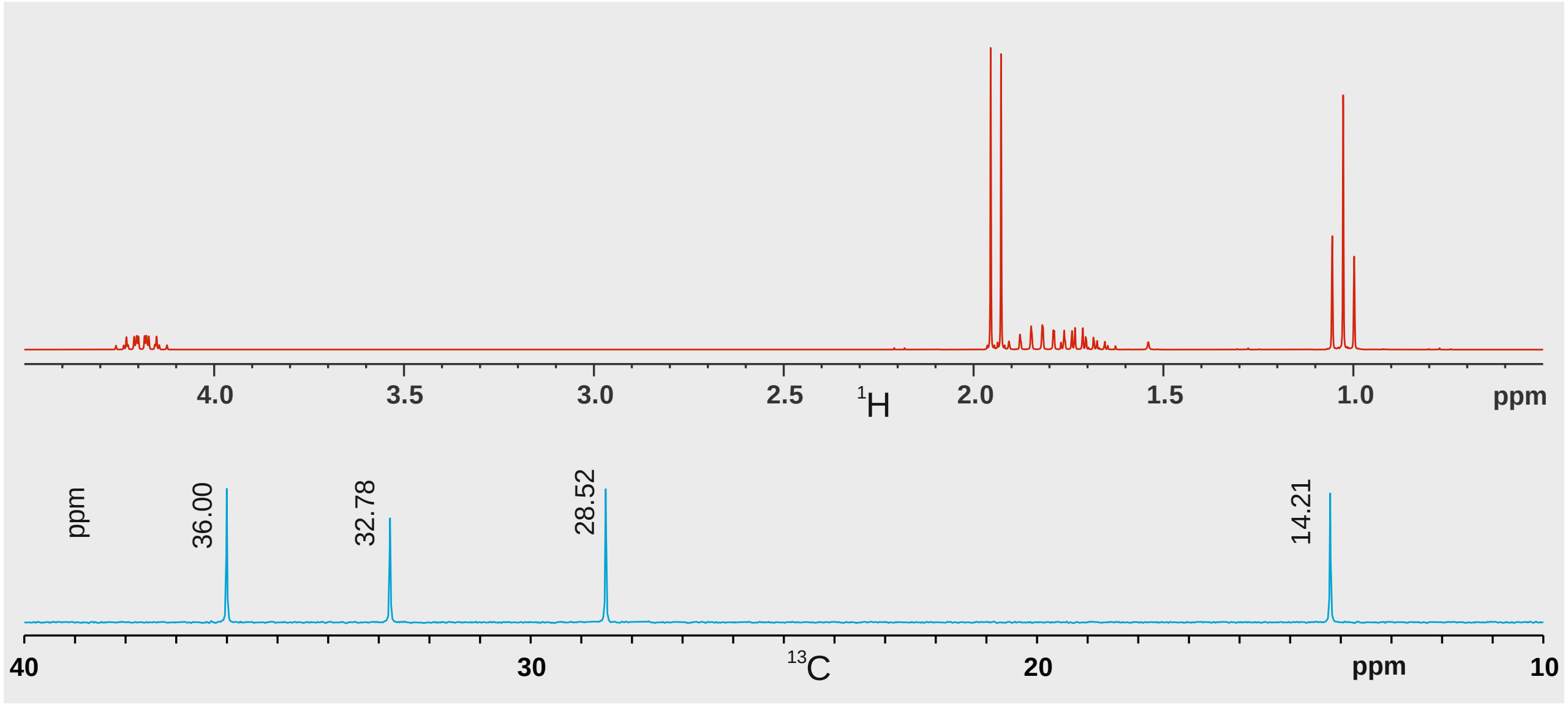
Exercise plus Solution – Quick overview

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.

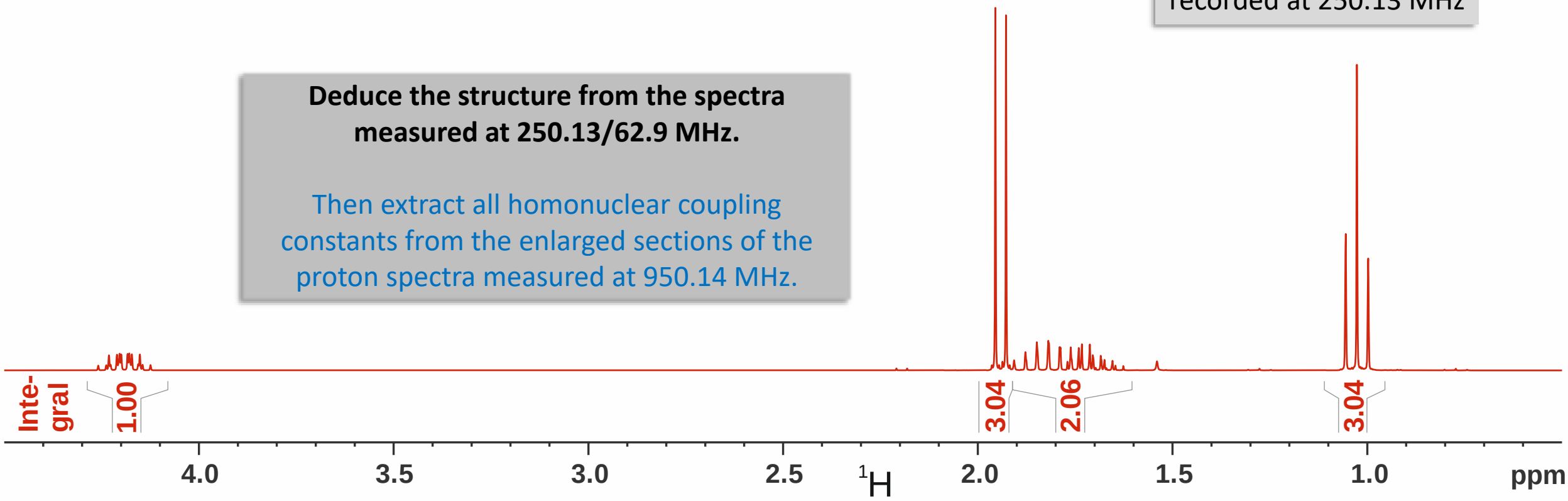


C_4H_9I in $CDCl_3$

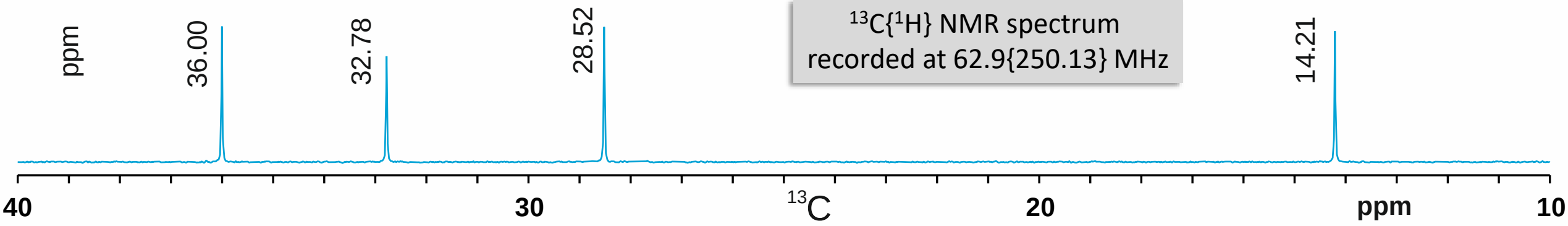
Deduce the structure from the spectra measured at 250.13/62.9 MHz.

Then extract all homonuclear coupling constants from the enlarged sections of the proton spectra measured at 950.14 MHz.

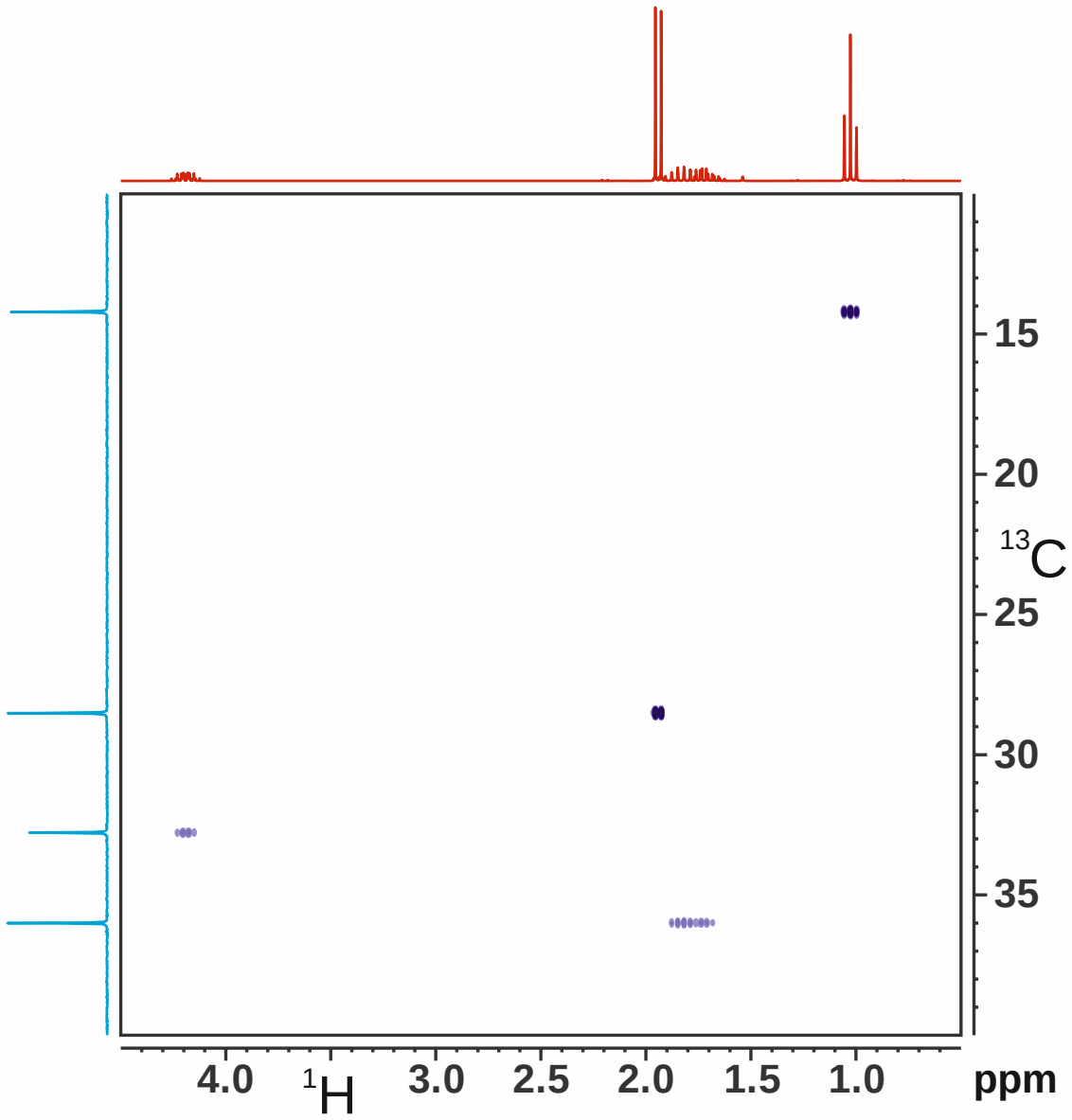
^{1}H NMR spectrum recorded at 250.13 MHz



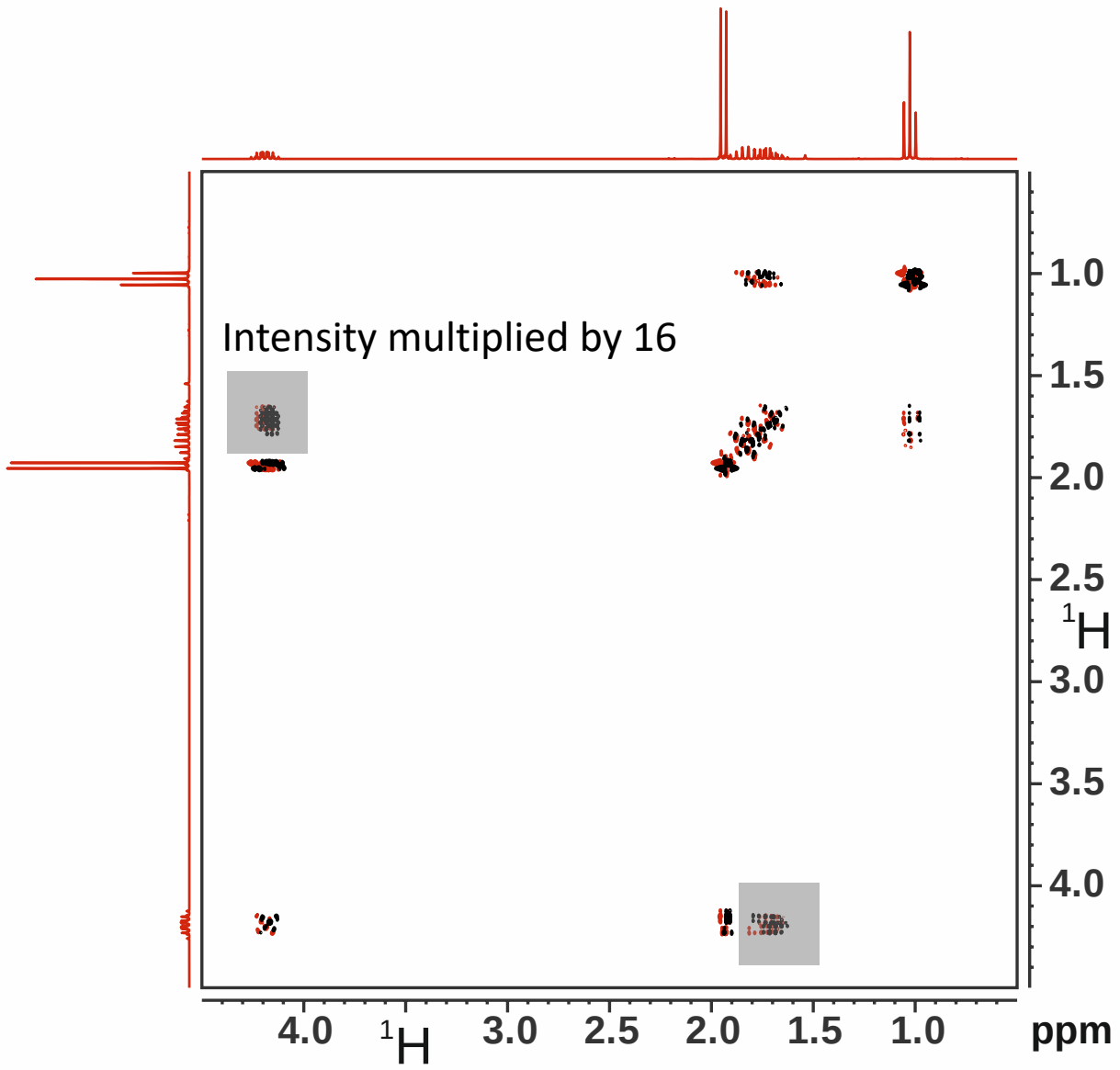
^{13}C{^{1}H} NMR spectrum recorded at 62.9{250.13} MHz

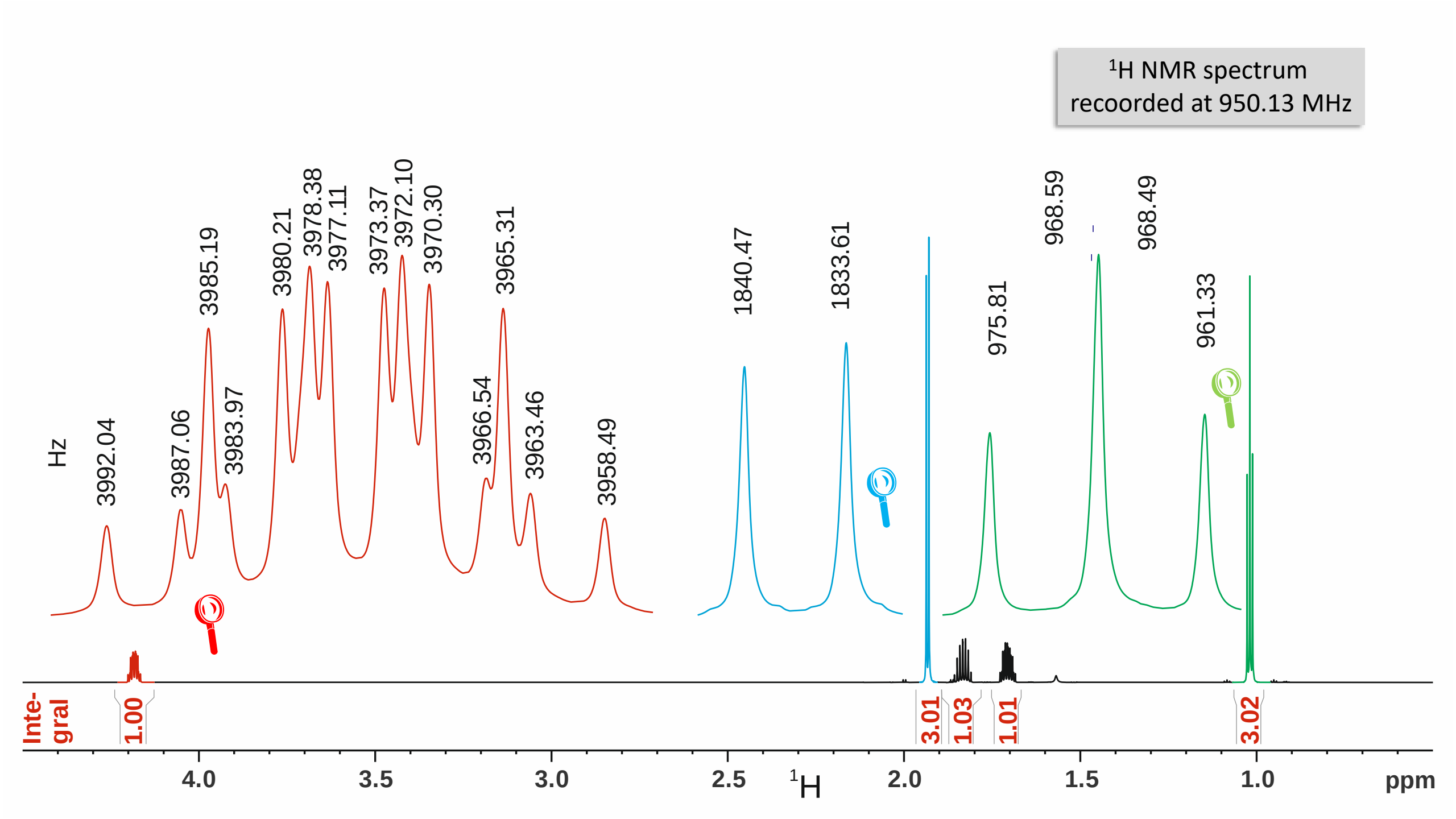


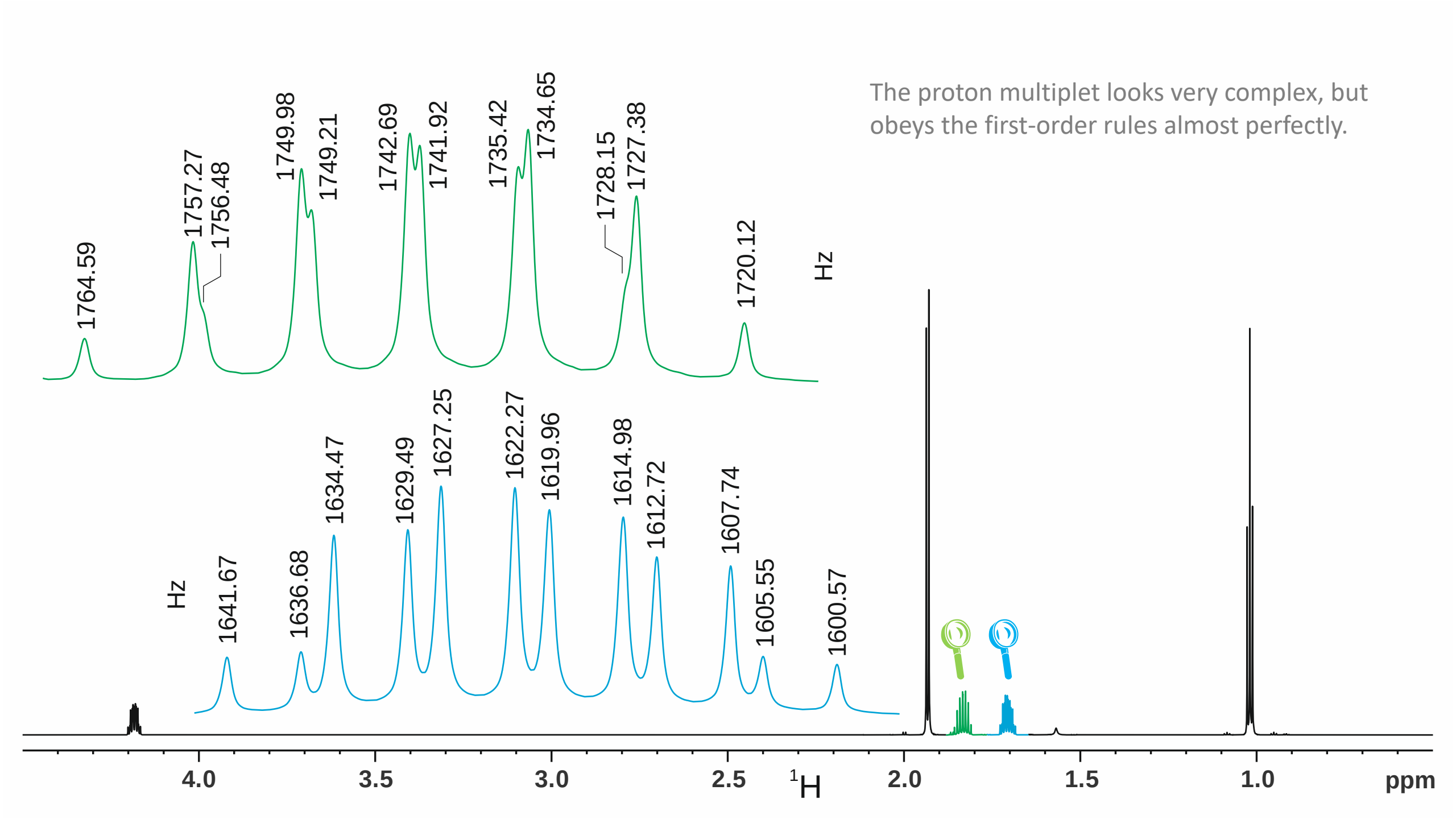
$^{1}H/^{13}C$ HSQC
recorded at 250.13/62.9 MHz



$^{1}H/^{1}H$ COSY
recorded at 250.13 MHz

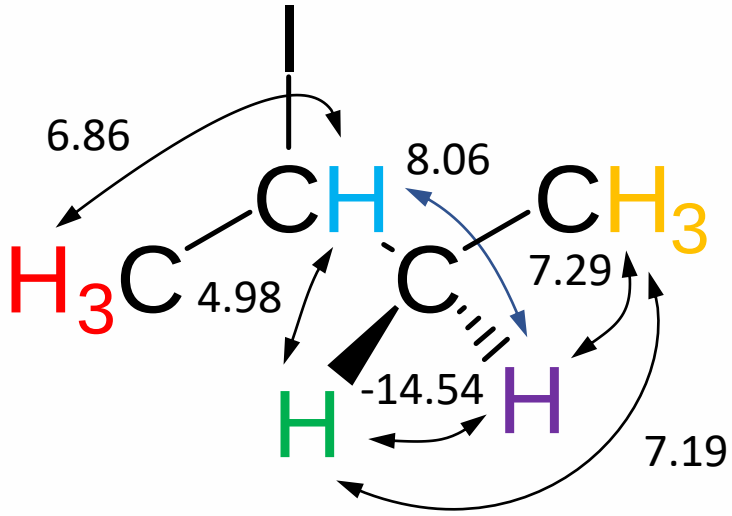



^{1}H NMR spectrum recoorded at 950.13 MHz
Hz
3992.04
3987.06
3985.19
3983.97
3980.21
3978.38
3977.11
3973.37
3972.10
3970.30
3966.54
3965.31
3963.46
3958.49
1840.47
1833.61
975.81
968.59
968.49
961.33
Inte-gral
1.00
3.01
1.03
1.01
3.02
4.0
3.5
3.0
2.5
2.0
1.5
1.0
^{1}H
ppm


The proton multiplet looks very complex, but obeys the first-order rules almost perfectly.
Hz
1764.59
1757.27
1756.48
1749.98
1749.21
1742.69
1741.92
1735.42
1734.65
1728.15
1727.38
1720.12
Hz
1641.67
1636.68
1634.47
1629.49
1627.25
1622.27
1619.96
1614.98
1612.72
1607.74
1605.55
1600.57
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
^{1}H

Solution at a glance

As soon as you see the green footprints on the problem icon, the step-by-step-solution is available



Contributions

Spectrometer time

TU Munich

Measurements

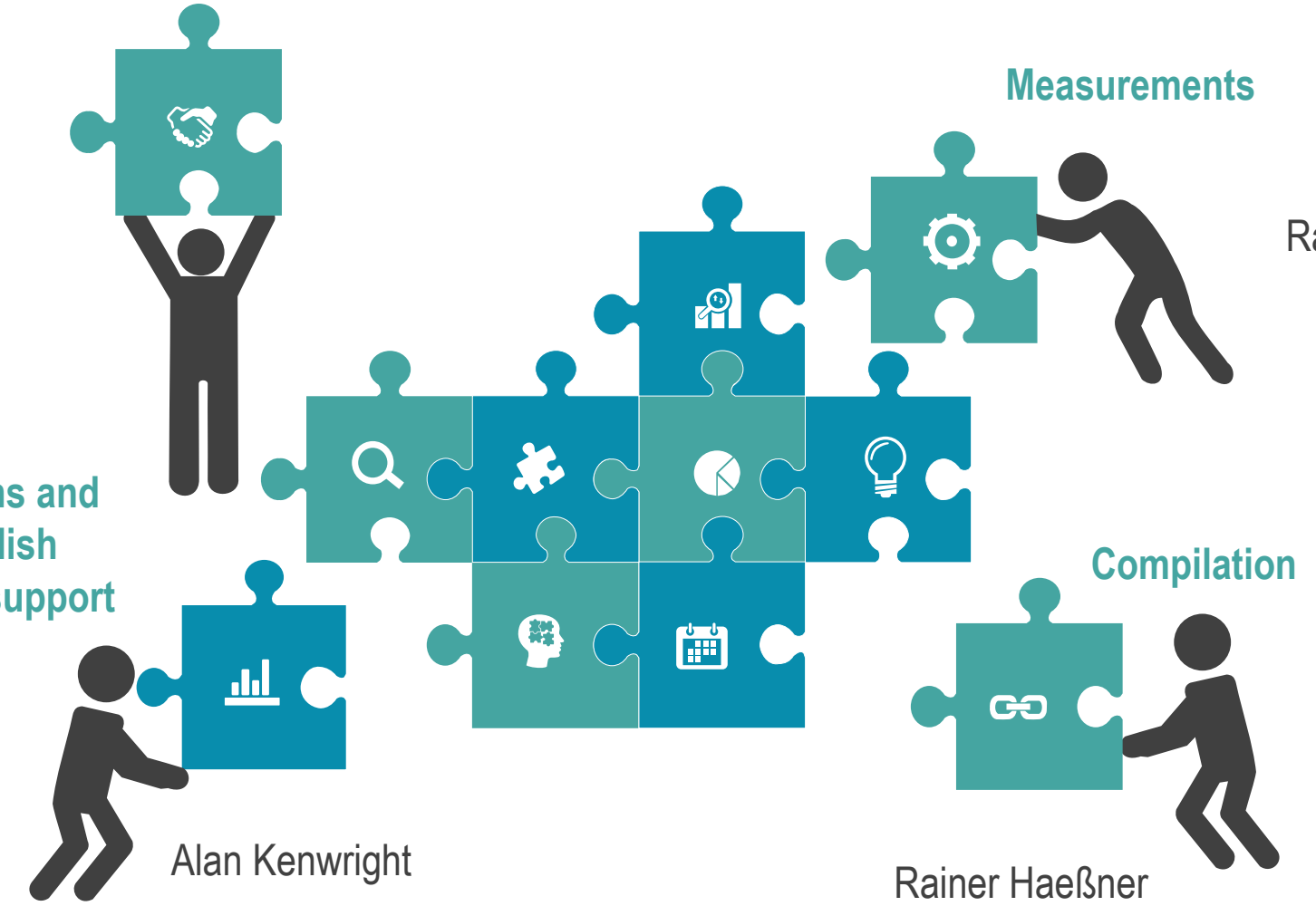
Rainer Haeßner

Discussions and native English language support

Alan Kenwright

Compilation

Rainer Haeßner



More exercises …