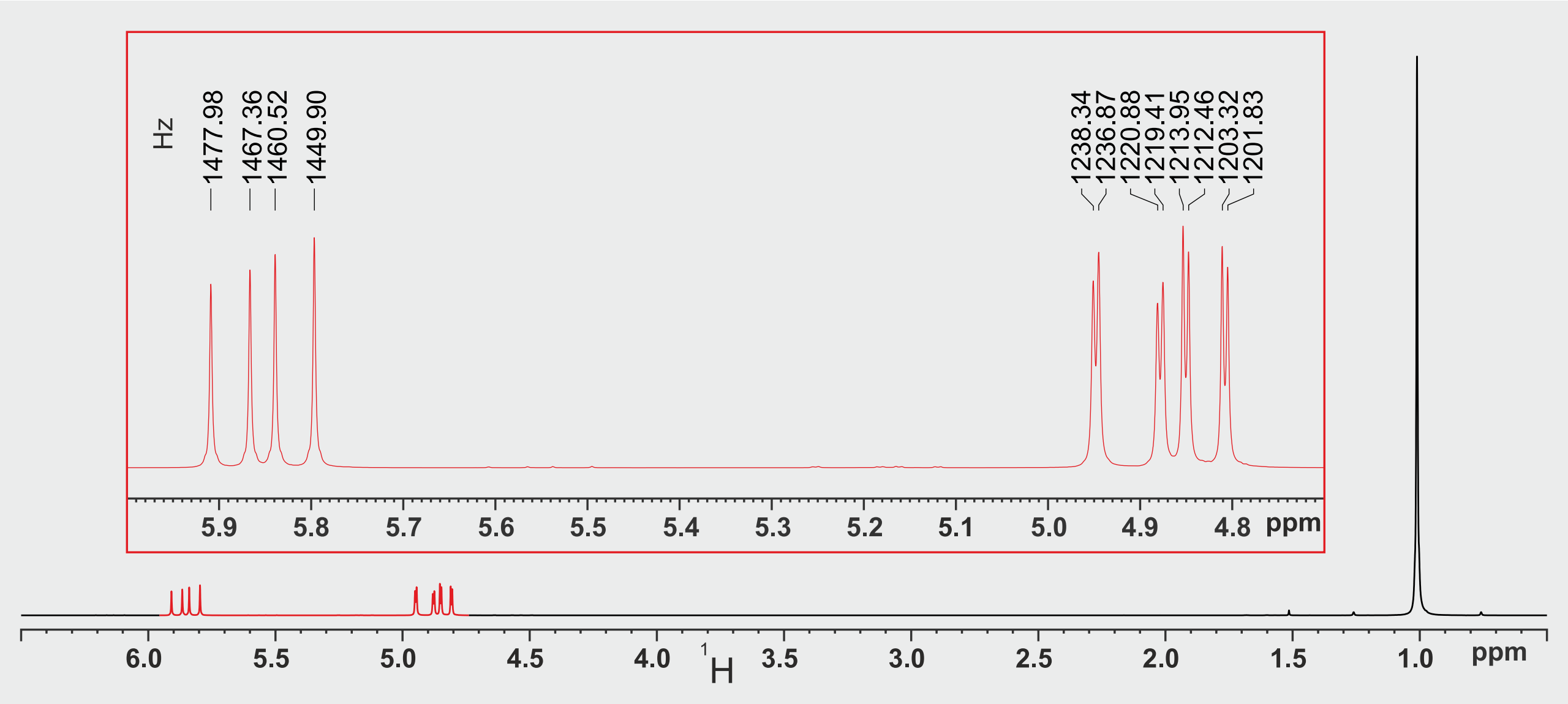
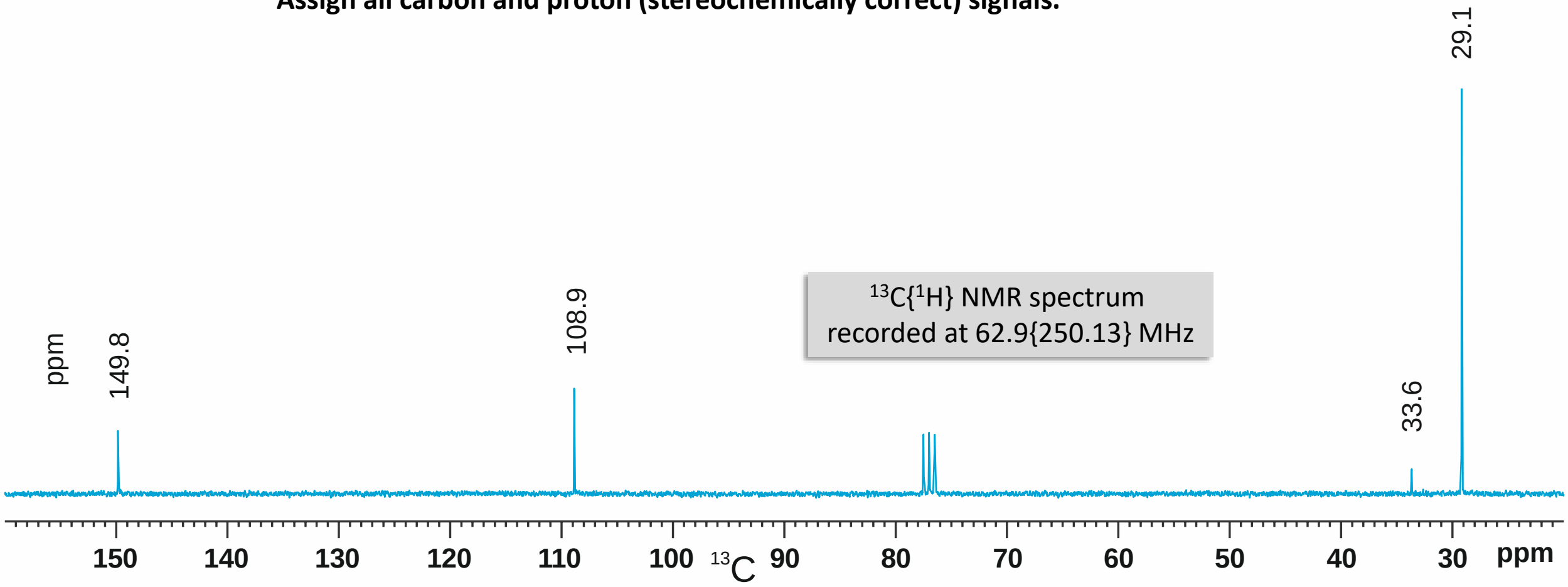
Exercise plus Solution – Quick overview

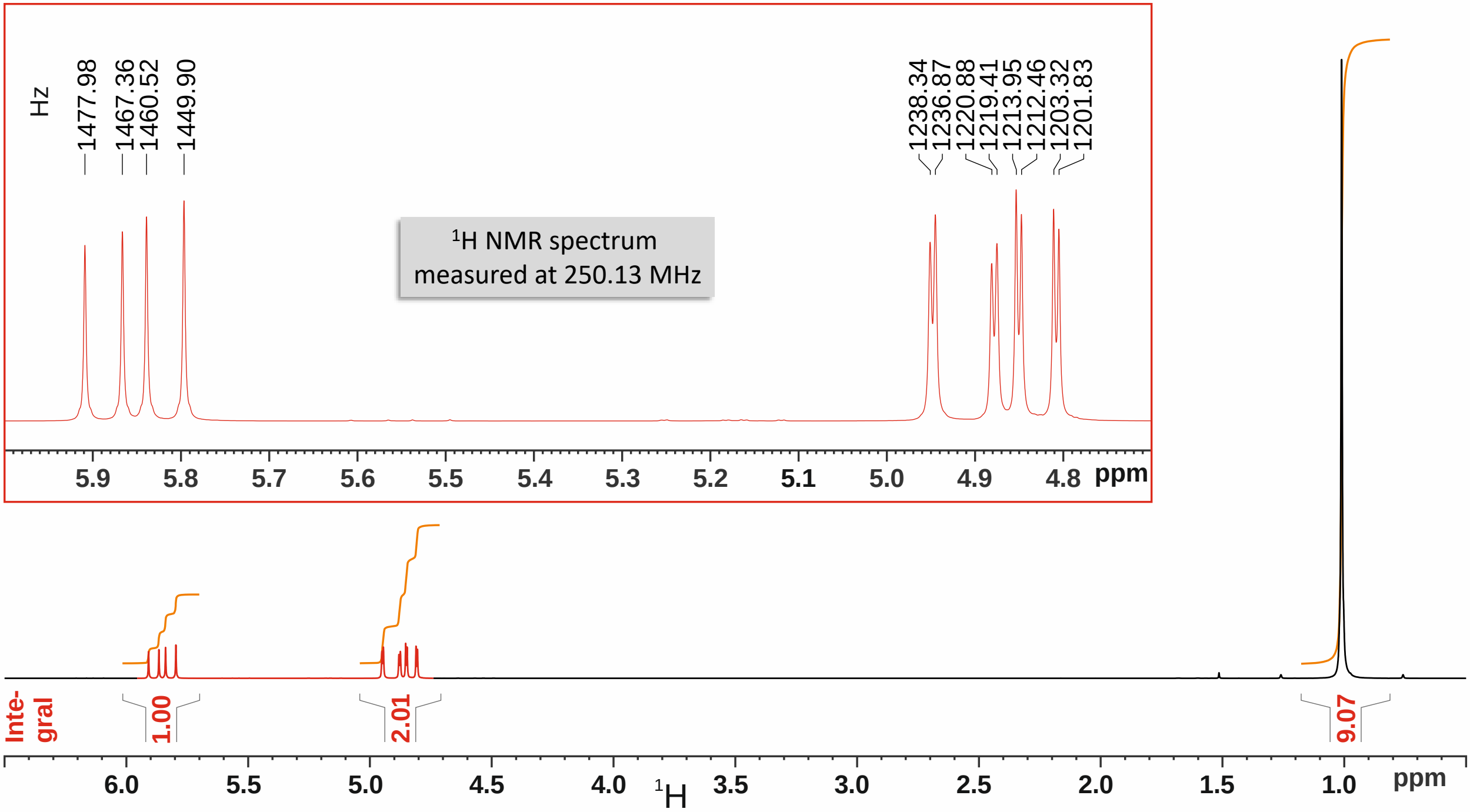
It is recommended to use this version only for a quick overview of the NMR challenge. All animations of the PowerPoint version are missing, under certain circumstances quality deficiencies may also occur.
The higher quality PowerPoint files are freely available for download at any time.



C_6H_{12} measured in $CDCl_3$

Deduce the structure and measure three homonuclear coupling constants.
Assign all carbon and proton (stereochemically correct) signals.

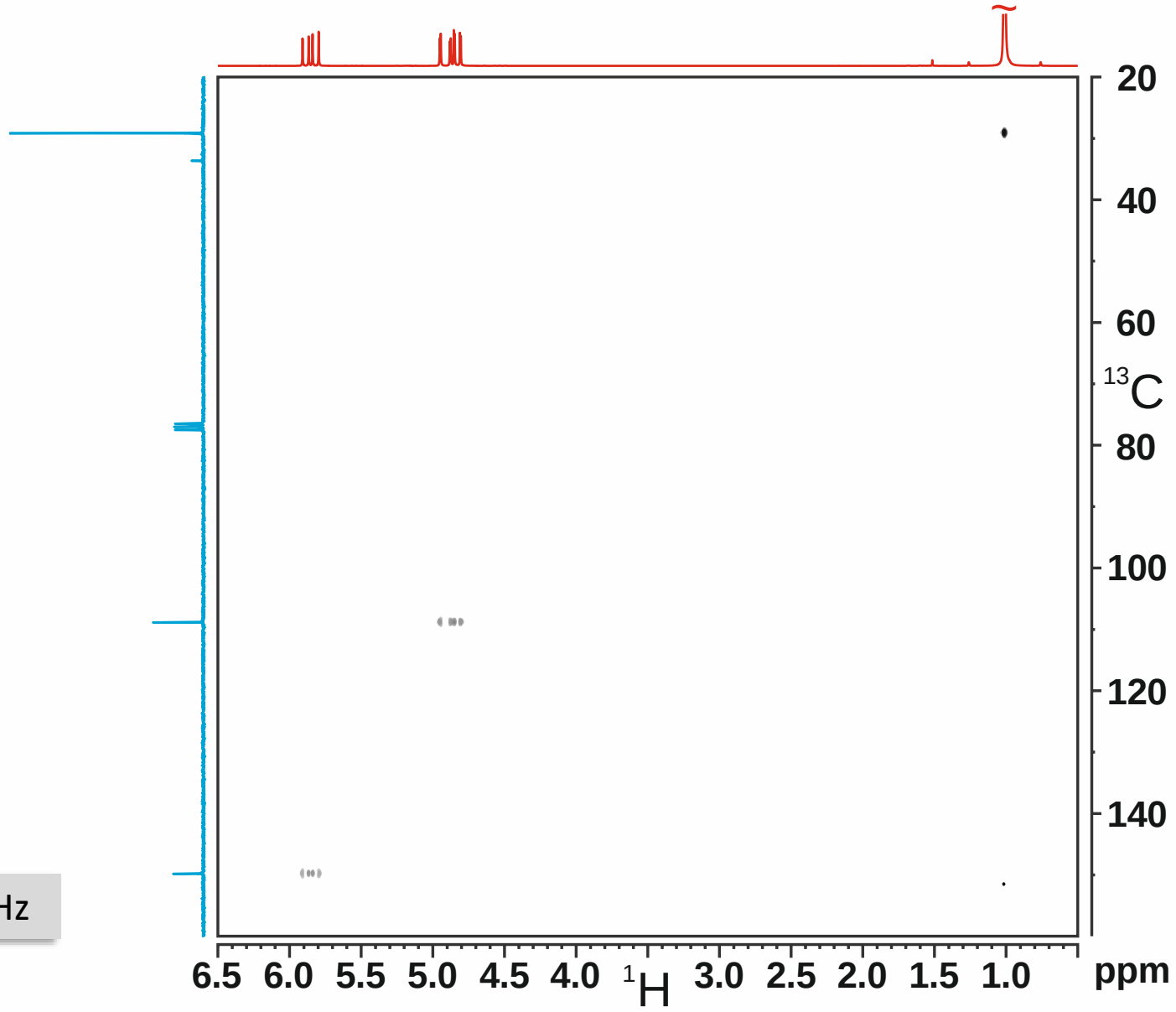



Hz
1477.98
1467.36
1460.52
1449.90
1238.34
1236.87
1220.88
1219.41
1213.95
1212.46
1203.32
1201.83
^{1}H NMR spectrum
measured at 250.13 MHz
5.9
5.8
5.7
5.6
5.5
5.4
5.3
5.2
5.1
5.0
4.9
4.8
ppm
Inte-
gral
1.00
2.01
9.07
6.0
5.5
5.0
4.5
4.0
^{1}H
3.5
3.0
2.5
2.0
1.5
1.0
ppm

Hints

(1) Always use the HSQC to get the building blocks.

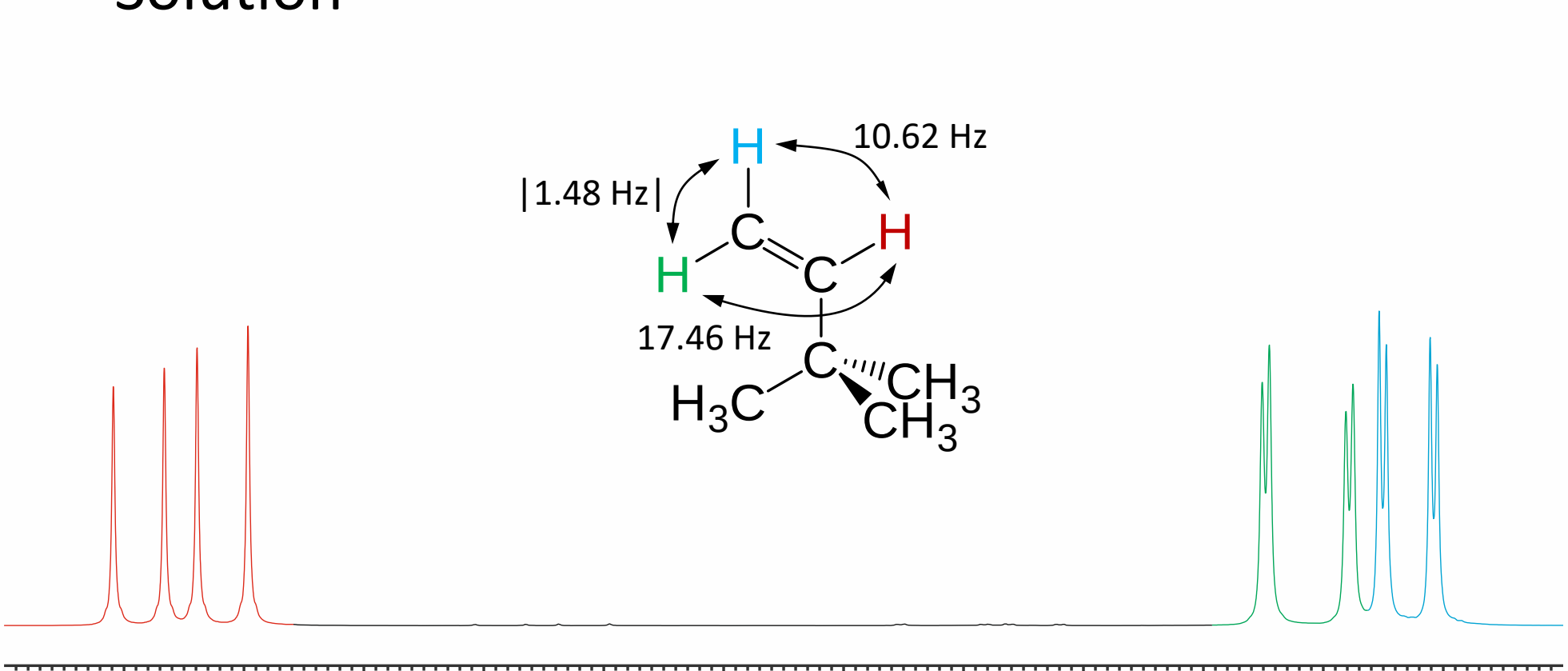
(2) It‘s a little bit tricky to separate the ^{1}H signals at 4.9 ppm. You might try to use either the integral or the „roof effect“ as a first attempt.



H,C-HSQC @ 250.13/62.9 MHz

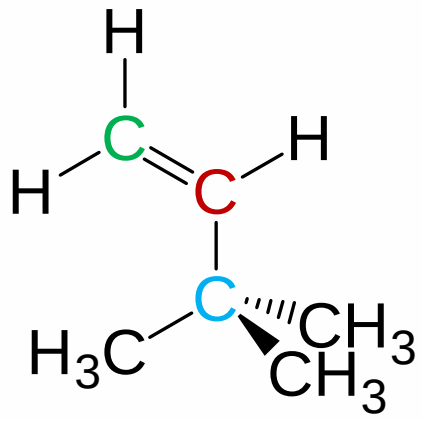
Solution

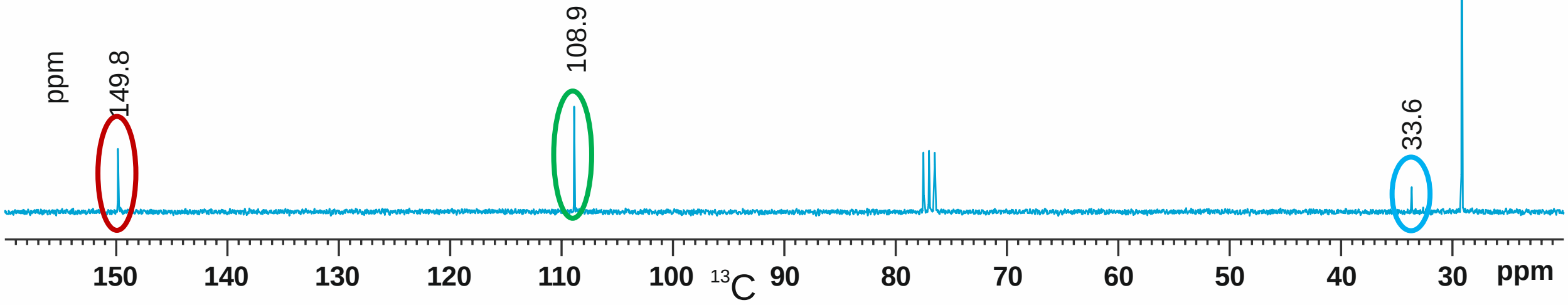
H
10.62 Hz
|1.48 Hz|
C
H
H
C
17.46 Hz
C
H3C
CH3
CH3


5.9
5.8
5.7
5.6
5.5
5.4
5.3
5.2
5.1
5.0
4.9
4.8
ppm

6.0
5.5
5.0
4.5
4.0
1H
3.5
3.0
2.5
2.0
1.5
1.0
ppm

There is no step by step solution available so far.





Contributions

Spectrometer time

TU Munich

Measurements

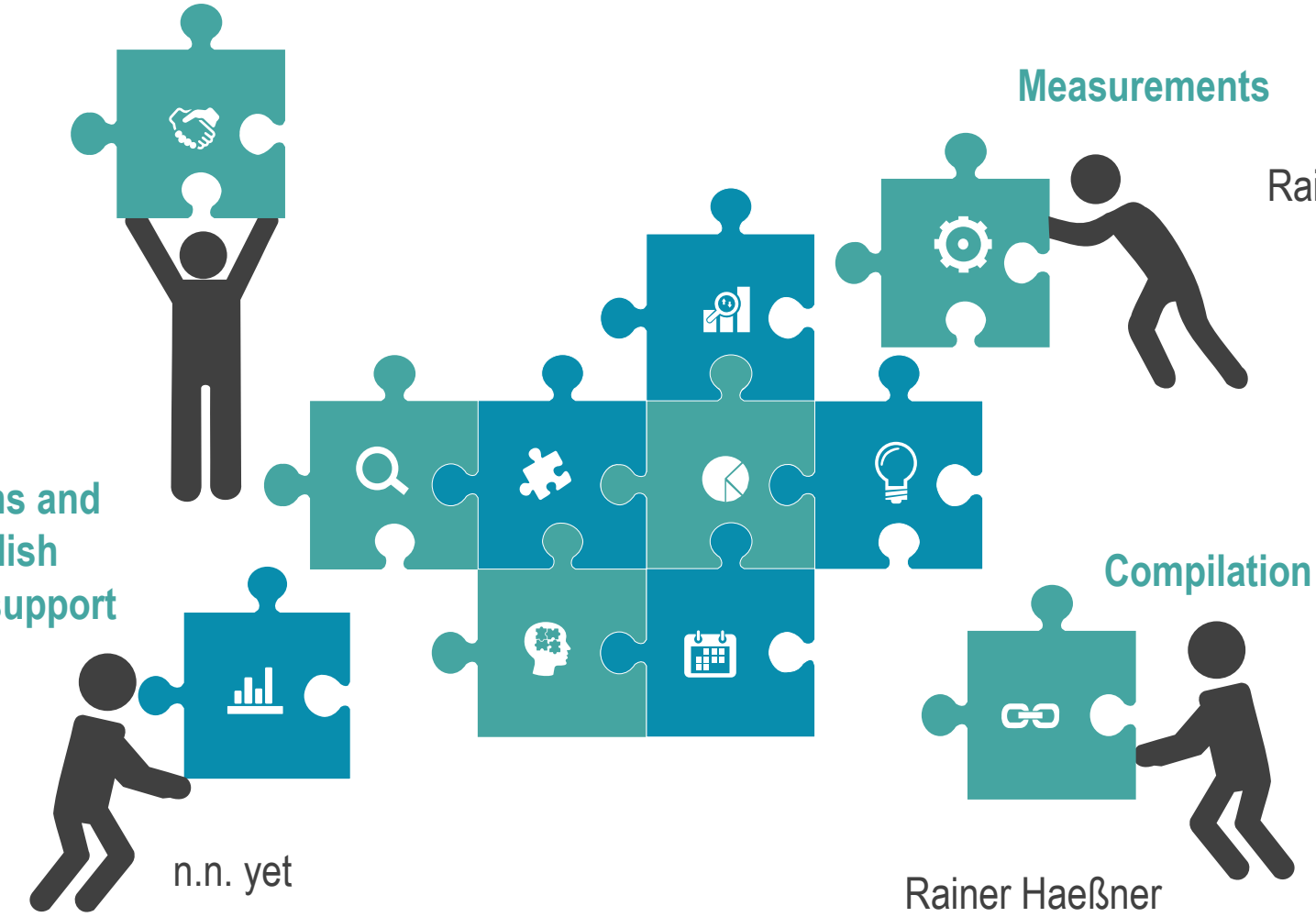
Rainer Haeßner

Discussions and native English language support

n.n. yet

Compilation

Rainer Haeßner



More exercises …