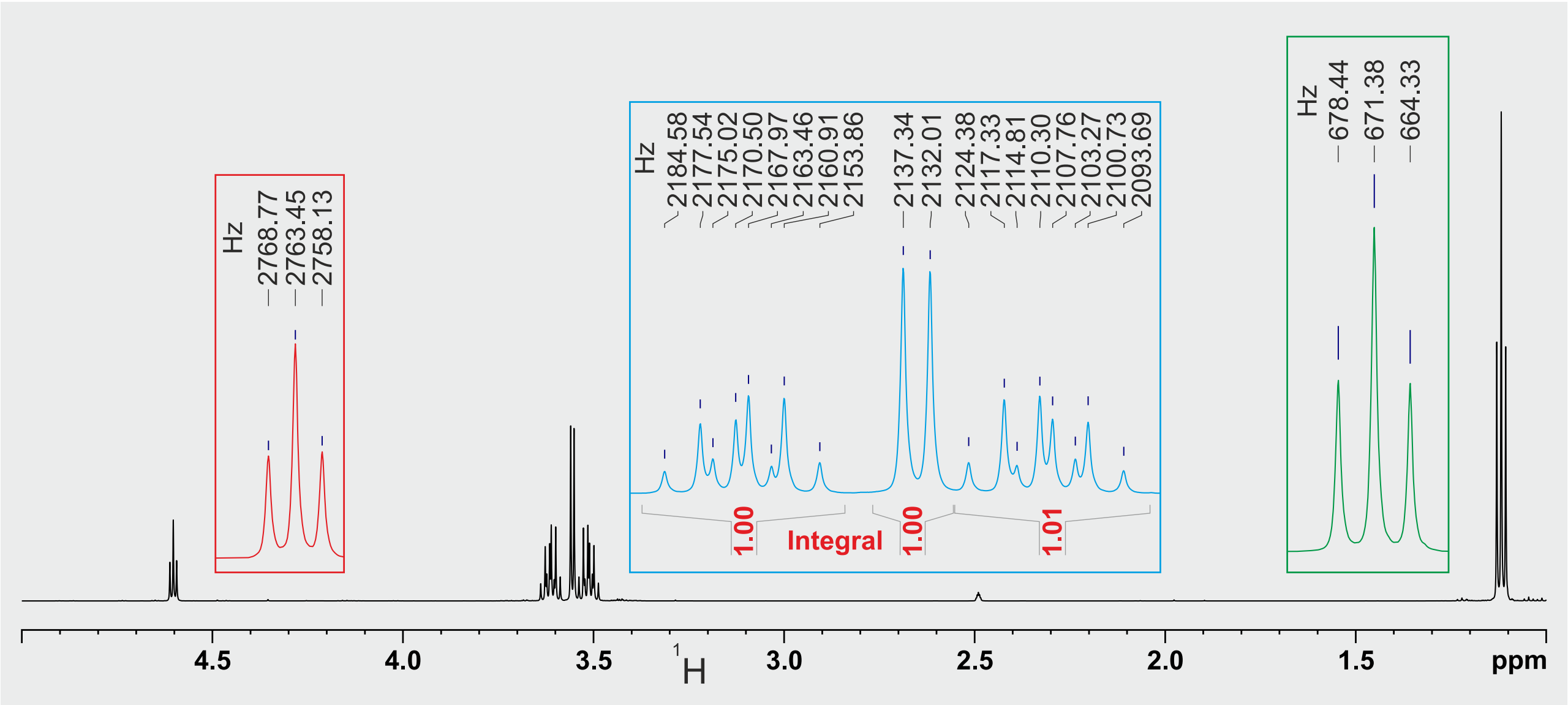
Exercise plus Solution – Quick overview

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.



$C_6H_{13}ClO_2$

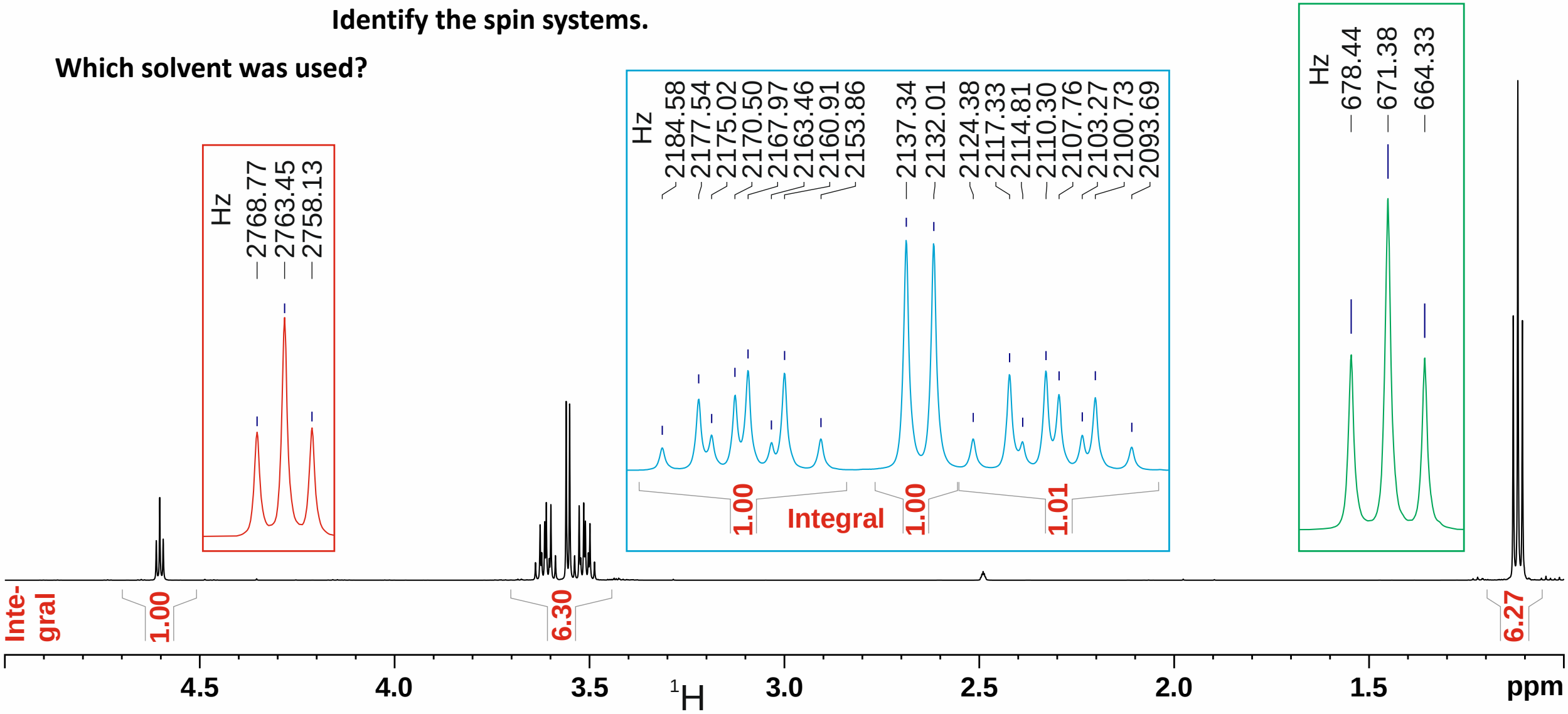
Deduce the structure and measure all homonuclear coupling constants.

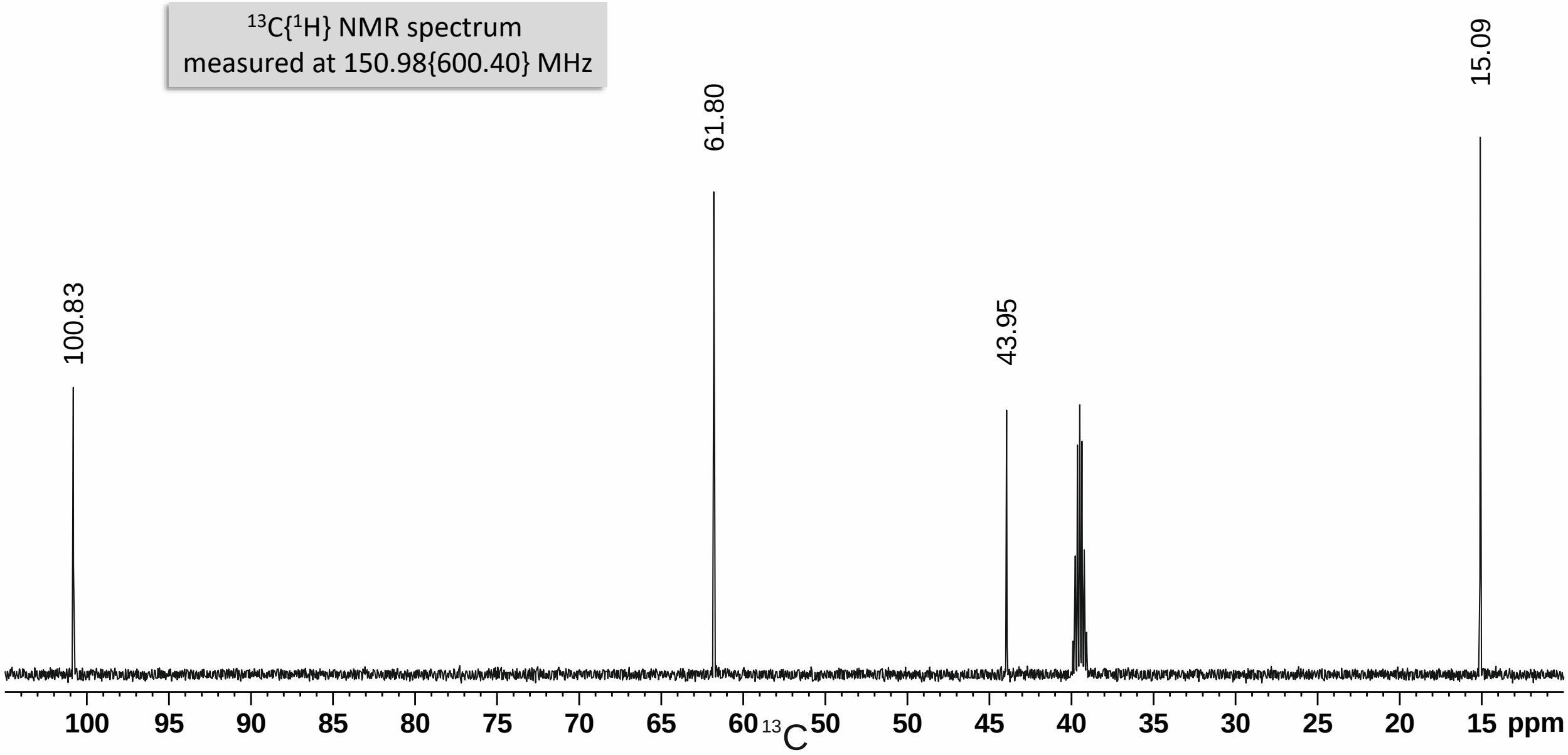
Assign all proton and carbon signals.

Identify the spin systems.

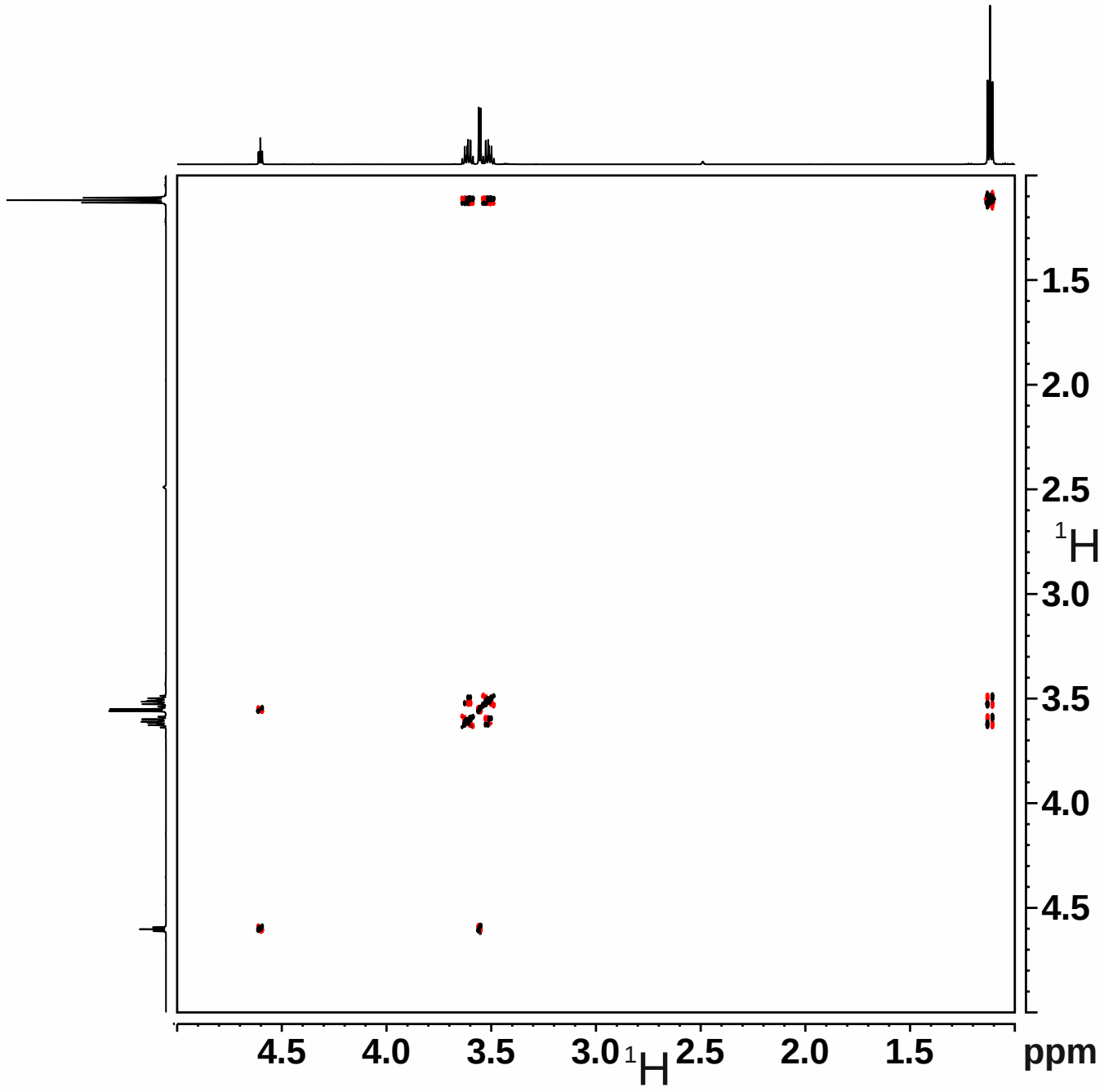
Which solvent was used?

^{1}H NMR spectrum measured at 600.40 MHz

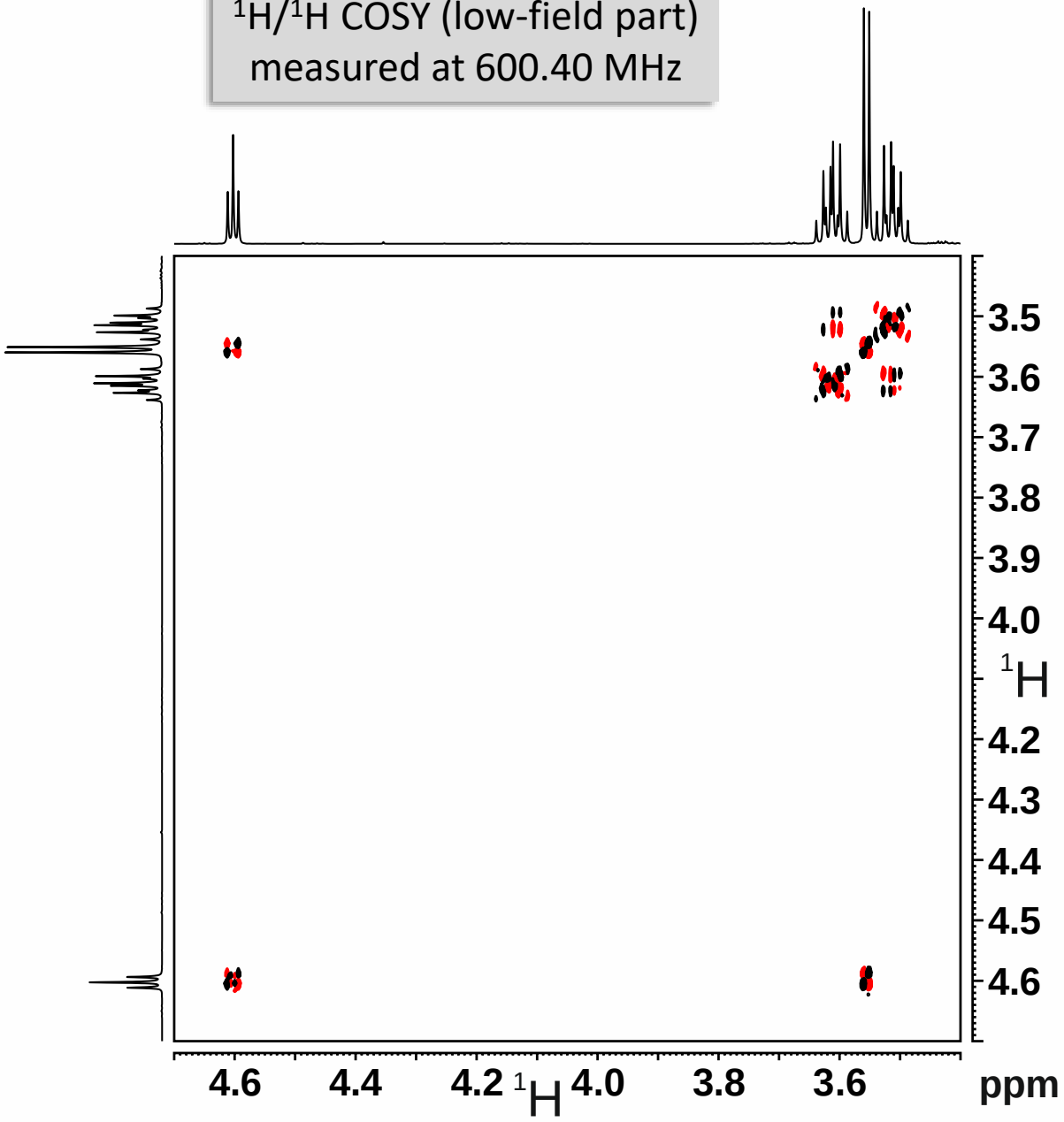



$^{13}C\{^{1}H\}$ NMR spectrum
measured at 150.98{600.40} MHz
100.83
61.80
43.95
15.09
100
95
90
85
80
75
70
65
60
50
50
45
40
35
30
25
20
15
ppm
^{13}C

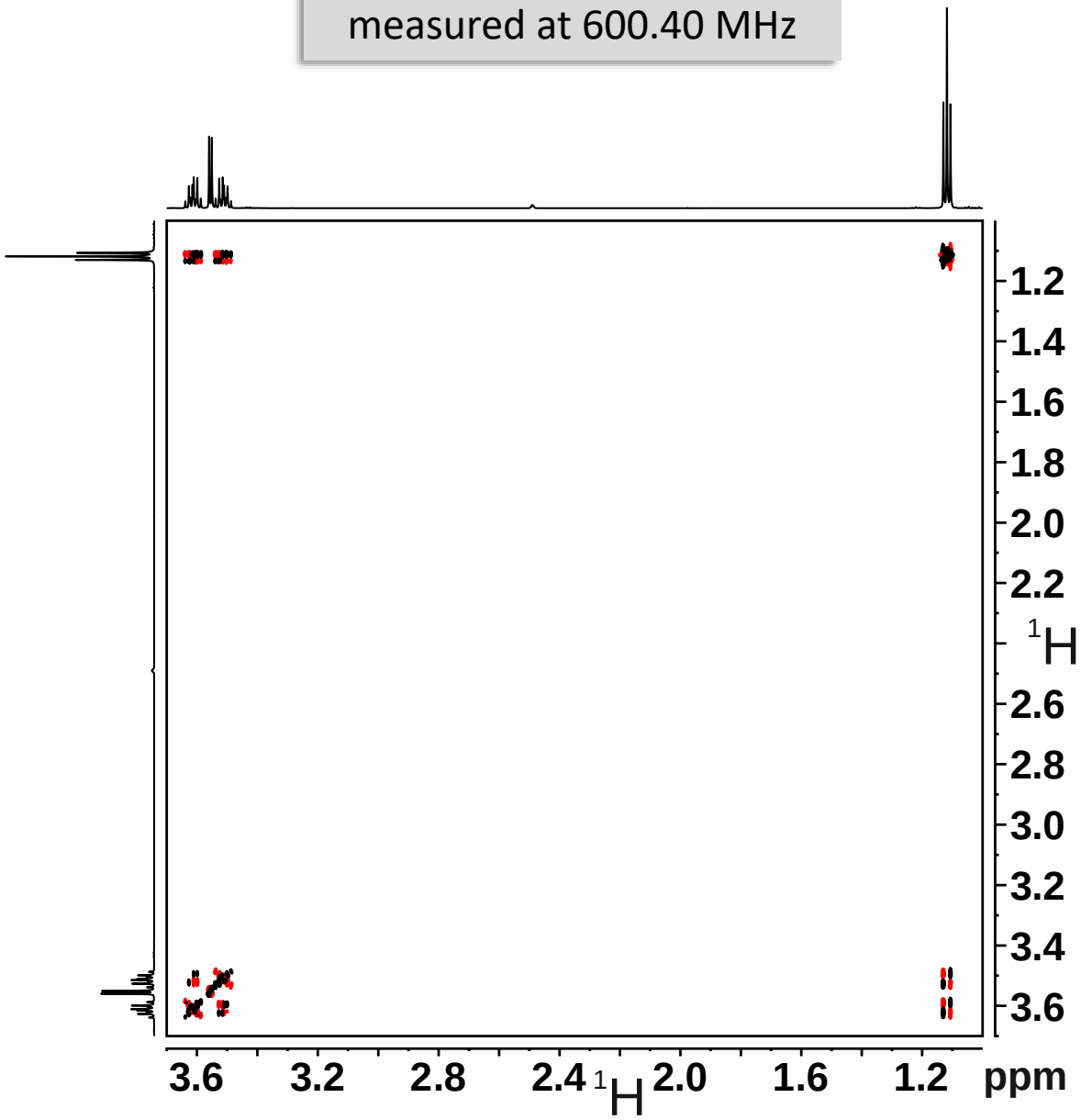
$^{1}H/^{1}H$ COSY (overview)
measured at 600.40 MHz



^{1}H/^{1}H COSY (low-field part)
measured at 600.40 MHz



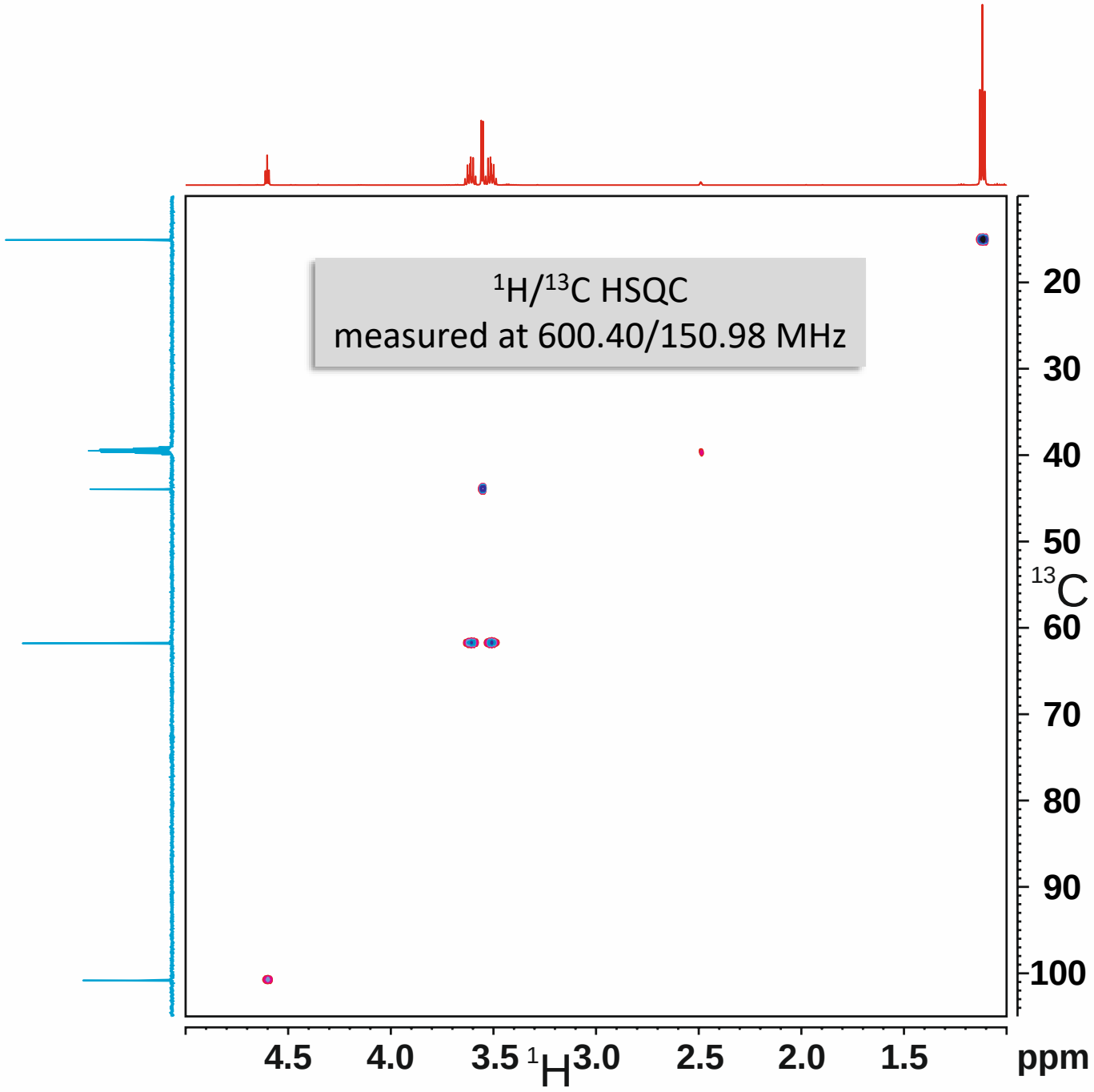
^{1}H/^{1}H COSY (high-field part)
measured at 600.40 MHz

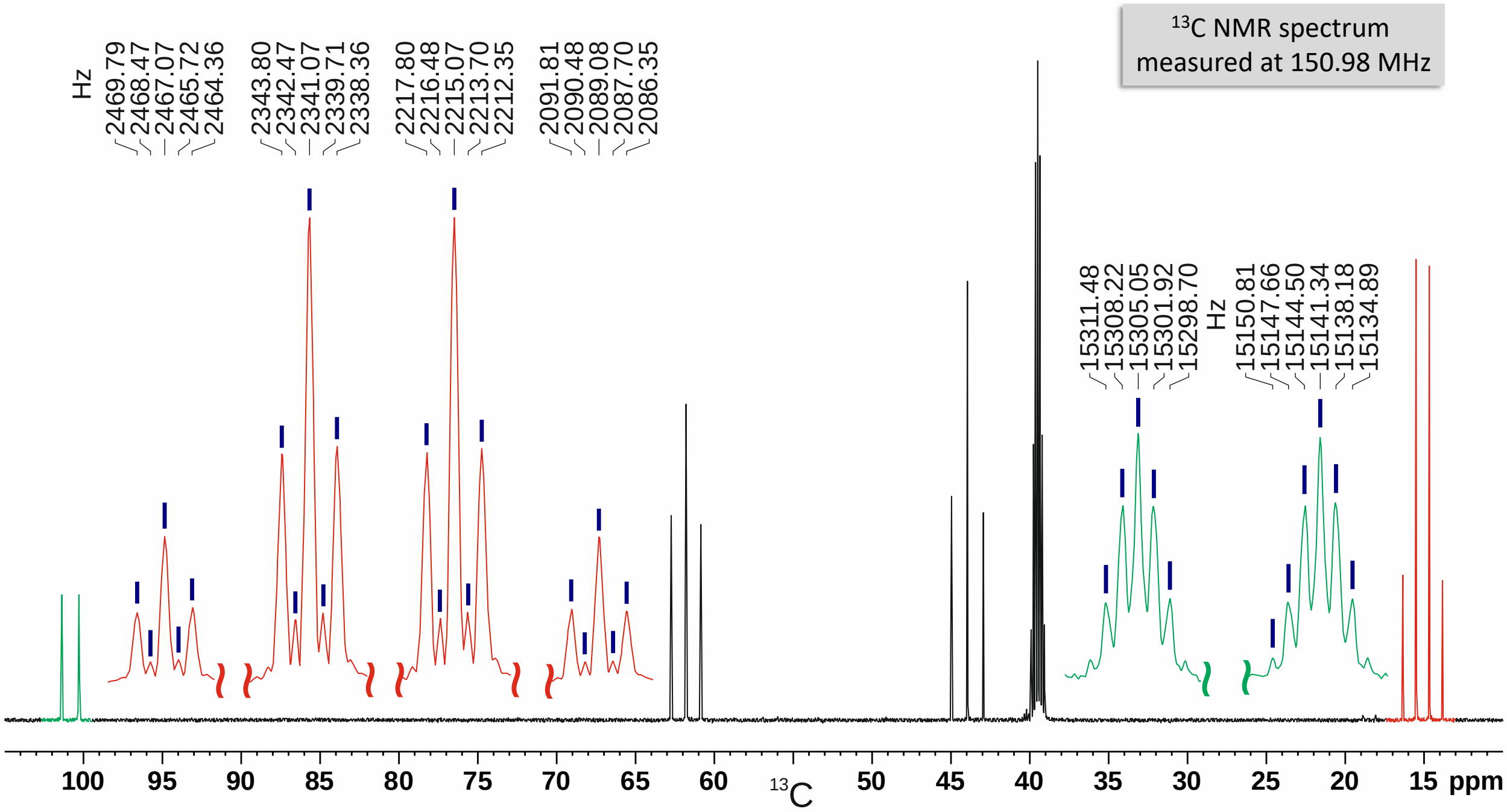


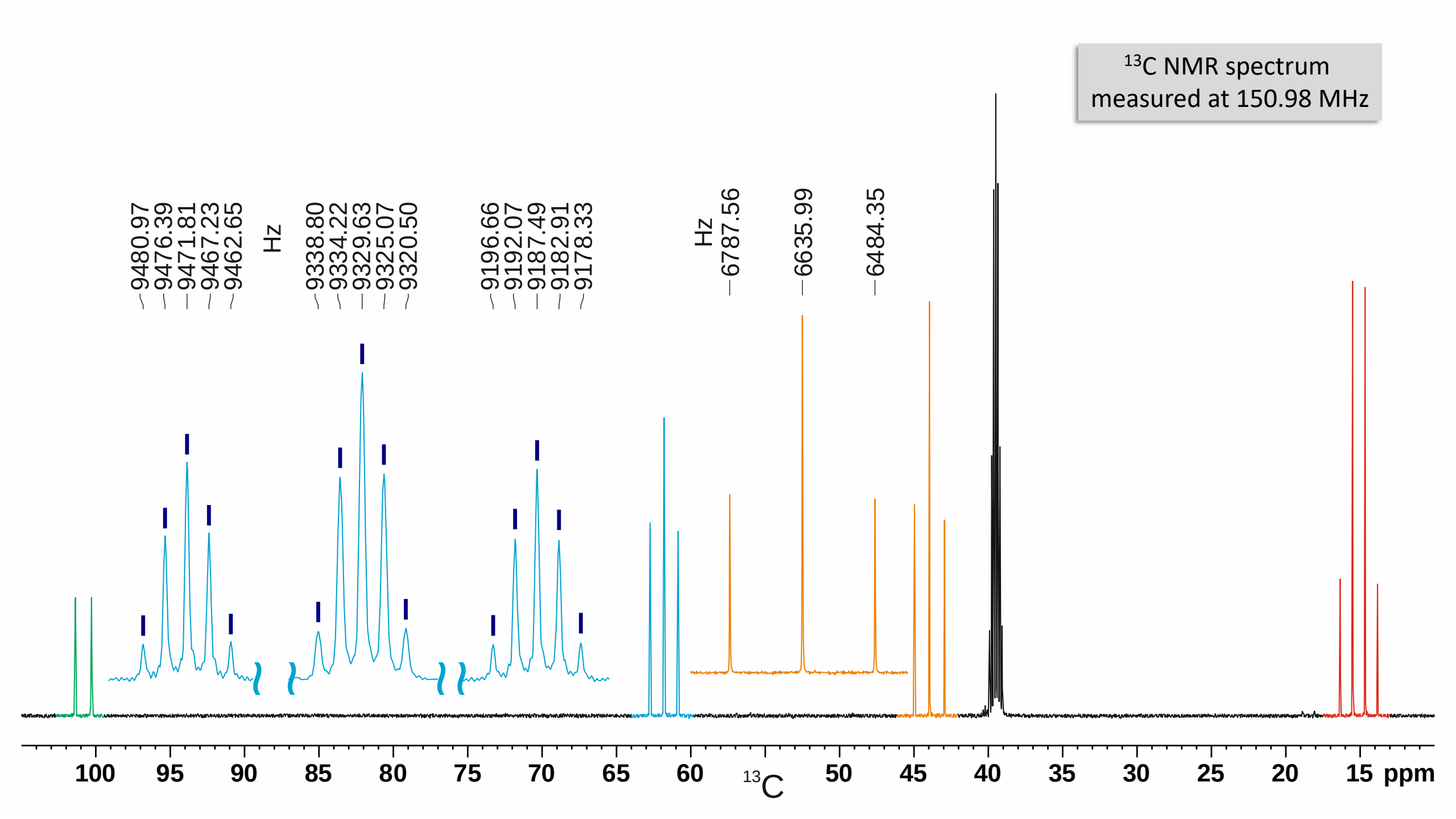
The ^{13}C spectrum on the next two pages is not necessary to solve the problem.
You can optionally try to understand the coupling patterns.

Same colours mean same parts of the spectrum.

Due to space restrictions, some areas within the enlarged multiplets containing noise only were removed.

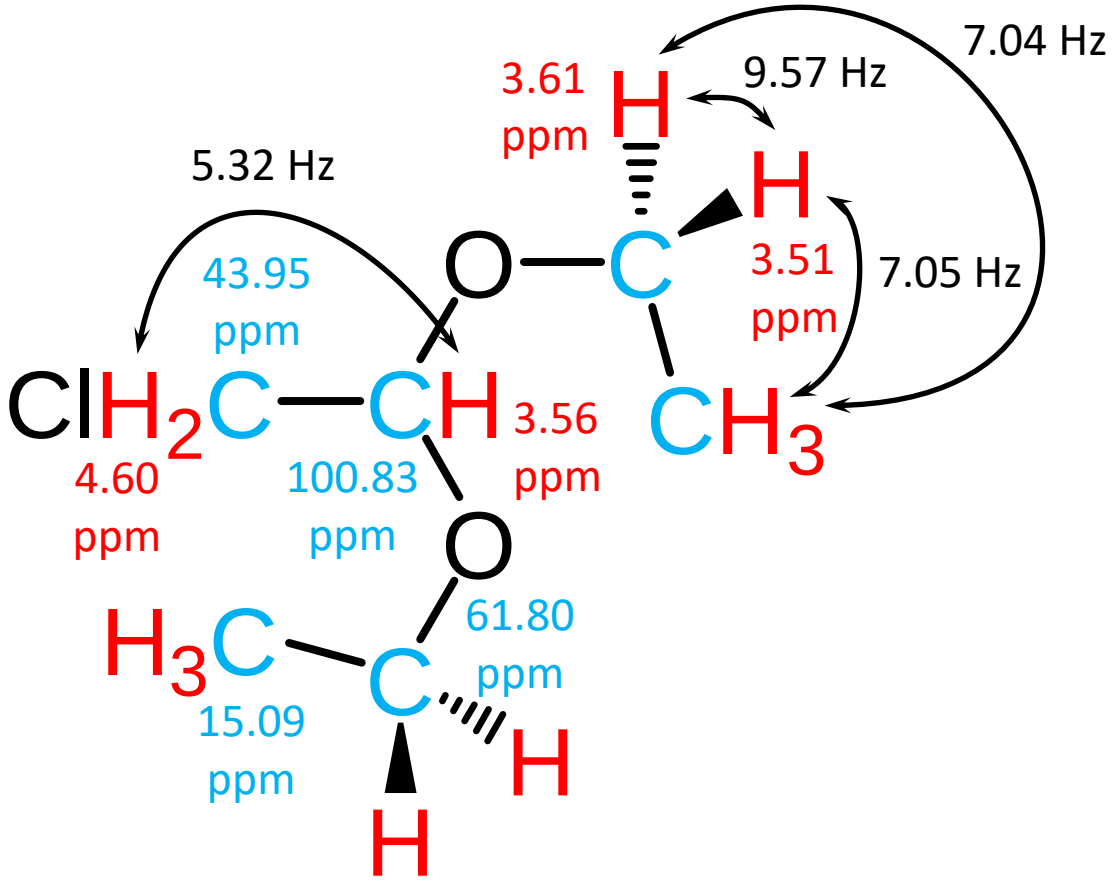



^{13}C NMR spectrum
measured at 150.98 MHz
Hz
2469.79
2468.47
2467.07
2465.72
2464.36
2343.80
2342.47
2341.07
2339.71
2338.36
2217.80
2216.48
2215.07
2213.70
2212.35
2091.81
2090.48
2089.08
2087.70
2086.35
15311.48
15308.22
15305.05
15301.92
15298.70
Hz
15150.81
15147.66
15144.50
15141.34
15138.18
15134.89
100
95
90
85
80
75
70
65
60
^{13}C
50
45
40
35
30
25
20
15
ppm


^{13}C NMR spectrum
measured at 150.98 MHz
9480.97
9476.39
9471.81
9467.23
9462.65
Hz
9338.80
9334.22
9329.63
9325.07
9320.50
9196.66
9192.07
9187.49
9182.91
9178.33
Hz
6787.56
6635.99
6484.35
100
95
90
85
80
75
70
65
60
^{13}C
50
45
40
35
30
25
20
15
ppm

Solution at a glance

There is no step by step solution available so far.



Contributions

Spectrometer time

TU Munich

Measurements

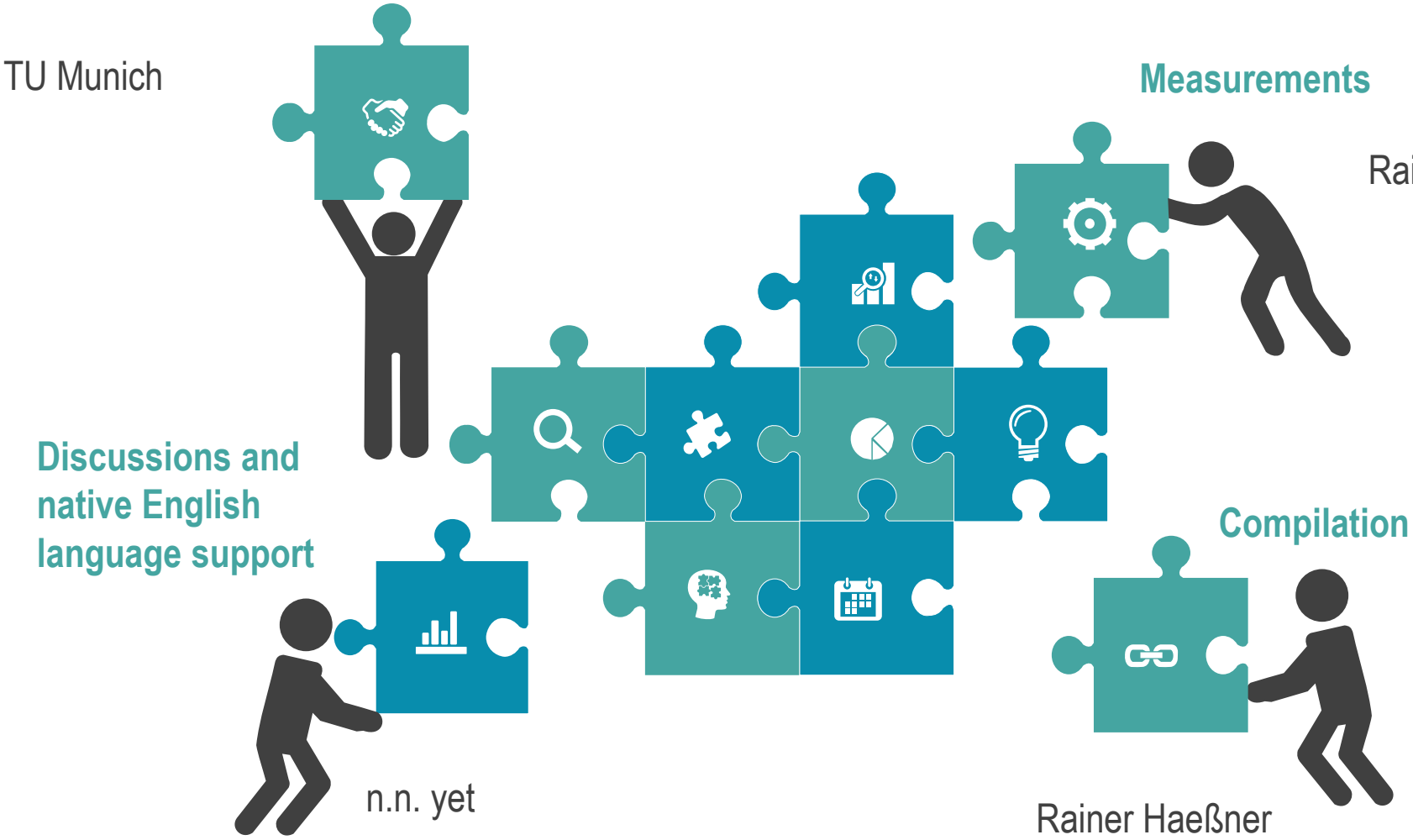
Rainer Haeßner

Discussions and native English language support

n.n. yet

Compilation

Rainer Haeßner



More exercises …