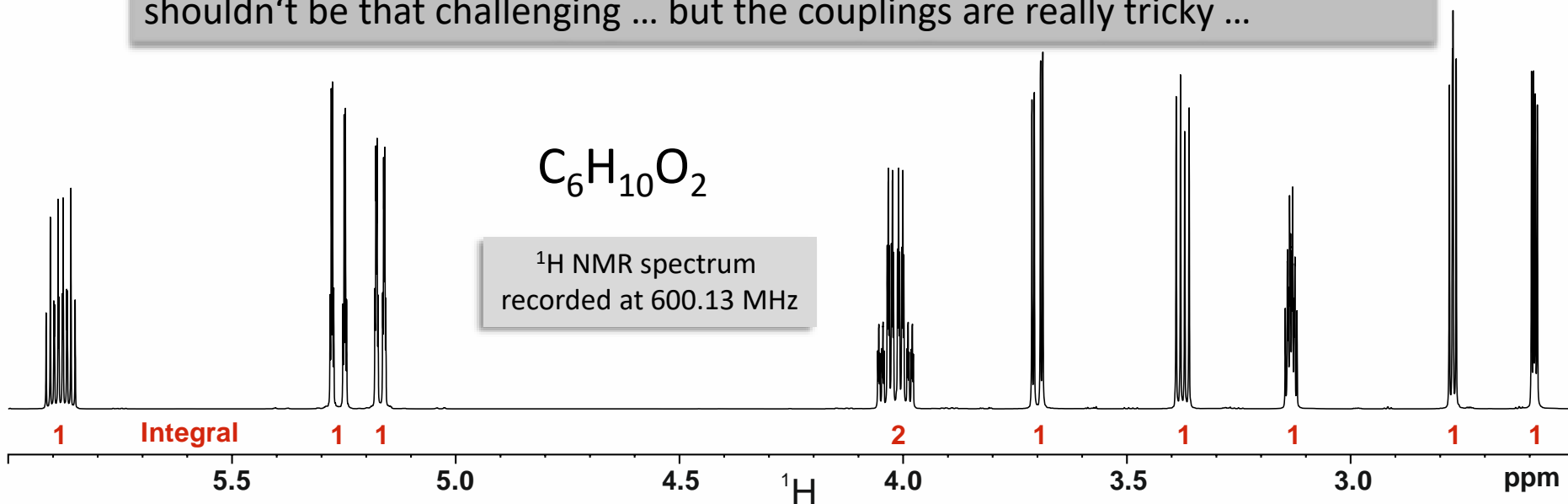


Problem of the Month:

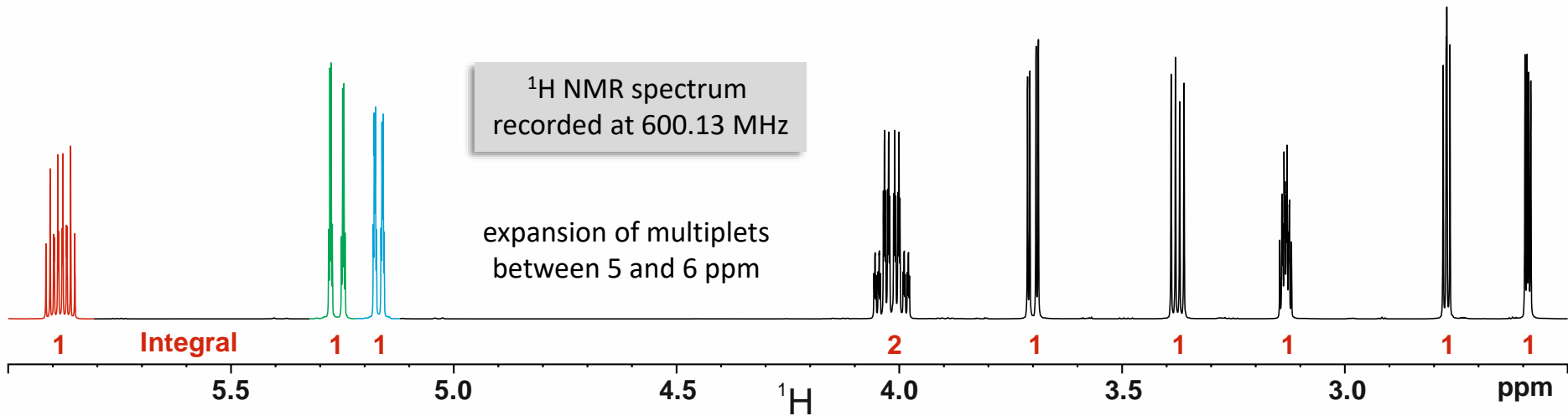
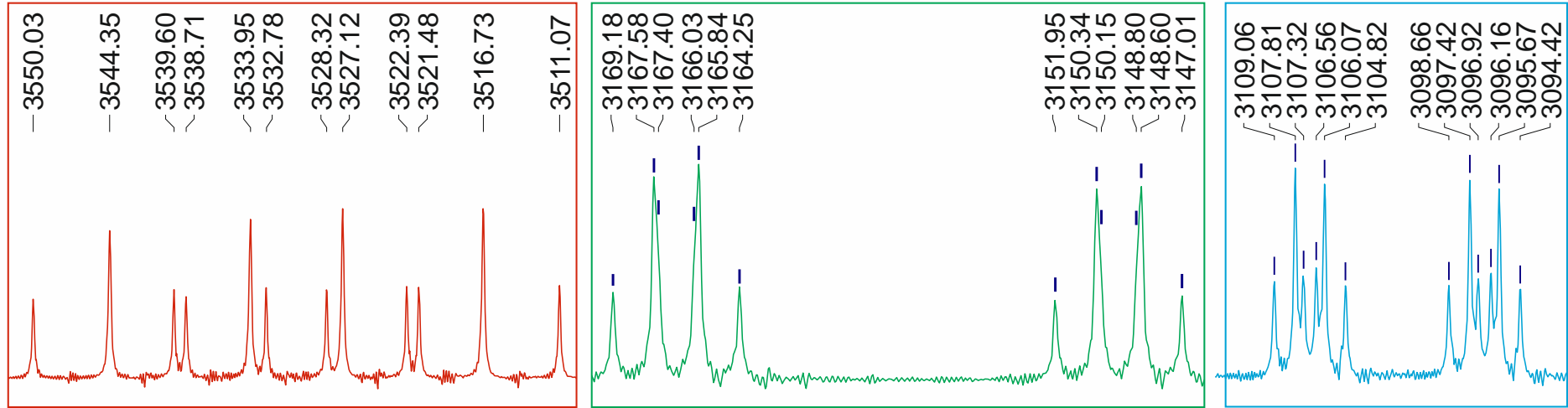
December 2020

Deduce the constitution, assign all nuclei (stereochemically correct as far as possible) and work out all proton-proton coupling constants

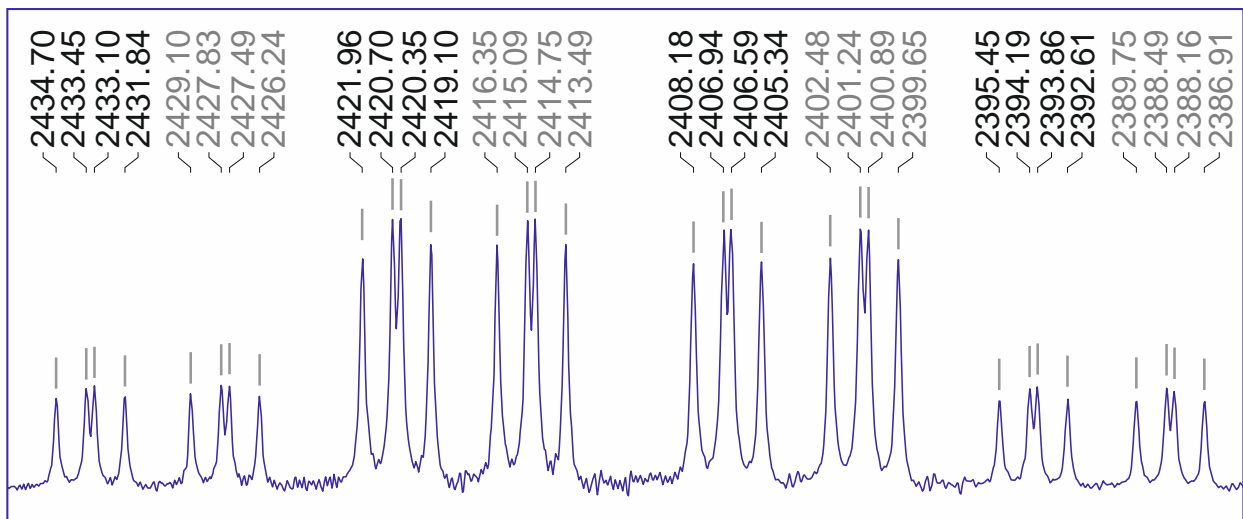
Finding the constitution using HSQC, COSY and the one dimensional spectra shouldn't be that challenging ... but the couplings are really tricky ...



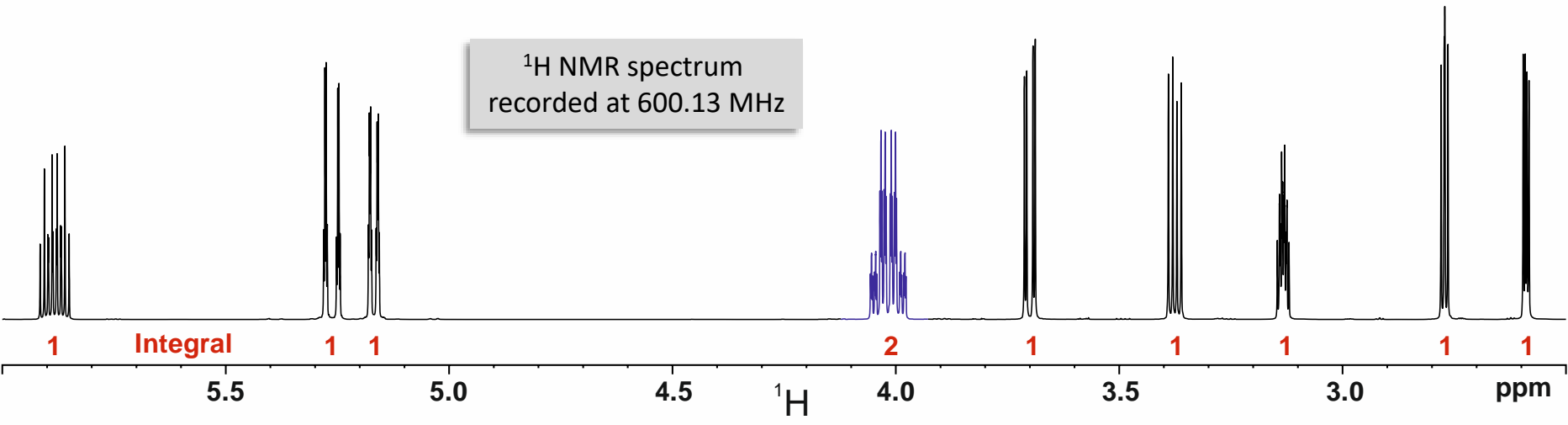
Problem of the Month:



Problem of the Month:

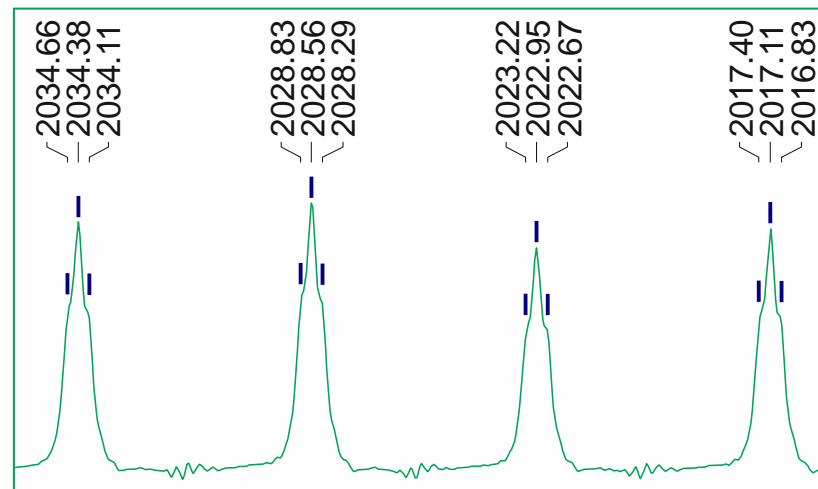
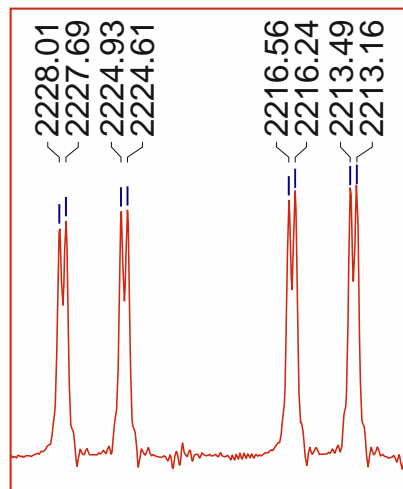


expansion of multiplet at 4 ppm

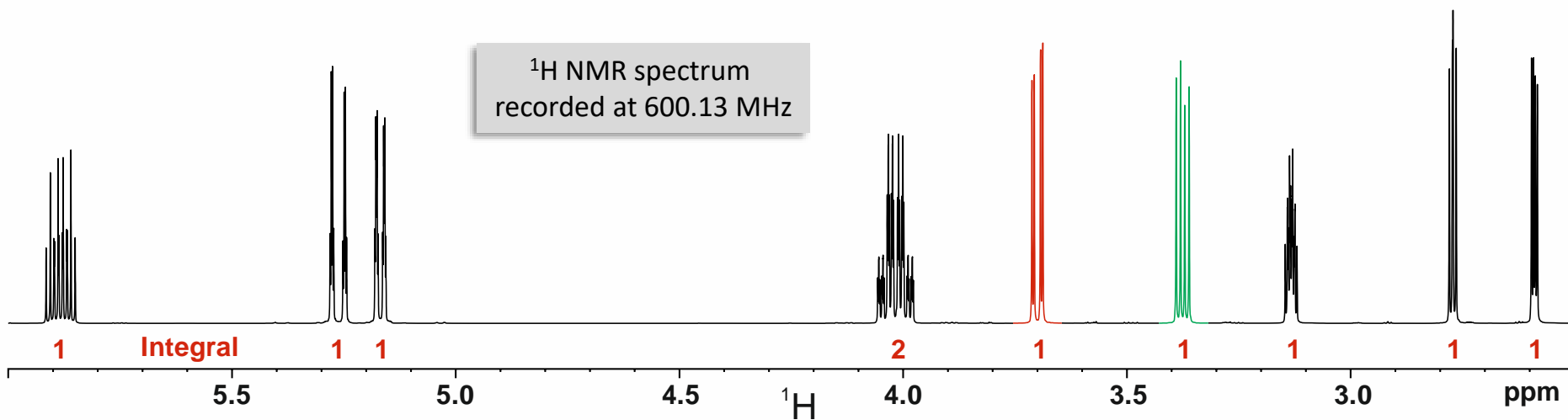


Problem of the Month:

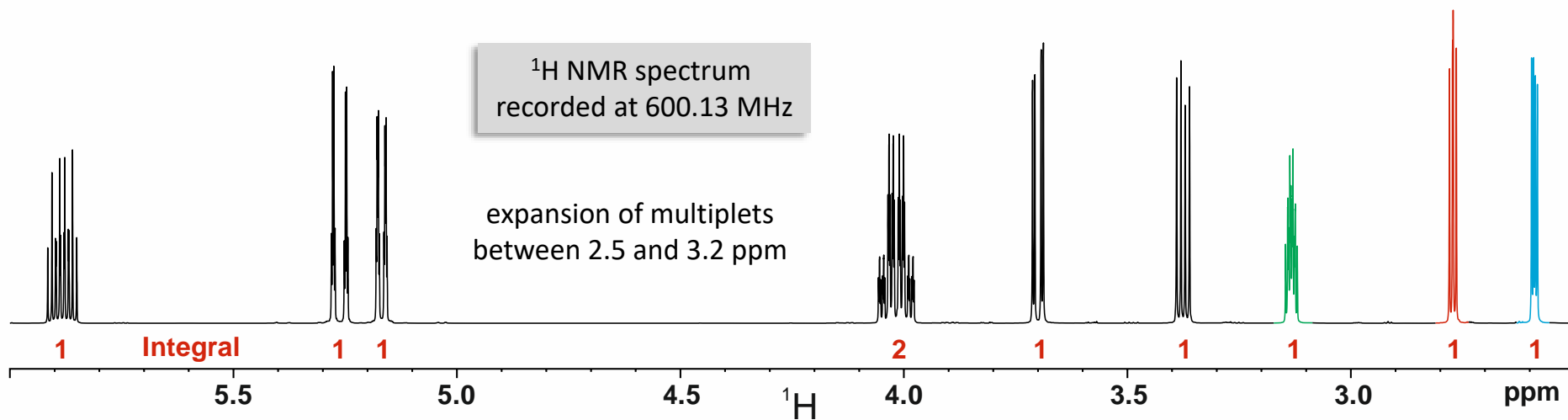
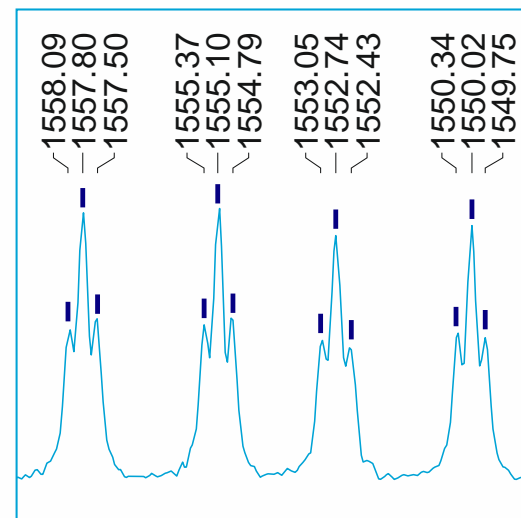
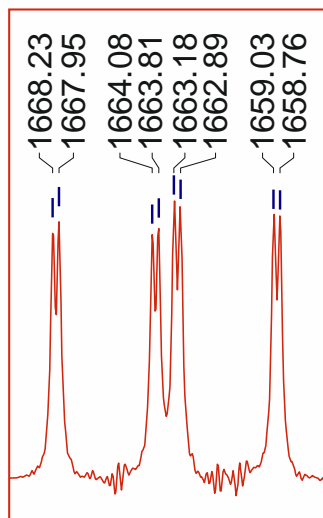
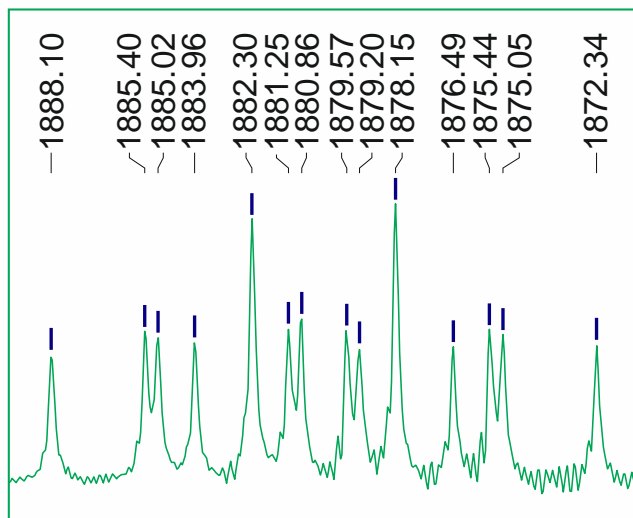
expansion of multiplets
between 3.3 and 3.8 ppm



^1H NMR spectrum
recorded at 600.13 MHz



Problem of the Month:



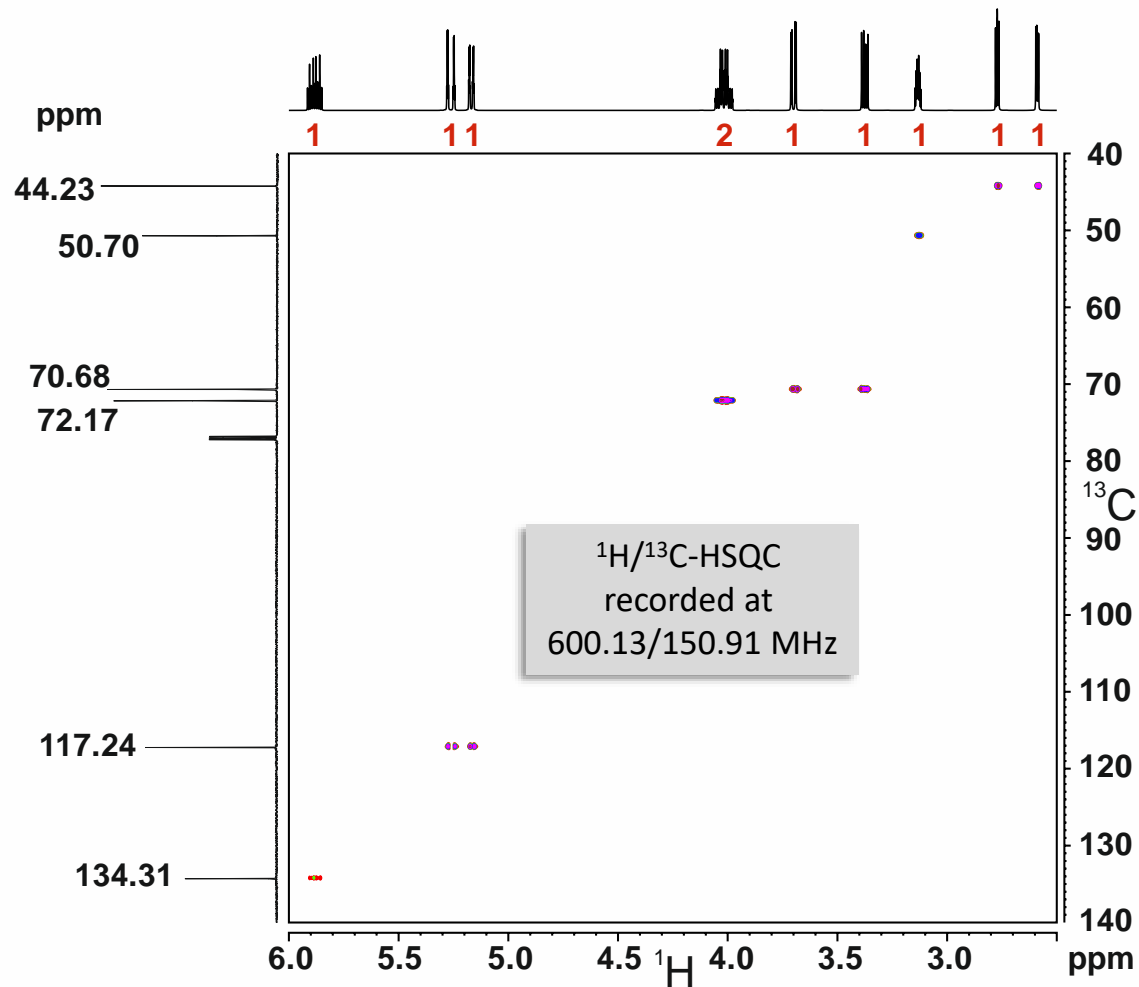
Problem of the Month:

December 2020

Step by step:

To get the constitution, initially you don't need to analyze the structure of the proton multiplets.

Use the ^{13}C projection to get all ^{13}C NMR signals. There are no quaternary carbon atoms as you see if you compare this HSQC with the molecular formula.



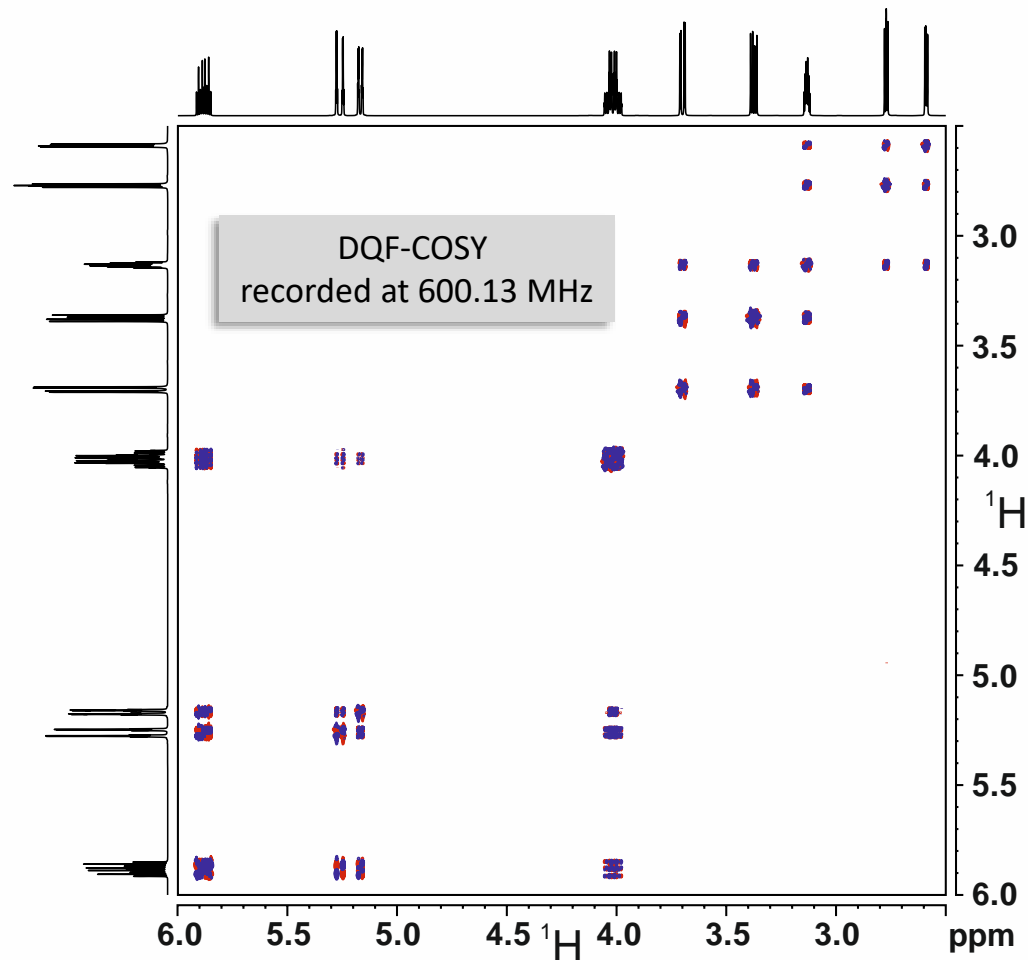
Problem of the Month:

December 2020

Step by step:

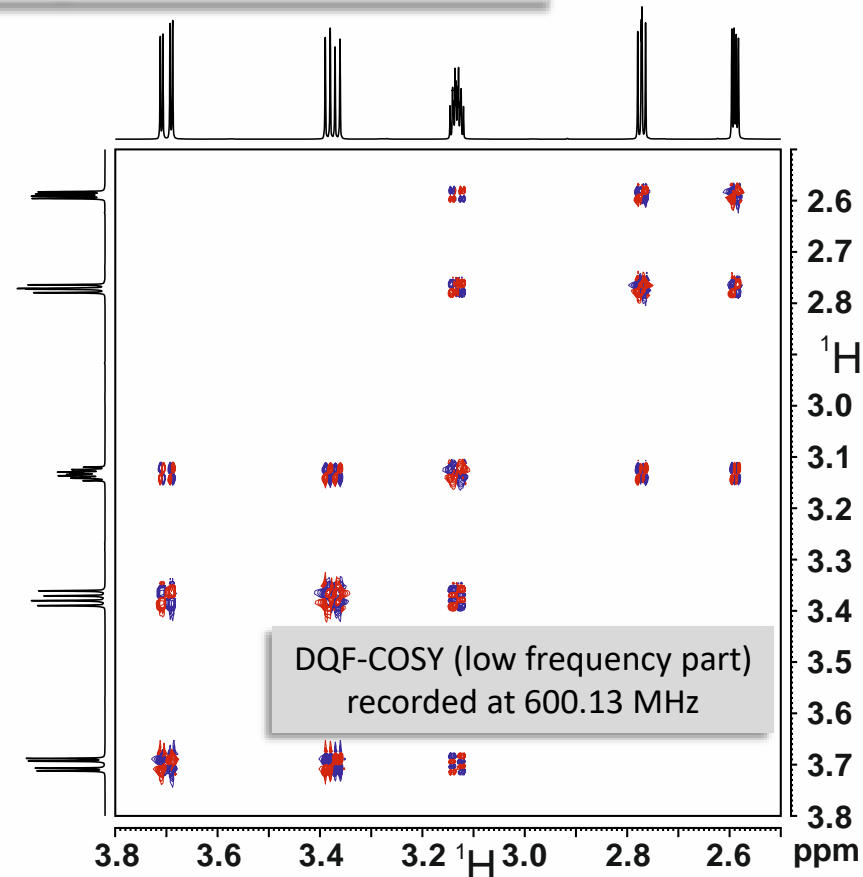
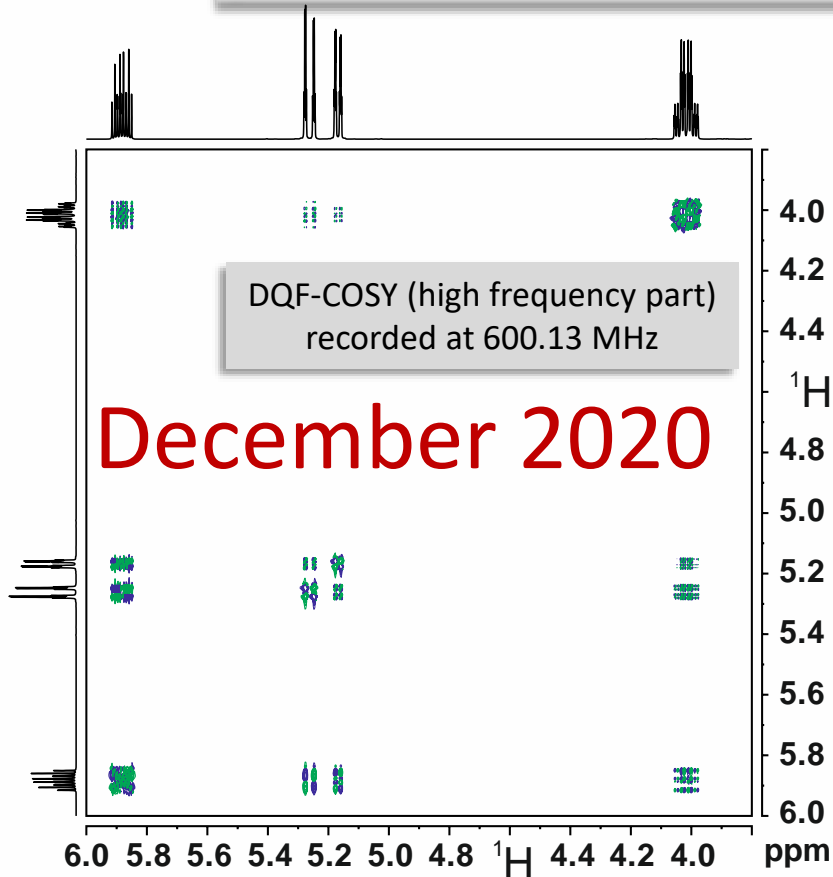
HSQC and COSY are enough to get the constitution.

The COSY can be separated into two independent subspectra.



Problem of the Month:

These are the somewhat easier to handle subspectra. No more pieces of information are necessary to get the constitution.



Problem of the Month:

December 2020

Strategy

- (1) Initially, you might calculate the degree of unsaturation (DBE) from the given molecular formula.
- (2) Find out which spin systems are available in the molecule. Use H,C HSQC and H,H COSY spectra for that purpose.
- (3) How are the fragments connected? A detailed analysis of the multiplets (including size of couplings) can be very helpful. There is a nice tool to simulate spin systems at nmr.cheminfo.org
- (4) In case that you are stuck (no HMBC) you can use [nmrshiftdb's prediction](http://nmrshiftdb.org) to check your structure proposals.