

¹H-NMR

Discussion

Part 1

March/2021

How to study

1] Elementary particles such as electrons and nucleus have magnetic feature.

- a) True
- b) False

2] What do you expect to observe in the ^1H NMR spectrum of chloroethane $\text{CH}_3\text{CH}_2\text{Cl}$?

- a) A doublet and a quartet
- b) Two doublets.
- c) A triplet and a quartet
- d) A doublet and a triplet.

3] Which of the following compounds contains one or more protons that could undergo exchange with D_2O

- a) CH_3OH
- b) $(\text{CH}_3)_3\text{N}$
- c) $(\text{CH}_3)_2\text{O}$
- d) CH_3Br

4] J-Coupling is _____ between adjacent peaks.

- a) Distance
- b) Distance ratio
- c) two-fold ratio
- d) All of these

- Predict the simple chemical structure of the molecular formula that matches the following spectrum ?
- Draw the HNMR spectrum of a given structure.
- Specify splitting patterns for a given structure.
- Explain why !!!!!
- How to distinguish between two compounds !!

Al-Azhar University
College of pharmacy
Pharmaceutical Chem. Dept.
Instrumental Analysis
Introduction , H-NMR

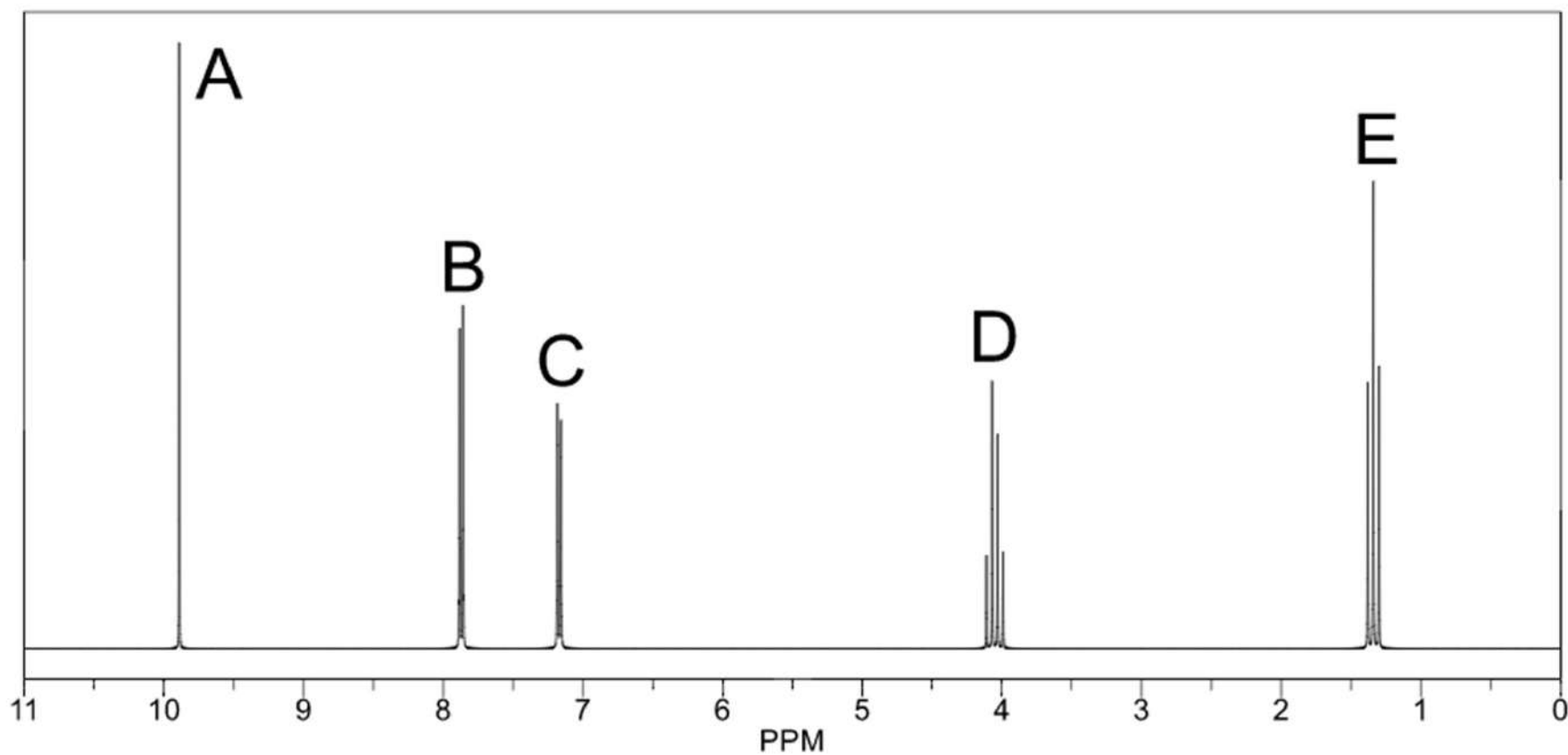
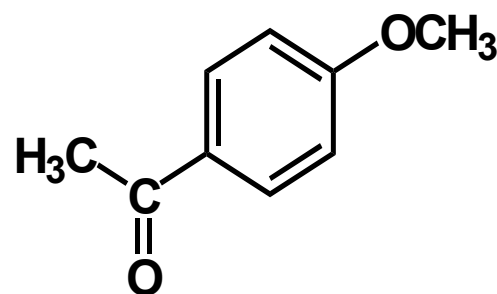
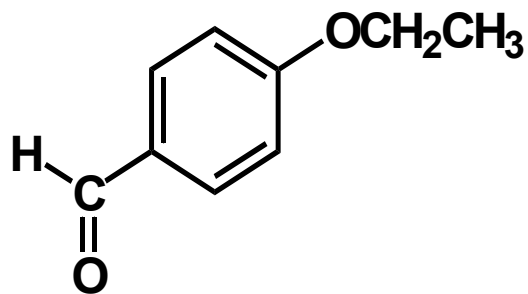
Dr. Kanan M. Al Wuhaidi



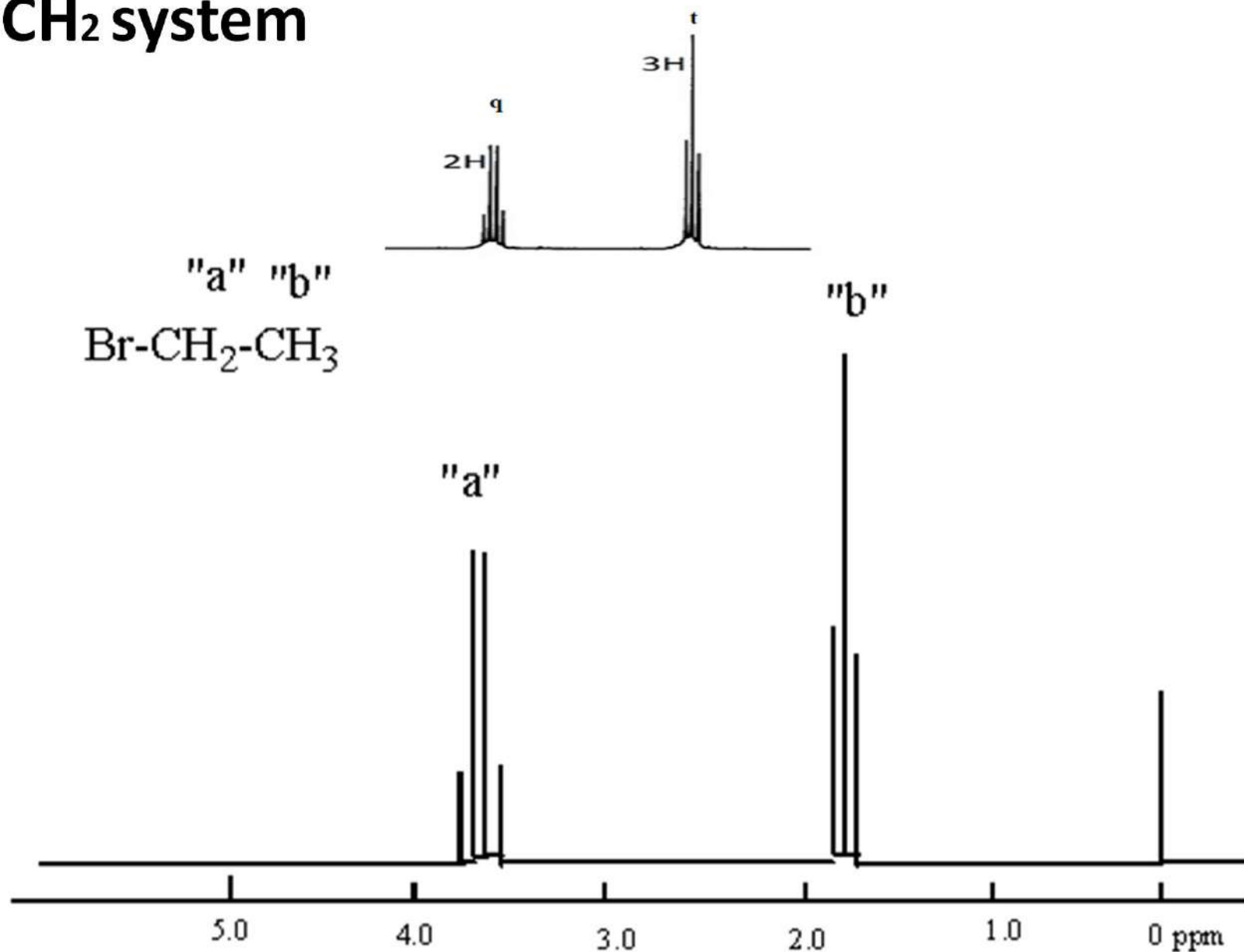
1. Explain in brief the difference between classic and modern methods for analysis
2. What is the difference between Precision and accuracy?
3. What is Spectroscopy?
4. What is the difference between Spectrum and spectrometer?
5. What is EMR?
6. Which part does the UV radiation affect in chemical structure?
7. Which part does the IR radiation use to investigate?

الرجوع الى الملزمة وفيها الاسئلة

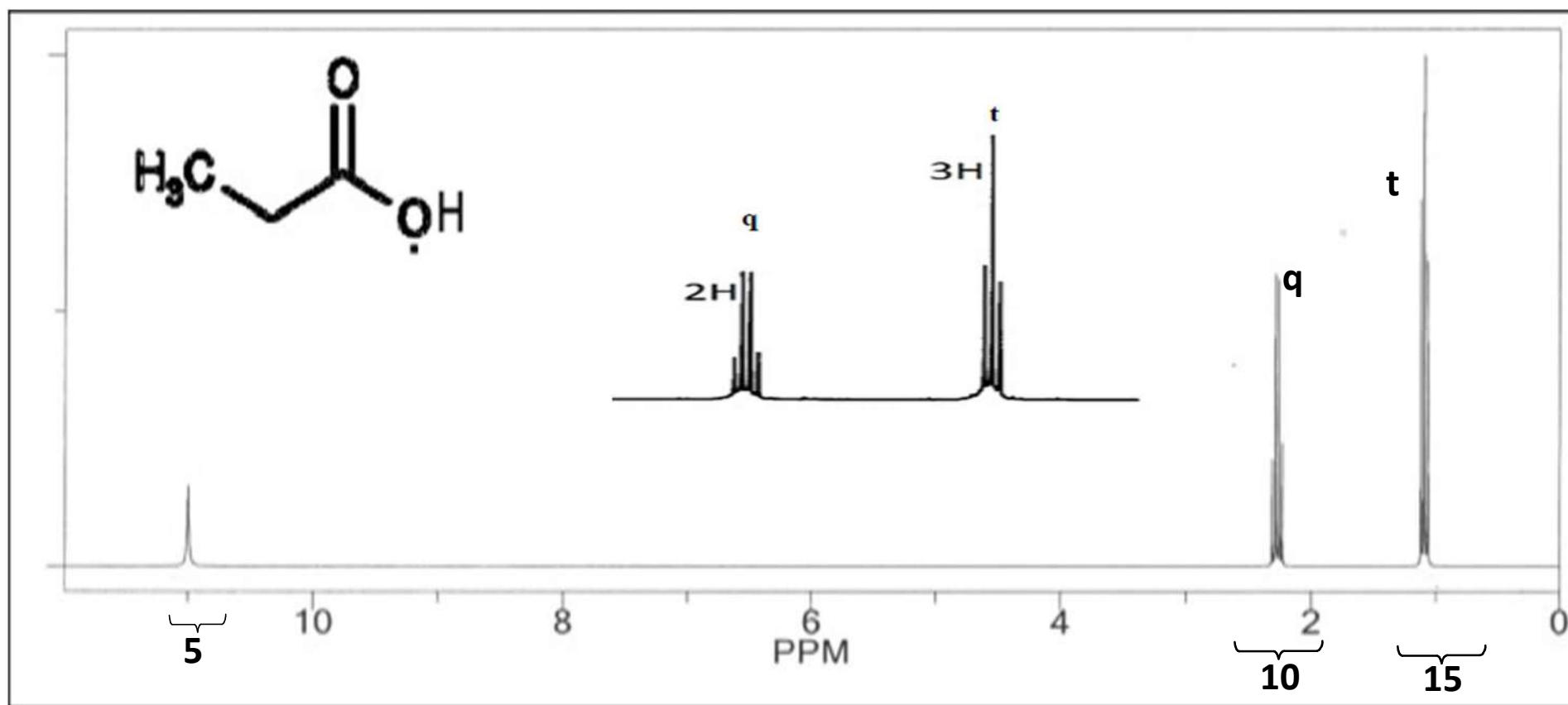
Distinguished Singlet C-H of aldehydes around 9 ppm.



Distinguished triplet and quartet peaks CH_3CH_2 system

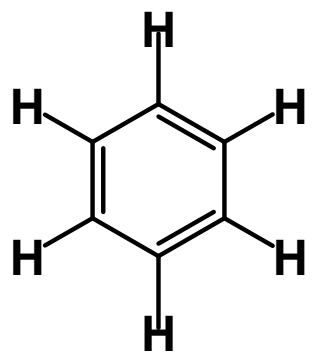


Propanoic acid

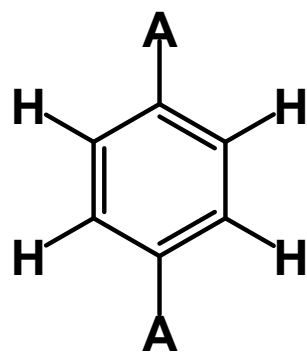


Ortho, meta and para disubstituted benzene (Distinguished para system)

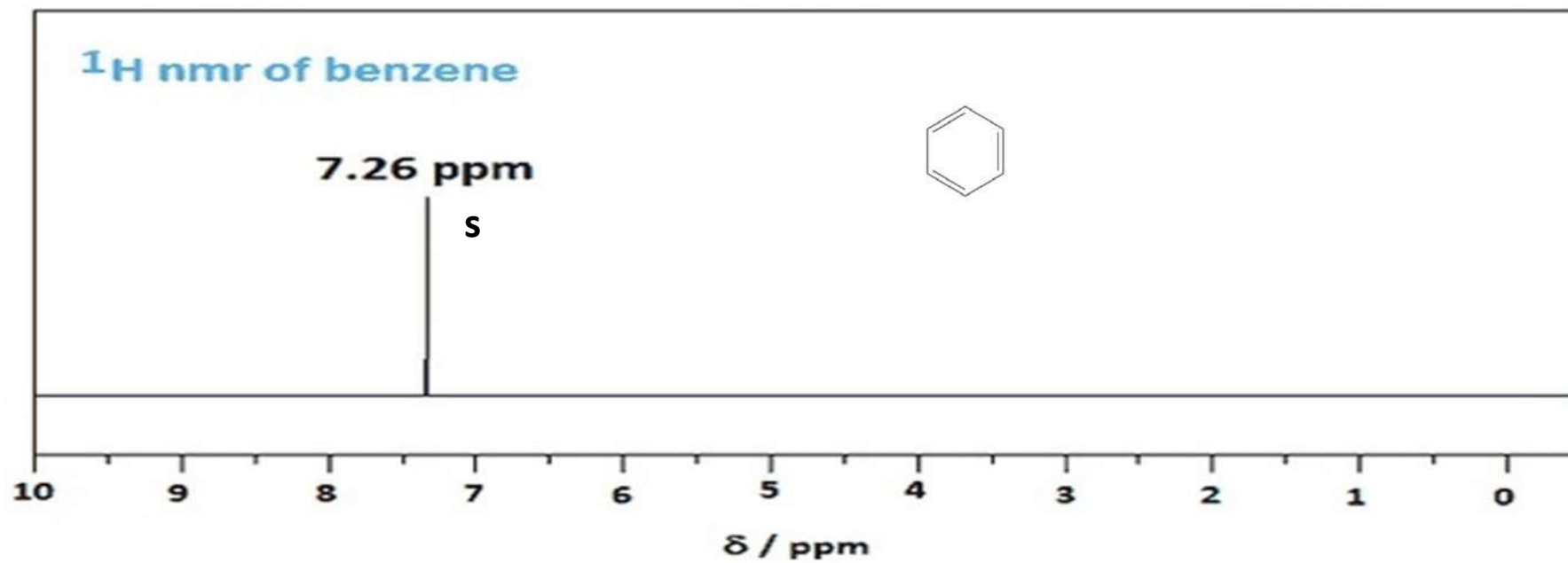
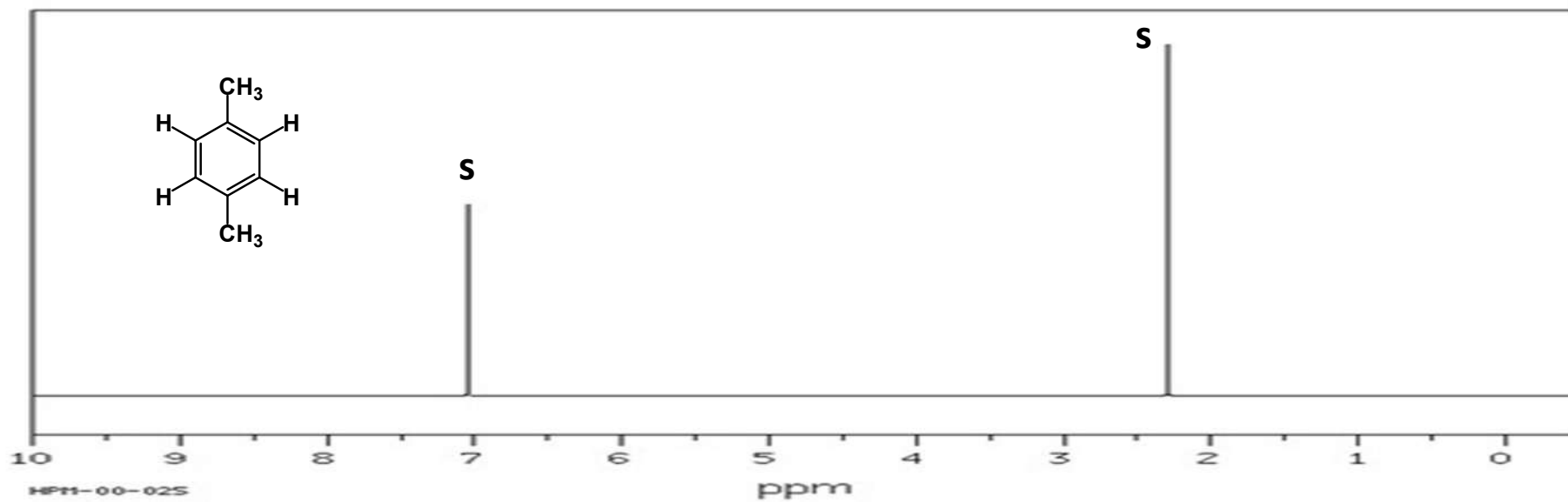
- The only aromatic that shows singlet; benzene and the para symmetrical one



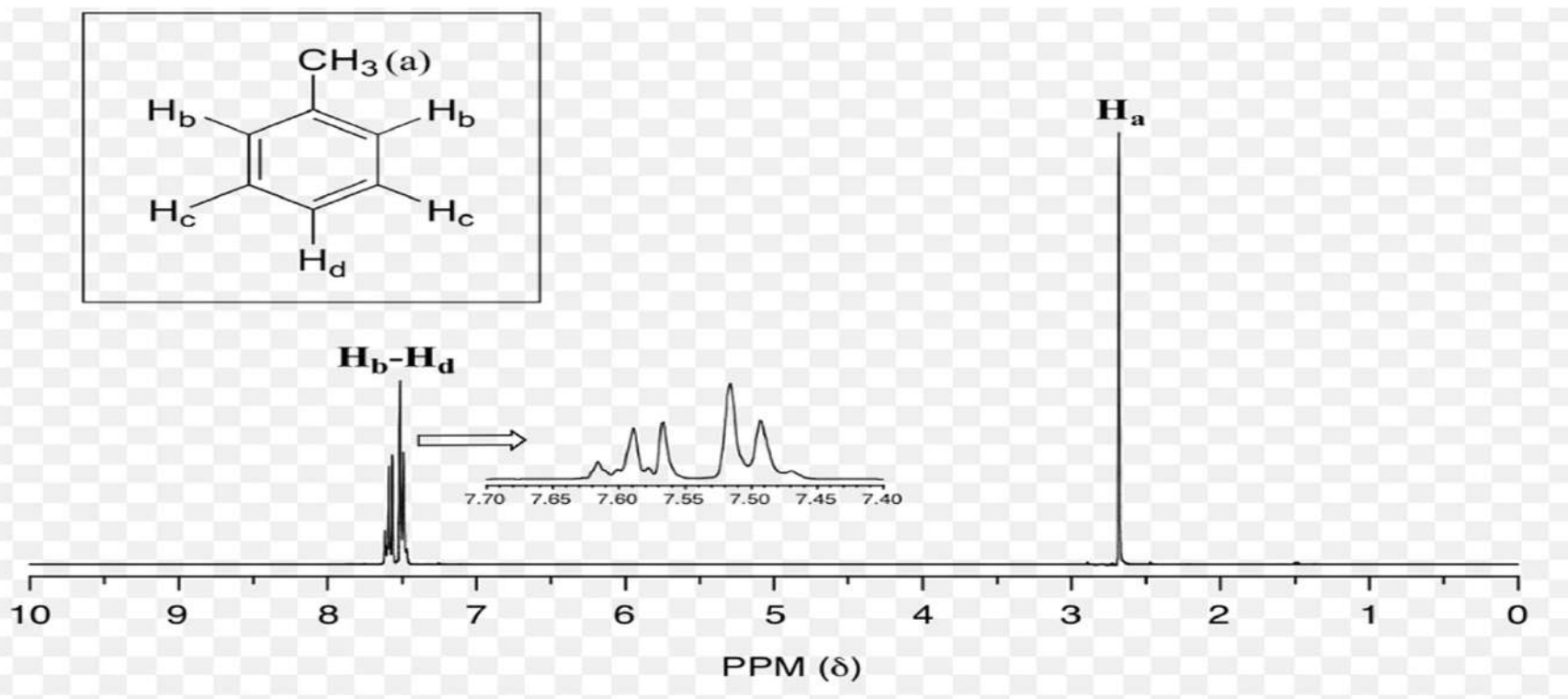
Singlet peak



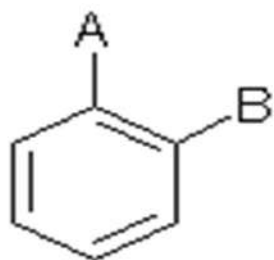
A=A (any substituent)
Singlet peak



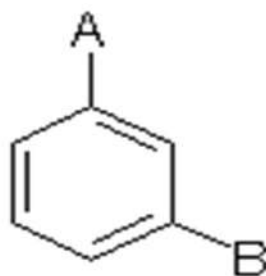
- Mono-substituted benzene shows multiplet (overlapped over each other appears upon expansion appears in aromatic region)



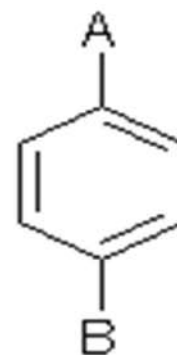
- By inspection; one can distinguish between (Ortho/Meta) from Para !!!!!!!!!!!!!



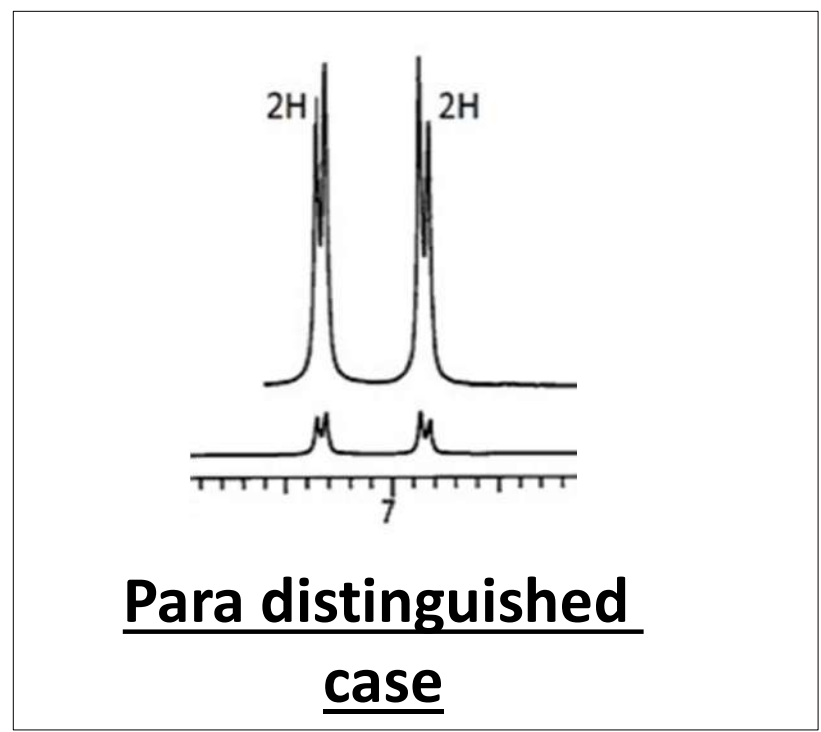
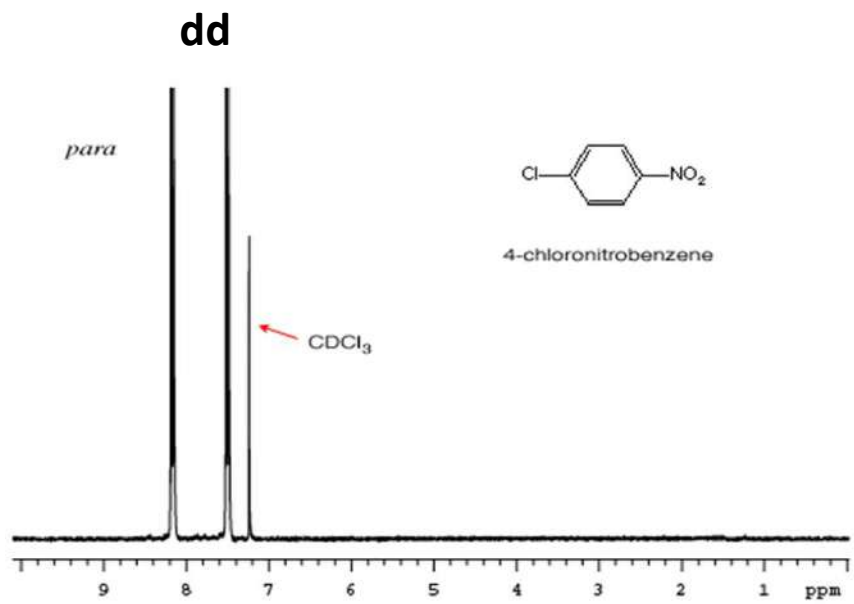
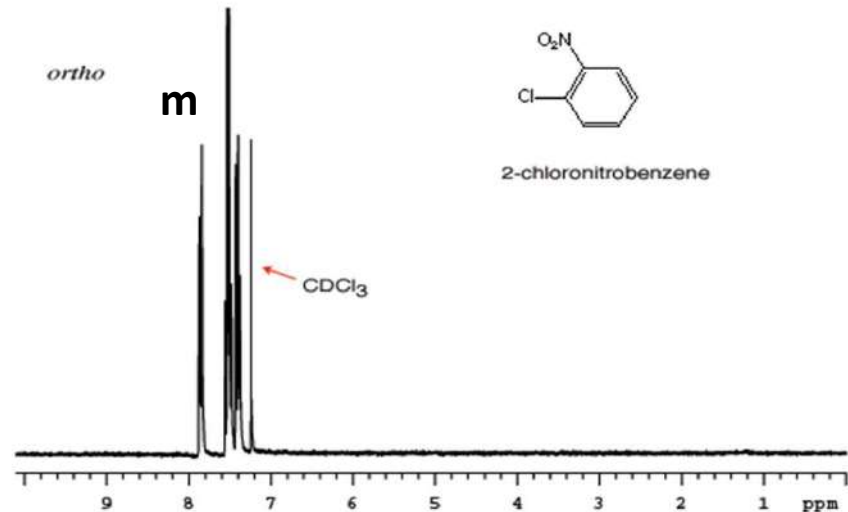
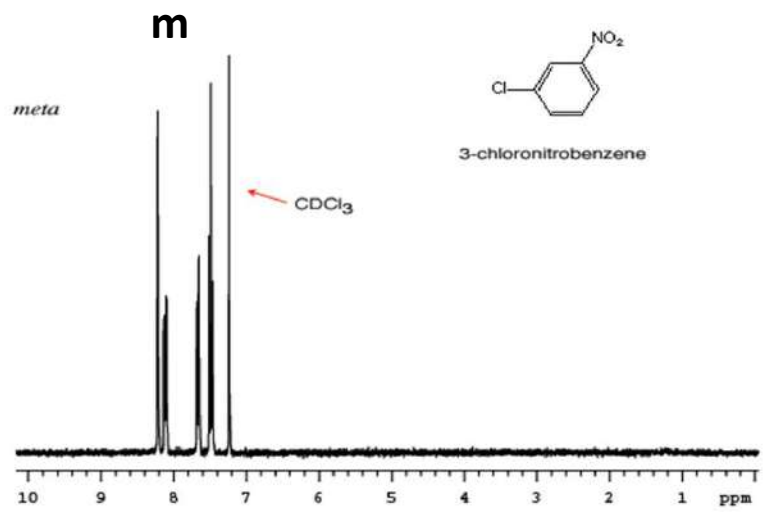
ortho-
1,2-



meta-
1,3-

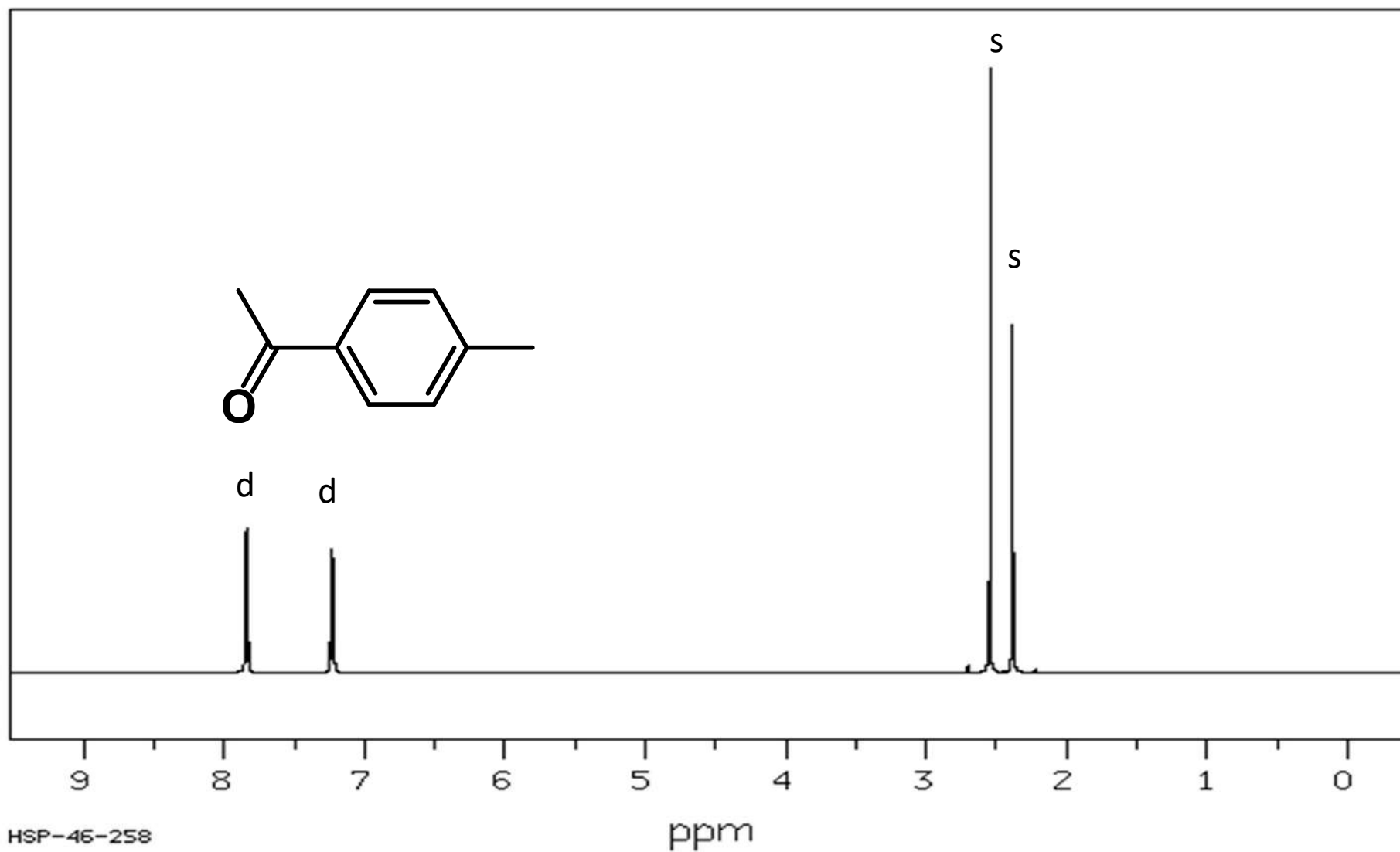


para-
1,4-

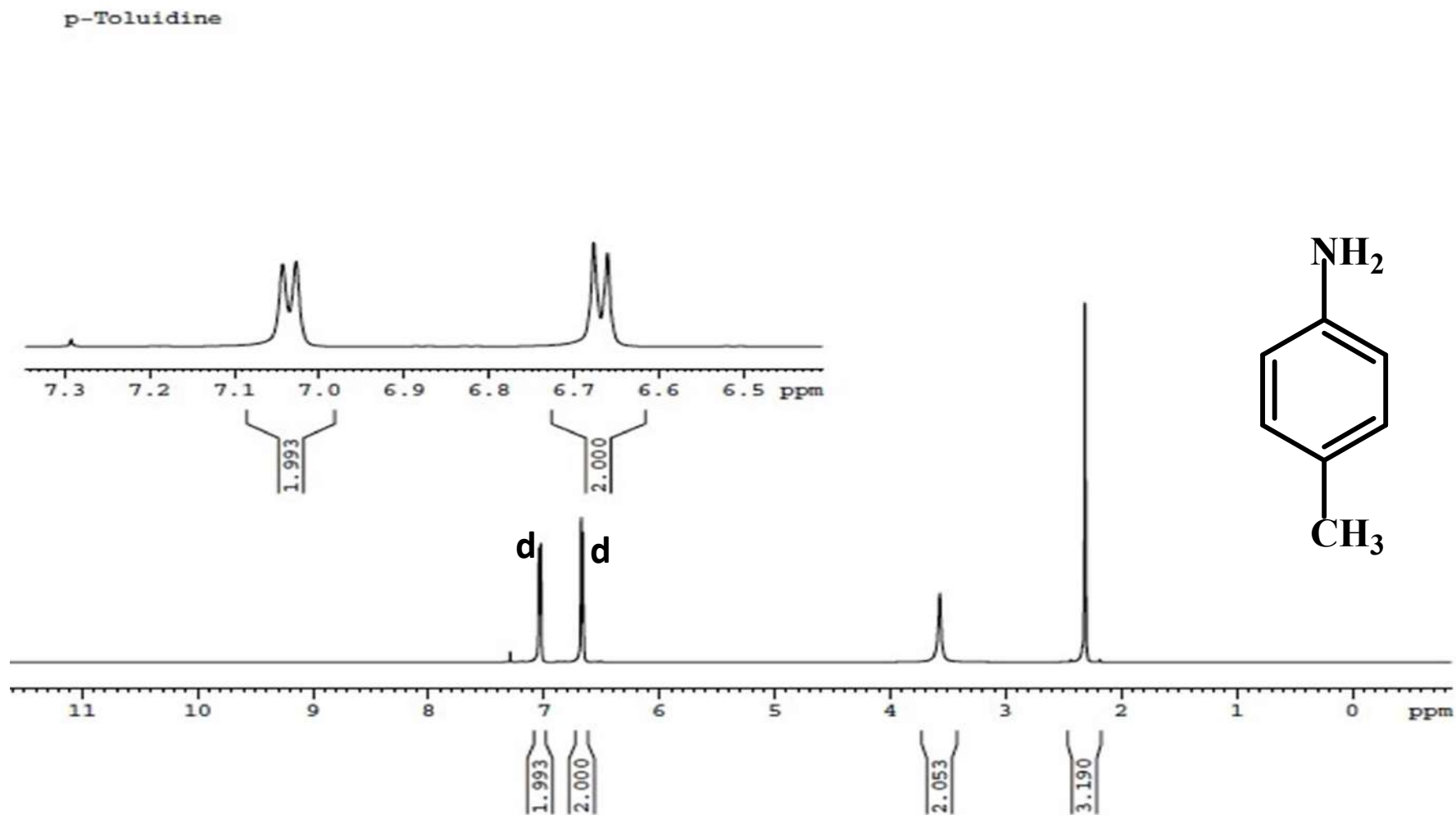


The distinctive pattern is the pair of doublets, can be widely spaced or closed

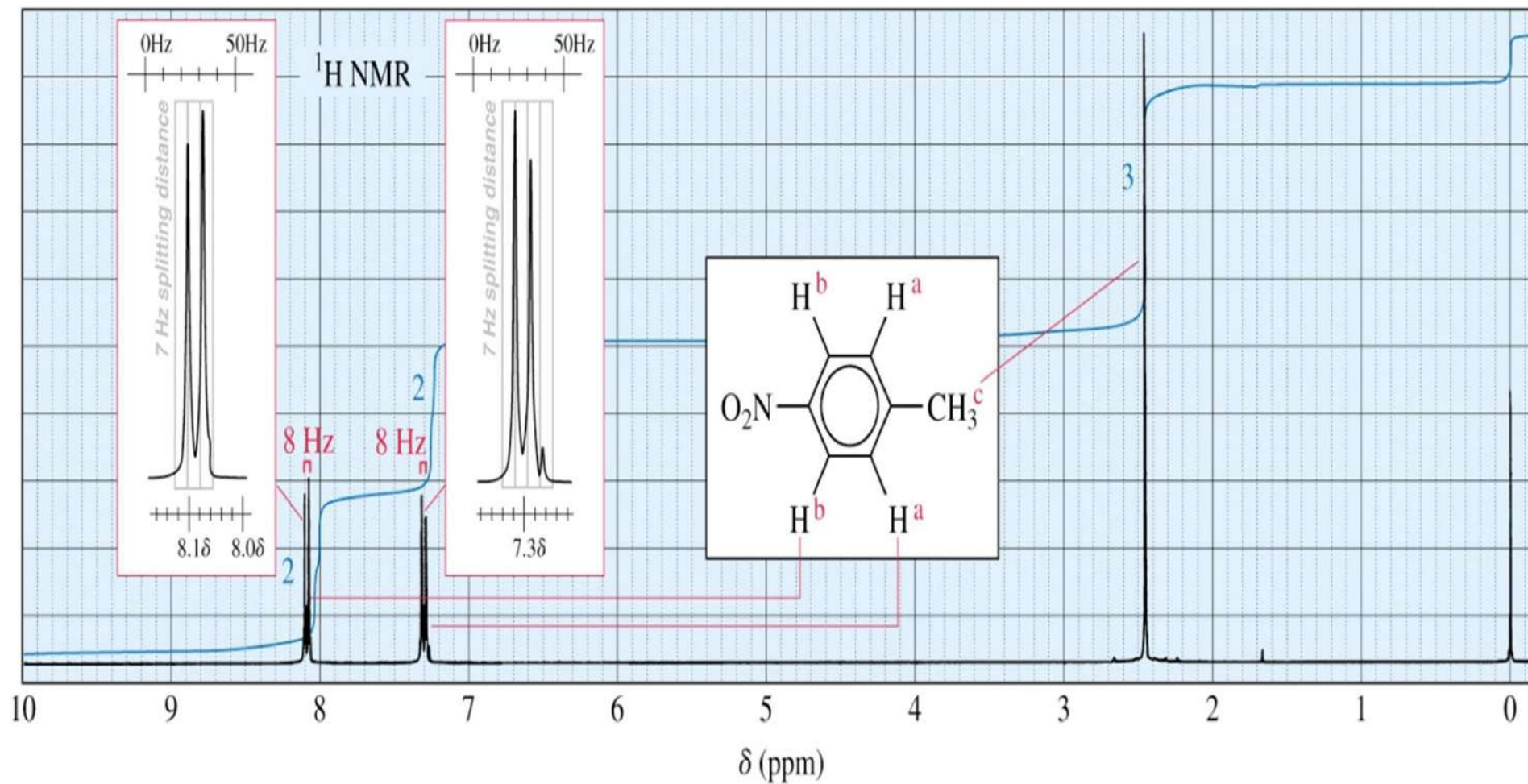
The distinctive pattern is the pair of doublets, can be widely spaced or closed



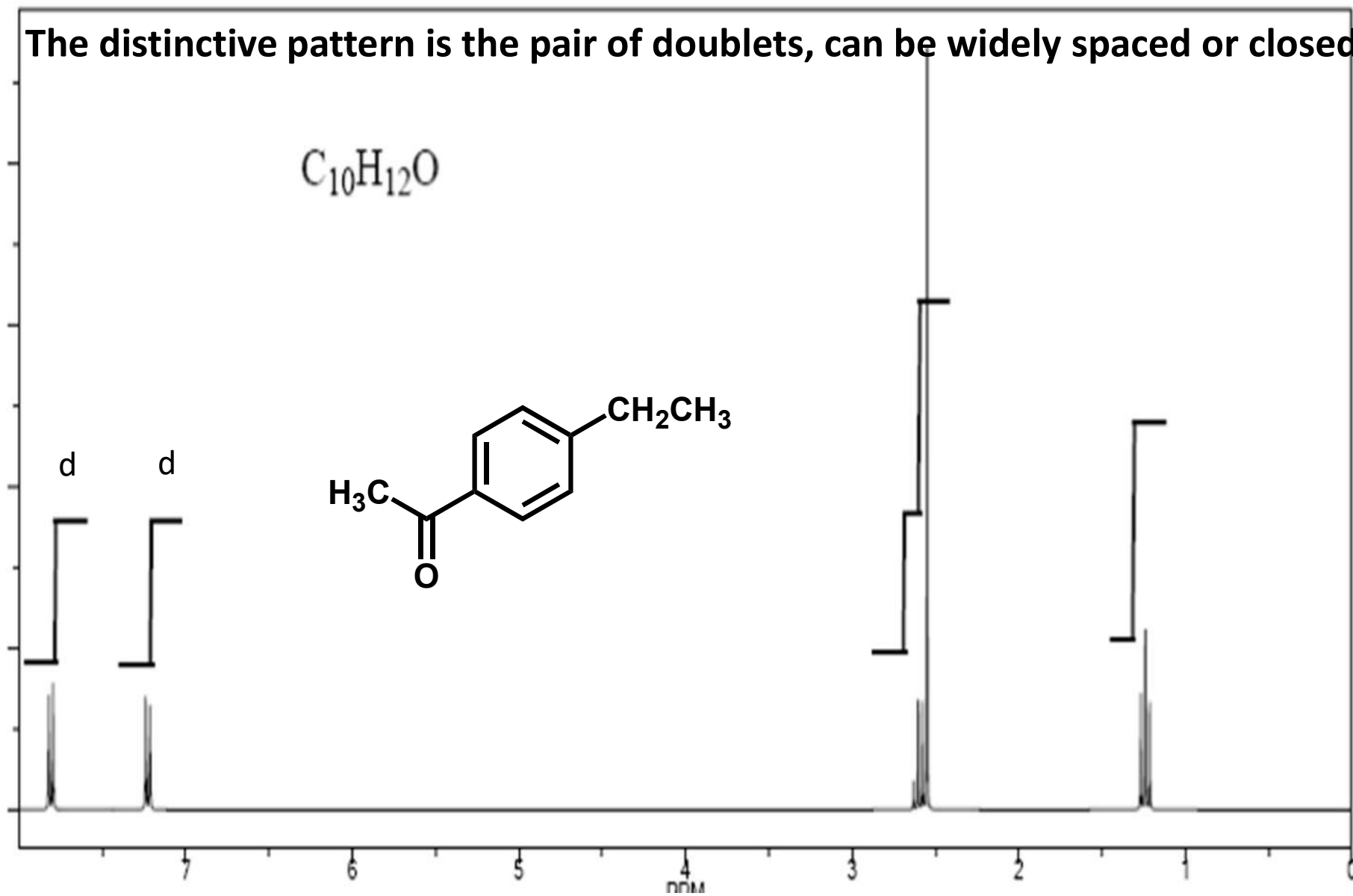
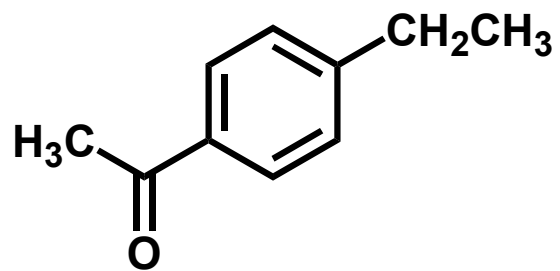
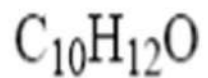
The distinctive pattern is the pair of doublets, can be widely spaced or closed



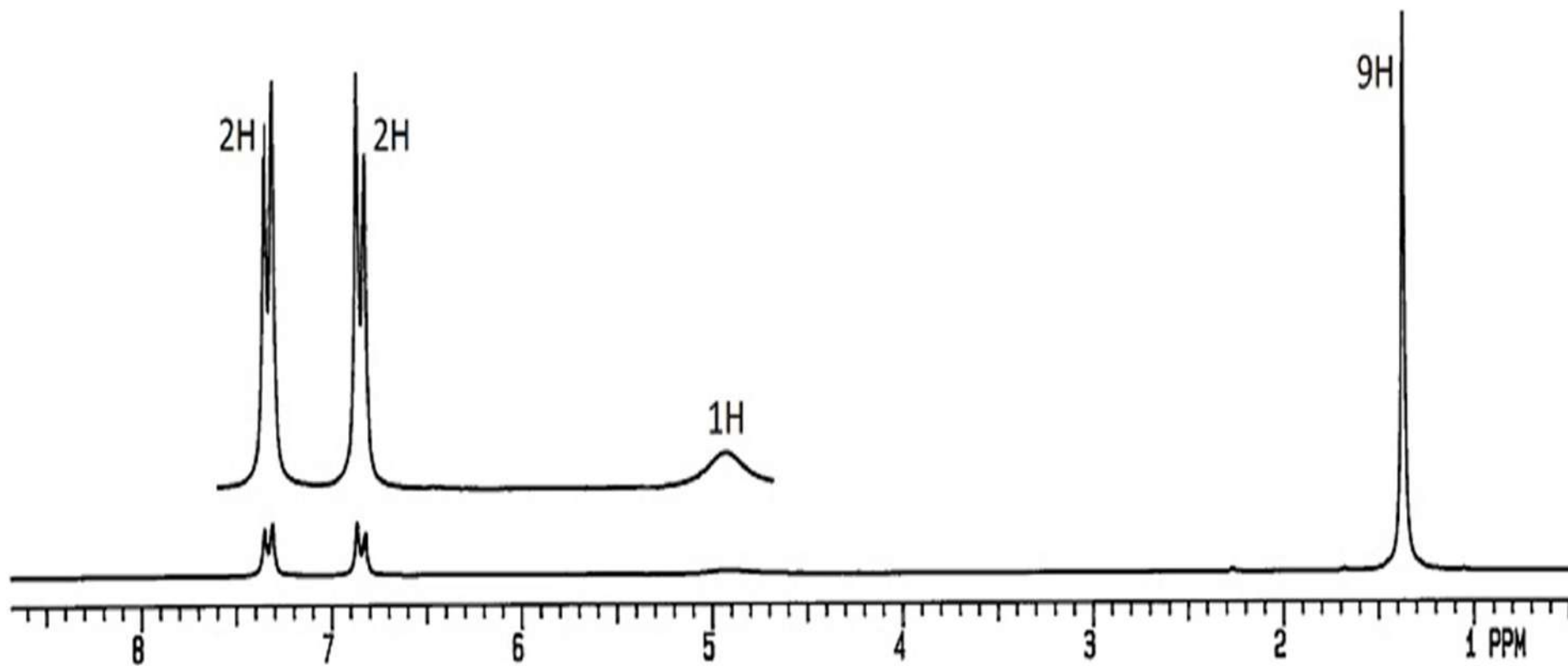
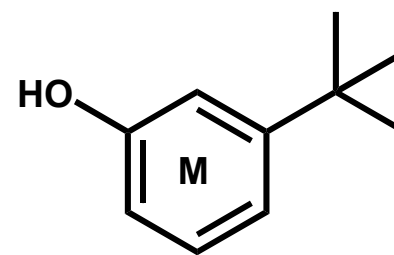
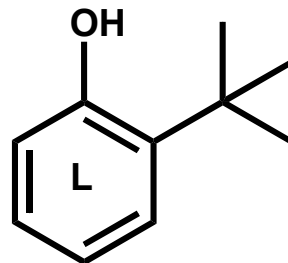
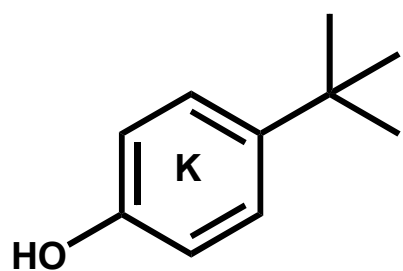
The distinctive pattern is the pair of doublets, can be widely spaced or closed



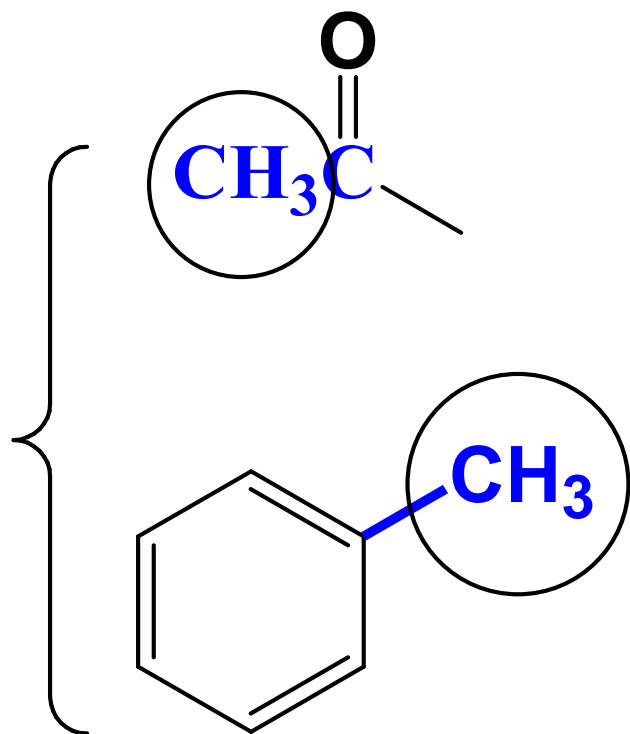
The distinctive pattern is the pair of doublets, can be widely spaced or closed



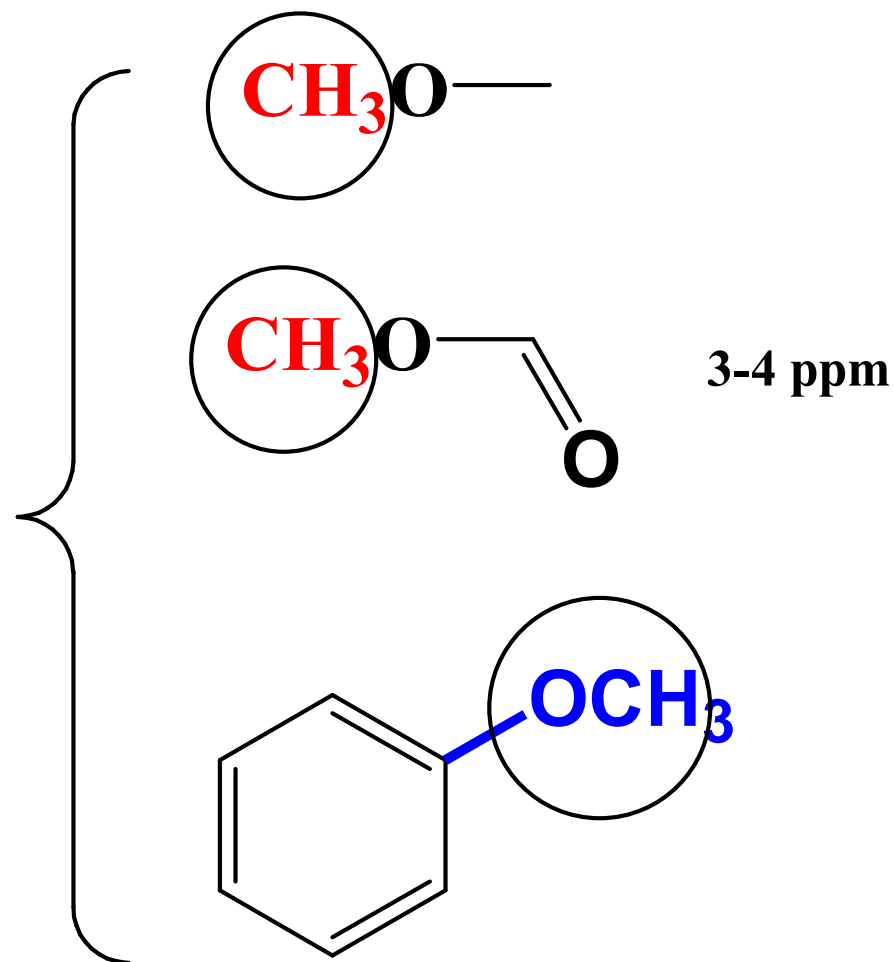
Match the correct structure



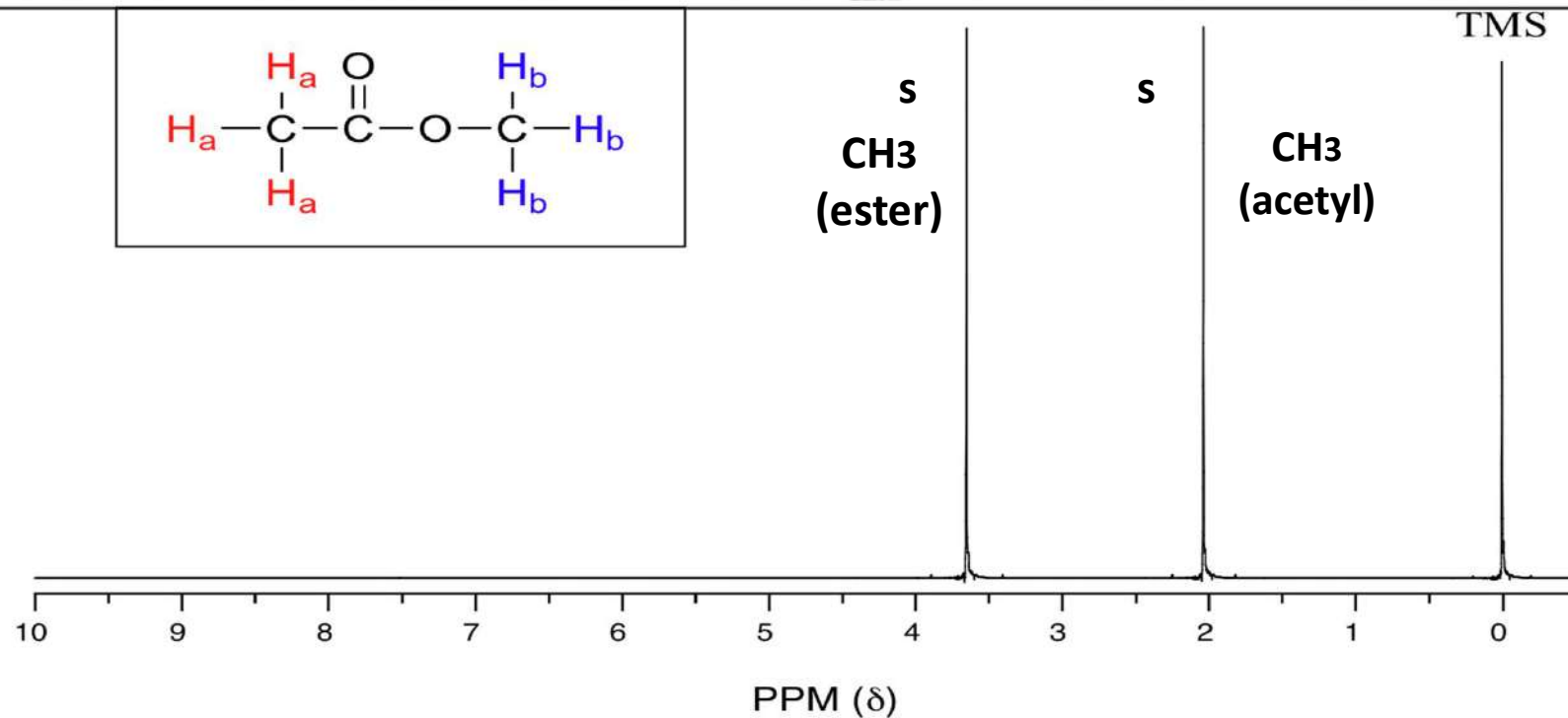
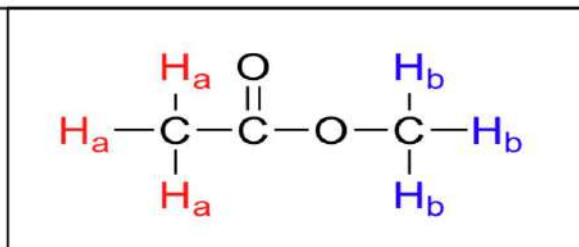
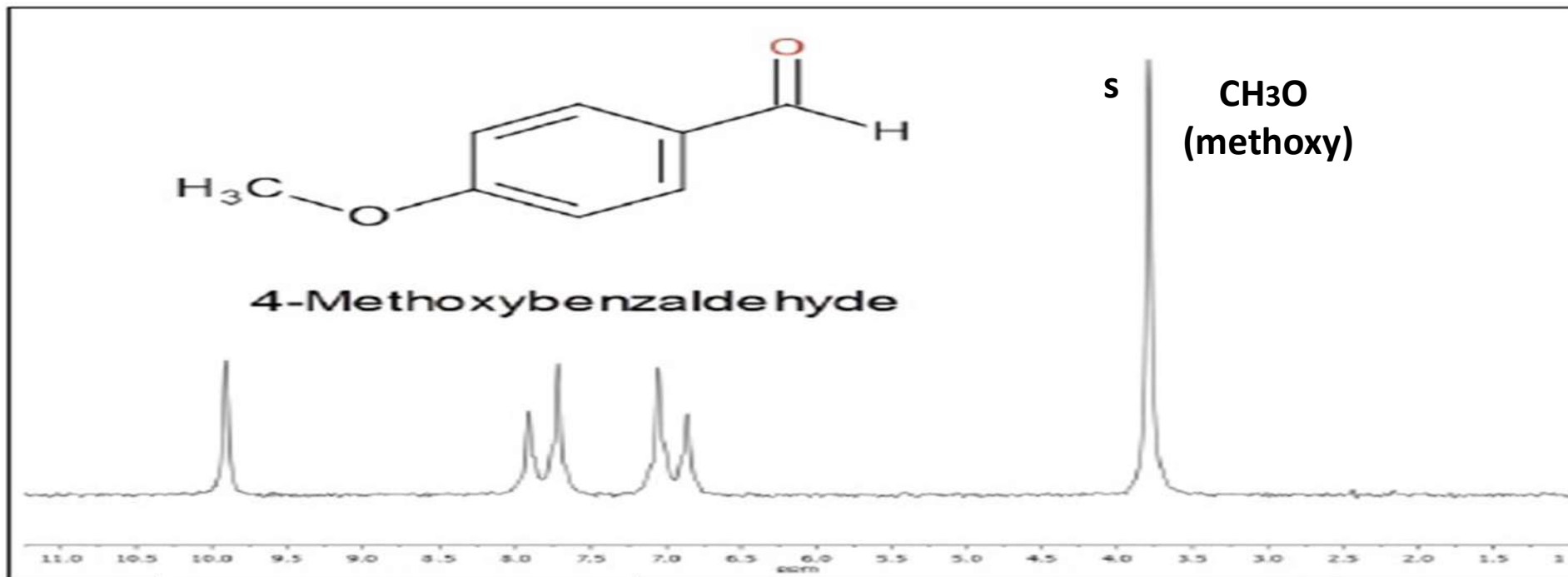
Distinguished Singlet methyl (CH₃)

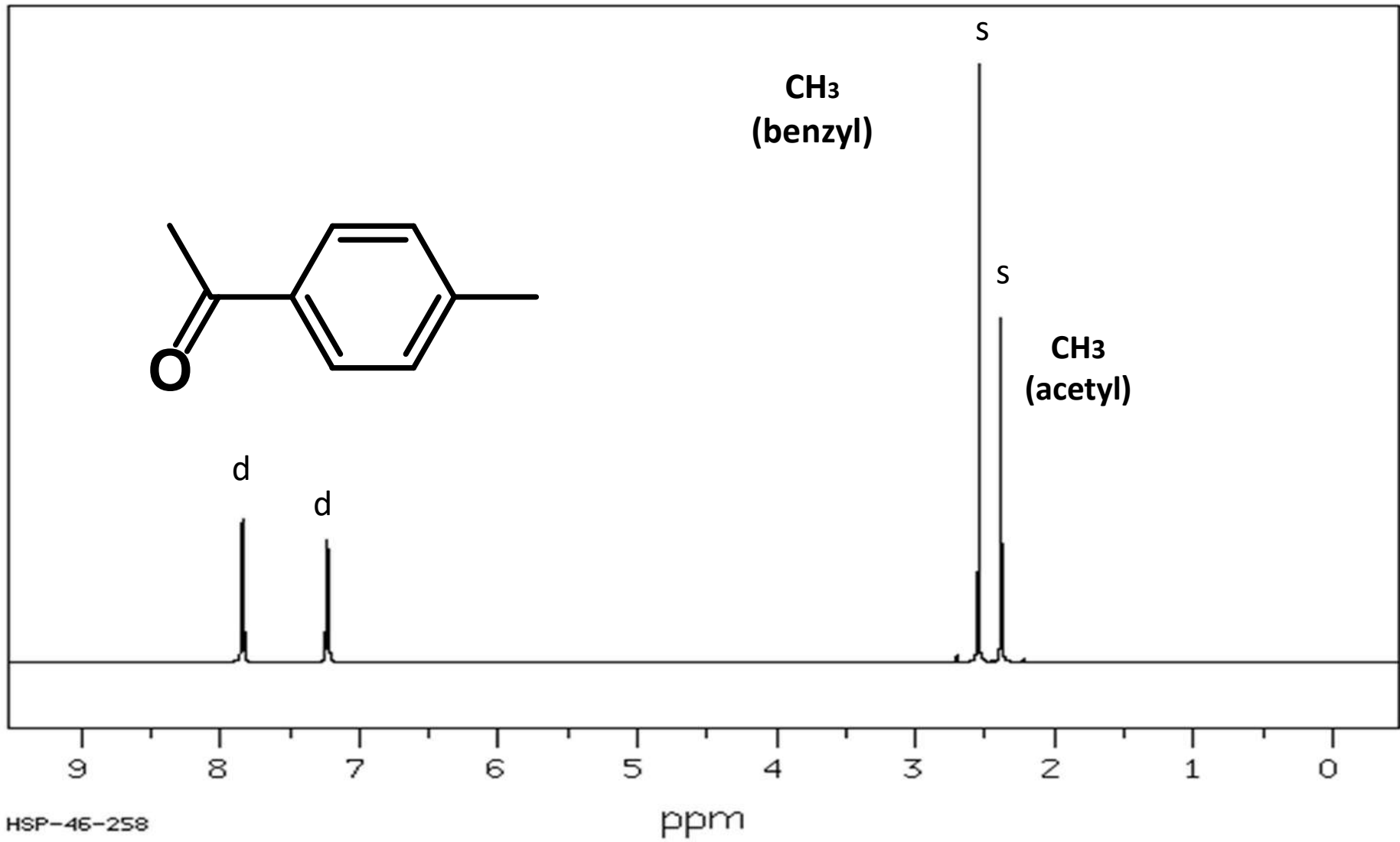


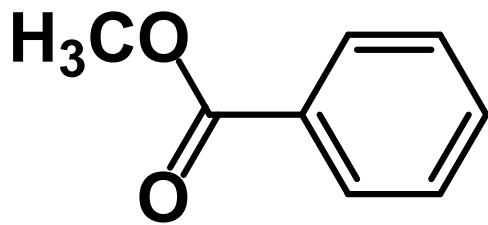
2-3 ppm



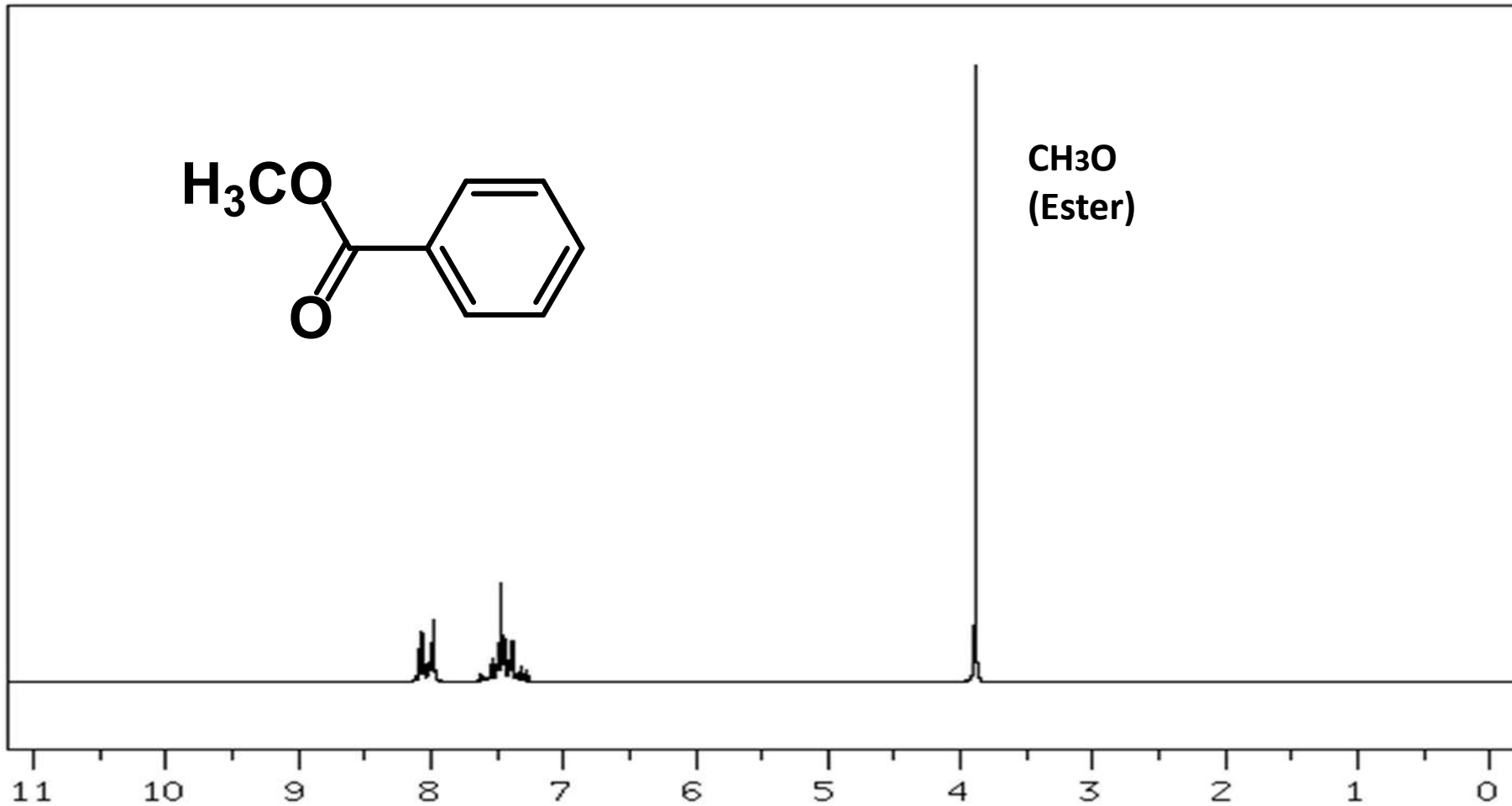
3-4 ppm







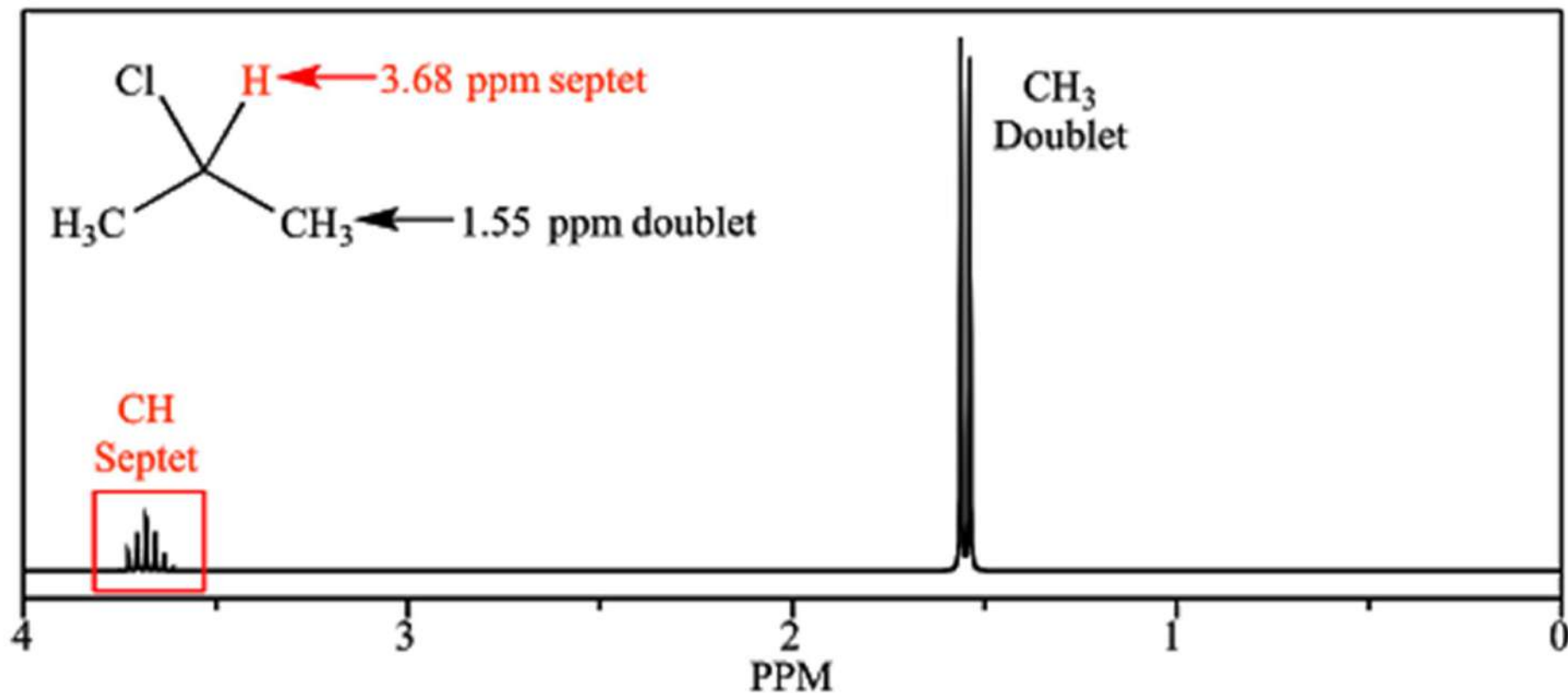
CH₃O
(Ester)

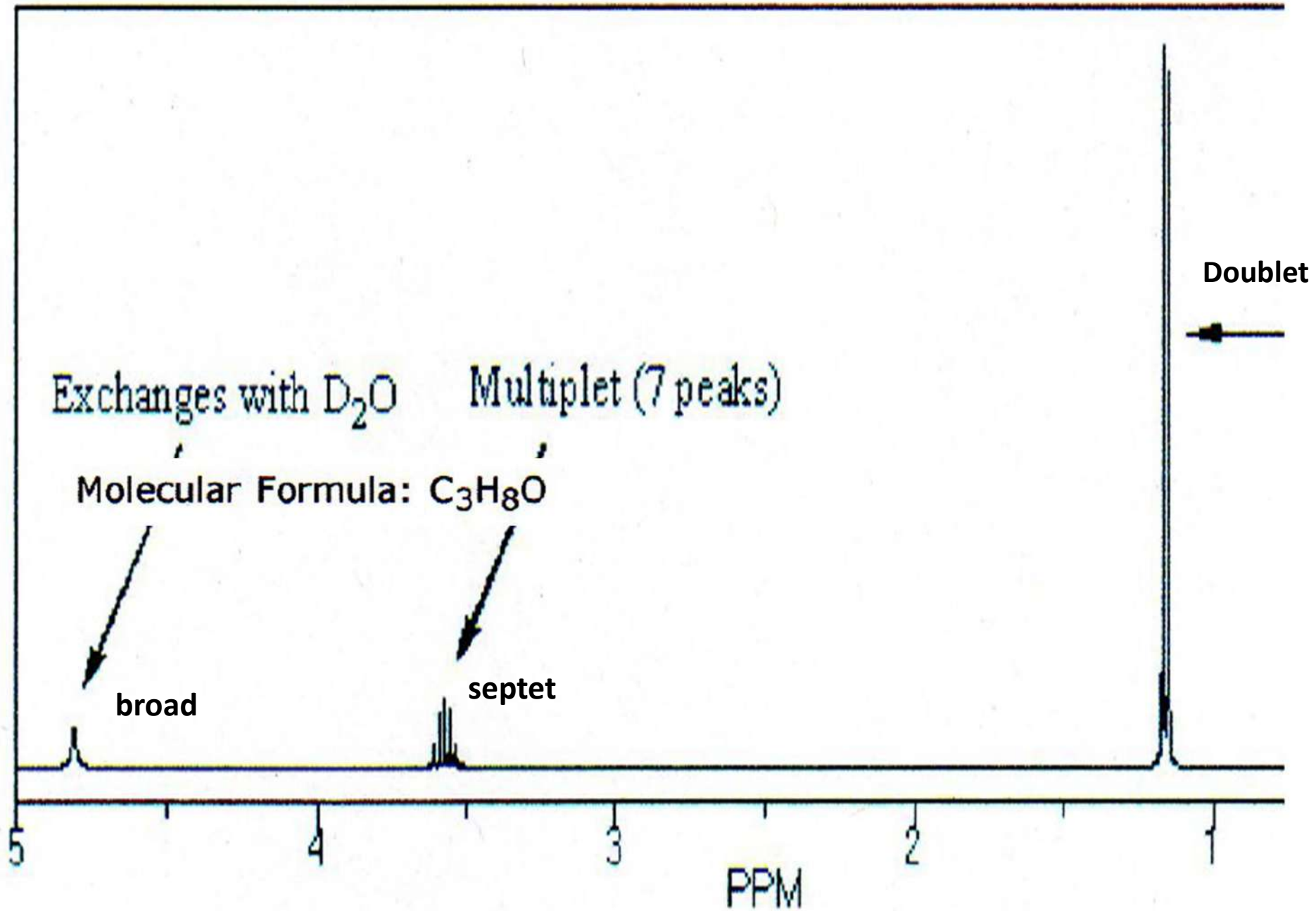


HSP-00-108

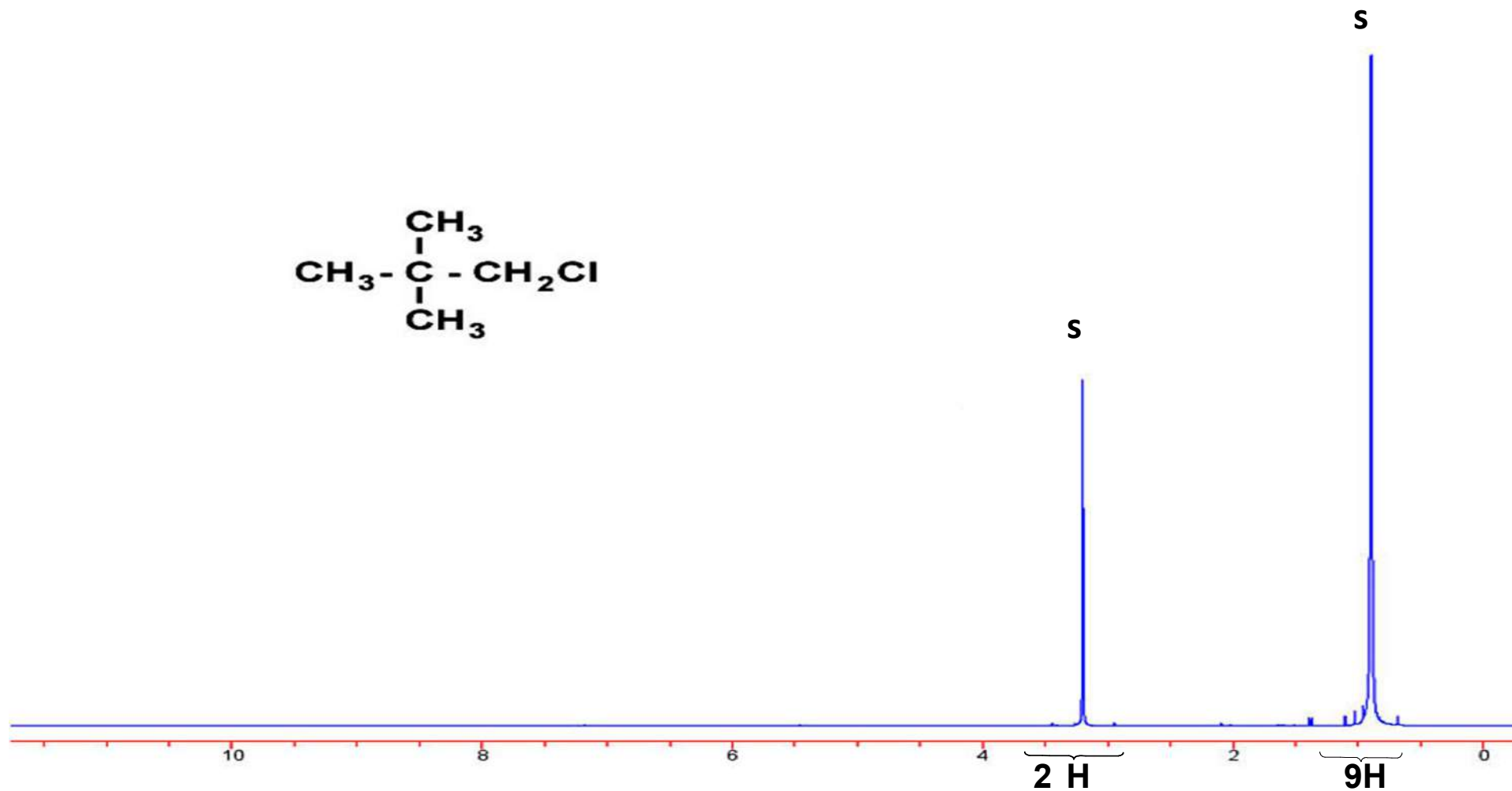
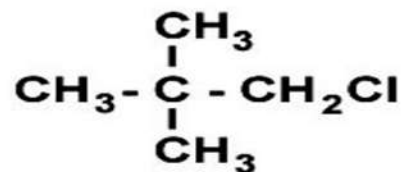
ppm

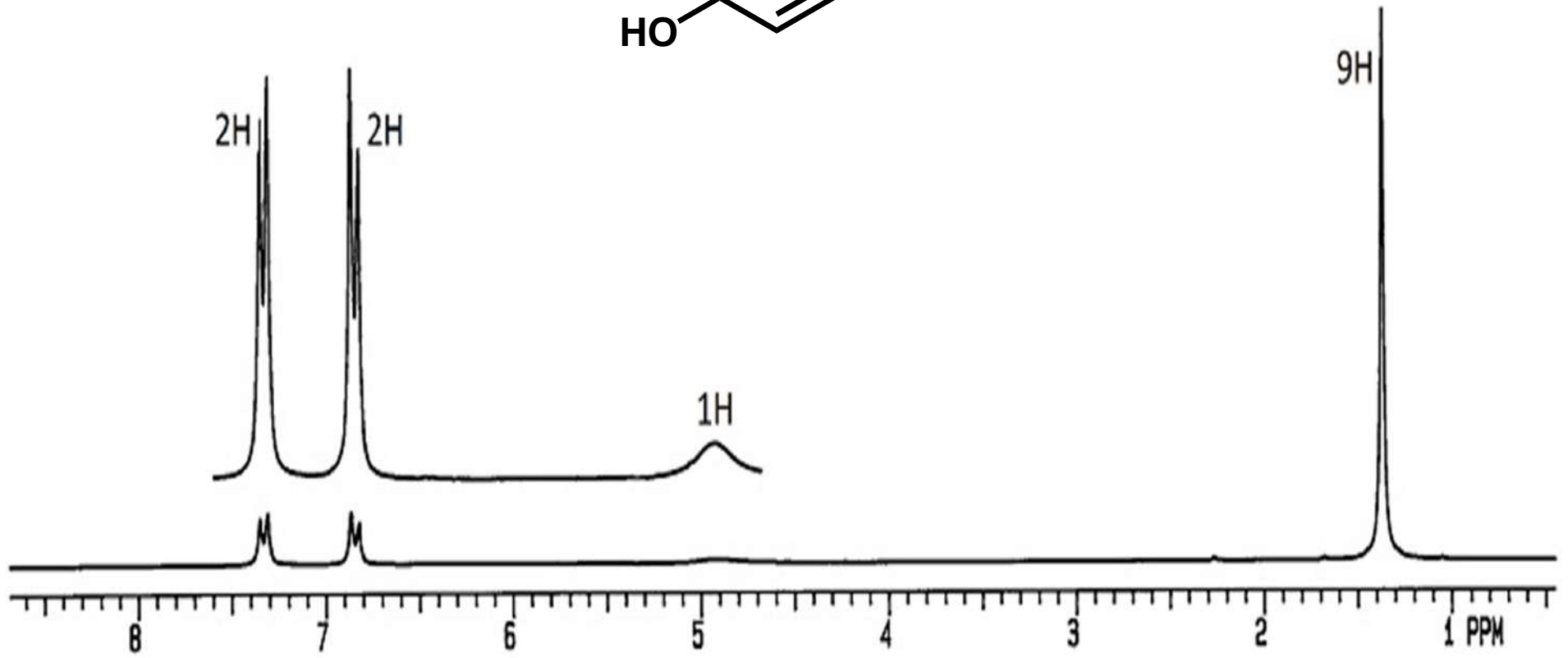
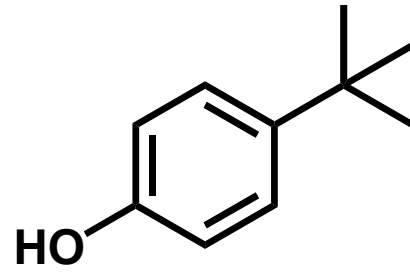
Distinguished doublet/septet system (Isopropyl group)





Distinguished singlet with 9H integration (tertiary butyl group) around 1-2 ppm





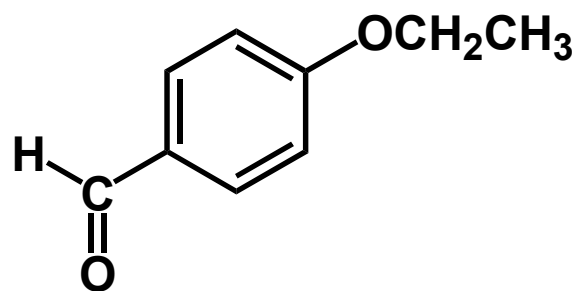
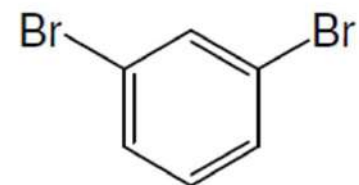
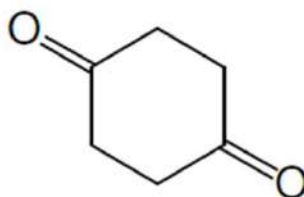
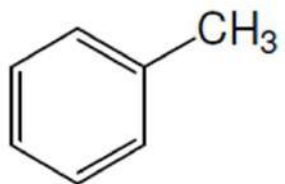
¹H-NMR

Discussion

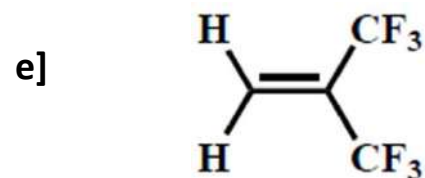
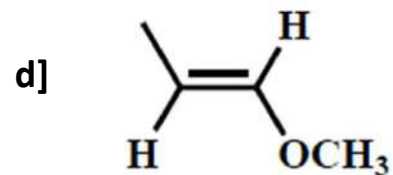
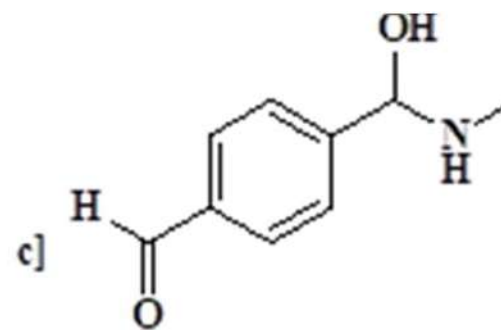
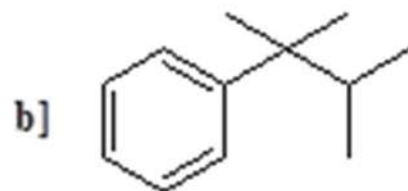
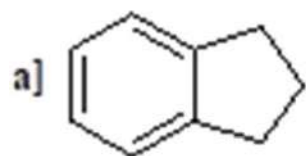
Part 2

March/2021

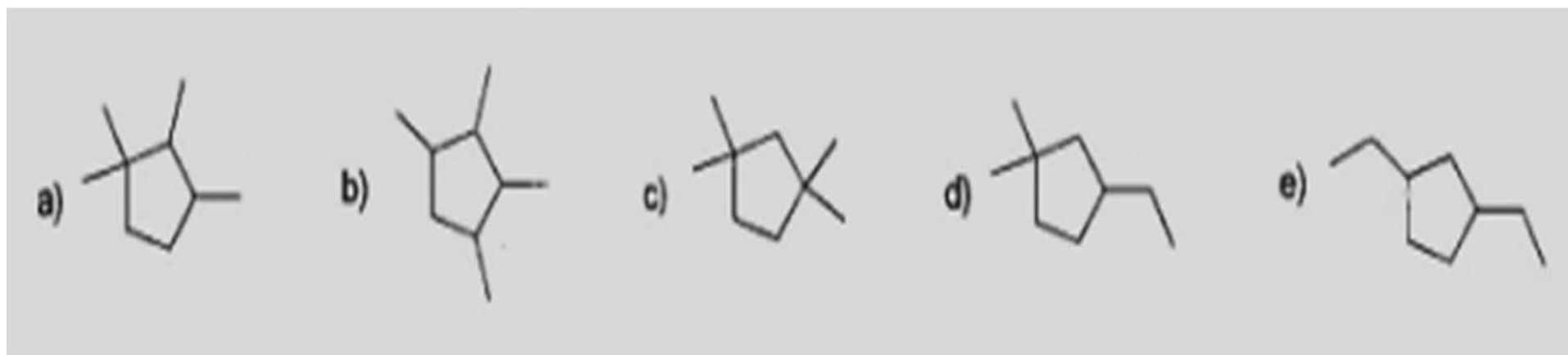
1] Predict how many hydrogen types (signals) in each of the following compounds



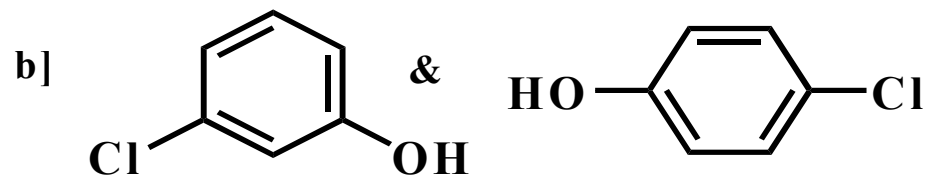
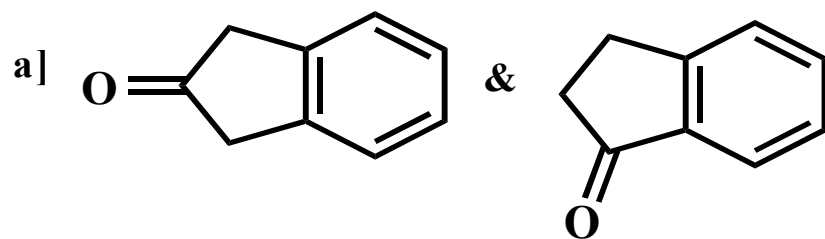
2] How many H-NMR signals would you expect to find in each of the following compounds?



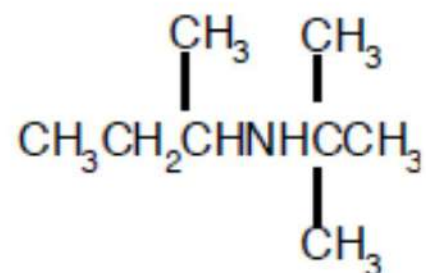
3] Which compound shows three signals (all singlets) in ^1H NMR spectrum



4] How would you use the H-NMR to distinguish between each of the following pairs of compounds? (Just tell how many peaks does each compound show)

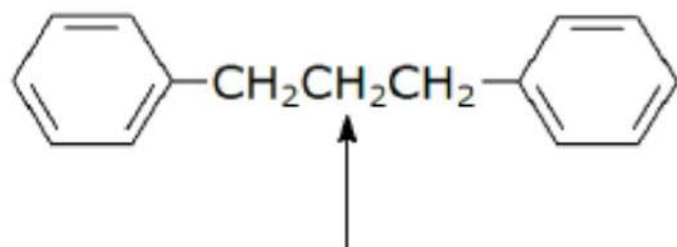


5] How many signals are predicted for the ^1H NMR of the following compound?



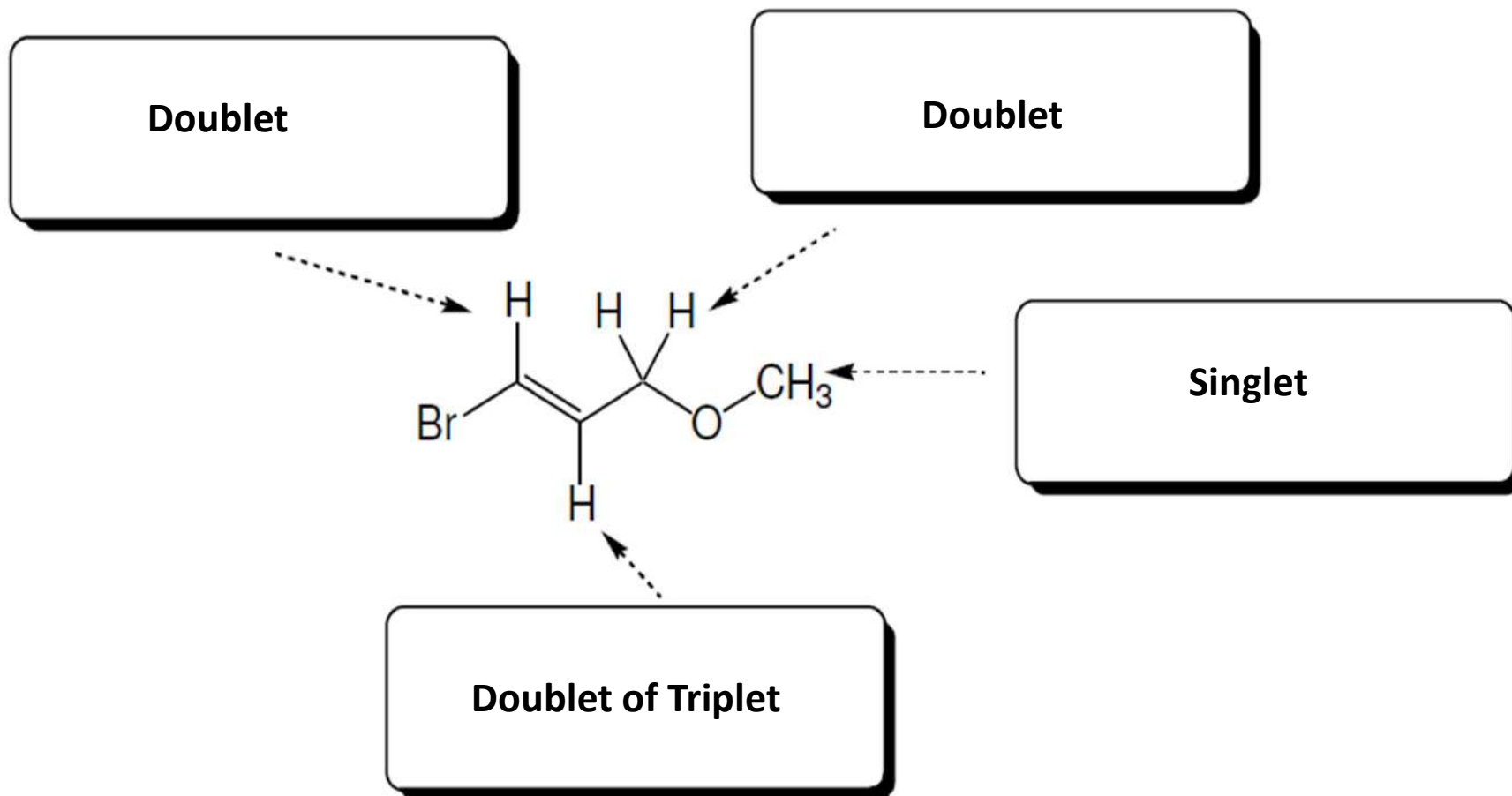
- A) 4 B) 5 C) 6 D) 7 E) 8

What is the multiplicity of the methylene hydrogens indicated in the proton NMR of the following compound?



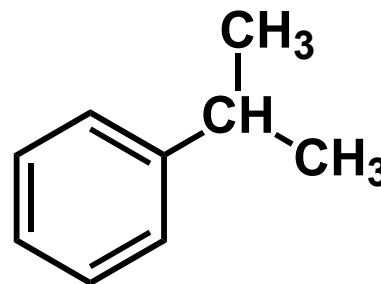
- A. singlet
B. doublet
C. triplet
D. quartet
E. pentet

6] The ^1H NMR of the given compound has four signals with the following multiplicities



7] Determine the most likely structure of a compound, with the molecular formula C_9H_{12} , which gave a 1H NMR spectrum consisting of:

- a doublet at 1.25 ppm
- a septet at 2.90 ppm and
- a multiplet at 7.25 ppm

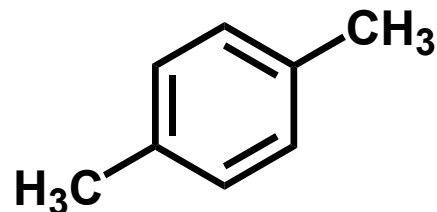


doublet and septet together ???? What does it mean (isopropyl group)

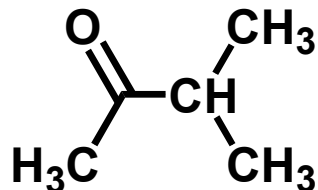
7.25 ppm means aromatic area

8] Propose the structure of a compound that exhibits the following H-NMR data.

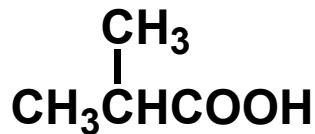
- C_8H_{10} [2.35 δ (6H, singlet) 7.09 (4H, singlet)].



- $C_5H_{10}O$ [1.09 δ (6H, doublet) 2.12(3H, singlet) 2.58 (1H, septet)]



- $C_4H_8O_2$ [1.21 δ (6H, doublet) 2.59 (1H, septet) 11.38 (1H, singlet)].



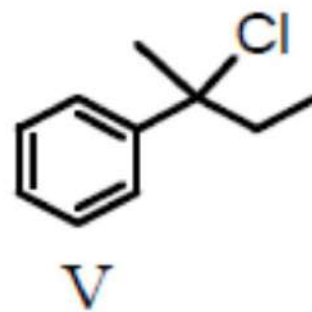
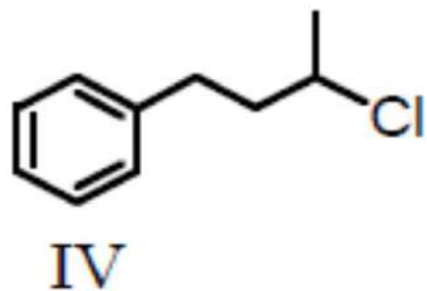
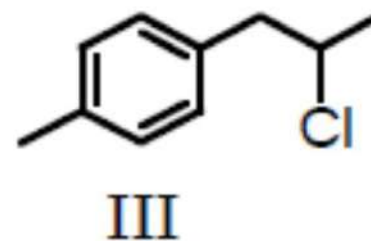
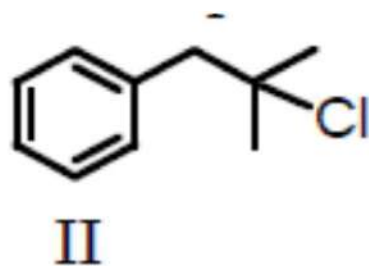
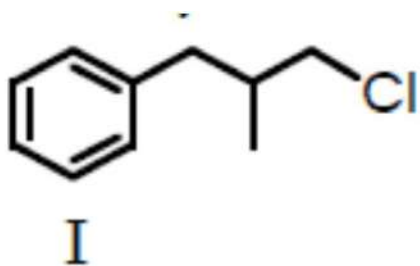
9] A compound with the molecular formula ($C_{10}H_{13}Cl$) gave the following 1H NMR spectrum:

singlet, 1.6 ppm

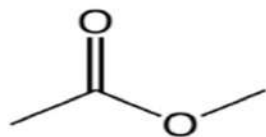
singlet, 3.1 ppm

multiplet, 7.2 ppm (5H)

The most likely structure for the compound is:



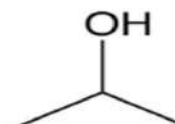
10] Choose the letter corresponding to the appropriate molecule that matches the spectrum.



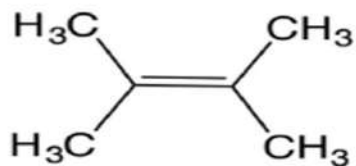
A



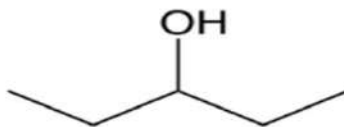
B



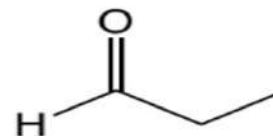
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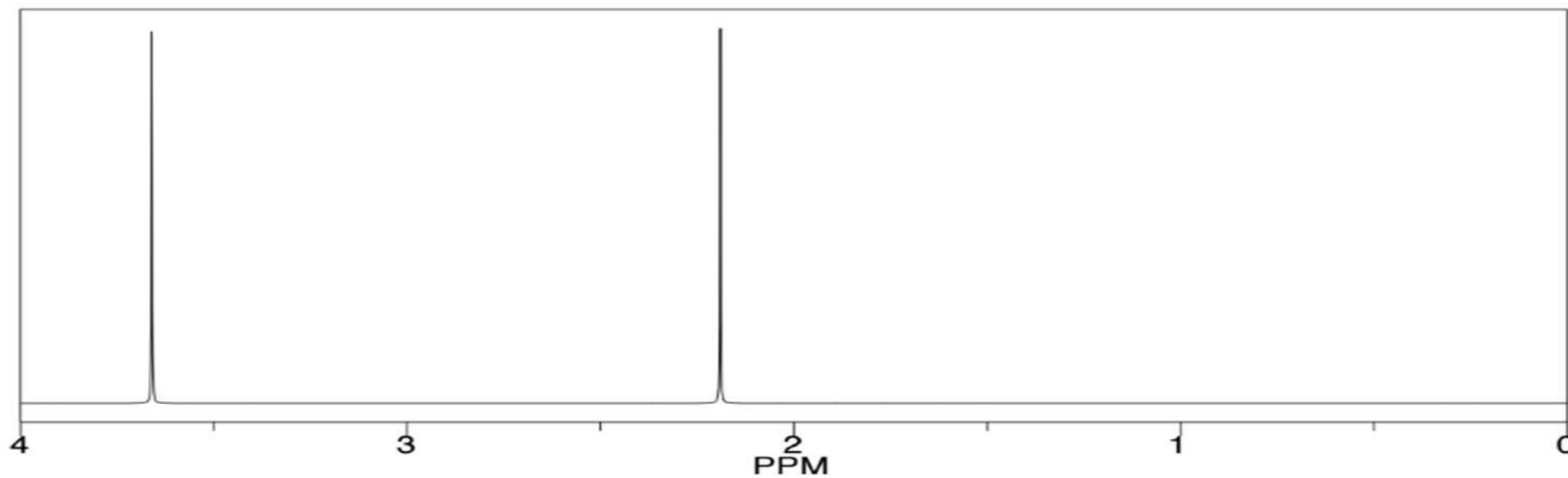
D



E



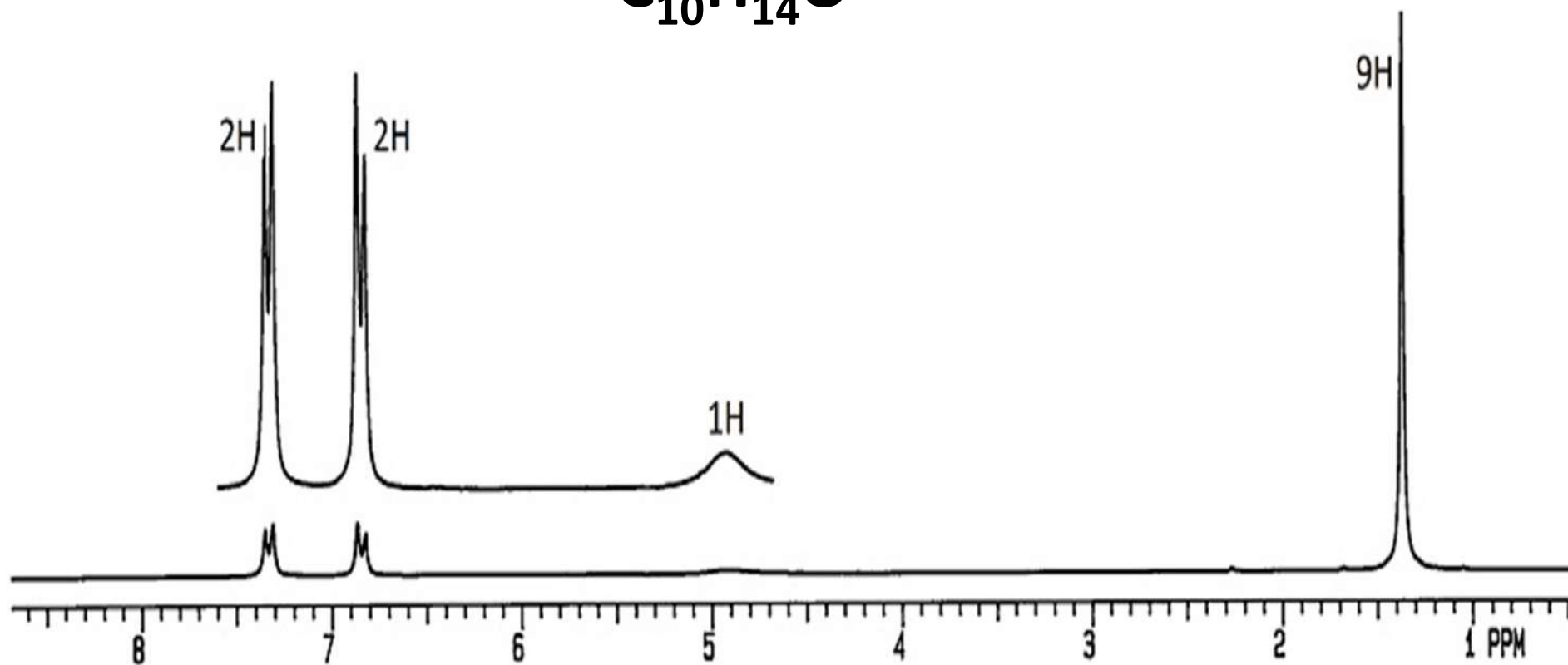
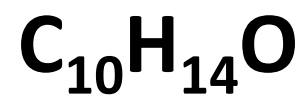
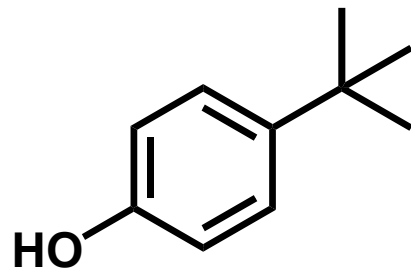
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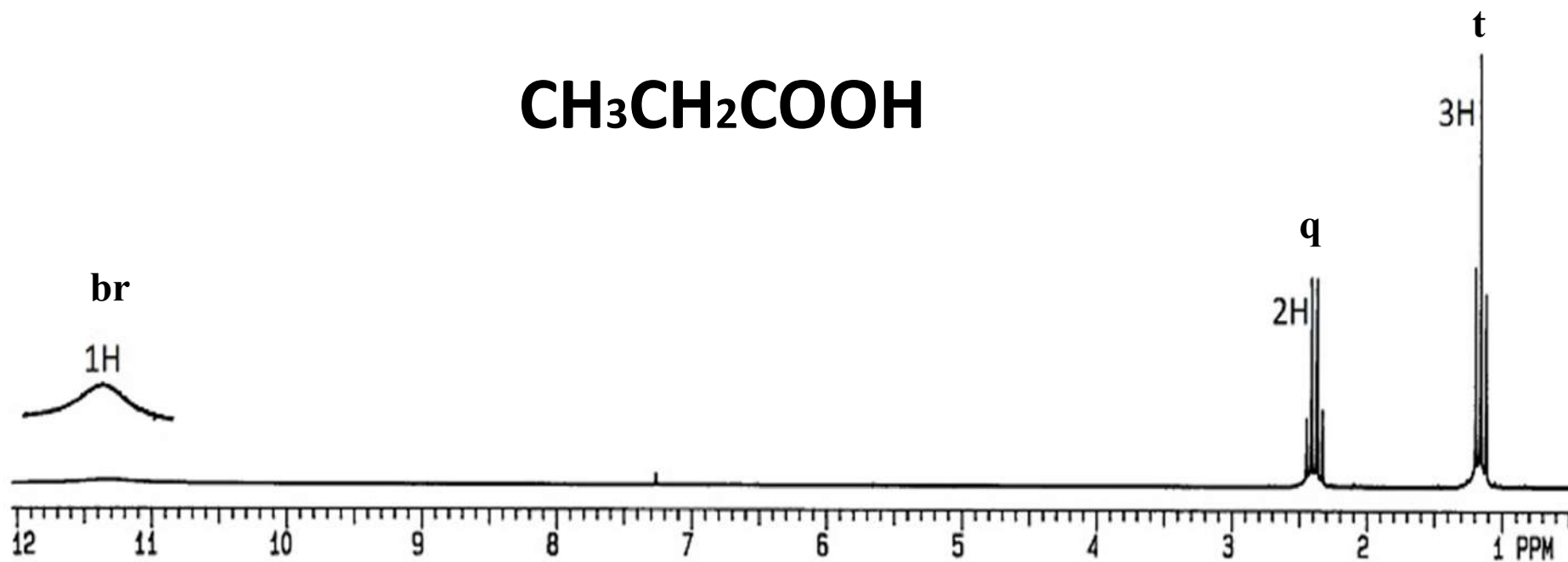
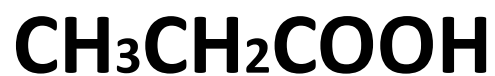
NMR

35

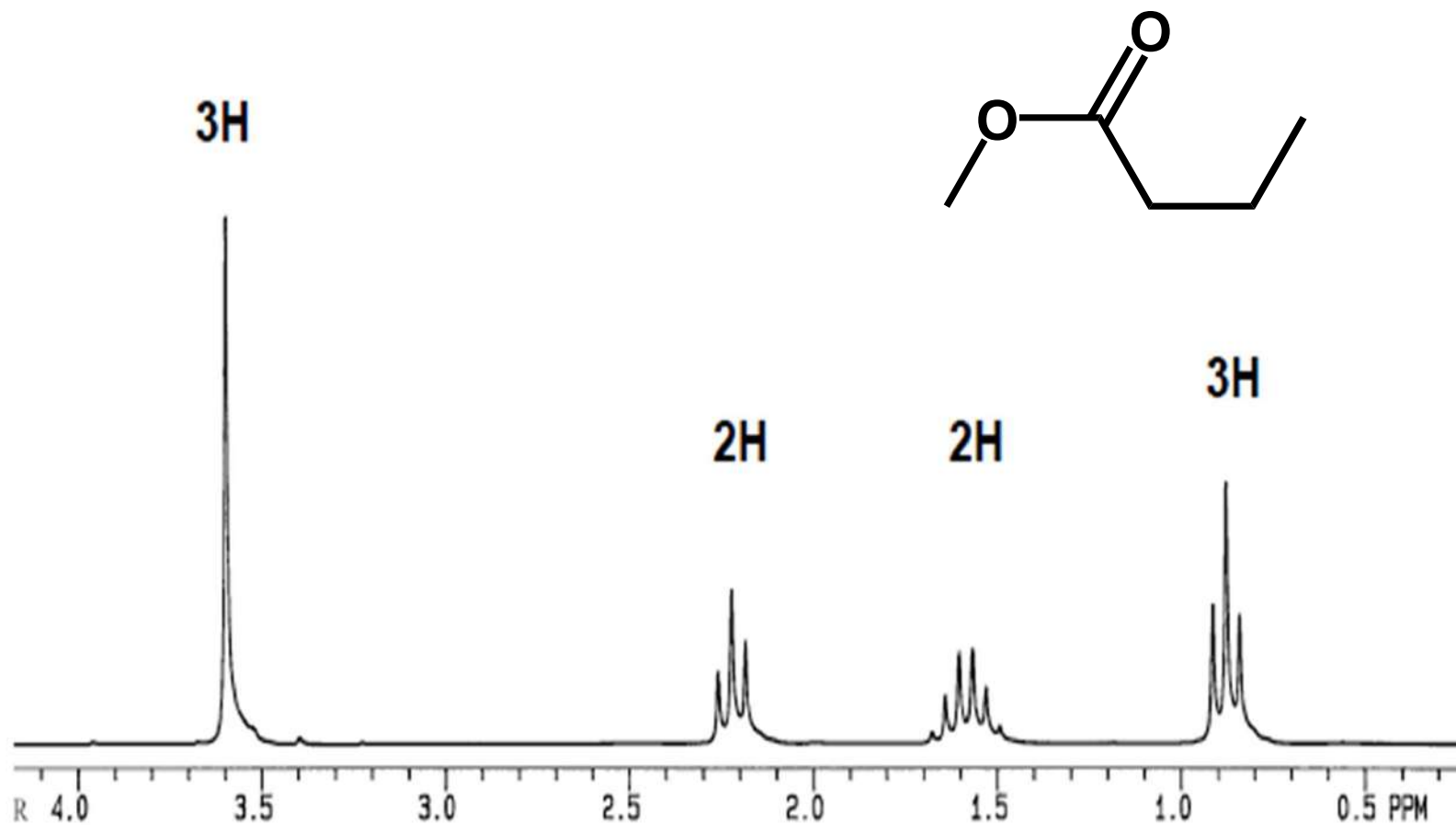
11] Using both given spectrum and molecular formula to identify the unknown compound



12] Using both given spectrum and molecular formula to identify the unknown compound?

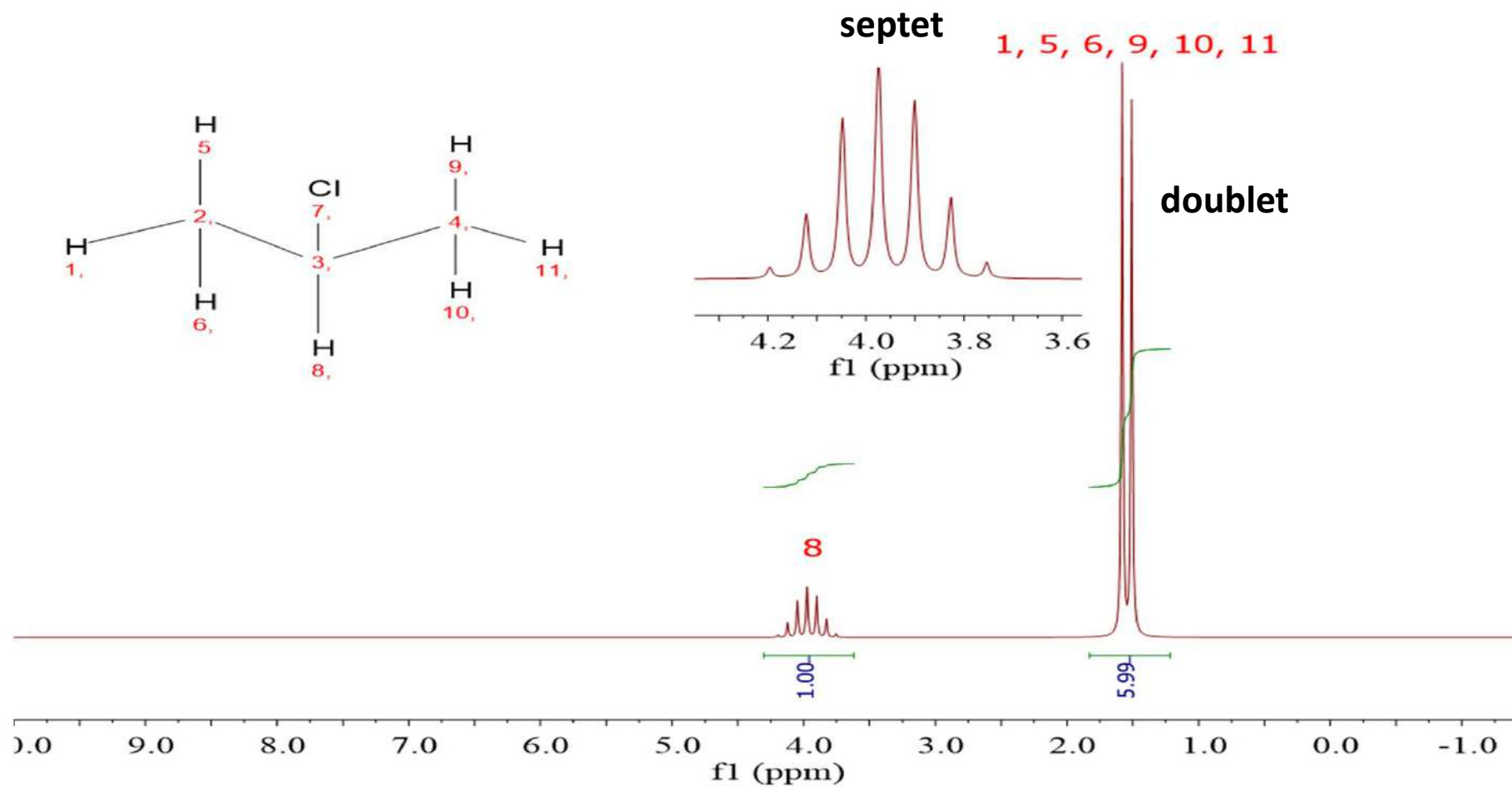


13] Using both given spectrum and molecular formula to identify the unknown compound?

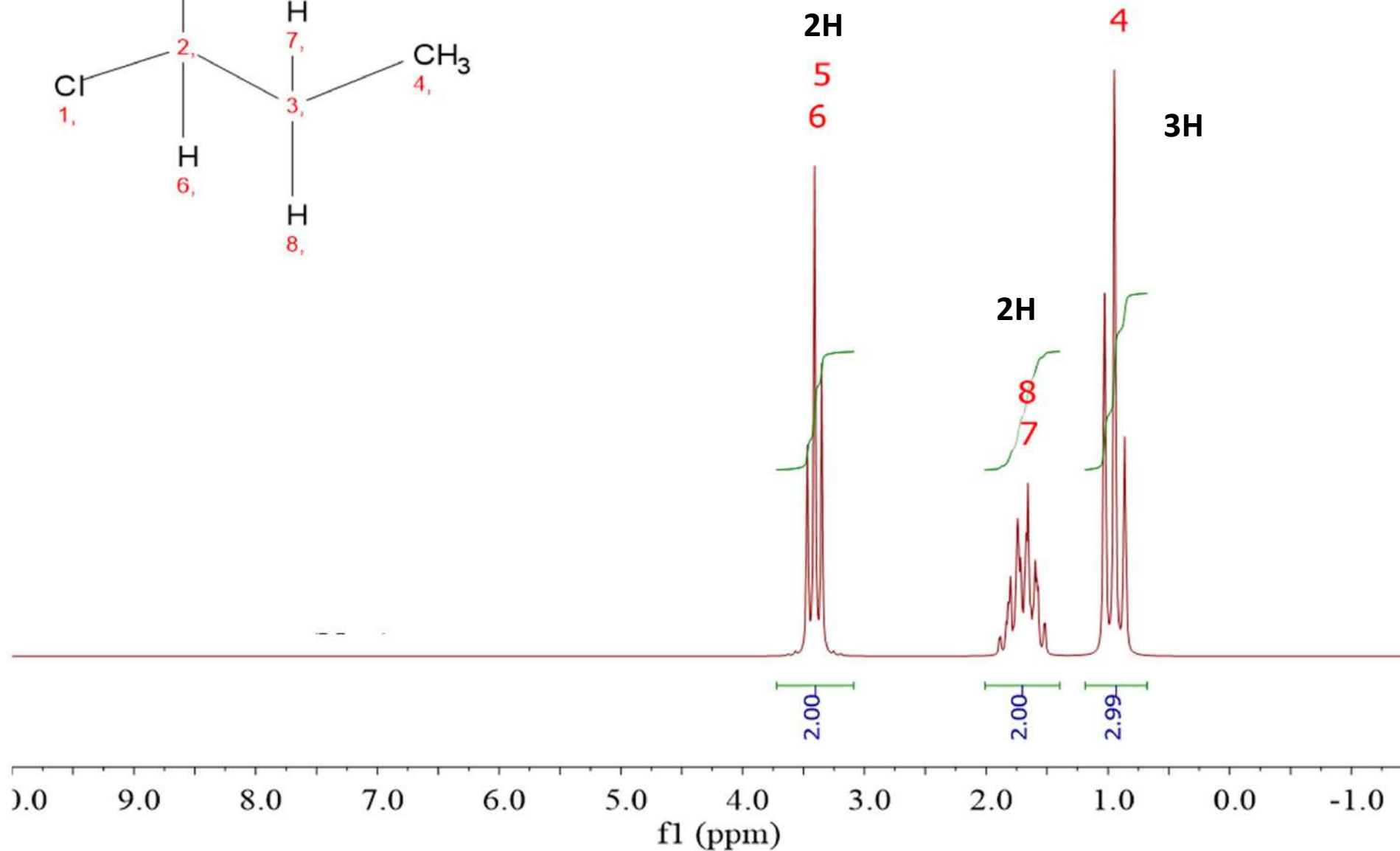
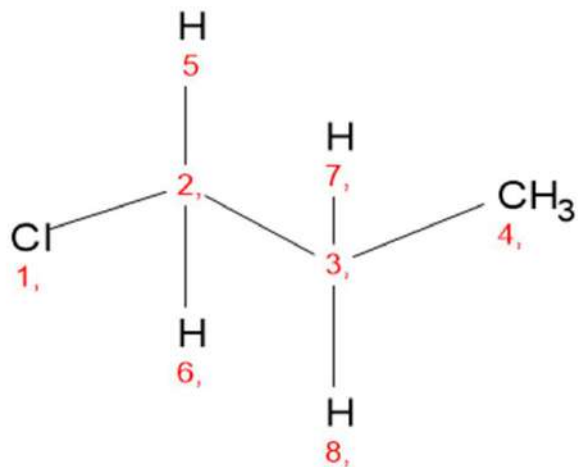


14] Using both given spectrum and molecular formula to identify the unknown compound?

A] C₃H₇Cl ???

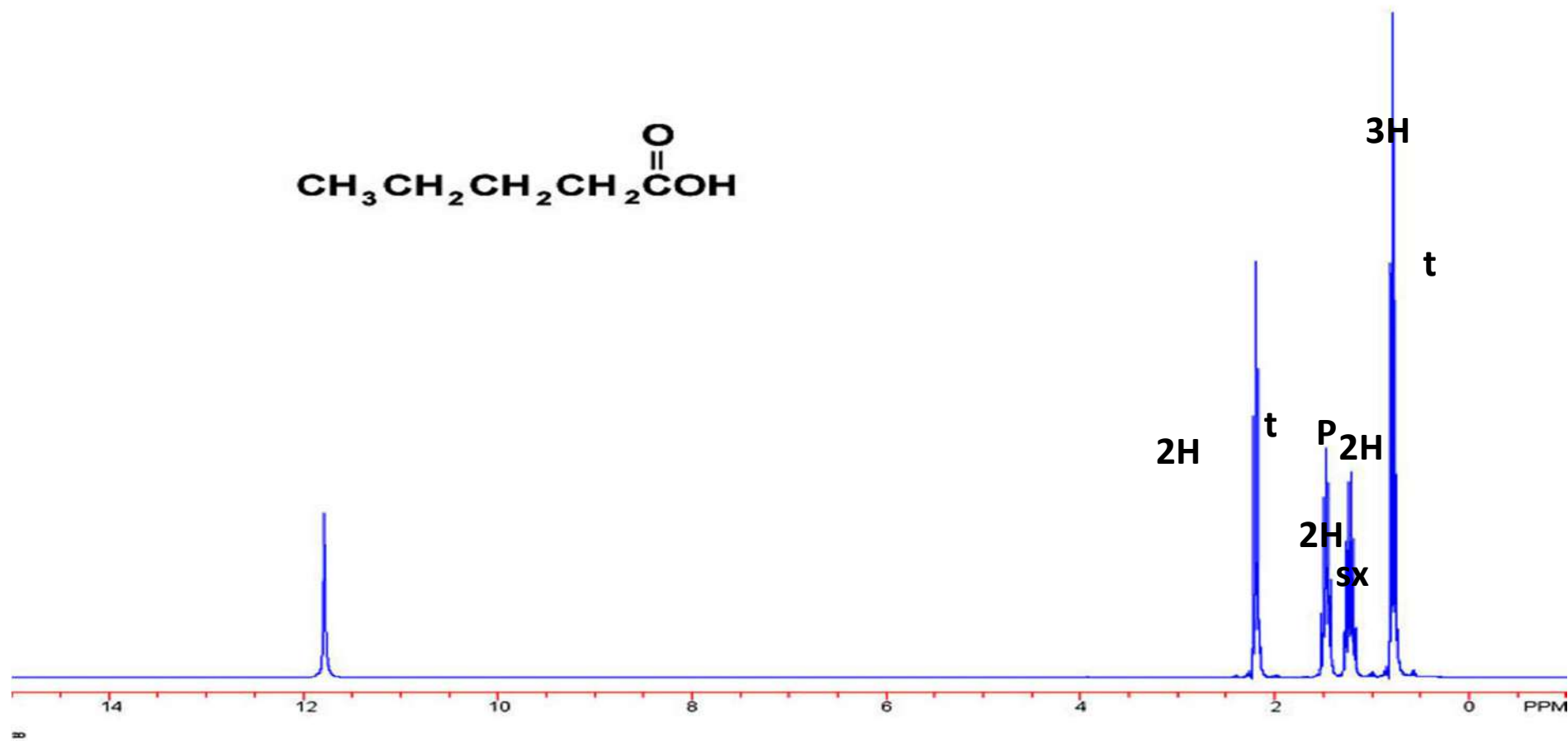


B] C₃H₇Cl ???

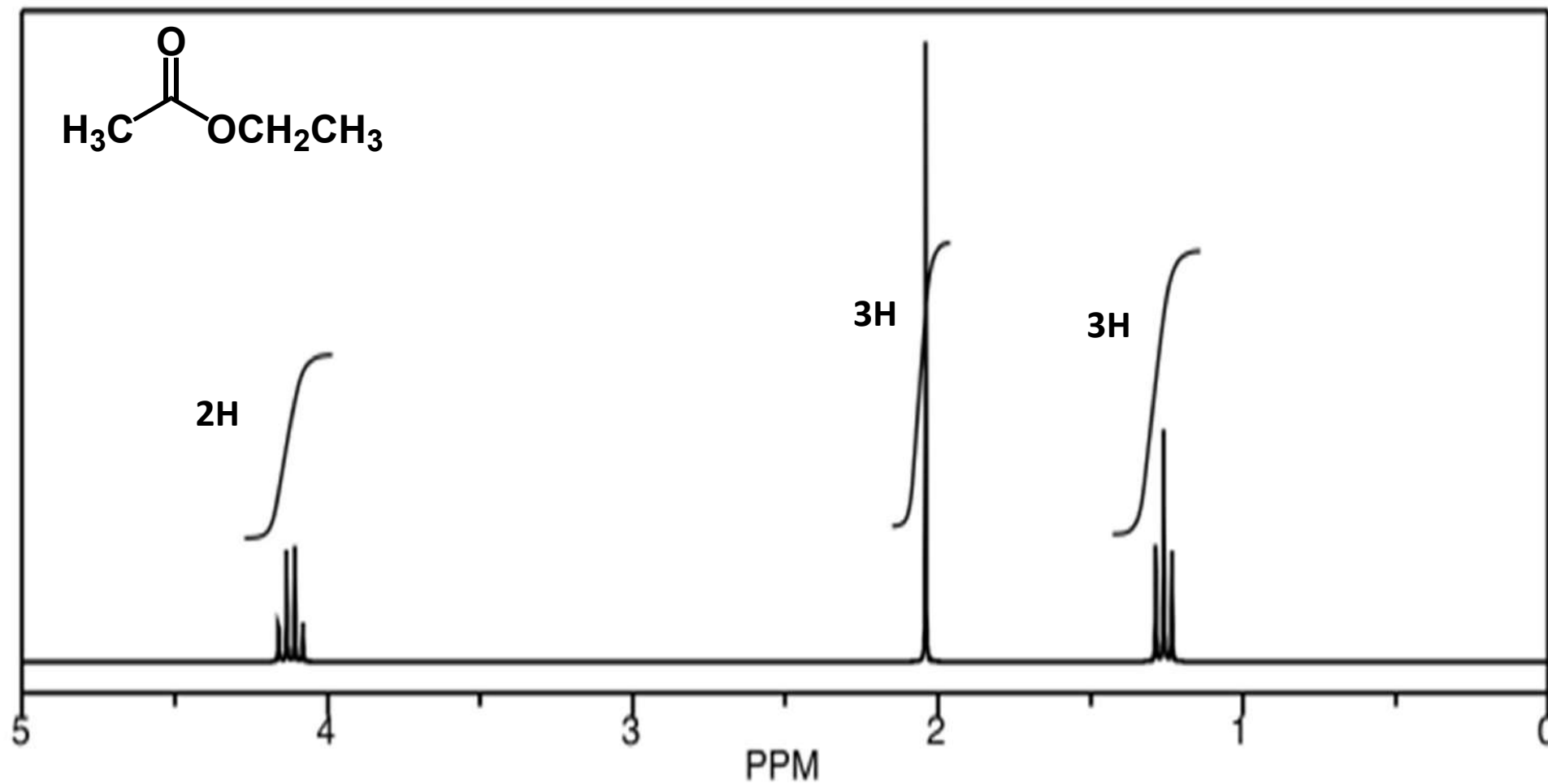
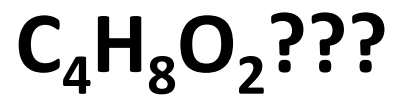


15] Using both given spectrum and molecular formula to identify the unknown compound?

$(C_5H_{10}O_2)$????

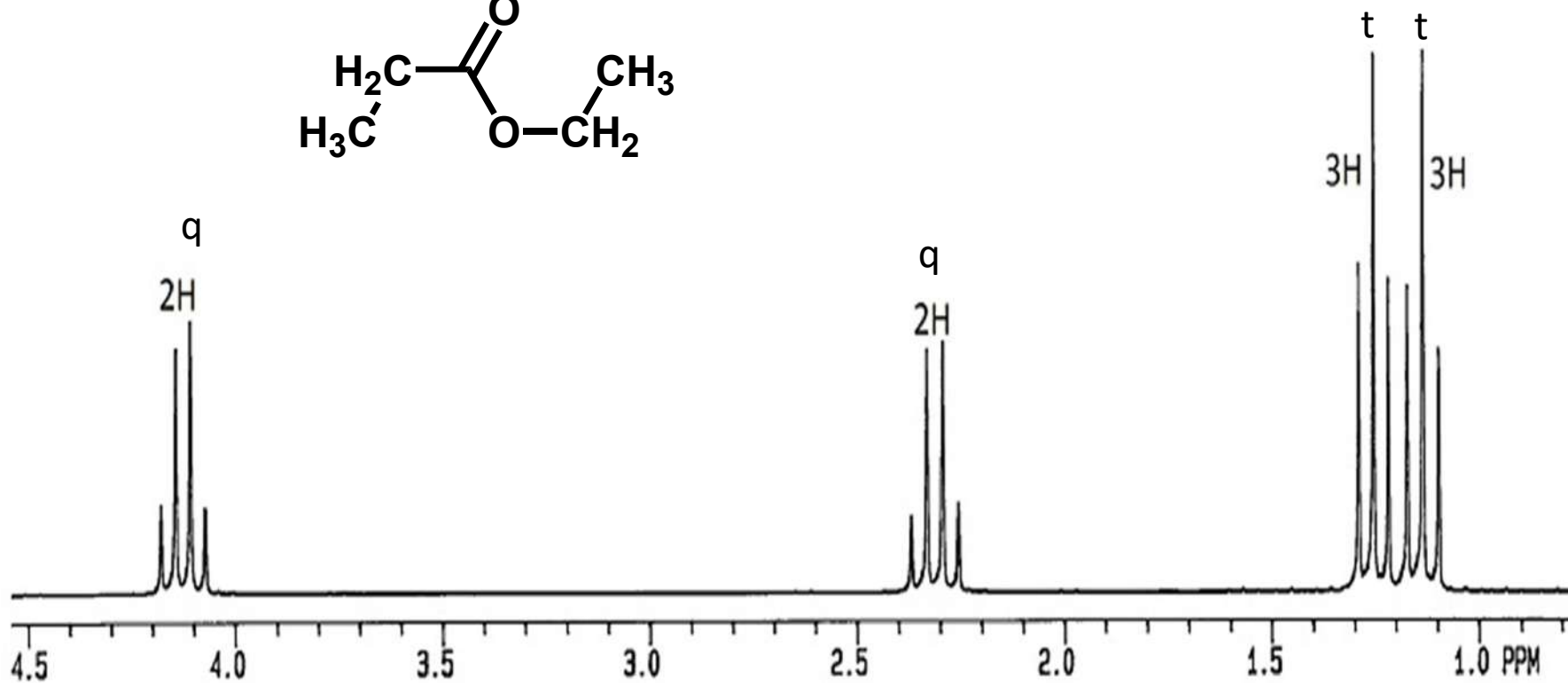
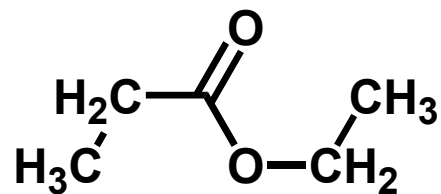


16] Predict the simple chemical structure of the molecular formula ($C_4H_8O_2$) that matches the following spectrum



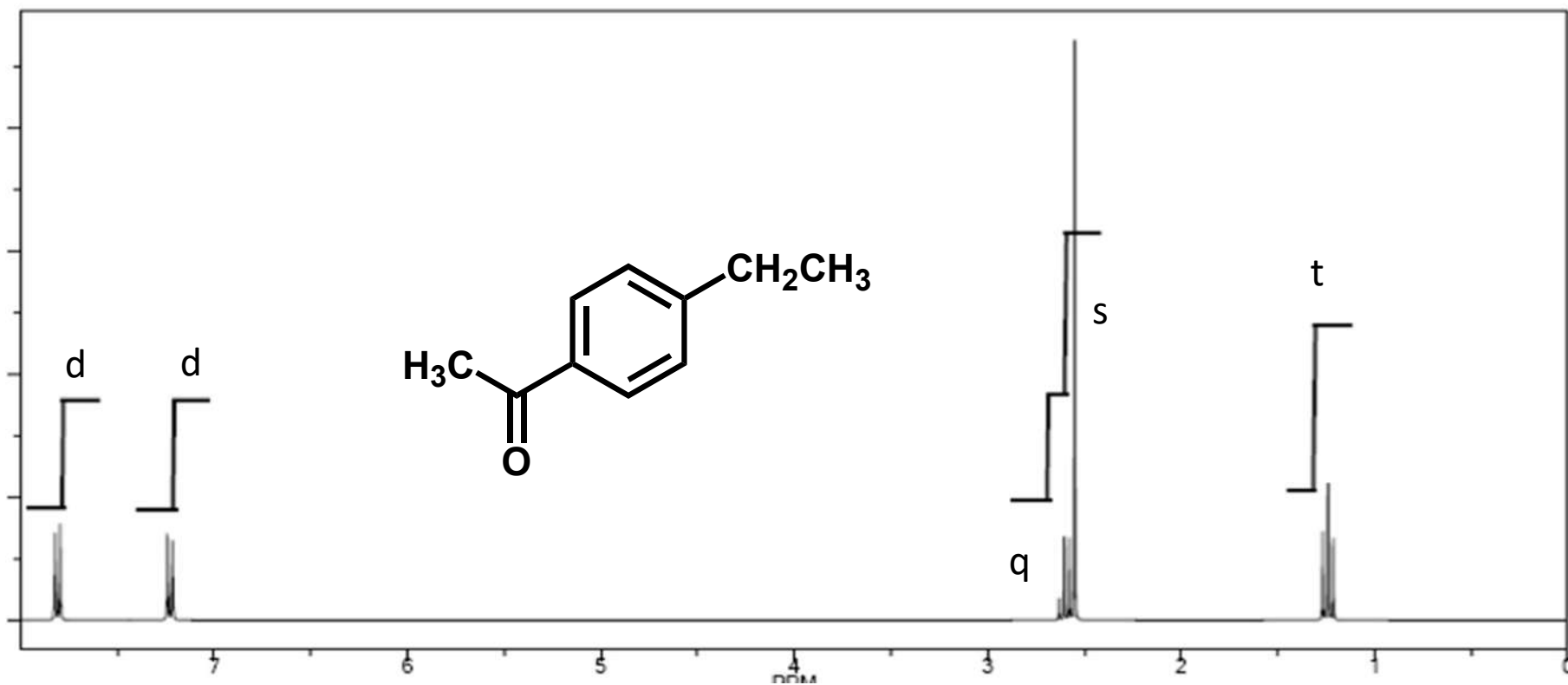
17] Predict the simple chemical structure of the molecular formula that matches the following spectrum ?

(C₅H₁₀O₂) ???

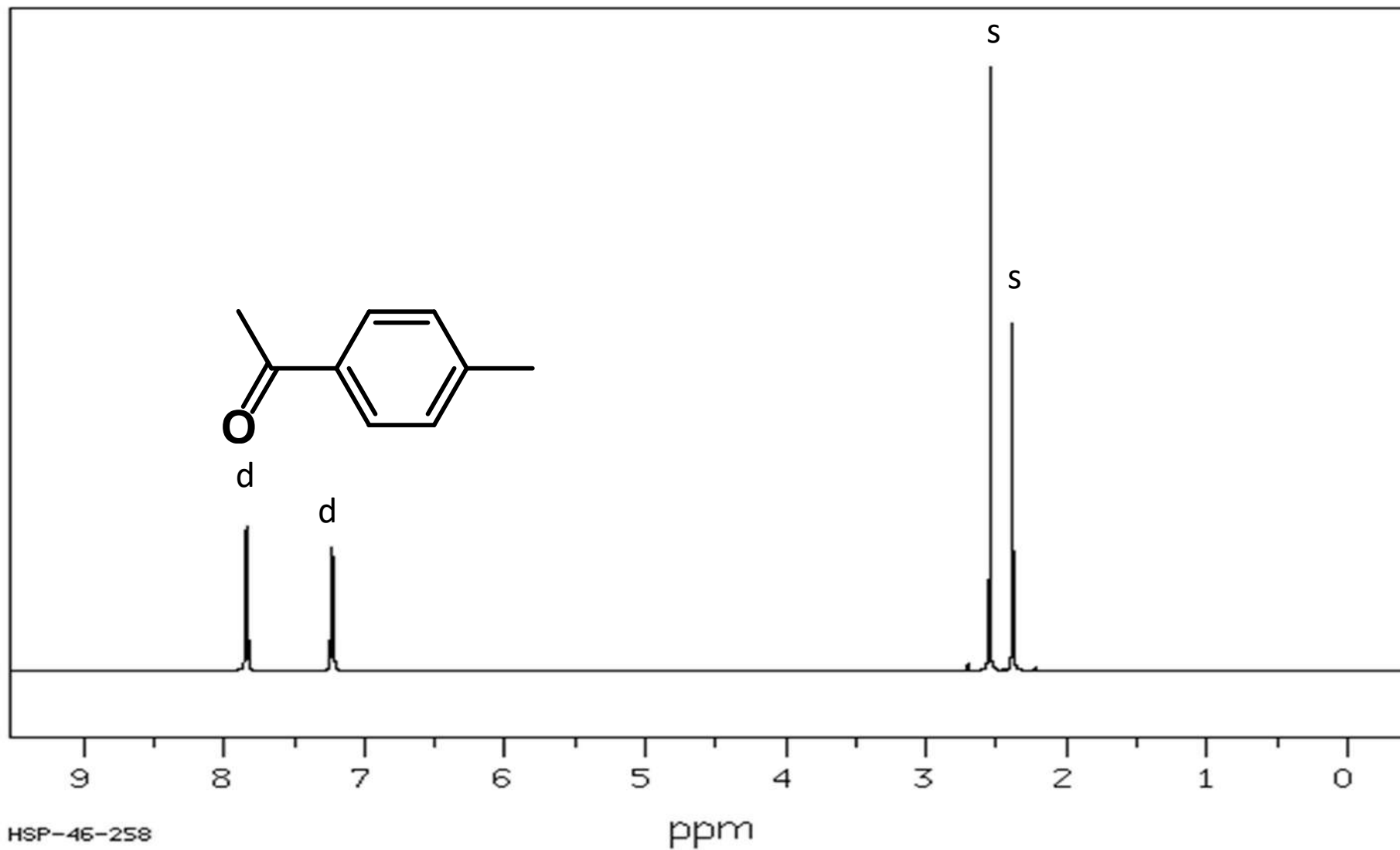


18] Predict the simple chemical structure of the molecular formula that matches the following spectrum?

(C₁₀H₁₂O) ?????

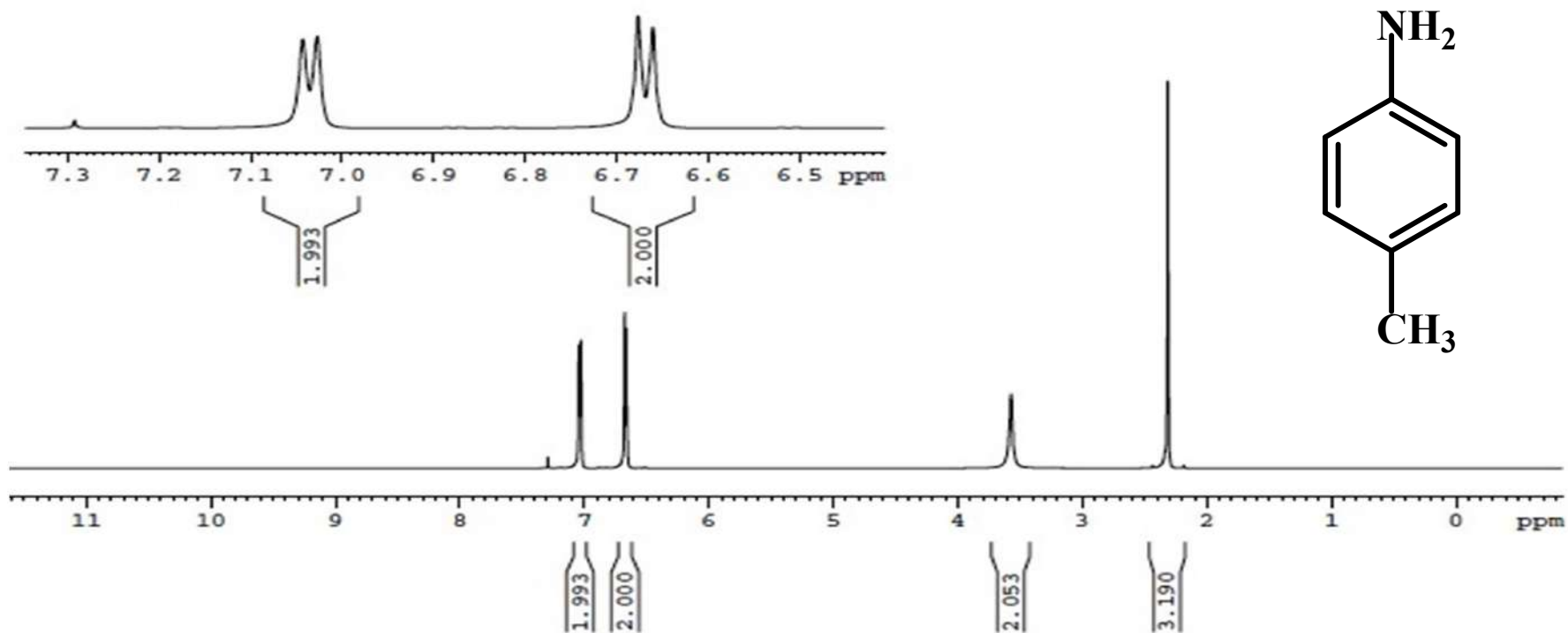


19] Correlate each signal to its hydrogen. Explain briefly

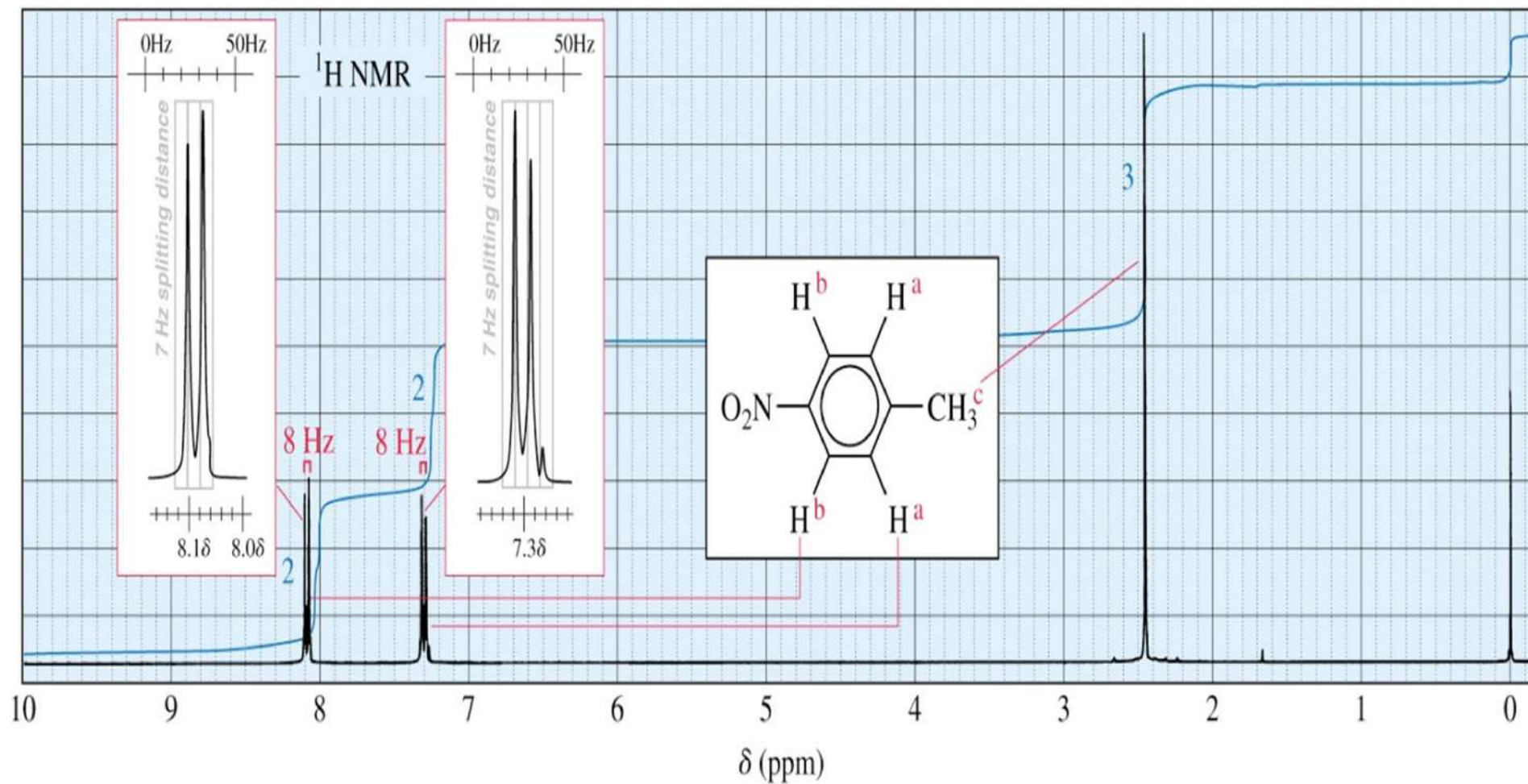


20] Correlate each signal to its hydrogen. Explain briefly

p-Toluidine

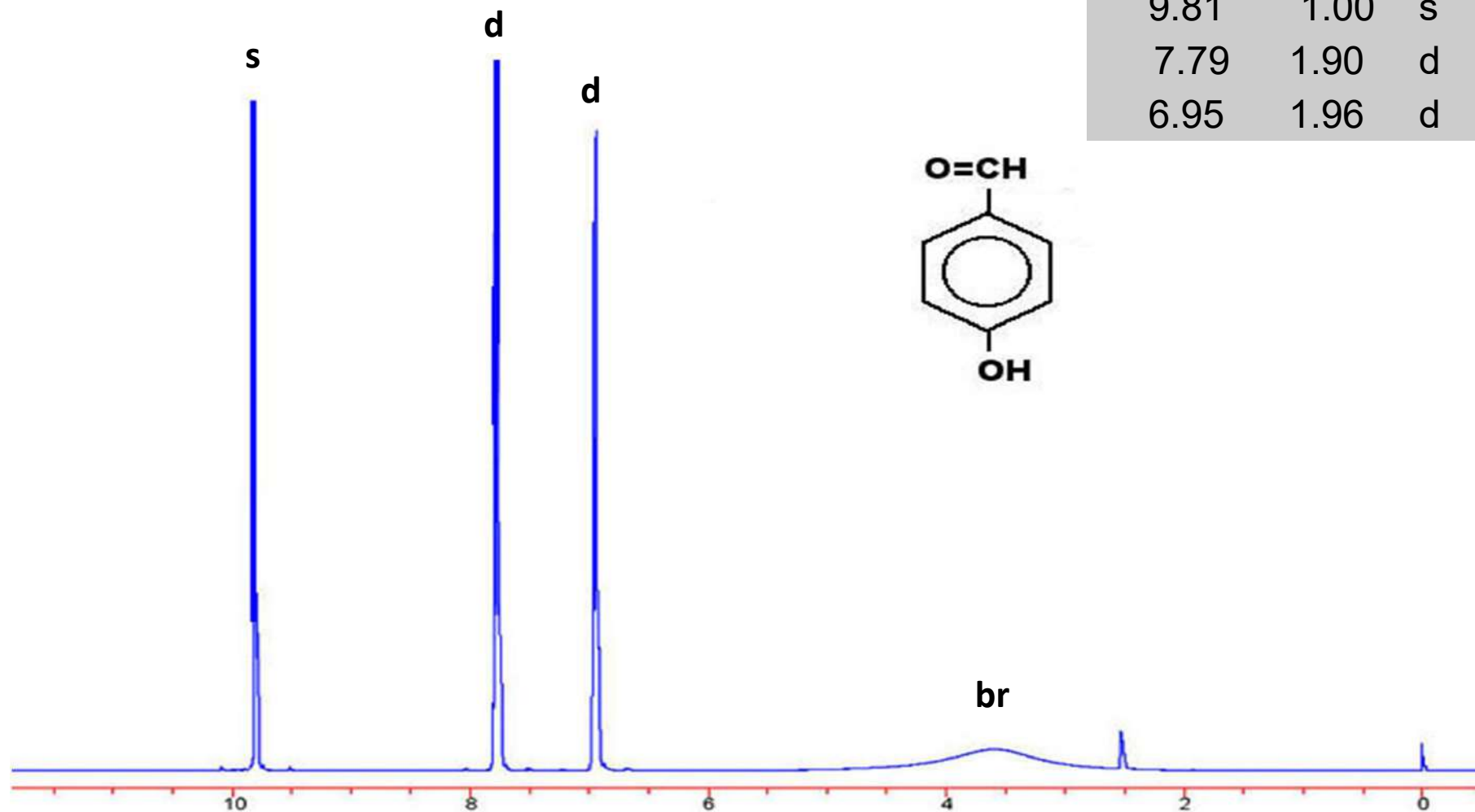


21] Explain complex splitting in the following aromatic compounds.

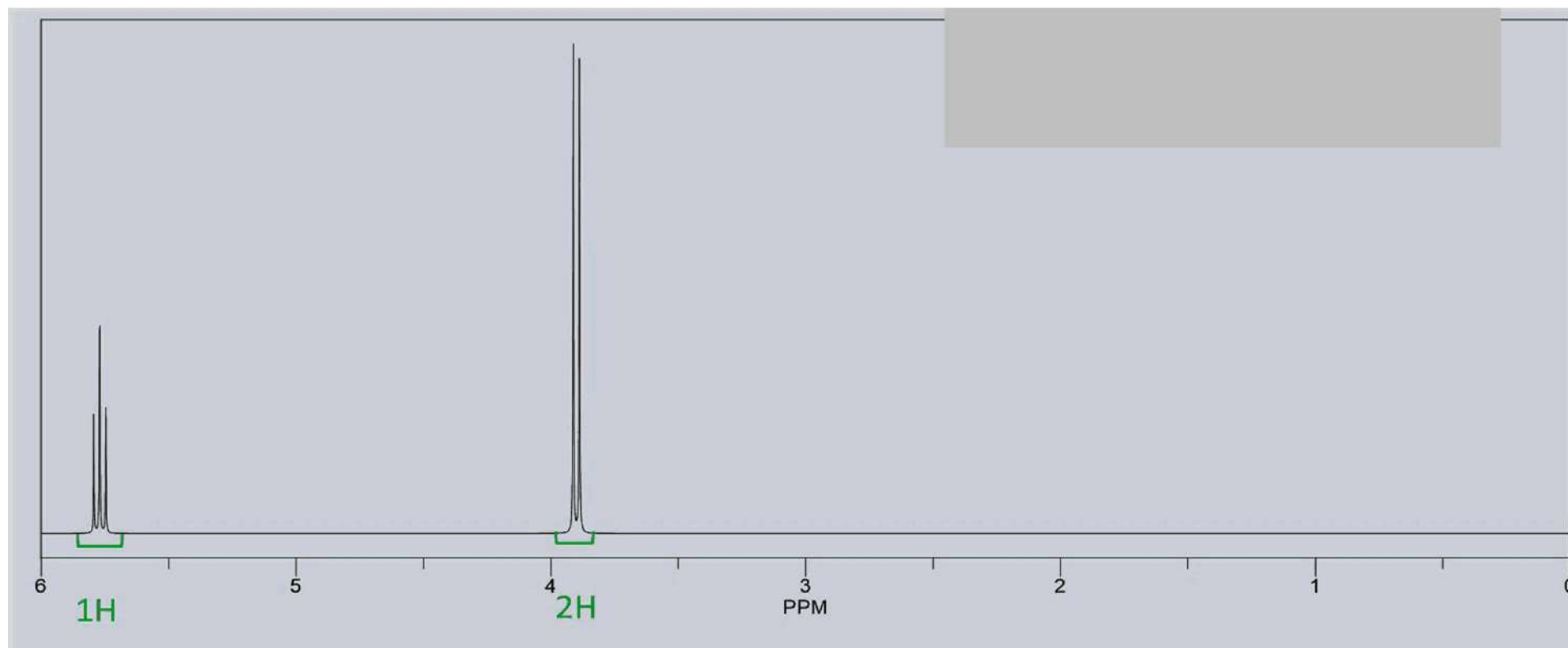
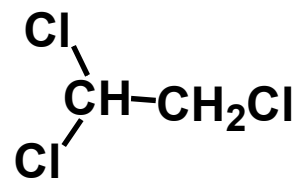
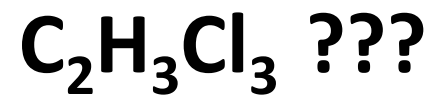


22] Predict the simple chemical structure of the molecular formula that matches the following spectrum ?

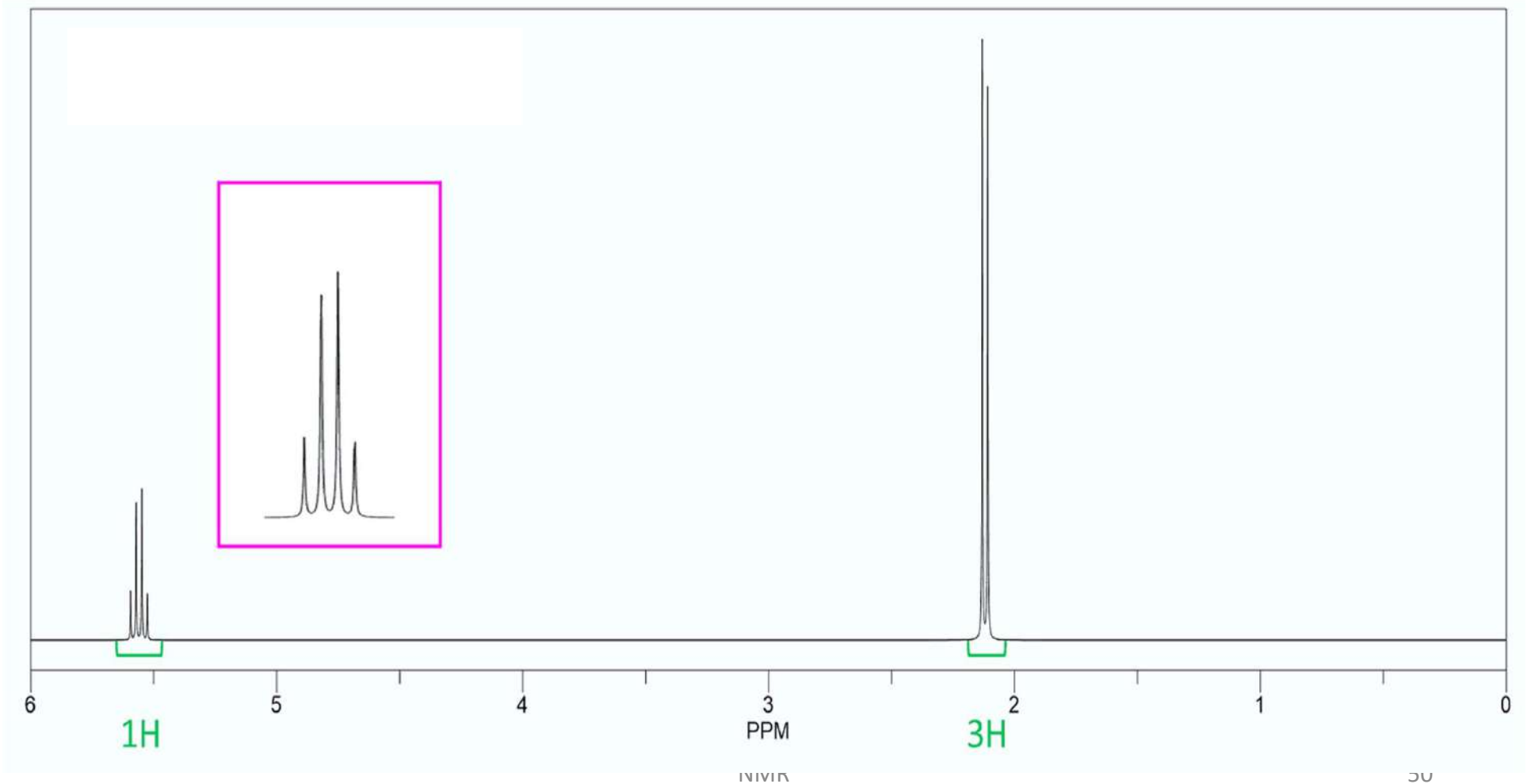
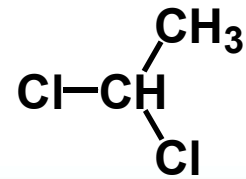
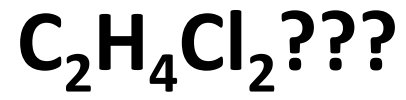
(C₇H₆O₂) ???



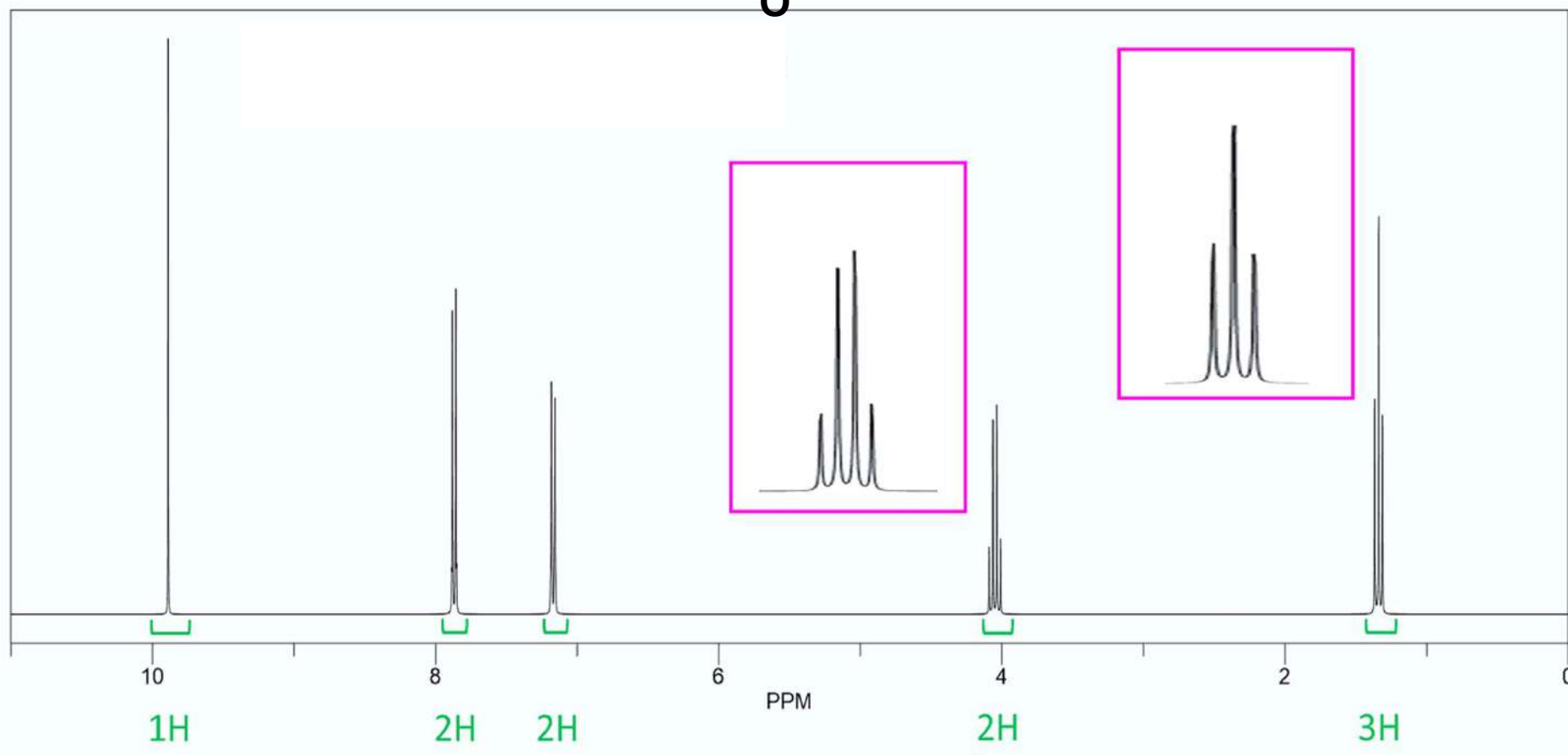
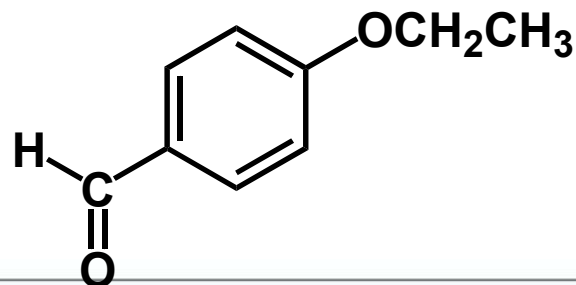
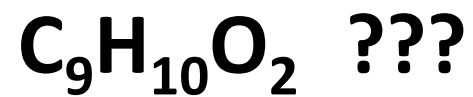
23] Predict the simple chemical structure of the molecular formula that matches the following spectrum ?



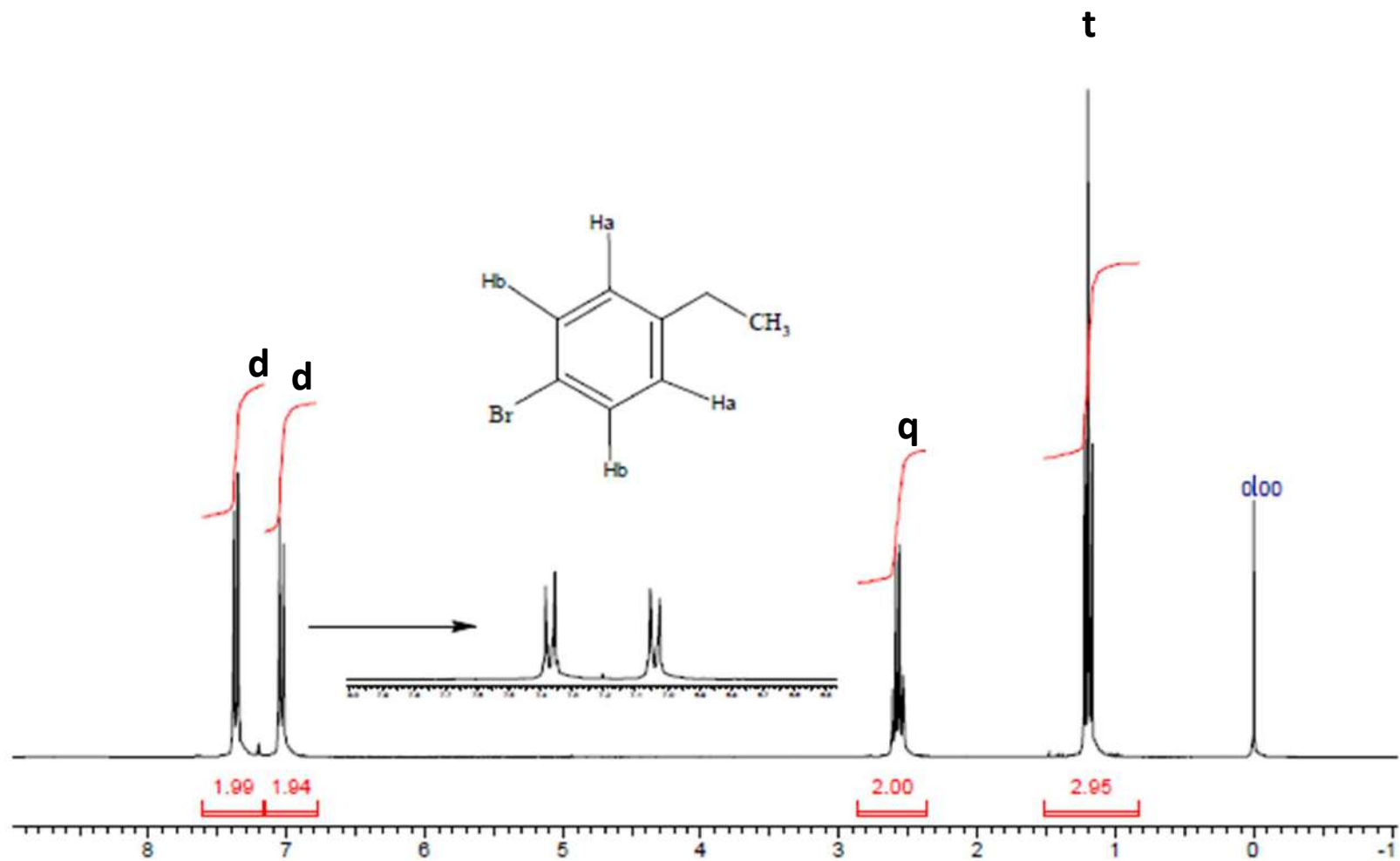
24] Predict the simple chemical structure of the molecular formula that matches the following spectrum ?



25] Predict the simple chemical structure of the molecular formula that matches the following spectrum ?



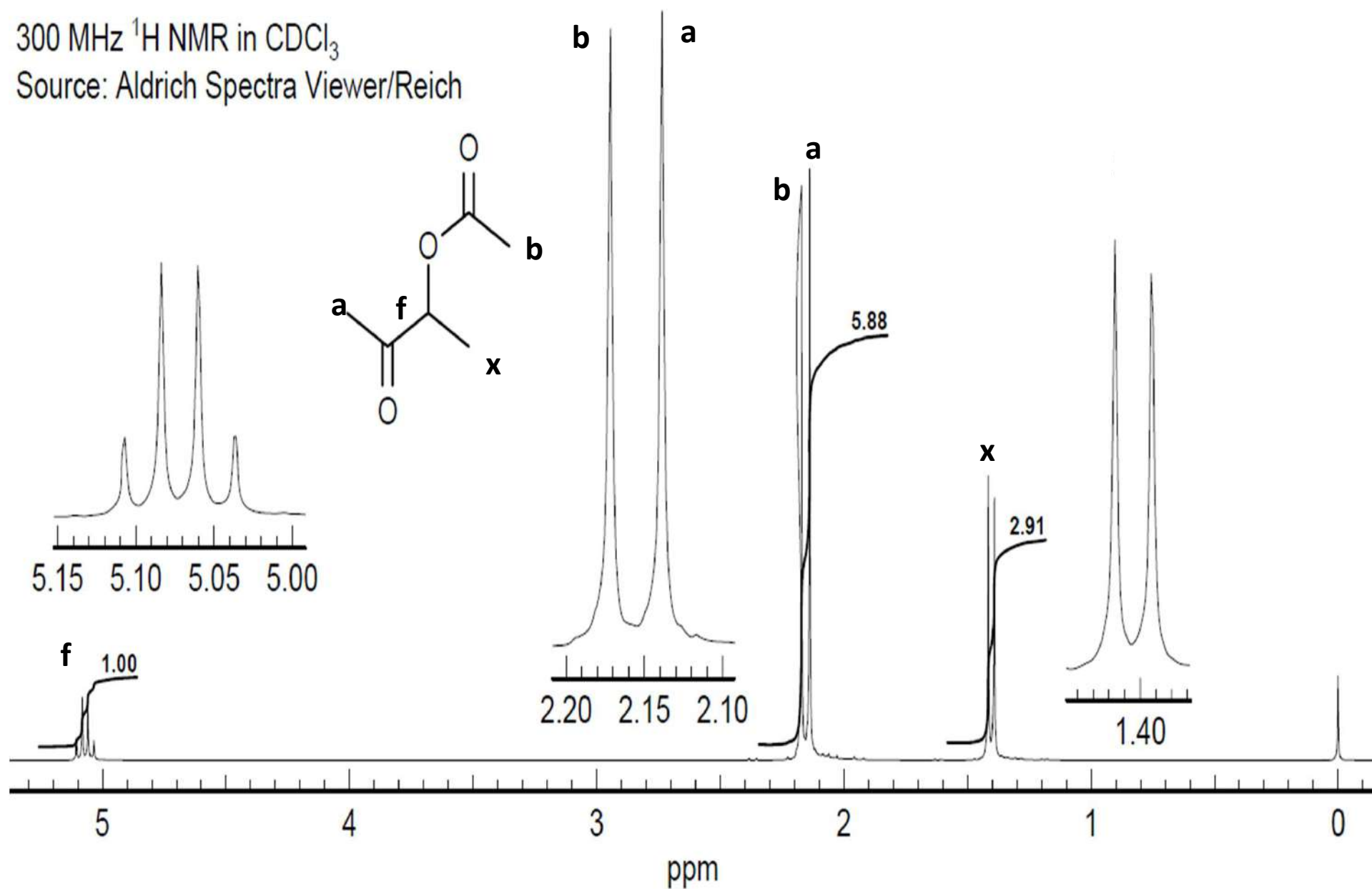
26] Correlate each signal to its hydrogen. Explain briefly



27] In the following spectra; Correlate each signal to its hydrogen. Explain briefly

300 MHz ^1H NMR in CDCl_3

Source: Aldrich Spectra Viewer/Reich



T **H** **E**

E **N** **D**