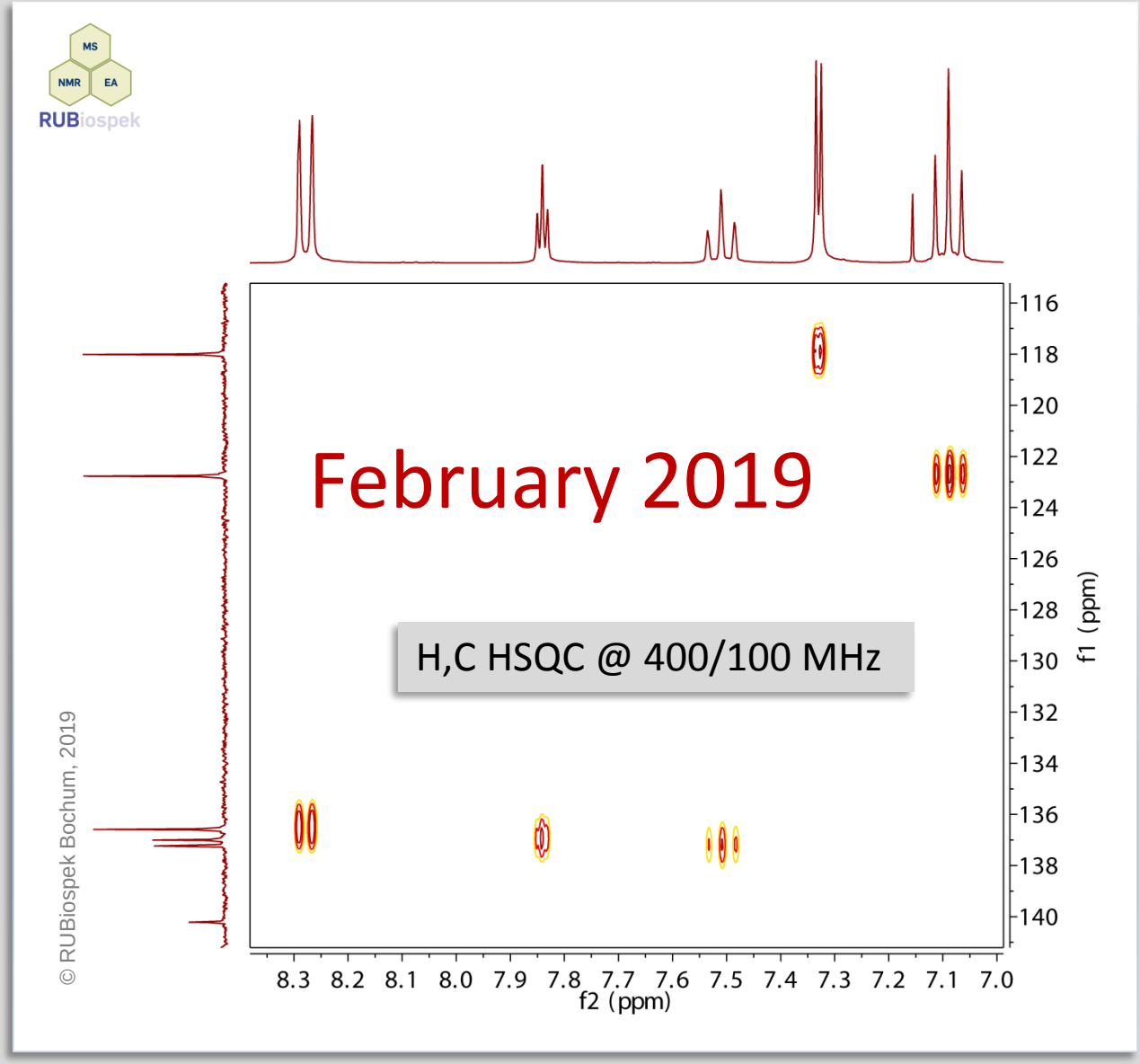
Problem of the Month:



Problem of the Month:
February 2019

Strategy

(1) The degree of unsaturation (DBE) can be derived from the molecular formula: $C_{10}H_8$.

(2) Check the number of distinct signals for carbon and hydrogen NMR: This will give you a clue.

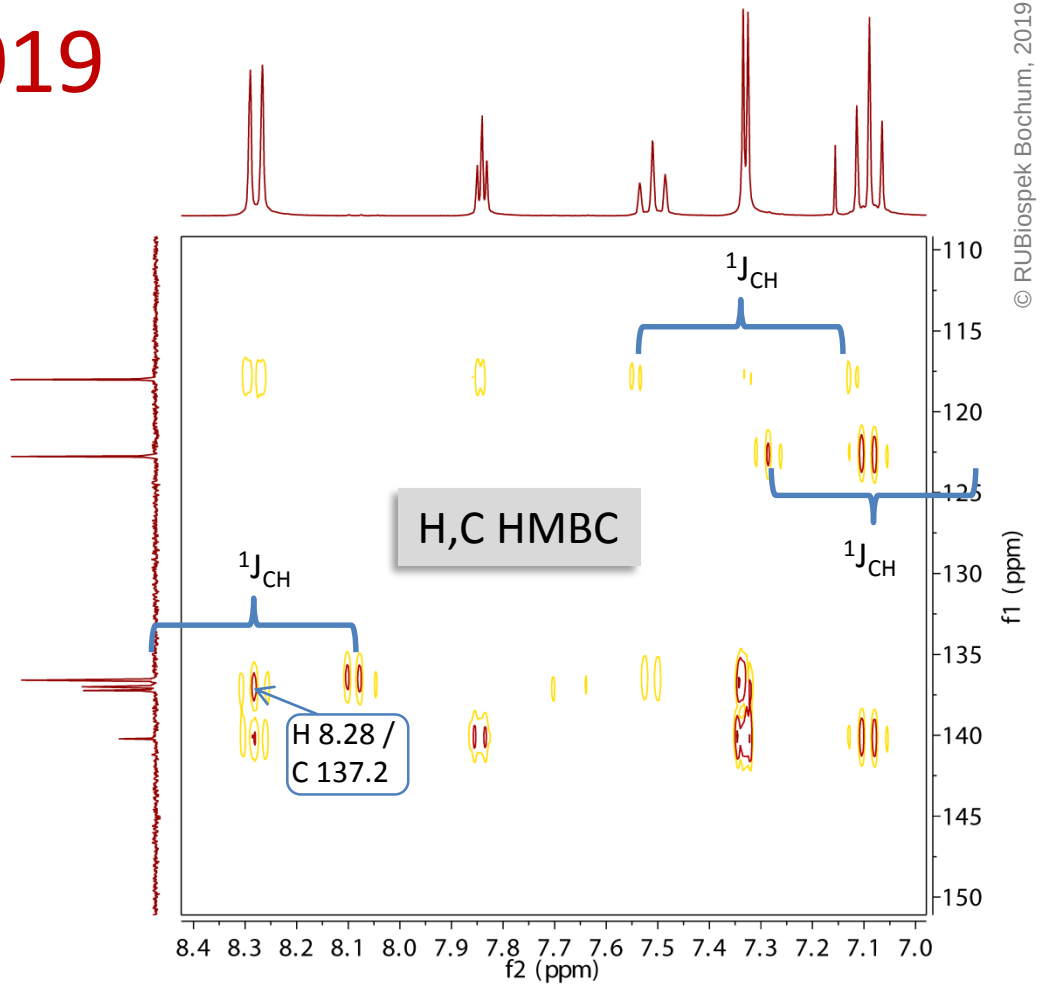
(3) Carefully analyse the structure of the multiplets visible in the 1D ^{1}H NMR spectrum - if you are struggling, there is a H,H COSY provided, too.

Problem of the Month:

February 2019

^{13}C chemical shifts:
140.2, 137.2, 137.0,
136.6, 122.8 , 118.0

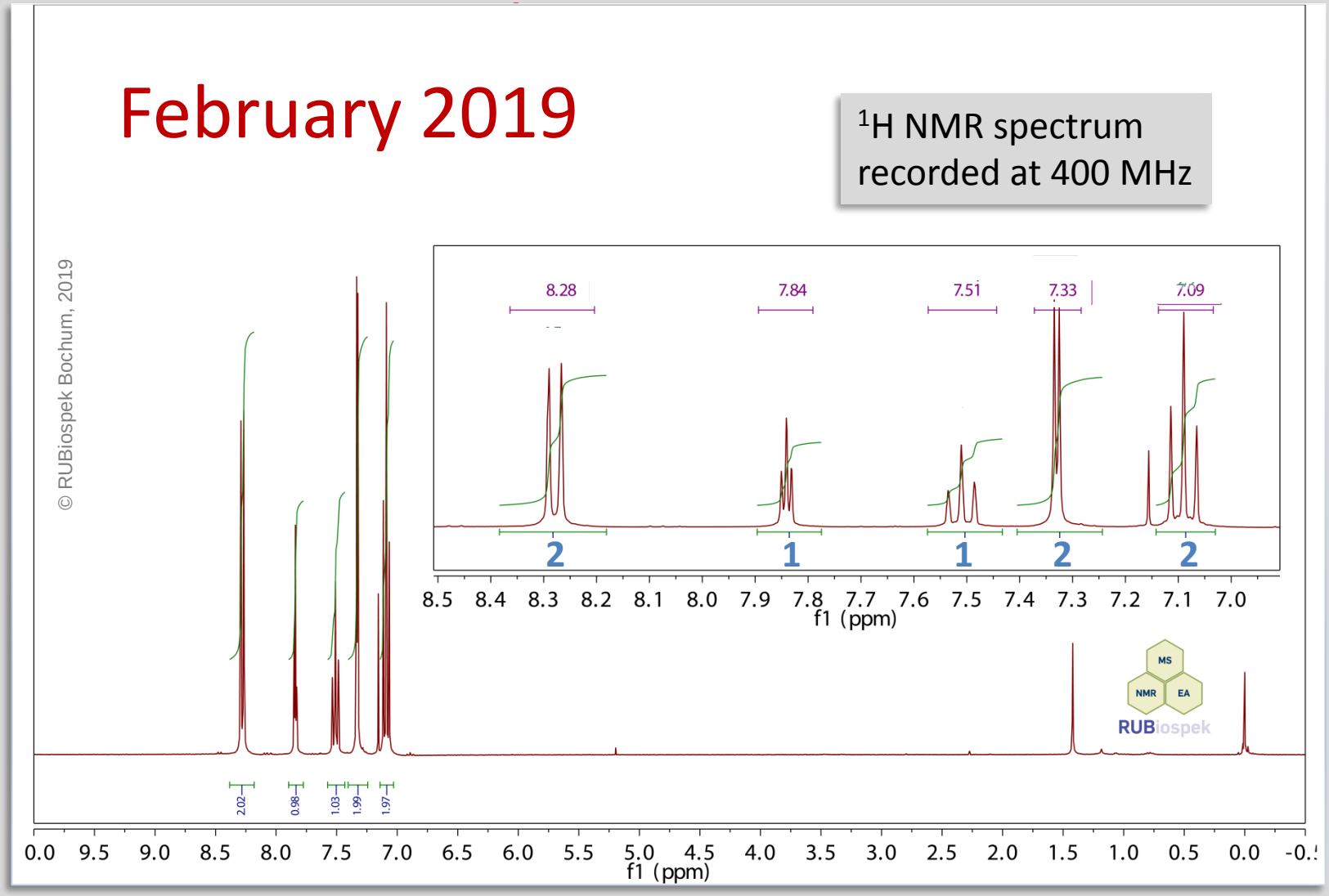
^{1}H chemical shifts:
8.28, 7.84, 7.51,
7.33, 7.09



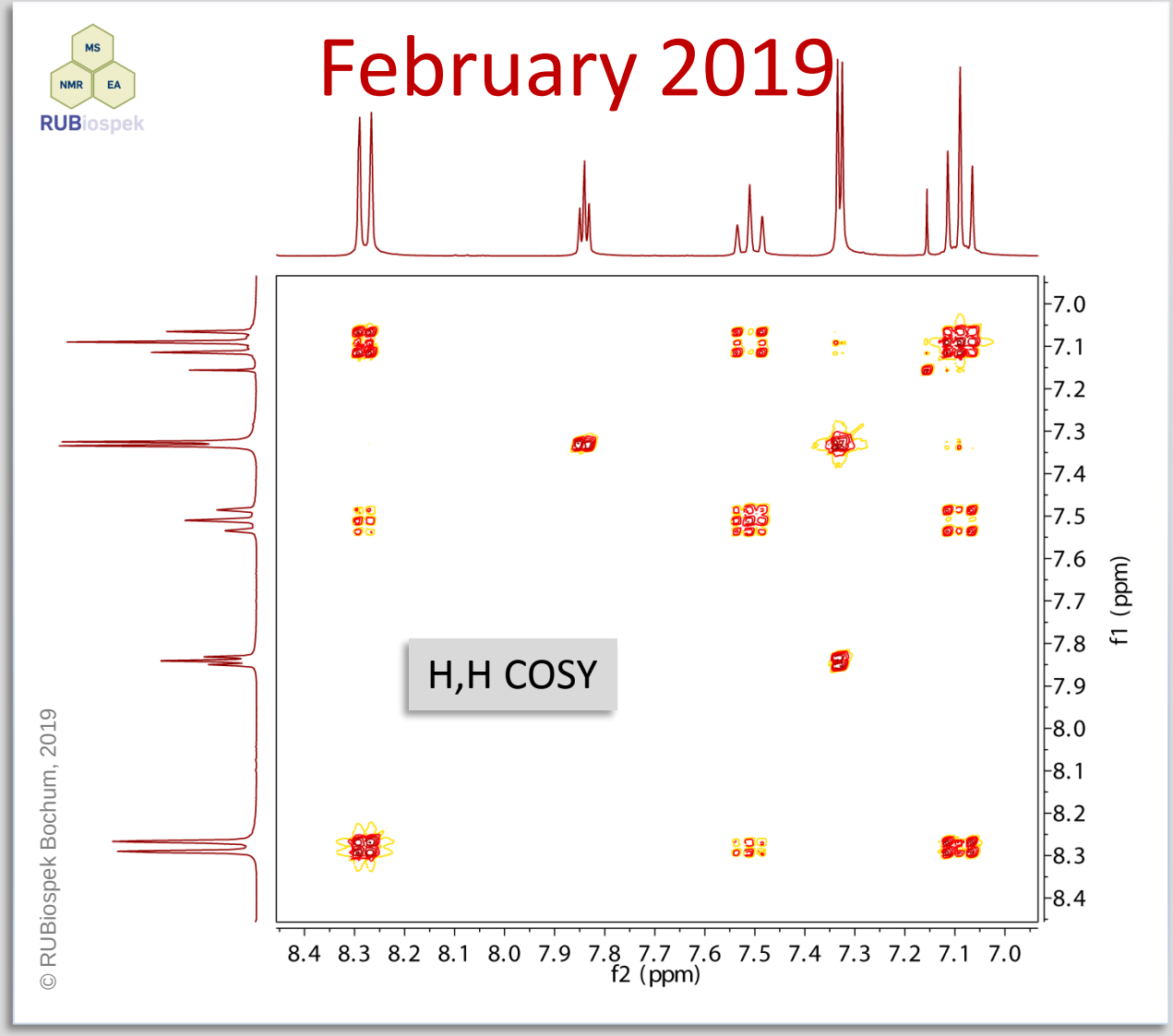
Problem of the Month:

February 2019

^{1}H NMR spectrum recorded at 400 MHz



Problem of the Month:



Problem of the Month:
February 2019

Hints

(1) It is most important to recognise the symmetry of the compound - all chemically equivalent atoms give rise to one common signal. Integration of proton signals is given below the corresponding peaks.

(2) In the HMBC, most of the cross peaks derive from $^{3}J_{CH}$ coupling. In the COSY experiment, two spin systems may be identified - caution, there are also long range correlations visible ($> {}^{3}J_{HH}$).

Problem of the Month:
February 2019

Solution

(1) The molecule of February is quite symmetric - there are four positions that exists twice. Also, it is an aromatic compound for the chemical shifts in the proton spectrum, it contains 7 DBE.

(2) The two spin systems are divided into an AX_2 and an AA‘MM‘X part. You may simulate such a 5-spin system at http://nmr.cheminfo.org (middle box in the ‚tools‘ section, choose ABCDE system and set δ 8.28 for A/B, 7.51 for C and 7.09 for D/E. Providing uniform ^3J couplings of 7 Hz between A/D, B/E, C/D and C/E is sufficiently accurate).

(3) Connecting the annulated system is feasible through HMBC correlations. If you are still in doubt - enter the chemical shifts of the ^{13}C signals (compare results with and without carbon multiplicities, i.e. S = no proton attached, D = proton attached) in nmrshiftdb2‘s search function.