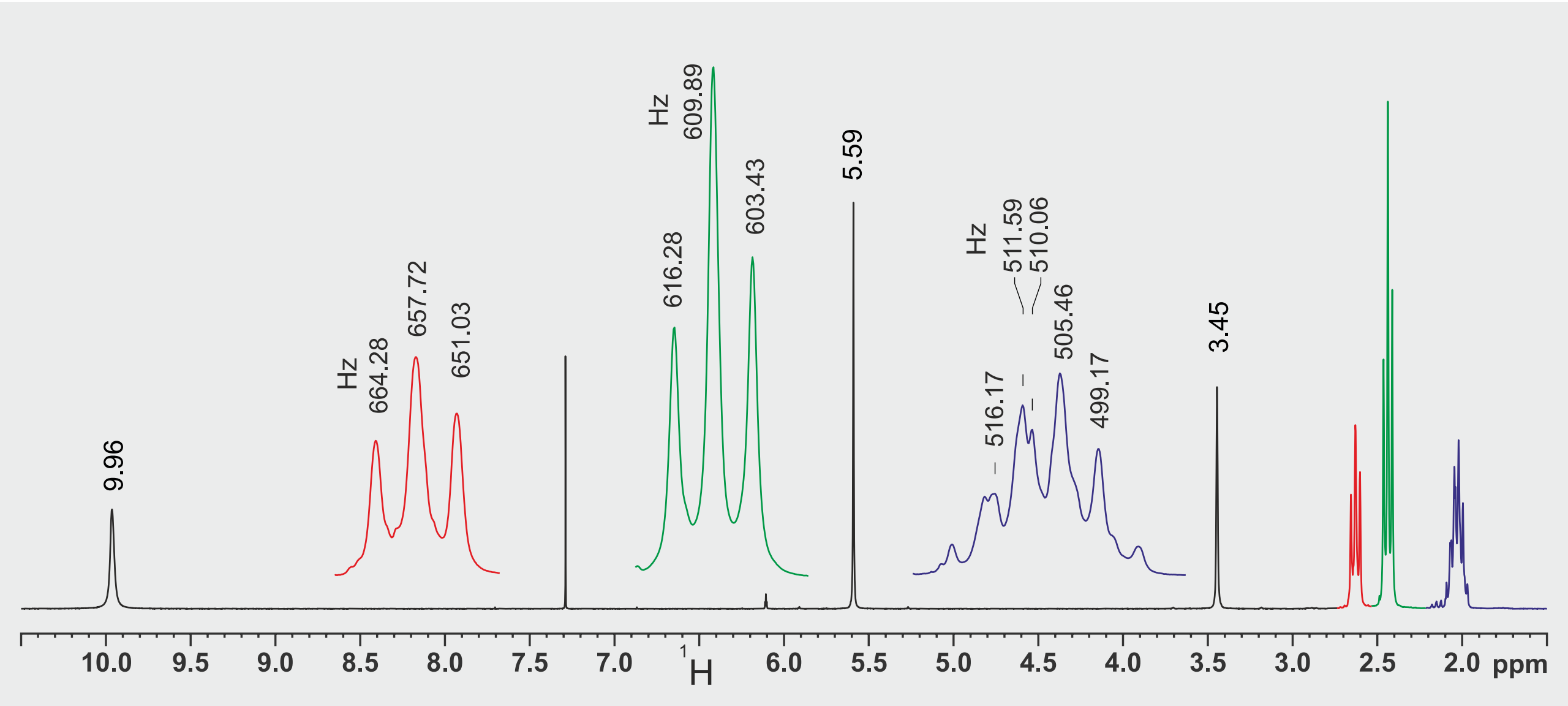
Exercise plus Solution – Quick overview

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.

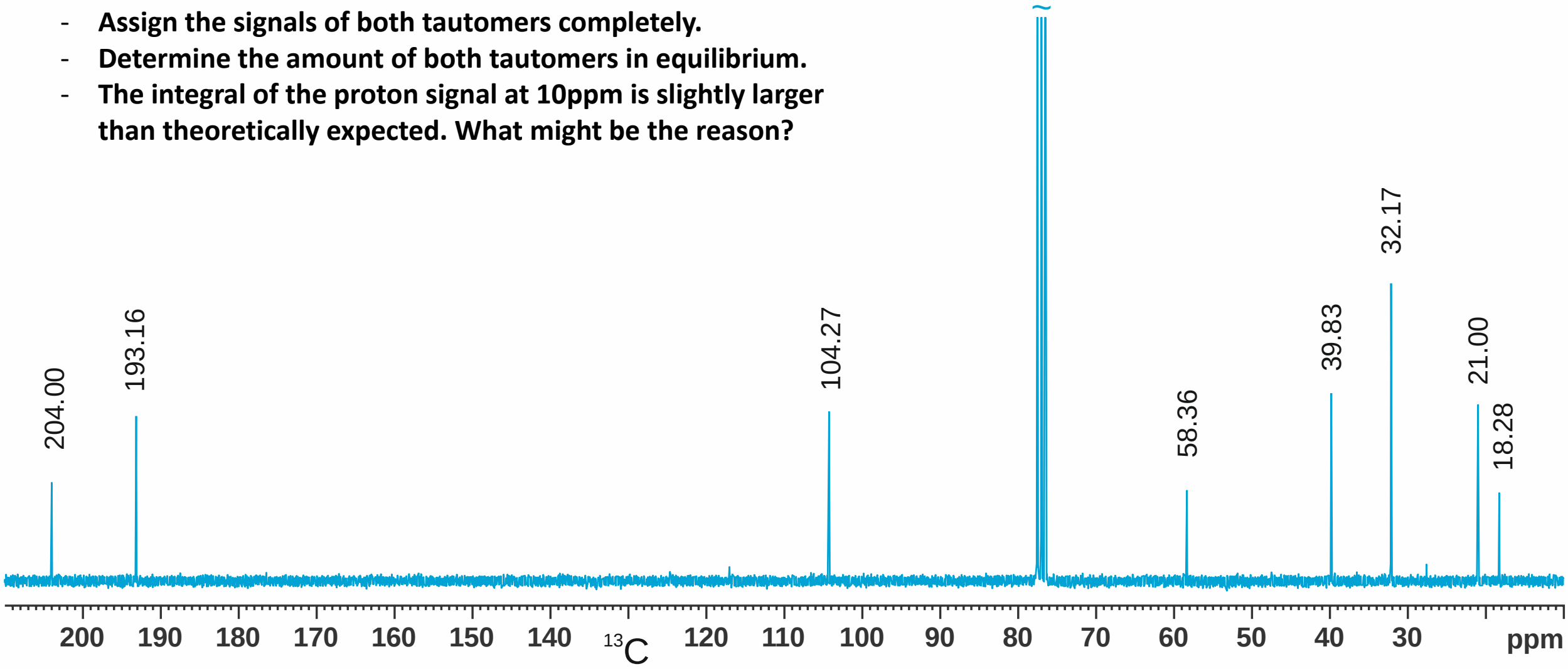


1,3-Cyclohexadion measured in $CDCl_3$

1,3-cyclohexadione exists in equilibrium with its enol form..

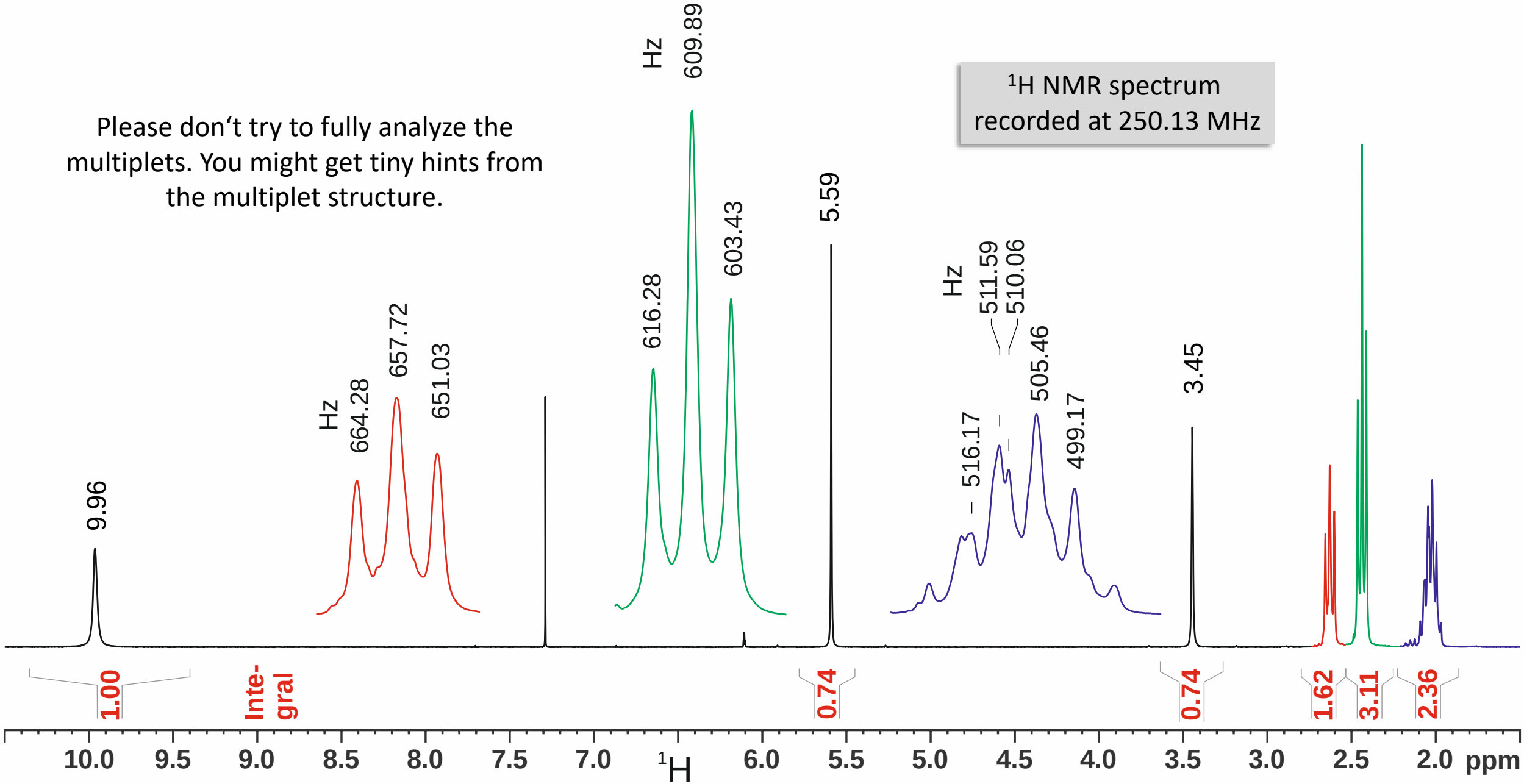
- **Assign the signals of both tautomers completely.**
- **Determine the amount of both tautomers in equilibrium.**
- **The integral of the proton signal at 10ppm is slightly larger than theoretically expected. What might be the reason?**

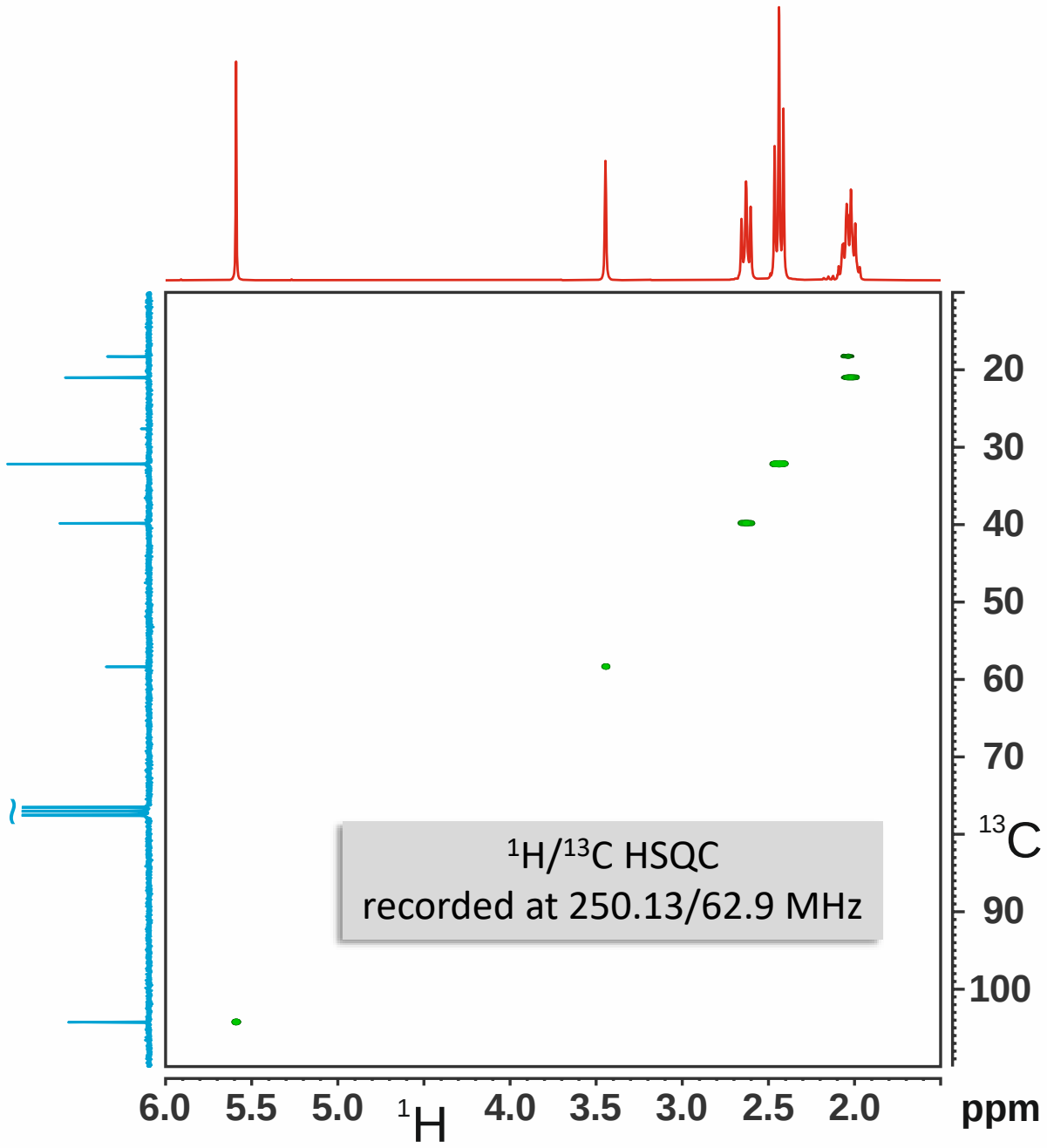
$^{13}C\{^{1}H\}$ NMR spectrum measured at 62.9{250.13} MHz

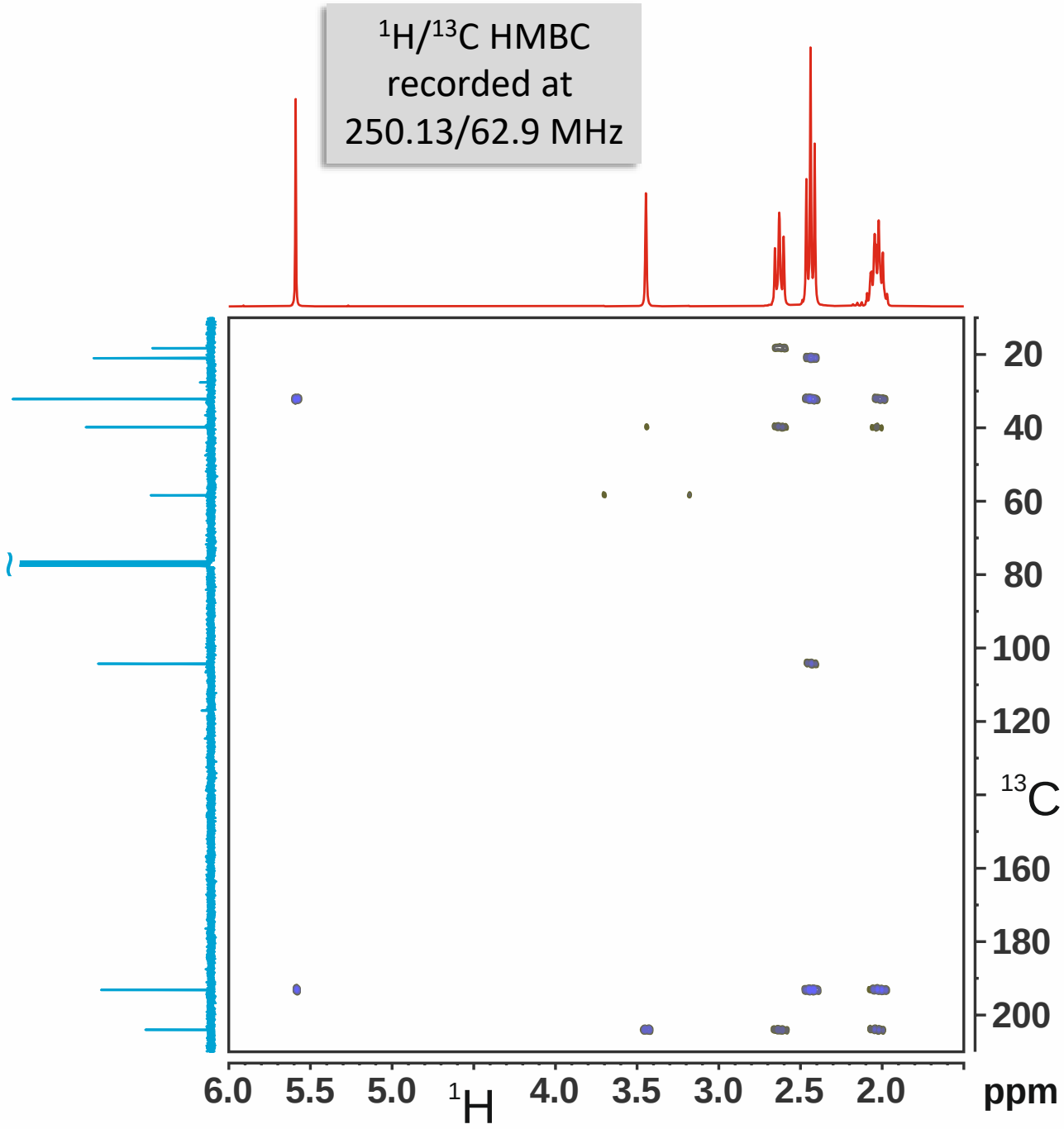


Please don‘t try to fully analyze the multiplets. You might get tiny hints from the multiplet structure.

^{1}H NMR spectrum recorded at 250.13 MHz

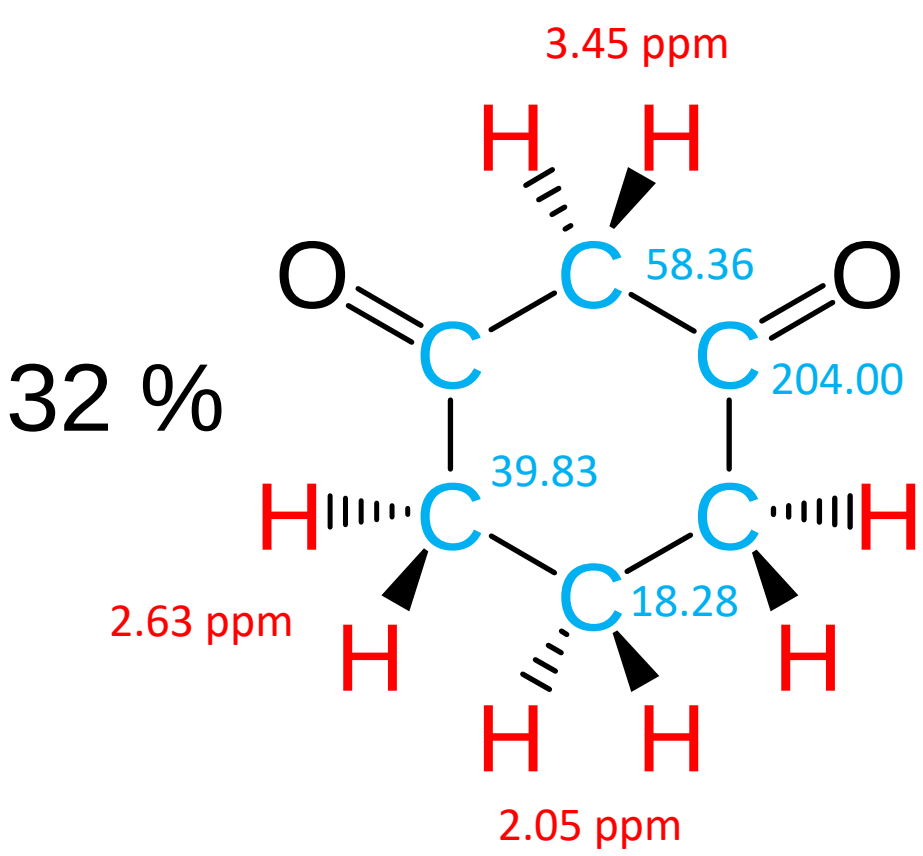


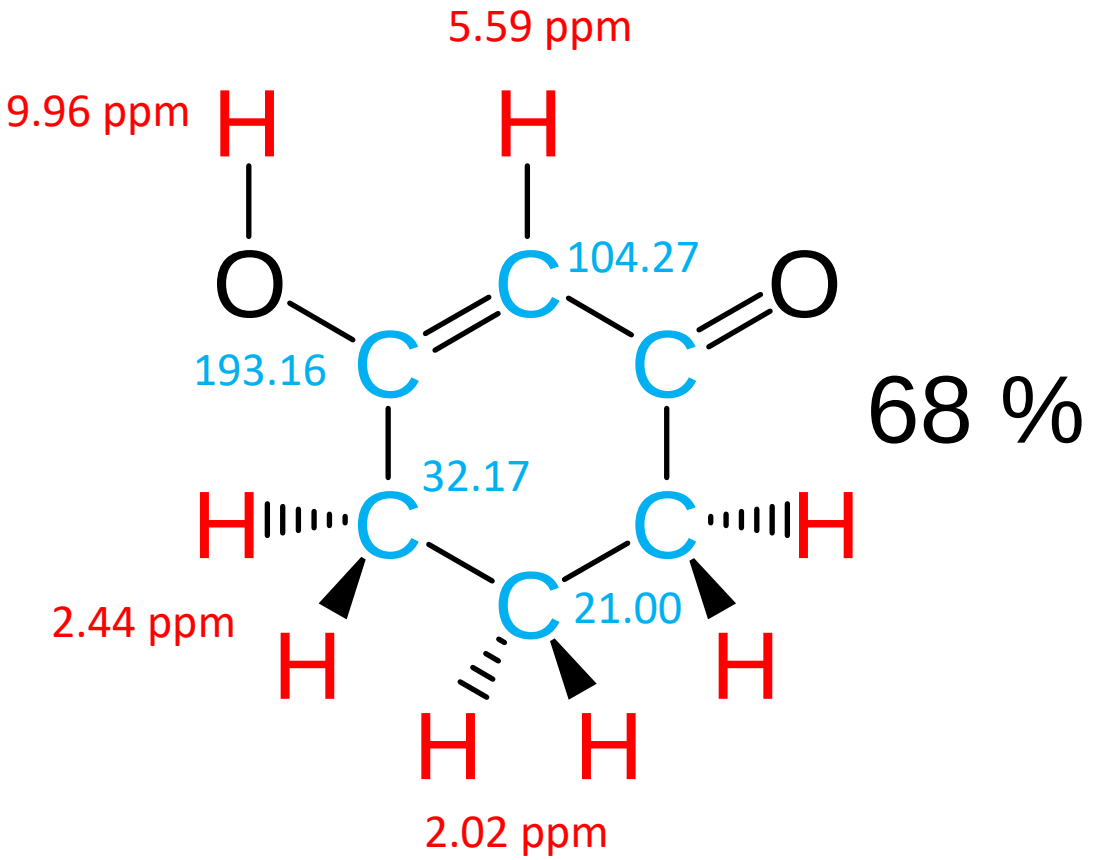

^{1}H/^{13}C HSQC
recorded at 250.13/62.9 MHz
20
30
40
50
60
70
90
100
^{13}C
6.0
5.5
5.0
^{1}H
4.0
3.5
3.0
2.5
2.0
ppm


^{1}H/^{13}C HMBC
recorded at
250.13/62.9 MHz
20
40
60
80
100
120
^{13}C
160
180
200
6.0
5.5
5.0
^{1}H
4.0
3.5
3.0
2.5
2.0
ppm

Solution at a glance

There is no step by step solution available so far.





Contributions

Spectrometer time

TU Munich

Measurements

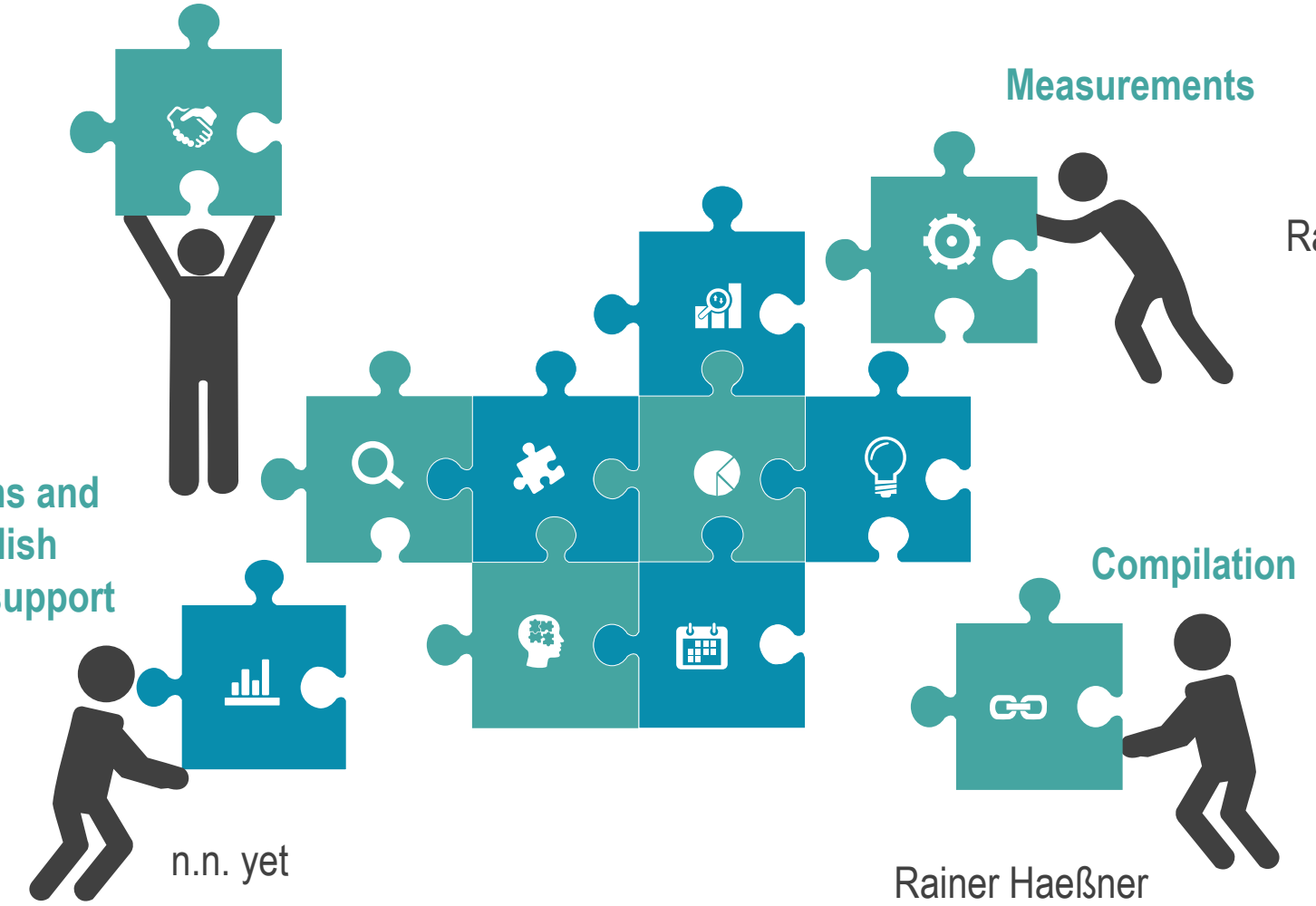
Rainer Haeßner

Discussions and native English language support

n.n. yet

Compilation

Rainer Haeßner



More exercises …