C8953
NMR strukturní analýza
seminář

Elucidating structure using NMR

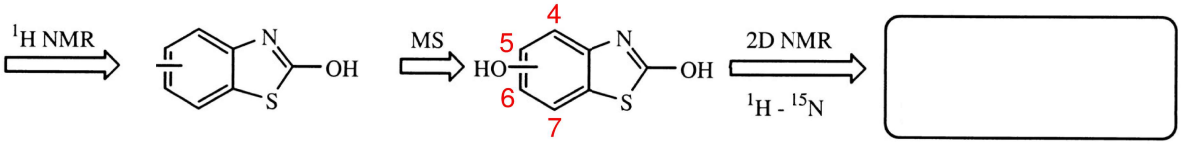
Jan Novotný, Ondřej Jurček
176003@is.muni.cz, ondrej.jurcek@ceitec.muni.cz

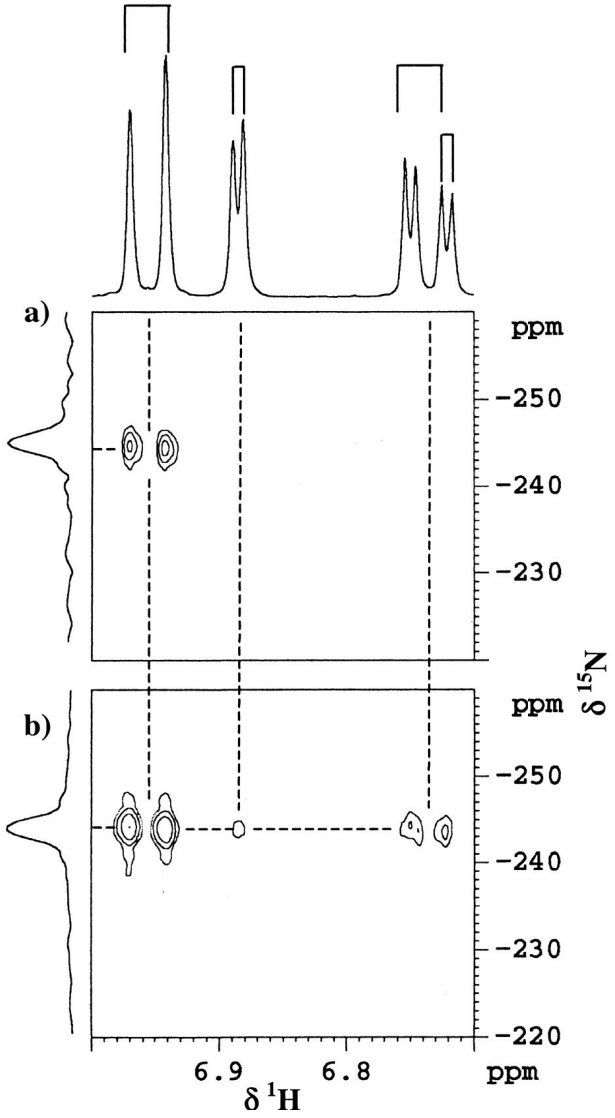
April 25, 2018

Isomerisms and NMR

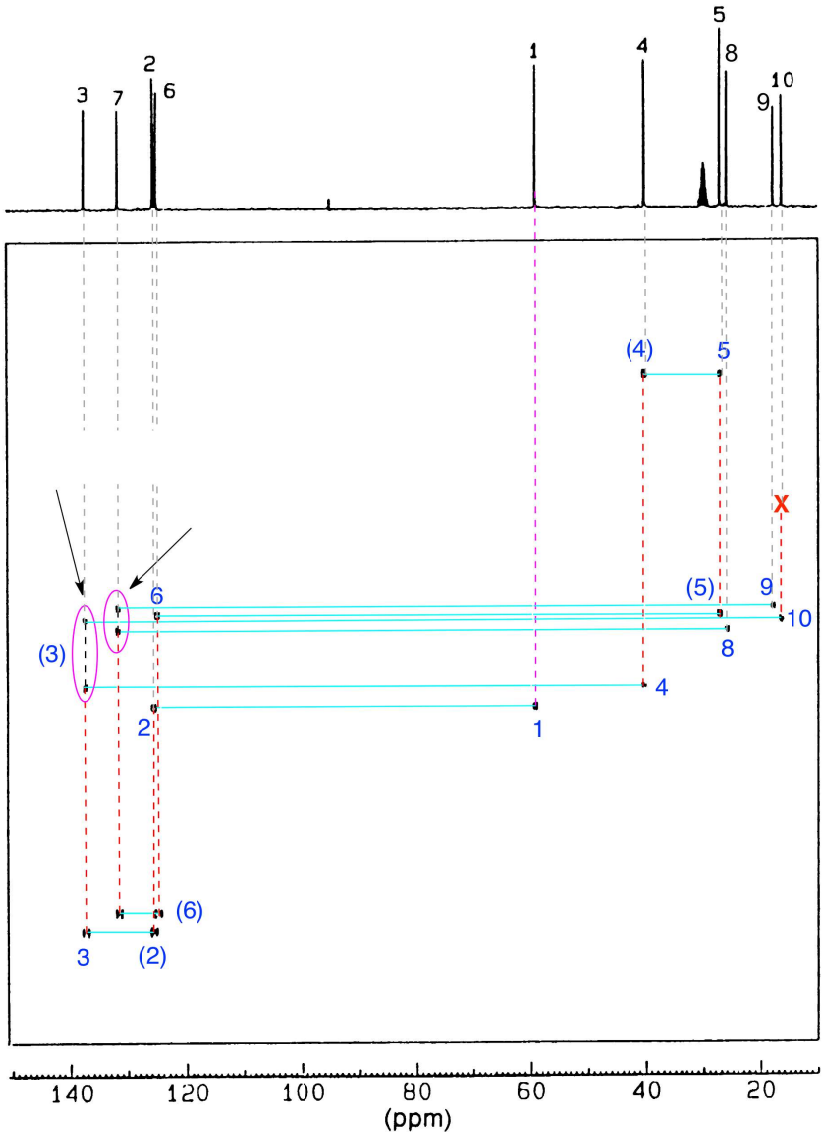
- Functional groups (constitution) - chemical shift
- Position of substituents - HMBC, NOESY/ROESY
- Relative configuration on double bonds or rings - *J*-coupling, NOESY/ROESY
- Absolute configuration - application of Chiral Derivatizing Agents (CDA)

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

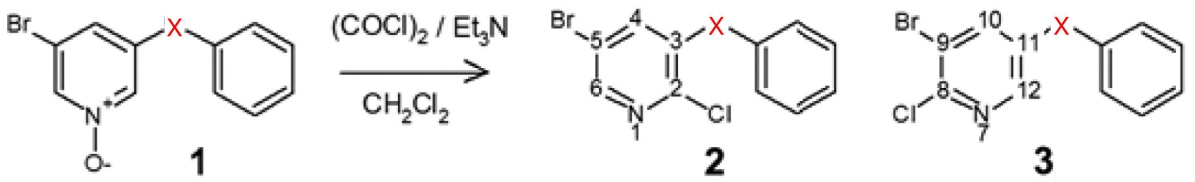




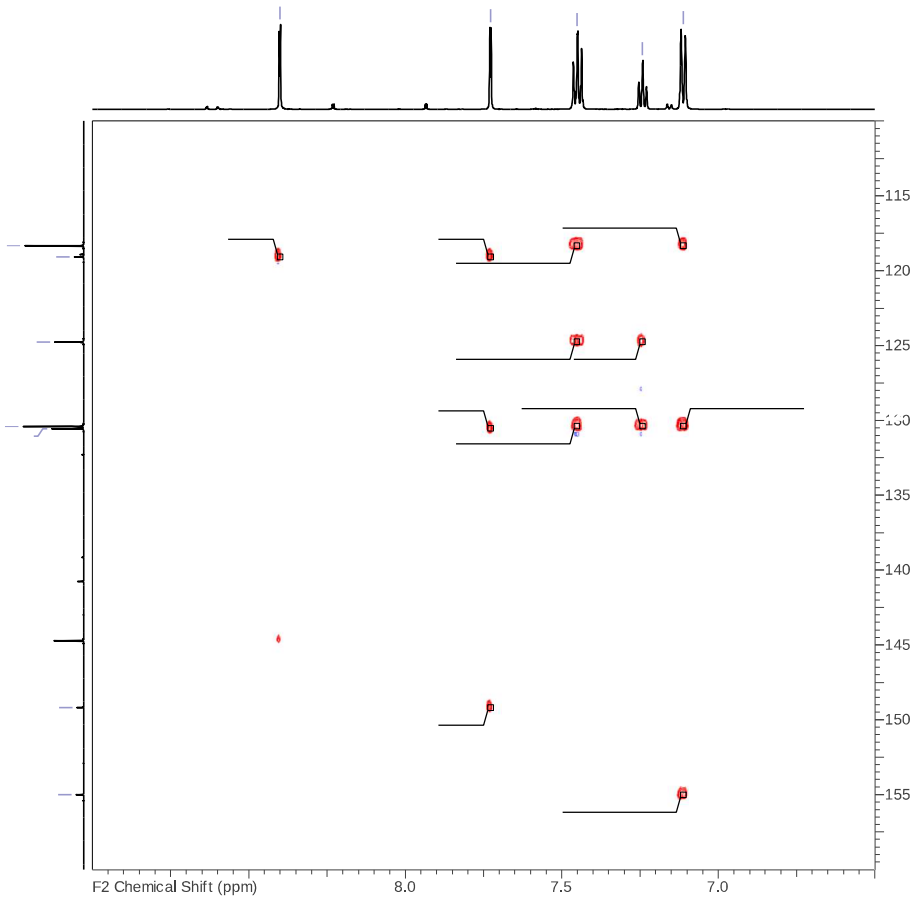
Determine the structure of $C_{10}H_{18}O$ using INADEQUATE exp.



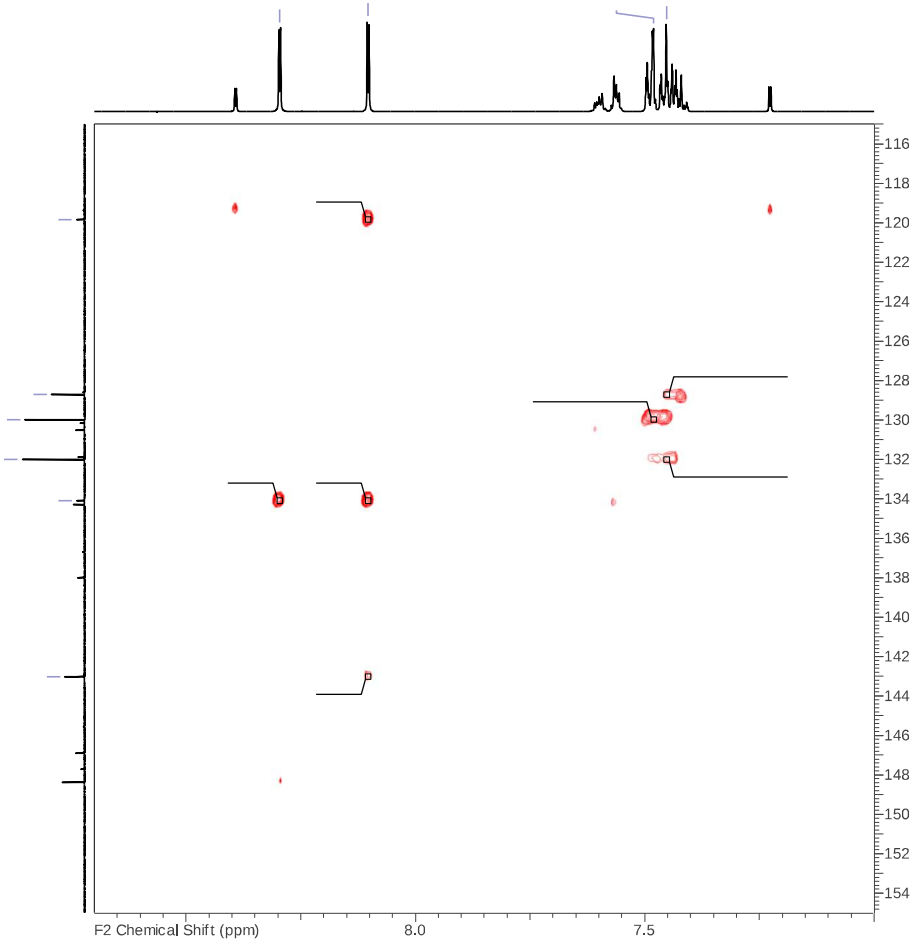
Regioselectivity in the Halogenation: 1,1-ADEQUATE (*Org. Lett.*, **2016**, 18, 19561959)



X = O

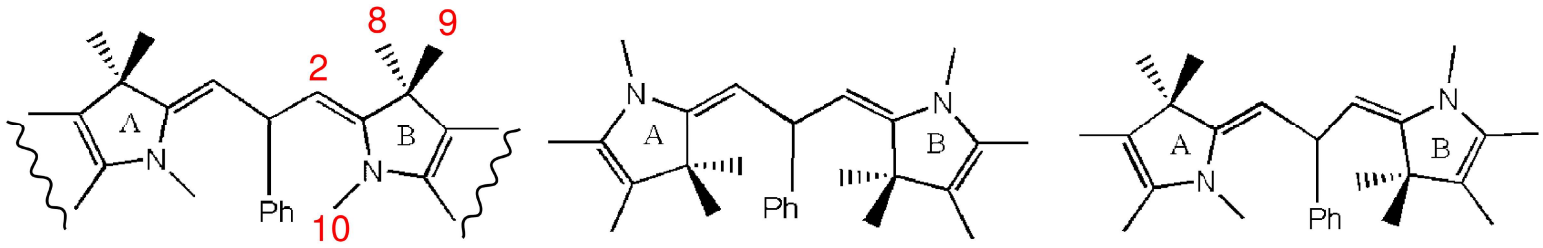


X = S

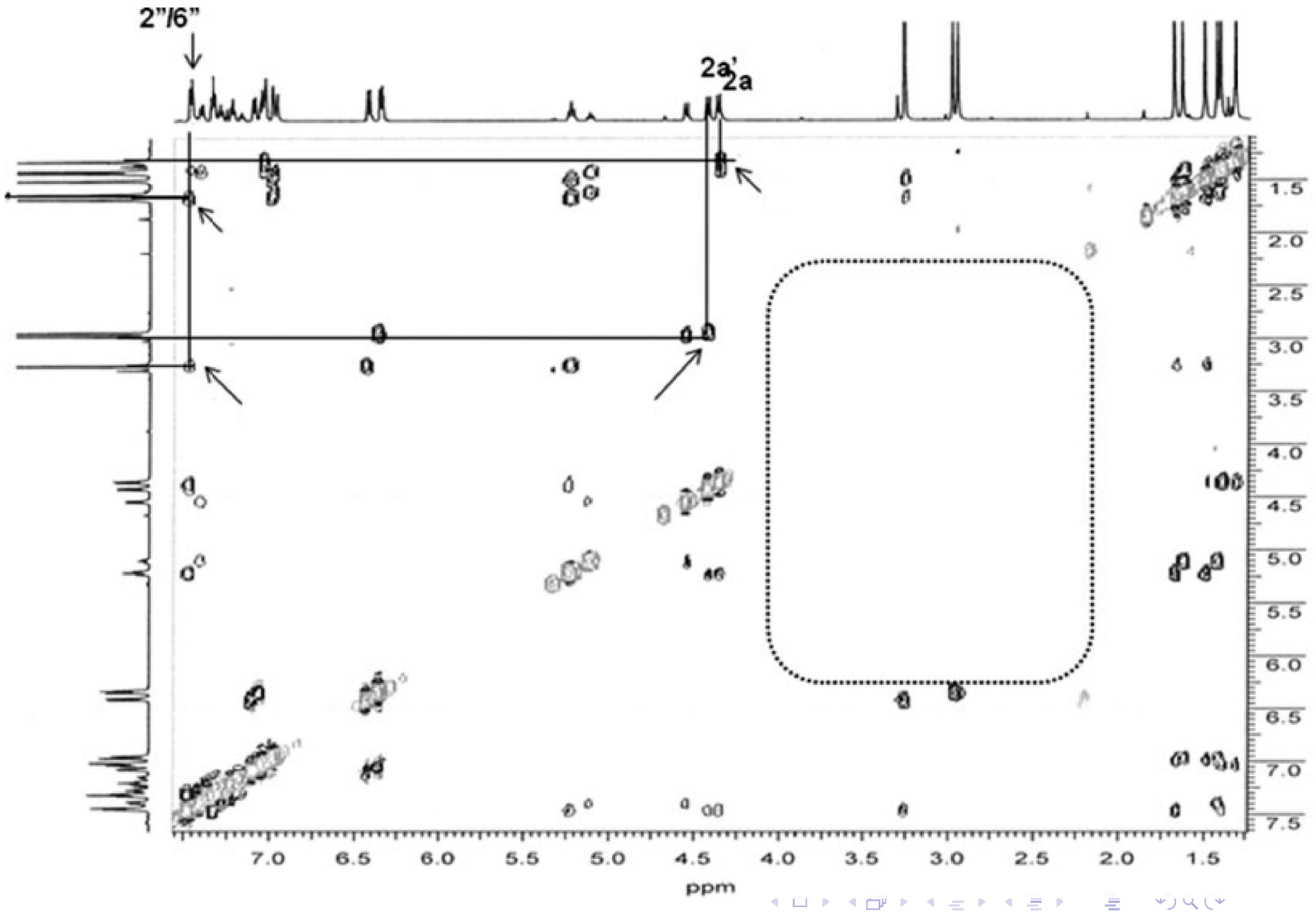


Configuration on double bonds (*Magn. Reson. Chem.* **2008**, 46, 872–877)

Describe the isomers of molecule shown bellow:

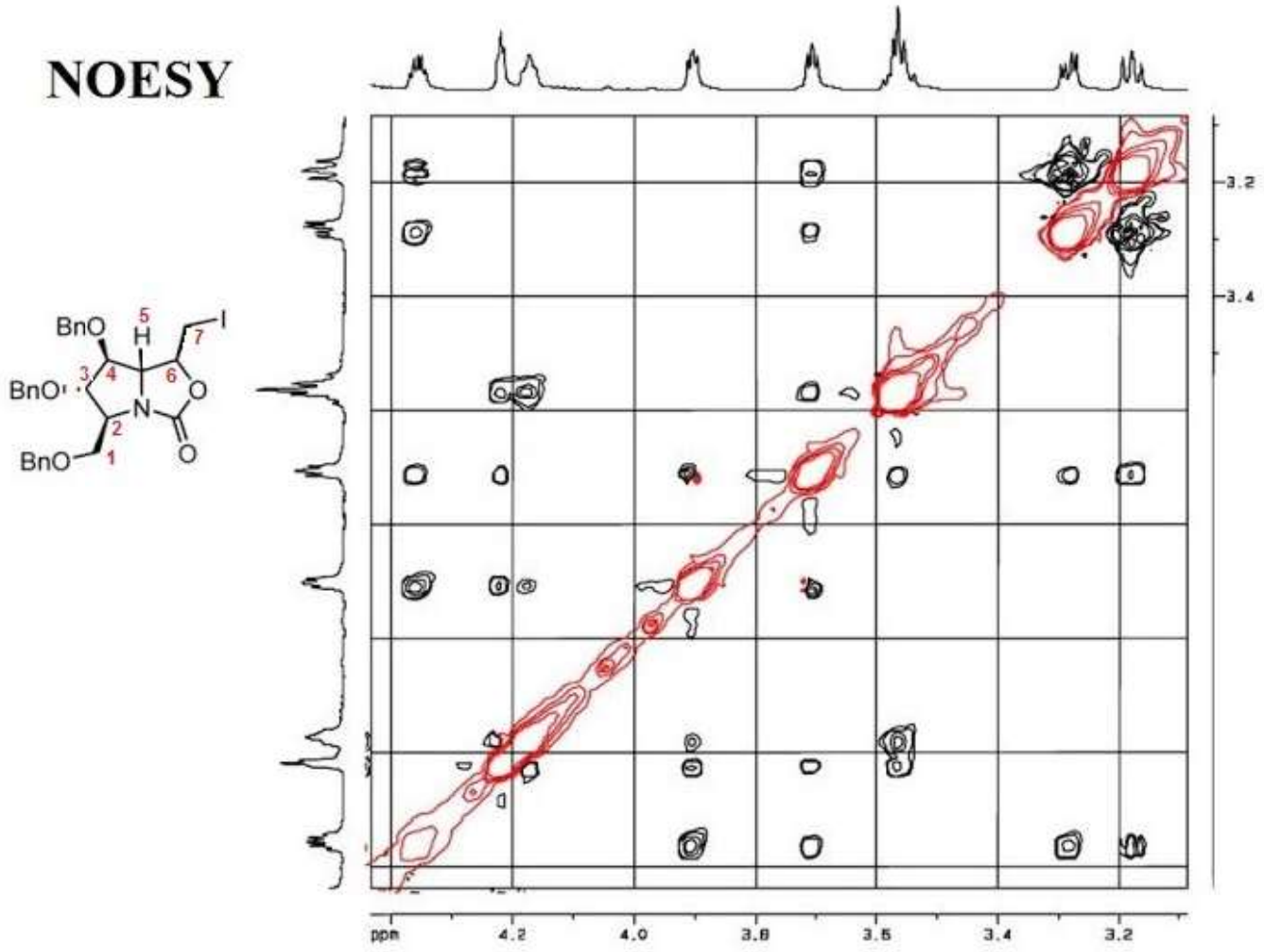


Configuration on double bonds: NOESY



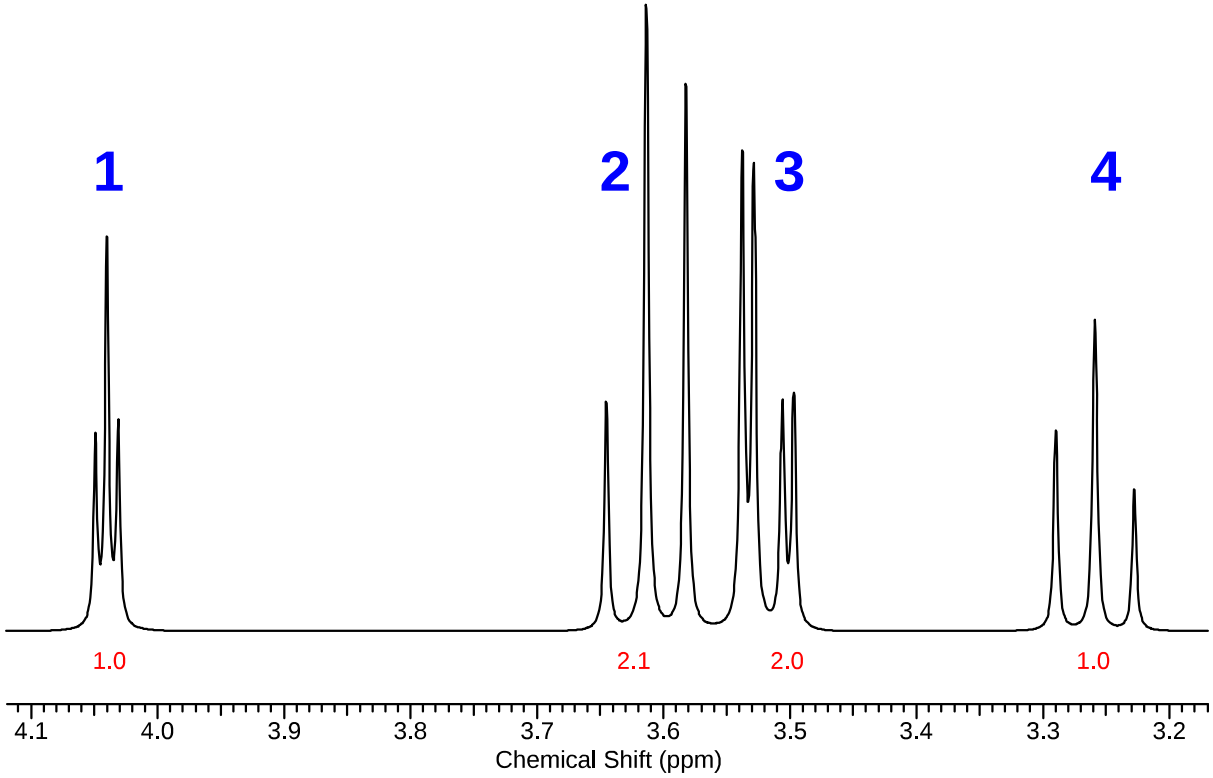
Relative stereochemistry on a ring: NOESY

Provide the complete assignment of ^{1}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**.