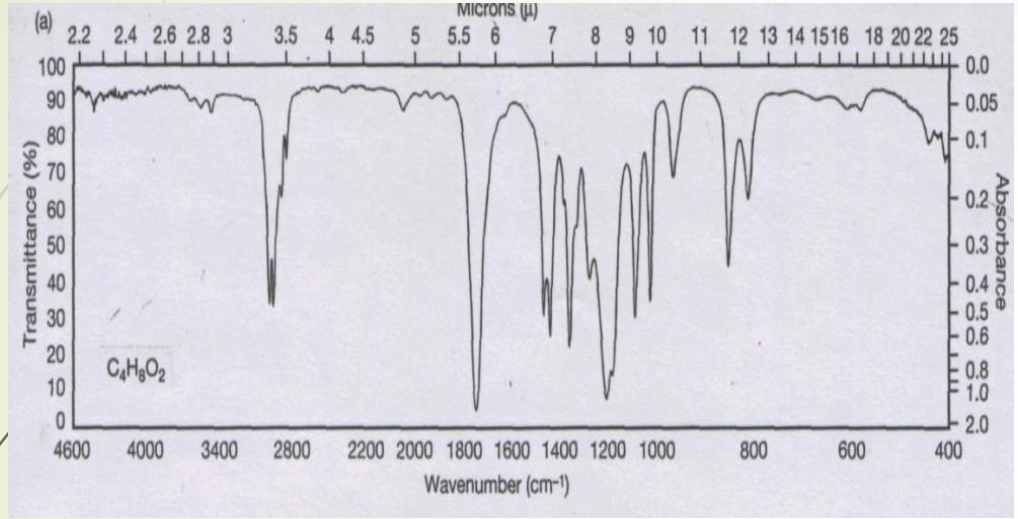
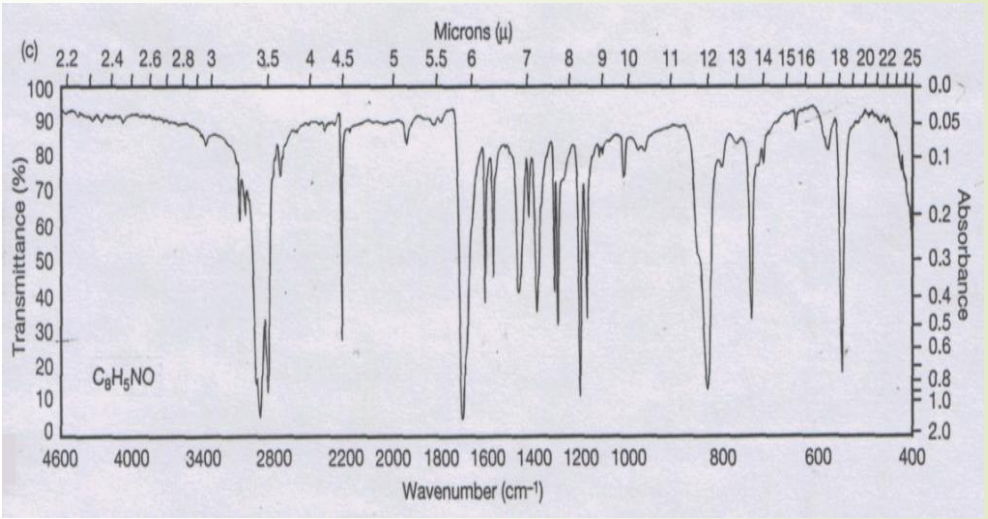
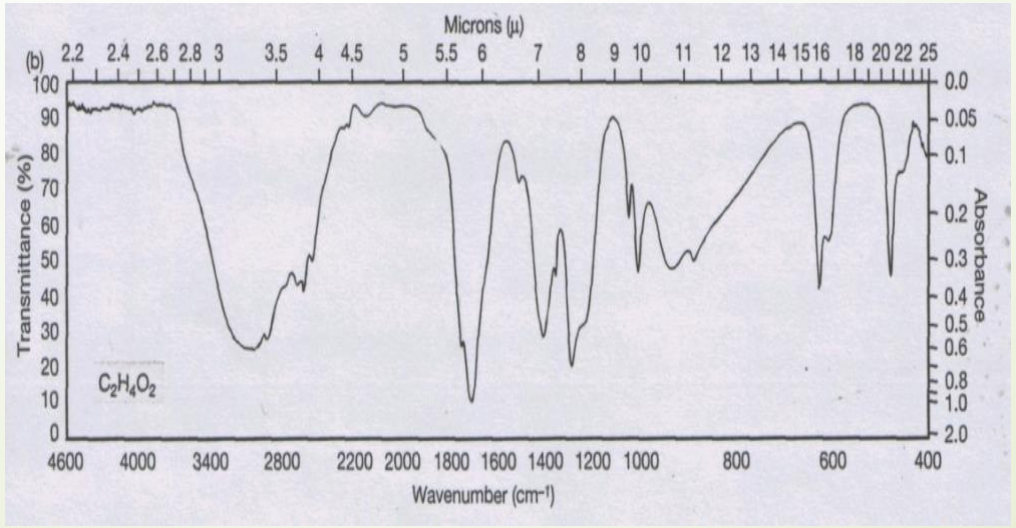
Pharmaceutical Chemistry III Practice

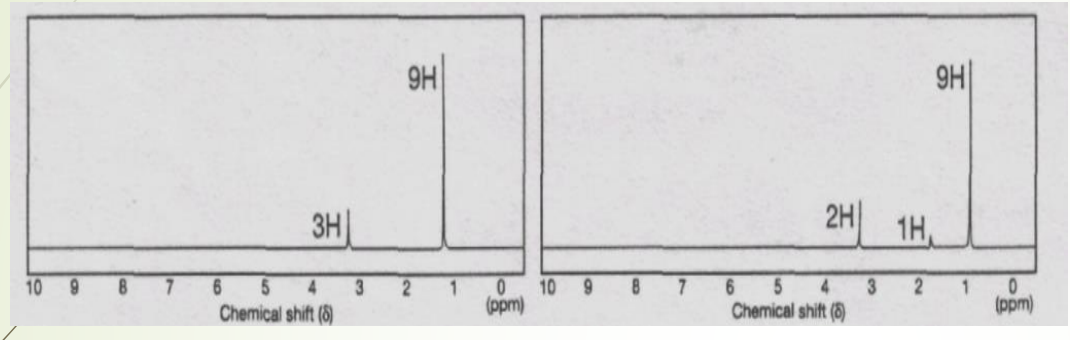
Practice 1. Define the functional groups based on the following IR spectra and draw the possible structures of the molecules based on the molecular formulas.

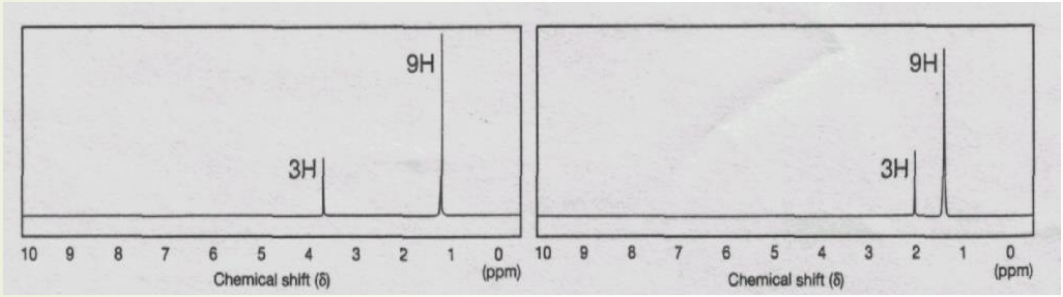


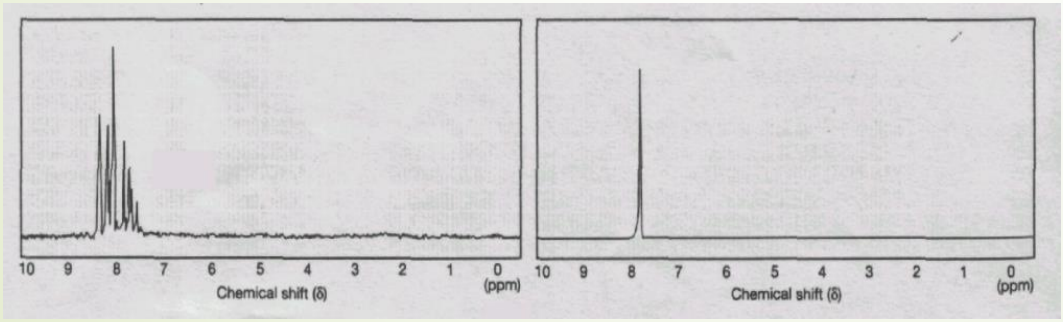


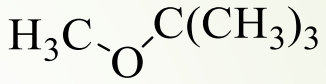


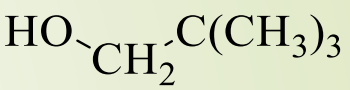
Practice 2. Match the organic compounds with the spectra.

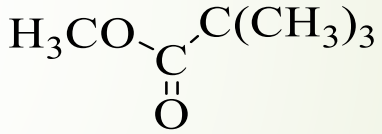


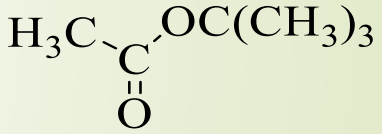


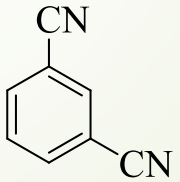


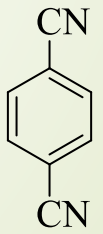




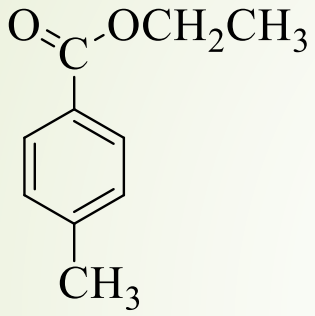




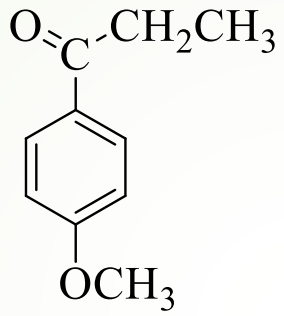




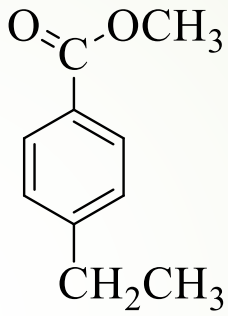
Practice 3. There are 4 bottles that each have a different substance. Match the spectral data of these substances given below. We have 4 bottles, each with a different substance. The spectral data of these substances are given below. Which data belong to which item?



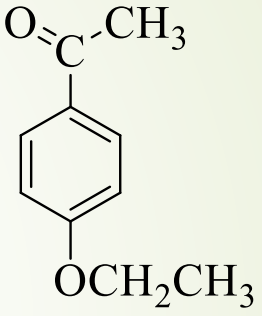
E



F



G

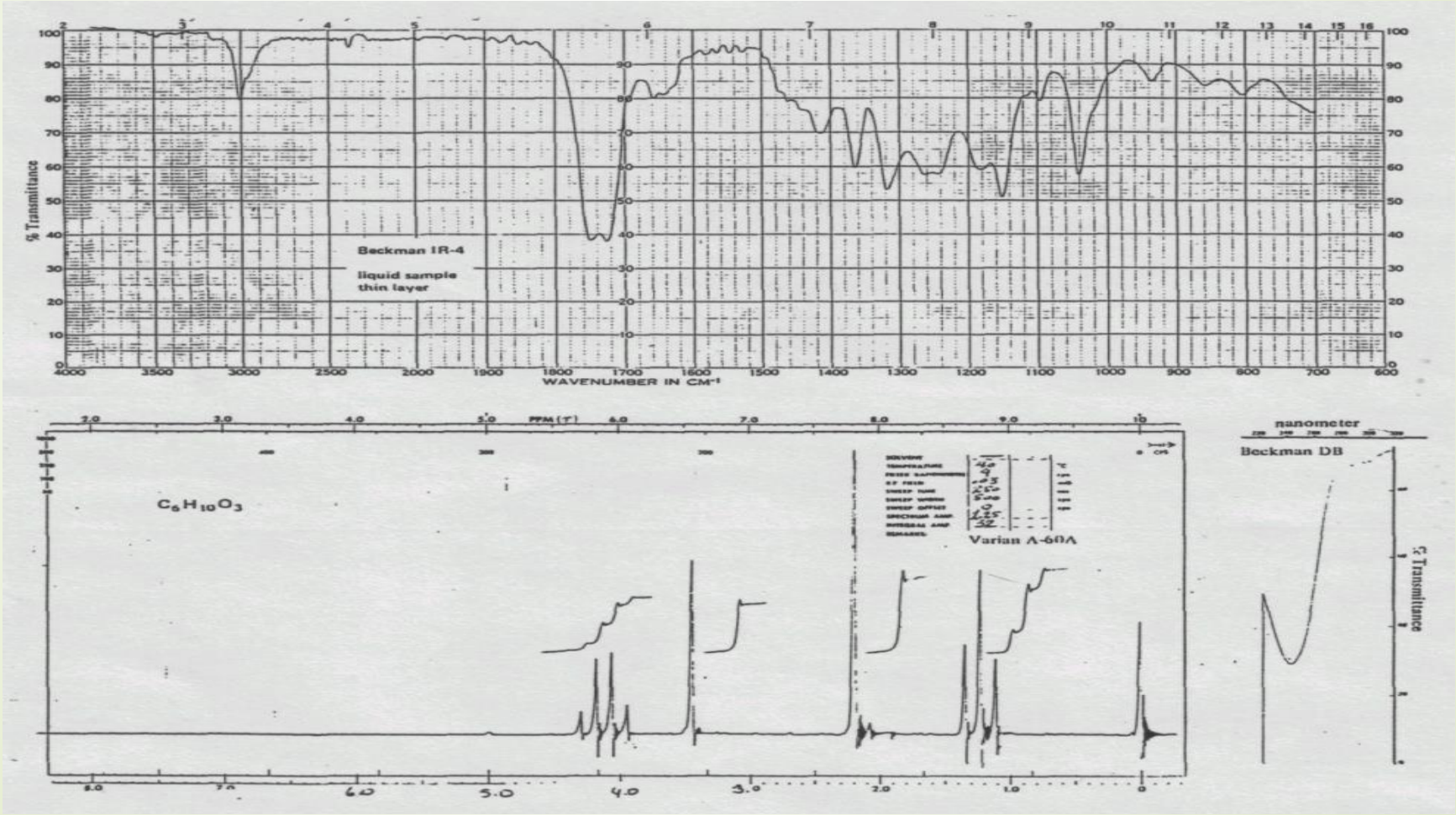


H

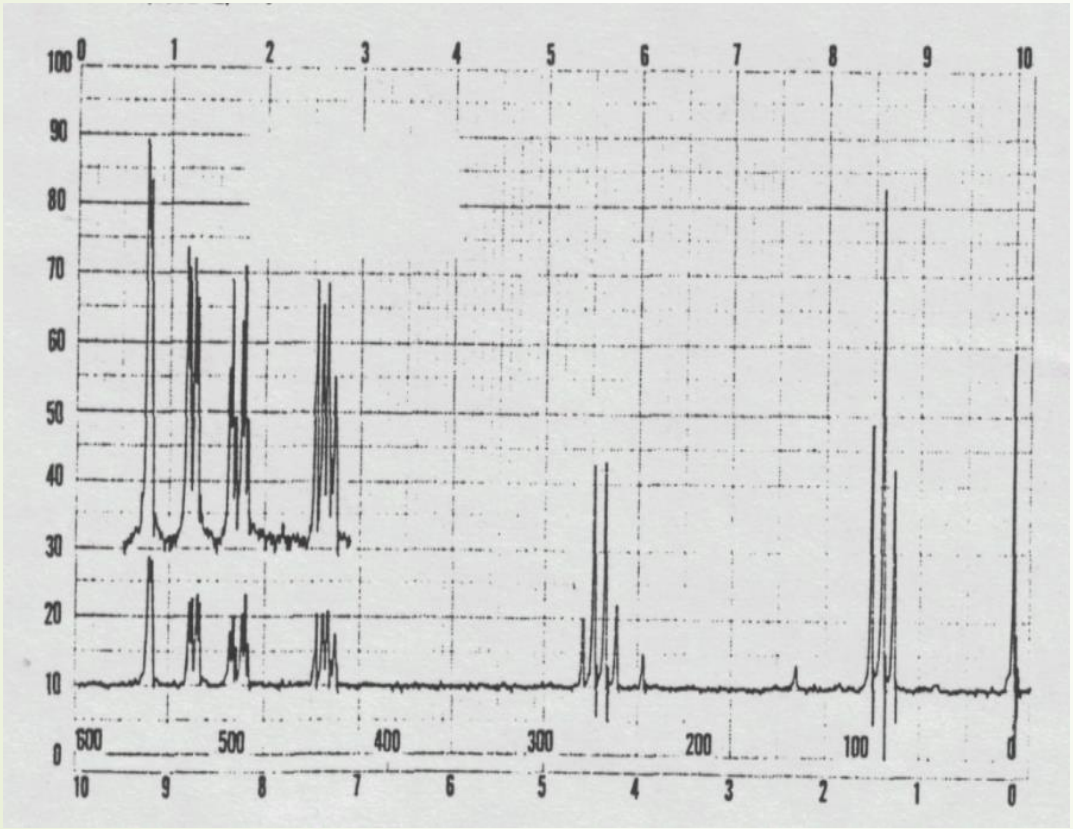
For all compounds, since 4H peaks are observed in the aromatic field, this information has not been used.

1. bottle: IR 1720 cm^{-1} ^1H NMR δ 1.38 (t, 3H), 2.40 (s, 3H), 4.36 (q, 2H)
2. bottle: IR 1688 cm^{-1} ^1H NMR δ 1.12 (t, 3H), 2.81 (q, 2H), 3.76 (s, 3H)
3. bottle: IR 1725 cm^{-1} ^1H NMR δ 1.21 (t, 3H), 2.65 (q, 2H), 3.85 (s, 3H)
4. bottle: IR 1680 cm^{-1} ^1H NMR δ 1.40 (t, 3H), 2.50 (s, 3H), 4.07 (q, 2H)

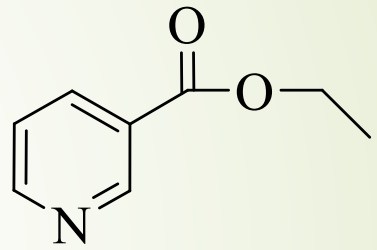
Practise 4. Draw the chemical formula of the compound which is the molecular formula $C_6H_{10}O_3$ and having the UV, IR, 1H NMR spectra recorded below and the m/e values 45, 29, 28 and 15 in the Mass spectrum. Find the open formula of the compound having the closed formula C6H10O3 and the UV, IR, 1H NMR spectra given below and the m / e values 45, 29, 28 and 15 in the Mass spectrum.



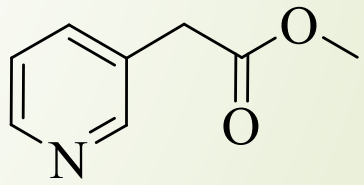
Practise 5. Choose the structure that fits the following ^{1}H-NMR spectrum.



a)



b)

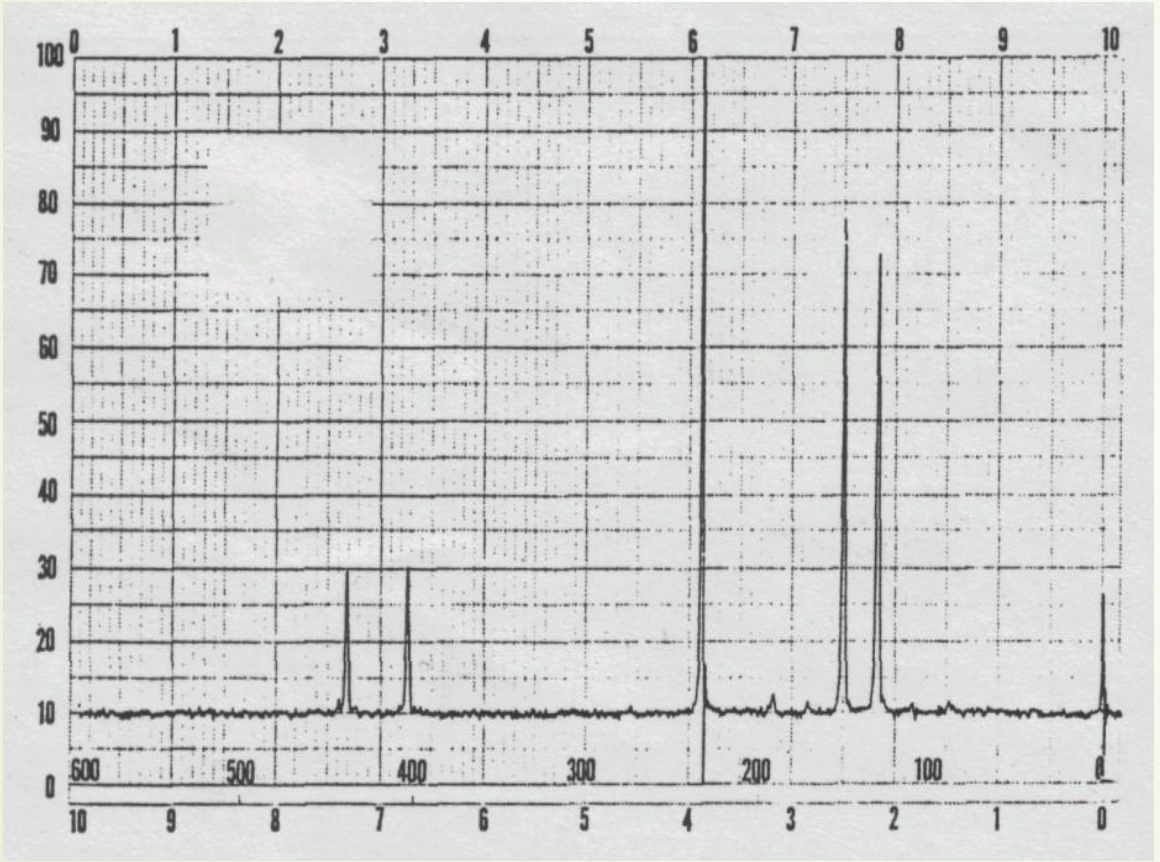


Practise 6. Draw the chemical structure of the compound (molecular formula, C_3H_6O) , based on the following data obtained from IR and ^1H NMR spectra.

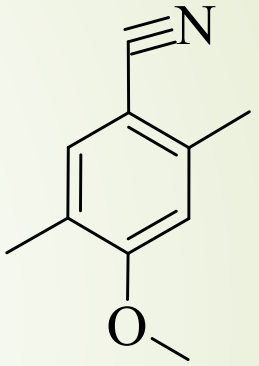
IR (cm^{-1})= 1720, 2800 (dublet)

NMR (δ ppm)= 1 (t, 3H), 2.5 (q, 2H), 9.77 (s, 1H)

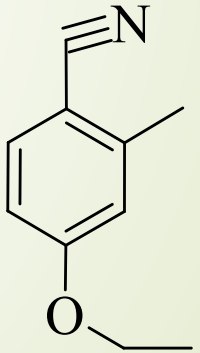
Question 1. Choose the structure that fits the following ^{1}H-NMR spectrum.



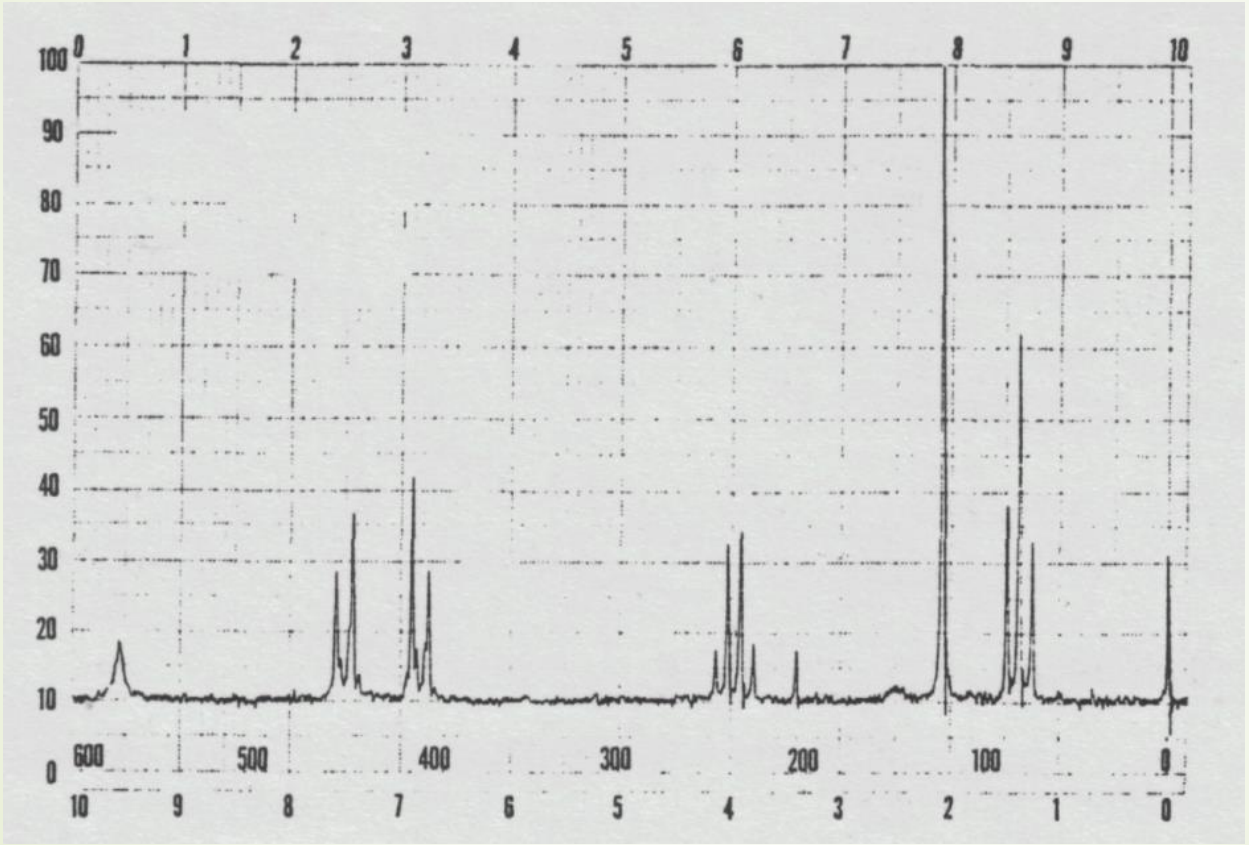
a)



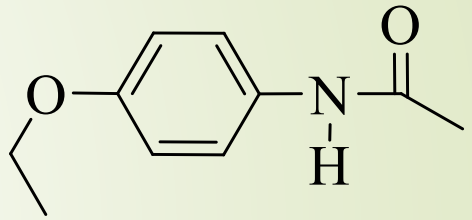
b)



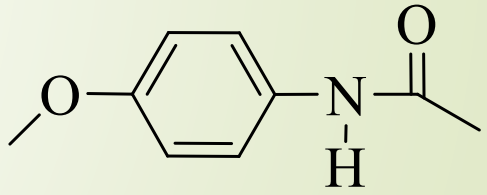
Question 2. Choose the structure that fits the following ^{1}H-NMR spectrum.



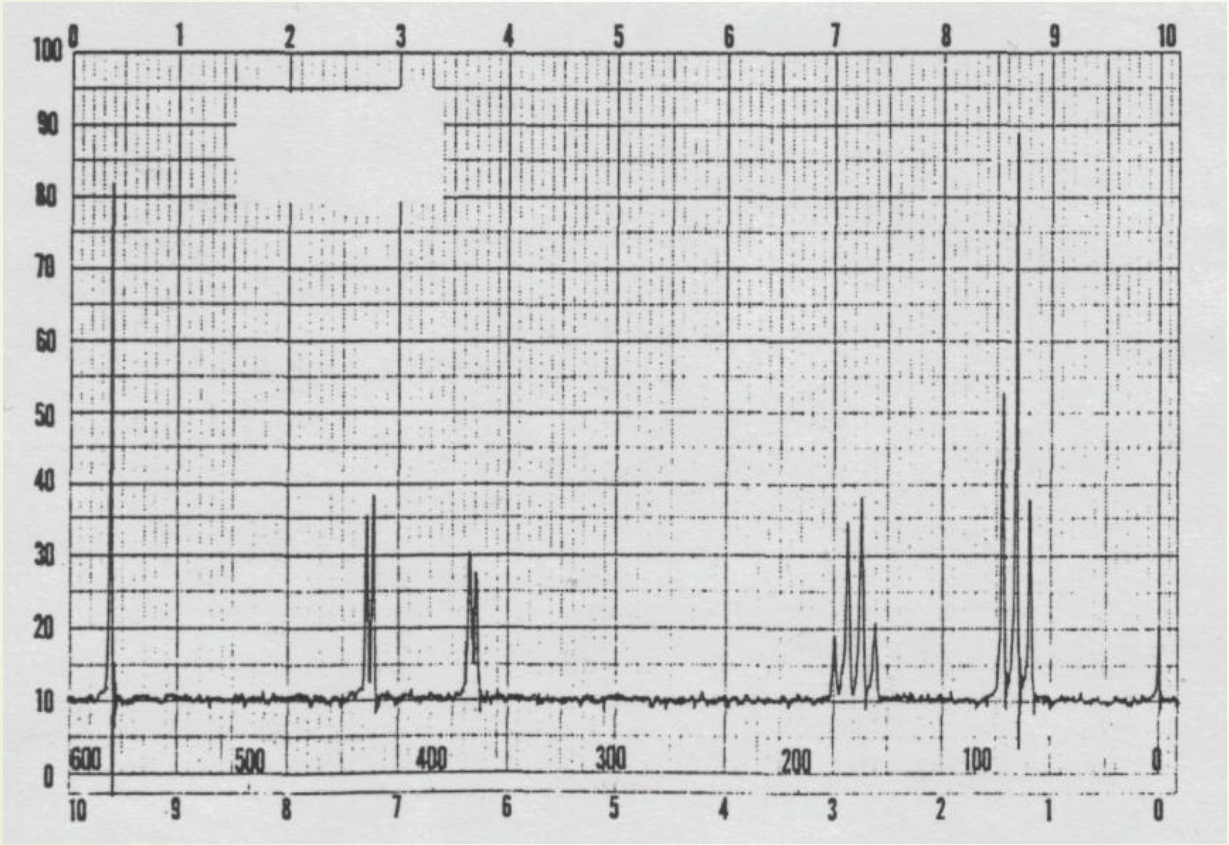
a)



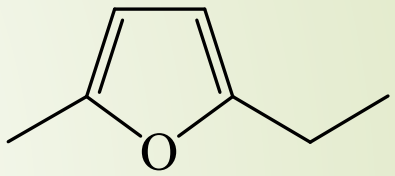
b)



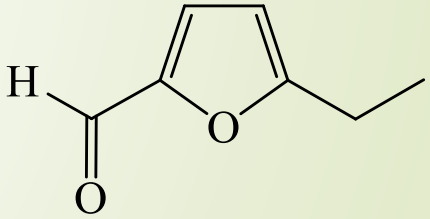
Question 3. Choose the structure that fits the following ^{1}H-NMR spectrum.



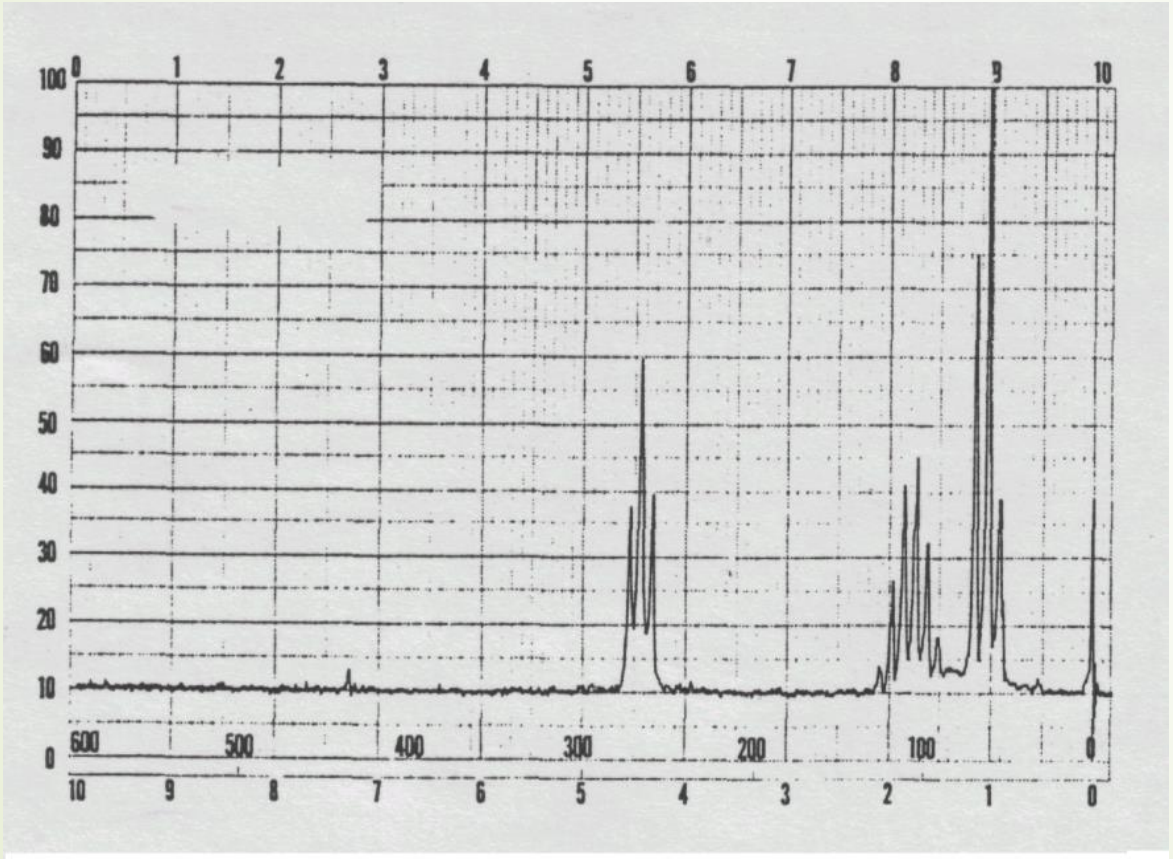
a)



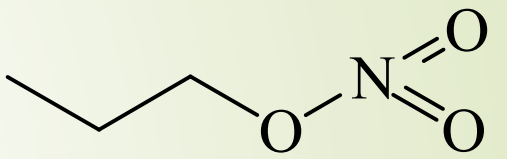
b)



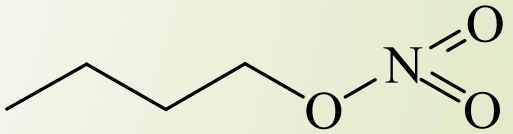
Question 4. Choose the structure that fits the following ^{1}H-NMR spectrum.



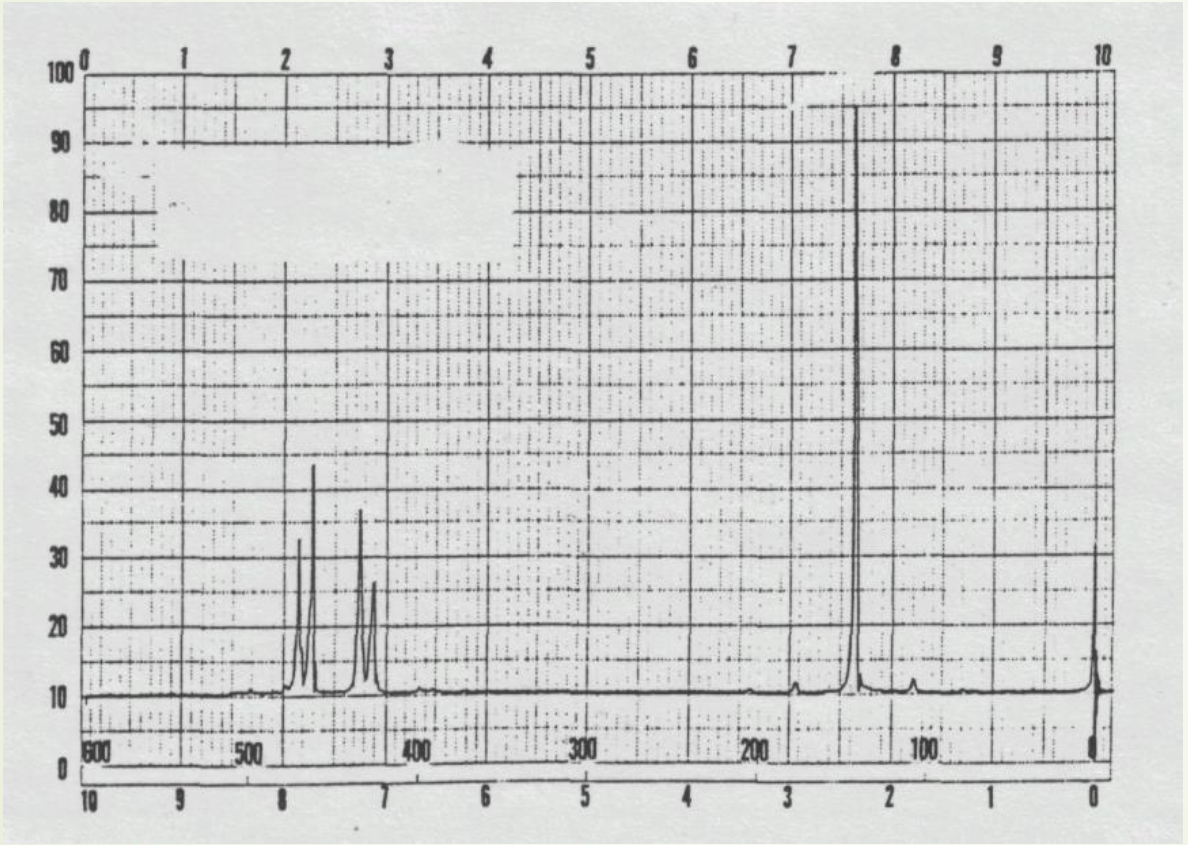
a)



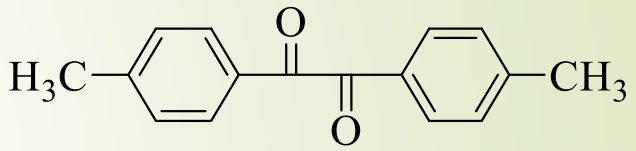
b)



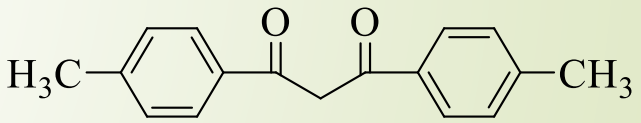
Question 5. Choose the structure that fits the following ^{1}H-NMR spectrum.



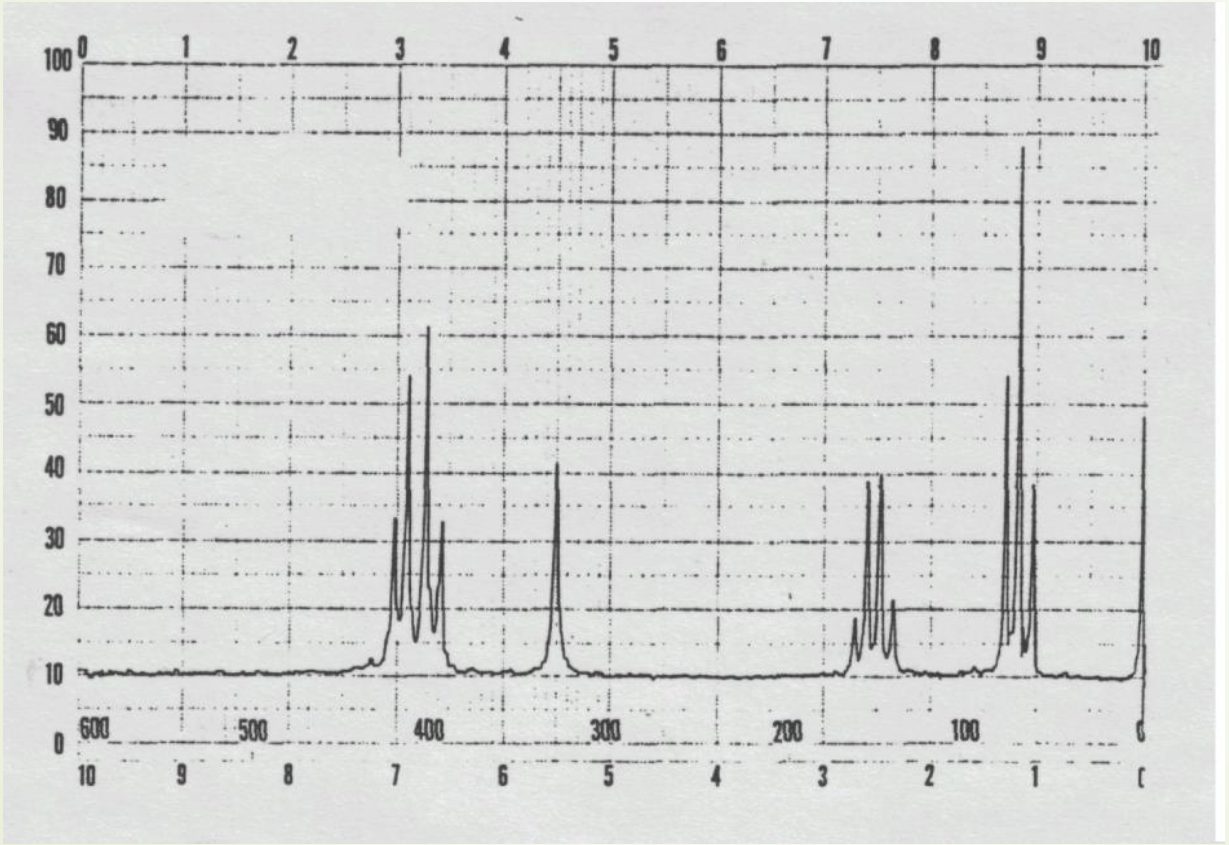
a)



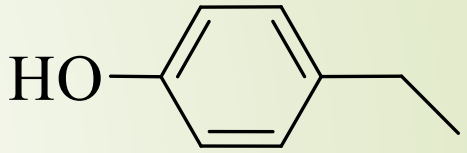
b)



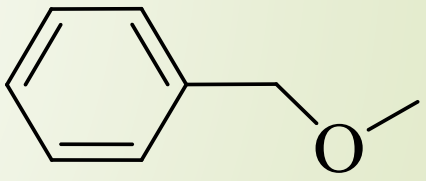
Question 6. Choose the structure that fits the following ^{1}H-NMR spectrum.



a)

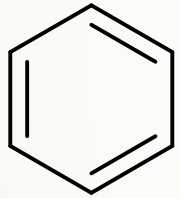


b)

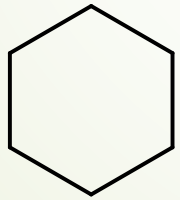


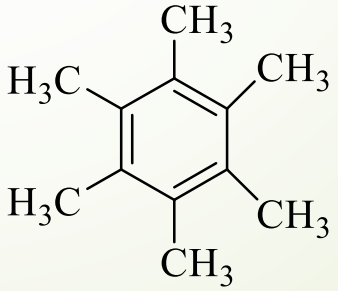
Question 7. Match the organic compounds with the appropriate δ ppm values.

- δ 2.25, 0.04, 1.42, 0.90, 7.37 ppm

a) 

b) $(H_3C)_3Si{-}Si(CH_3)_3$

c) 

d) 

e) $C(CH_3)_4$

Question 8. In ^{1}H NMR spectrum, it is seen that α-hydrogen attached to amine group ($R-\underline{CH_2}NH_2$) is at higher field than α-hydrogen attached to hydroxyl group ($R-\underline{CH_2}OH$). Explain why.

Question 9. Find the chemical structure of the compound which is molecular formula, C_3H_6O , based on the following data obtained from IR, Mass and ^1H NMR spectra.

- IR (cm^{-1})= 1710
- NMR (δ ppm)= 2.2 (s, 6H)
- Mass (m/e)= 43, 15

a) H_3CCOCH_3 b) HO-CH=CH-CH_3

Question 10. Find the chemical structure of the compound which is molecular formula, $C_3H_6O_2$, based on the following data obtained from IR, Mass and ^1H NMR spectra.

- IR (cm^{-1})= 1740
- NMR (δ ppm)= 2.1 (s, 3H), 3.7 (s, 3H)
- Mass (m/e)= 59, 43, 31, 15

a) $HO\text{-}CH_2\text{-}C(OH)=CH_2$ b) $H_3CCOOCH_3$

Question 11. Find the chemical structure of the compound which is molecular formula, C_2H_5NO , based on the following data obtained from IR, Mass and ^1H NMR spectra.

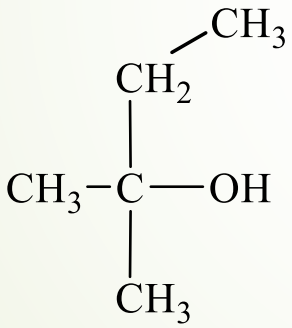
- IR (cm^{-1})= 3530, 1690
- NMR (δ ppm)= 2.0 (s, 3H), 4.7 (s, 2H)
- Mass (m/e)= 44, 15

a) H_3C-NH-COH b) H_3CCONH_2

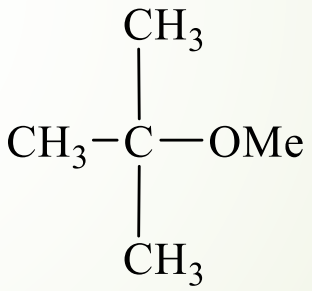
Question 12. Find the chemical structure of the compound which is molecular formula, $C_5H_{12}O$, based on the following data obtained from ^1H NMR spectrum.

- NMR (δ ppm)= 1.0 (s, 9H), 3.0 (s, 3H)

a)



b)



Question 13. Find the chemical structure of the compound which is molecular formula, $C_4H_{10}O$, based on the following data obtained from ^1H NMR spectrum.

- NMR (δ ppm)= 0.9 (t, 6H), 3.4 (q, 4H)

a) $H_3CCH_2CH(OH)CH_3$

b) $CH_3CH_2OCH_2CH_3$

c) $H_3COCH_2CH_2CH_3$

d) $H_3CCH_2CH_2CH_2OH$

Question 14. Find the chemical structure of the compound which is molecular formula, $C_2H_3Cl_3$, based on the following data obtained from ^1H NMR spectrum.

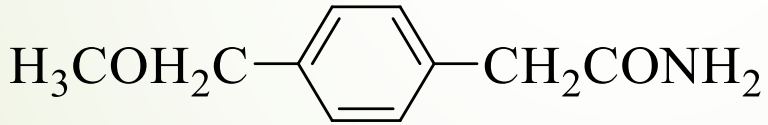
- NMR (δ ppm)= 3.9 (d, 2H), 5.2 (t, 1H)

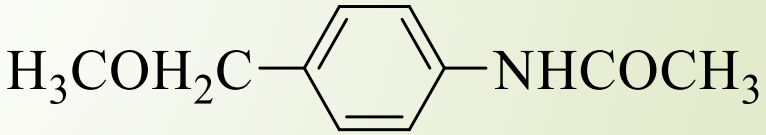
a) $H_3C\text{-}CCl_3$

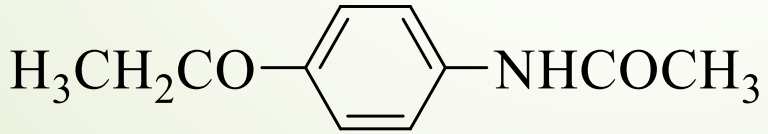
b) $ClCH_2CHCl_2$

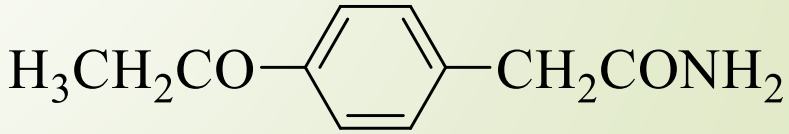
Question 15. Find the chemical structure of the compound which is molecular formula, C_3H_6O , based on the following data obtained from IR, Mass and ^1H NMR spectra.

- IR (cm^{-1})= 3500, 1650
- NMR (δ ppm)= 1.2 (t, 3H), 2.0 (s, 3H), 4.0 (q, 2H), 7.0 (d, 2H), 7.5 (d, 2H), 7.9 (s, 1H)
- Mass (m/e)= 179, 164, 137, 109, 108

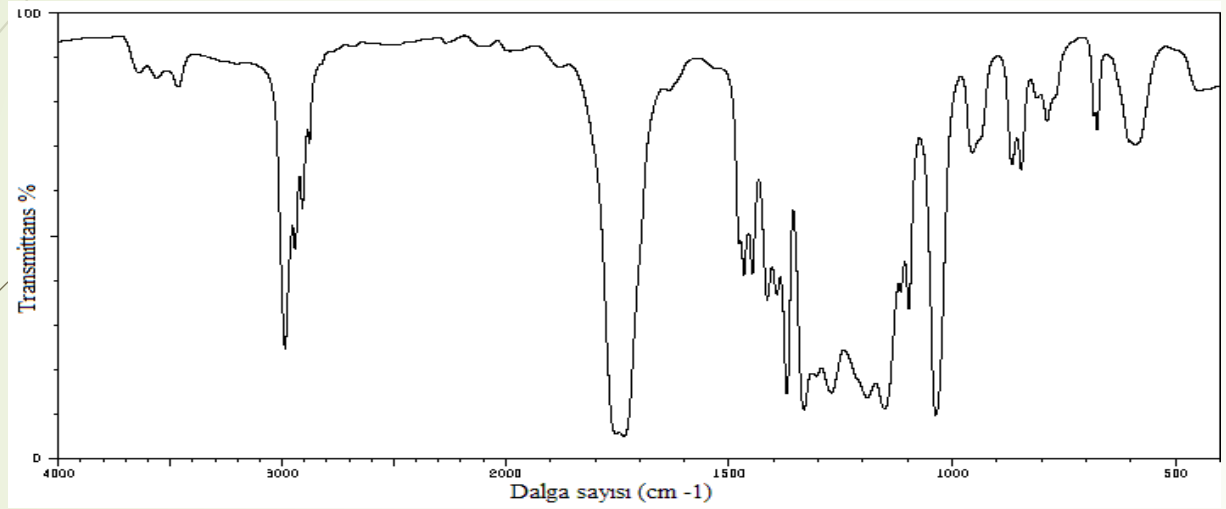
a) 

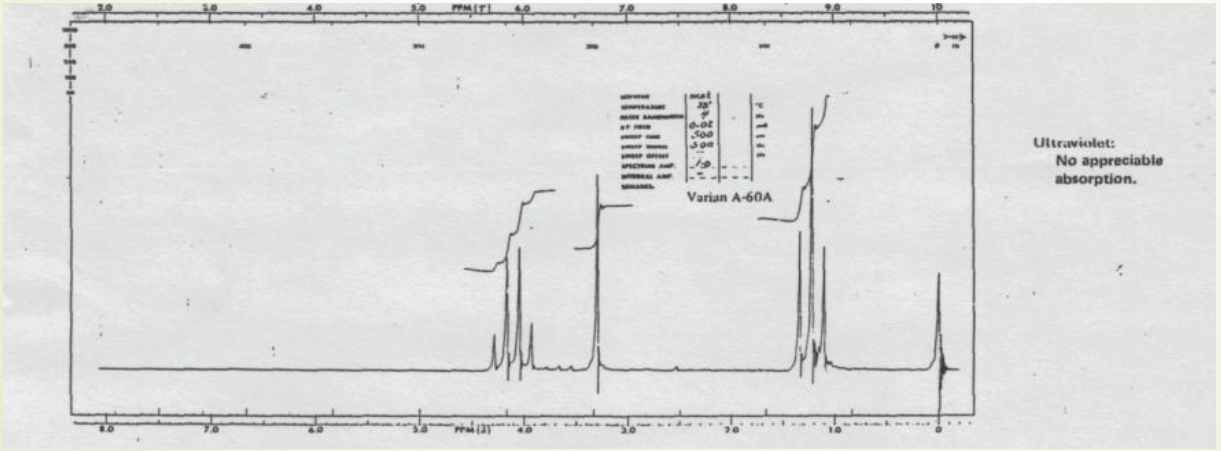
b) 

c) 

d) 

Question 16. Find the chemical structure of the compound which is molecular formula, C_3H_6O , based on the following data obtained from IR and ^1H NMR spectra.

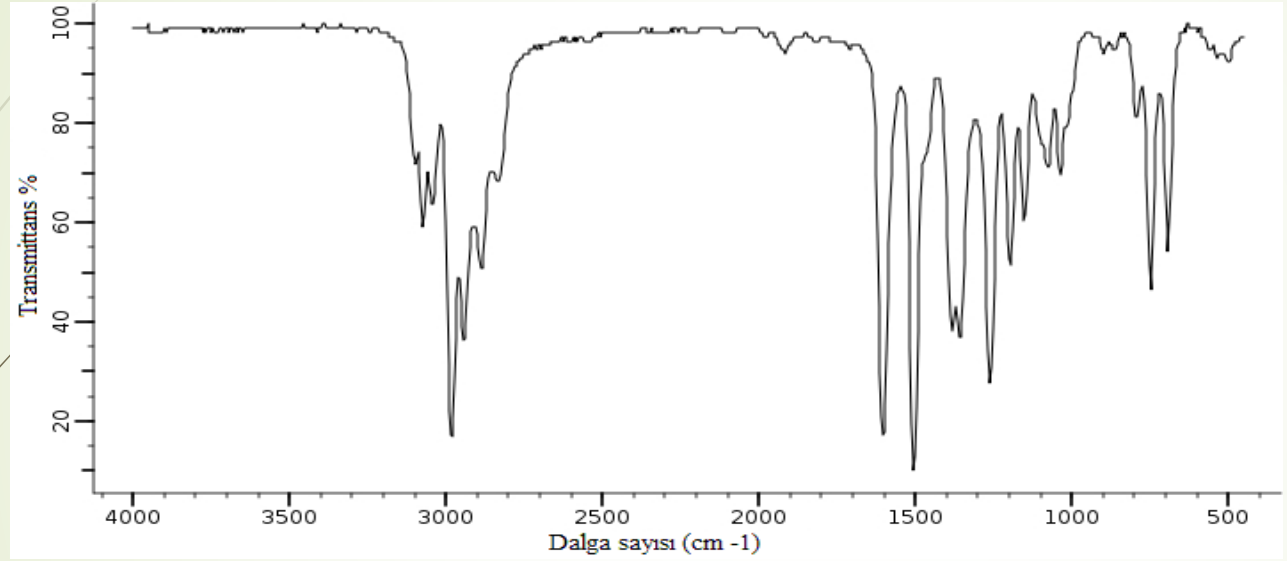




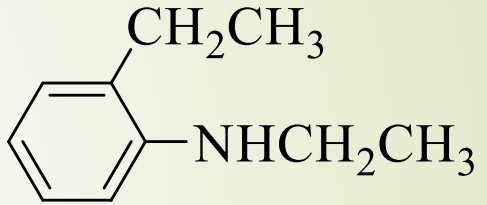
a) $COOCH_2CH_3$
CH_2
$COOCH_2CH_3$

b) $COOCH_2CH_3$
$COOCH_2CH_2CH_3$

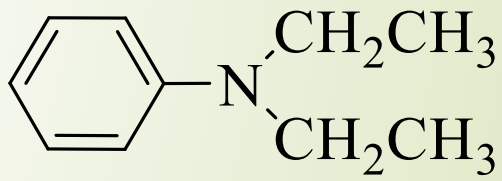
Question 17. Find the chemical structure of the compound, which molecular weight is 149 ± 3, IR and ^{1}H NMR spectra given below, known to be carrying nitrogen, not containing sulfur and halogen and soluble in dilute HCl.

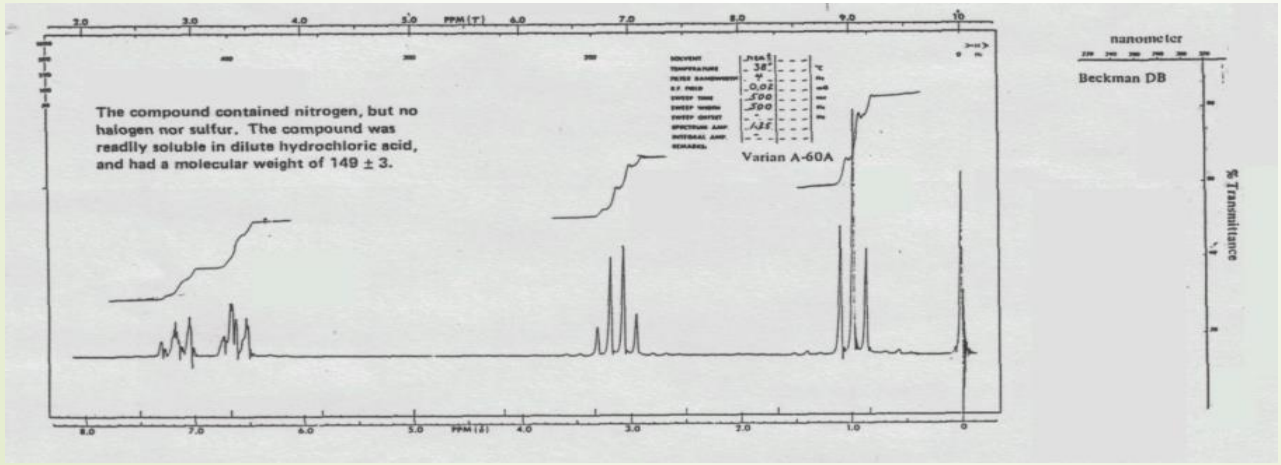


a)

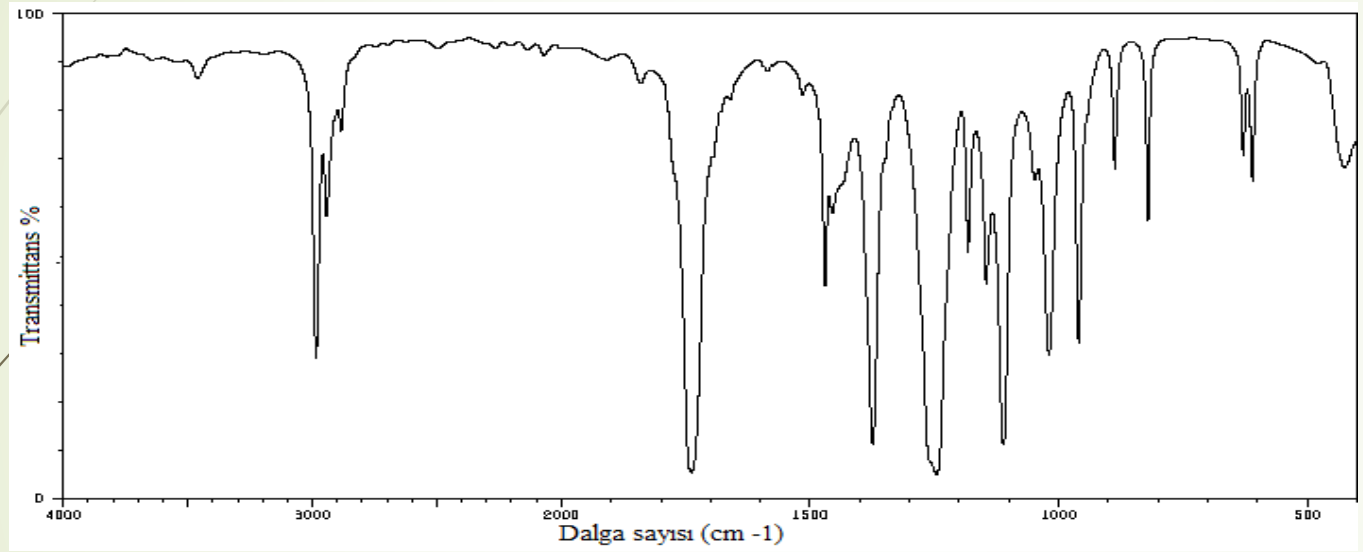


b)



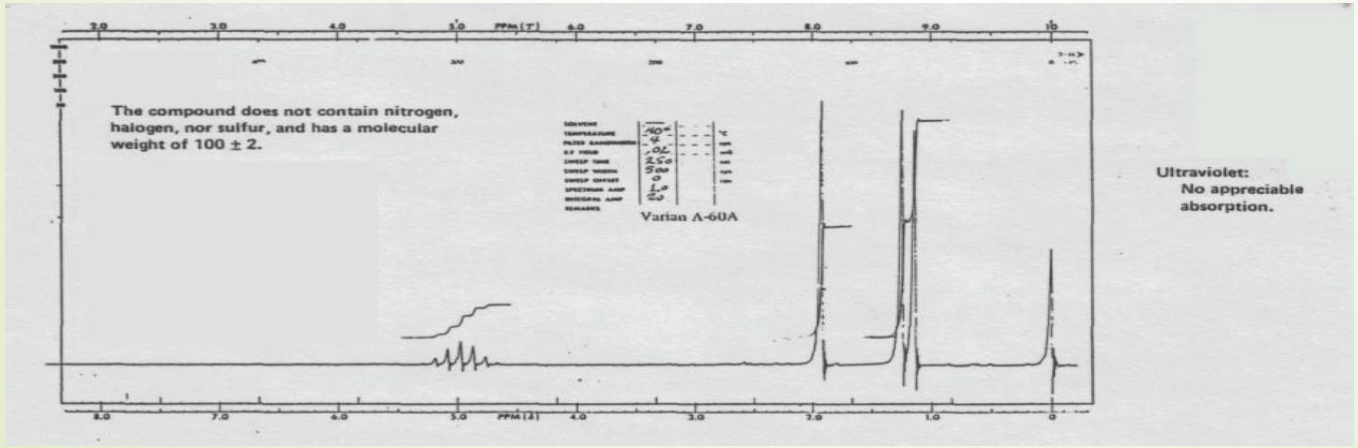


Question 18. Find the chemical structure of the compound, which is molecular formula $C_5H_{10}O_2$ and IR, ^1H NMR spectra given below, not containing nitrogen, sulfur and halogen.

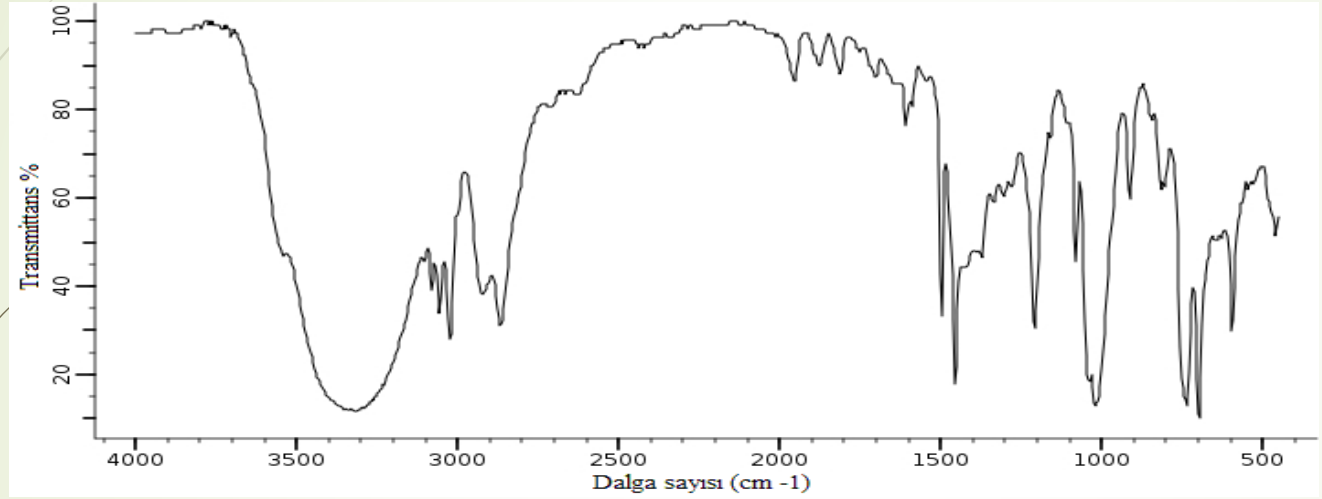


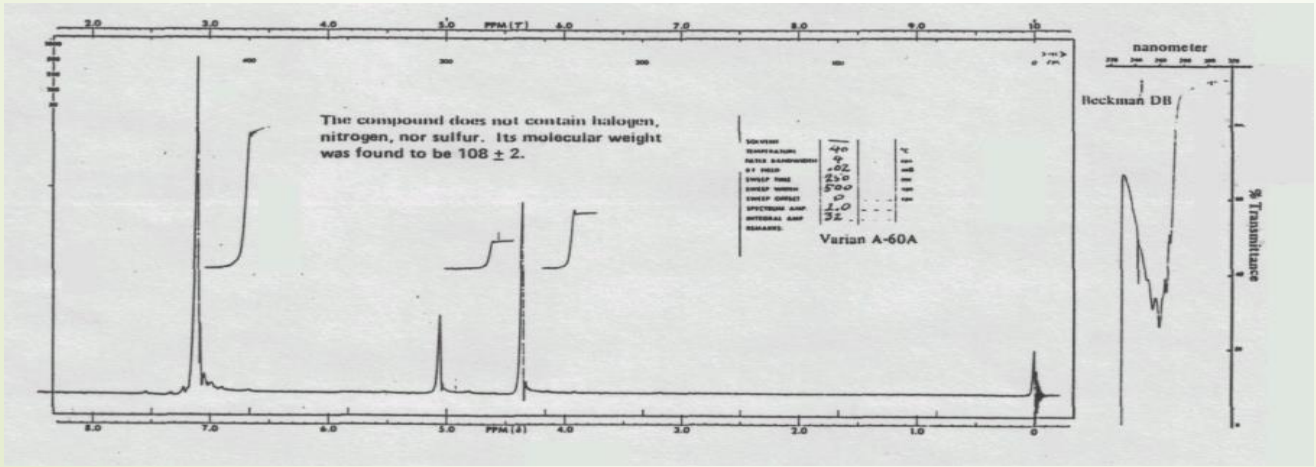
a) $H_3CCOOCH(CH_3)_2$

b) $(H_3C)_2CHCH_2COOH$

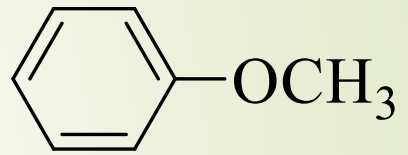


Question 19. Find the chemical structure of the compound, which is molecular formula C_7H_8O and UV, IR, ^1H NMR spectra given below, not containing nitrogen, sulfur and halogen.

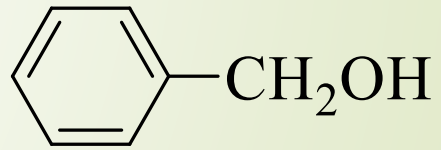




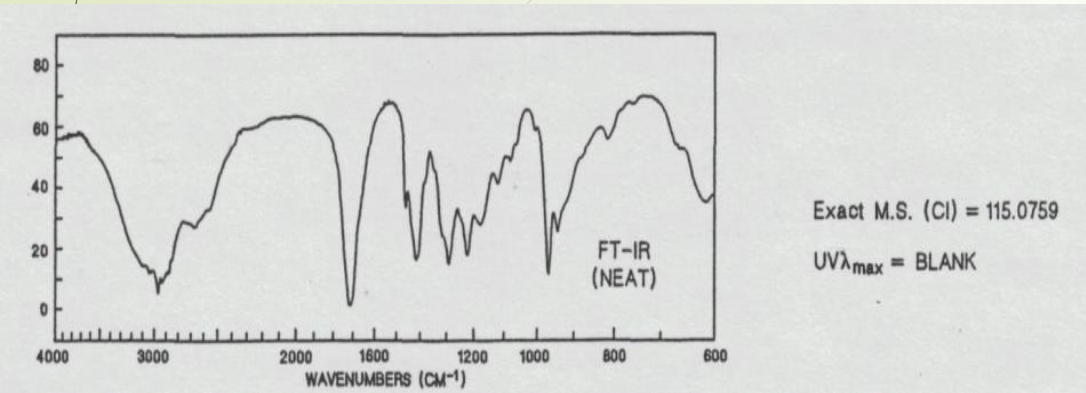
a)

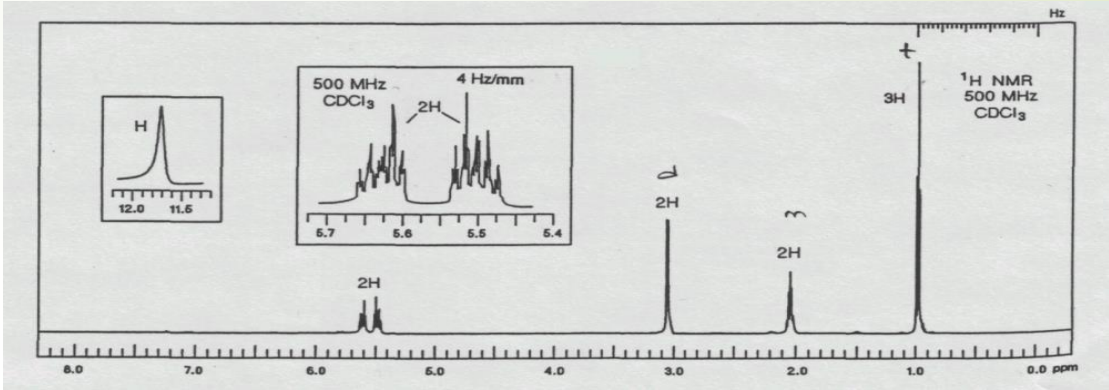


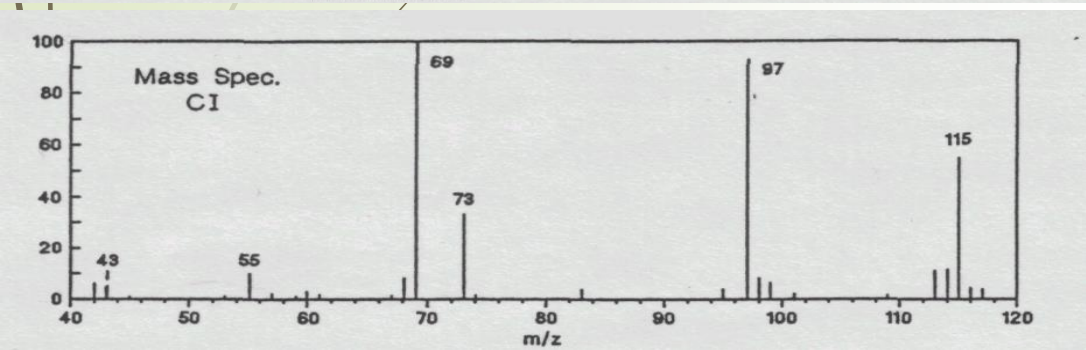
b)

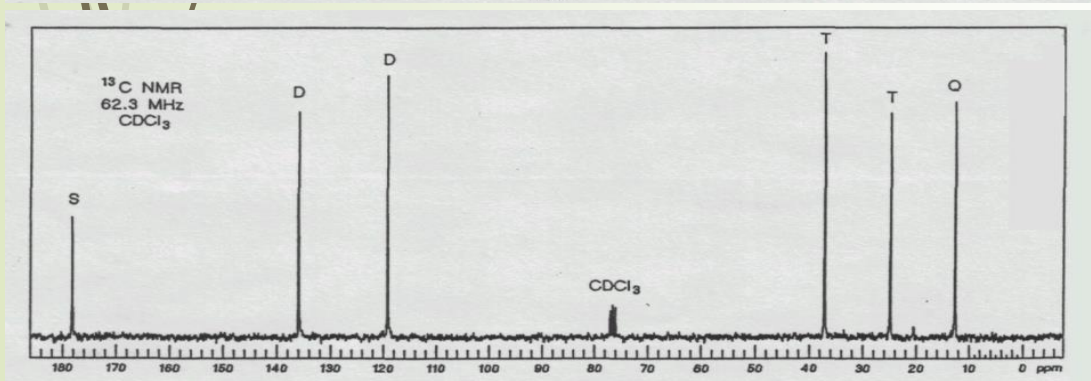


Question 20. Find the chemical structure of the compound, which is molecular formula $C_6H_{10}O_2$ and IR, Mass, ^{13}C ve ^{1}H NMR spectra given below, not containing nitrogen, sulfur and halogen.









a) $H_3CCH{=}C(CH_3)CH_2COOH$

b) $H_3CCH_2CH{=}CHCH_2COOH$

c) $H_3CCH_2CH{=}CHCOCH_2OH$