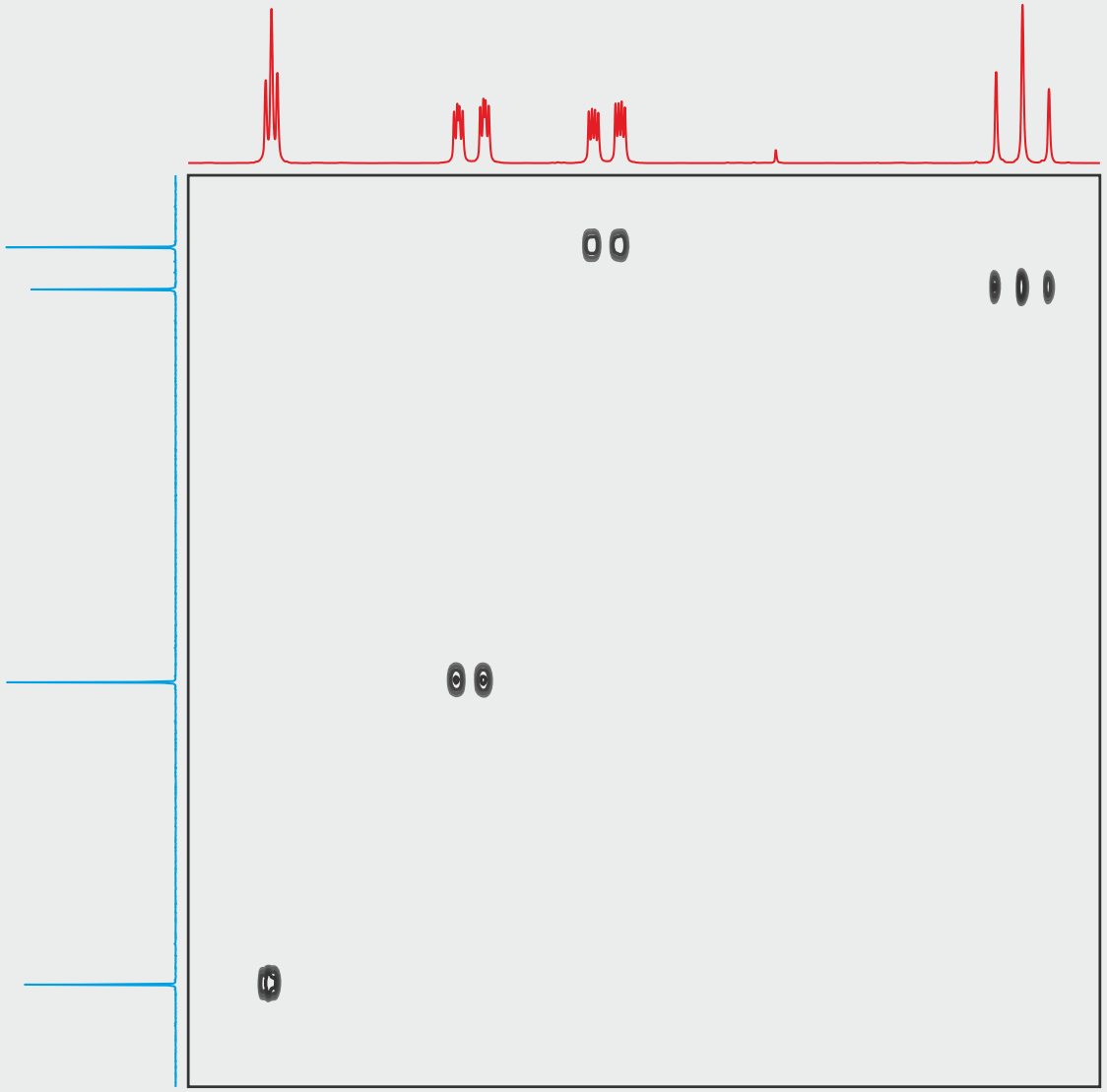
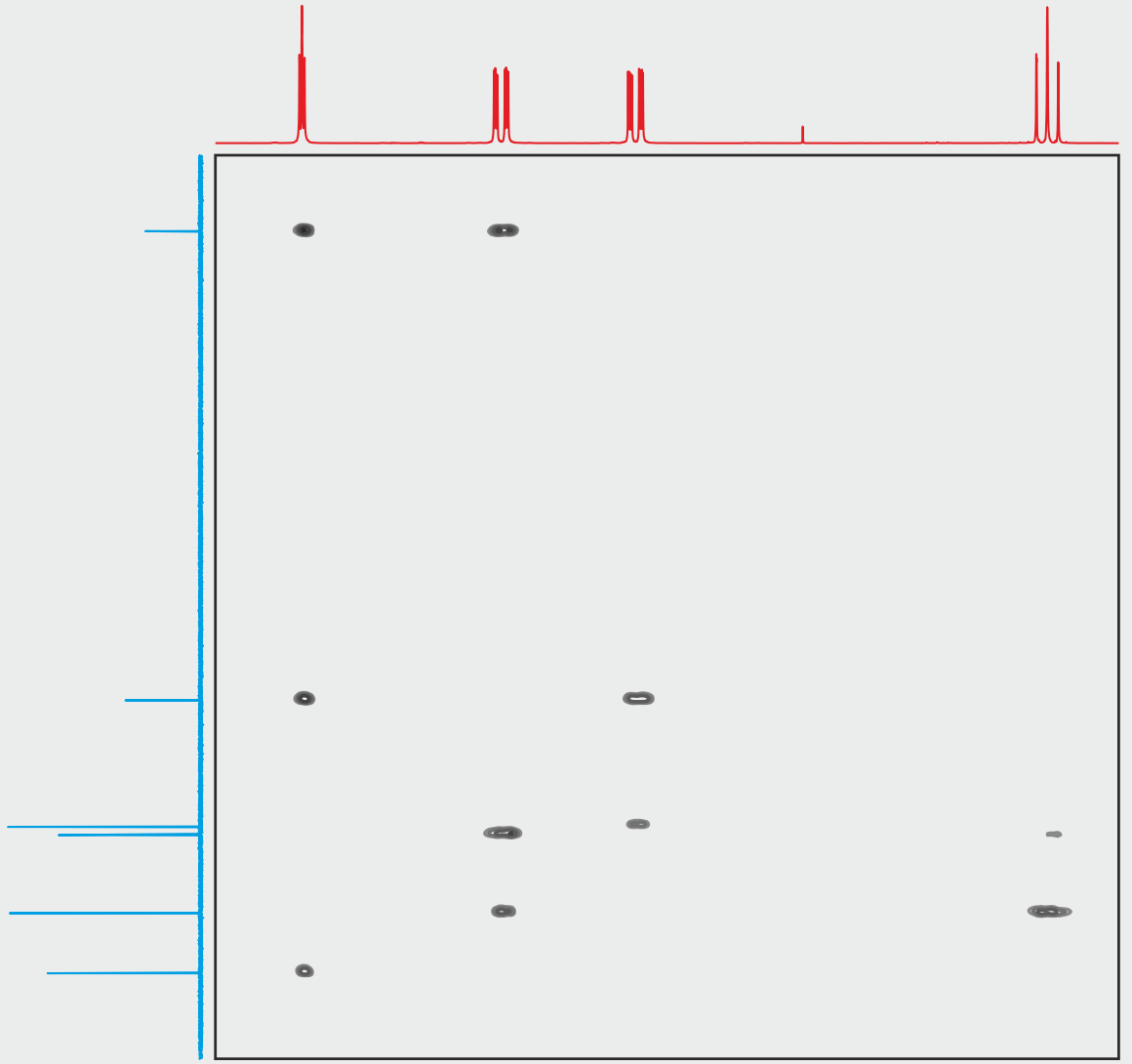
Exercise plus Solution – Quick PDF overview

It is recommended to use this PDF 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.





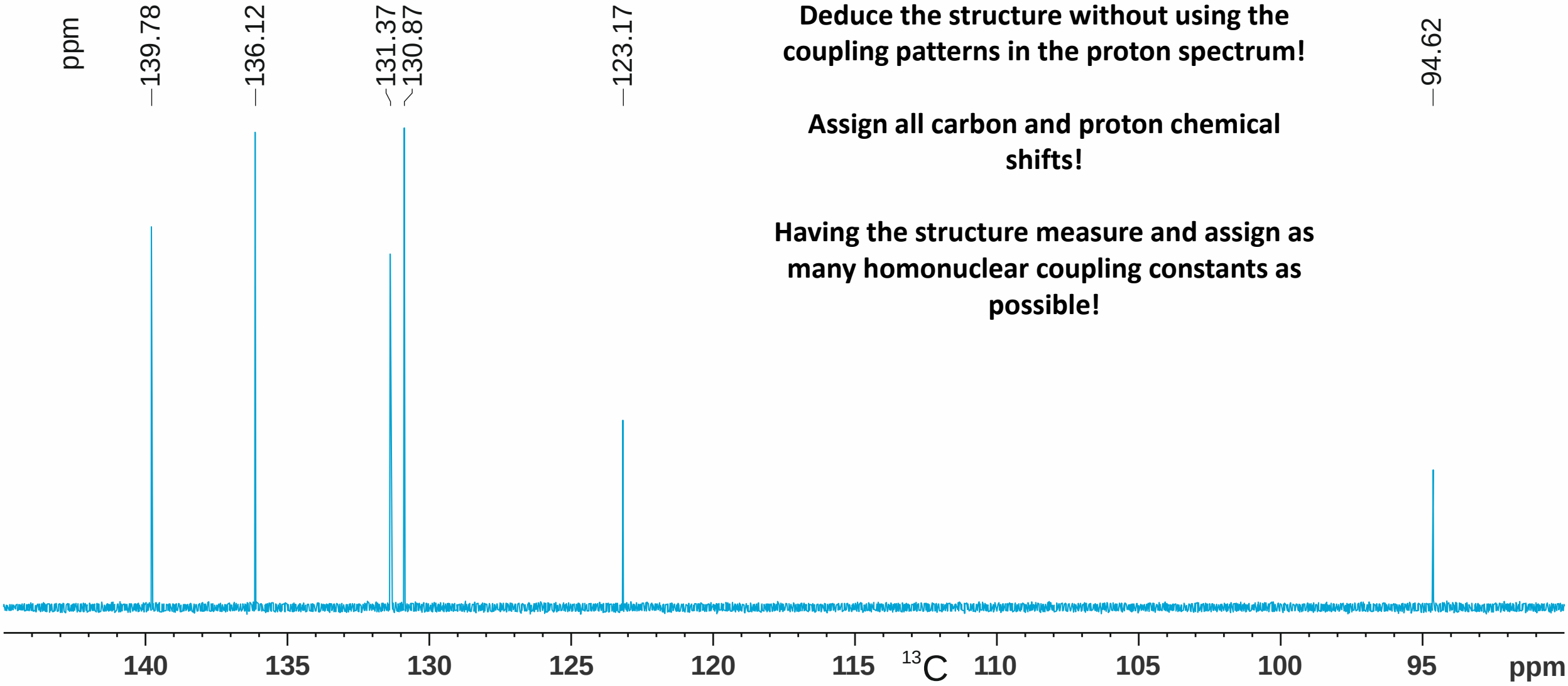
$^{13}C\{^{1}H\}$ NMR spectrum measured at 151.05{600.66} MHz

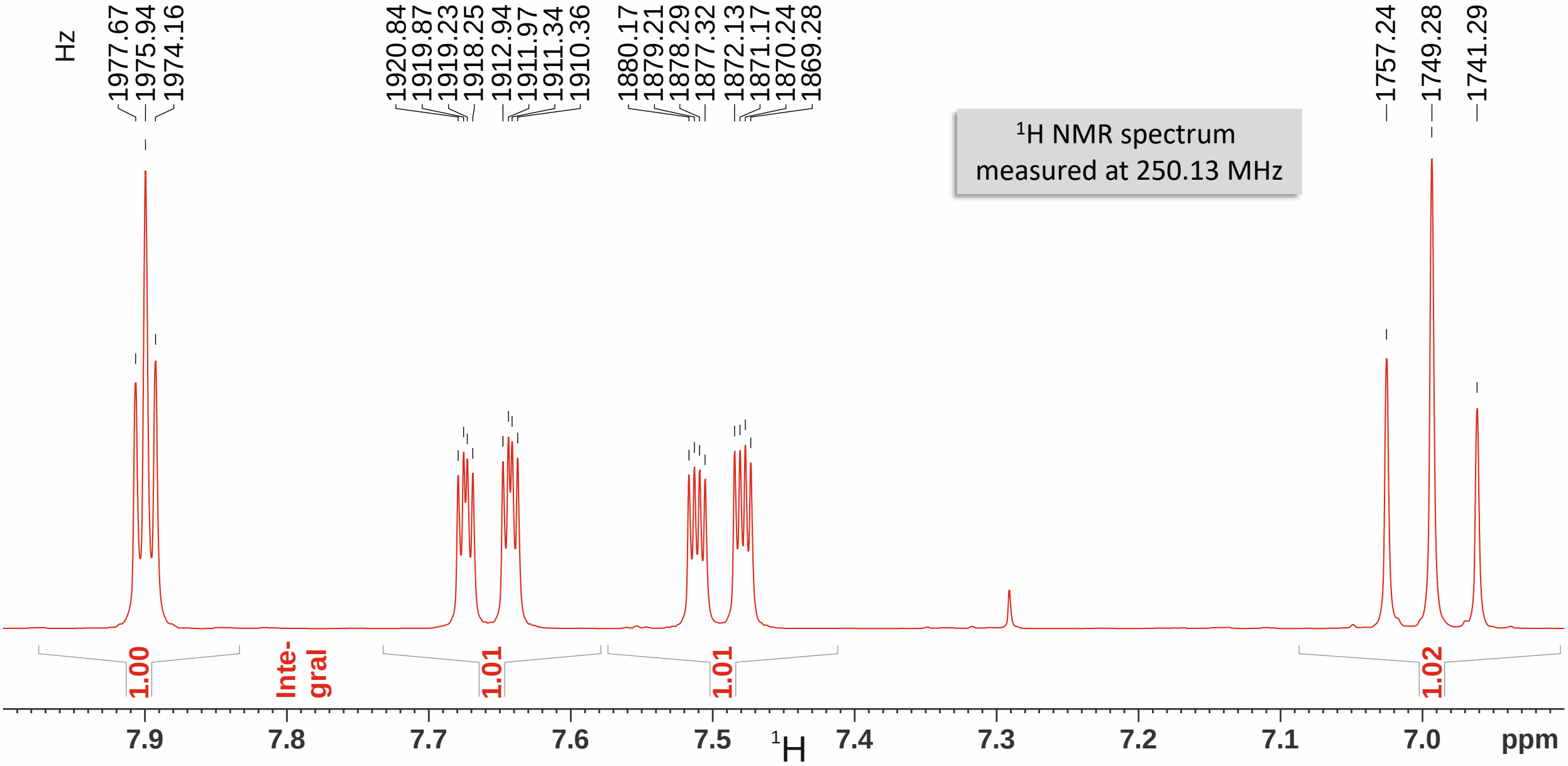
C_6H_4BrI measured in $CDCl_3$

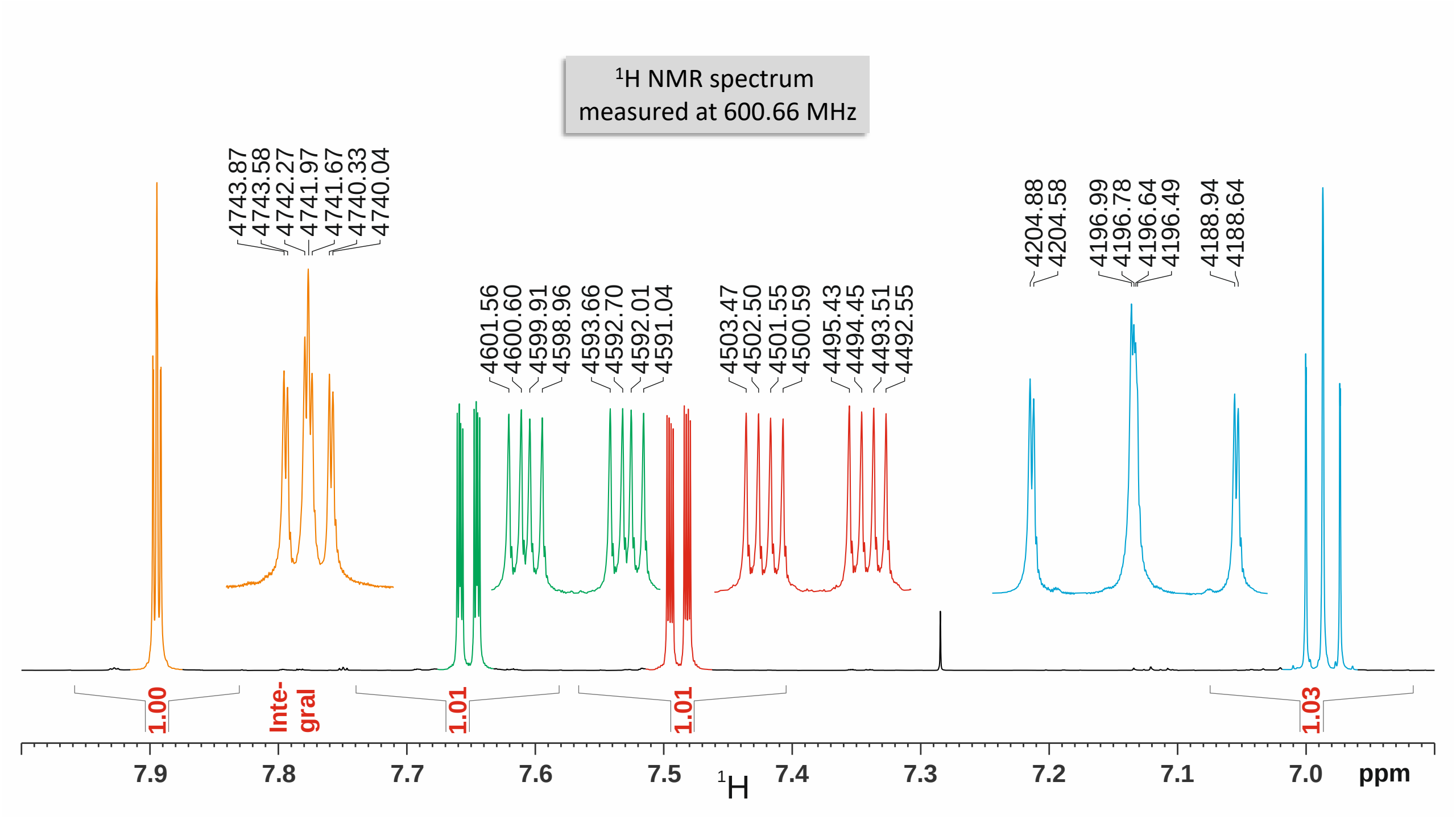
Deduce the structure without using the coupling patterns in the proton spectrum!

Assign all carbon and proton chemical shifts!

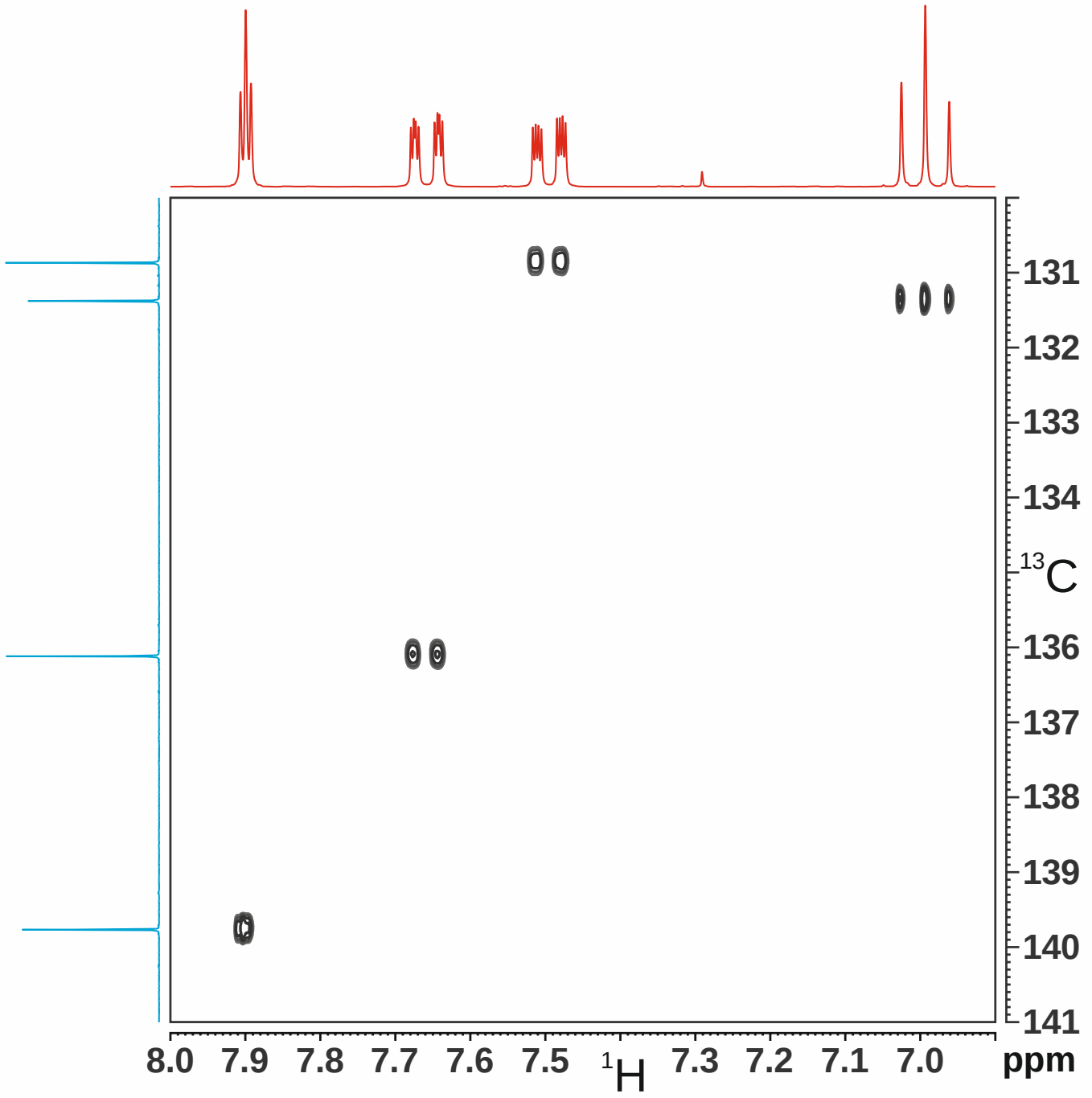
Having the structure measure and assign as many homonuclear coupling constants as possible!




Hz
1977.67
1975.94
1974.16
1920.84
1919.87
1919.23
1918.25
1912.94
1911.97
1911.34
1910.36
1880.17
1879.21
1878.29
1877.32
1872.13
1871.17
1870.24
1869.28
1757.24
1749.28
1741.29
^{1}H NMR spectrum
measured at 250.13 MHz
1.00
Inte-
gral
1.01
1.01
1.02
7.9
7.8
7.7
7.6
7.5
^{1}H
7.4
7.3
7.2
7.1
7.0
ppm


^{1}H NMR spectrum
measured at 600.66 MHz
4743.87
4743.58
4742.27
4741.97
4741.67
4740.33
4740.04
4601.56
4600.60
4599.91
4598.96
4593.66
4592.70
4592.01
4591.04
4503.47
4502.50
4501.55
4500.59
4495.43
4494.45
4493.51
4492.55
4204.88
4204.58
4196.99
4196.78
4196.64
4196.49
4188.94
4188.64
1.00
Inte-
gral
1.01
1.01
1.03
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
ppm
^{1}H

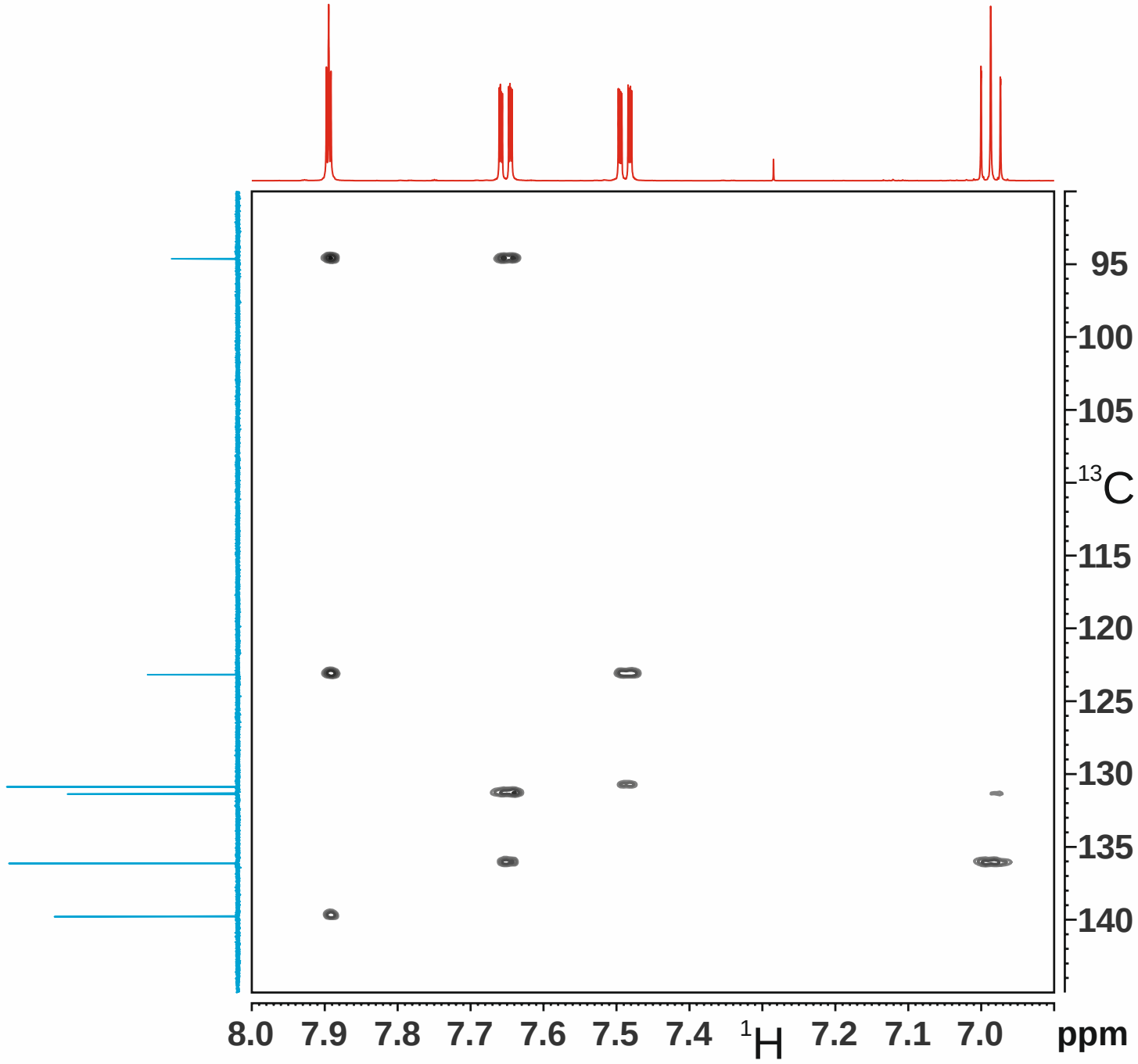
$^{1}H/^{13}C$ HSQC
measured at 250.13/62.90 MHz



1,1-ADEQUATE spectrum
measured at 151.05{600.66} MHz

Carefully watch the frequencies given for the individual spectra.

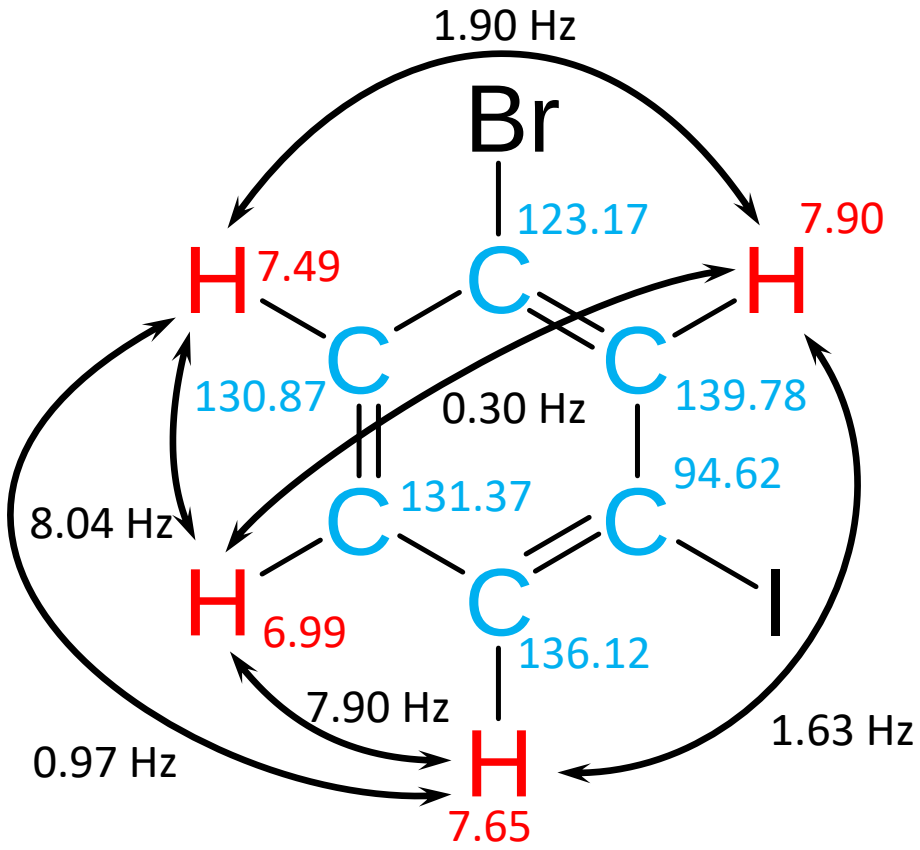
The spectra became measured using two different magnetic fields.



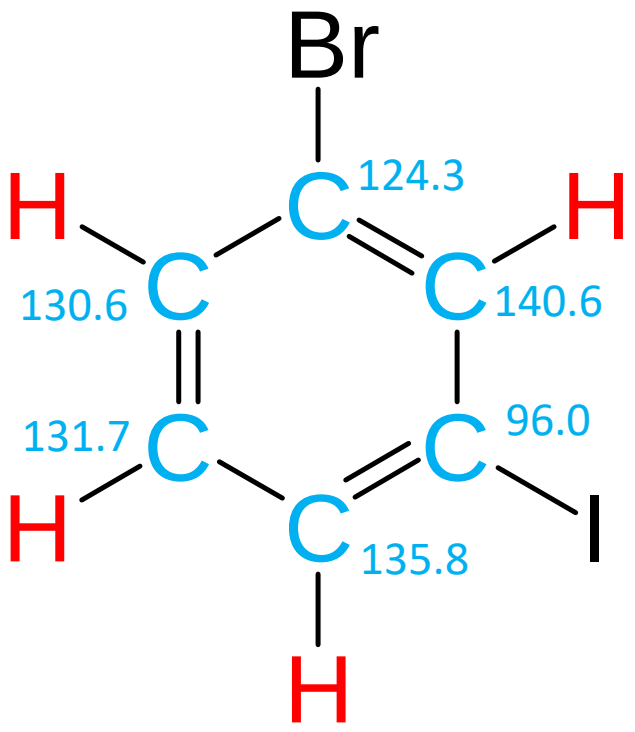
Solution at a glance

(no step by step solution so far)

Measured chemical shifts and coupling constants



Calculated carbon chemical shifts using a simple incremental scheme



Contributions

Spectrometer time

TU Munich

Measurements

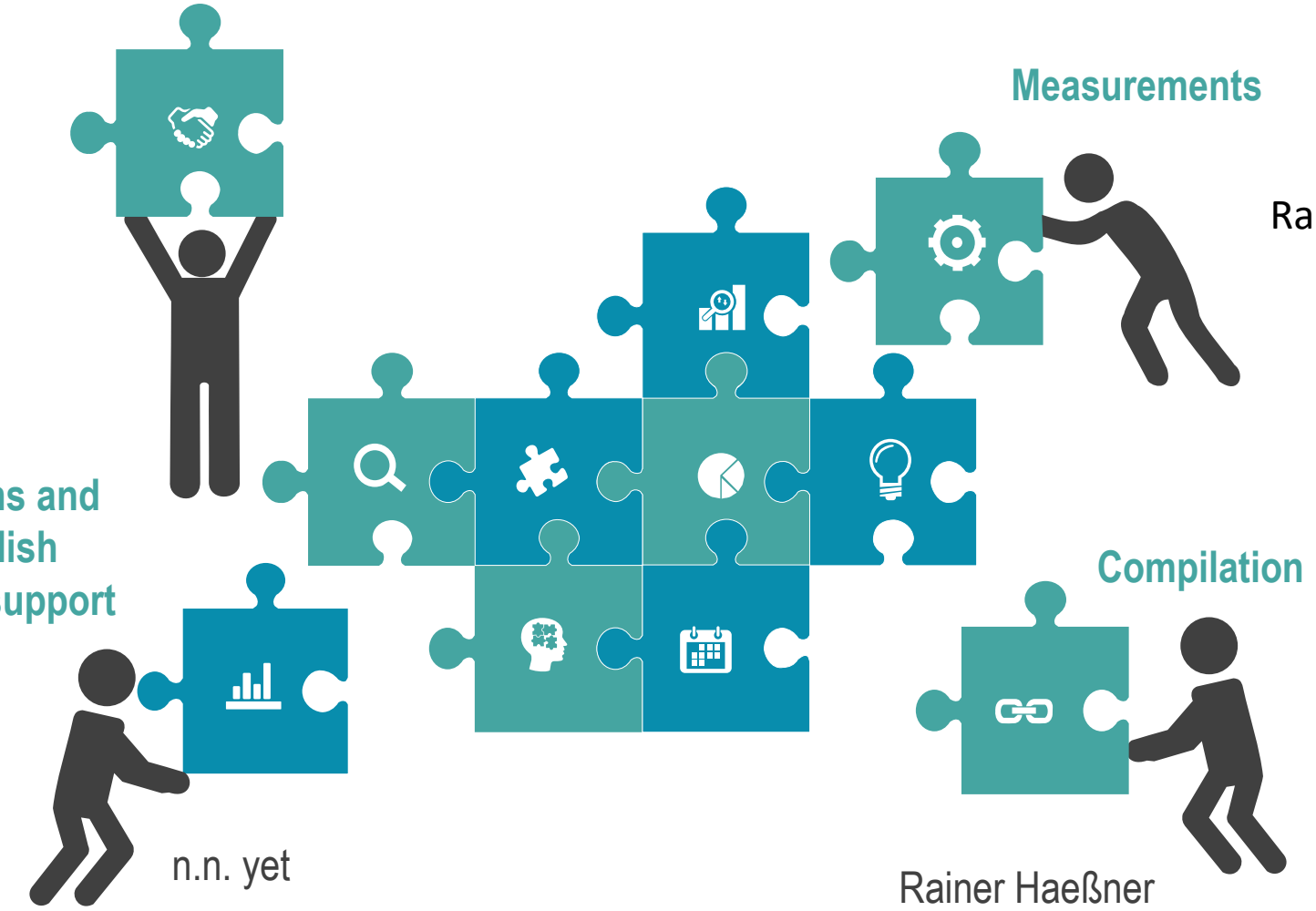
Rainer Haeßner

Discussions and native English language support

n.n. yet

Compilation

Rainer Haeßner



More exercises …