ÚOCHB AV ČR
IOCB PRAGUE

MAGNETIC RESONANCE DAY

Tips and tricks for NMR structural analysis

NMR structural analysis

NMR SPECTROSCOPY
RESEARCH-SERVICE GROUP
IOCB PRAGUE

- We encourage everyone to learn how to interpret NMR spectra
- We offer a wide range of support
  - Self-training materials
  - Workshops
  - Individual consultations

1D NMR problems – self training

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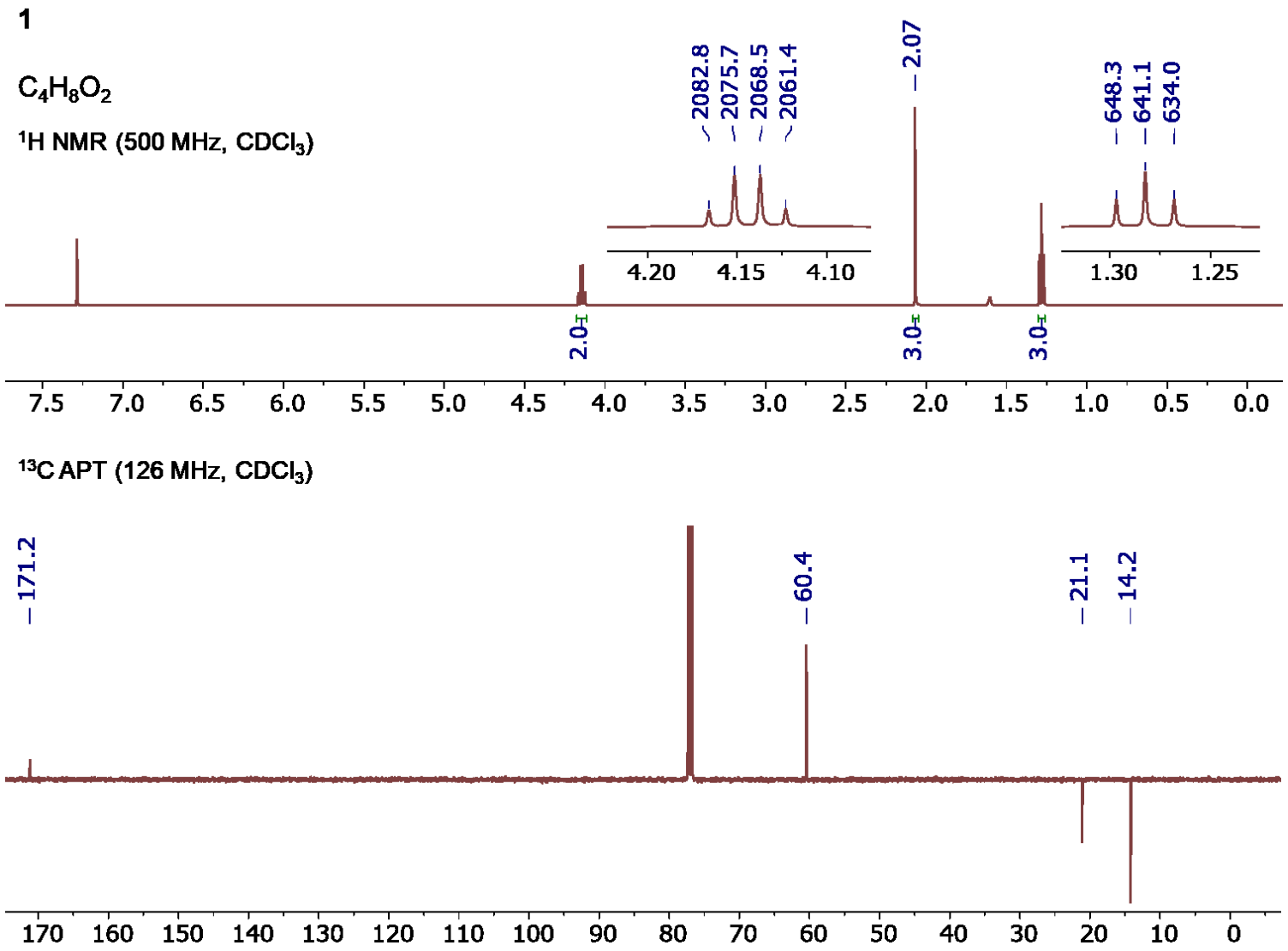
- Set of 90 1D spectra (^{1}H and ^{13}C) at
  https://nmr.group.uochb.cz/en/1d-2d-nmr-problems



1D NMR problems – self training

- Set of 90 1D spectra (^{1}H and ^{13}C) at
  https://nmr.group.uochb.cz/en/1d-2d-nmr-problems

- 1D Spectra - Test Answers
  Excel sheet where you can check your answers

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Spectrum No.	Level	Compound Name	Result	Points
1	1	ethyl acetate	Correct	1.00
2	1		No answer	-
3	1		No answer	-
4	3		No answer	-
5	2		No answer	-

2D NMR problems – self training

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- $C_9H_{10}O_2$ challenge
  - Set of 37 compounds with the same molecular formula
  - ^{1}H, ^{13}C APT, COSY, HSQC, HMBC

$C_9H_{10}O_2$ challenge

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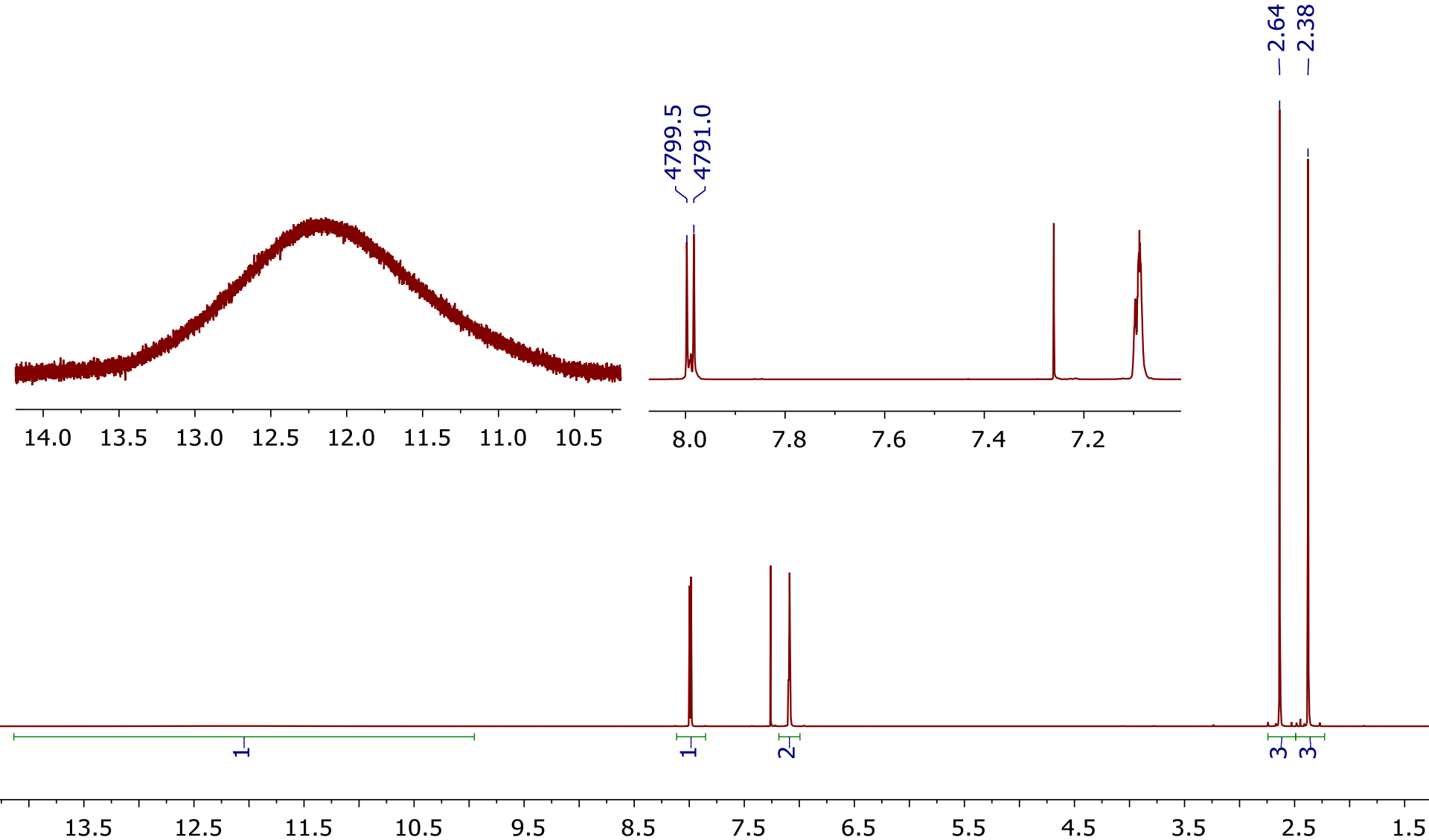

$C_9H_{10}O_2$ challenge

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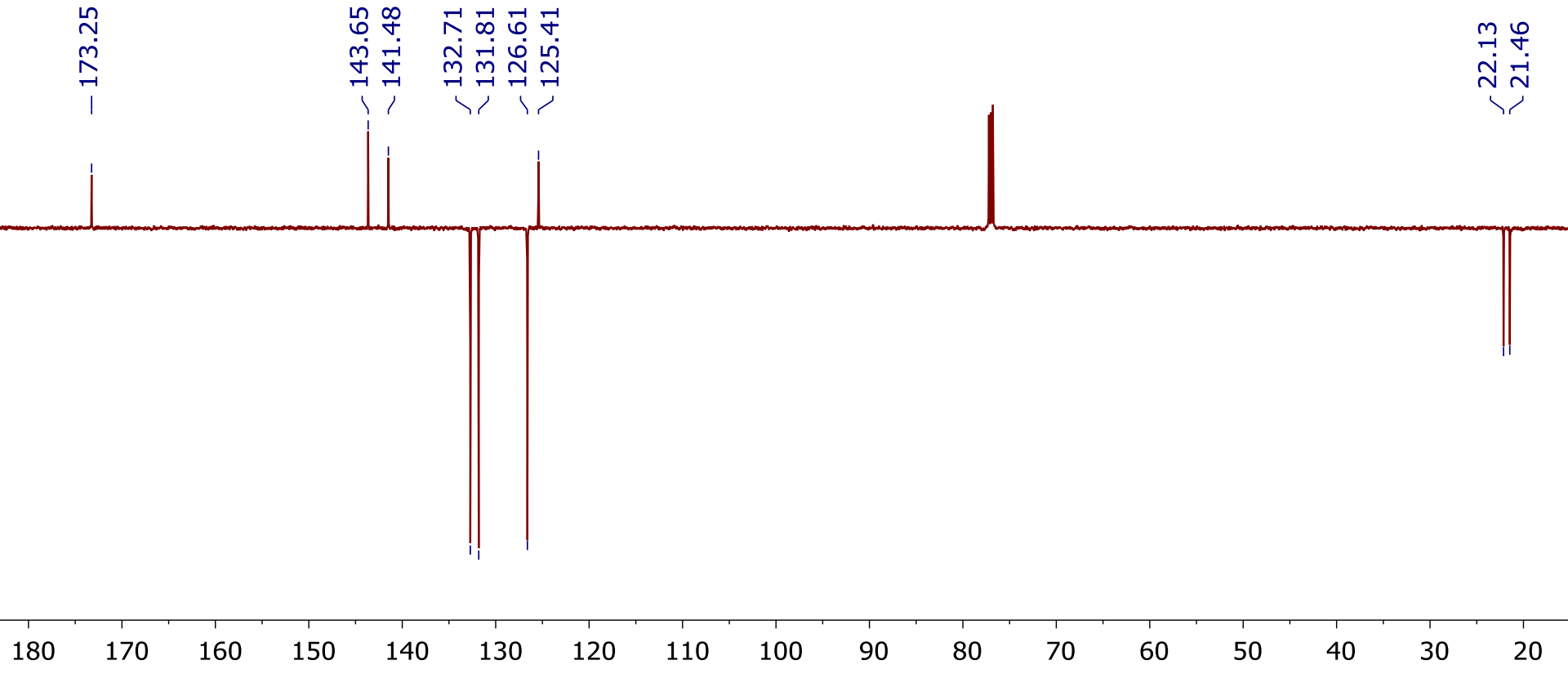
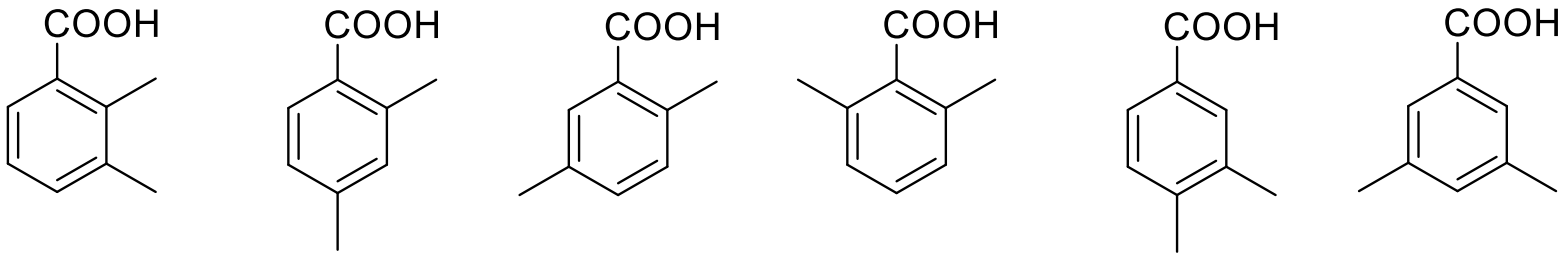
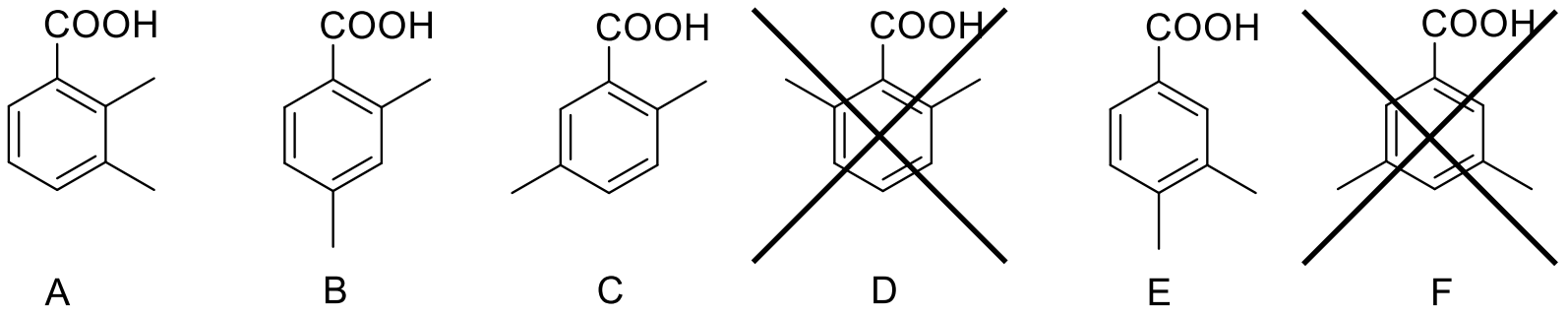


$C_9H_{10}O_2$ challenge



A B C D E F

$C_9H_{10}O_2$ challenge



$C_9H_{10}O_2$ challenge

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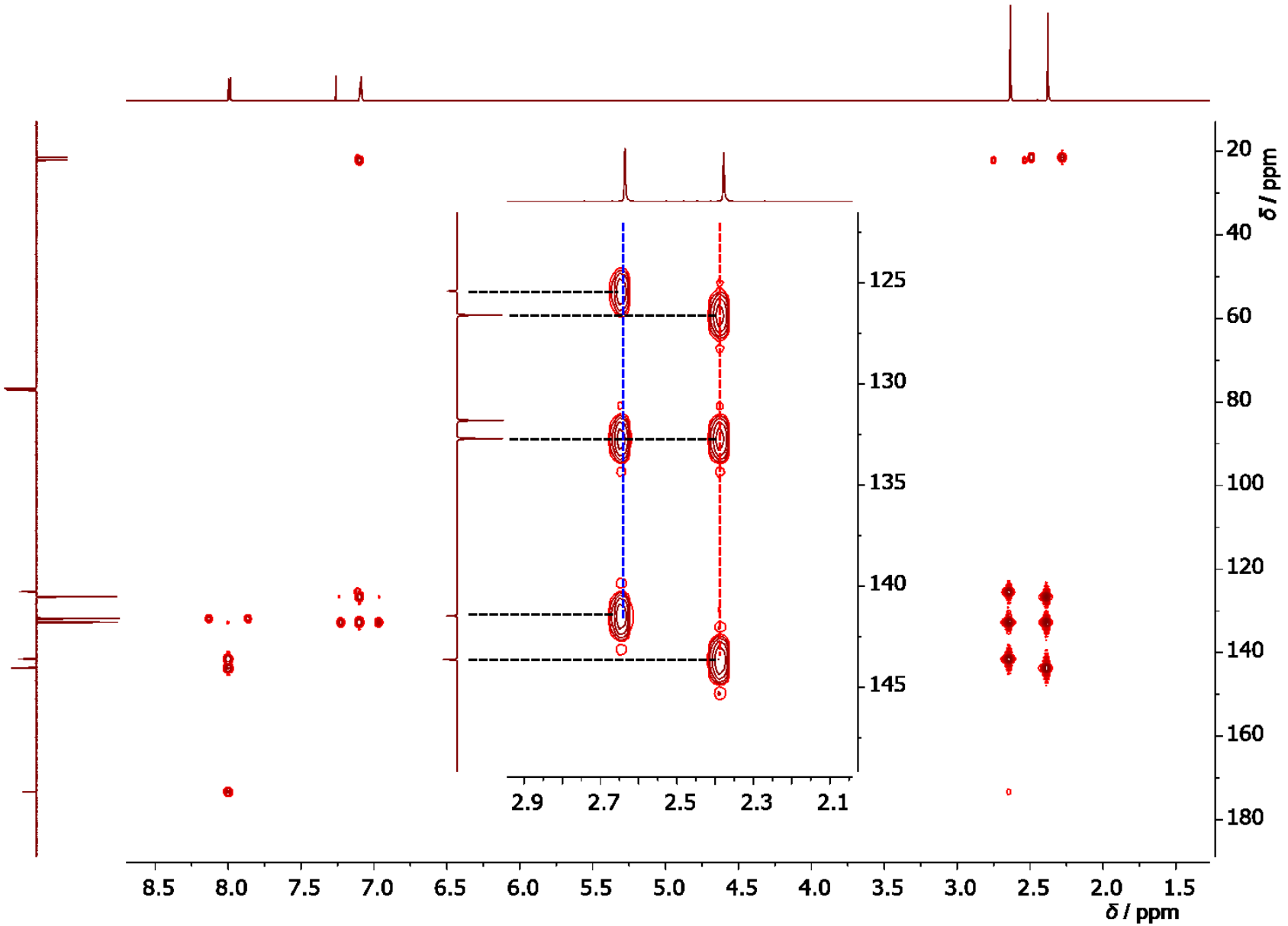
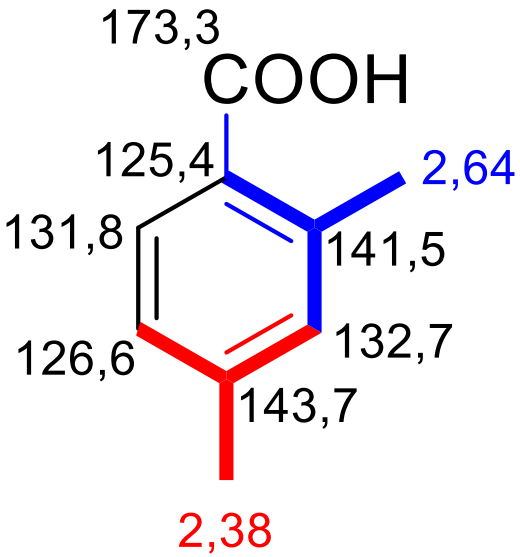
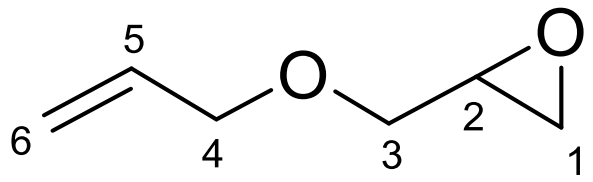


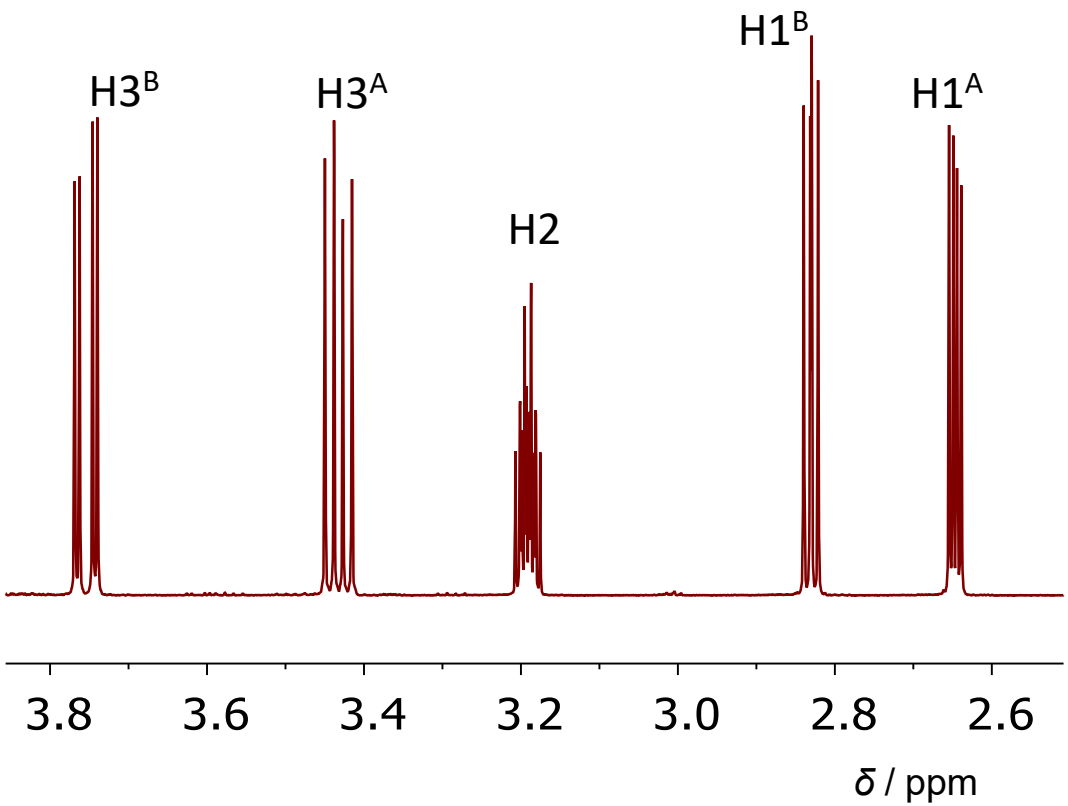
$C_9H_{10}O_2$ challenge

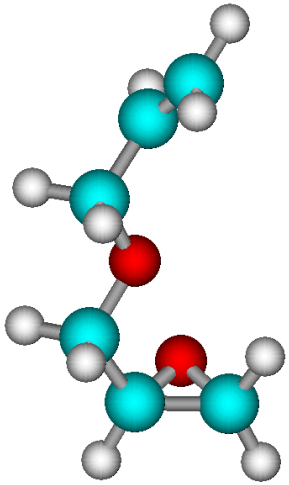


Topicity

- Homotopic (equivalent)
- Enantiotopic (equivalent under usual conditions)
- Diastereotopic (non-equivalent)



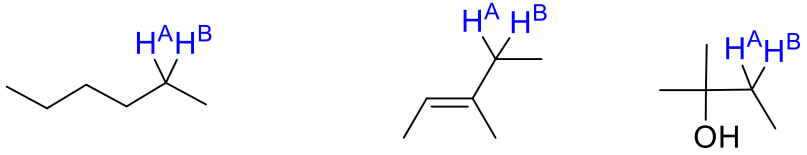




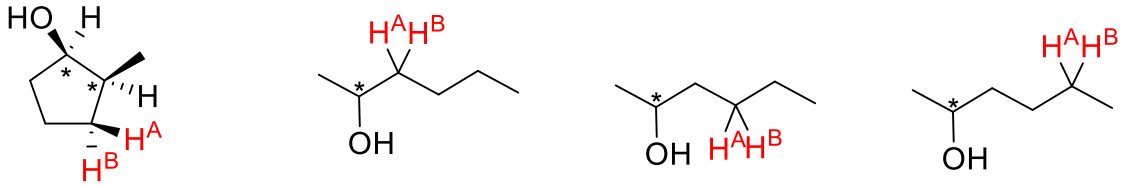
Topicity

- Homotopic (equivalent)

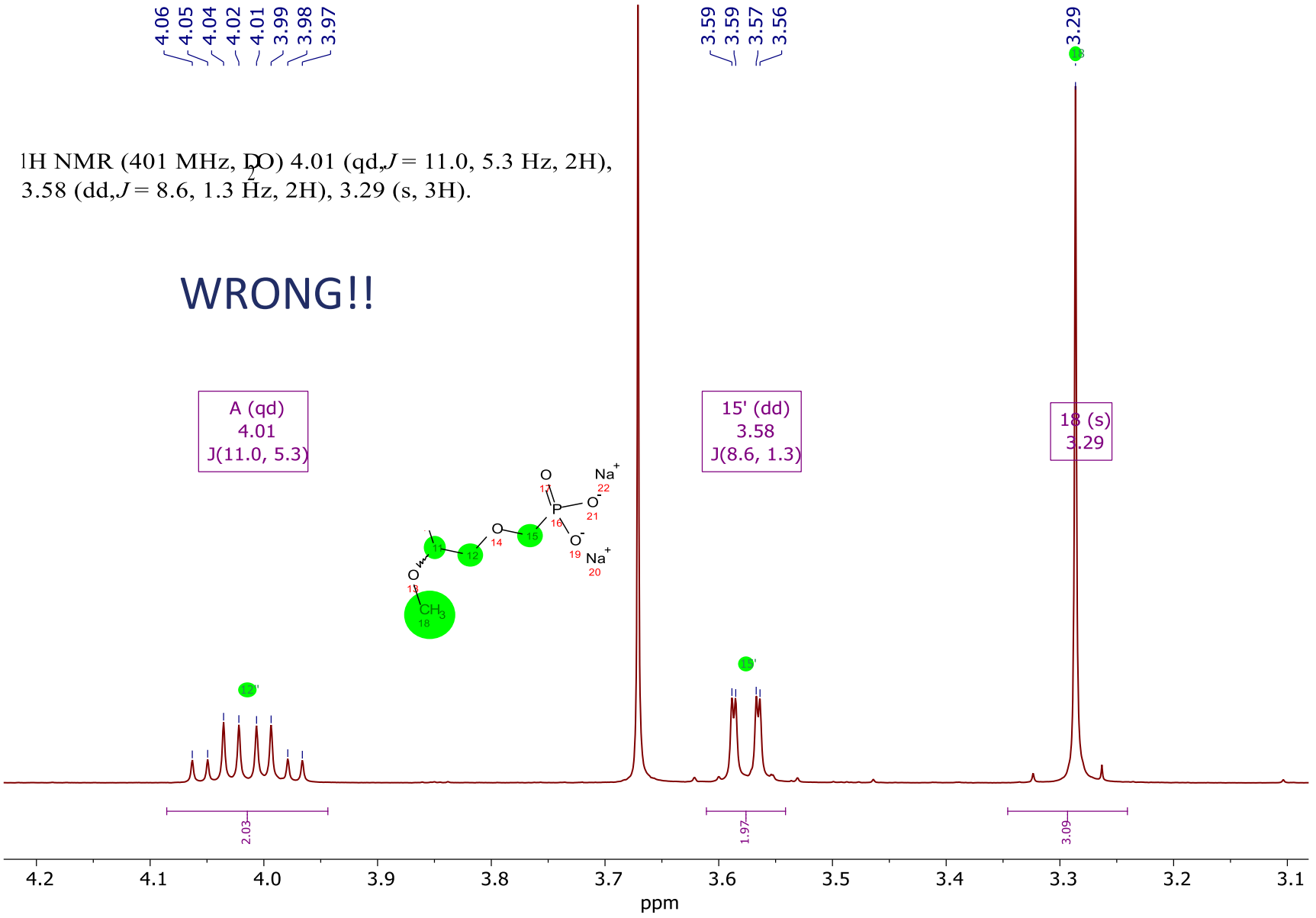
- Enantiotopic (equivalent)



- Diastereotopic (non-equivalent)

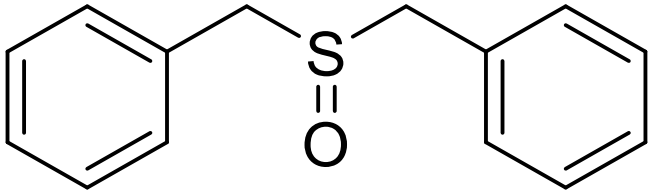


Topicity


4.06
4.05
4.04
4.02
4.01
3.99
3.98
3.97
3.59
3.59
3.57
3.56
3.29
1H NMR (401 MHz, D2O) 4.01 (qd, J = 11.0, 5.3 Hz, 2H), 3.58 (dd, J = 8.6, 1.3 Hz, 2H), 3.29 (s, 3H).
WRONG!!
A (qd)
4.01
J(11.0, 5.3)
15' (dd)
3.58
J(8.6, 1.3)
18 (s)
3.29
2.03
1.97
3.09
4.2
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
ppm

Topicity

- CH_2 hydrogen atoms in dibenzylsulfoxide are diastereotopic



Topicity

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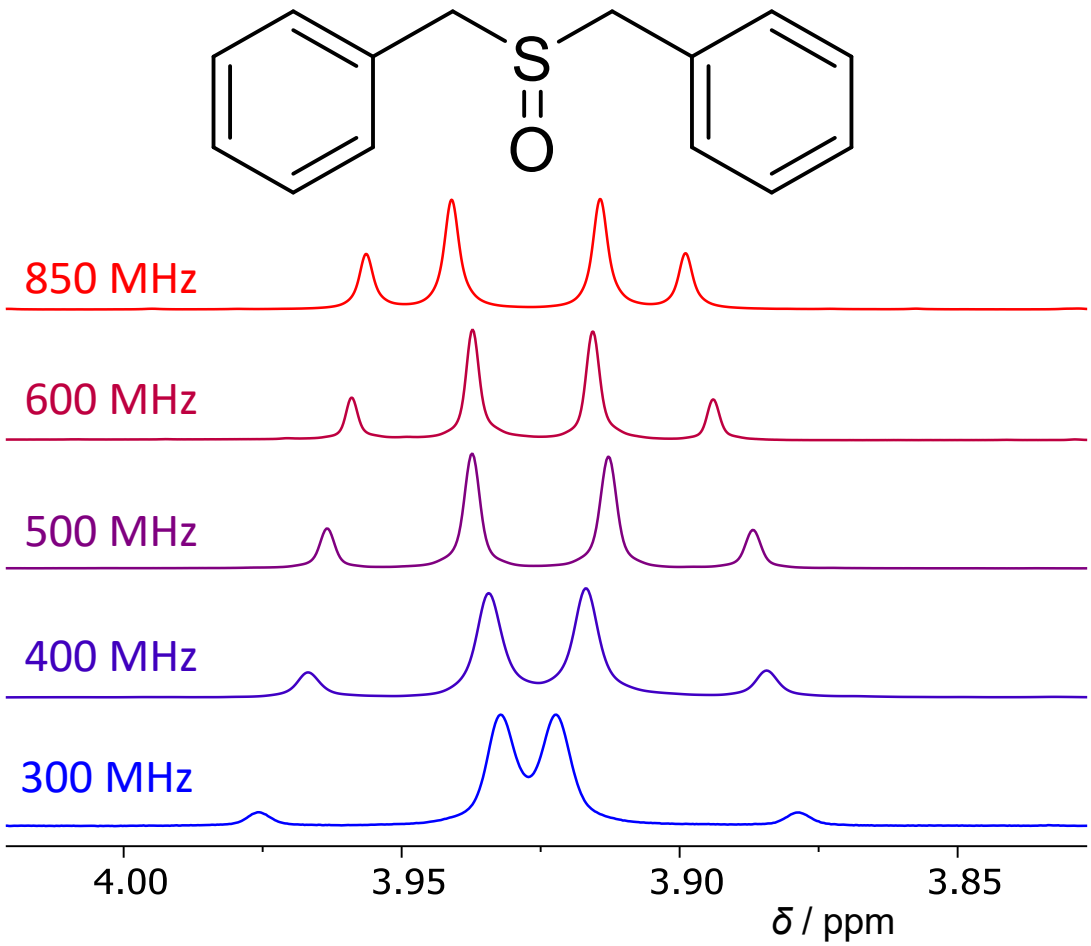
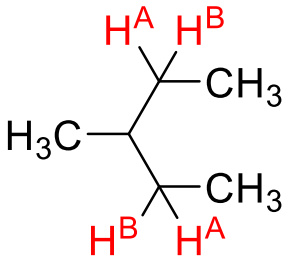
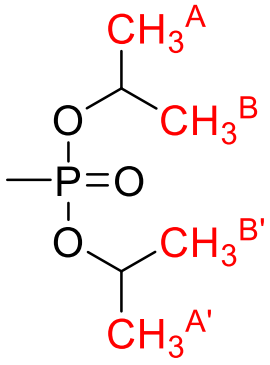


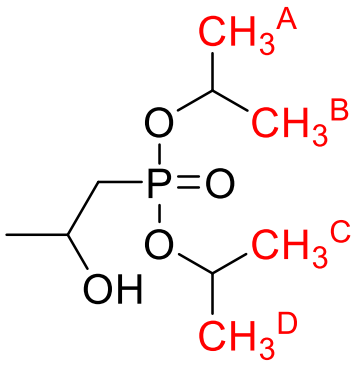
Topicity

- CH_2 hydrogen atoms in 3-methylpentane are diastereotopic



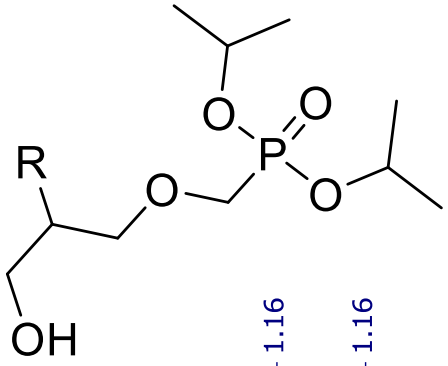
- Methyl groups in diisopropyl esters are diastereotopic



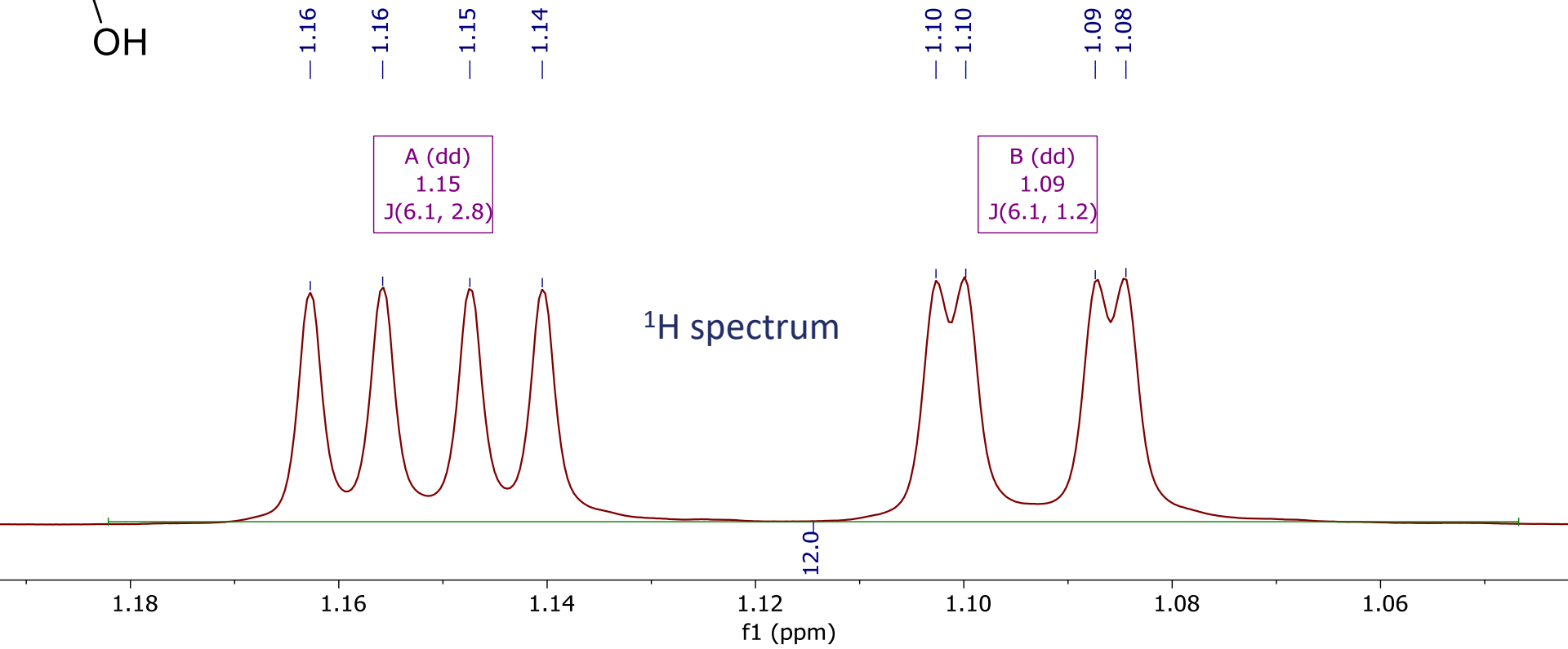


Topicity

- Methyl groups in di*iso*propyl esters are diastereotopic
- Expect four doublets in ^{1}H spectrum (coupling with CH proton)



WRONG!!



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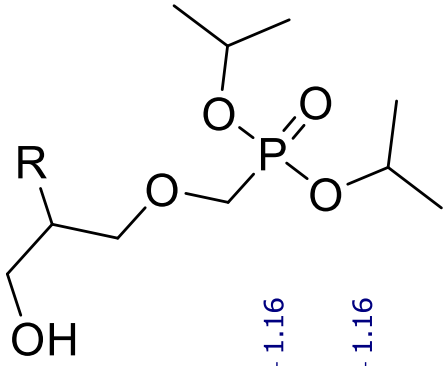
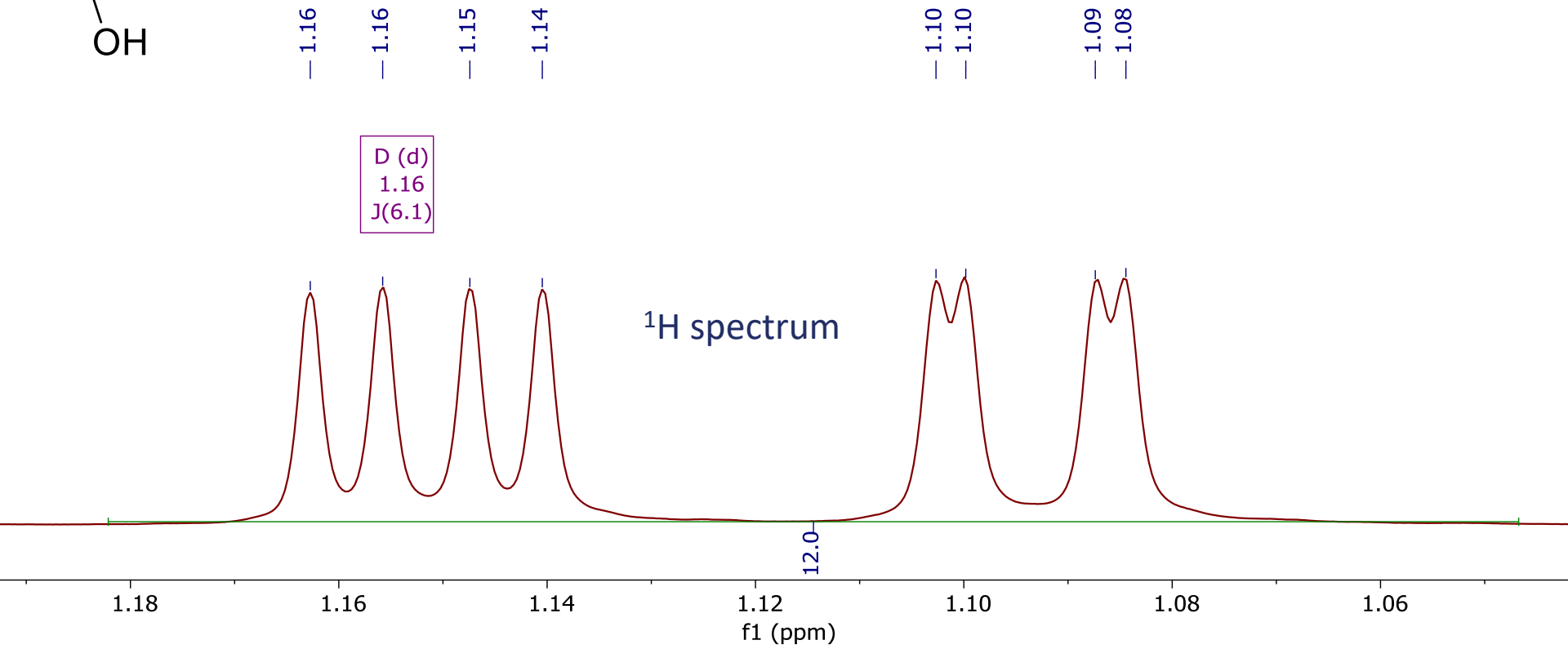
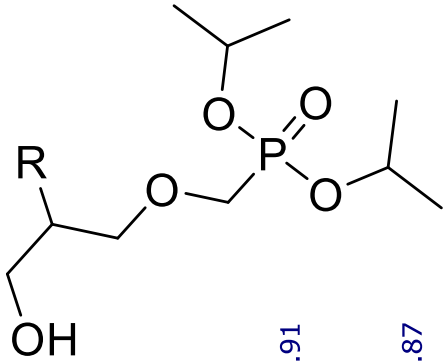
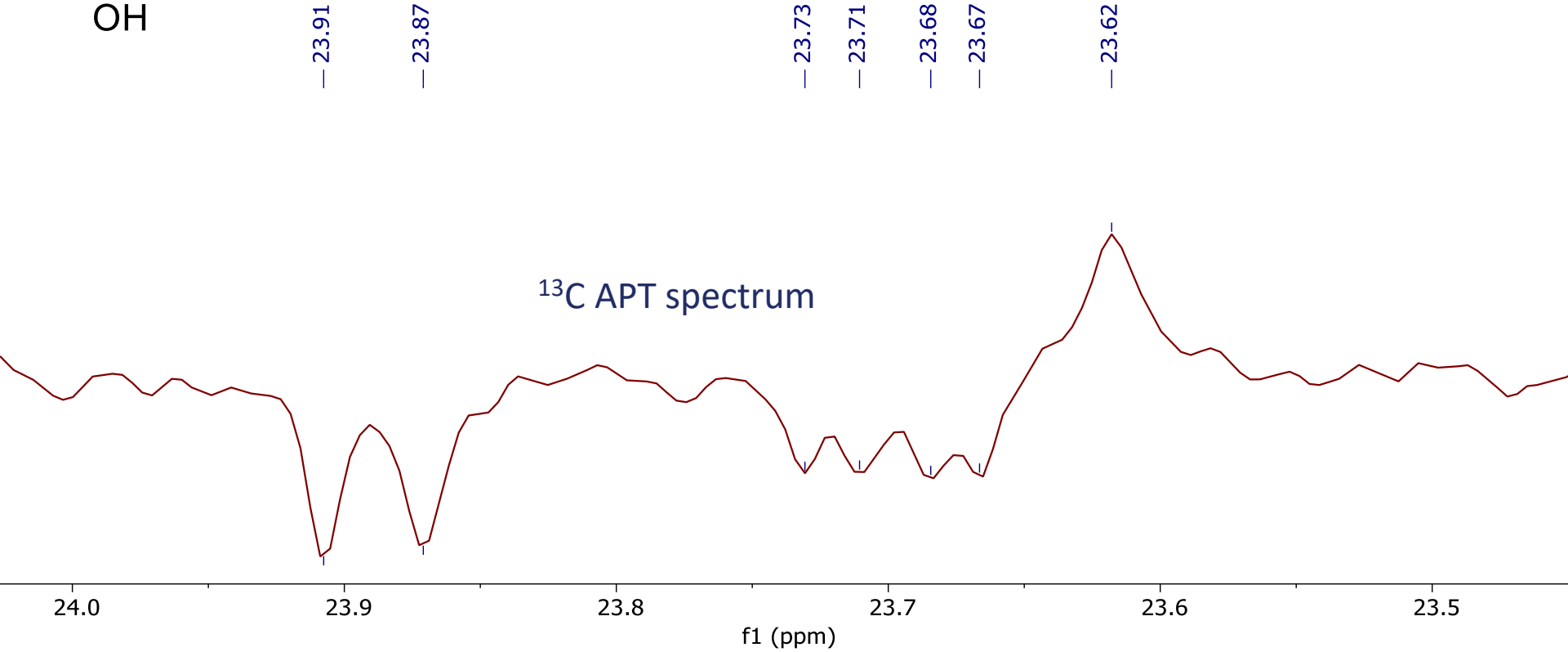




Topicity

- Methyl groups in diisopropyl esters are diastereotopic
- Expect four doublets in ^{13}C spectrum (coupling with phosphorus)





Workshops?

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- Would you like to attend hands-on workshops?

  Tell us!

  dracinsky@uochb.cas.cz or any member of NMR Spectroscopy group