

EXAMPLE 2: Camphour: HSQC/COSY/HMBC

STEP 1: 1D spectra

^{13}C : number of carbons, 1 C=O

^1H : number of protons

combine with mass to get molecular formula

STEP 2: HSQC

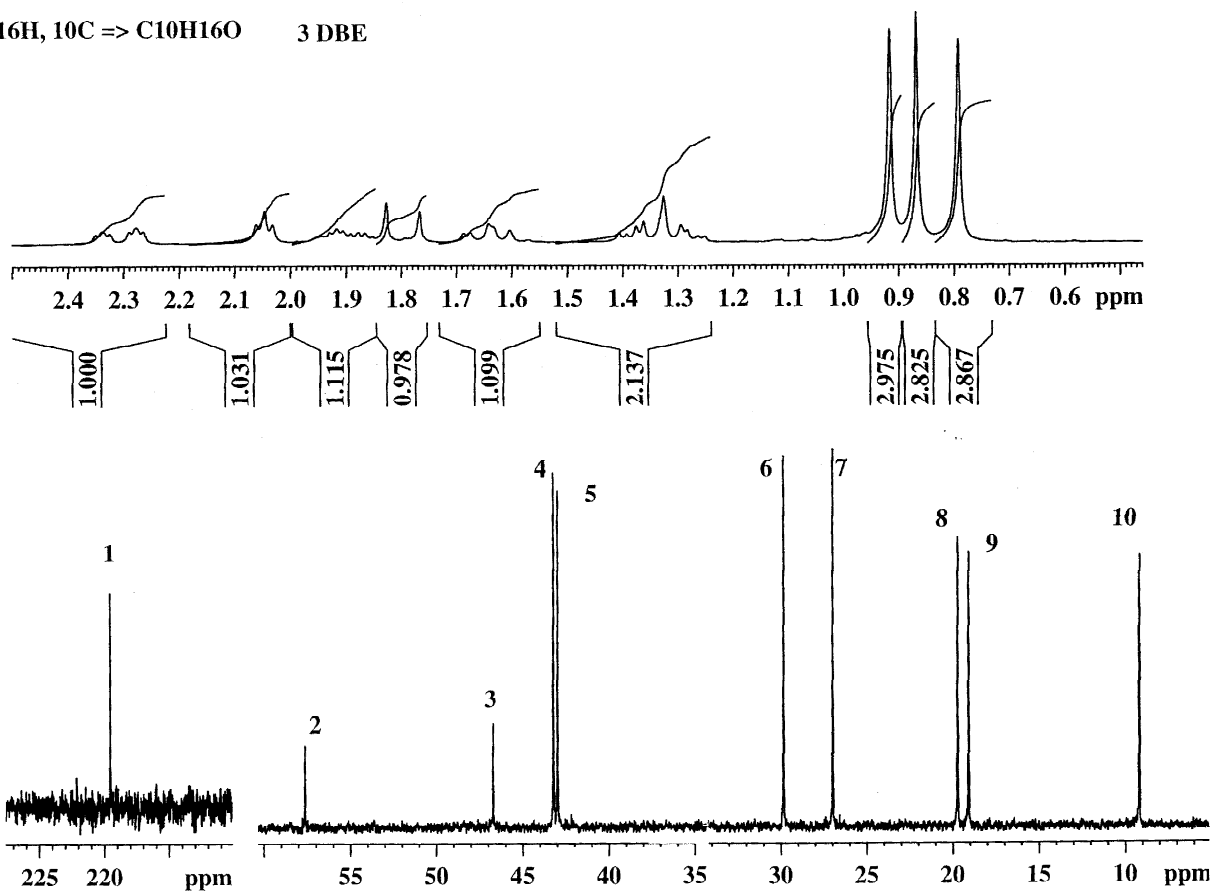
- identify diastereotopic pairs of protons
- relate protons to carbon atoms

STEP 3: COSY

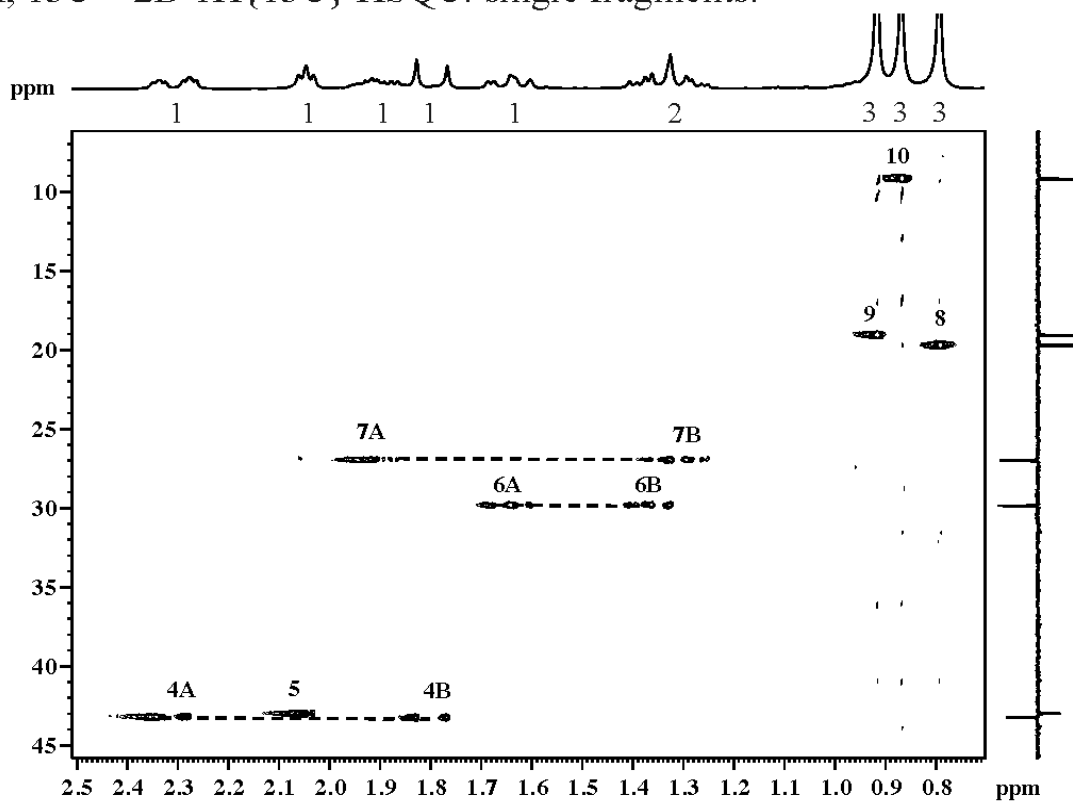
- connect neighbored CH fragments

M = 152.2

16H, 10C \Rightarrow C₁₀H₁₆O 3 DBE



1D ¹H, ¹³C + 2D ¹H{¹³C} HSQC: single fragments:



C₁₀H₁₆O
MW: 152.2358

*1
219.54

*2
57.61

*3
46.71

*4
43.23 (1.80) (2.30)

*5
42.98 (2.05)

*6
29.84 (1.38) (1.65)

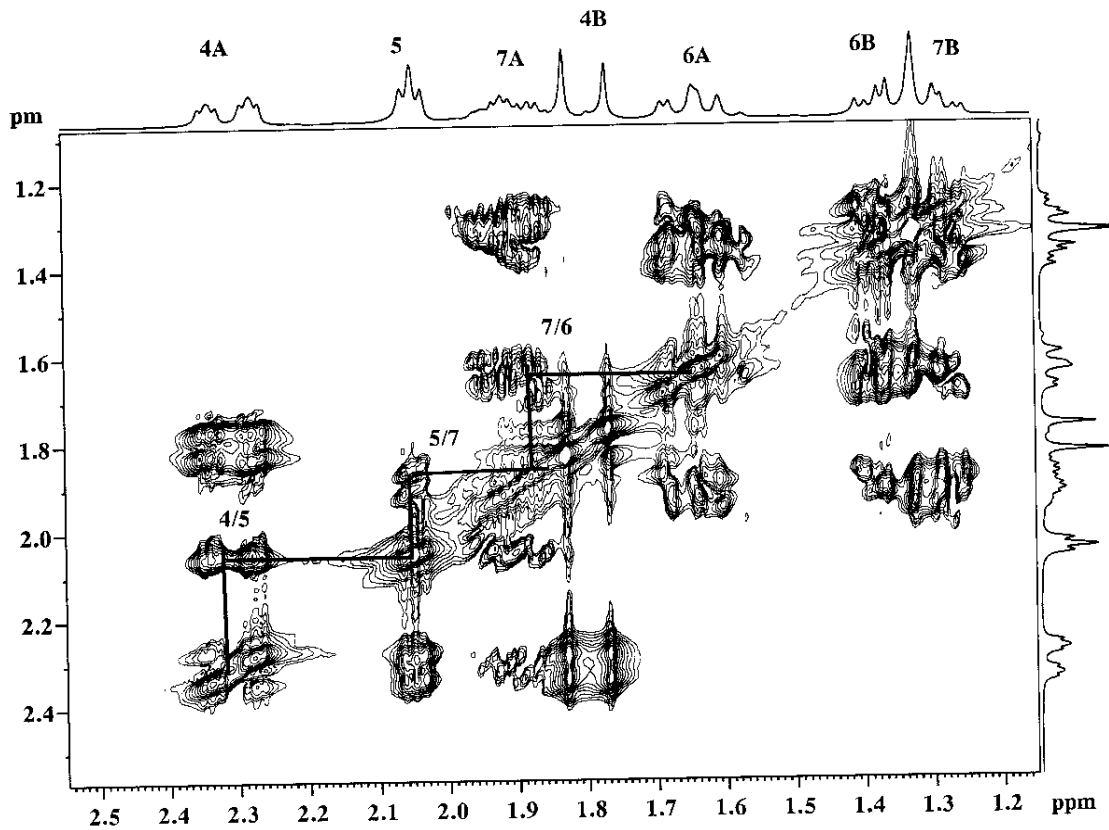
*7
26.98 (1.28) (1.91)

*8
19.71 (0.79)

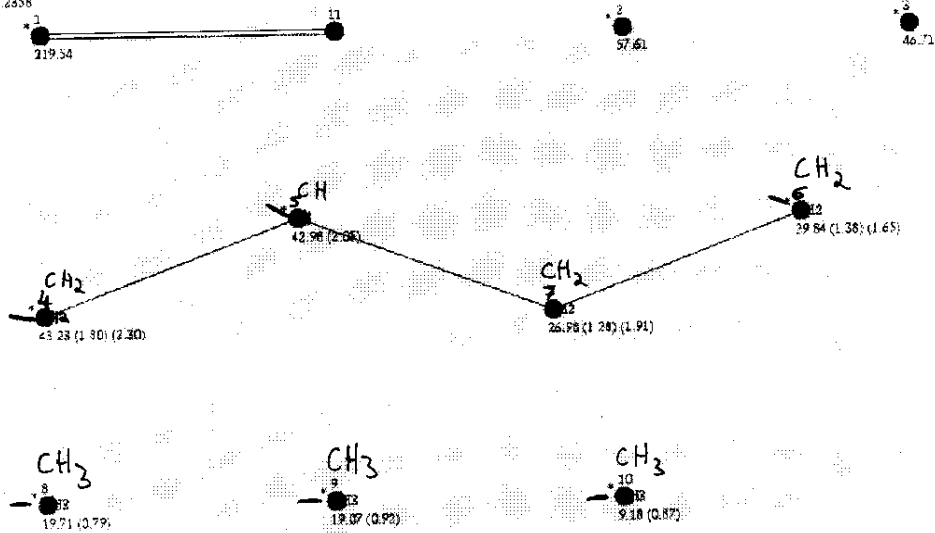
*9
19.07 (0.92)

*10
9.18 (0.87)

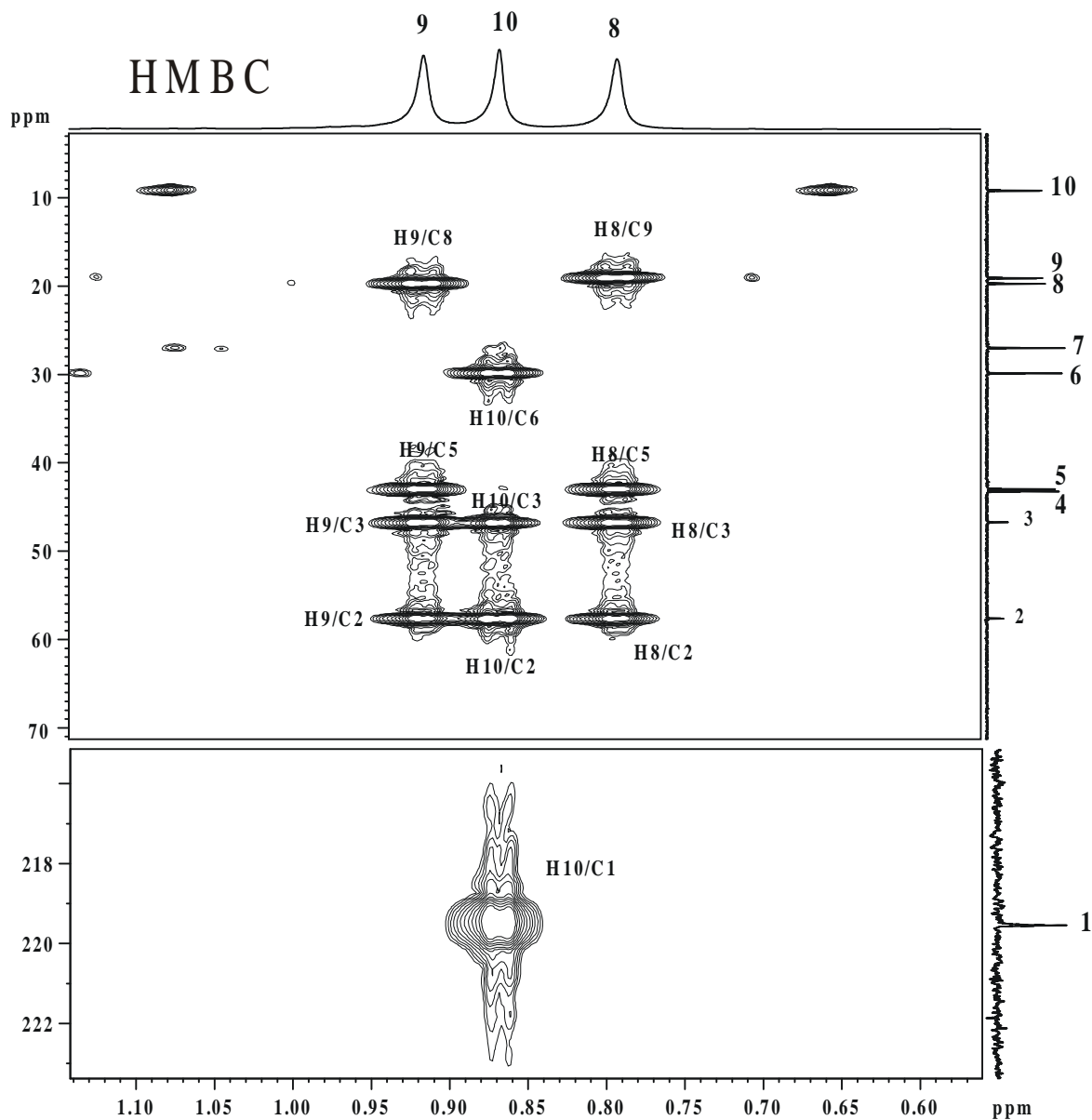
*11



C10H16O
MW 152.2358



It becomes evident that COSY is very limited in completing the structure elucidation in this case. In particular the location of the methyl groups is still unknown, and the connectivity across tertiary C atoms is not available from COSY => HMBC will be necessary.

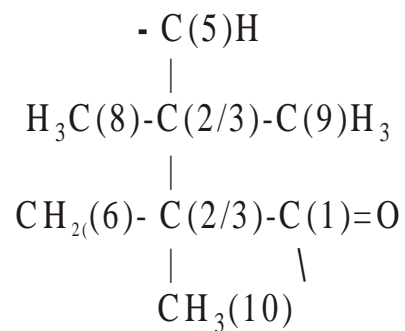


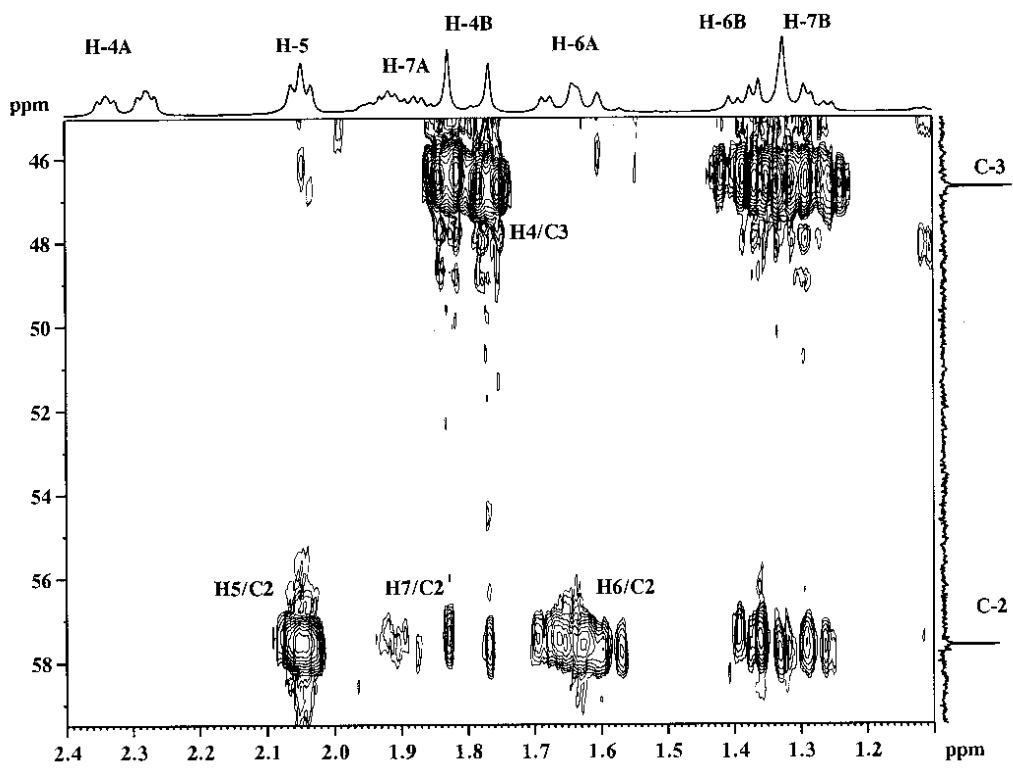
- only H-10 is coupled to C-1 (CO)

- methyl groups 9 and 8 see each other

- all methyl groups coupled to tertiary carbons C-2 and C-3

- Methyl group 10 coupled to CH₂-6, 9 and 8 to CH₂-5





C₁₀H₁₆O
MW: 152.2358

