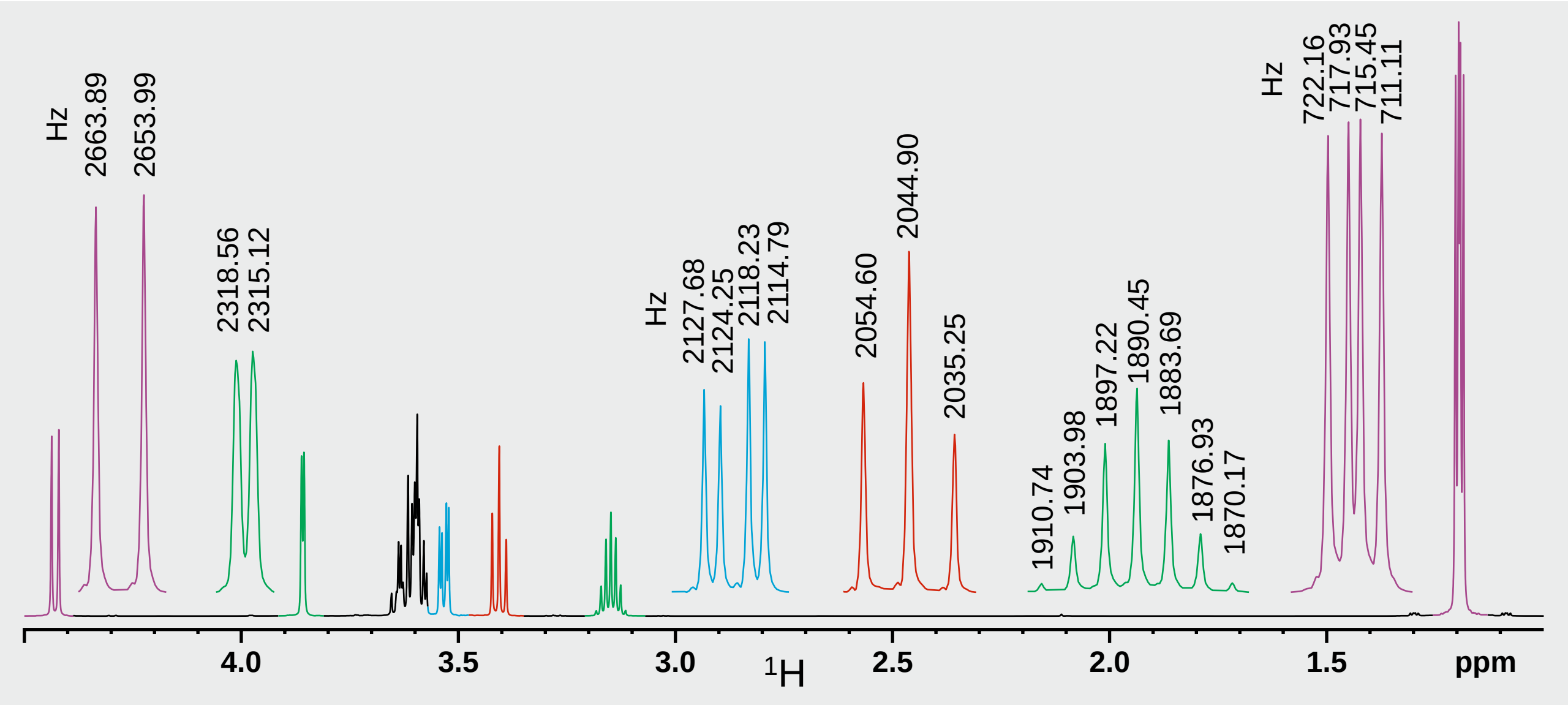
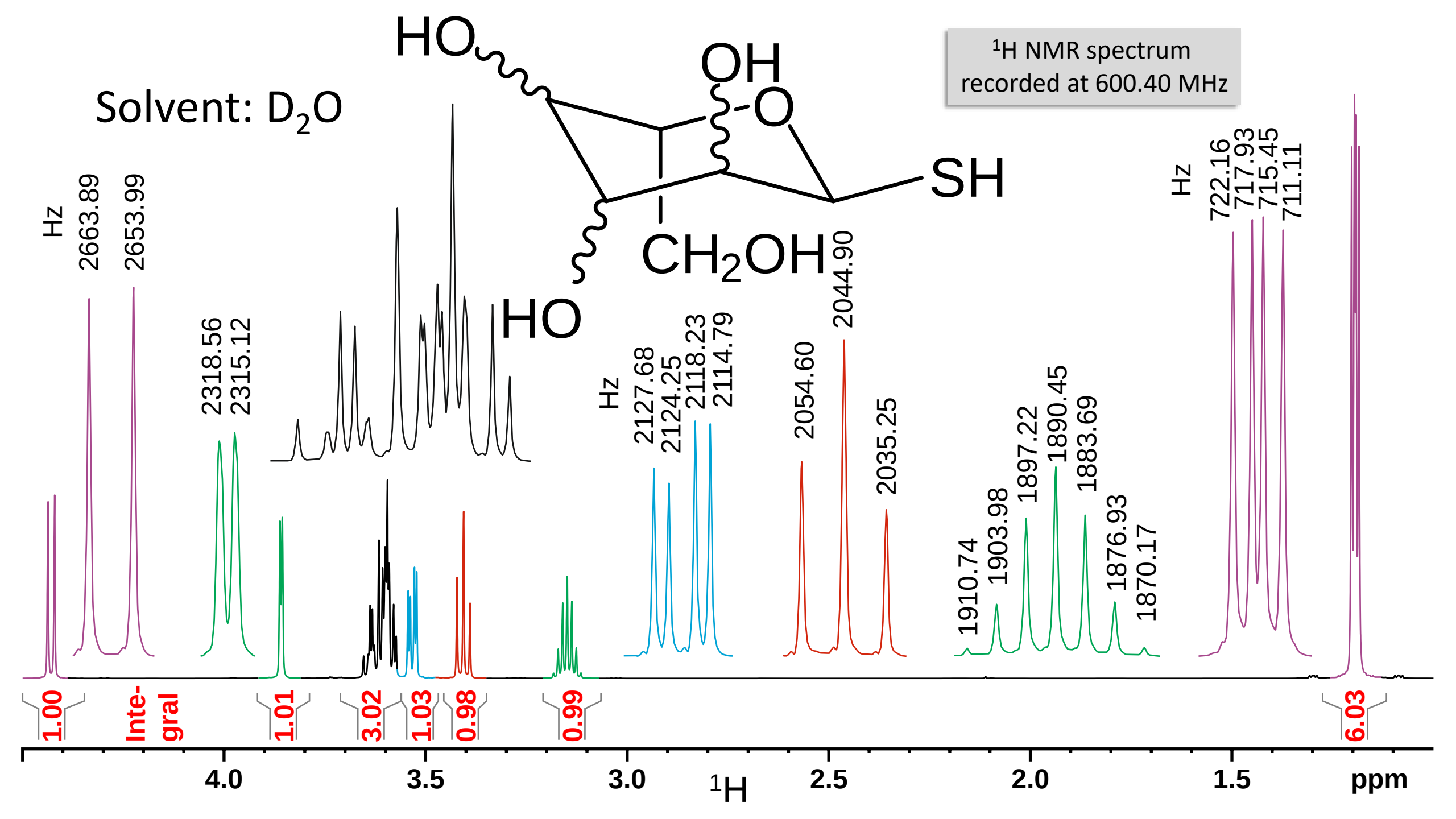
Exercise plus Solution – Quick overview

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.




Solvent: D2O
HO
OH
O
SH
CH2OH
HO
1H NMR spectrum recorded at 600.40 MHz
Hz
2663.89
2653.99
2318.56
2315.12
Hz
2127.68
2124.25
2118.23
2114.79
2054.60
2044.90
2035.25
1910.74
1903.98
1897.22
1890.45
1883.69
1876.93
1870.17
Hz
722.16
717.93
715.45
711.11
1.00
Inte-
gral
1.01
3.02
1.03
0.98
0.99
6.03
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1H

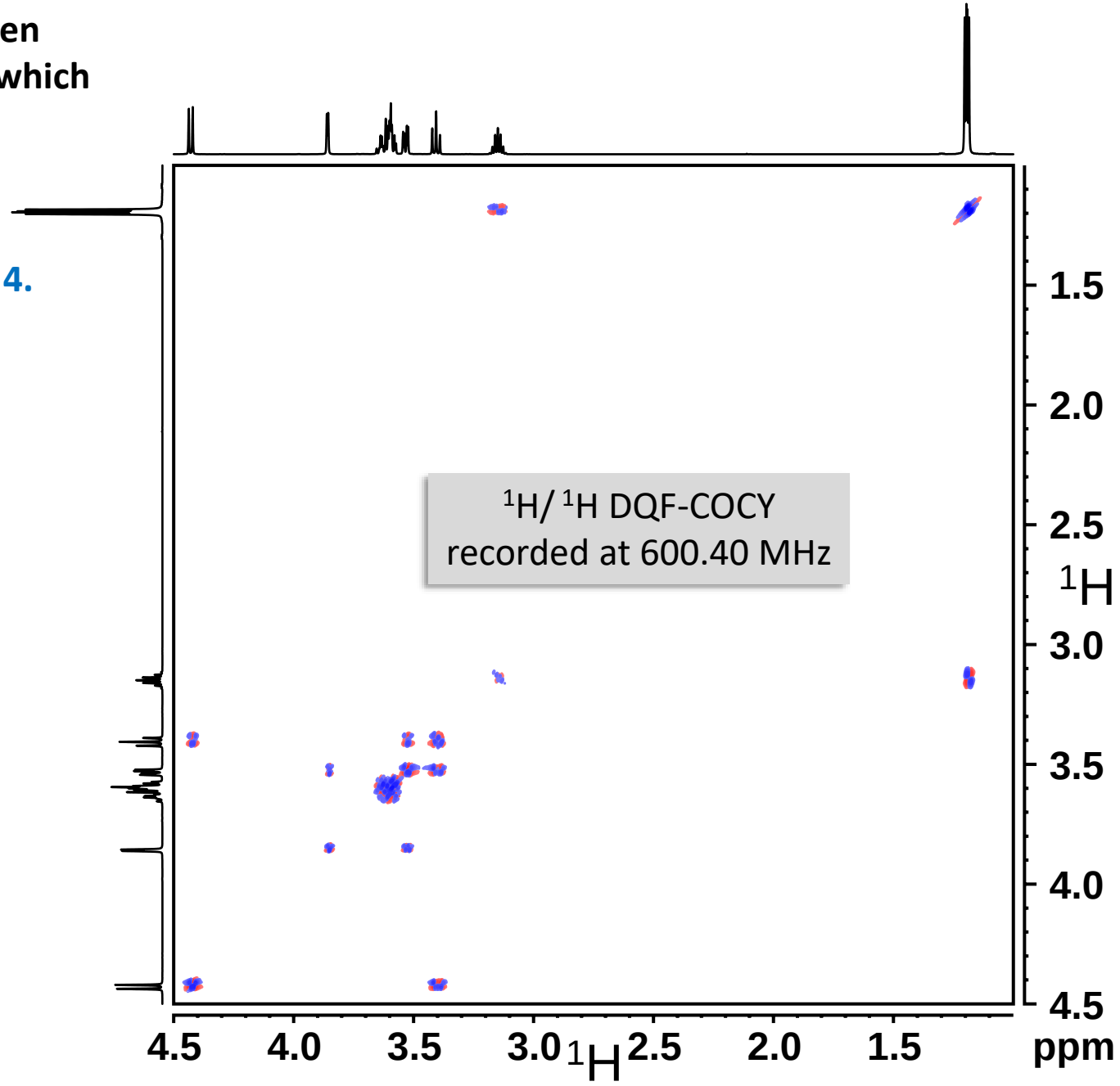
One of the exchangeable protons of the sugar has been substituted with an alkyl group. Which alkyl group is in which position?

Determine the stereochemistry in positions 2, 3 und 4.

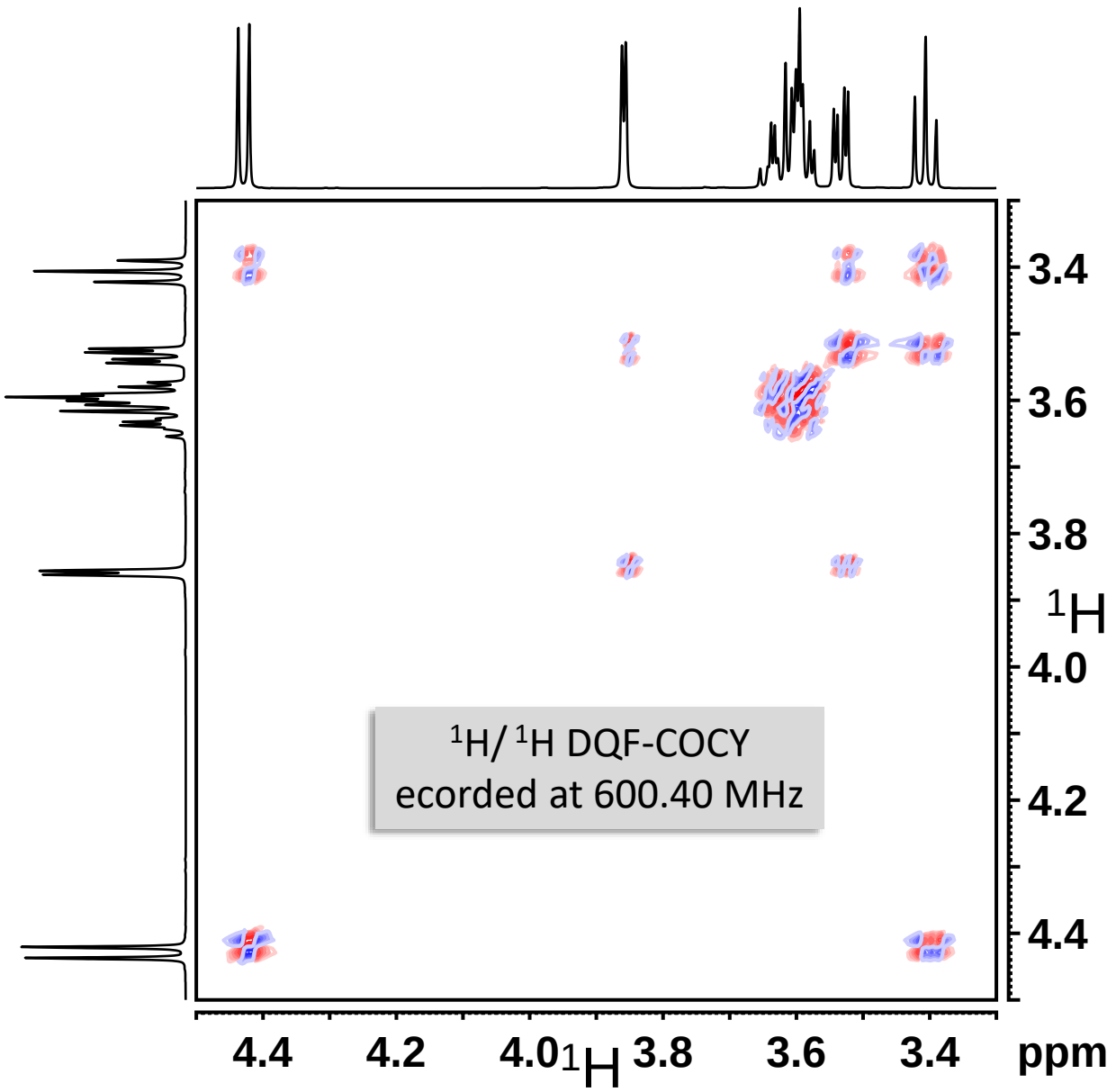
Assign all proton and carbon signals.

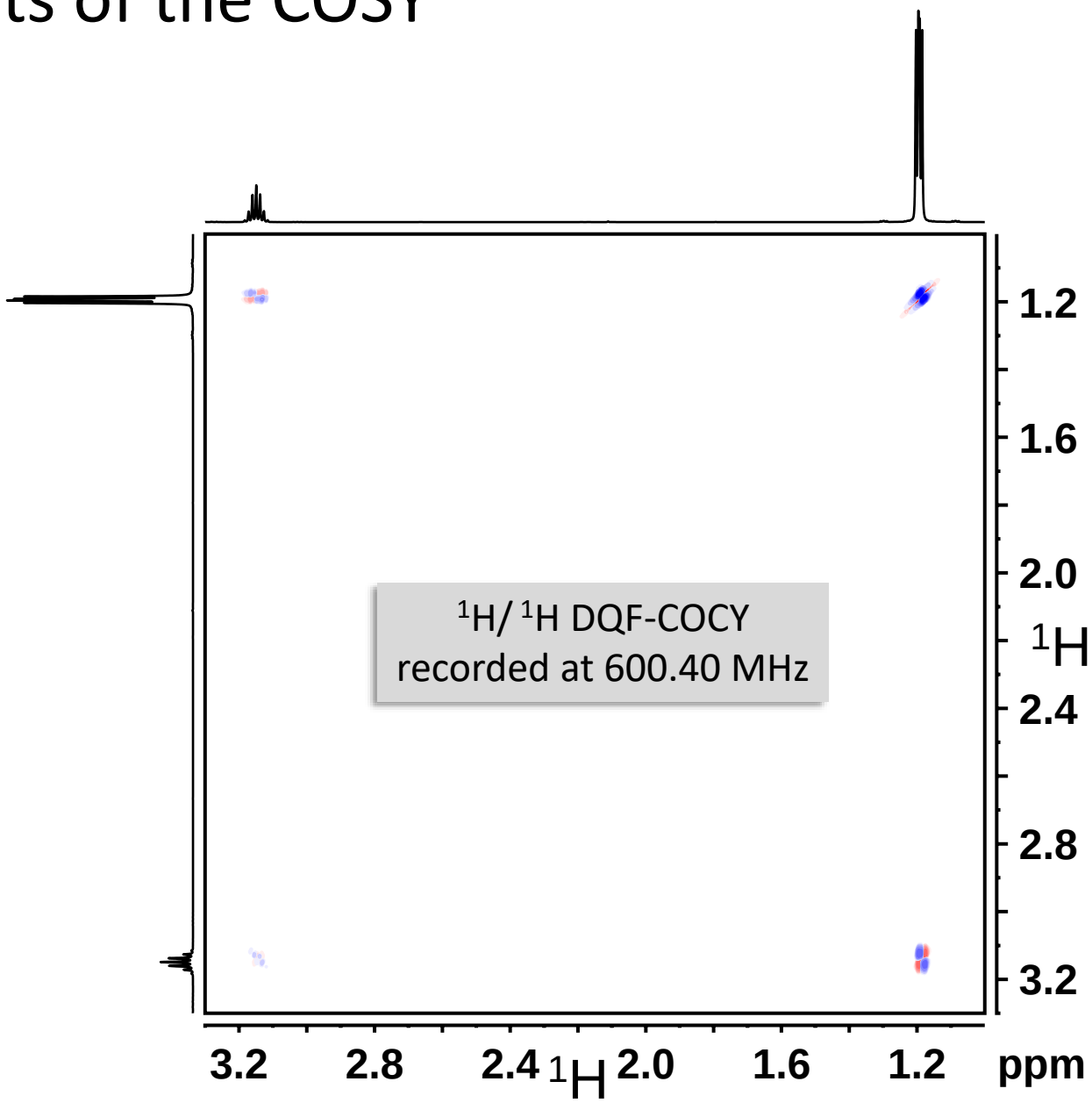
Name the spin systems.

Explain the multiplet structure at about 1.2 ppm.

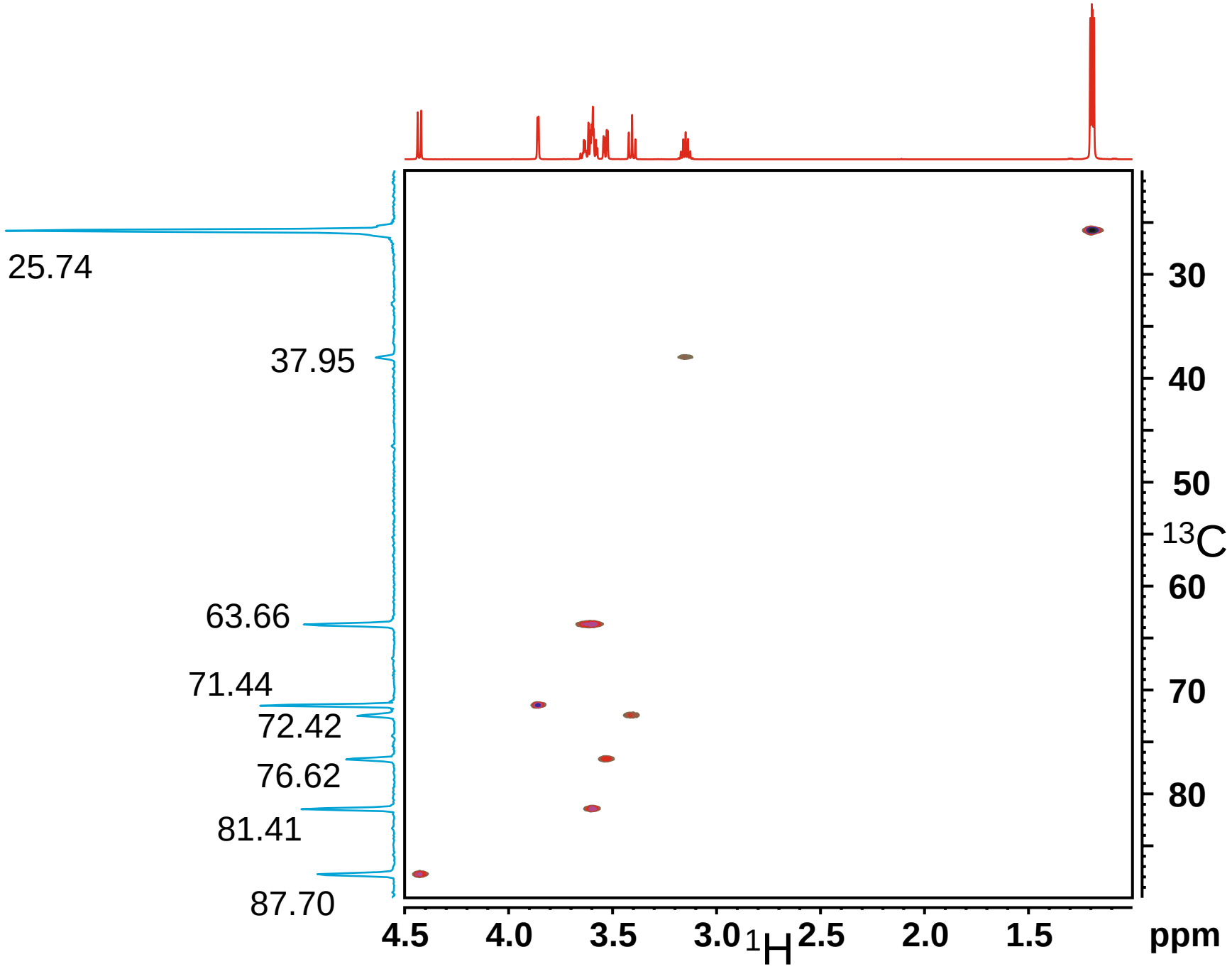


Parts of the COSY

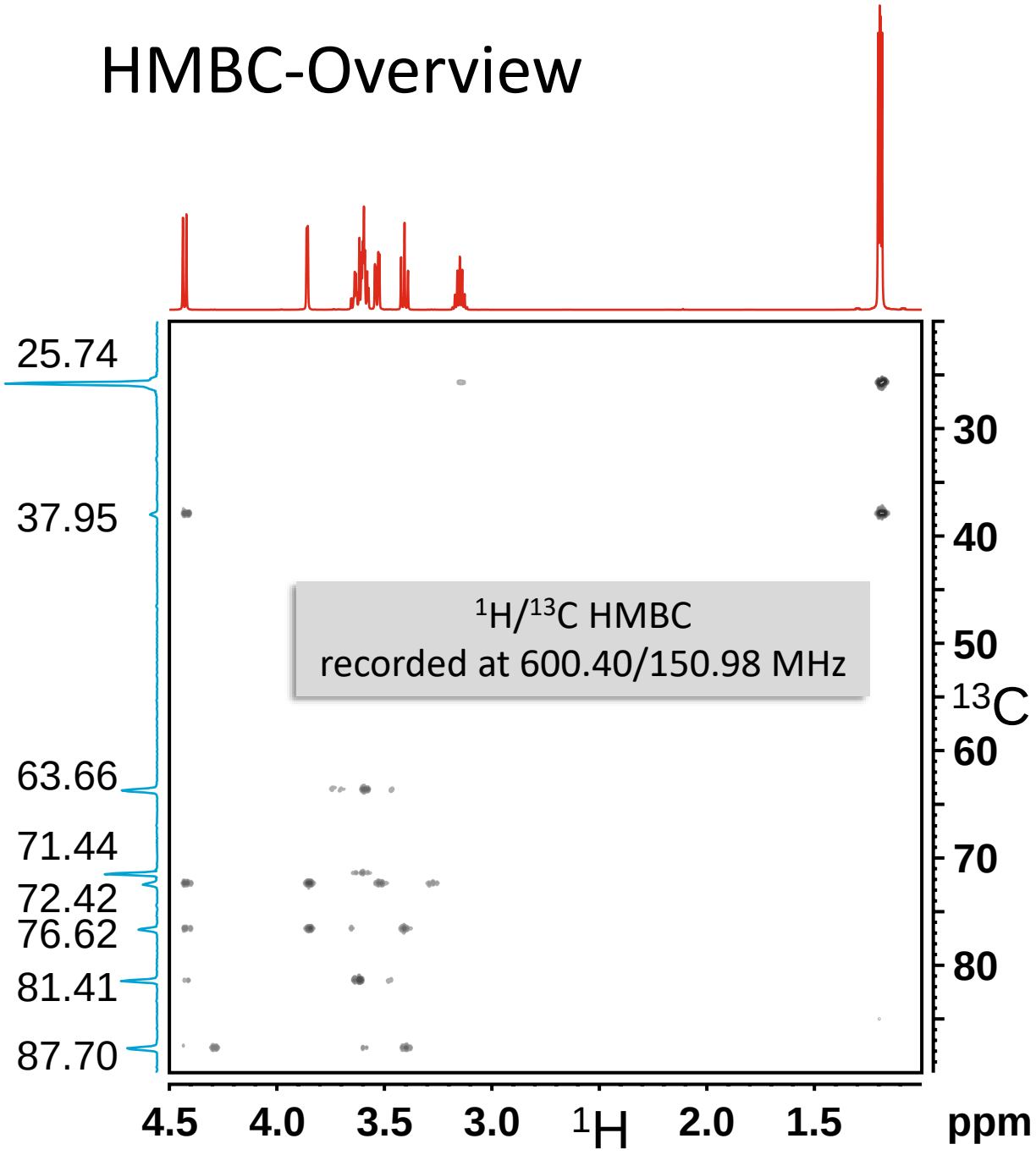




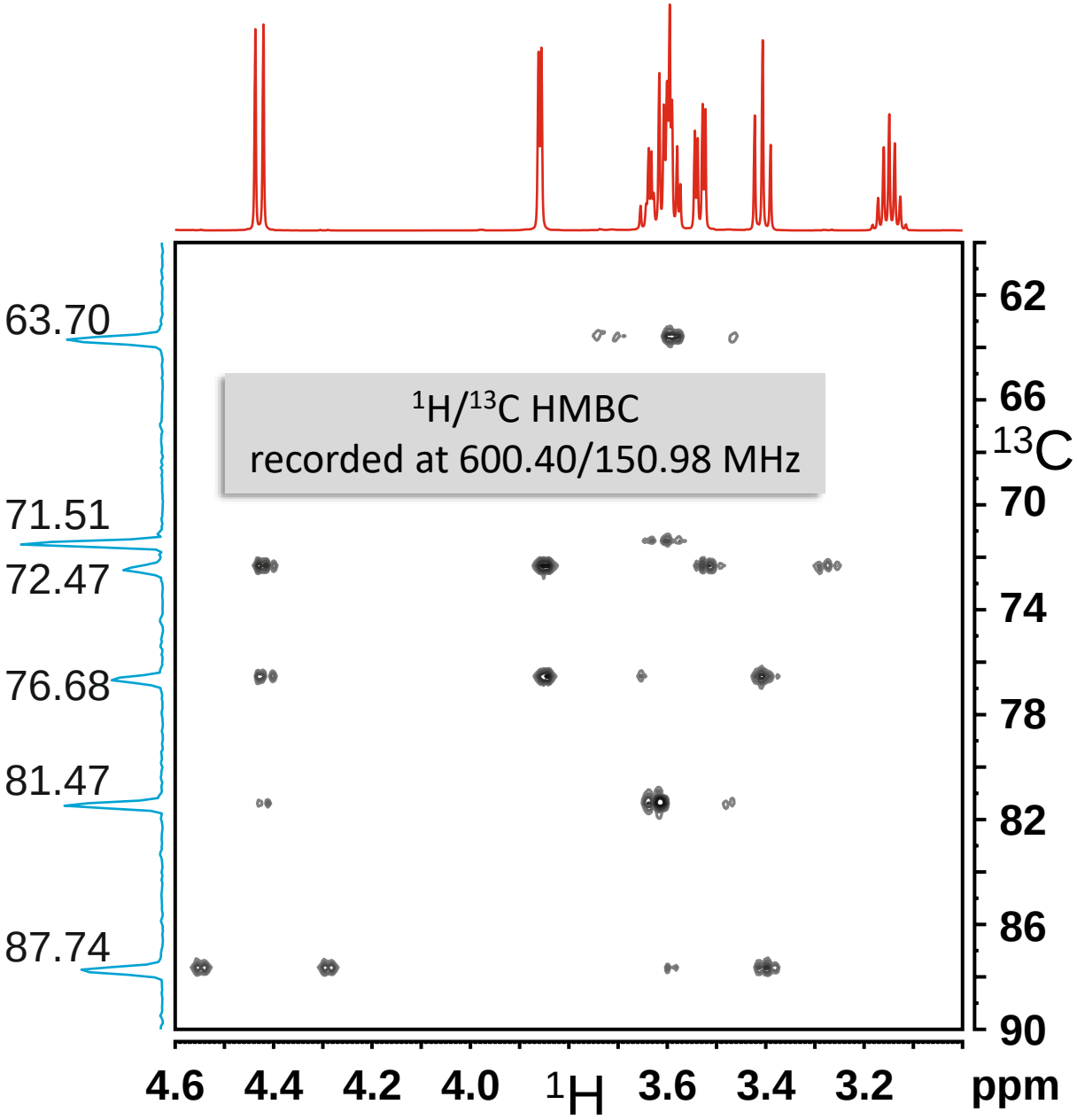
$^{1}H/^{13}C$ HSQC
recorded at 600.40/150.98 MHz



HMBC-Overview

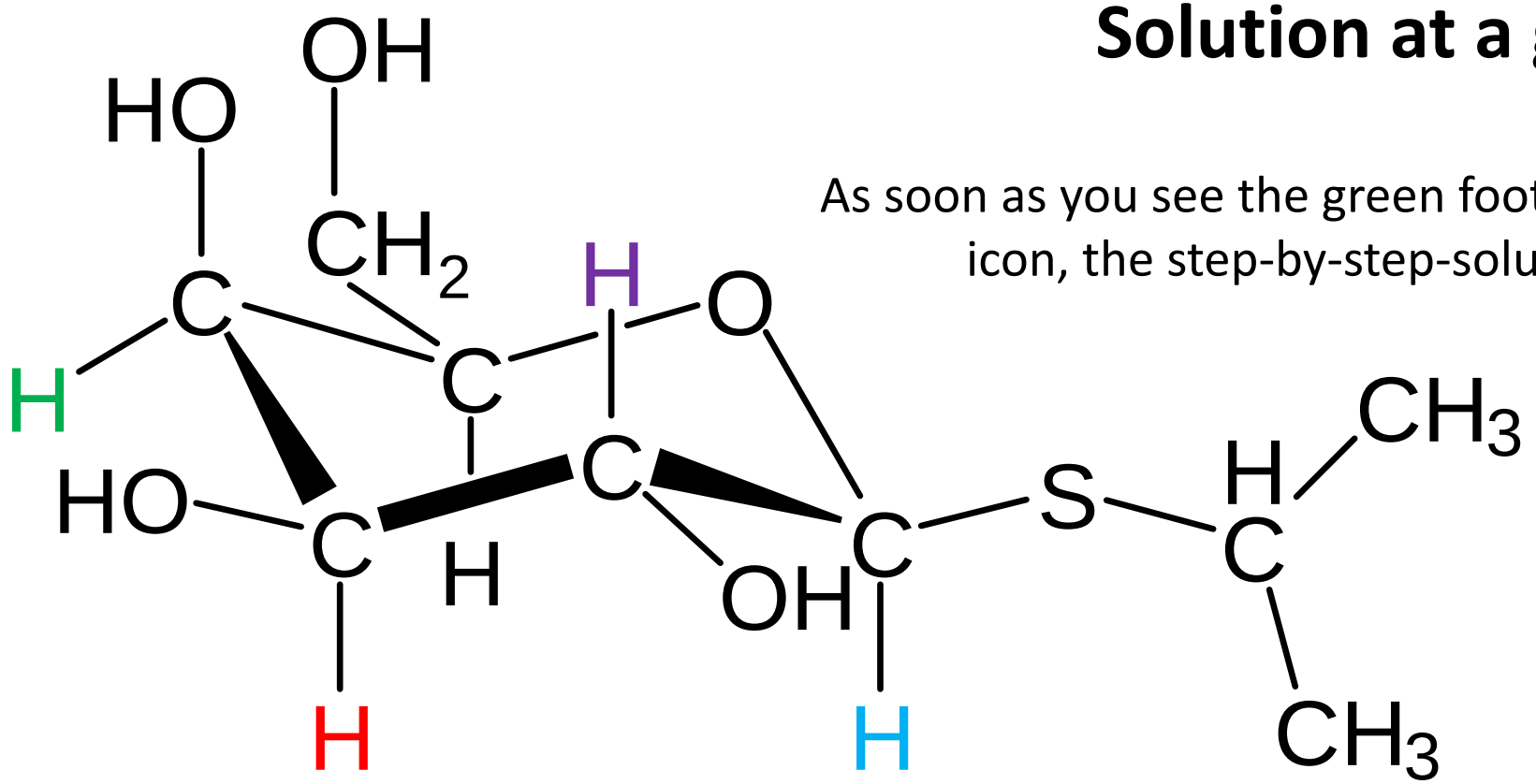


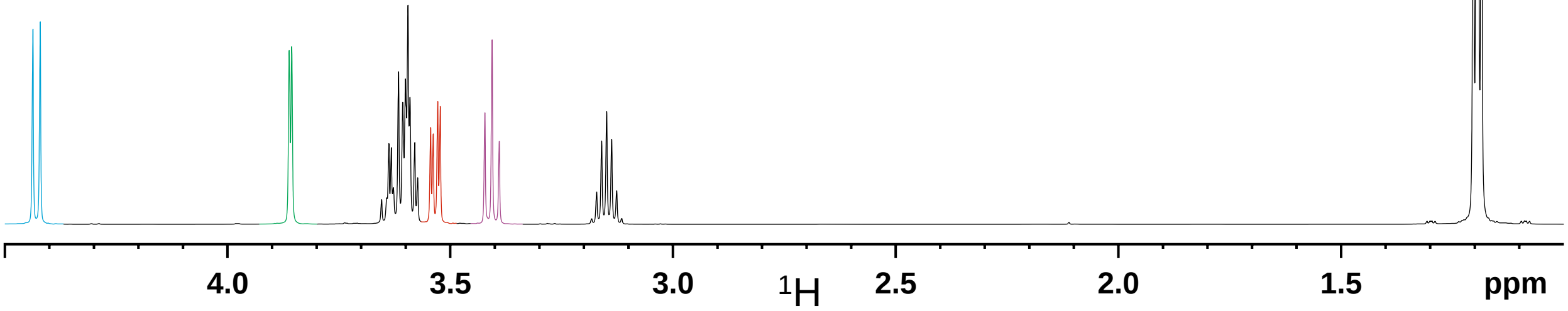
Part of the HMBC



Solution at a glance

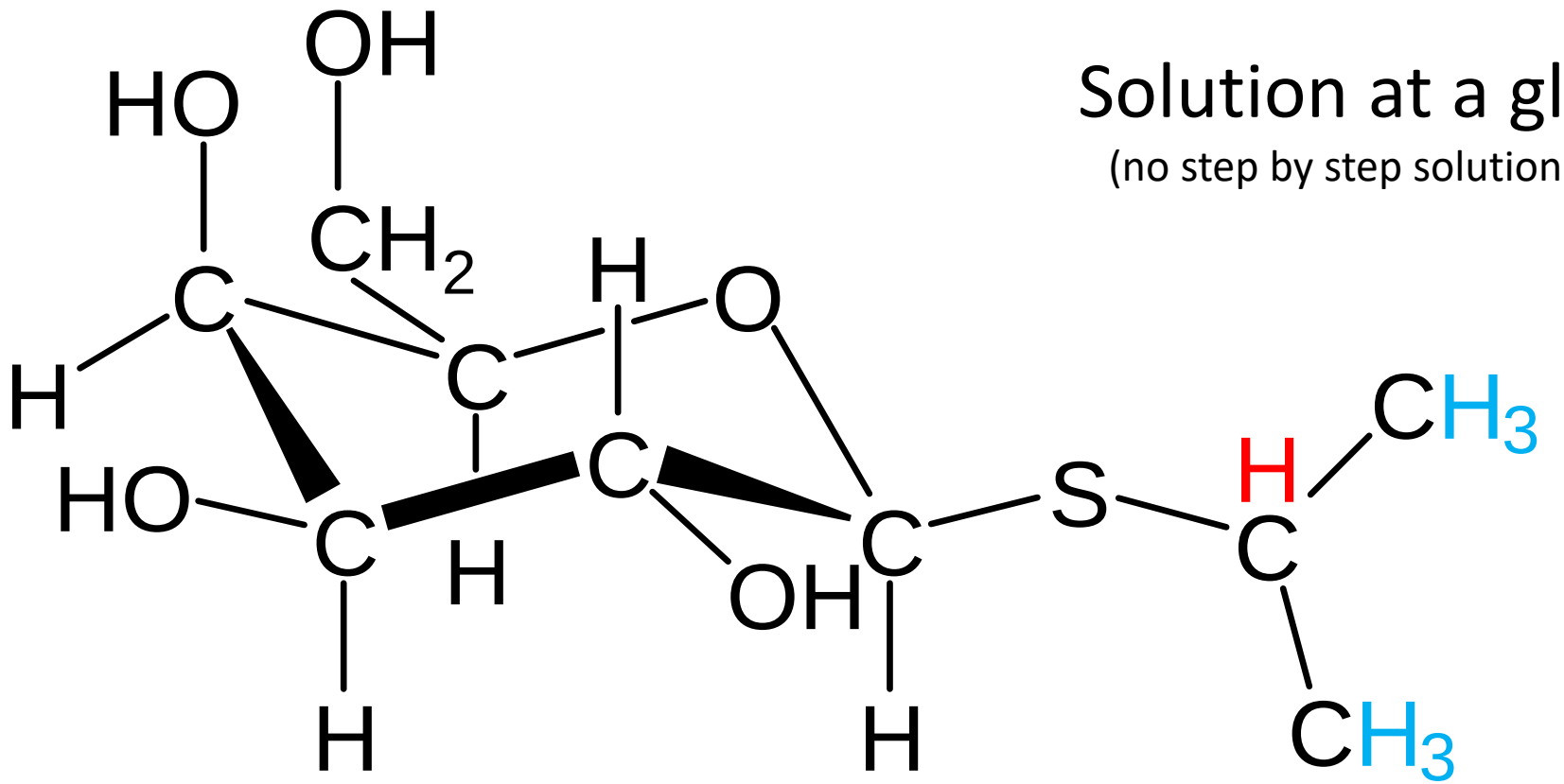
As soon as you see the green footprints on the problem icon, the step-by-step-solution is available

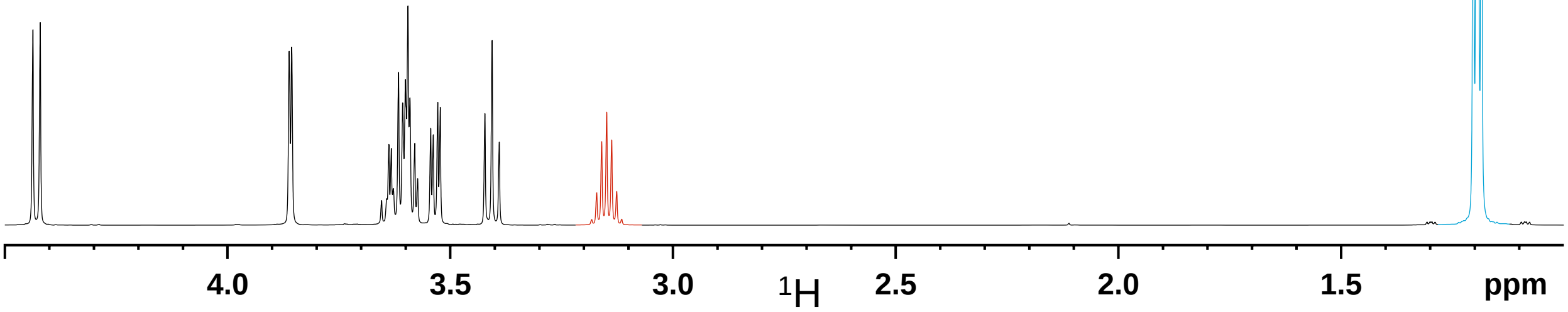




Solution at a glance

(no step by step solution so far)





Contributions

Spectrometer time

TU Munich

Measurements

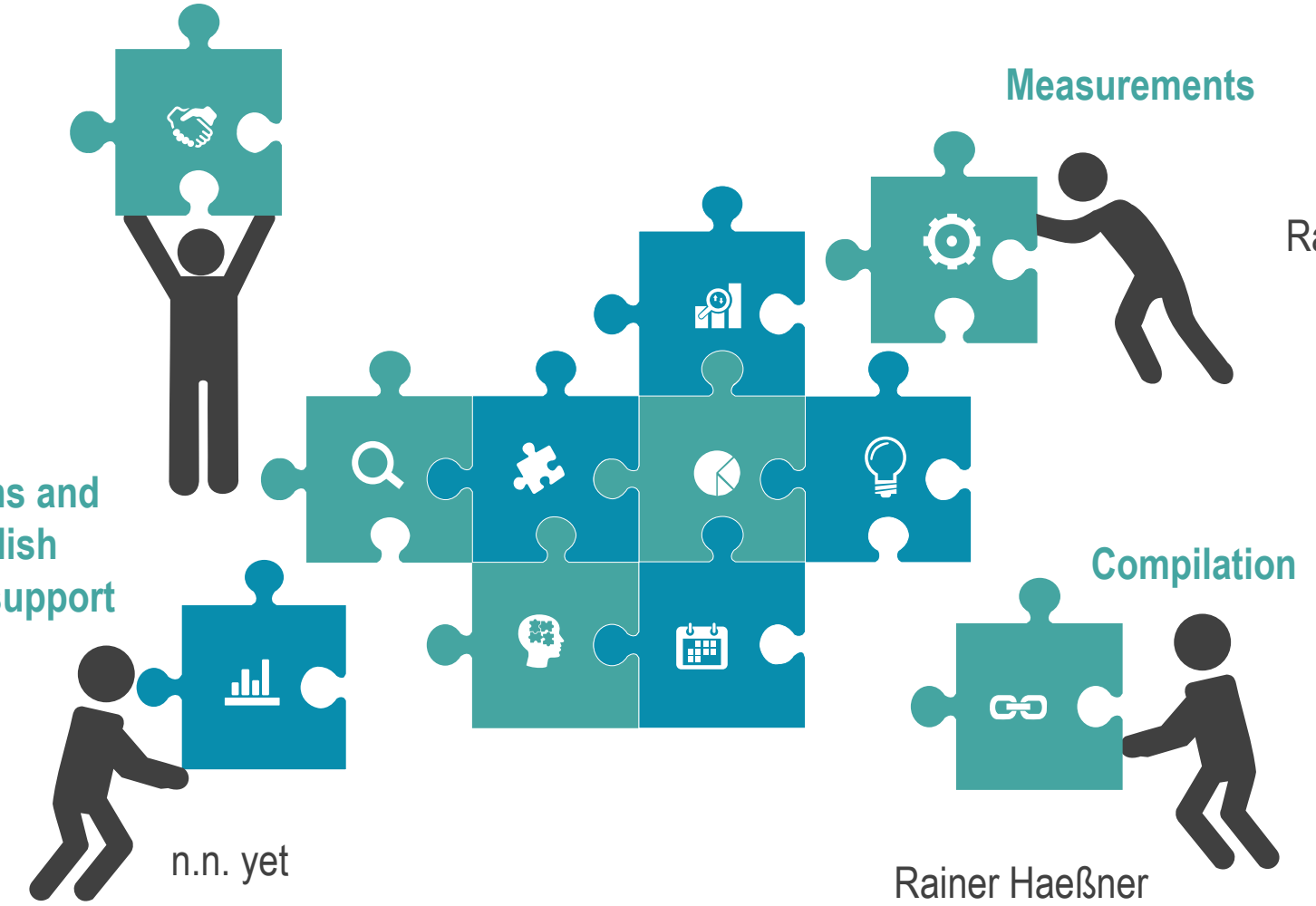
Rainer Haeßner

Discussions and native English language support

n.n. yet

Compilation

Rainer Haeßner



More exercises …