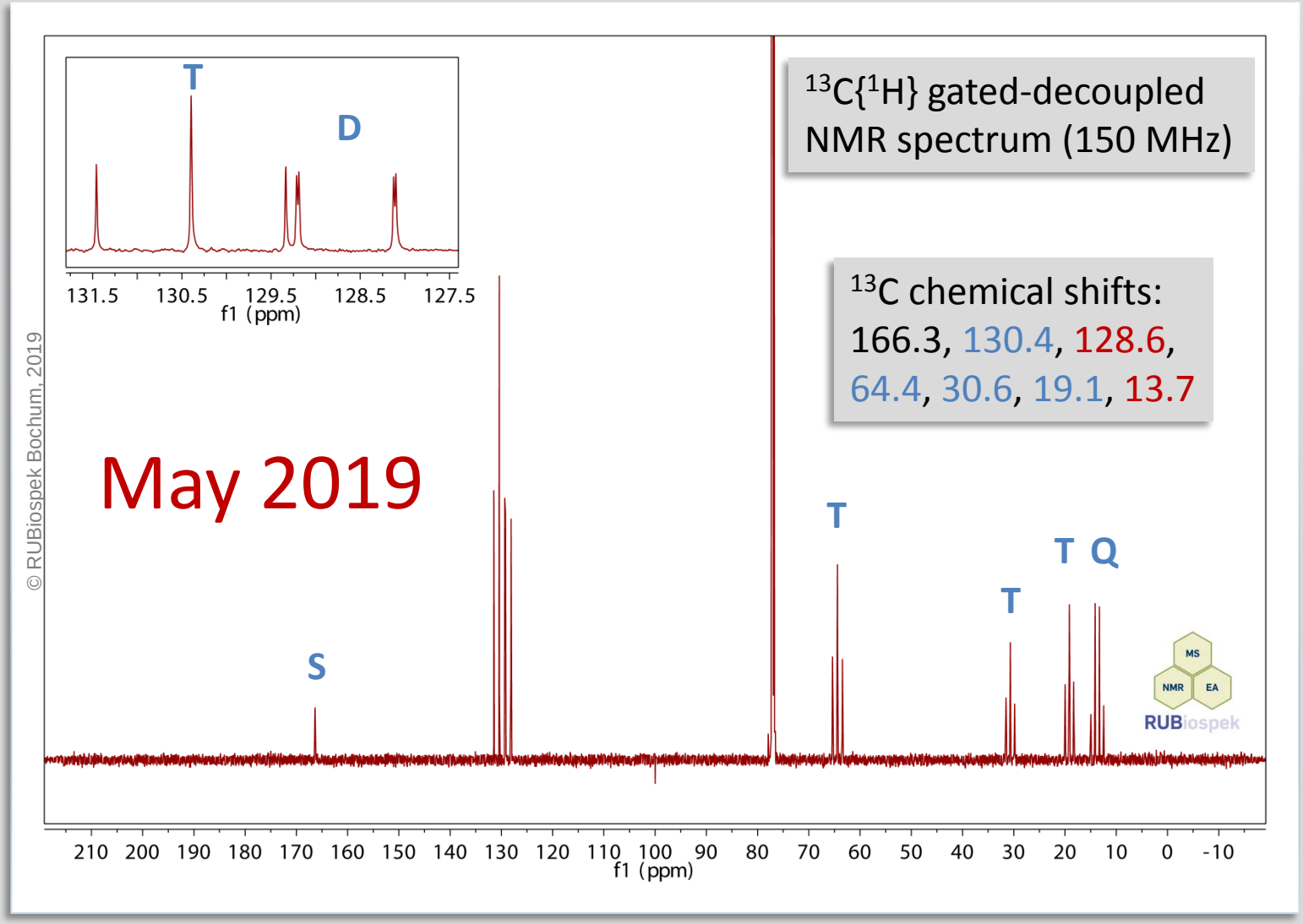
Problem of the Month:



Problem of the Month:
May 2019

Strategy

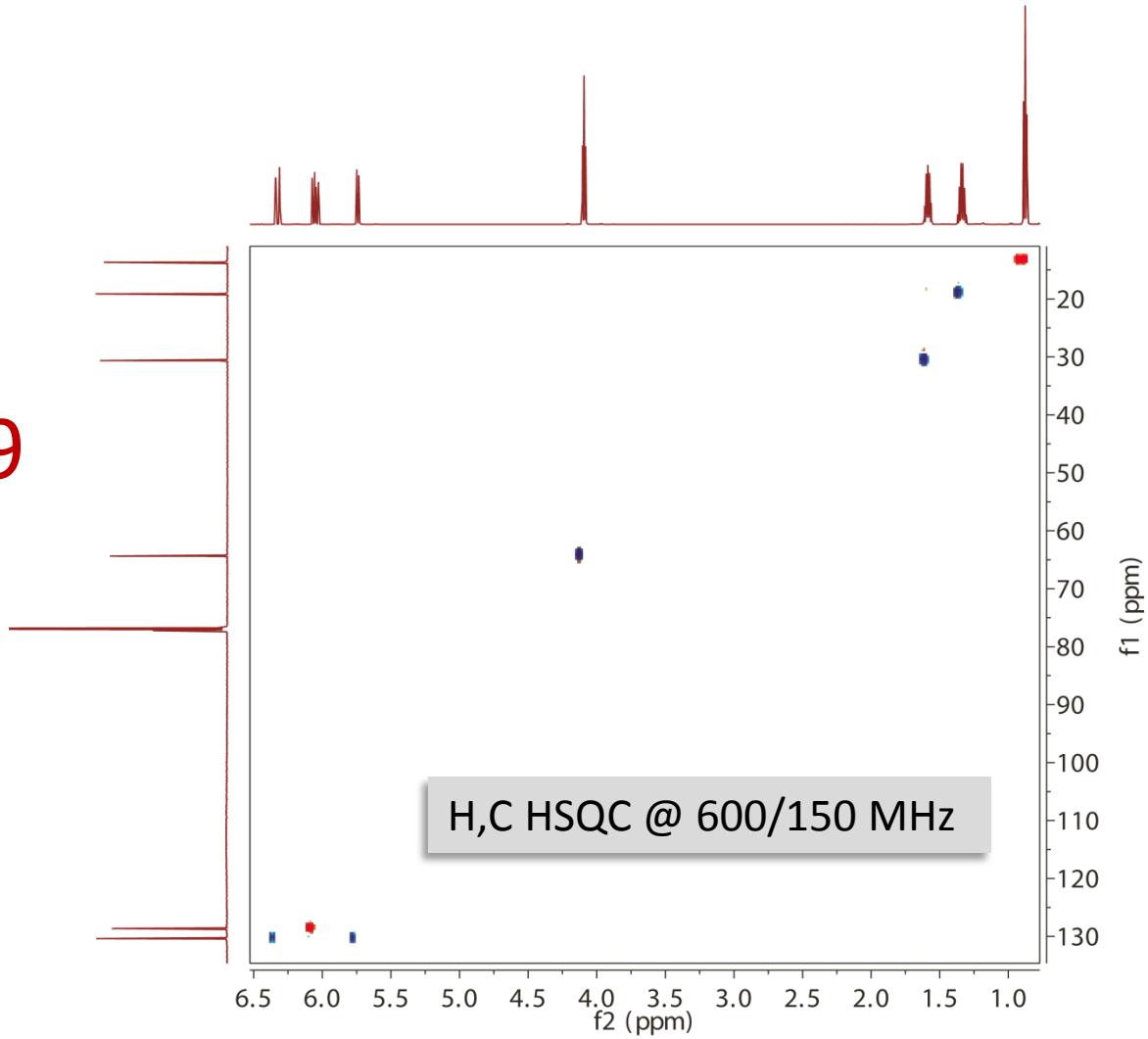
(1) Our 'cover' shows a type of ^{13}C NMR experiment which preserves coupling to ^{1}H. Thus, it is possible to identify the multiplicity of carbon atoms [note, however that this experiment is insensitive as compared to ^{1}J H,C correlations]

(2) On the next page, you will see the ‚modern' version of the same experiment [CH and CH_3 groups give positive cross peaks (red), CH2 groups give negative cross peaks (blue). Quaternary carbons, as well as OH protons, do not yield any crosspeaks].

(3) As always, it is helpful to calculate the degree of unsaturation (DBE) from the molecular formula: $C_7H_{12}O_2$.

Problem of the Month:

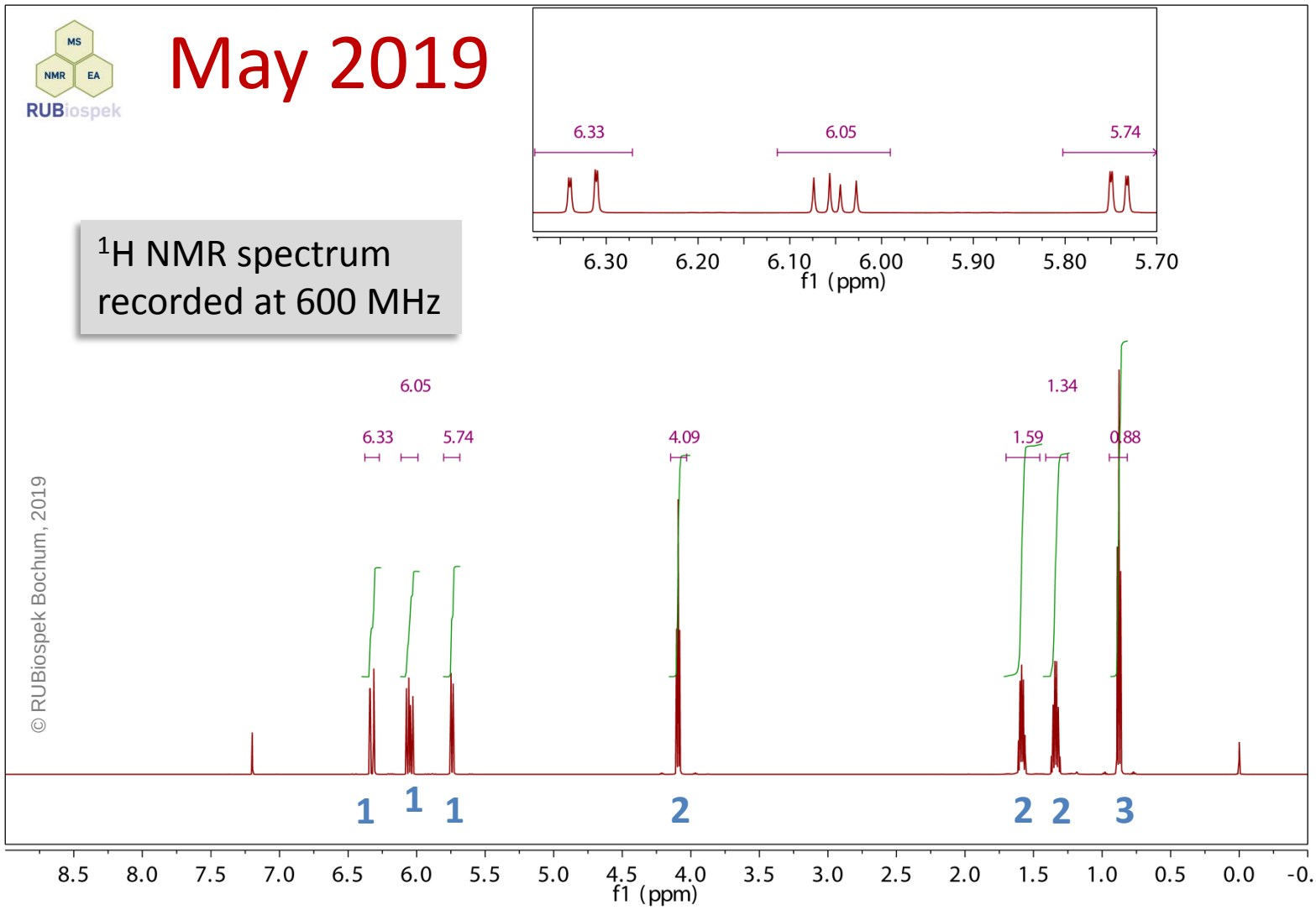
May 2019



Problem of the Month:

May 2019

^{1}H NMR spectrum recorded at 600 MHz



Problem of the Month:

May 2019

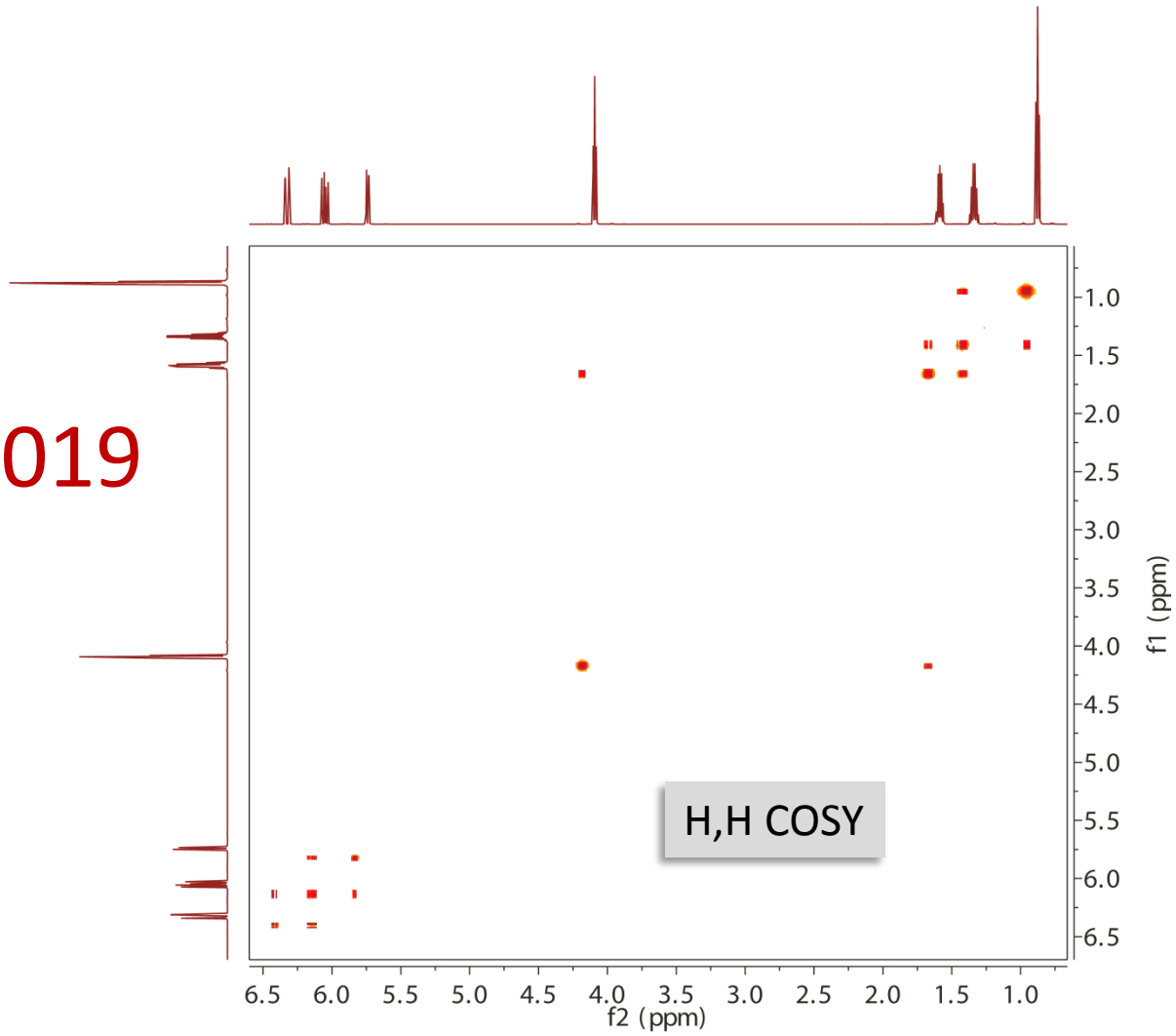
Hints

(1) There are two groups of spin systems in this molecule - they can be verified conveniently with a H,H COSY spectrum (next page).

(2) Even though there is no HMBC correlation provided here, chemical shifts and H,H correlations help to connect the fragments across the only existing quaternary carbon.

Problem of the Month:

May 2019



Problem of the Month:
May 2019

Solution

(1) The molecule of May could be almost solely elucidated through proton experiments. The only carbon that does not connect to any proton is typical for carboxylic acids and their derivatives.

(2) The two spin systems are divided into an olefinic AMX and an aliphatic $A_2M_2P_2X_3$ part. The olefinic couplings may be estimated, since 1 ppm corresponds to 600 Hz at the field strength employed for these experiments.

(3) On www.nmr.cheminfo.org, there is a nice tool to simulate the ^{1}H NMR spectrum: In the third row, select ‚predict 1H' and simply draw the assumed structure with the editor and compare [if you got real spectra, you may even superimpose them as a jcamp file via drag-and-drop].

(4) If you are still in doubt - the correct structure is found at http://www.nmrshiftdb.org/molecule/60004995.