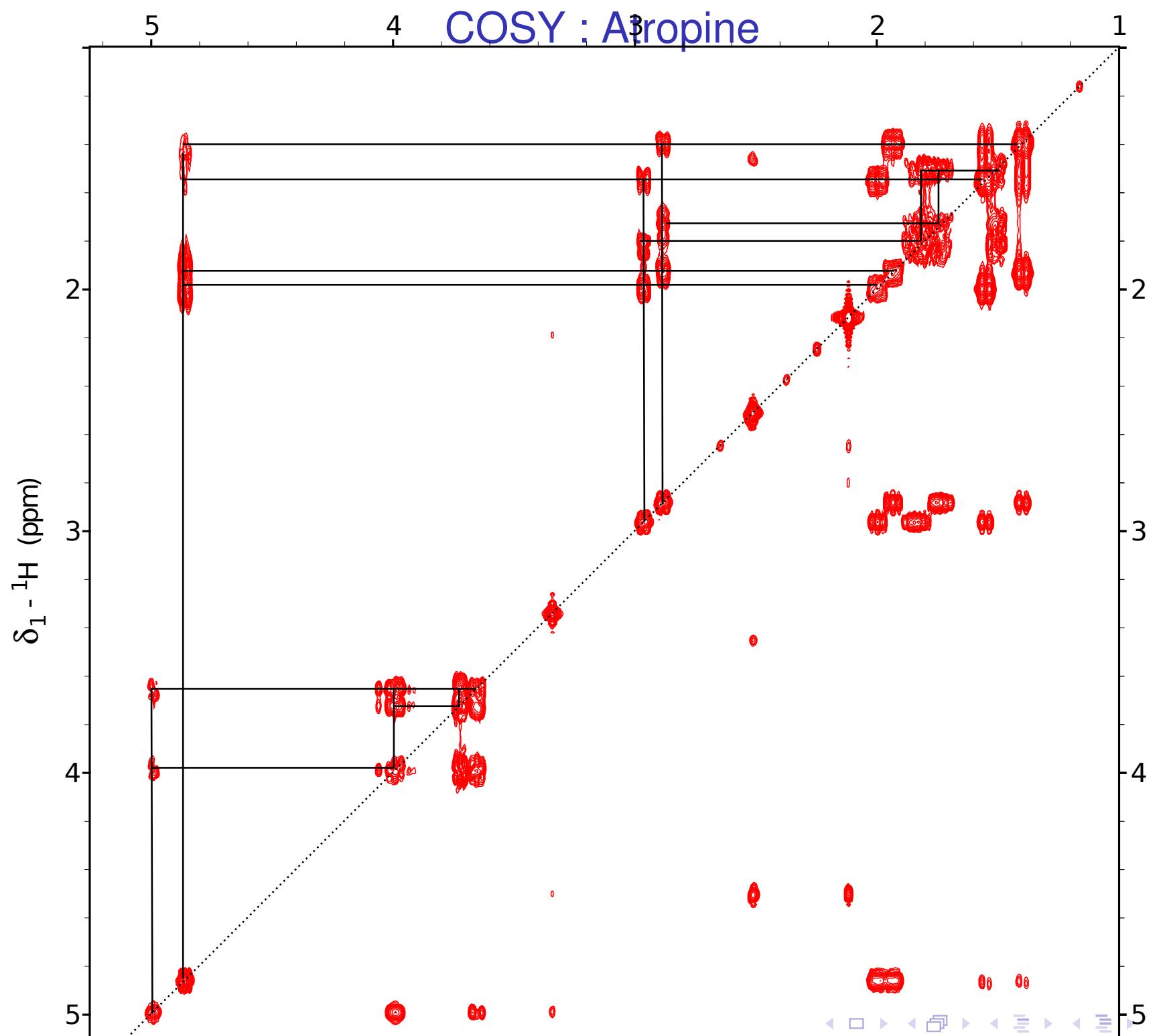
March 27, 2019

# COSY : Atropine



# COSY : Atropine





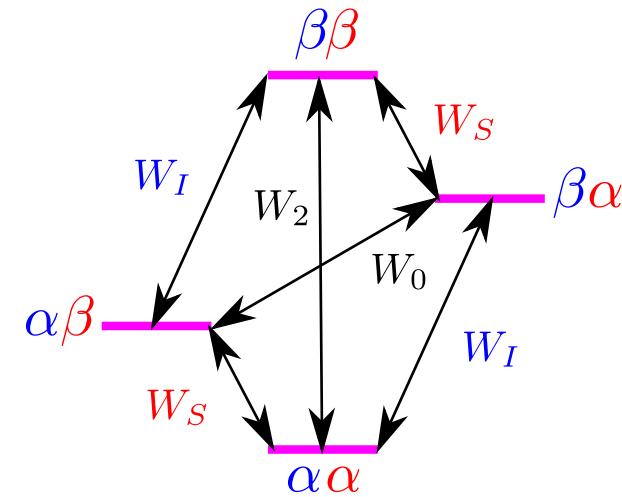
# NOESY - introduction

## Nuclear Overhauser effect

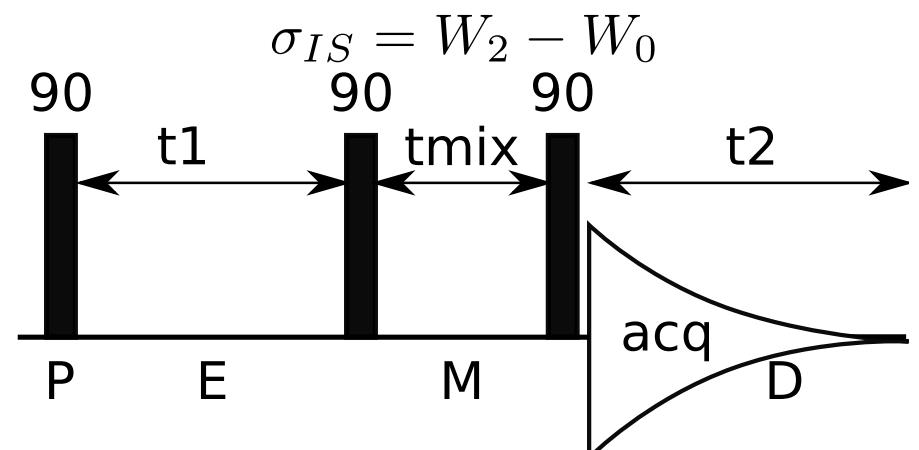
- ▶ dipol-dipol interaction
- ▶ magnetisation transfer **THROUGH SPACE** as a consequence of cross-relaxation

## NOESY

- ▶ correlates nuclei if their distance is **smaller than 5 Å**



$$\frac{d\Delta I_z}{dt} = -\rho_I(I_z - I_z^0) - \sigma_{IS}(S_z - S_z^0)$$

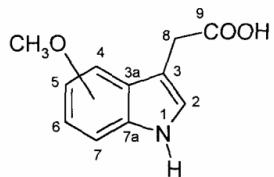


# NOE differential experiment

## PROBLEM 4

### NOE- Difference Spectroscopy

Figure 4.1 shows the  $^1\text{H}$  NMR and a  $^1\text{H}$  NOE difference spectrum of a 3-indolylacetic acid derivative **13** bearing a methoxy group at the benzenoid ring.



What is the position of the methoxy group?

(400 MHz  $^1\text{H}$ )

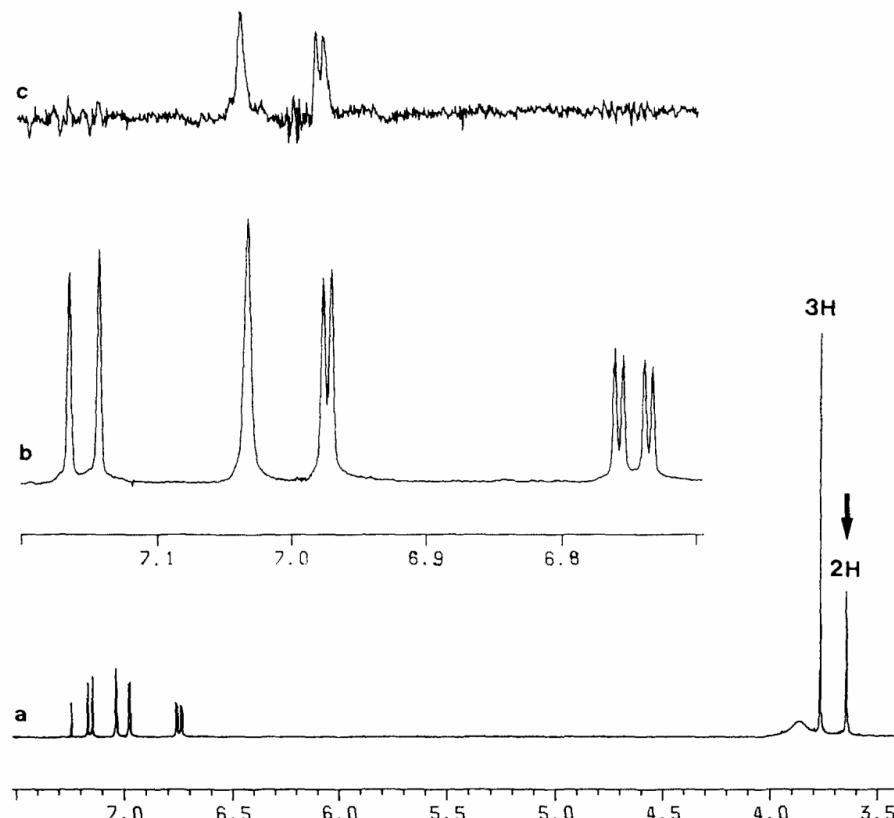
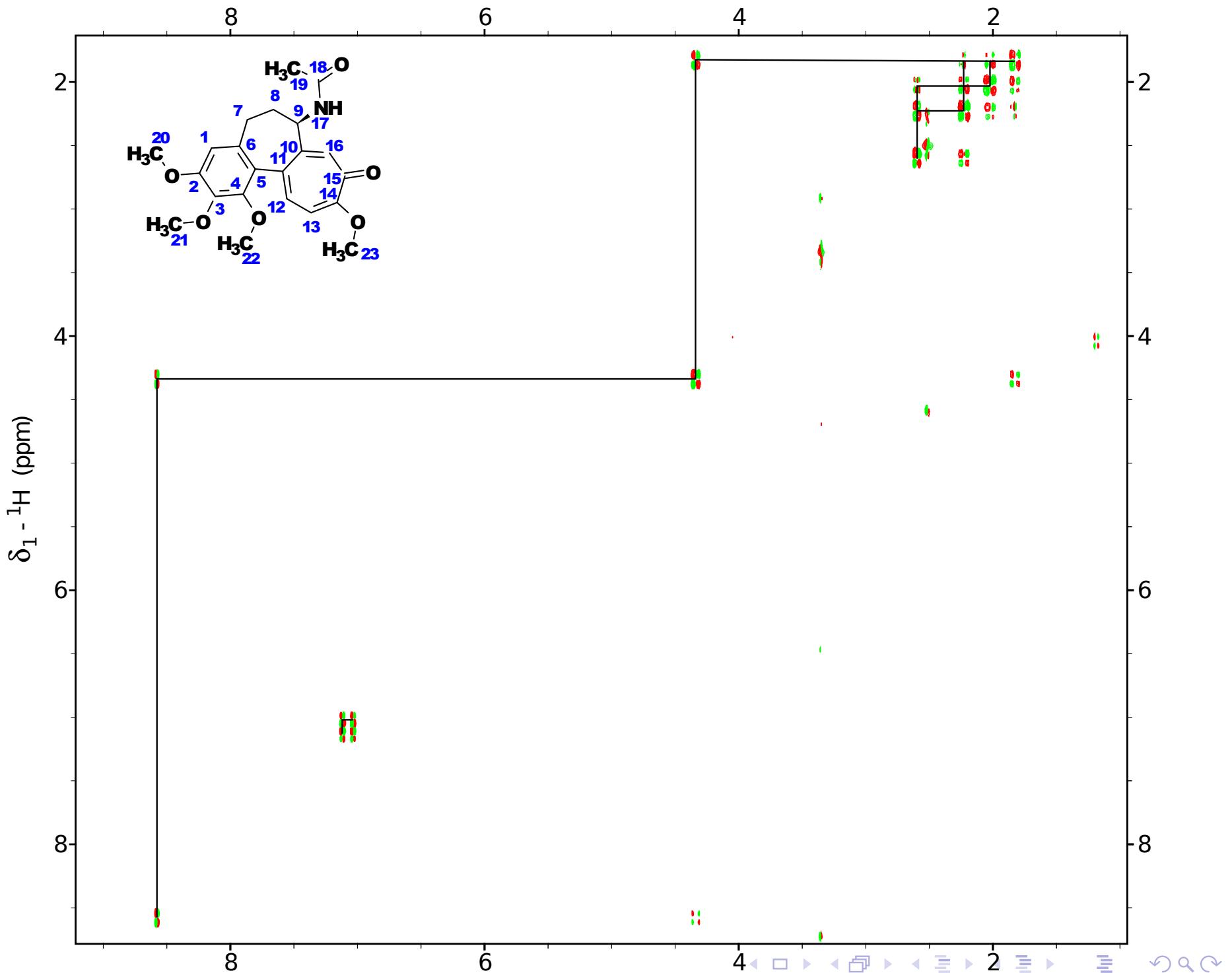
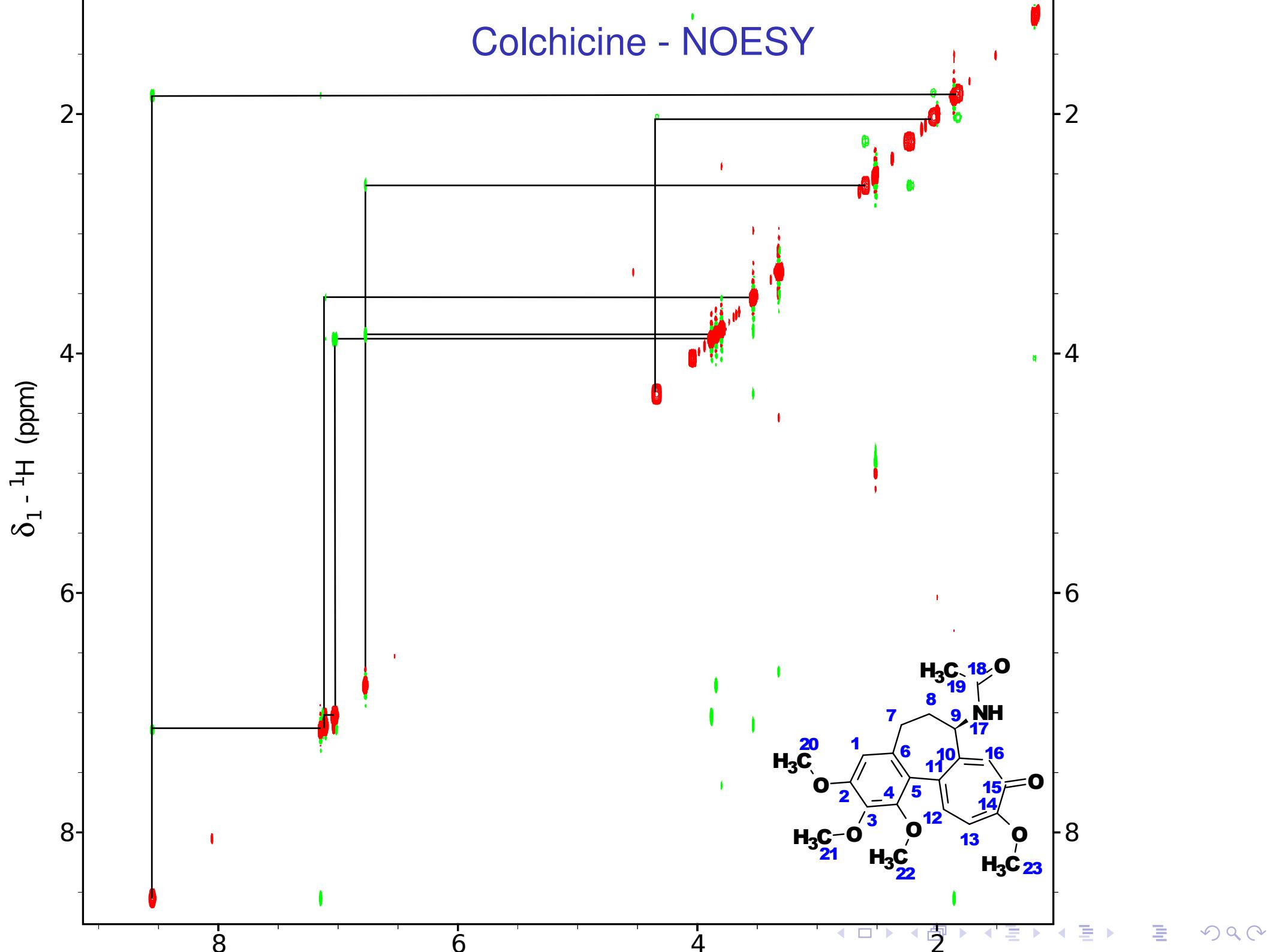


Fig. 4.1. 400 MHz  $^1\text{H}$  NMR spectrum of **13** in a mixture of  $\text{CDCl}_3$  and  $\text{CD}_3\text{OD}$ . **a** Full spectrum; **b** expanded section of the aromatic proton signals; **c**  $^1\text{H}$  NOE difference spectrum, same section as in **b**, irradiation position at  $\delta = 3.64$ .

# Colchicine - DQF-COSY



# Colchicine - NOESY



Next session:

Midterm Test, Heteronuclear correlations