

Trabajo Práctico de Laboratorio 1

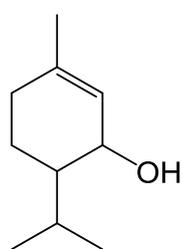
Resolución de problemas integrados de espectroscopía y espectrometría de masas. Dilucidación estructural

1. Las levaduras son microorganismos eucariotas que pueden metabolizar sustratos xenobióticos. Entre otras enzimas poseen diferentes tipos de reductasas. Al suministrar 2-ciclohexenona a un medio de cultivo donde se desarrolló la cepa de levaduras AX22 se obtuvo un producto de reducción. En base al análisis de sus espectros de RMN señalar si se redujo el carbonilo, el doble enlace o ambos.

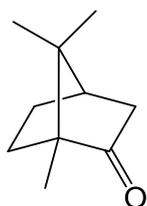
$^1\text{H RMN}$: $\delta = 3,17$ ppm (q, $J=7\text{Hz}$, 1H); 2,00 ppm (s ancho, 1H); 1,60 ppm (m, 4H); 1,47 ppm (m, 6H).

$^{13}\text{C RMN}$: $\delta = 72,7$ ppm (CH); 36,5 ppm ($2\times\text{CH}_2$); 28,3 ppm (CH_2); 21,8 ppm ($2\times\text{CH}_2$).

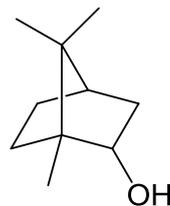
2. Un químico de productos naturales ha aislado un monoterpeno oxigenado a partir de la especie vegetal *Salvia officinalis*. En base al análisis de sus datos espectroscópicos definir de cuál de los siguientes monoterpenos se trata. Justificar adecuadamente su respuesta.



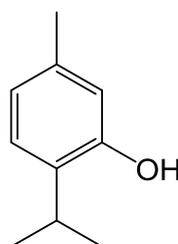
Terpineol



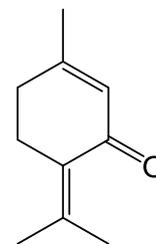
Camphor



Borneol

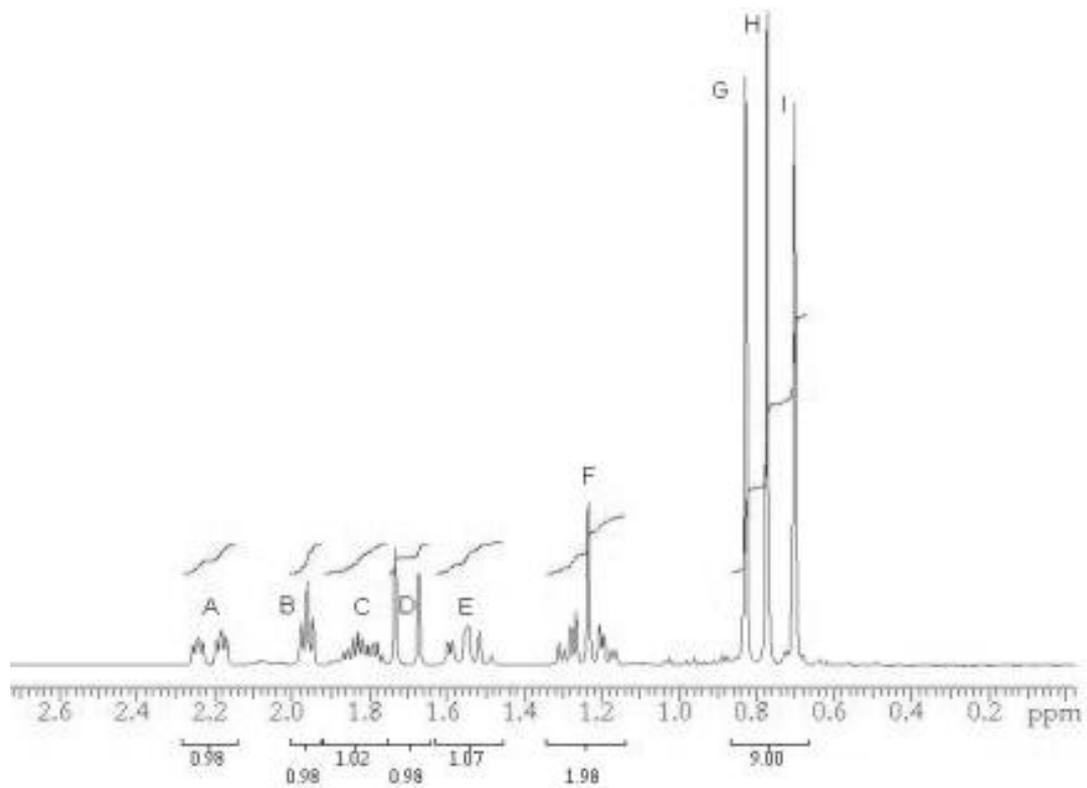


Thymol

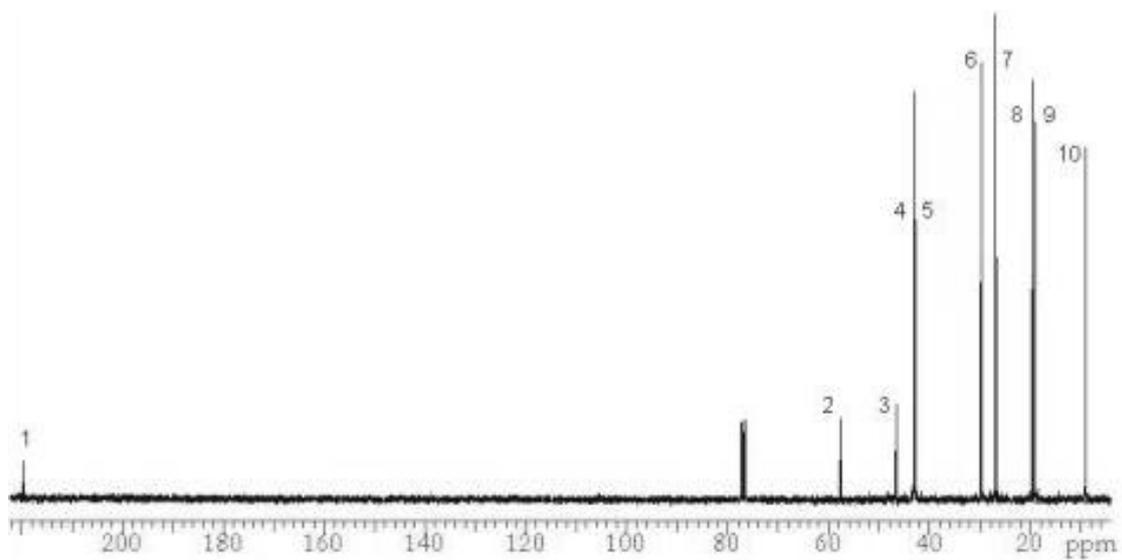


Pulegona

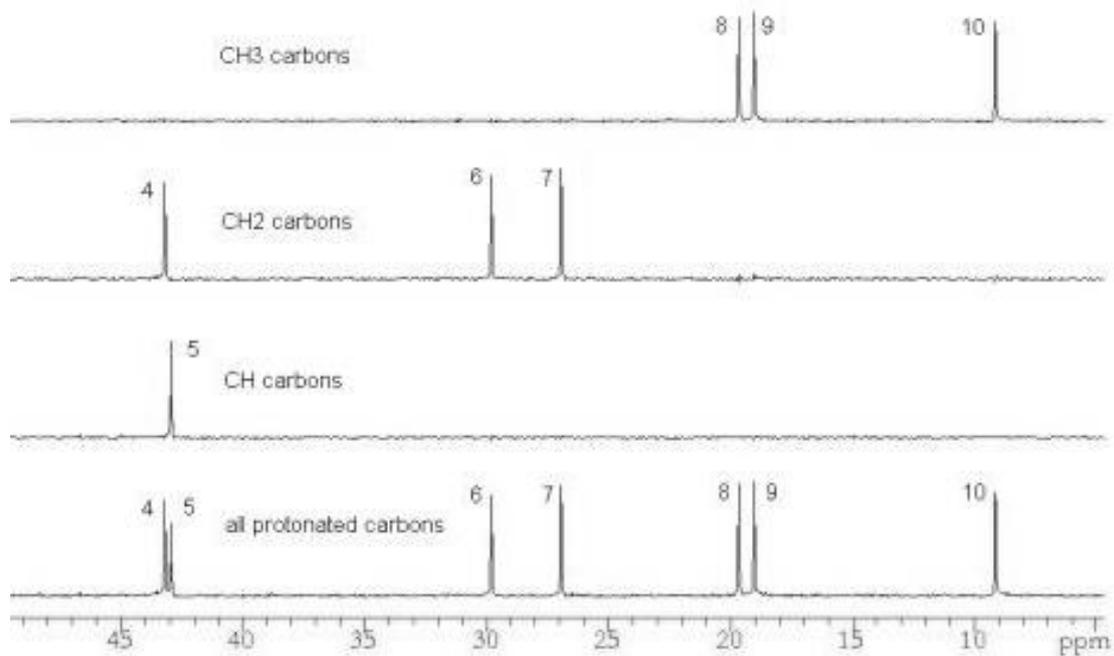
^1H RMN



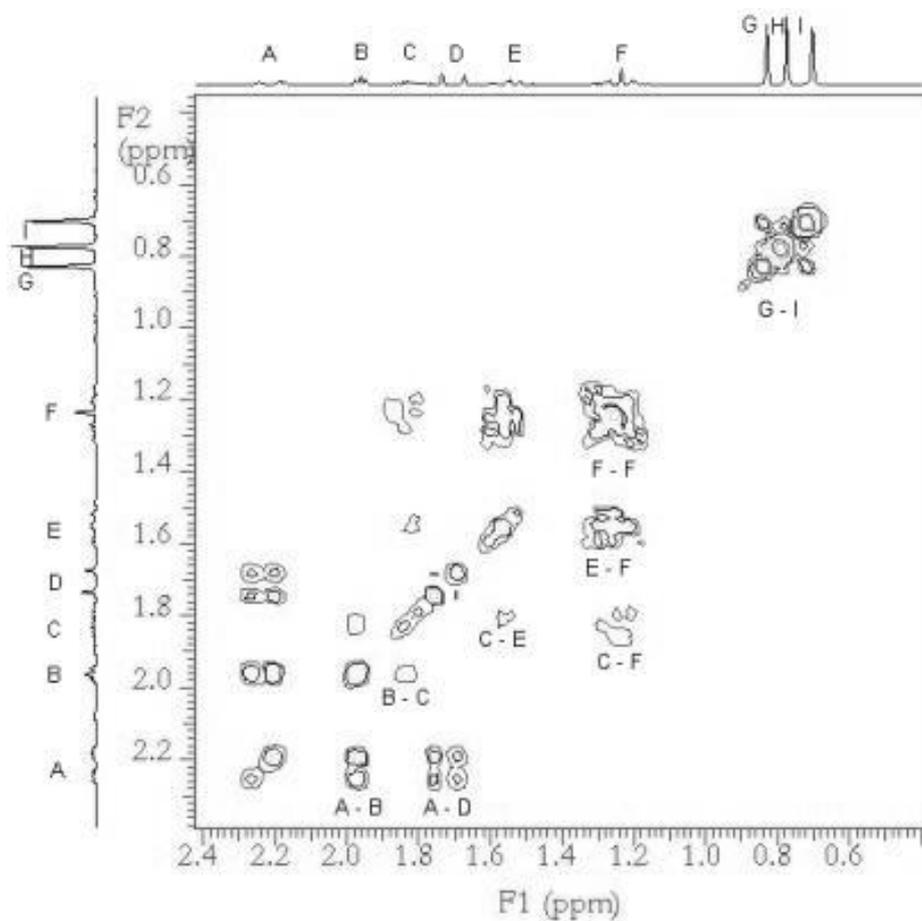
^{13}C RMN



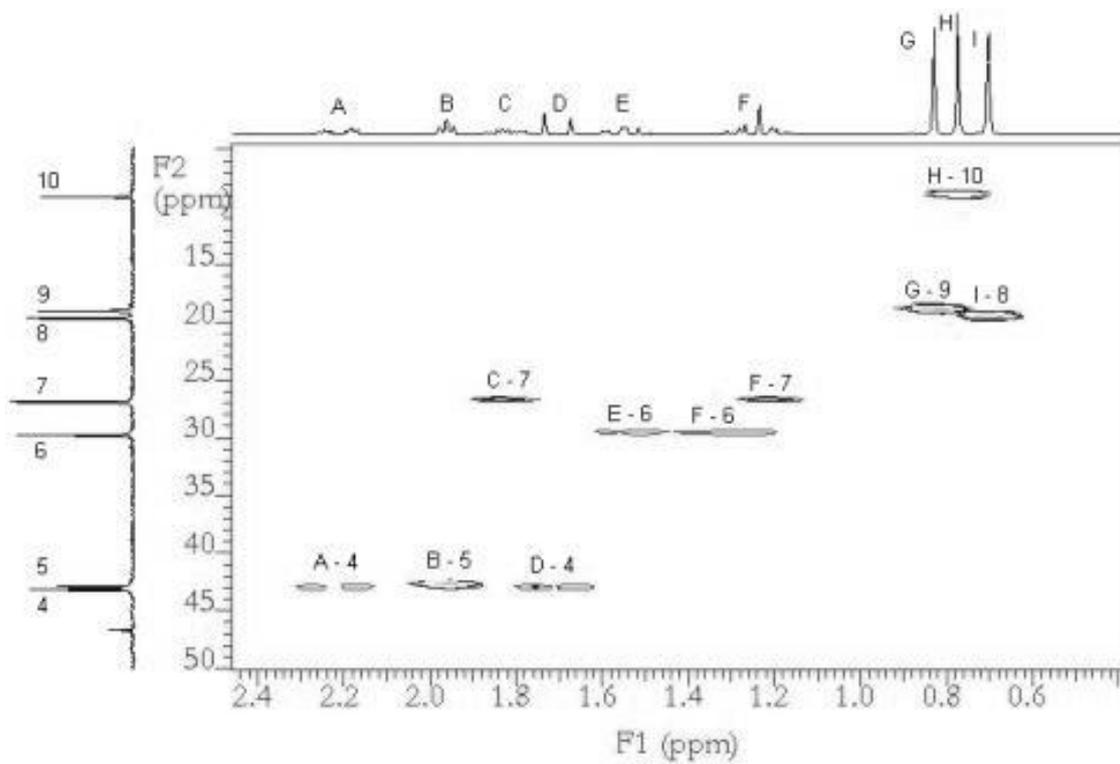
DEPT



COSY

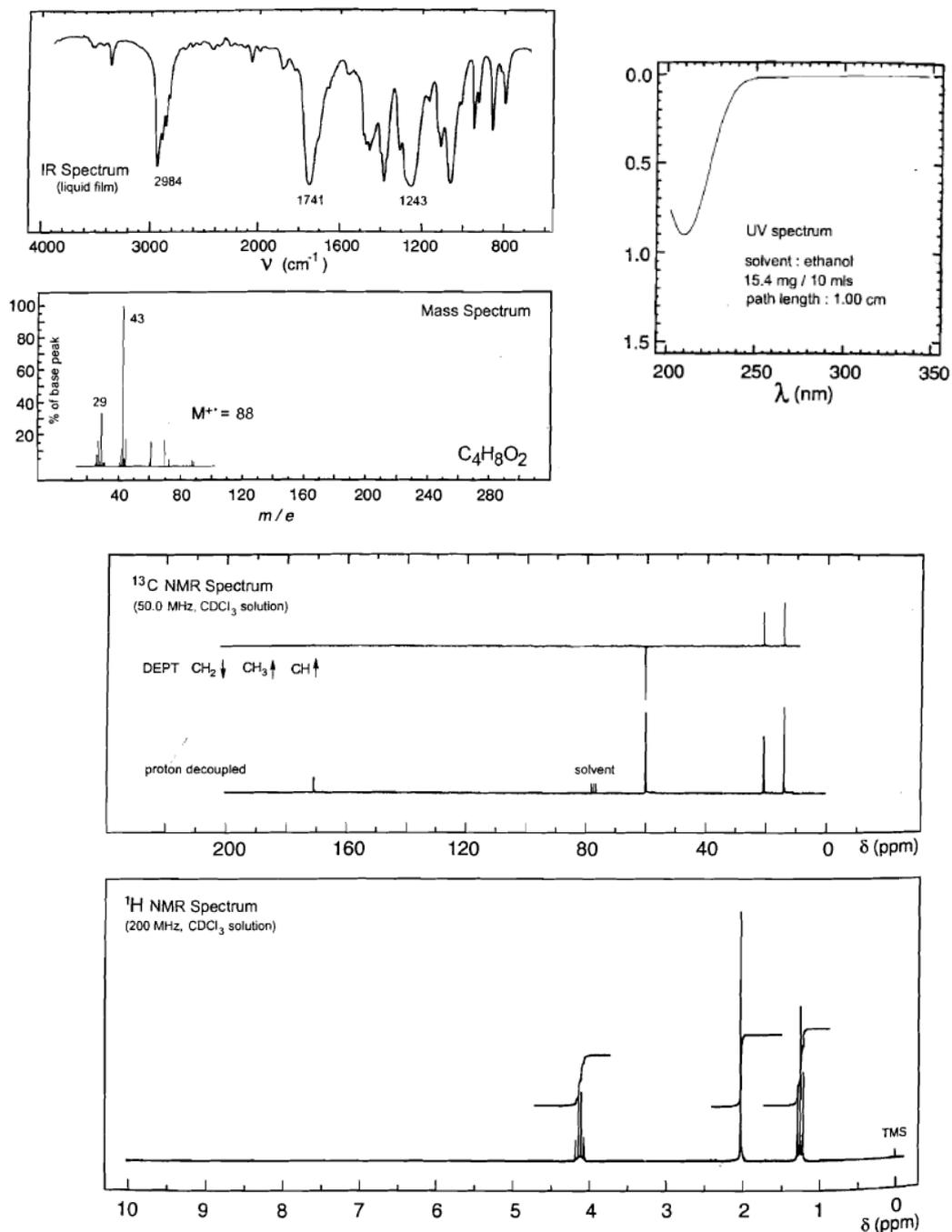


HETCOR

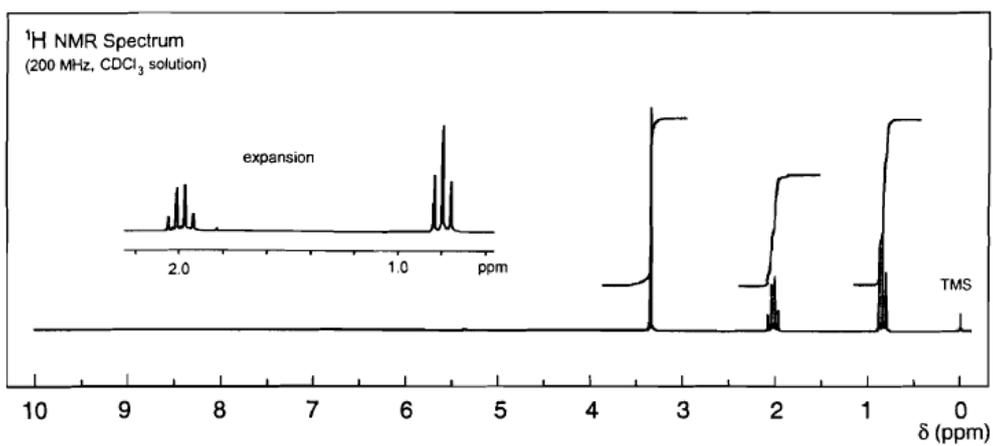
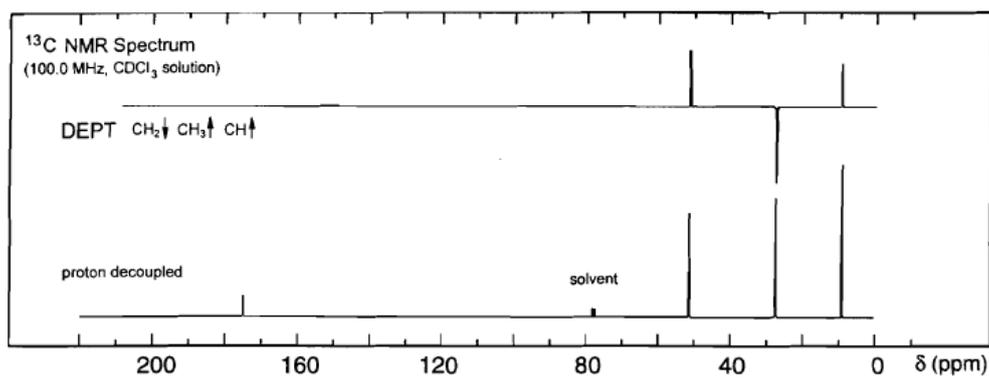
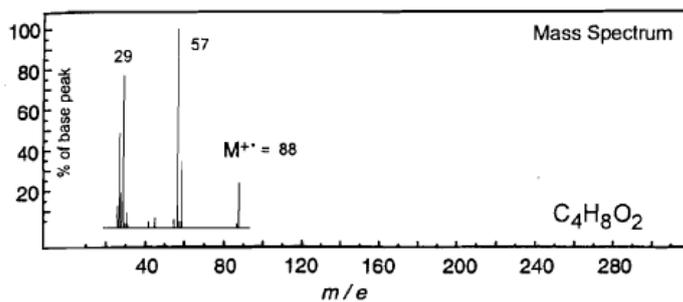
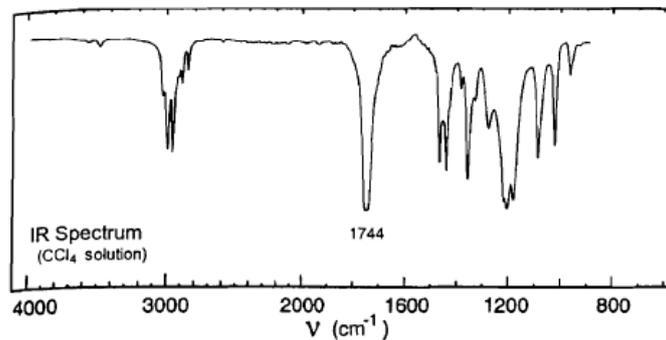


3. Ambos isómeros del compuesto $C_4H_8O_2$ presentan los siguientes datos espectroscópicos y espectrométricos. Proponer la estructura de cada isómero y justificar las asignaciones correspondientes.

A)

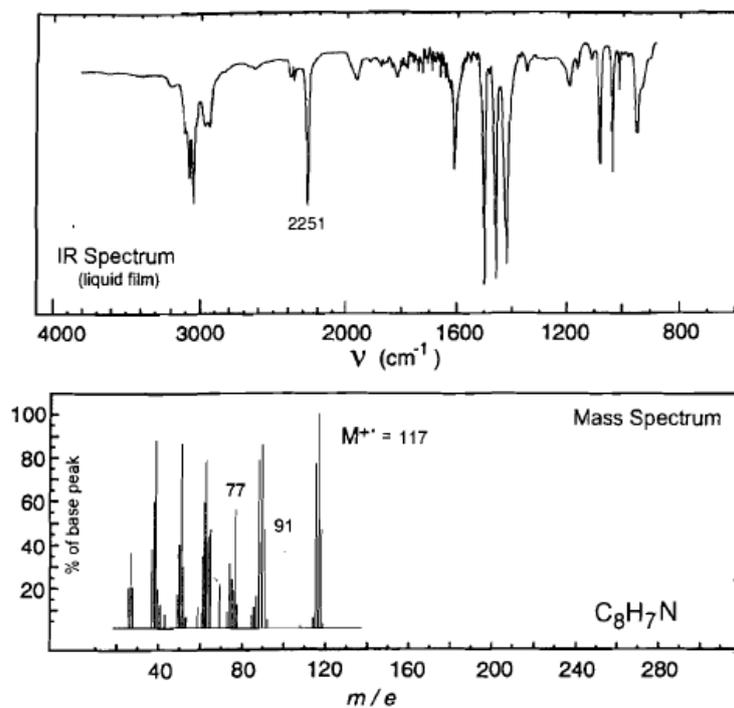


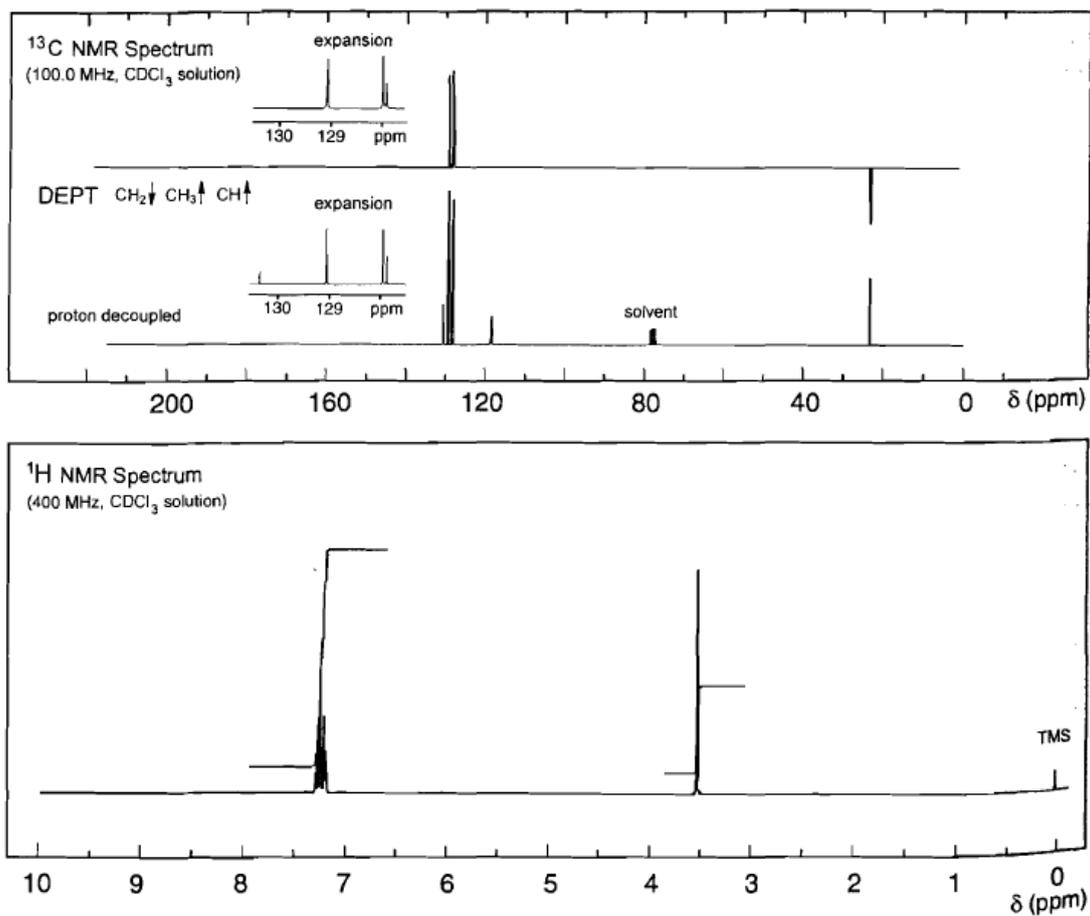
B)



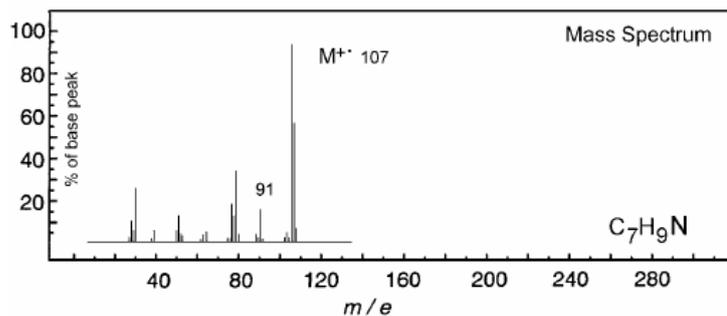
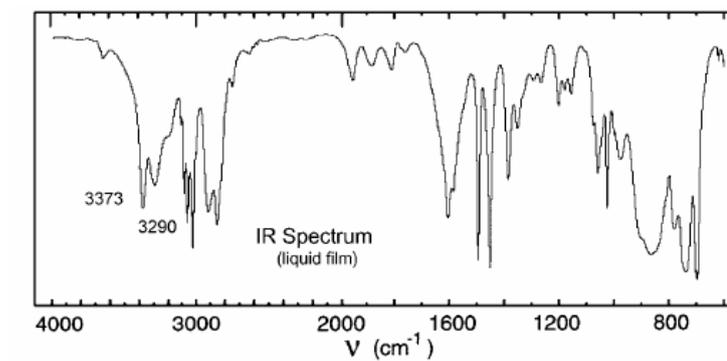
4. Los siguientes datos espectroscópicos pertenecen a derivados de bencenos monosustituídos. Asignar la estructura correspondiente a cada uno de ellos.

A)





B)

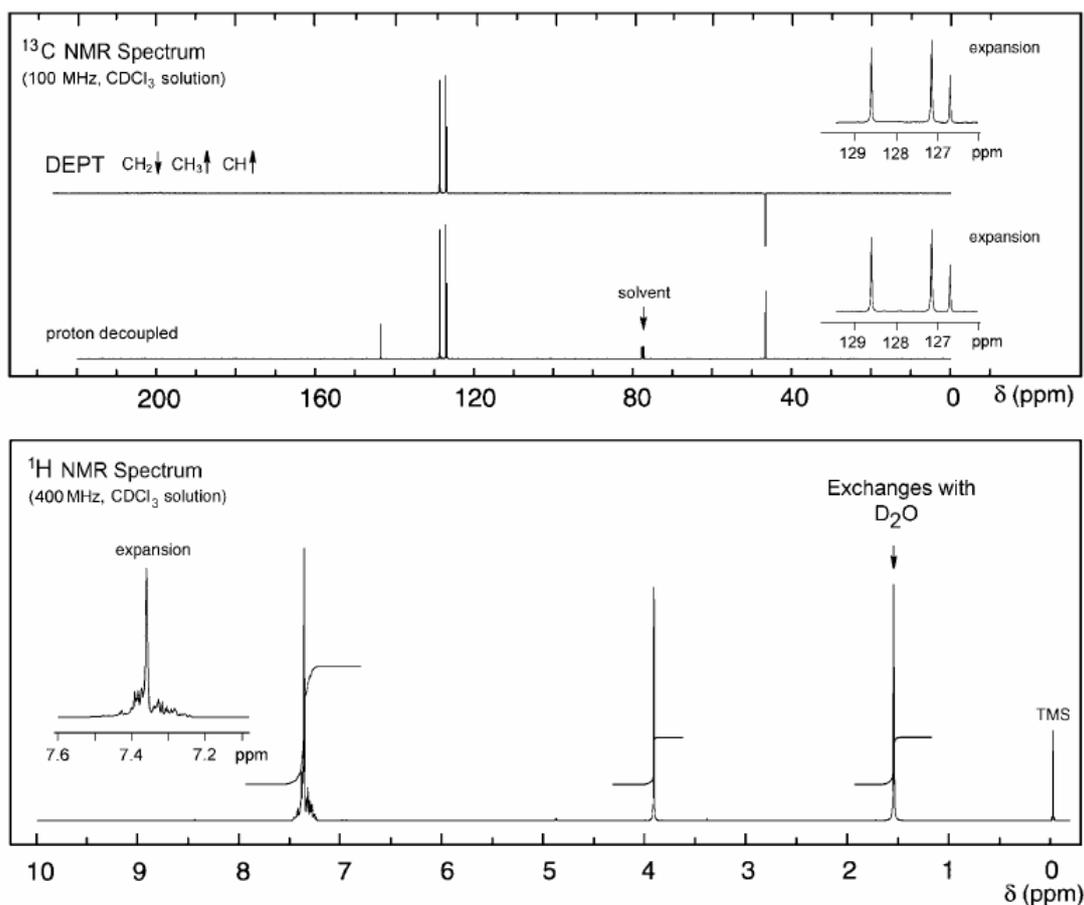


UV Spectrum

λ_{\max} 256 nm ($\log_{10} \epsilon$ 2.2)

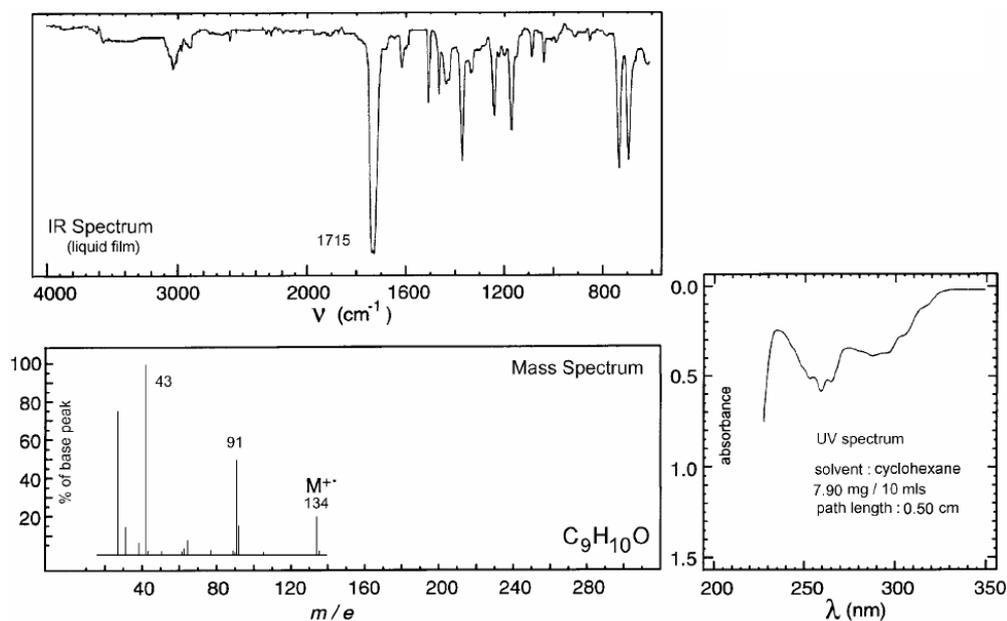
λ_{\max} 264 nm ($\log_{10} \epsilon$ 2.1)

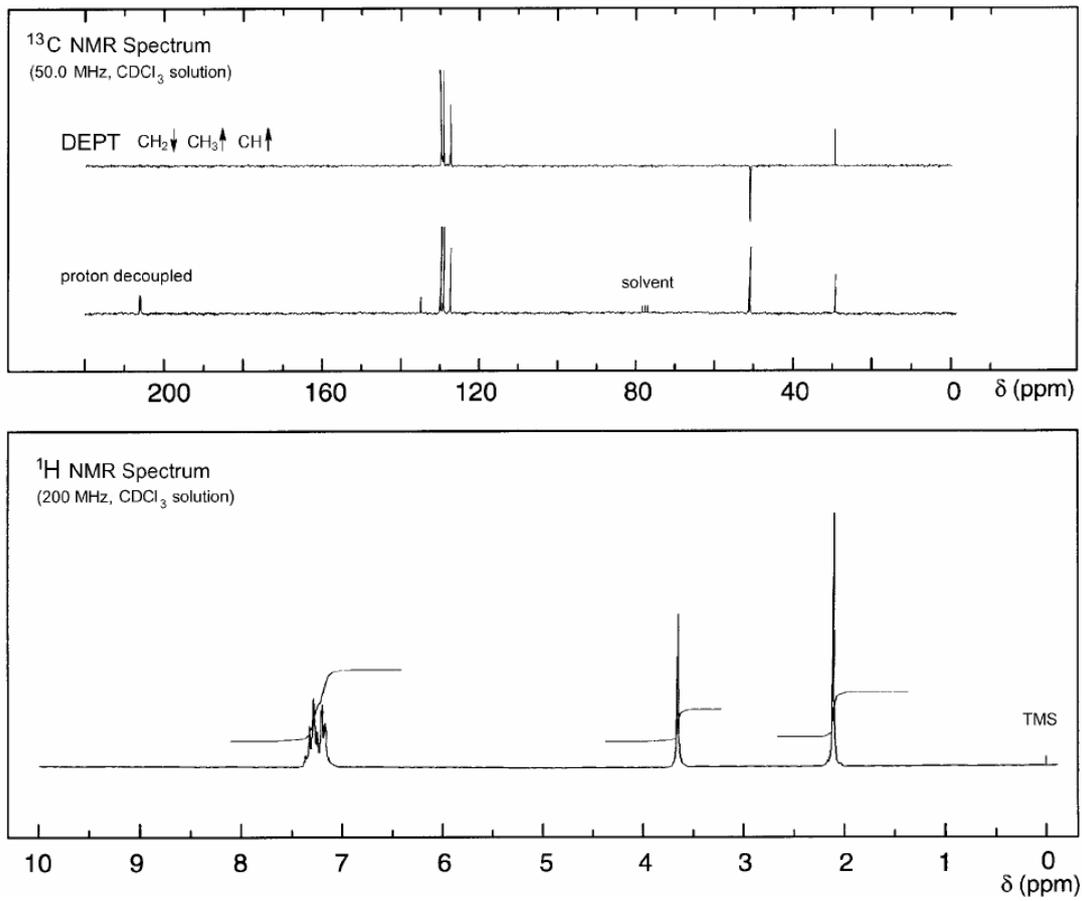
solvent : ethanol



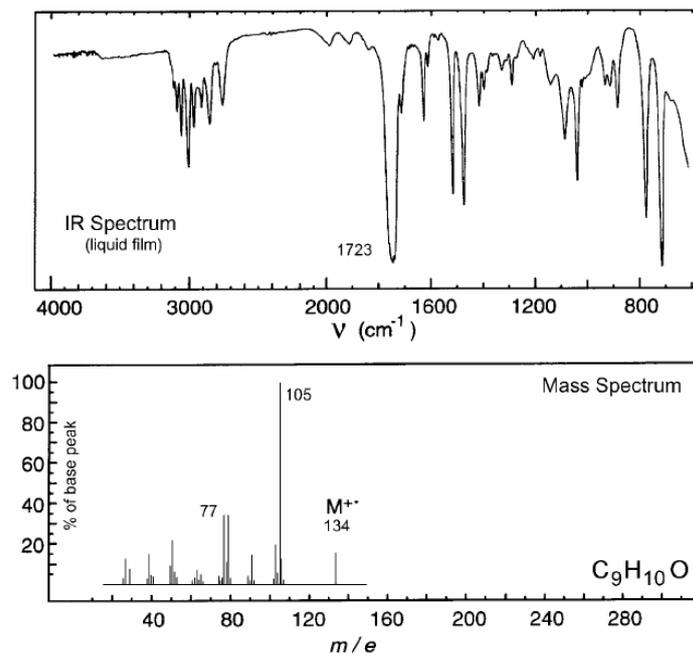
5. La fórmula molecular C₉H₁₀O es compartida por dos compuestos (A y B) que presentan los siguientes datos espectroscópicos. A partir del análisis comparativo de los espectros correspondientes asignar las estructuras y compararlas con las señales del compuesto D de fórmula molecular C₁₀H₁₂O.

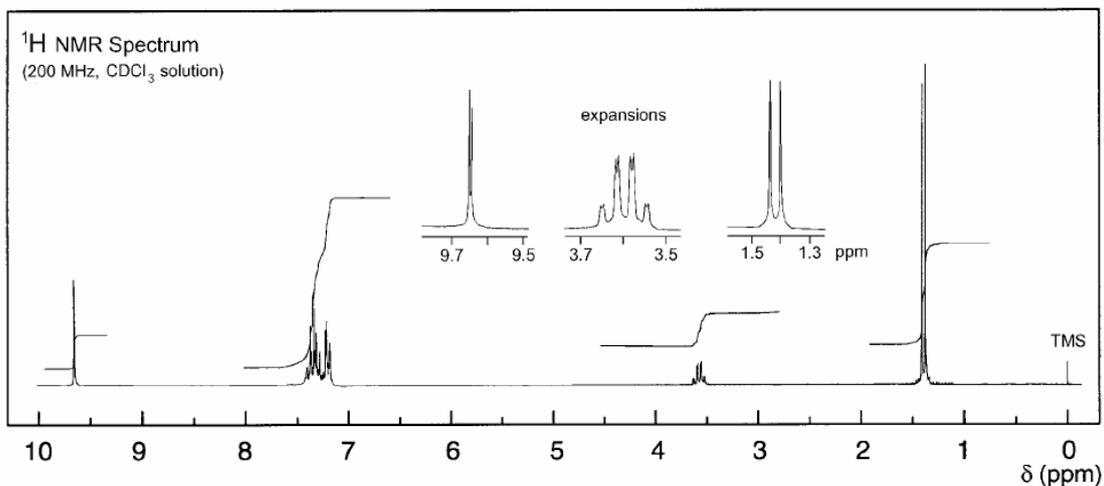
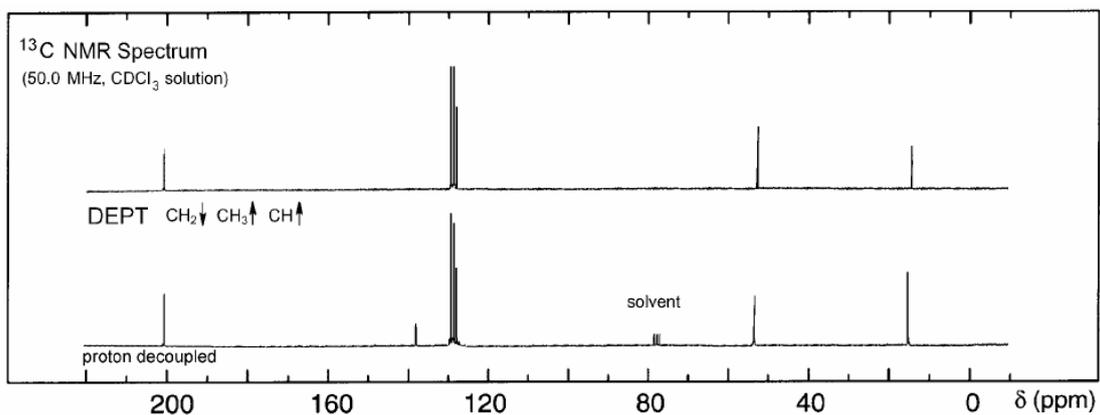
A)



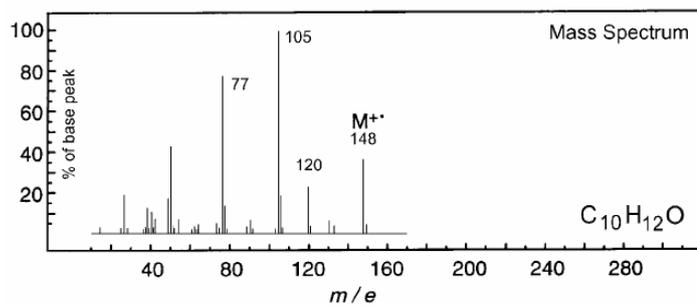
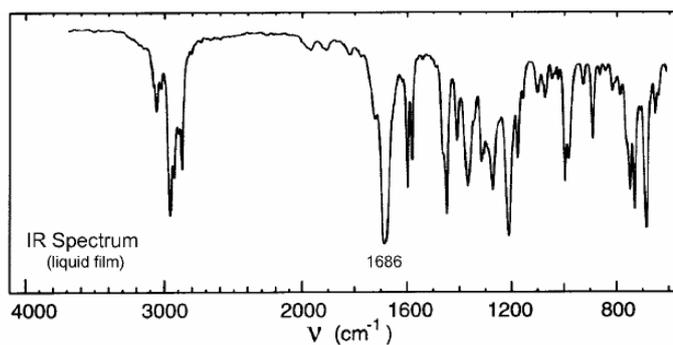


B)





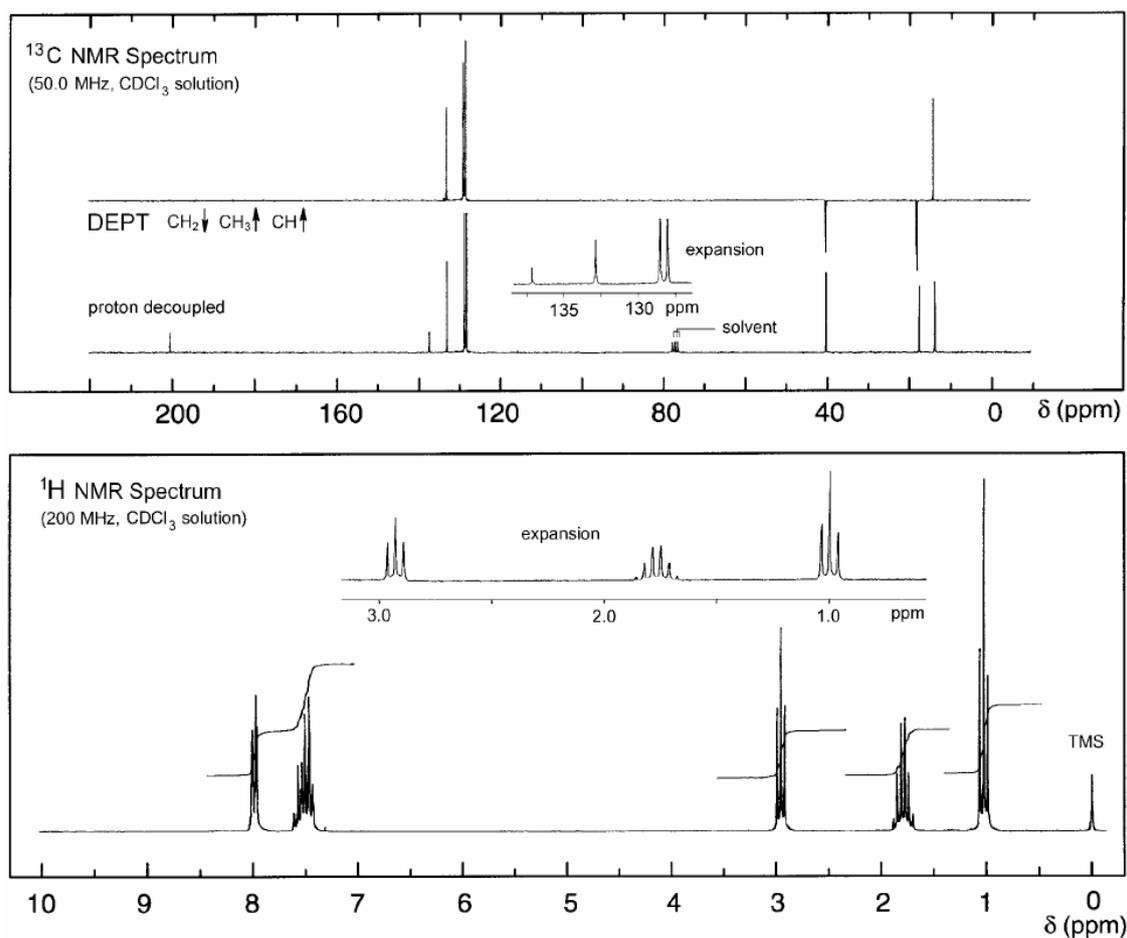
D)



UV Spectrum

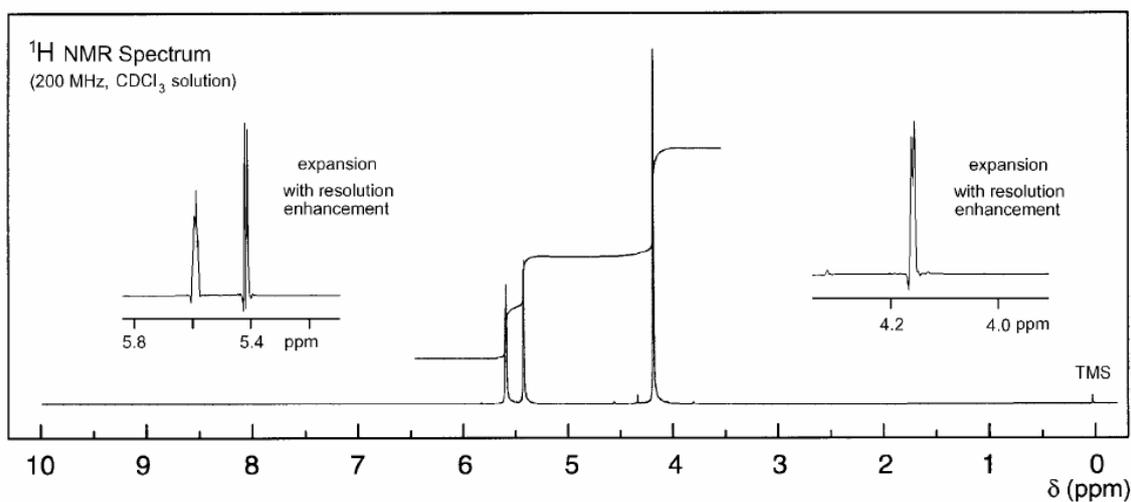
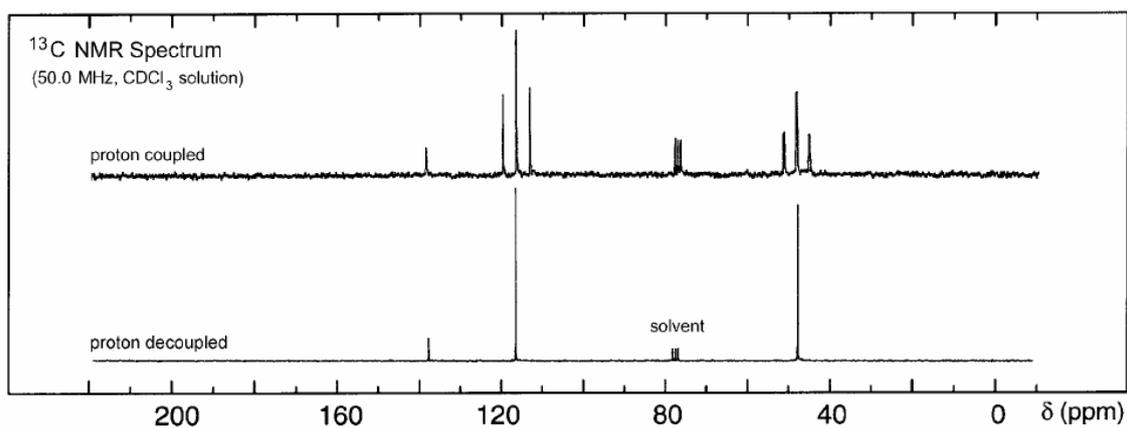
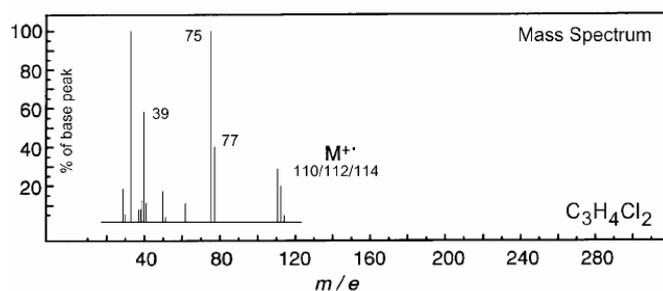
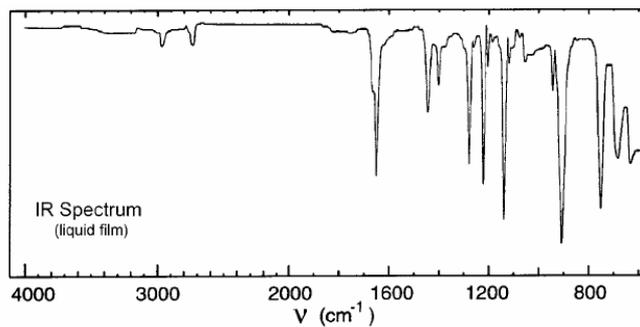
λ_{\max} 241 nm ($\log_{10} \epsilon$ 4.1)

solvent : methanol

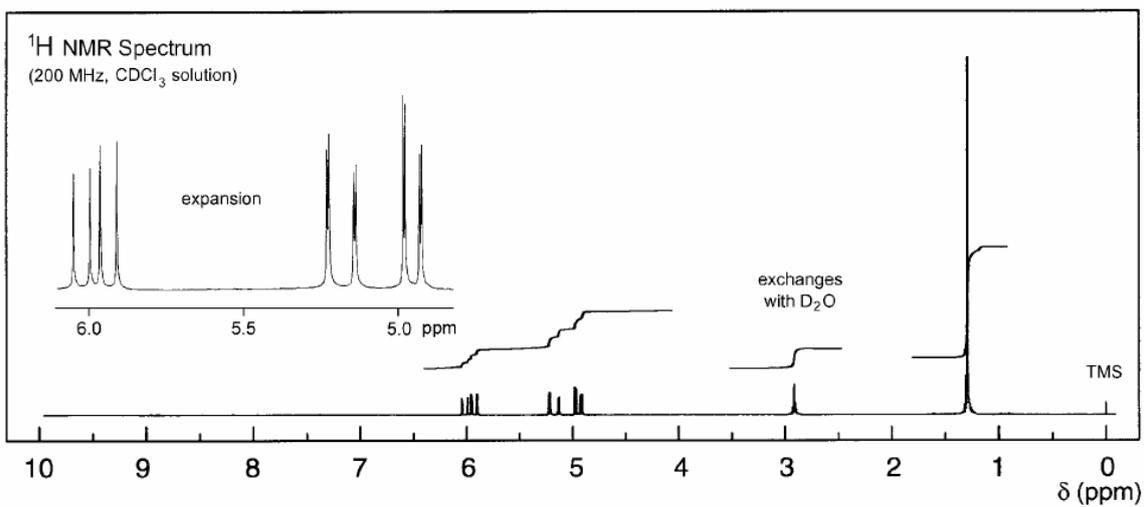
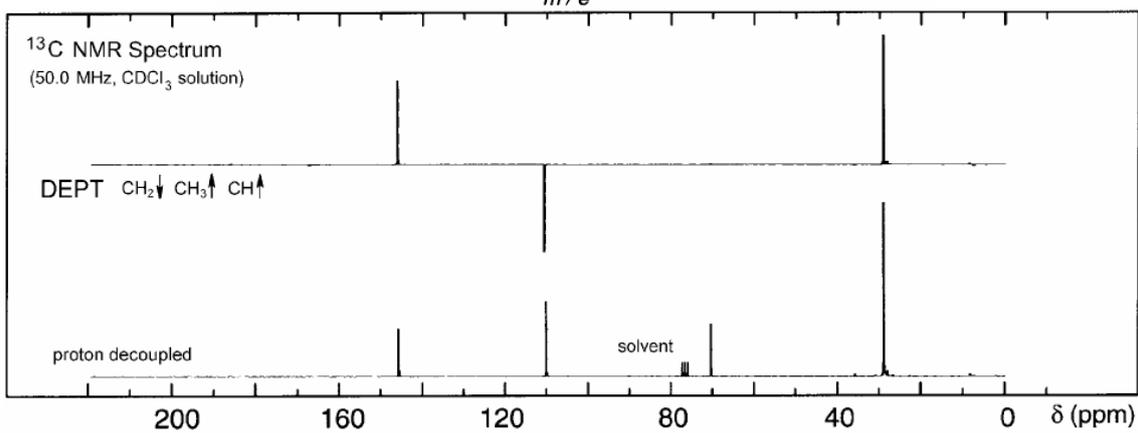
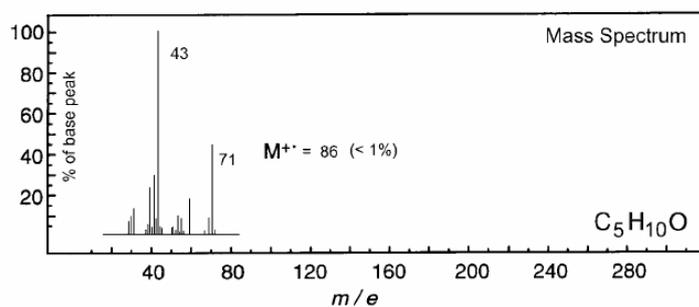
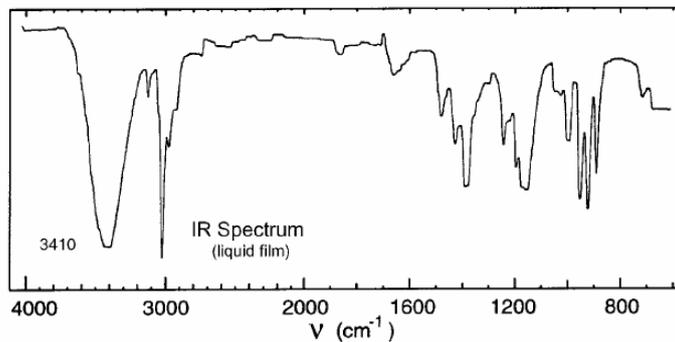


6. Los siguientes juegos de espectros pertenecen a dos derivados vinílicos. Asignar las estructuras correspondientes.

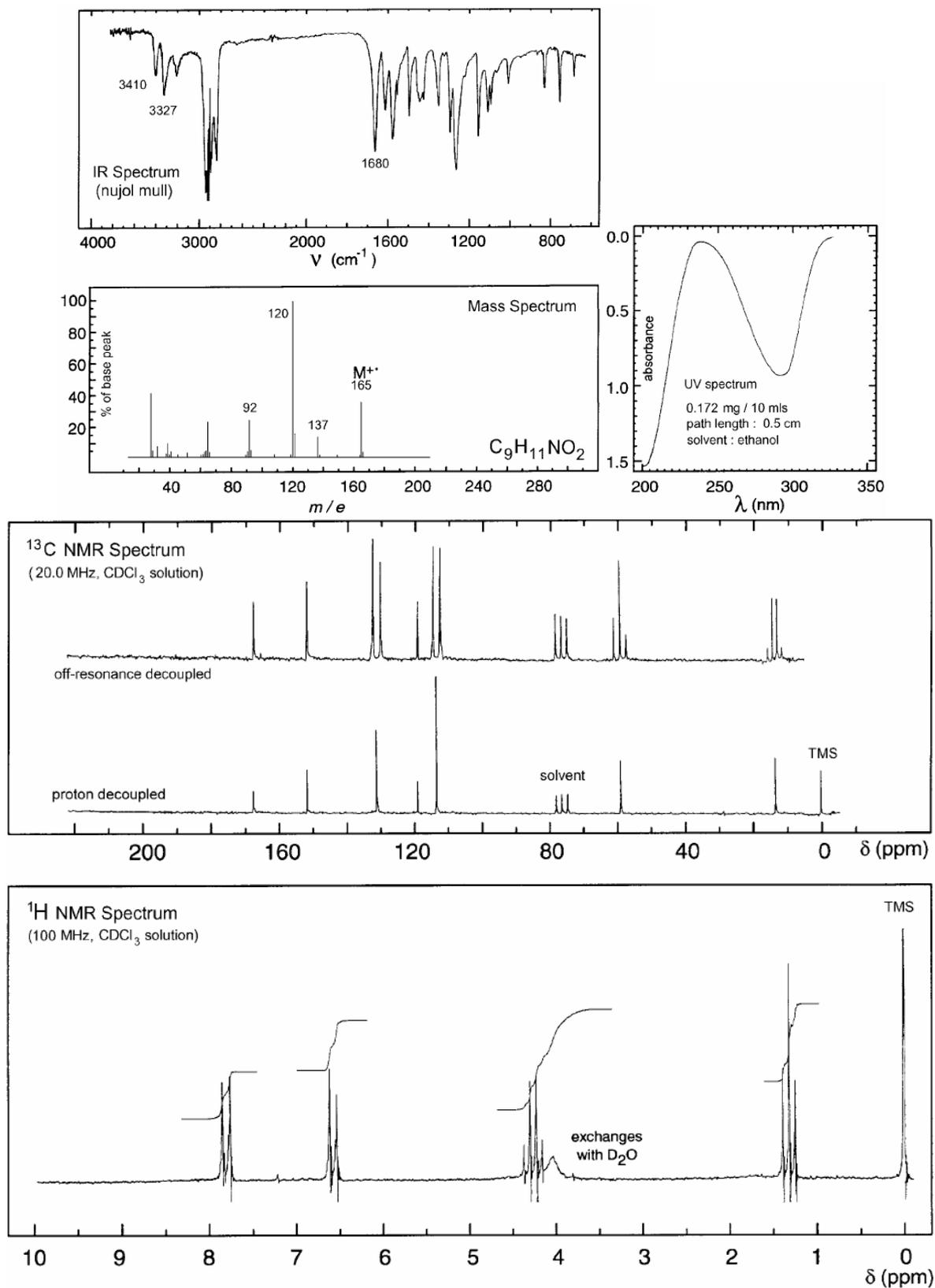
A) $C_3H_4Cl_2$



B) C₅H₁₀O



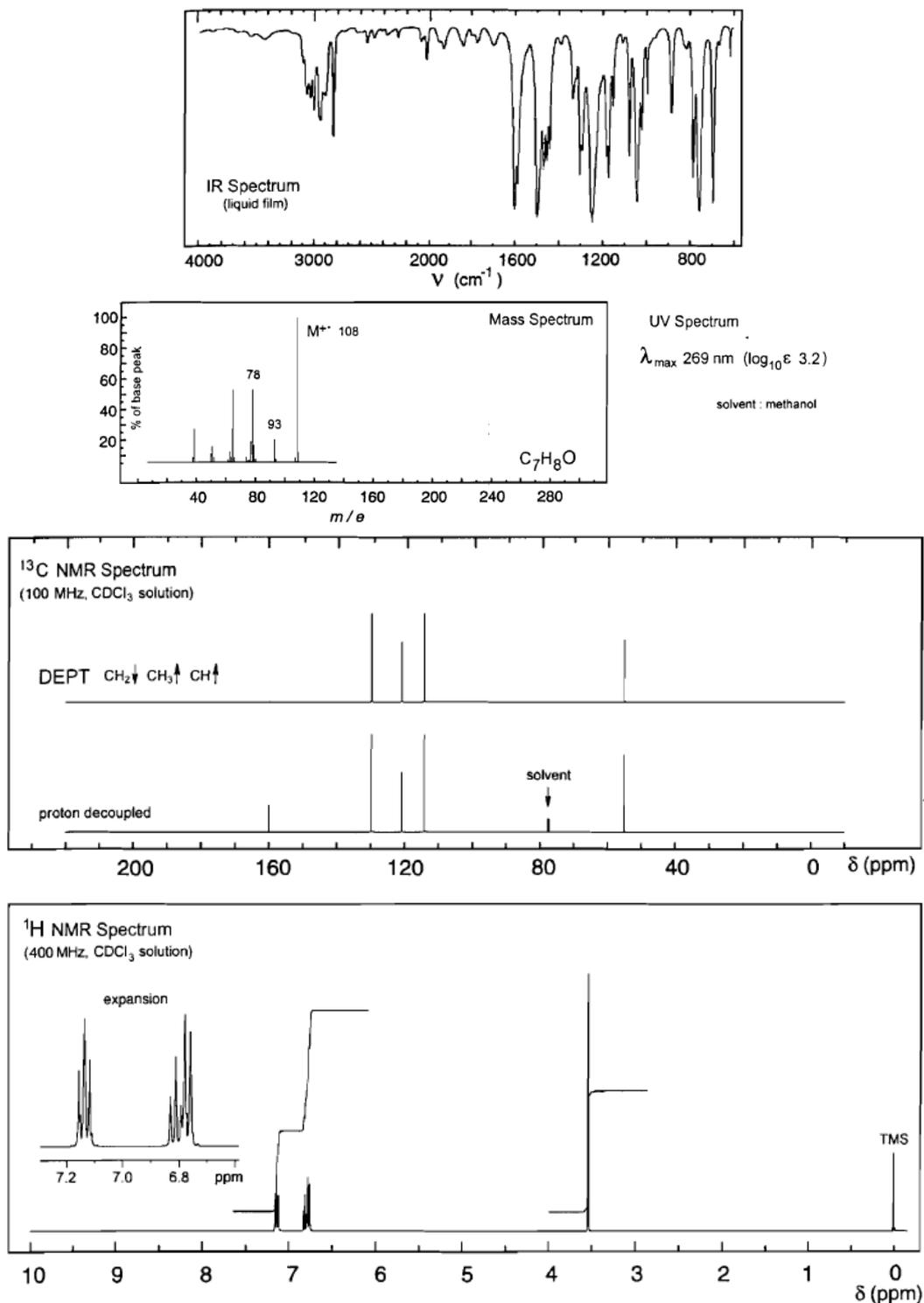
7. Proponer la estructura correspondiente al compuesto aromático de fórmula molecular $C_9H_{11}NO_2$.



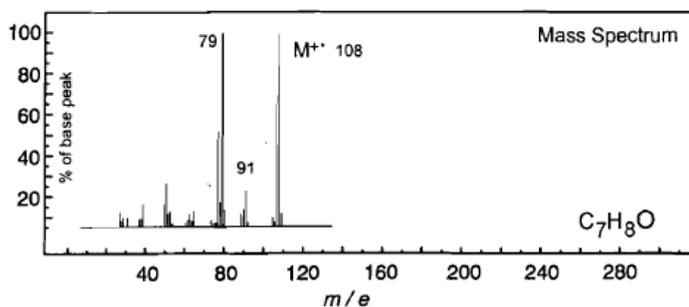
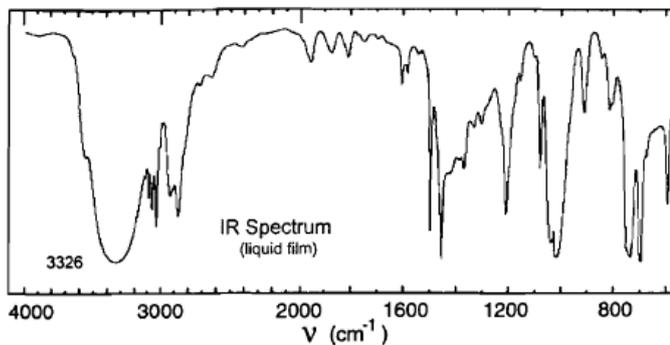
EJERCICIOS COMPLEMENTARIOS

1. Los siguientes datos espectroscópicos pertenecen a derivados de bencenos monosustituídos. Asignar la estructura correspondiente a cada uno de ellos.

A)



B)



UV Spectrum

λ_{max} 243 nm ($\log_{10} \epsilon$ 1.9)

λ_{max} 248 nm ($\log_{10} \epsilon$ 2.1)

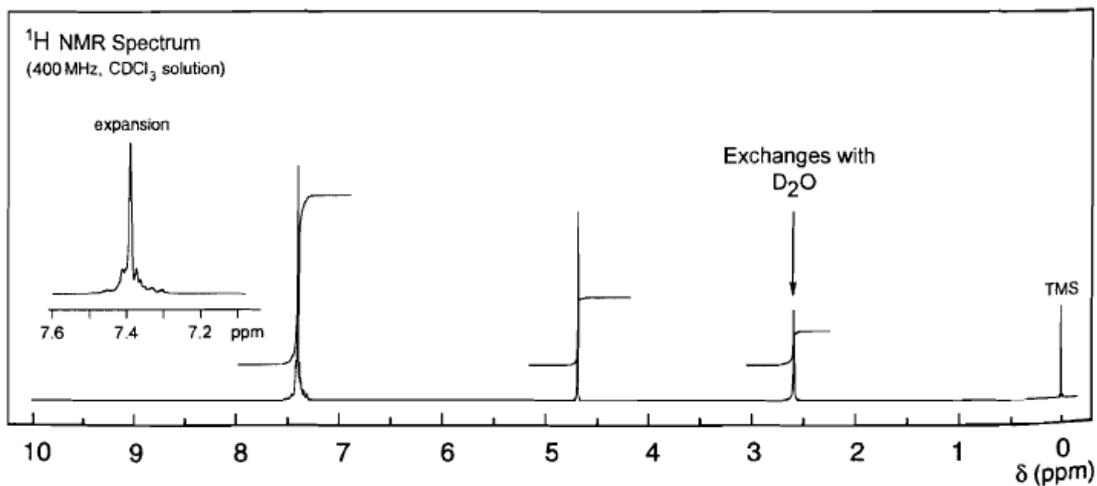
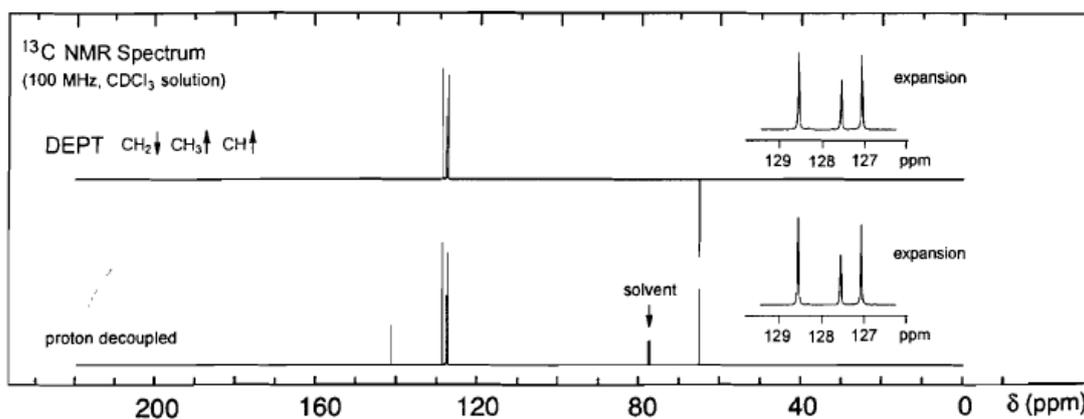
λ_{max} 252 nm ($\log_{10} \epsilon$ 2.2)

λ_{max} 258 nm ($\log_{10} \epsilon$ 2.3)

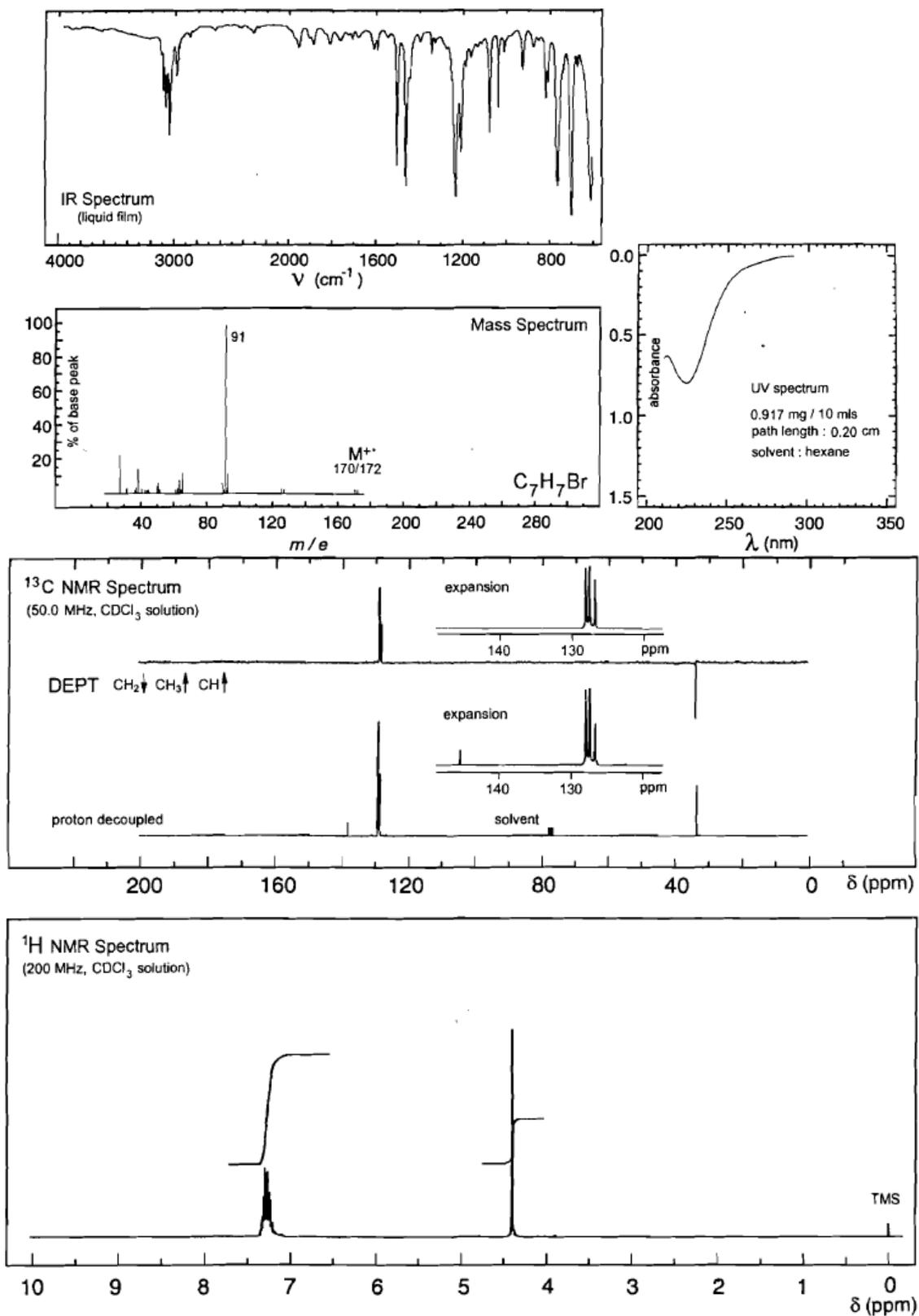
λ_{max} 264 nm ($\log_{10} \epsilon$ 2.1)

λ_{max} 268 nm ($\log_{10} \epsilon$ 1.9)

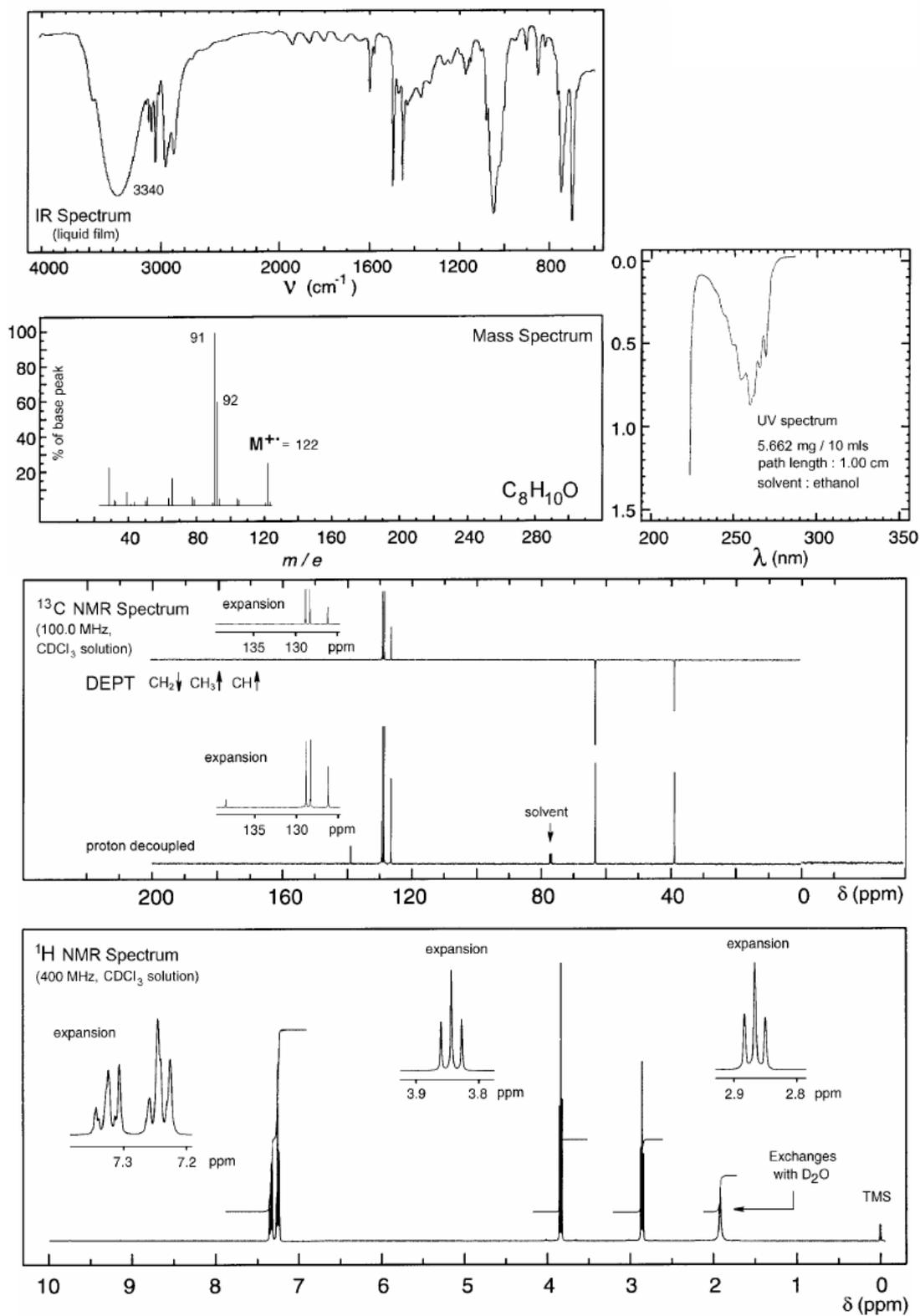
solvent: ethanol



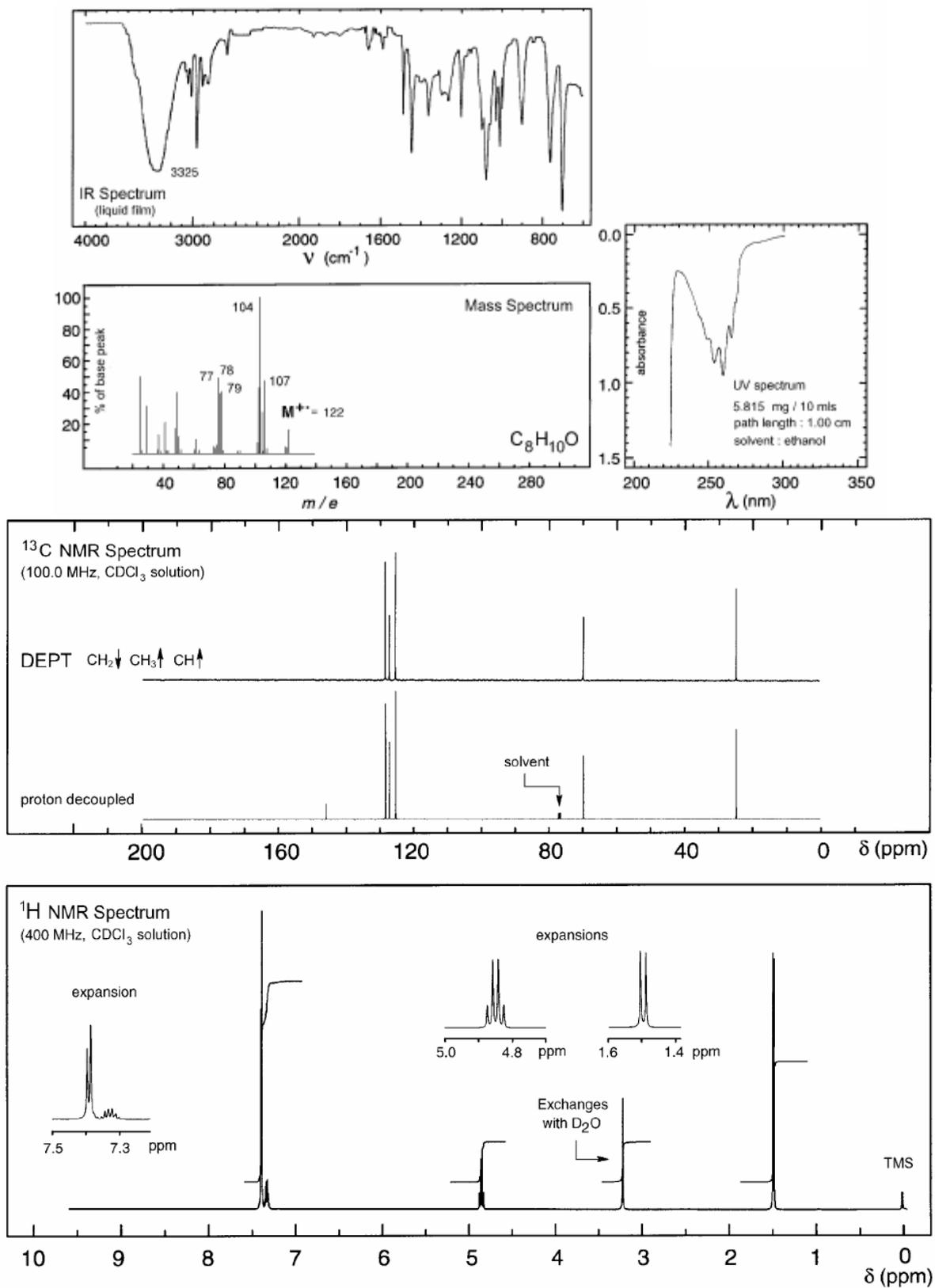
C)



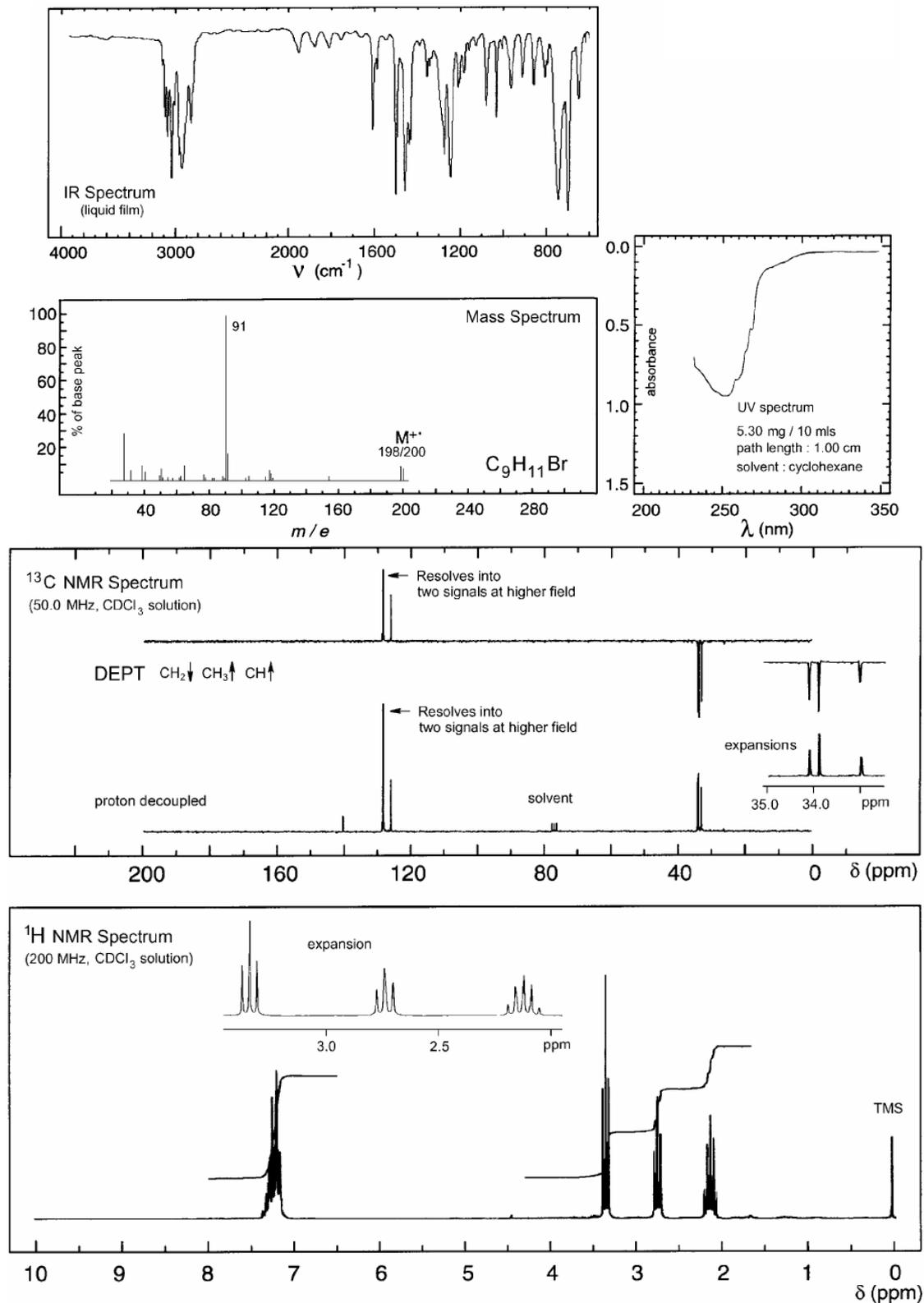
D)



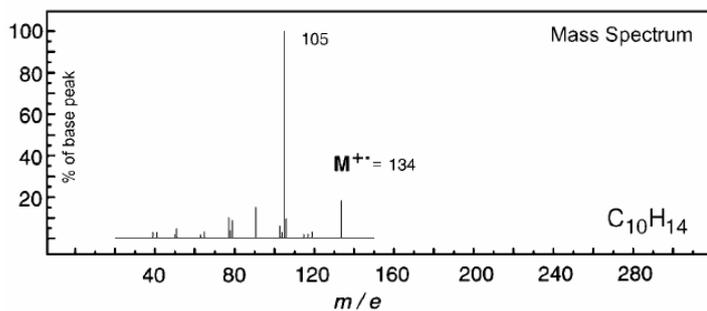
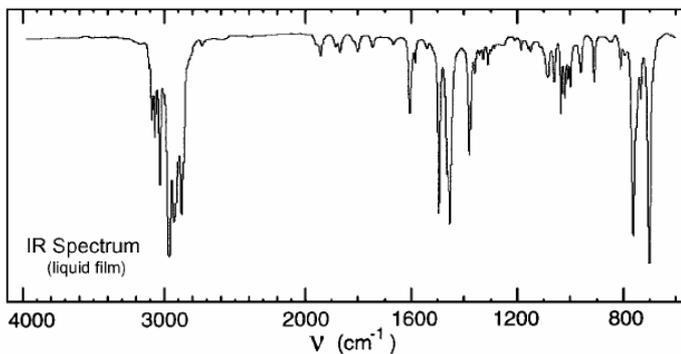
E)



F)

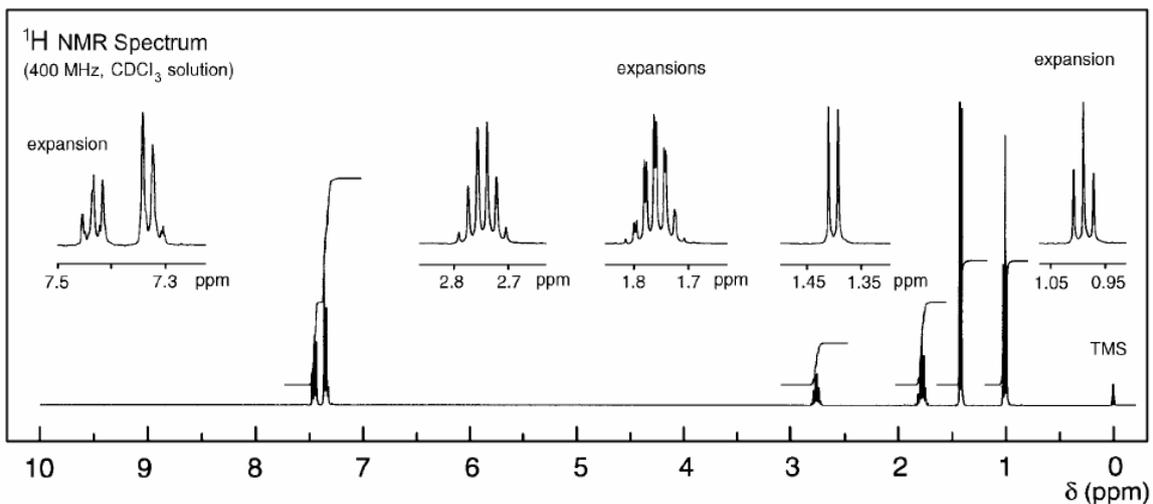
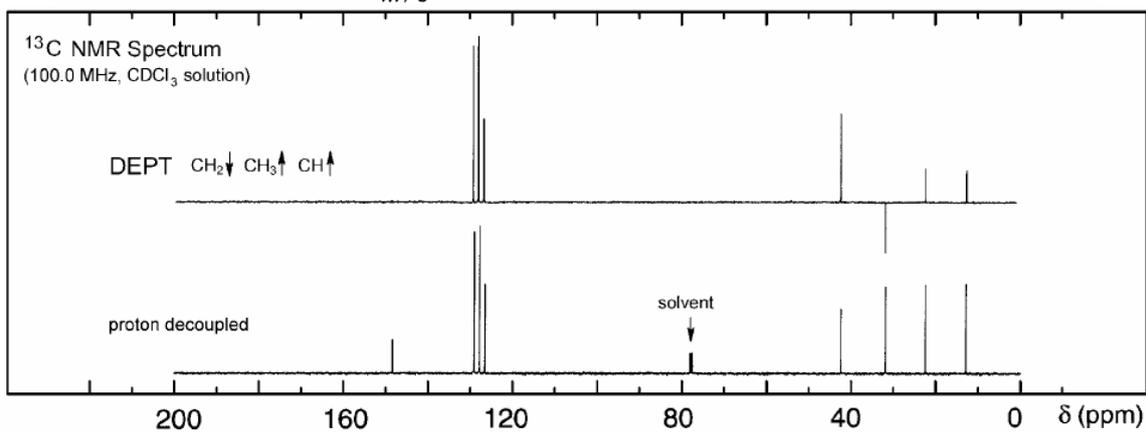


G)



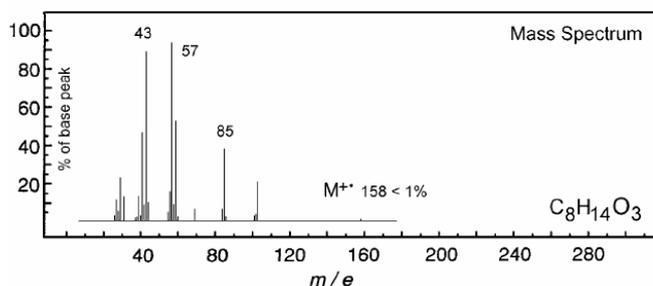
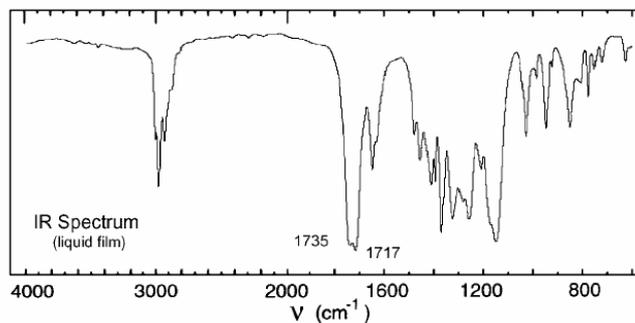
UV Spectrum

$$\lambda_{\max} \approx 260 \text{ nm} \quad (\log_{10} \epsilon \approx 2.5)$$

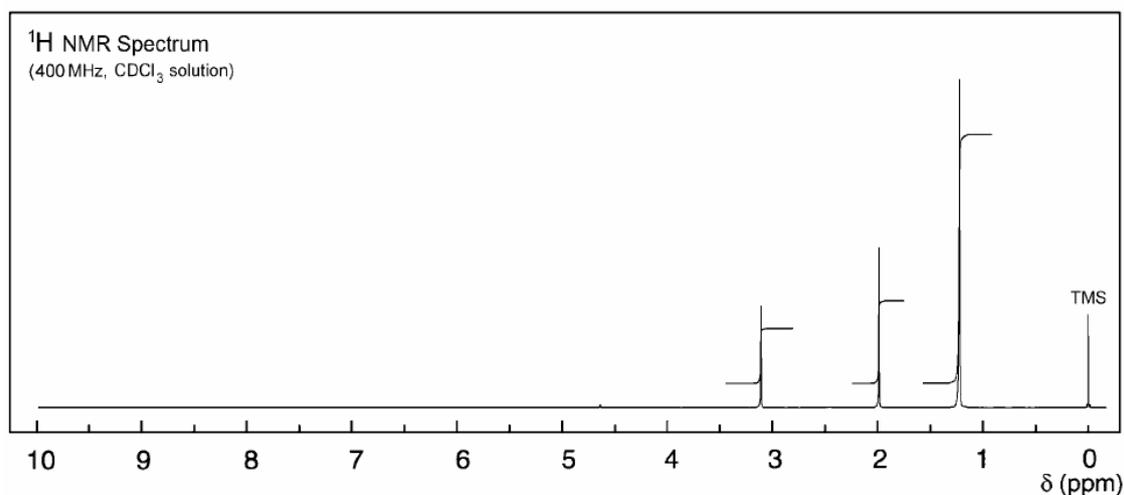
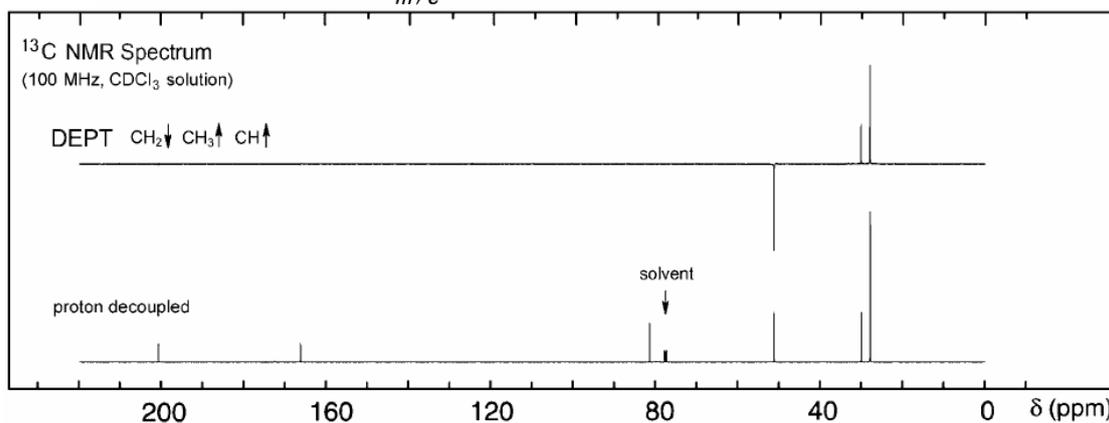


2. Dos compuestos carbonílicos de fórmula molecular $C_8H_{14}O_3$ presentan los siguientes espectros. Asignar las estructuras correspondientes.

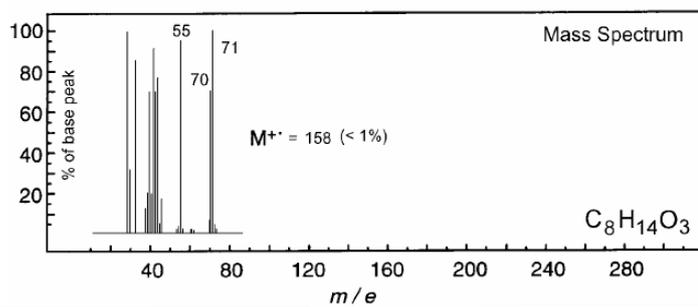
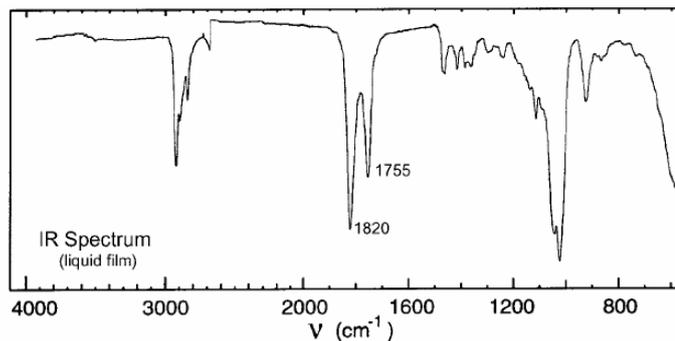
A)



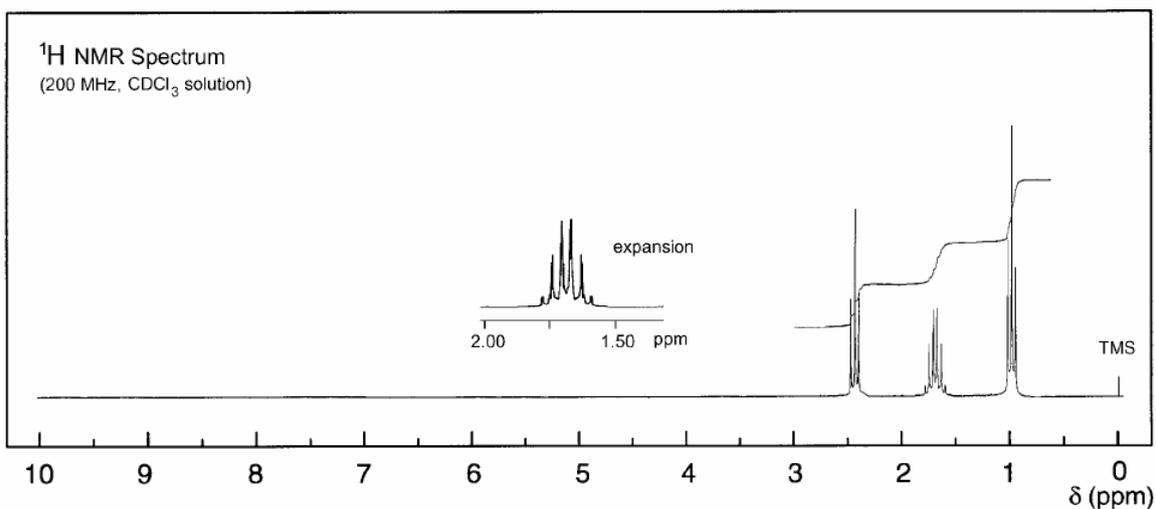
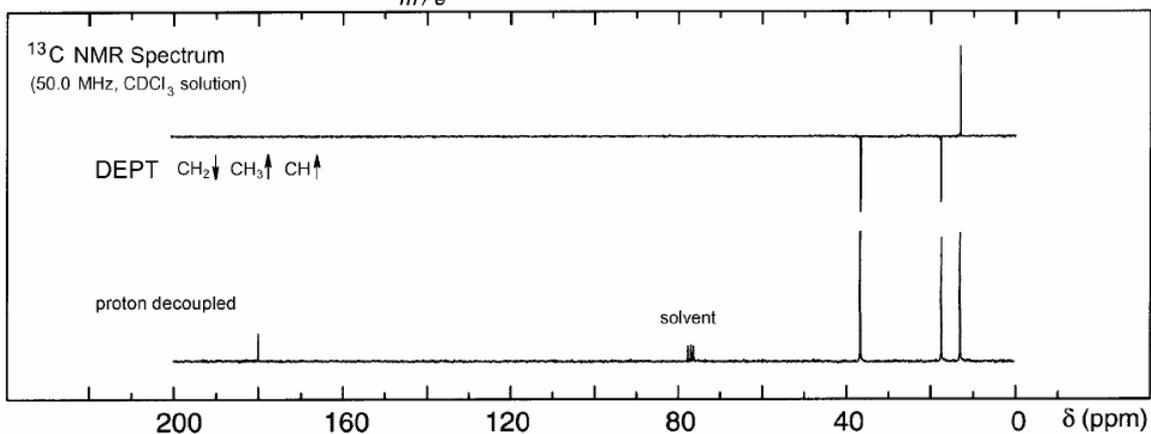
No significant UV absorption above 220 nm



B)

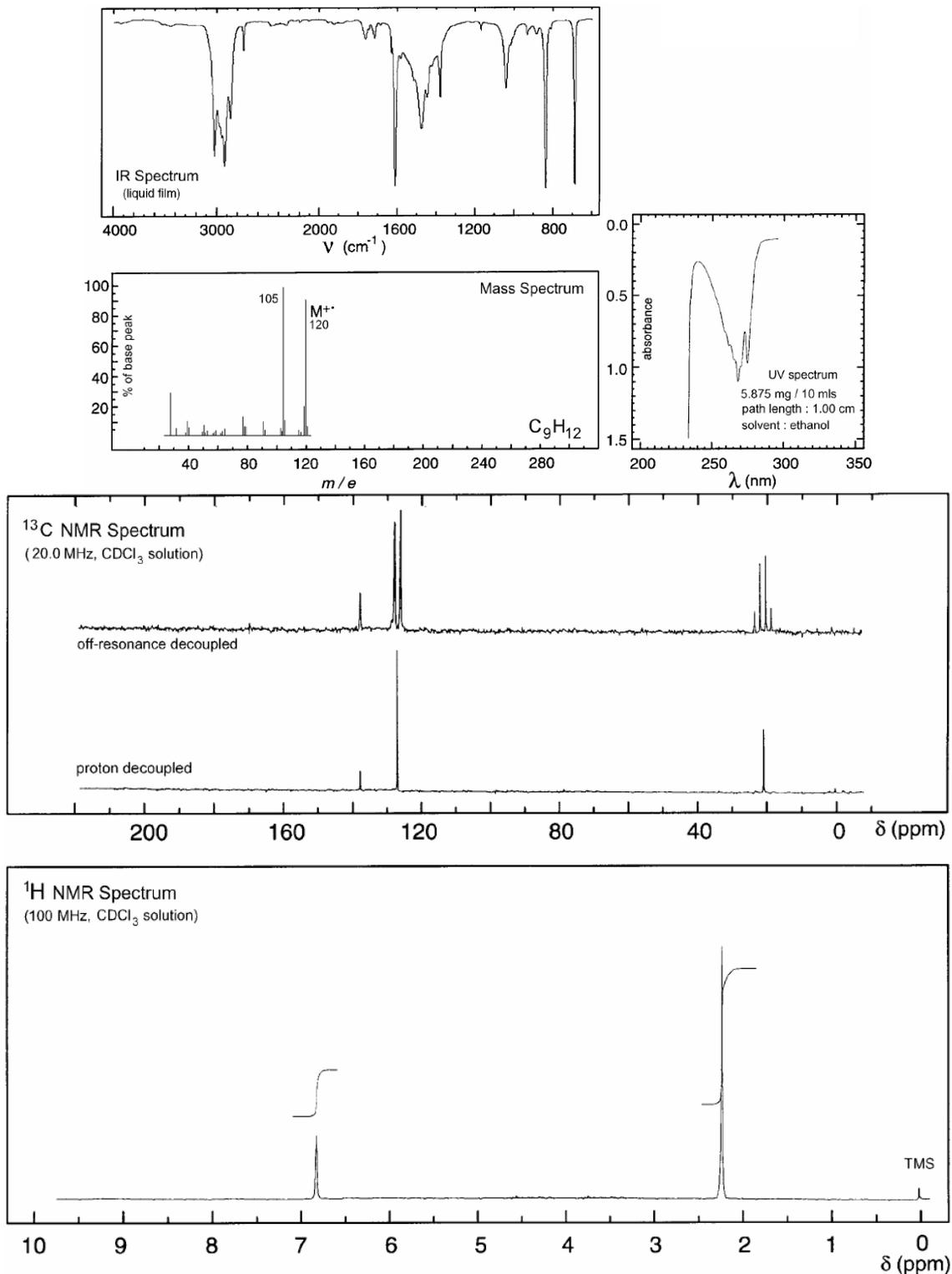


No significant UV absorption above 220 nm

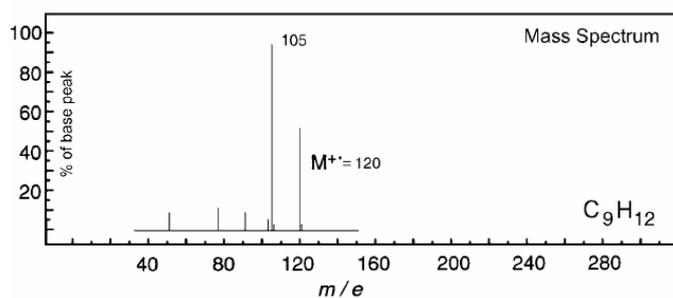
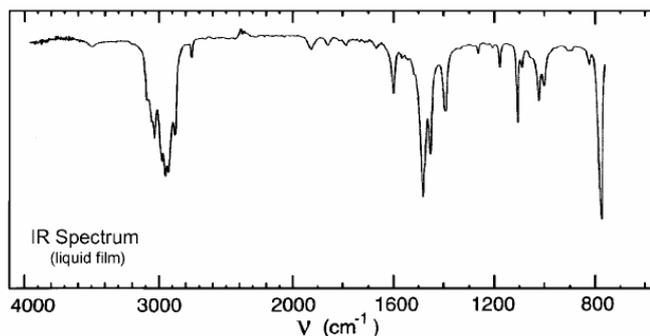


3. El siguiente grupo de espectros corresponde a tres compuestos isoméricos de trimetilbenceno. Asignar las estructuras correspondientes a cada uno de ellos.

A)



B)

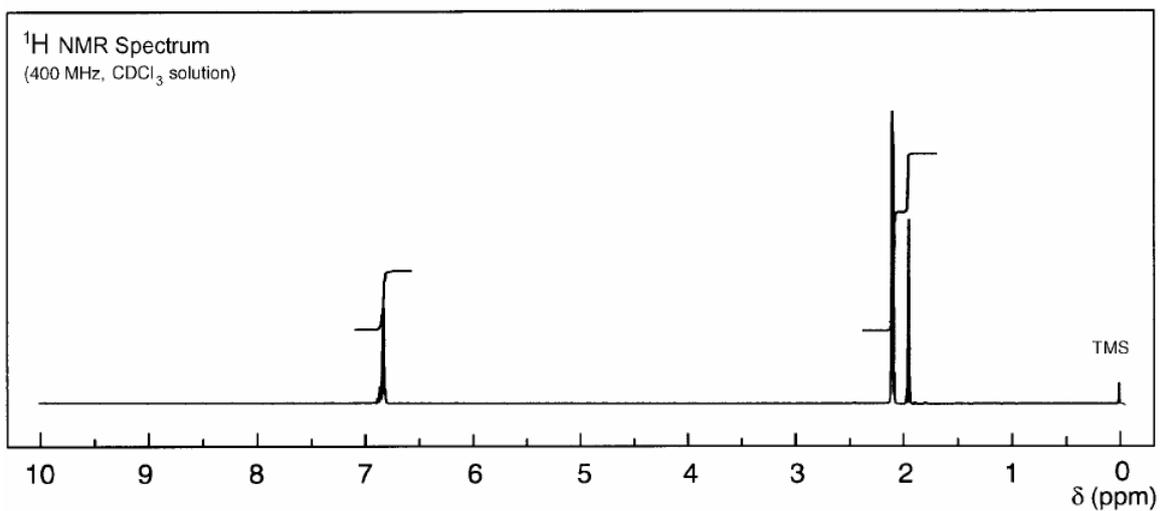
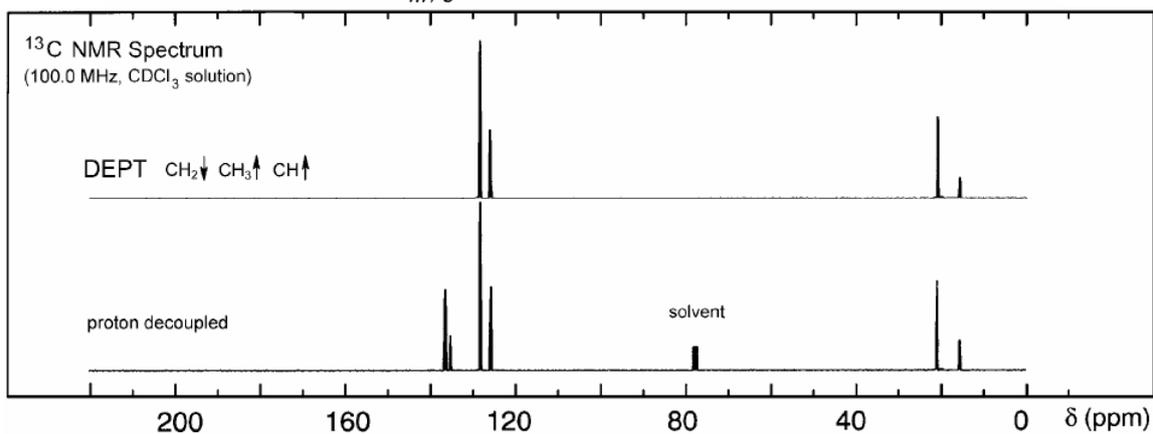


UV Spectrum

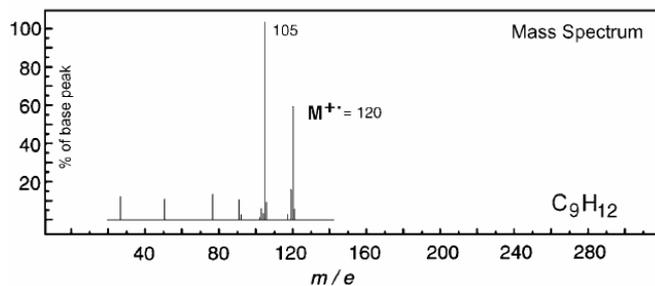
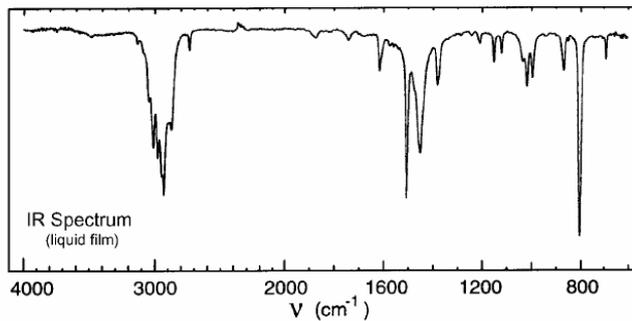
$\lambda_{\text{max}} 261 \text{ nm}$ ($\log_{10} \epsilon 2.7$)

$\lambda_{\text{max}} 269 \text{ nm}$ ($\log_{10} \epsilon 2.5$)

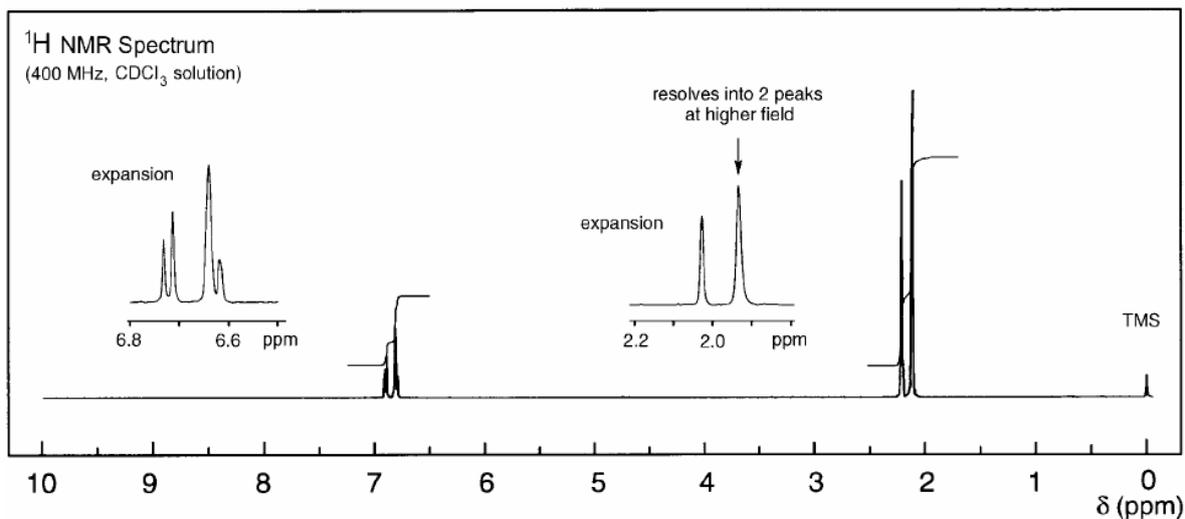
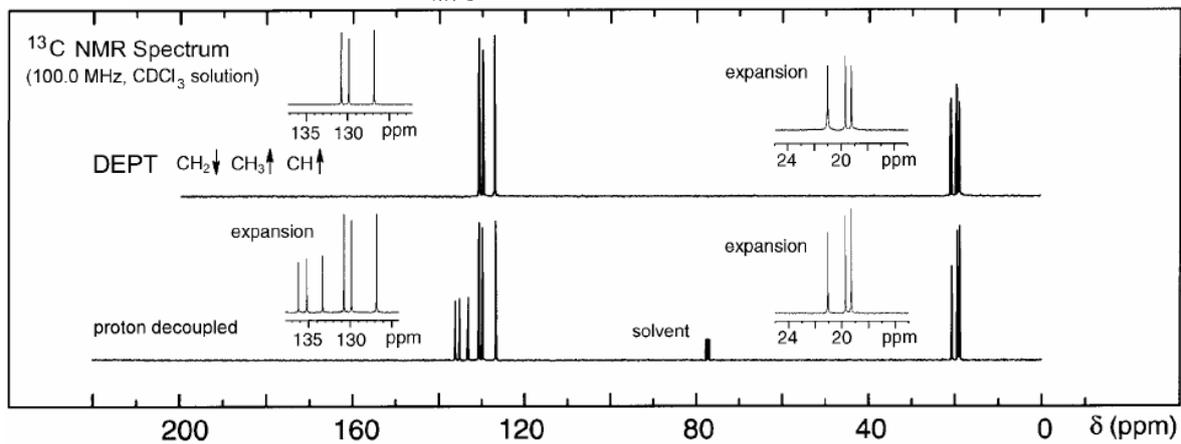
solvent: methanol



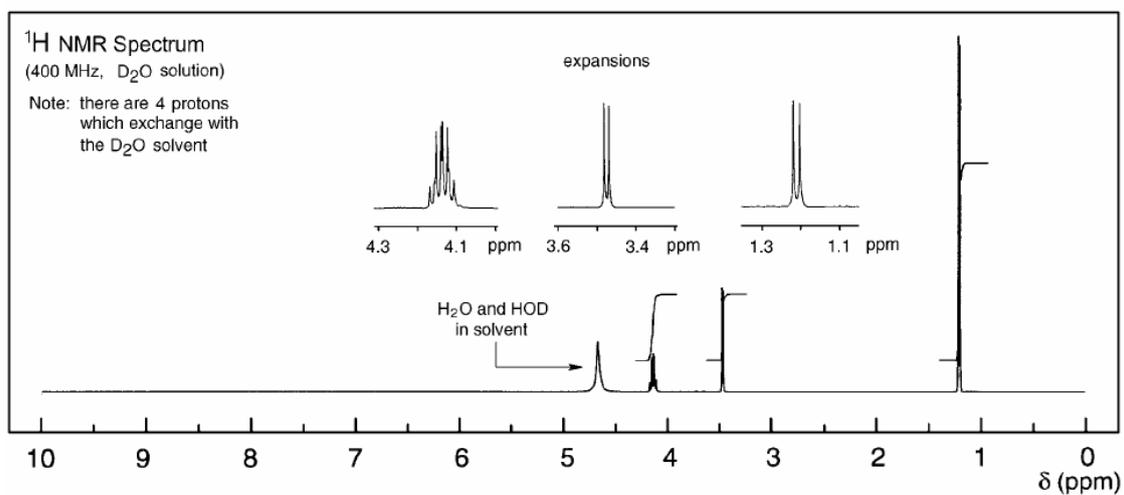
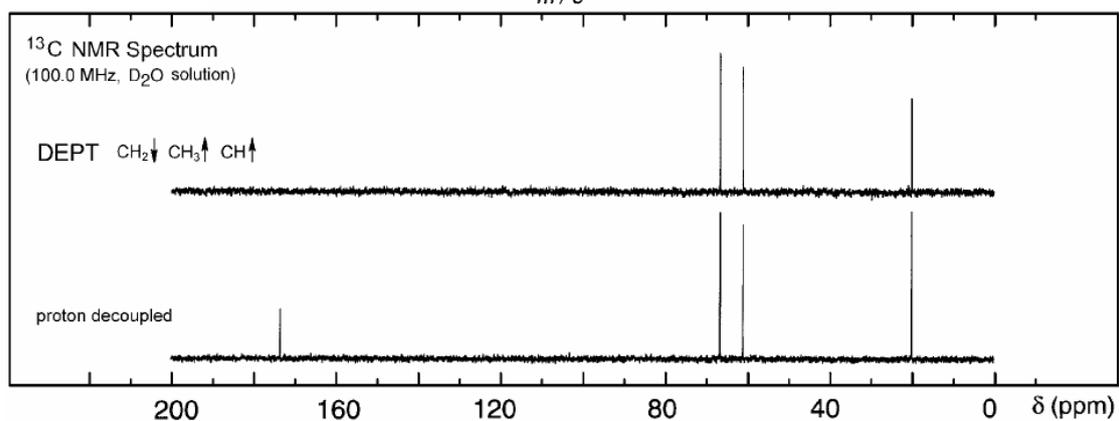
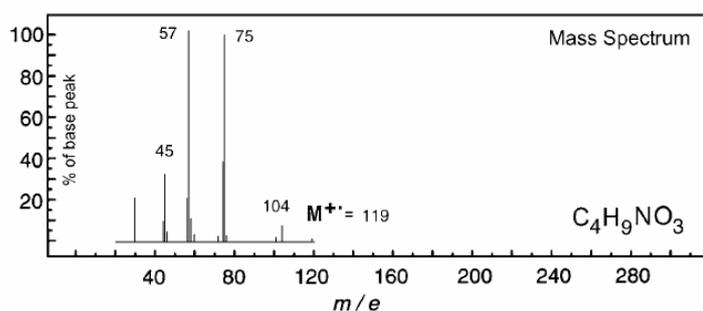
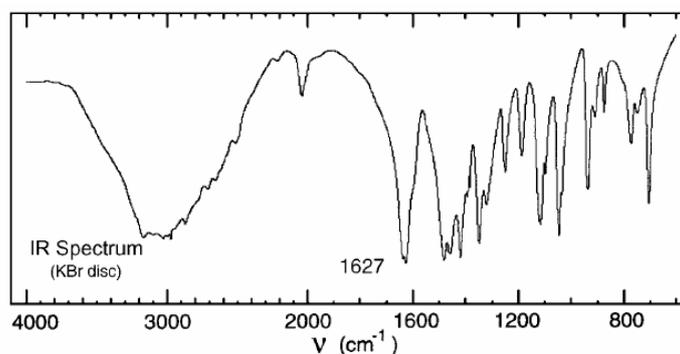
C)



UV Spectrum
λ_{max} 270 nm (log₁₀ ε 2.6)
solvent: methanol

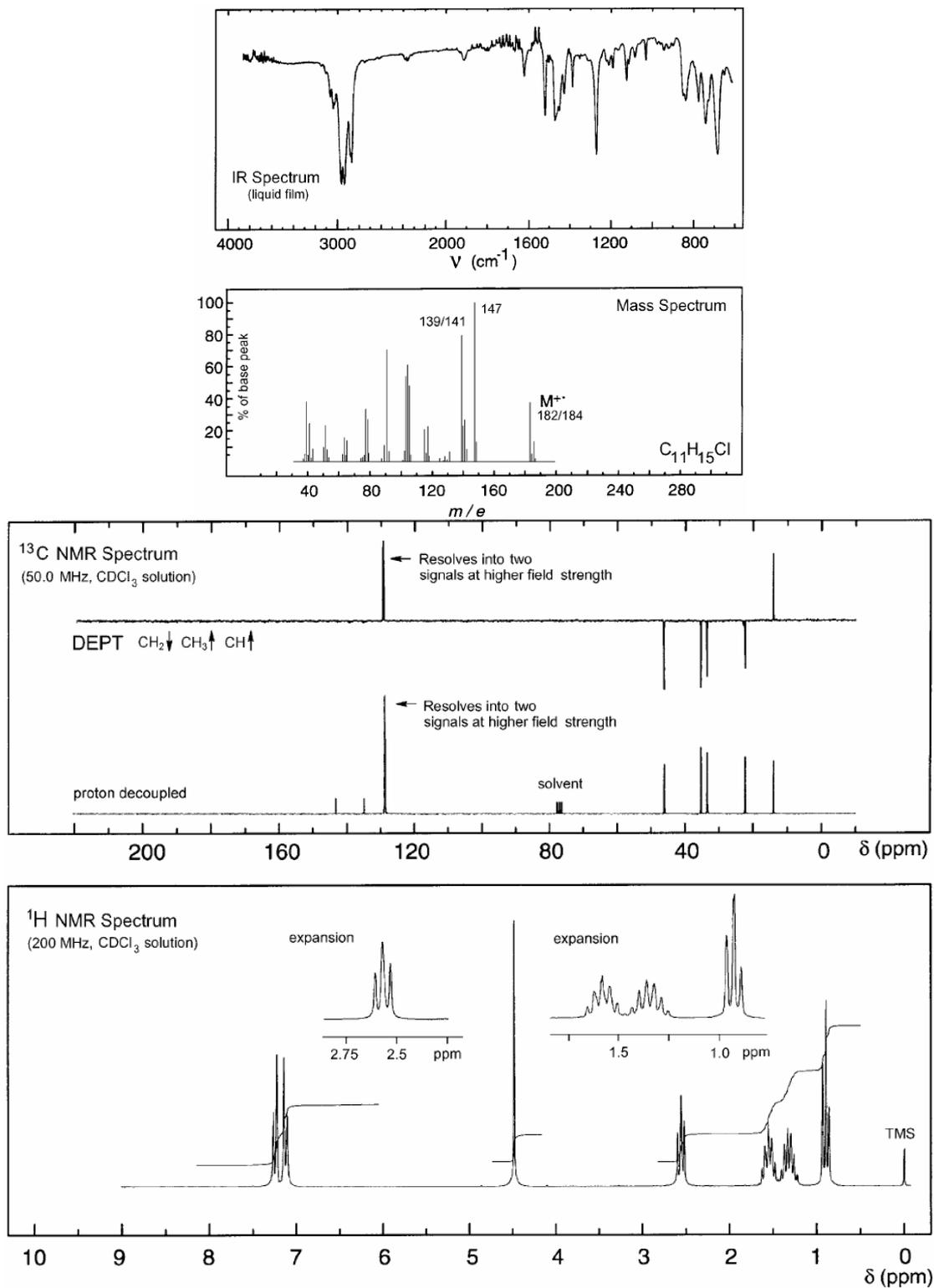


4. Un compuesto polifuncionalizado de fórmula molecular $C_4H_9NO_3$ presenta el siguiente espectro. Asignar su estructura.

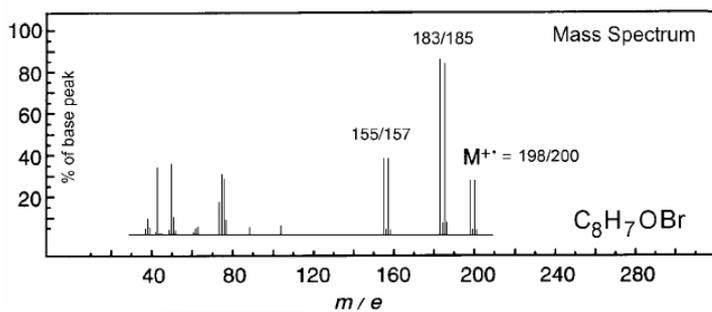
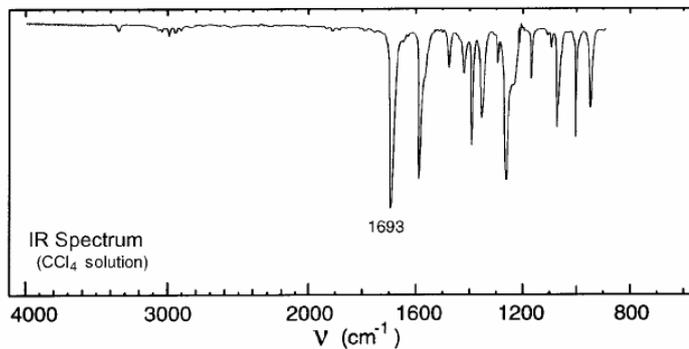


5. Los siguientes compuestos comparten la característica de ser bencenos con el mismo modelo de sustitución. Proponer la estructura de cada uno de ellos.

A: $C_{11}H_{15}Cl$



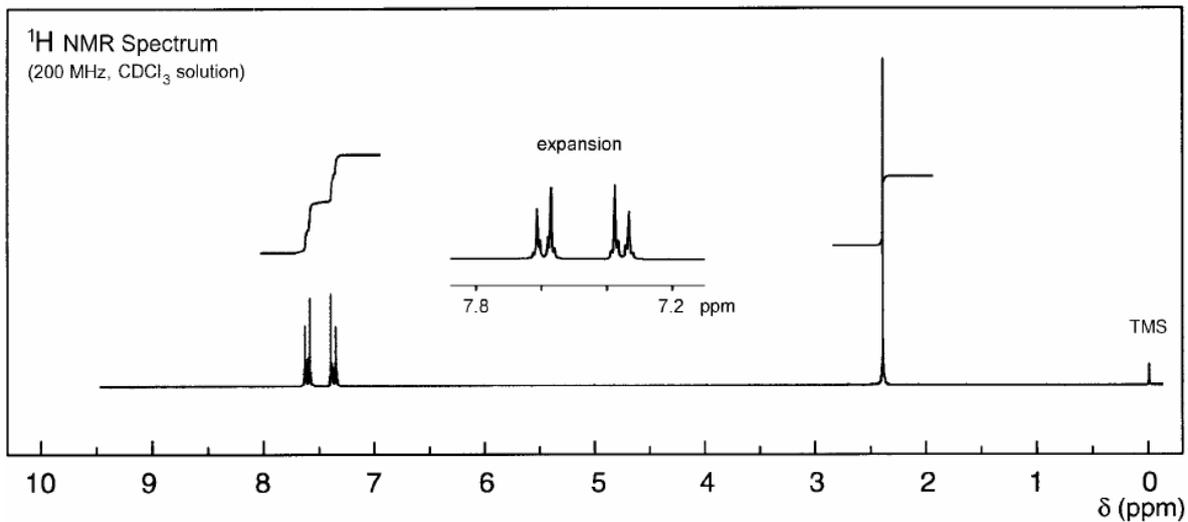
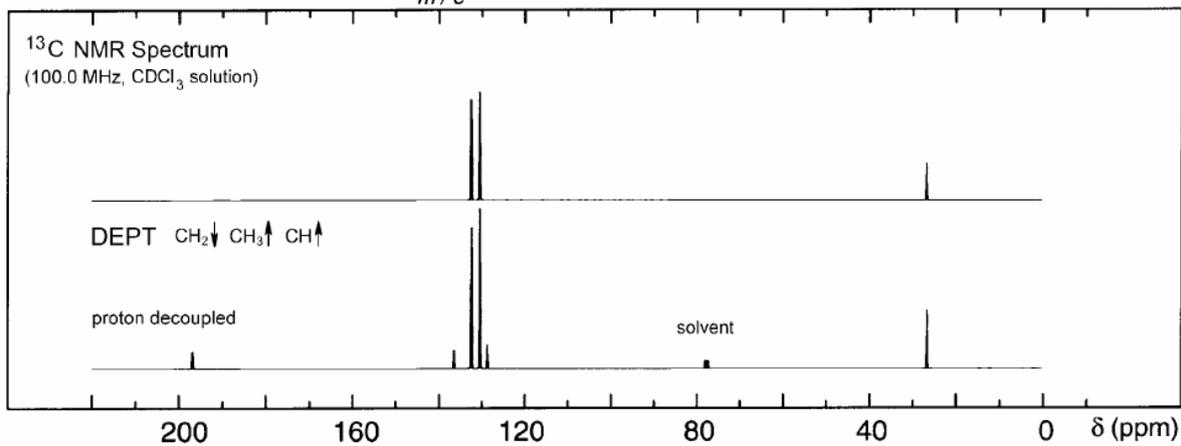
B: C_8H_7OBr



UV Spectrum

λ_{max} 258 nm ($\log_{10}\epsilon$ 4.2)

solvent: ethanol



C: C_8H_7OCl

