

C8953  
NMR structural analysis  
seminar

Elucidating the 3D structure

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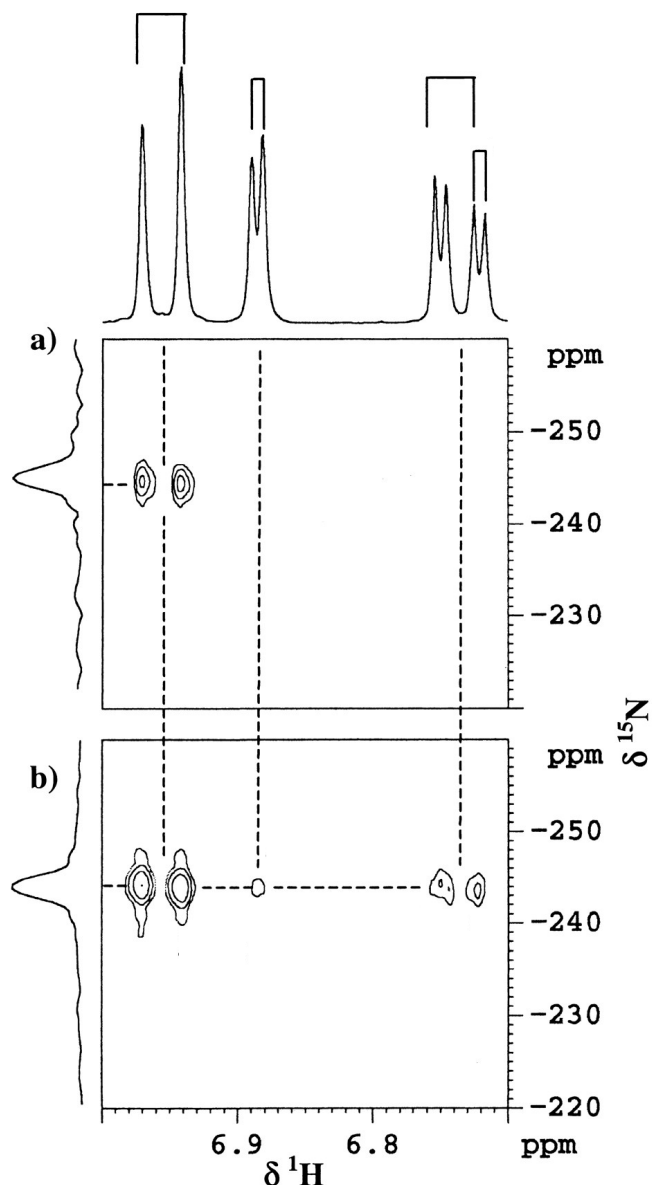
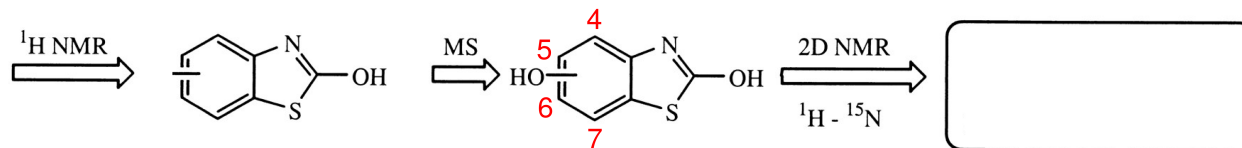
441648@mail.muni.cz, 176003@mail.muni.cz

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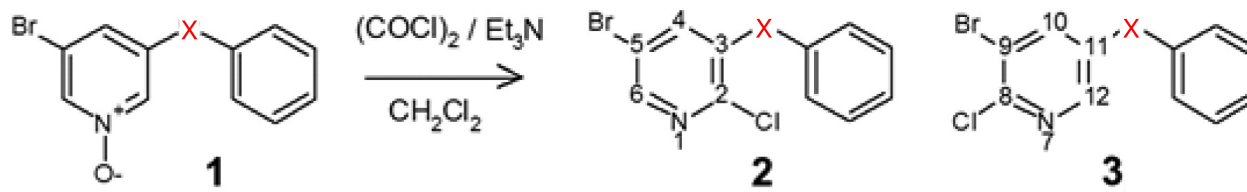
# Isomerisms and NMR

- ▶ Functional groups (constitution) - chemical shift
- ▶ Position of substituents - HMBC, NOESY/ROESY
- ▶ Relative configuration on double bonds or rings - *J*-coupling, NOESY/ROESY
- ▶ Absolute configuration - application of Chiral Derivatizing Agents (CDA)

# Benzothiazole Biodegradation: $^1\text{H}$ - $^{15}\text{N}$ HMBC (*Appl. Environ. Microbiol.*, 2001, 67)

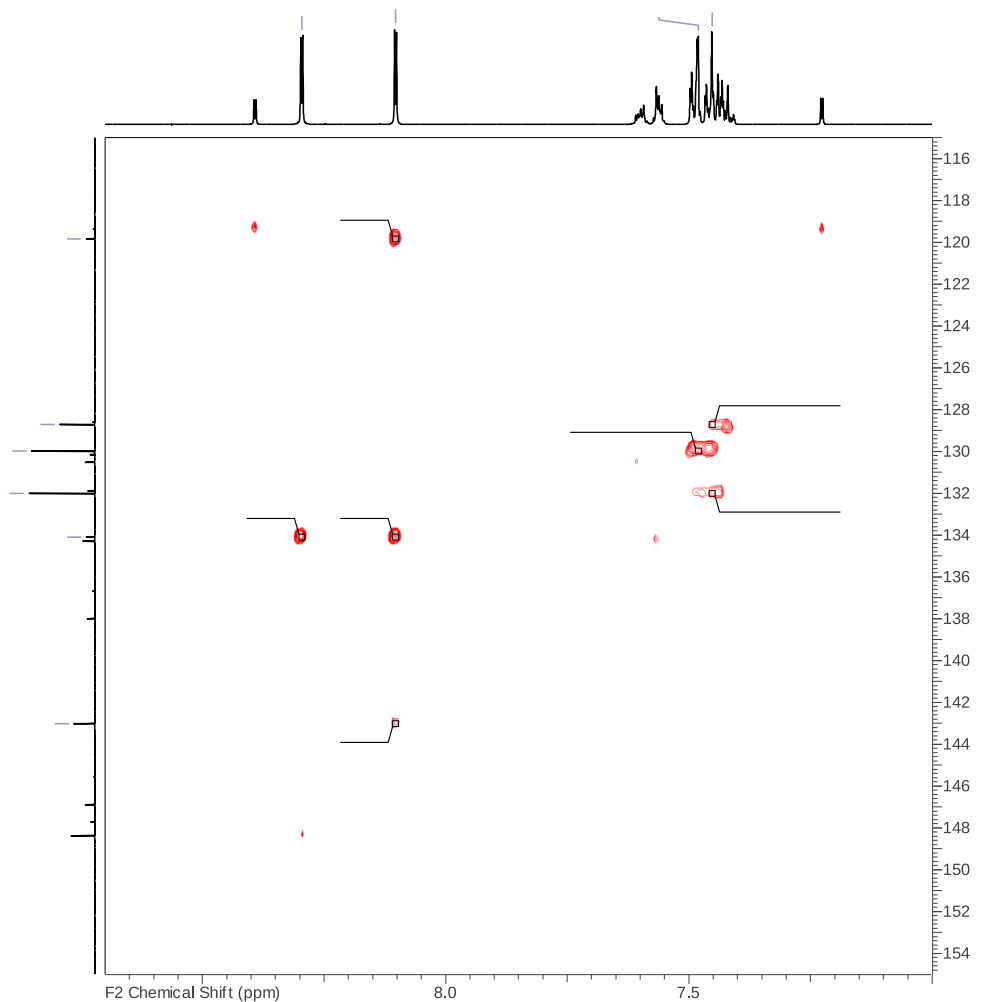
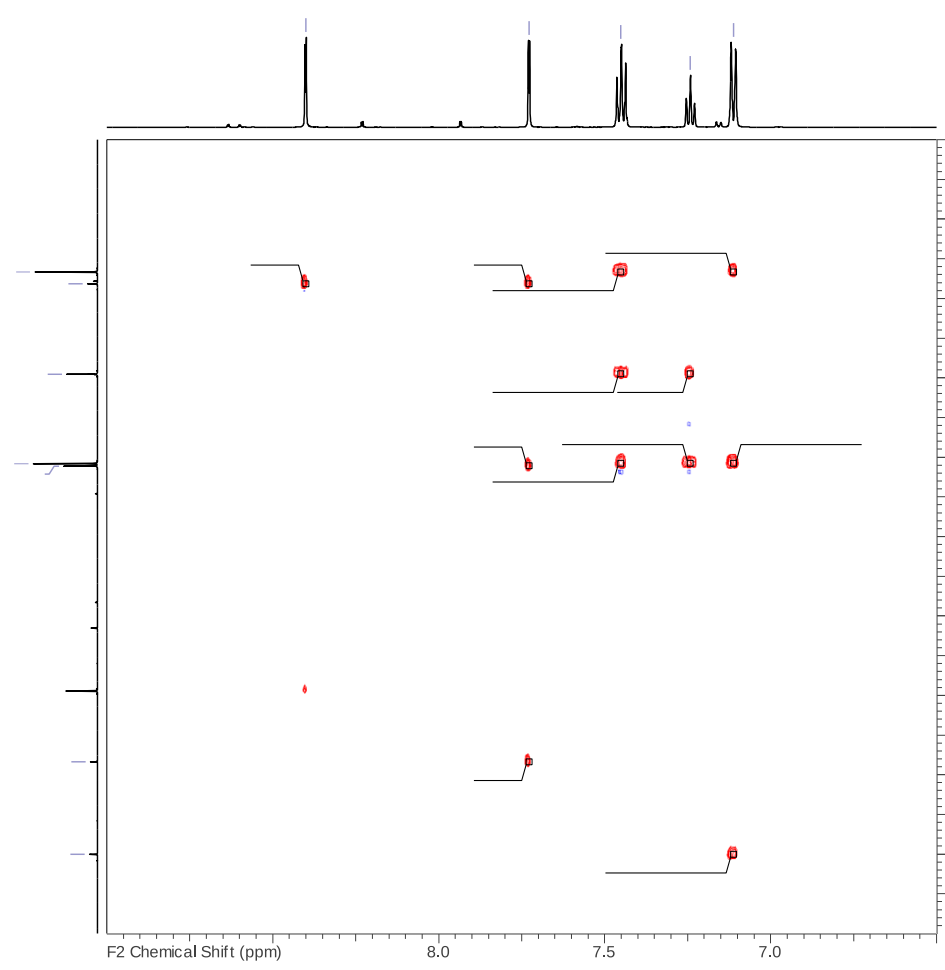


# Regioselectivity in the Halogenation: 1,1-ADEQUATE (*Org. Lett.*, **2016**, 18, 19561959)



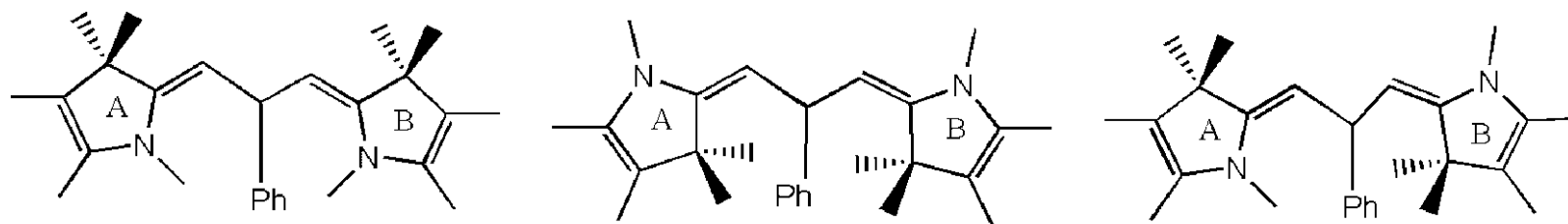
X = S

X = O

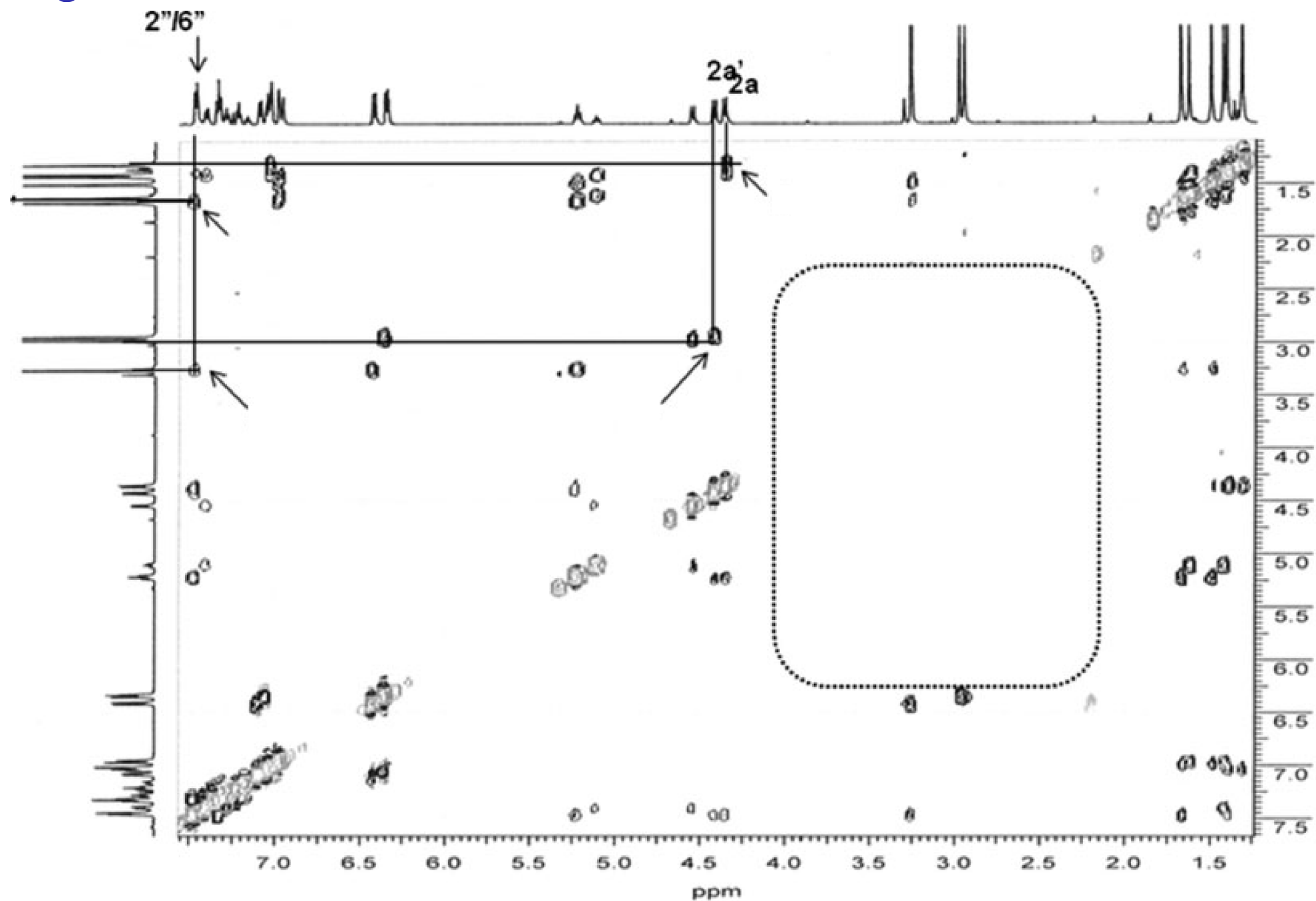


# Configuration on double bonds

Describe the isomers of molecule shown below:

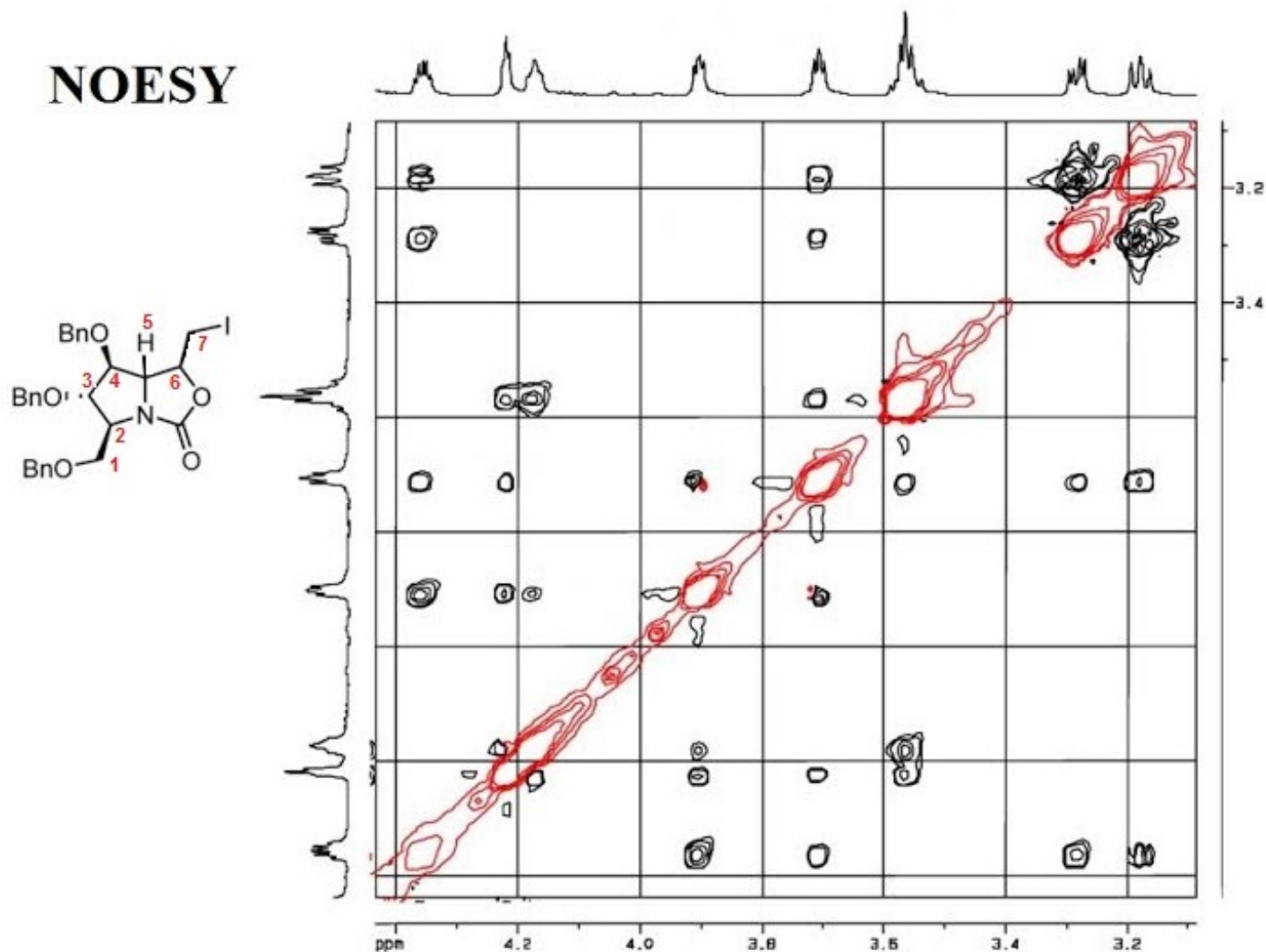


# Configuration on double bonds: NOESY



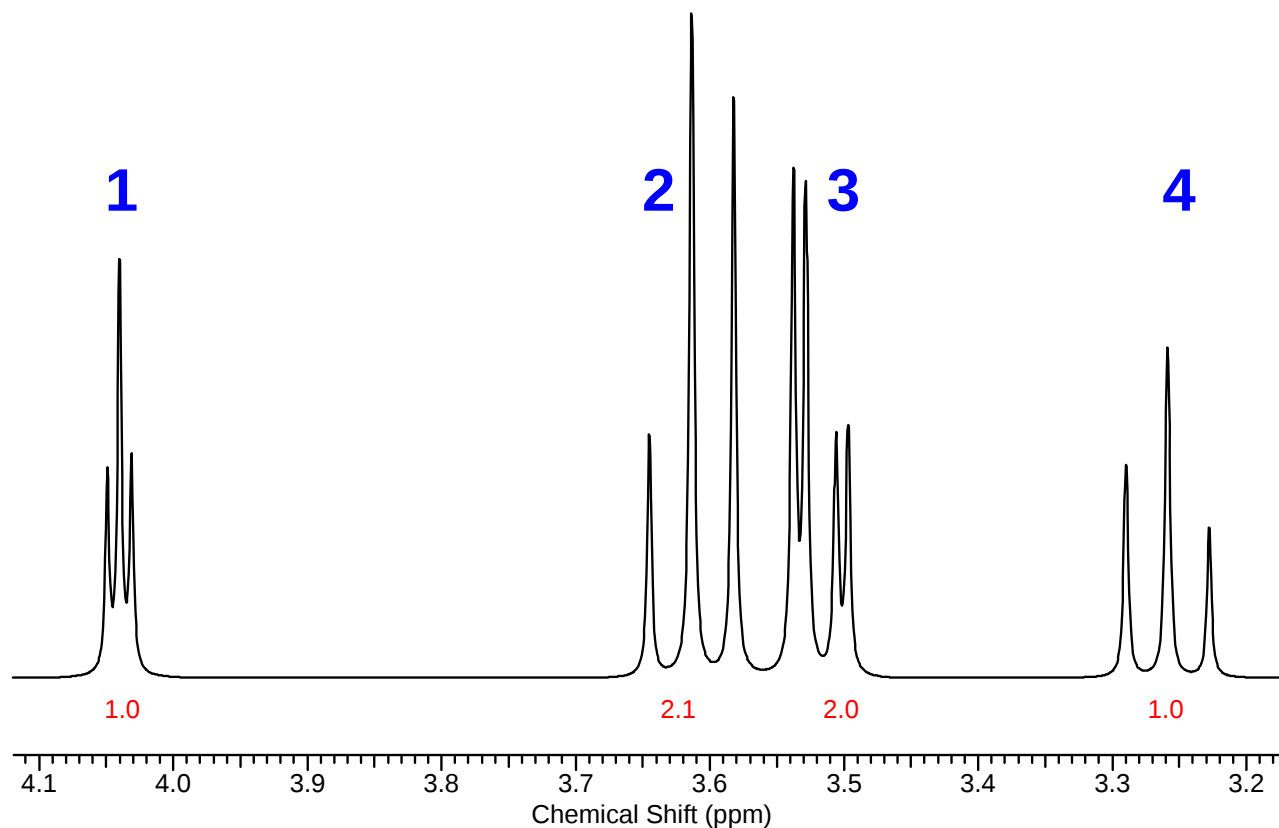
# Relative stereochemistry on a ring: NOESY

Provide the full assignment of  $^1\text{H}$  resonances and determine the orientation of H5 and H6.



# Interpretation of $J$ -coupling

**Unknown compound  $C_6H_{12}O_6$  measured in  $D_2O$**   
Detected  $J_{HH}$ -couplings: (2x9.6), (2.8, 9.6), (2x9.6), (2x2.8)



1D  $^{13}C$  NMR spectrum contains **4 signals in the range 71-75 ppm.**