

ANALITIČKA KEMIJA II

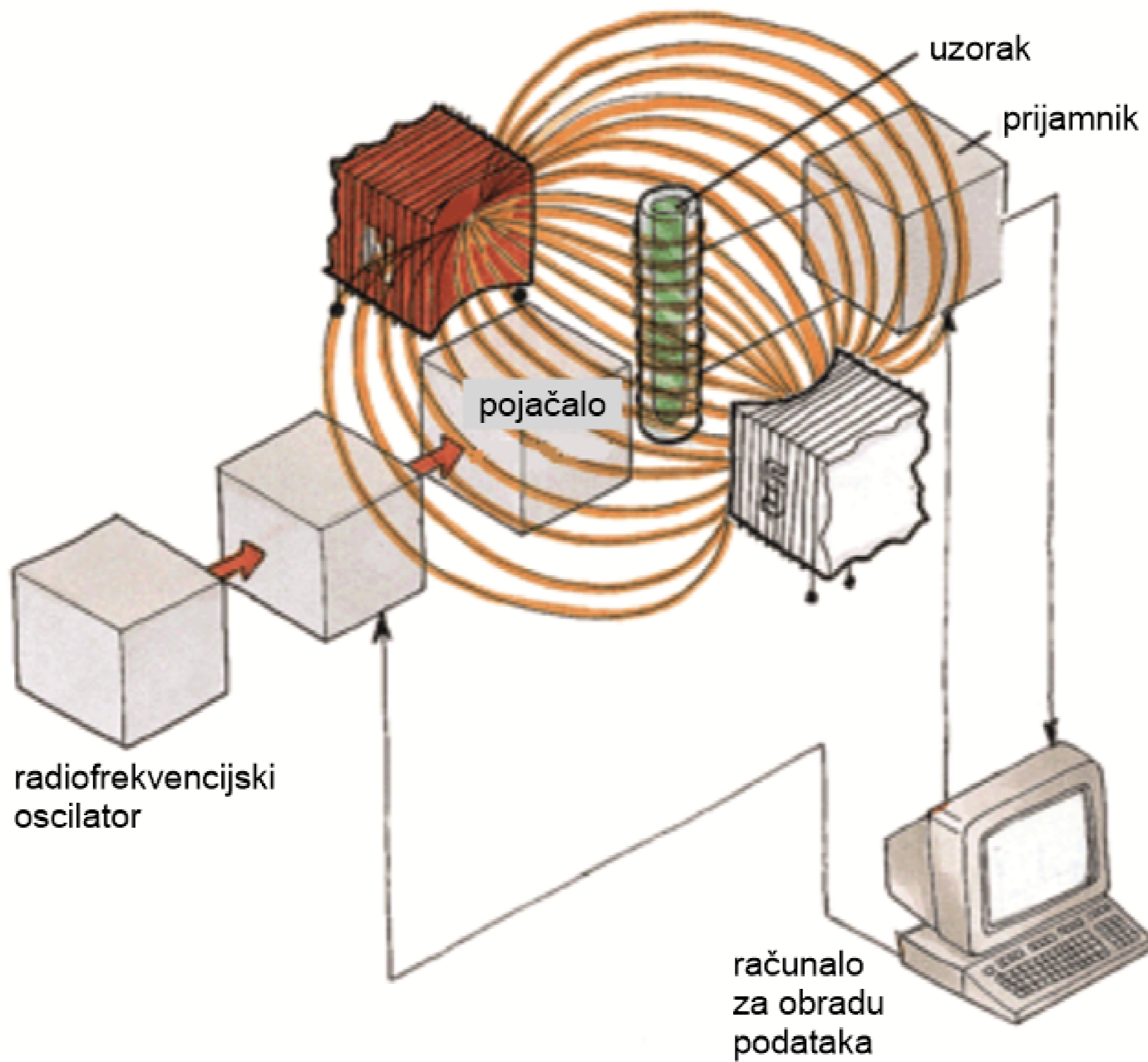
- uvod; normizacija; mjeriteljstvo; intelektualno vlasništvo
- osnove statistike
- Boltzmannova raspodjela
- atomska spektroskopija
- infracrvena (IR) i Ramanova spektroskopija
- **spektroskopija nuklearne magnetne rezonancije (NMR)**

SPEKTROMETAR NUKLEARNE MAGNETNE REZONANCIJE (NMR)

- uređaj koji se koristi za snimanje spektara NMR
- omogućava snimanje spektara otopina, tekućih i čvrstih uzoraka
- dvije izvedbe:
 - **CV (engl. *continuous wave*) NMR spektrometar**
 - **FT (engl. *Fourier transform*) NMR spektrometar**

- **CV-NMR spektrometar**

- temelji se na tehnici kontinuiranog vala
- u tehnici kontinuiranog vala pobuda se može izvoditi:
 - **promjenom frekvencije ν_1 pri konstantnom vanjskom magnetnom polju B_0**
 - **promjenom vanjskog magnetnog polja B_0 pri konstantnoj frekvenciji ν_1**
- snima se spektar u frekvencijskoj domeni



Shematski prikaz CV-NMR spektrometra

- **FT-NMR spektrometar**

- pobuda kratkim radiofrekvencijskim pulsevima

spektar u vremenskoj domeni (t),
FID (engl. *free induction decay*)

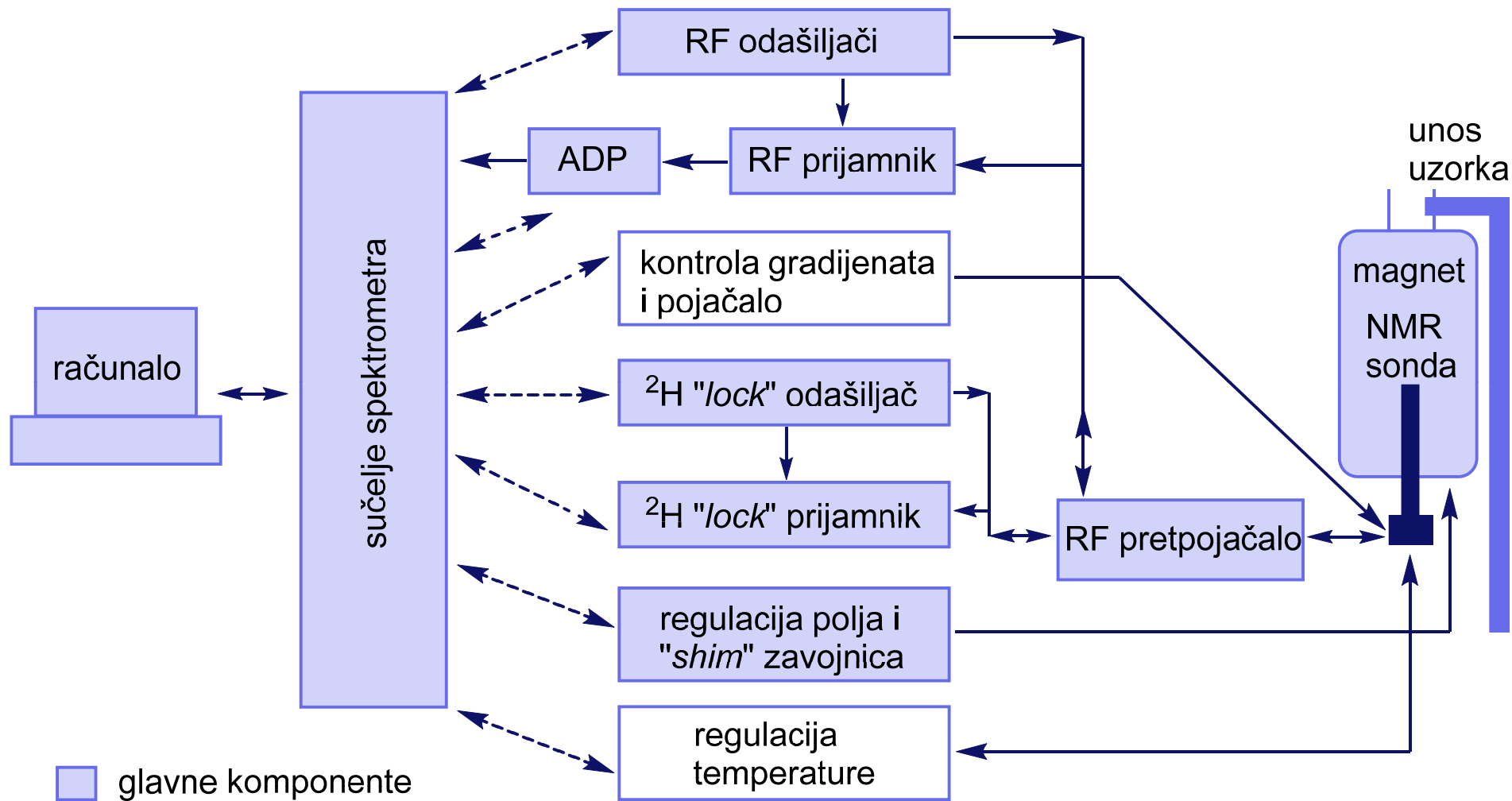


**Fourierova
transformacija**

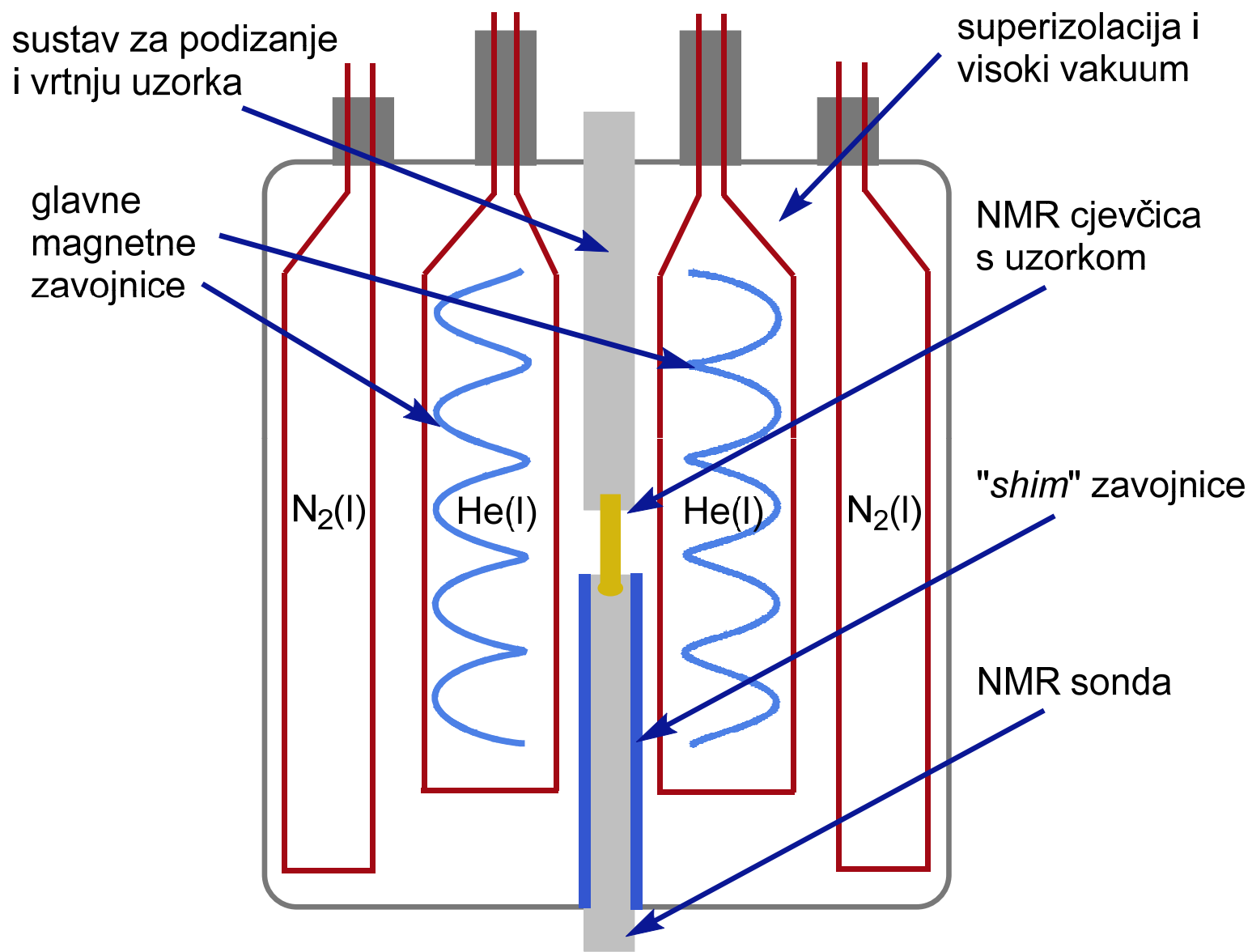


spektar u frekvencijskoj domeni (ν)

- koristi se u suvremenim tehnikama NMR



Shematski prikaz modernog FT-NMR spektrometra



Presjek unutrašnjosti magneta FT-NMR spektrometra

1. Koja je energijska razlika između 2 spinska stanja ^1H u magnetnom polju od 5,87 T?

$$B_0 = 5,87 \text{ T}$$

$$\gamma = 267,512 \cdot 10^6 \text{ rad T}^{-1} \text{ s}^{-1}$$

$$\Delta E = \frac{\gamma \hbar B_0}{2\pi}$$

$$\Delta E = \frac{267,512 \cdot 10^6 \text{ rad T}^{-1} \text{ s}^{-1} \cdot 6,626 \cdot 10^{-34} \text{ Js} \cdot 5,87 \text{ T}}{2 \cdot 3,14 \text{ rad}} = 1,66 \cdot 10^{-25} \text{ J}$$

2. a) Koja je frekvencija precesije ^{13}C jezgre pri 5,87 T?

$$B_0 = 5,87 \text{ T}$$

$$\nu = \frac{\gamma B_0}{2\pi} = \frac{67,2640 \cdot 10^6 \text{ rad T}^{-1} \text{ s}^{-1} \cdot 5,87 \text{ T}}{2 \cdot 3,14 \text{ rad}}$$

$$\nu = 6,29 \cdot 10^7 \text{ Hz} = 62,9 \text{ MHz}$$

b) Kojem području elektromagnetnog spektra odgovara zračenje tih frekvencija?

Odgovara radiofrekvencijskom području.

3. Pri kojoj jakosti magnetnog polja protoni (jezgre ^1H) precesiraju frekvencijom od 300 MHz?

$$\nu = 300 \text{ MHz}$$

$$B_0 = \frac{2\pi\nu}{\gamma}$$

$$B_0 = \frac{2 \cdot 3,14 \text{ rad} \cdot 300 \cdot 10^6 \text{ s}^{-1}}{267,512 \cdot 10^6 \text{ rad T}^{-1} \text{ s}^{-1}} = 7,04 \text{ T}$$

4. Koji se udio ^1H jezgara pri $25\text{ }^\circ\text{C}$ i jakosti magnetnog polja od $5,87\text{ T}$ nalazi u višem odnosno nižem stanju?

$$\theta = 25\text{ }^\circ\text{C}$$

$$T = 298\text{ K}$$

$$B_0 = 5,87\text{ T}$$

$$\frac{N_{(m=-1/2)}}{N_{(m=1/2)}} = \exp\left(-\frac{\Delta E}{kT}\right)$$

$$\frac{N_{(m=-1/2)}}{N_{(m=1/2)}} = \exp\left(-\frac{1,66 \cdot 10^{-25}\text{ J}}{1,381 \cdot 10^{-23}\text{ J K}^{-1} \cdot 298\text{ K}}\right) = 0,99996$$

Budući da postoje samo 2 spinska stanja:

$$P_{(m=-1/2)} = 1 - P_{(m=1/2)}$$

$$P_{(m=-1/2)} = 0,49999$$

$$P_{(m=1/2)} = 0,50001$$

Razlika u populacijama ^1H spinskih stanja iznimno je mala, reda veličine 20 ppm.

5. Ako se magnetno polje spektrometra promijeni za +0,00001 T (oko 2 ppm), koliki je iznos promjene frekvencije rezonancije ^1H jezgara pri 5,87 T?

$$\Delta B_0 = +0,00001 \text{ T}$$

$$B_0 = 5,87 \text{ T}$$

$$\nu = \frac{\gamma B_0}{2\pi} = \frac{267,512 \cdot 10^6 \text{ rad T}^{-1} \text{ s}^{-1} \cdot 5,87 \text{ T}}{2 \cdot 3,14 \text{ rad}}$$

$$= 2,50 \cdot 10^8 \text{ s}^{-1} = 250 \text{ MHz}$$

$$\frac{0,00001 \text{ T}}{5,87 \text{ T}} = \frac{\Delta \nu}{250 \text{ MHz}}$$

$$\nu = 0,000430 \text{ MHz} = 430 \text{ Hz}$$

6. ^1H NMR spektar toluena snimljen na spektrometru frekvencije 80 MHz pokazuje signale na 188 Hz i 578 Hz, pri nižem polju u odnosu na TMS.

a) Izračunajte kemijske pomake navedenih signala.

b) Koliki su kemijski pomaci ovih signala na instrumentu od 250 MHz?

a) $\nu_1 - \nu_{\text{ref}} = 188 \text{ Hz}$ $\nu_0 = 80 \text{ MHz}$

$$\delta = \frac{\nu_i - \nu_{\text{ref}}}{\nu_0} \cdot 10^6 \text{ ppm}$$

$$\delta_1 = \frac{\nu_1 - \nu_{\text{ref}}}{\nu_0} \cdot 10^6 \text{ ppm} = \frac{188 \text{ Hz}}{80 \text{ MHz}} \cdot 10^6 \text{ ppm} = 2,35 \text{ ppm}$$

$$\nu_2 - \nu_{\text{ref}} = 578 \text{ Hz}$$

$$\nu_o = 80 \text{ MHz}$$

$$\delta_2 = \frac{\nu_2 - \nu_{\text{ref}}}{\nu_o} \cdot 10^6 \text{ ppm} = \frac{578 \text{ Hz}}{80 \text{ MHz}} \cdot 10^6 \text{ ppm} = 7,23 \text{ ppm}$$

b) Isti! Kemijski pomak ne ovisi o frekvenciji instrumenta.

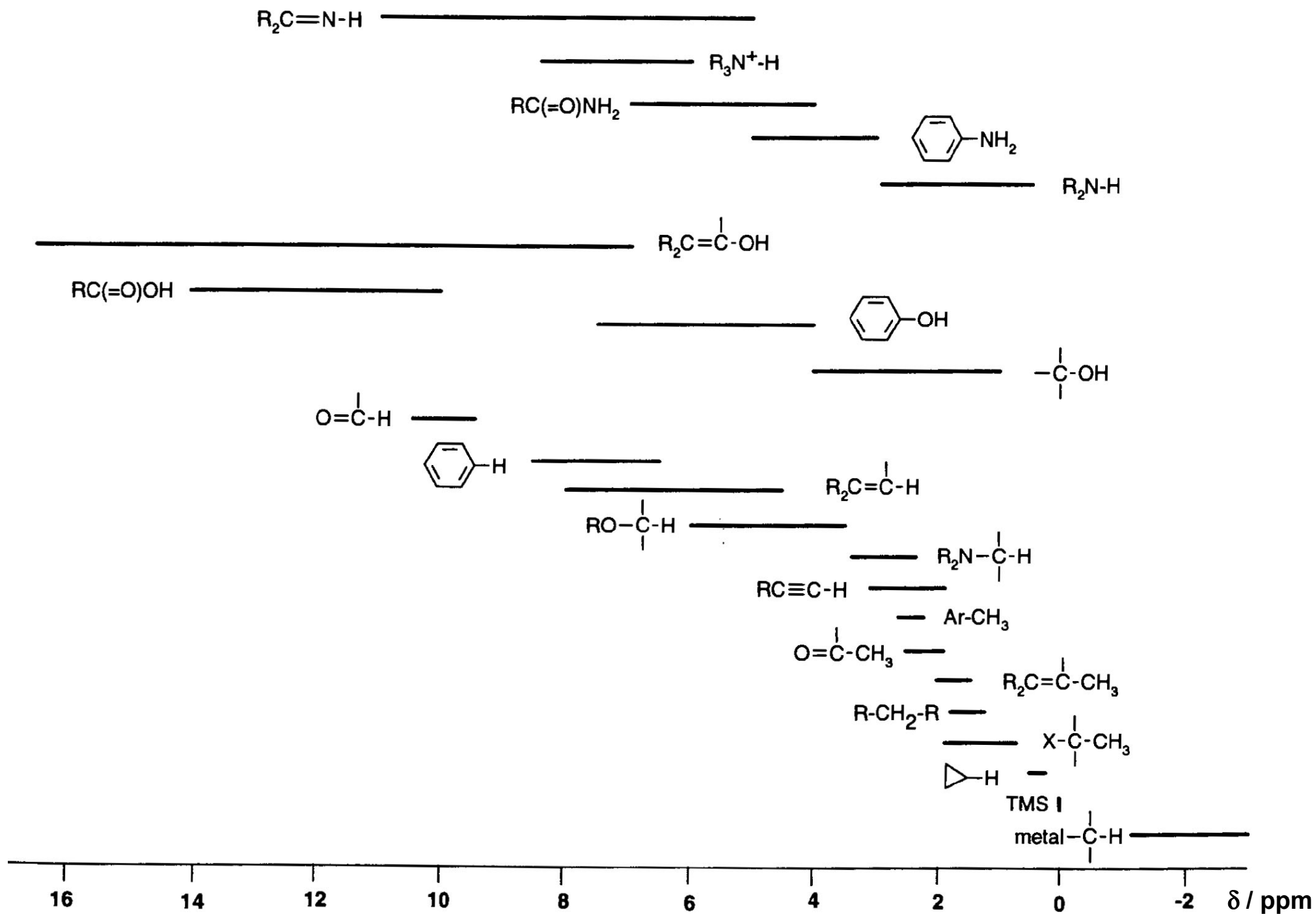
7. ^1H NMR spektar metilijata CH_3Li snimljen na spektrometru frekvencije 250 MHz pokazuje signal na 525 Hz, **pri višem polju** u odnosu na TMS. Koliki je njegov kemijski pomak?

$$\nu_o = 250 \text{ MHz}$$

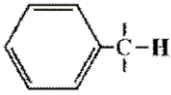
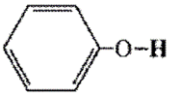
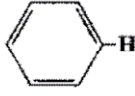
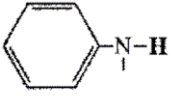
$$\nu_i - \nu_{\text{ref}} = -525 \text{ Hz}$$

$$\delta(\text{CH}_3\text{Li}) = \frac{\nu_i - \nu_{\text{ref}}}{\nu_o} \cdot 10^6 \text{ ppm}$$

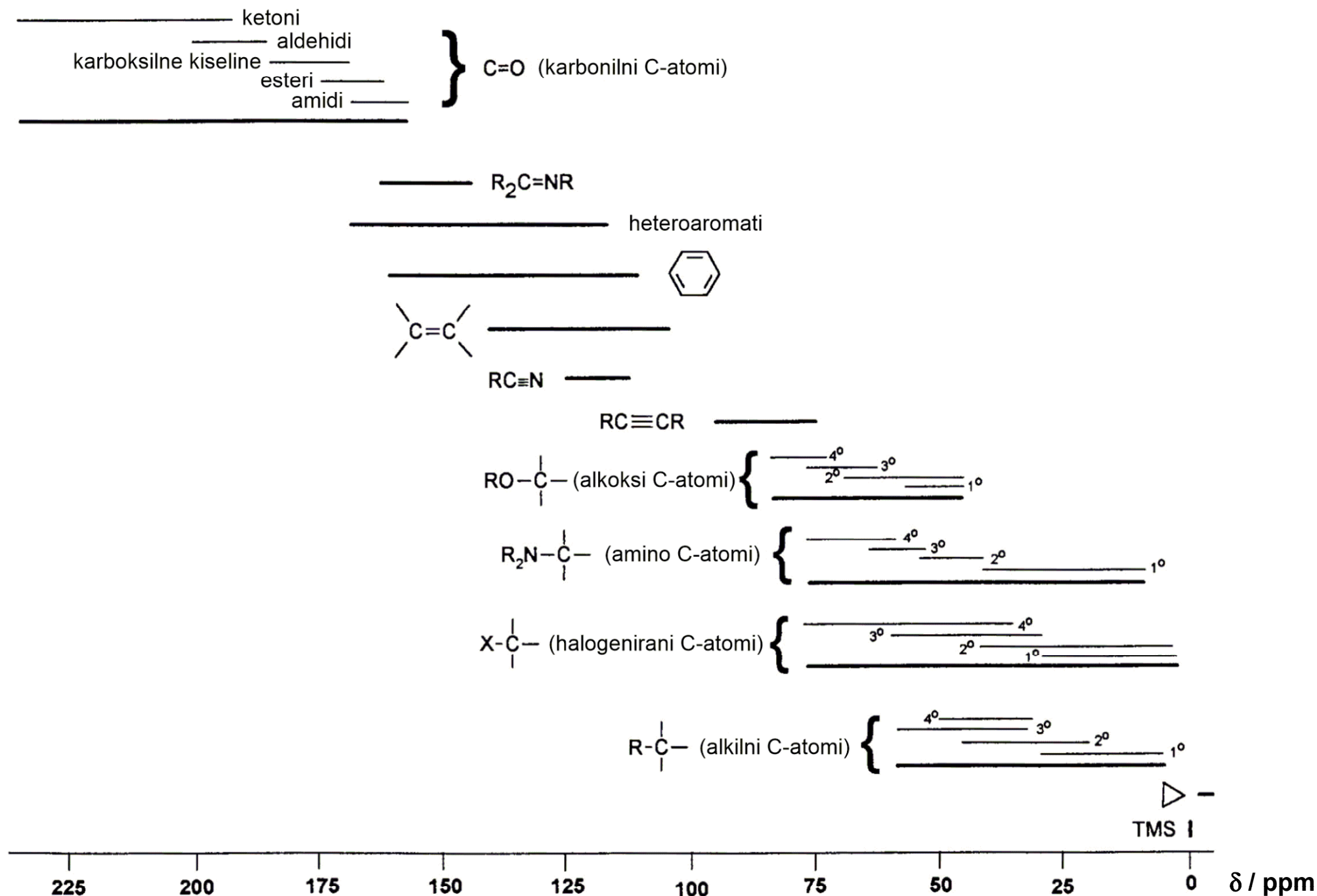
$$\delta(\text{CH}_3\text{Li}) = -\frac{525 \text{ Hz}}{250 \text{ MHz}} \cdot 10^6 \text{ ppm} = -2,10 \text{ ppm}$$



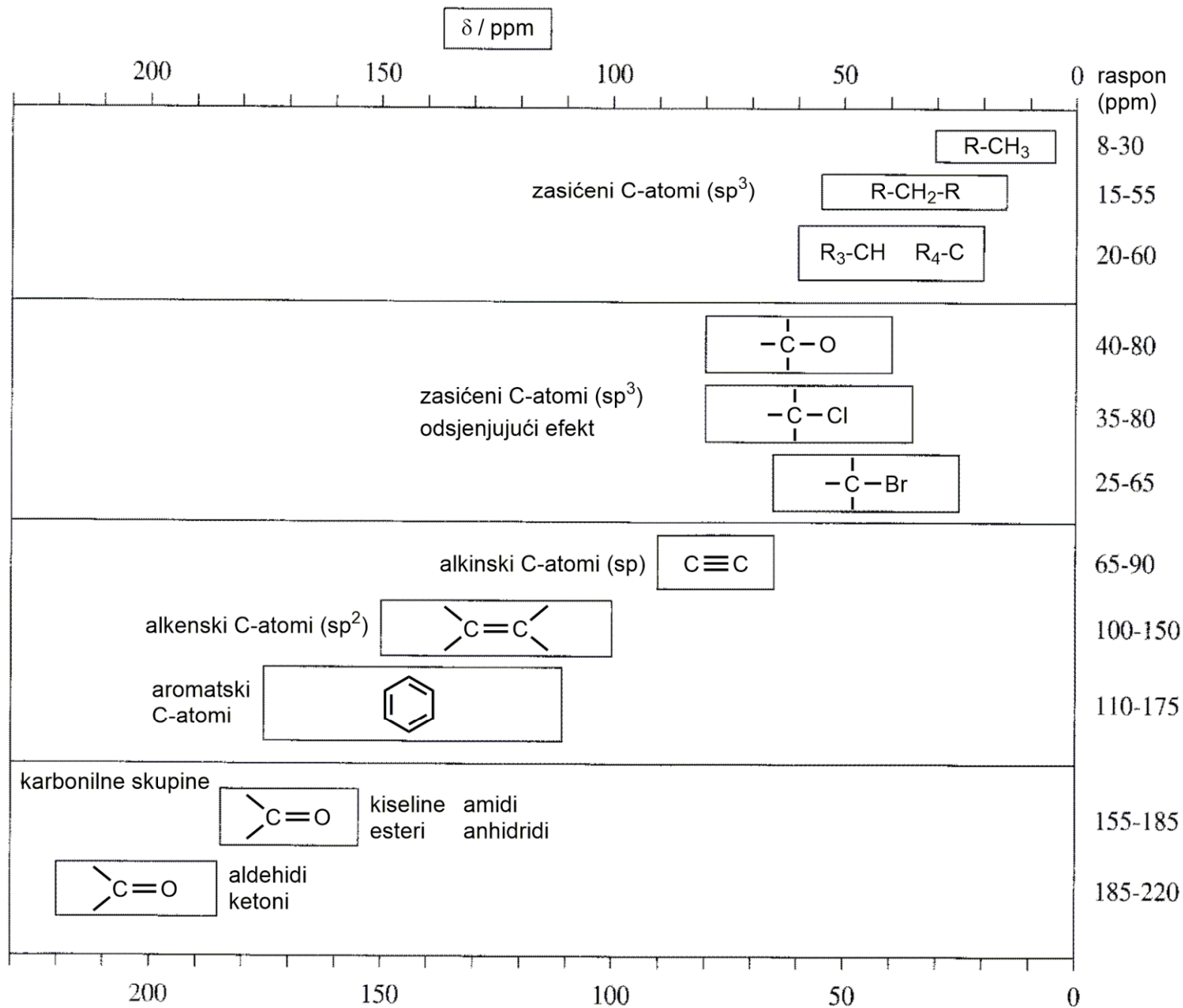
Područje kemijskog pomaka u 1H NMR spektrima

$R-CH_3$		0.7 – 1.3	$R-\overset{ }{N}-\overset{ }{C}-H$	2.2 – 2.9
$R-CH_2-R$		1.2 – 1.4	$R-\overset{ }{S}-\overset{ }{C}-H$	2.0 – 3.0
R_3CH		1.4 – 1.7	$I-\overset{ }{C}-H$	2.0 – 4.0
$R-\overset{ }{C}=\overset{ }{C}-\overset{ }{C}-H$		1.6 – 2.6	$Br-\overset{ }{C}-H$	2.7 – 4.1
$R-\overset{O}{\parallel}{C}-\overset{ }{C}-H, H-\overset{O}{\parallel}{C}-\overset{ }{C}-H$		2.1 – 2.4	$Cl-\overset{ }{C}-H$	3.1 – 4.1
$RO-\overset{O}{\parallel}{C}-\overset{ }{C}-H, HO-\overset{O}{\parallel}{C}-\overset{ }{C}-H$		2.1 – 2.5	$R-\overset{O}{\parallel}{S}-\overset{O}{\parallel}{O}-\overset{ }{C}-H$	ca. 3.0
$N\equiv C-\overset{ }{C}-H$		2.1 – 3.0	$RO-\overset{ }{C}-H, HO-\overset{ }{C}-H$	3.2 – 3.8
		2.3 – 2.7	$R-\overset{O}{\parallel}{C}-O-\overset{ }{C}-H$	3.5 – 4.8
$R-C\equiv C-H$		1.7 – 2.7	$O_2N-\overset{ }{C}-H$	4.1 – 4.3
$R-S-H$	var	1.0 – 4.0 ^b	$F-\overset{ }{C}-H$	4.2 – 4.8
$R-\overset{ }{N}-H$	var	0.5 – 4.0 ^b		
$R-O-H$	var	0.5 – 5.0 ^b	$R-\overset{ }{C}=\overset{ }{C}-H$	4.5 – 6.5
	var	4.0 – 7.0 ^b		6.5 – 8.0
	var	3.0 – 5.0 ^b	$R-\overset{O}{\parallel}{C}-H$	9.0 – 10.0
$R-\overset{O}{\parallel}{C}-\overset{ }{N}-H$	var	5.0 – 9.0 ^b	$R-\overset{O}{\parallel}{C}-OH$	11.0 – 12.0

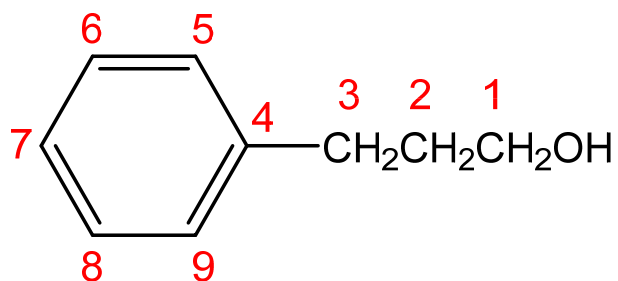
Približna područja kemijskih pomaka (ppm) za odabrane vrste protona



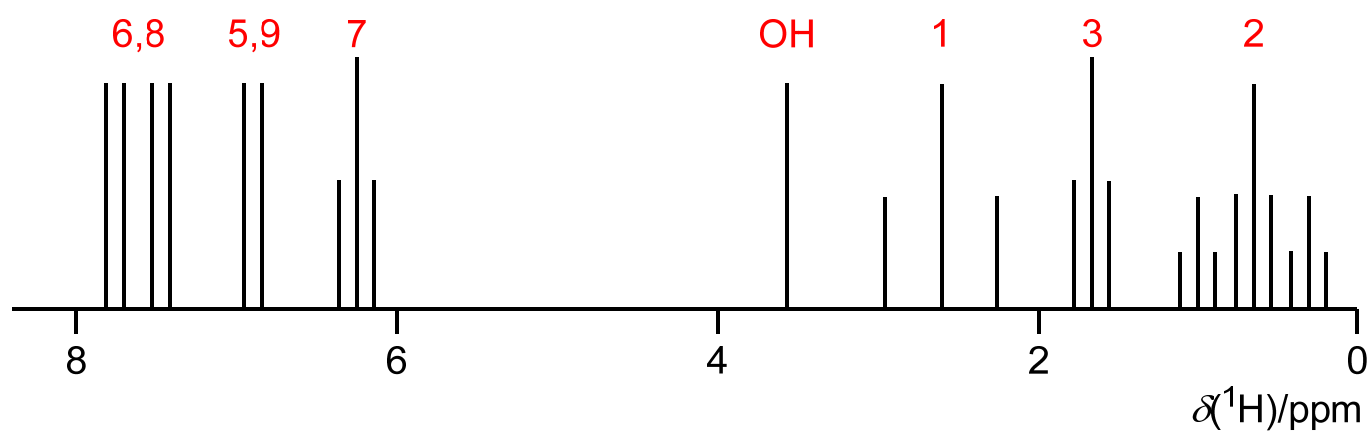
Područje kemijskog pomaka u ^{13}C NMR spektrima



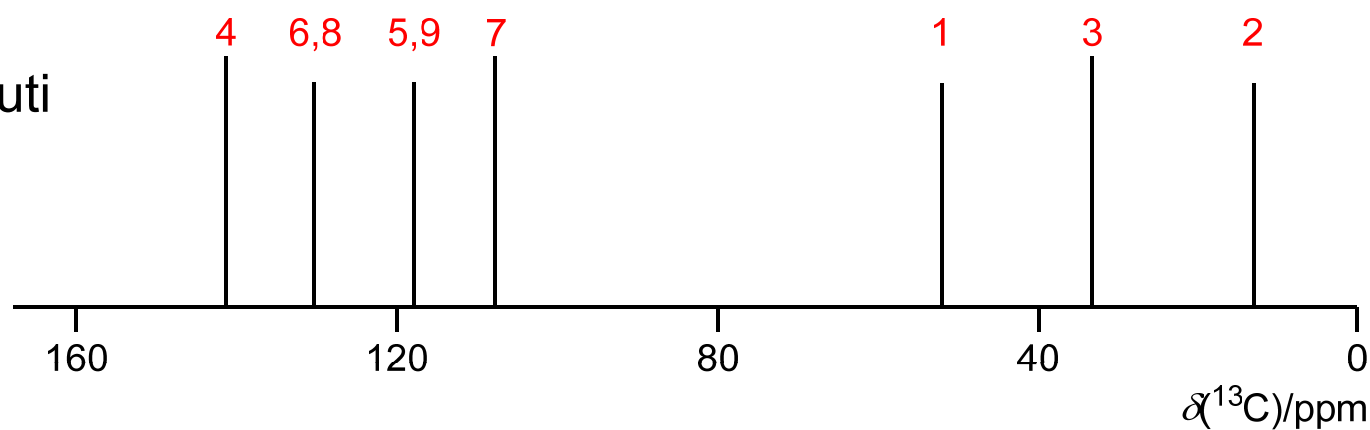
8. Skicirajte ^1H i potpuno raspregnuti ^{13}C NMR spektar 3-fenilpropan-1-ola.



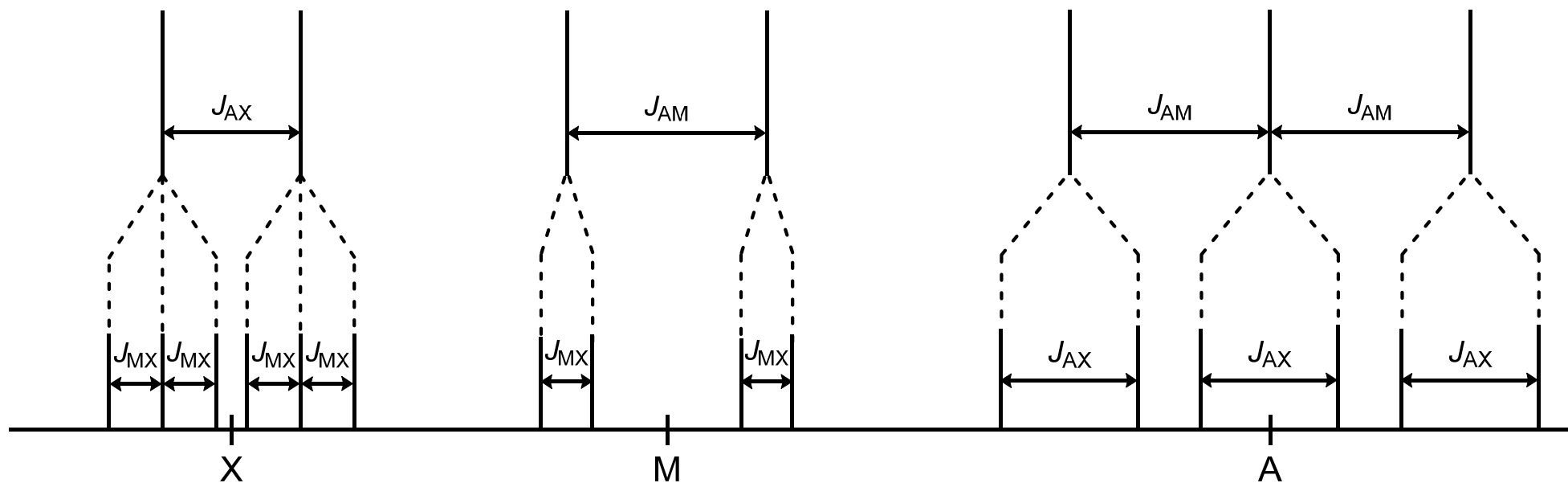
^1H NMR



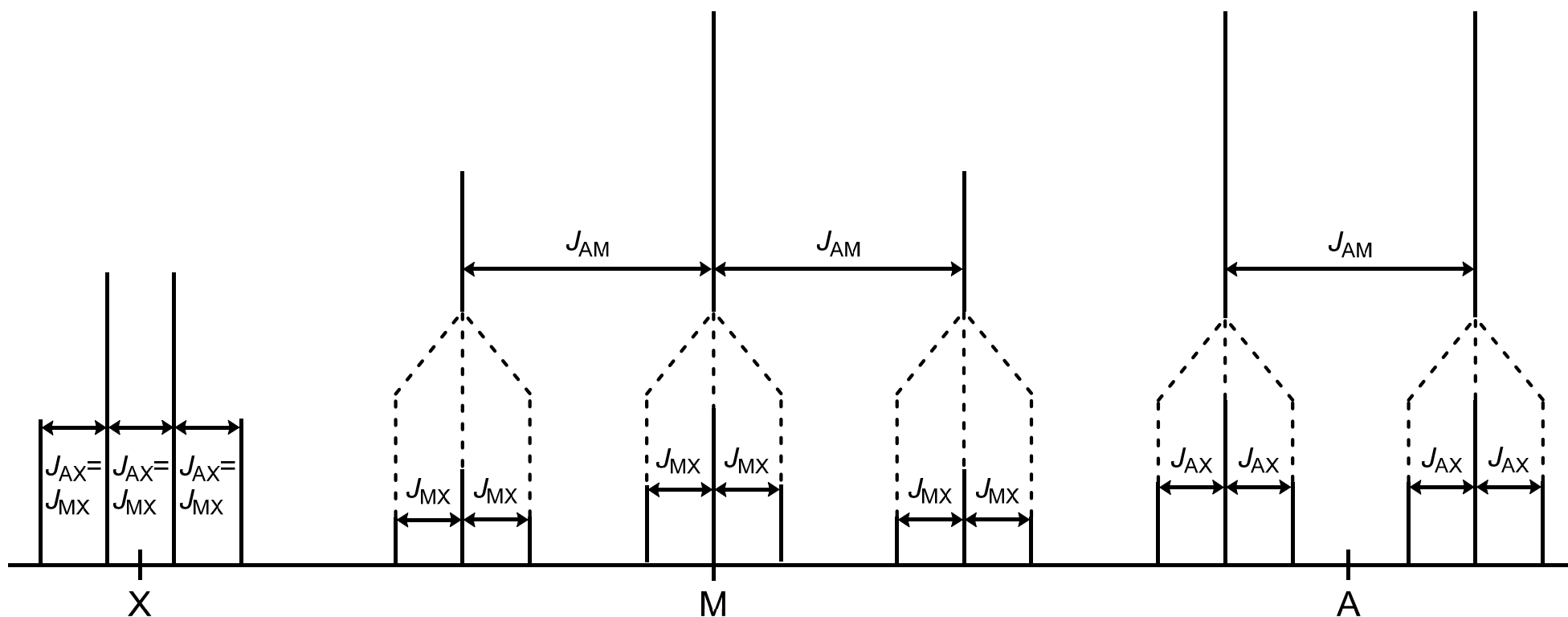
Potpuno
raspregnuti
 ^{13}C NMR



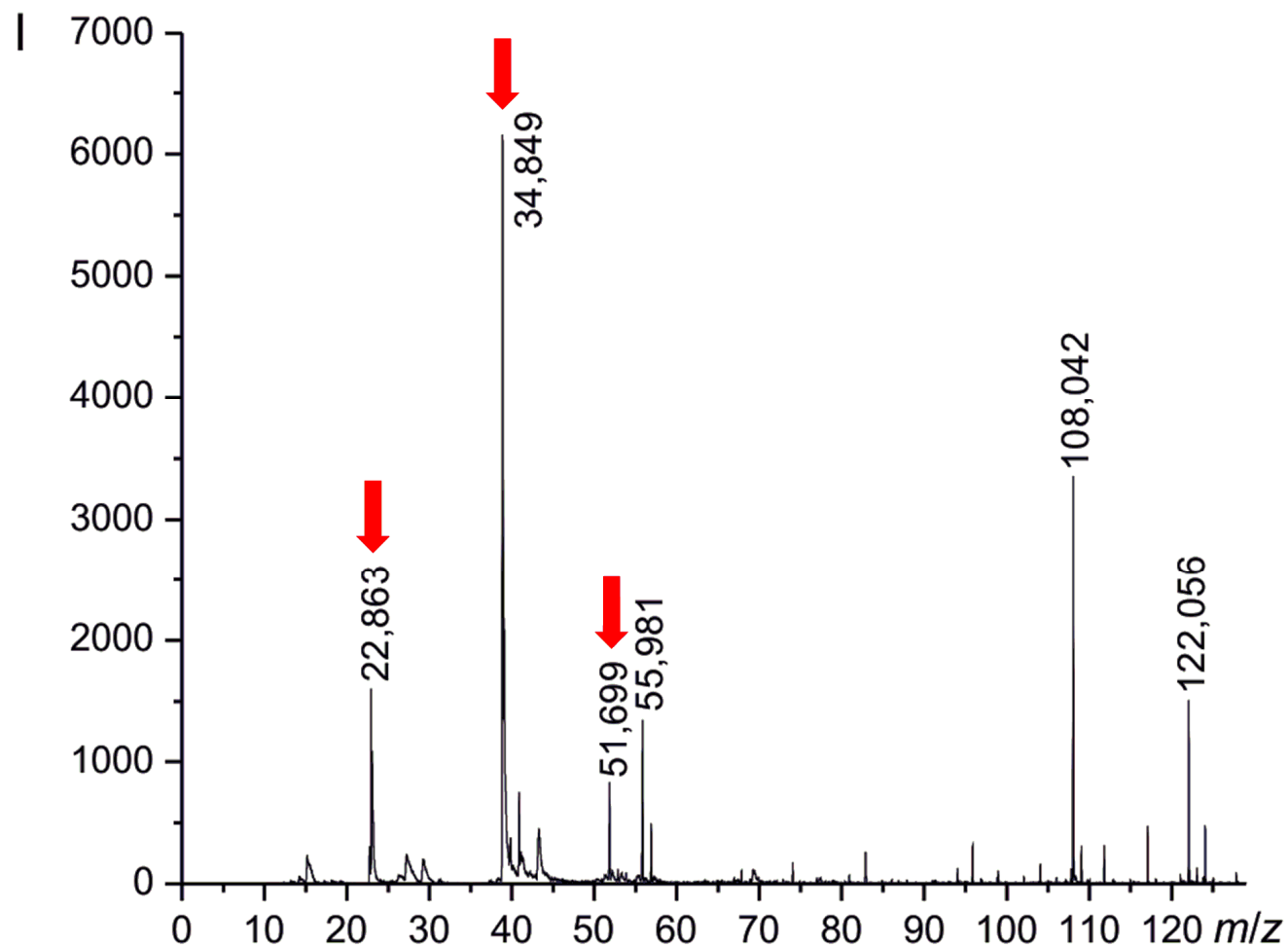
9. Razmotrimo spinski sustav AMX, gdje je $I_A=1/2$, $I_M=1$, a $I_X=1/2$. Skicirajte signale spinova A, M i X u spektru NMR, ako je $J_{AM} > J_{AX} > J_{MX}$.



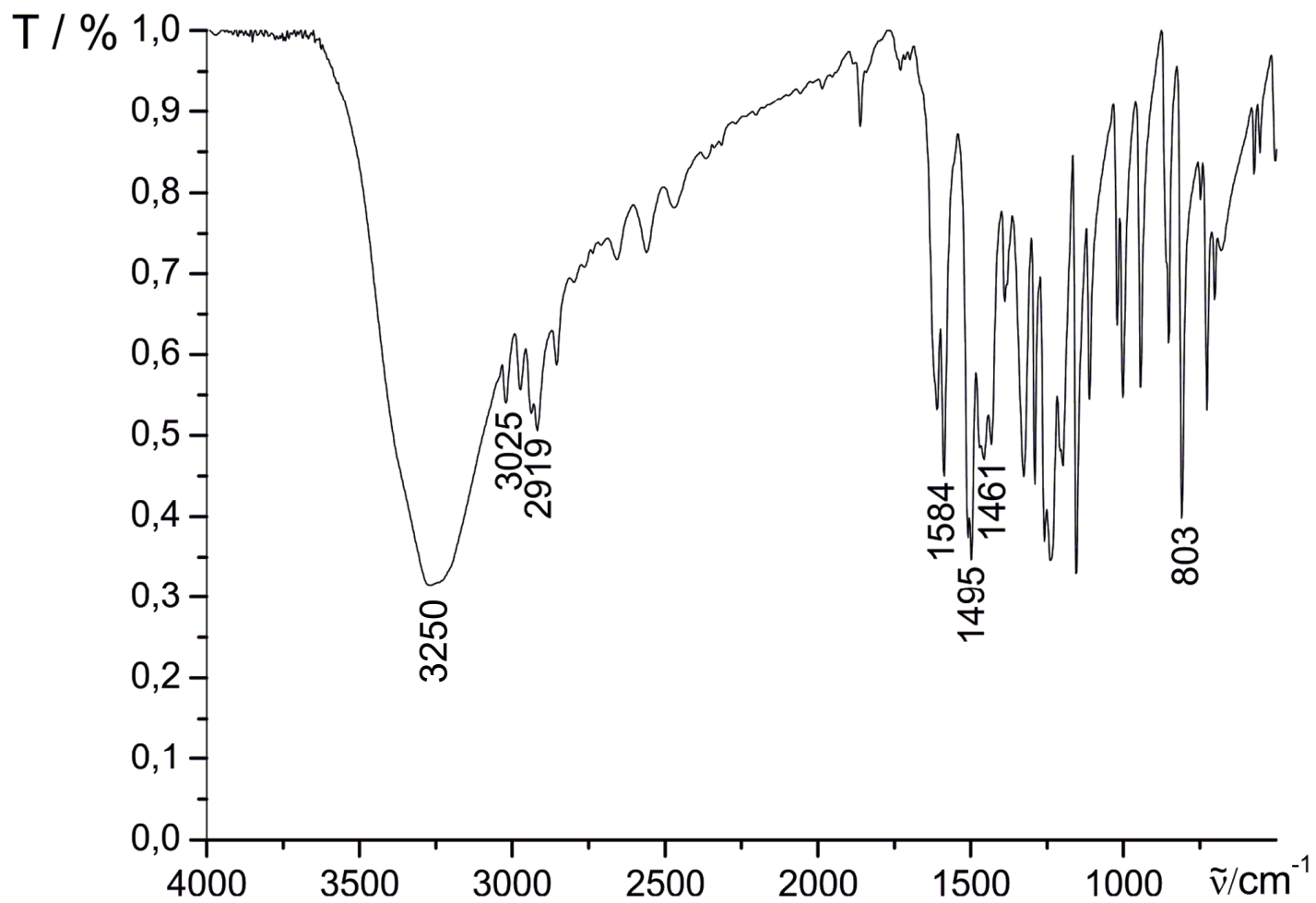
10. Razmotrimo spinski sustav A_2MX_2 , gdje je $I_A = I_M = I_X = 1/2$. Skicirajte signale spinova A, M i X u spektru NMR, ako je $J_{AM} > J_{AX} = J_{MX}$.



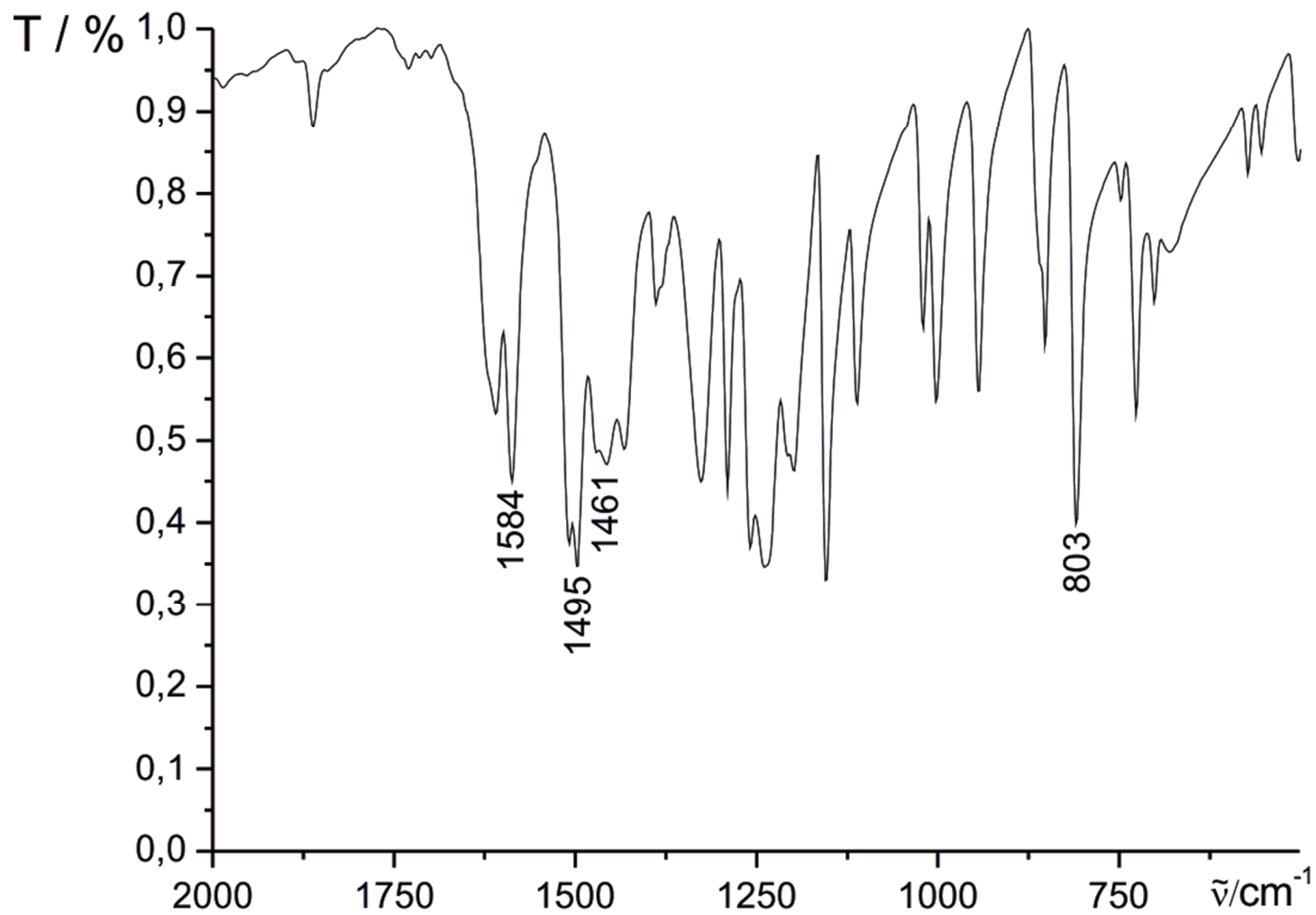
Primjer: Odredite strukturu analiziranog spoja na temelju njegovog spektra masa, infracrvenog, ^1H NMR, APT, HSQC i HMBC spektra



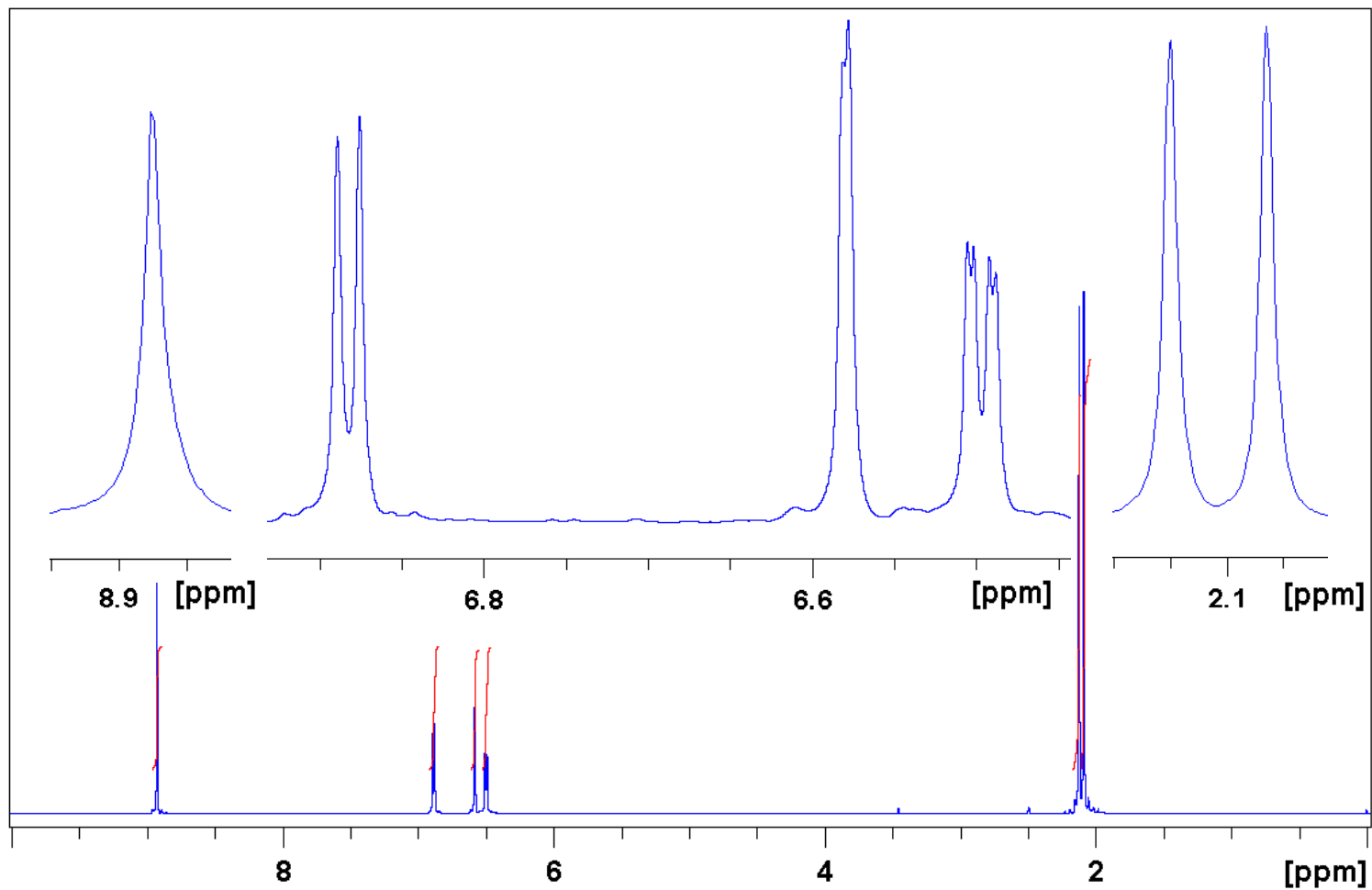
Spektar masa analiziranog spoja dobiven tehnikom MALDI-TOF. Uzorak je otopljen u smjesi acetona i vode (v/v=1:1). Signali označeni crvenim strelicama odgovaraju ionima Na^+ , K^+ i Cl^- koji su prisutni u matrici uzorka te njihovim aduktima.



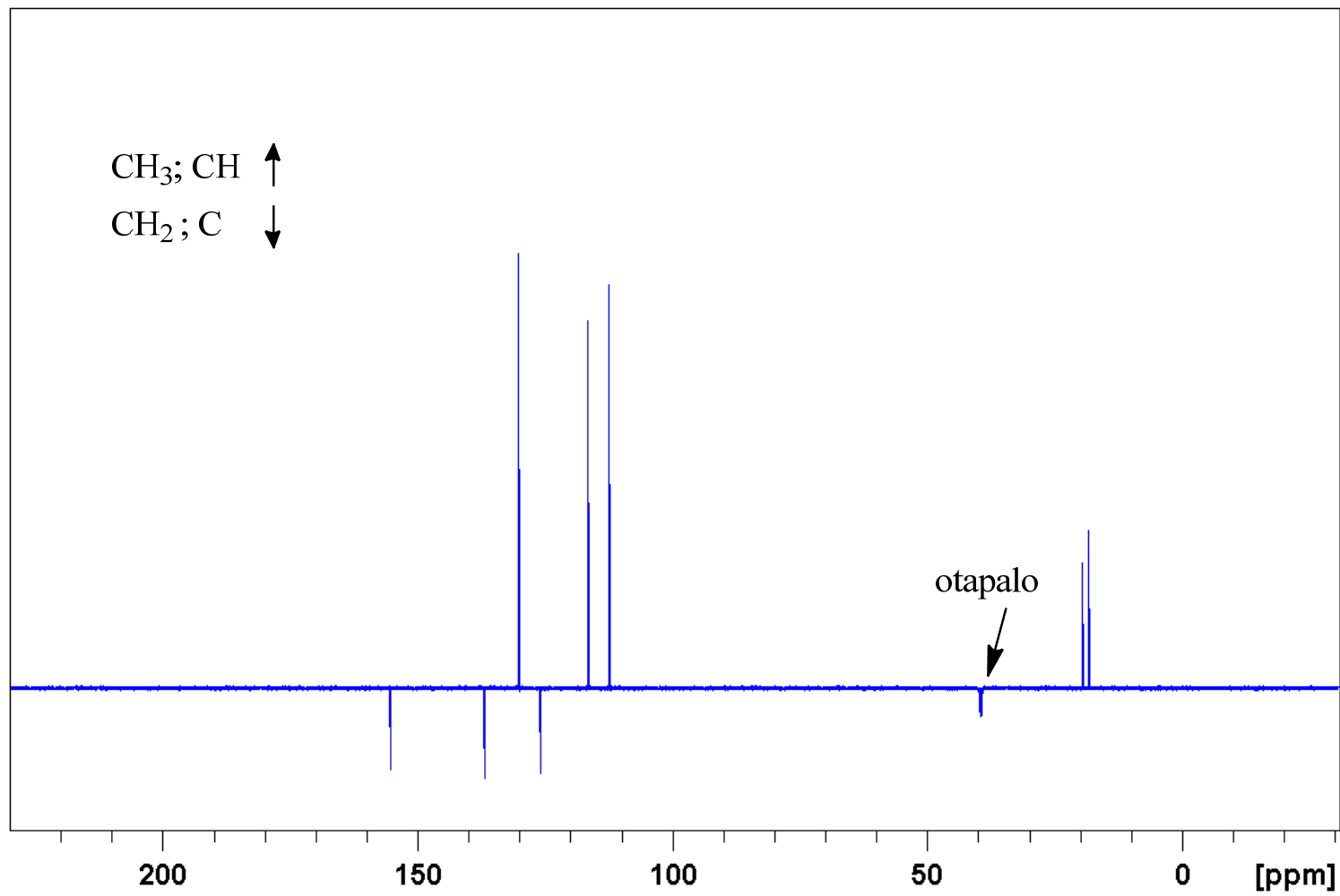
Infracrveni spektar analiziranog spoja snimljen tehnikom KBr pastile



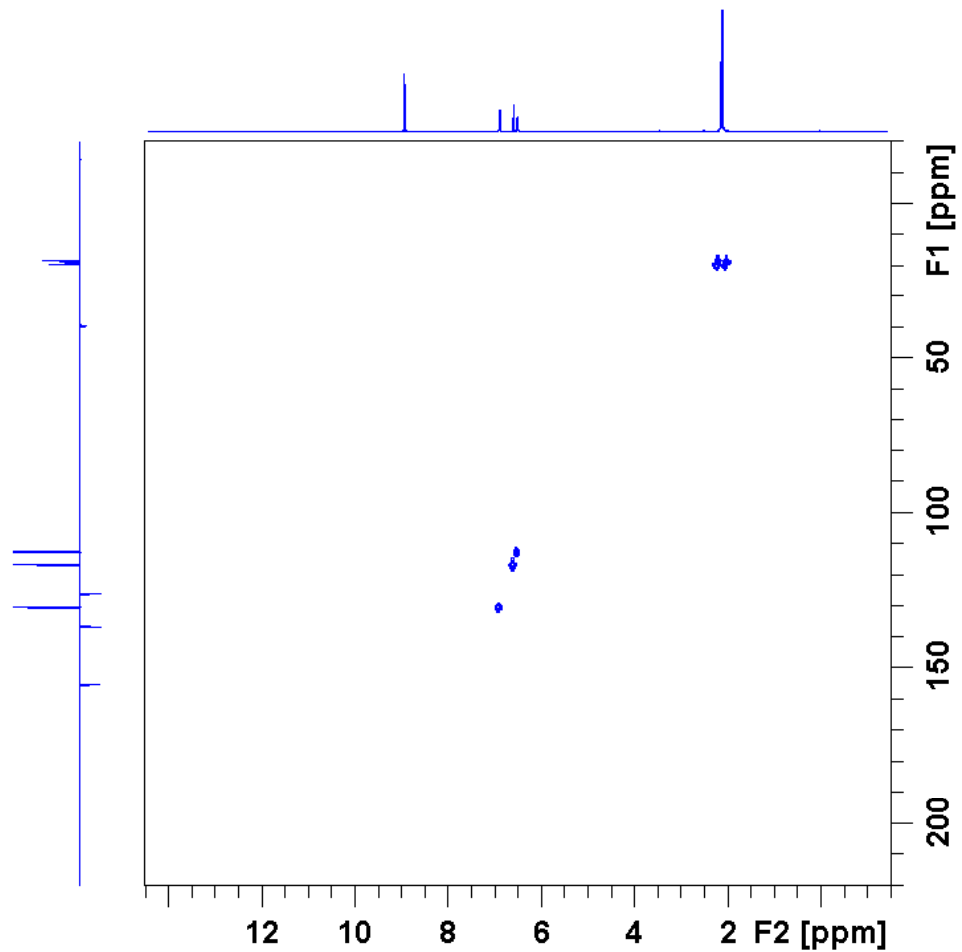
Uvećani prikaz infracrvenog spektra analiziranog spoja snimljen tehnikom KBr pastile u području od 2000 cm⁻¹ do 400 cm⁻¹



^1H NMR spektar analiziranog spoja snimljen u DMSO-d_6 uz uvećani prikaz područja koja odgovaraju pojedinim signalima

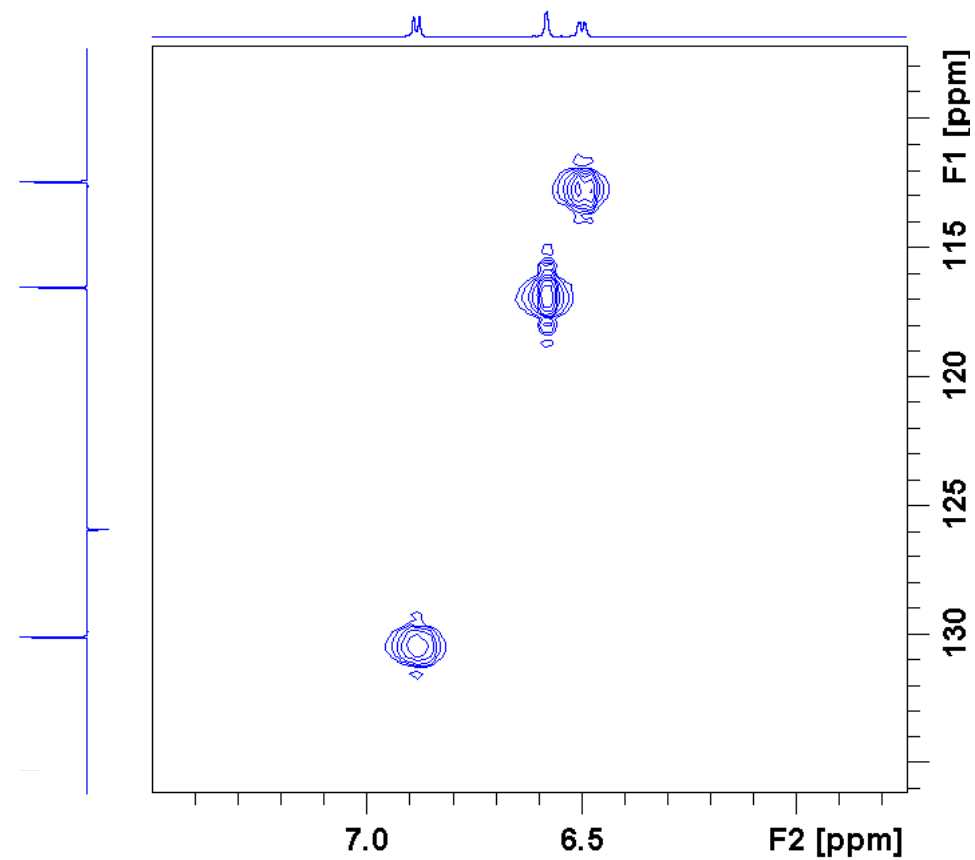


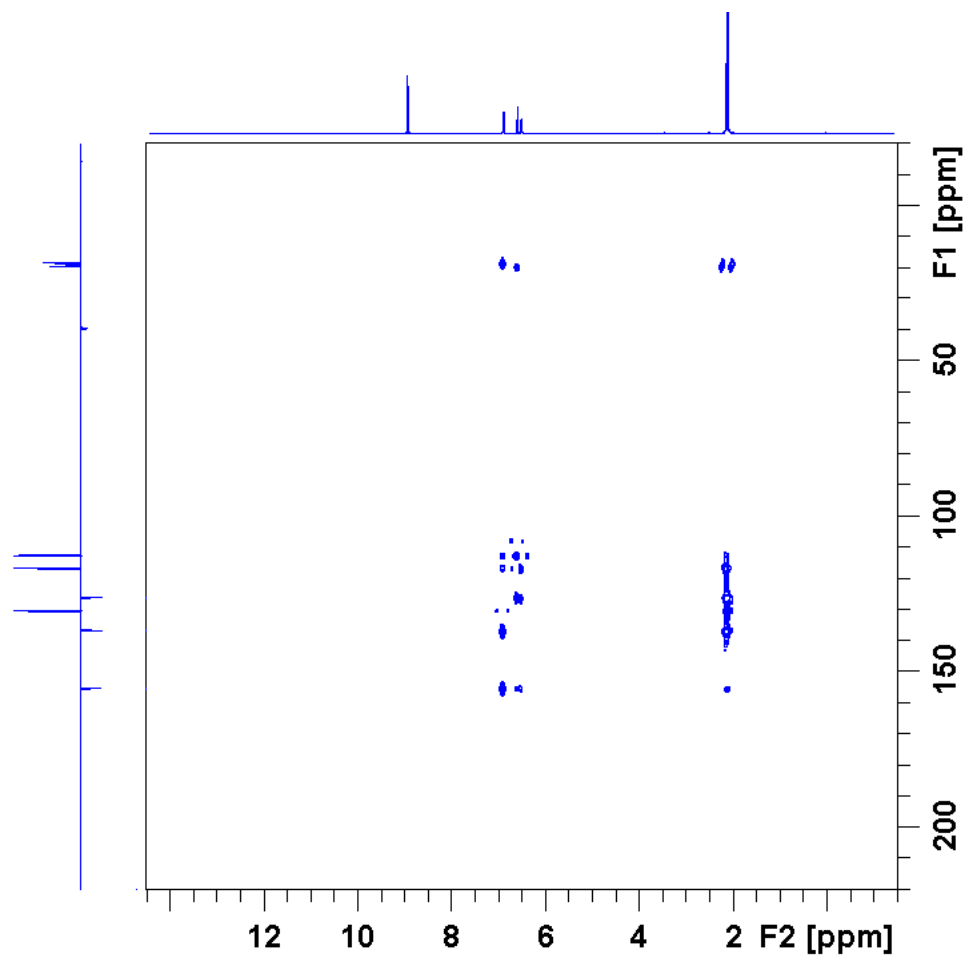
APT spektar analiziranog spoja snimljen u DMSO-d₆ uz uvećani prikaz područja koja odgovaraju pojedinim signalima



HSQC spektar analiziranog spoja
snimljen u DMSO-d₆

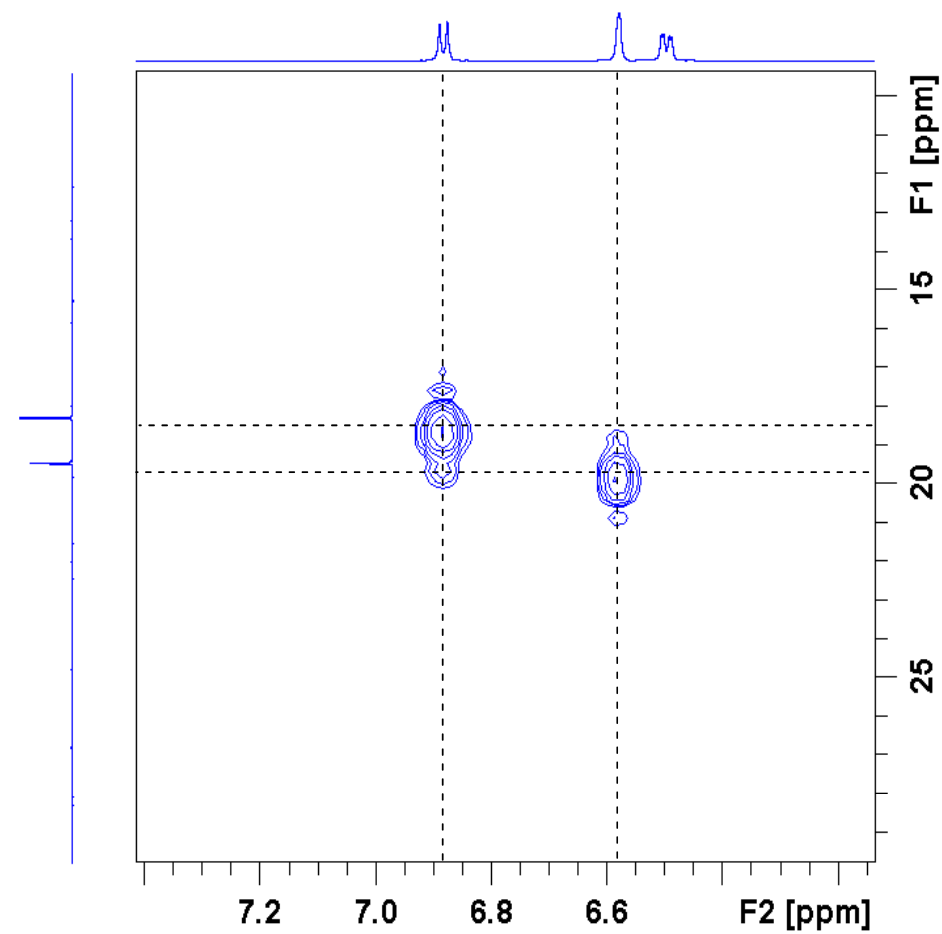
Uvećani prikaz HSQC korelacija između
aromatskih protona i ugljikovih atoma

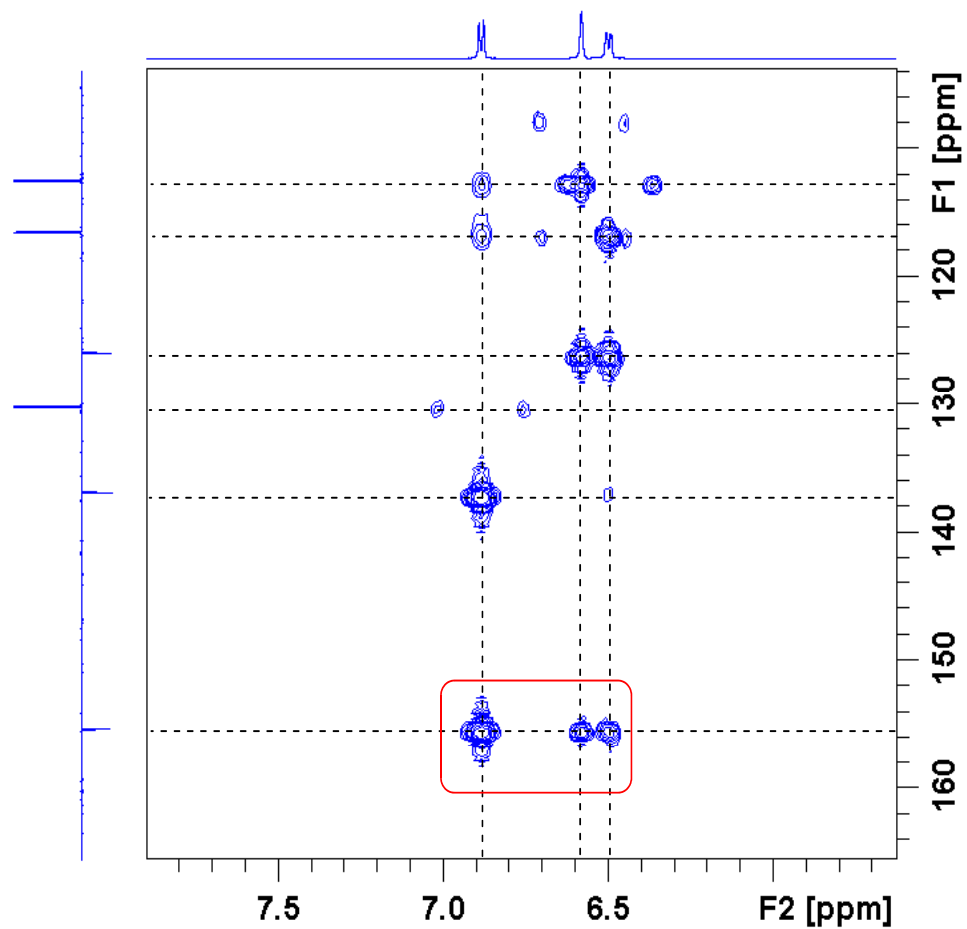




HMBC spektar analiziranog spoja
snimljen u DMSO-d₆

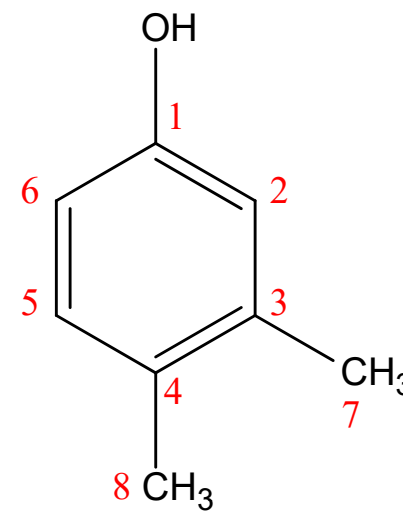
Uvećani prikaz HMBC korelacija metilnih
ugljikovih atoma s aromatskim protonima





Uvećani prikaz HMBC korelacija između aromatskih protona i ugljikovih atoma

Struktura analiziranog spoja i brojanje atoma



Asignacija karakterističnih fragmenata u spektru masa analiziranog spoja

Signal	m/z
bazni signal	34,849
Na ⁺	22,863
Cl ⁺	34,849
NaC ₂ H ₅ ⁺	51,699
C ₃ H ₄ O ⁺	55,981
C ₇ H ₈ O ⁺	108,042
M ⁺	122,056

Karakteristične vibracijske vrpce u infracrvenom spektru analiziranog spoja

ν / cm^{-1}	Način vibracije
3550 – 2750	ν (O–H)
3025	$\nu_{\text{aromatsko}}$ (C–H)
2919	$\nu_{\text{alifatsko}}$ (C–H)
1584; 1495; 1461	$\nu_{\text{aromatsko}}$ (C=C)
803	γ (=CH) _{izvan ravnine}
3550 – 2750	ν (O–H)
3025	$\nu_{\text{aromatsko}}$ (C–H)

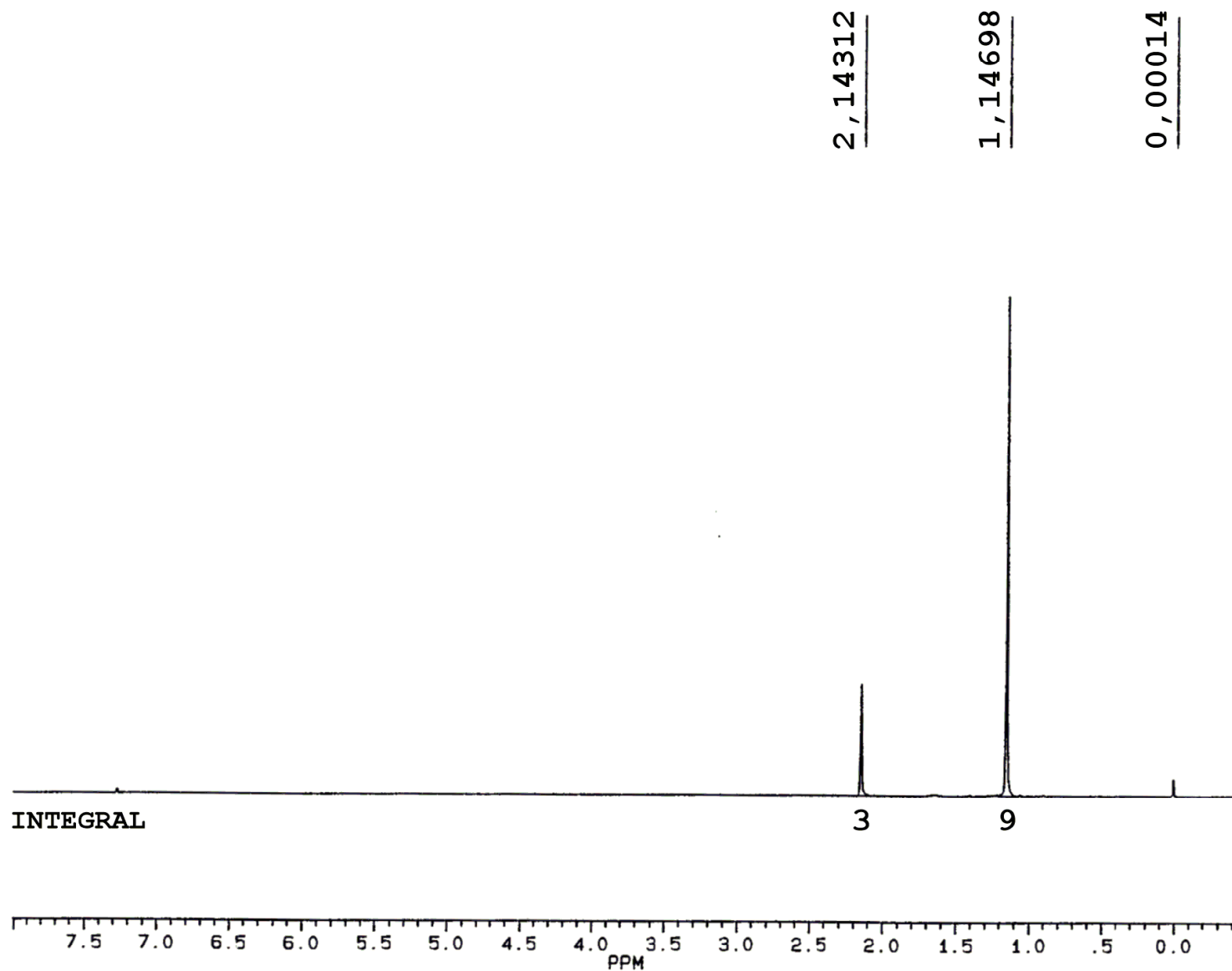
Asignacija ^1H NMR kemijskih pomaka analiziranog spoja

δ / ppm	Integral	Multipletnost	H-atom
6,58	1	s	2
6,88	1	d	5
6,50	1	dd	6
2,12	3	s	7
2,08	3	s	8
8,85	1	s	OH

Asignacija ^{13}C NMR kemijskih pomaka analiziranog spoja

δ / ppm	C-atom
155	1
117	2
137	3
125	4
130	5
112	6
20	7
19	8

11. Odredite strukturu spoja čiji je ^1H NMR spektar prikazan na slici. Molekulska formula navedenog spoja je $\text{C}_6\text{H}_{12}\text{O}$.



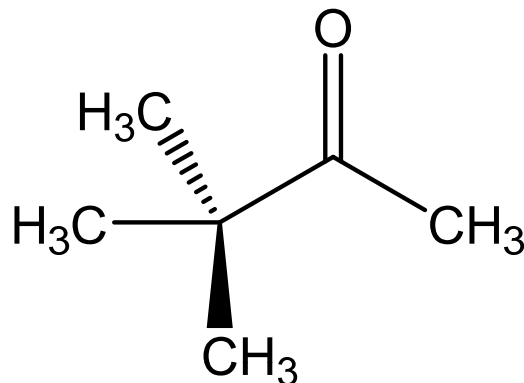
^1H NMR spektar analiziranog spoja snimljen u CDCl_3

- indeks manjka vodika, engl. *index of hydrogen deficiency* (IHD):

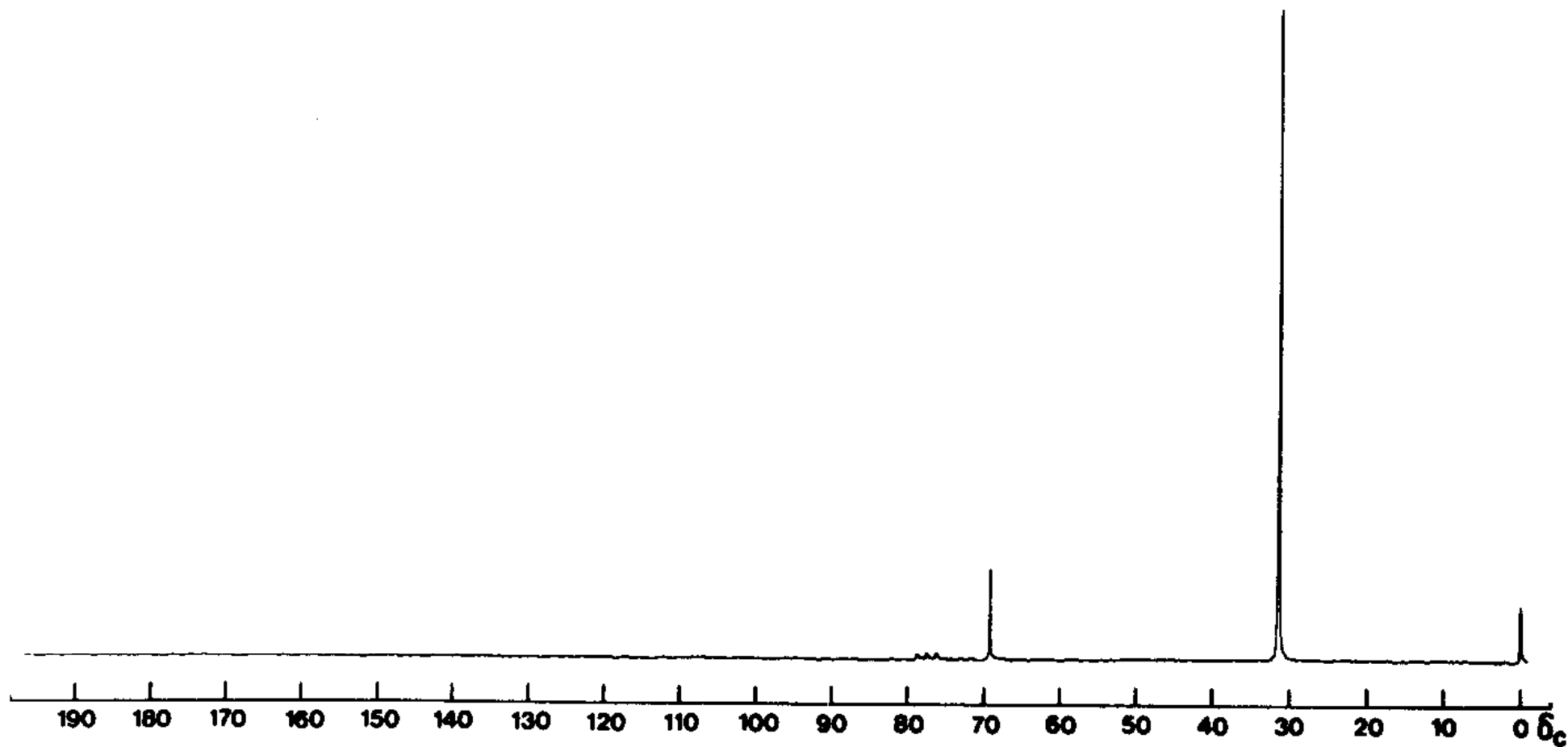
$$\text{IHD} = \frac{1}{2}[2C + 2 + N - (H + X)]$$

- za ovaj spoj: $\text{IHD} = [2 \cdot 6 + 2 - 12] / 2 = 1$
- jedan prsten ili dvostruka veza
- 12 H atoma
- 9 ekvivalentnih H atoma pri 1,15 ppm i 3 ekvivalentna H atoma pri 2,14 ppm
- *tert*-butilna skupina, $(\text{CH}_3)_3\text{C}-$, pri 1,15 ppm
- metilna skupina, CH_3- , vezana za karbonilnu, $\text{C}=\text{O}$, pri 2,14 ppm

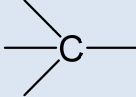
rješenje:



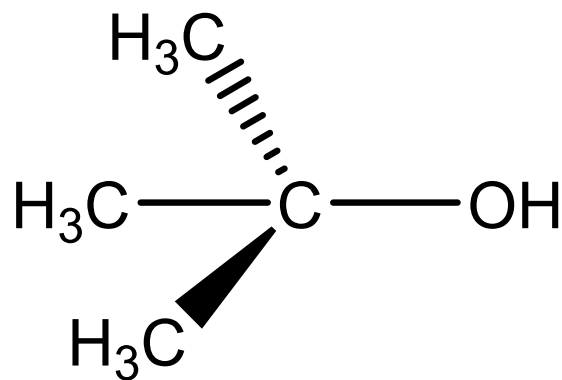
12. Odredite strukturu spoja čiji je ^{13}C NMR spektar prikazan na slici. Molekulska formula navedenog spoja je $\text{C}_4\text{H}_{10}\text{O}$.



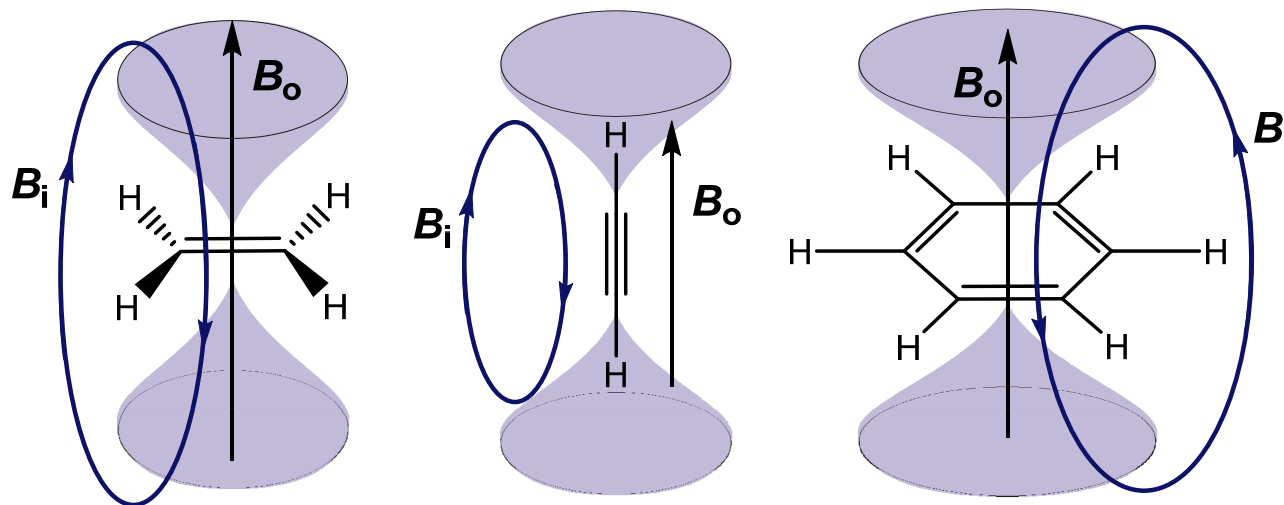
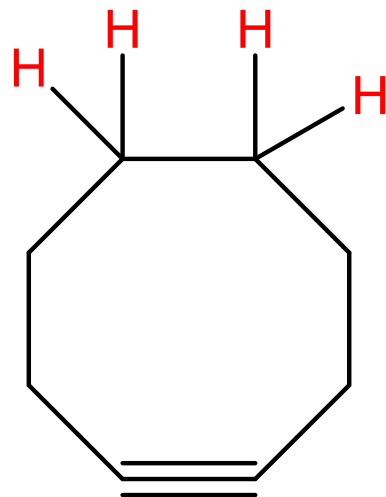
$$\text{IHD} = [2 \cdot 4 + 2 - 10] / 2 = 0$$

$\delta(^{13}\text{C})/\text{ppm}$	C-atom
30,1	-CH ₃
60,9	

rješenje:

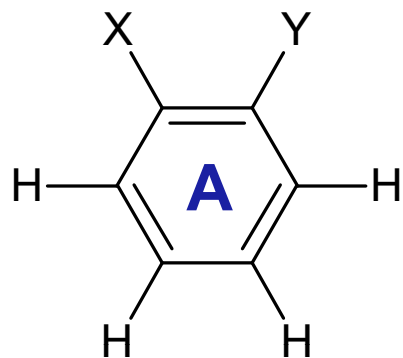


13. Kako će na protone u ciklooktinskom prstenu označene **crveno** utjecati inducirano magnetno polje trostruke veze?

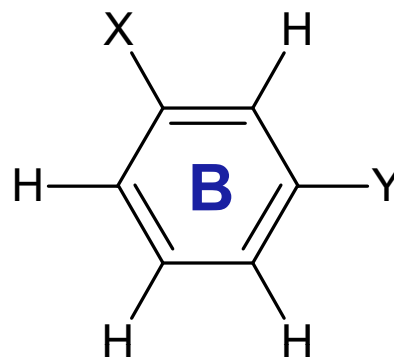


Djelovat će odsjenjujuće, tj. signali protona bit će pri višim frekvencijama, odnosno imat će viši kemijski pomak.

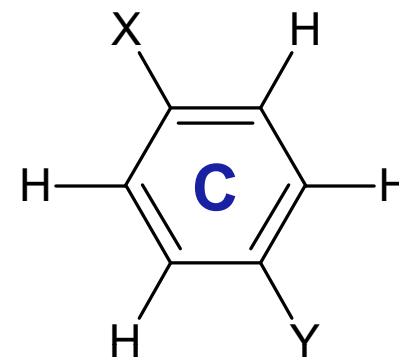
14. Koliko signala u ^1H i ^{13}C NMR spektrima očekujete za svaku navedenu strukturu ako je: a) $X = Y \neq \text{H}$; b) $X \neq Y \neq \text{H}$?



orto



meta



para

a) ^1H
 ^{13}C

2
3

3
4

1
2

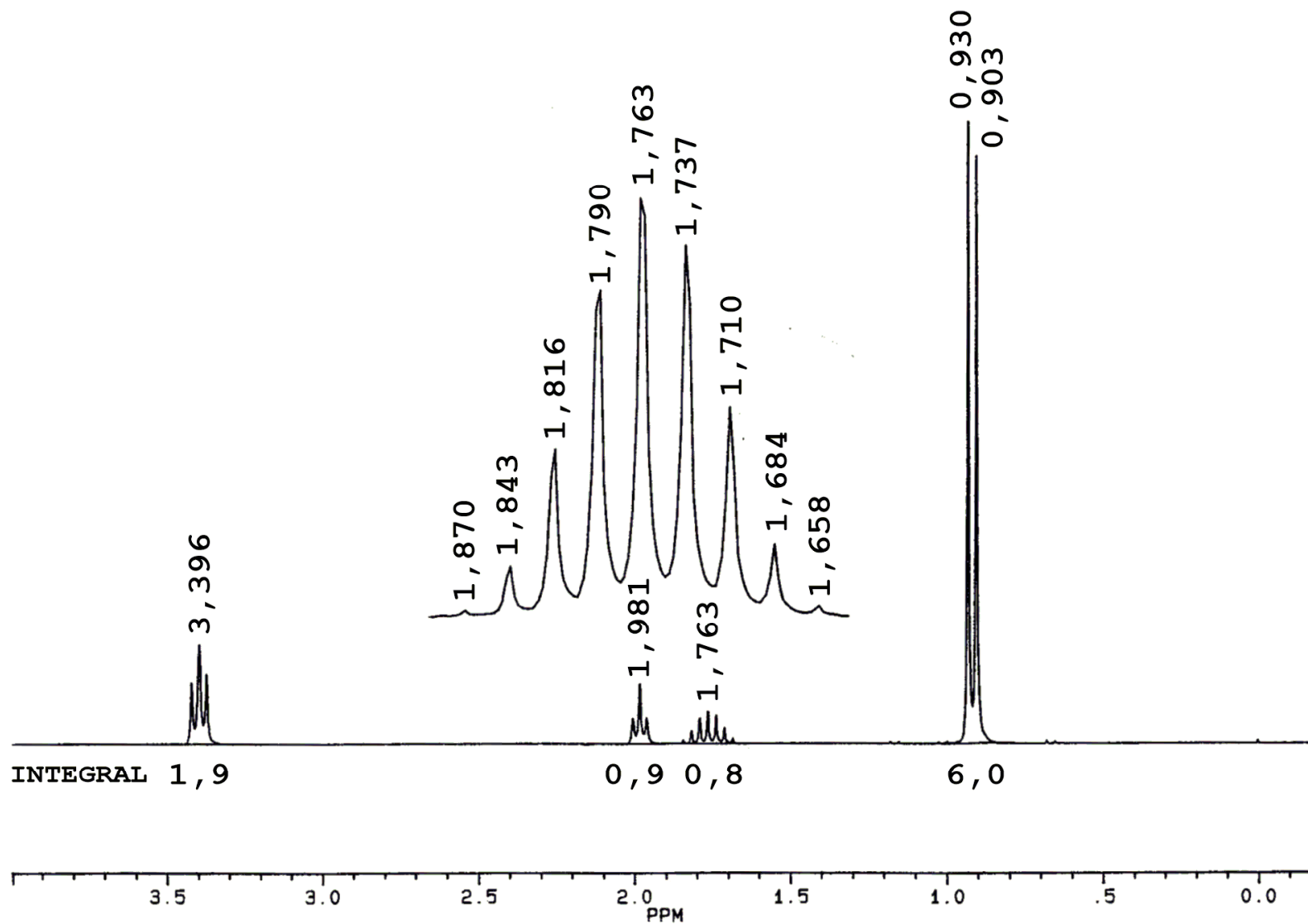
b) ^1H
 ^{13}C

4
6

4
6

2
4

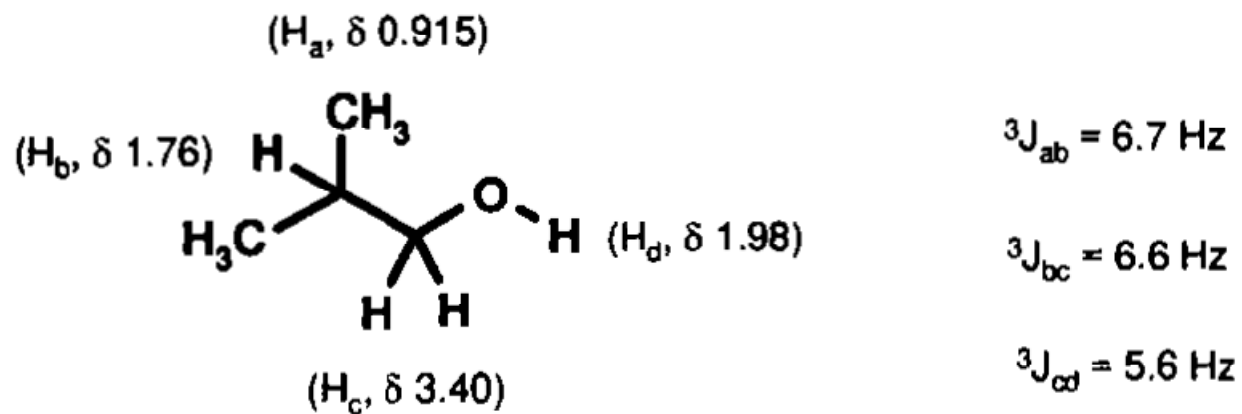
15. Prikazani spektar pripada organskom spoju molarne mase 74 g/mol, koji sadrži ugljik, vodik i kisik. Identificirajte spoj.



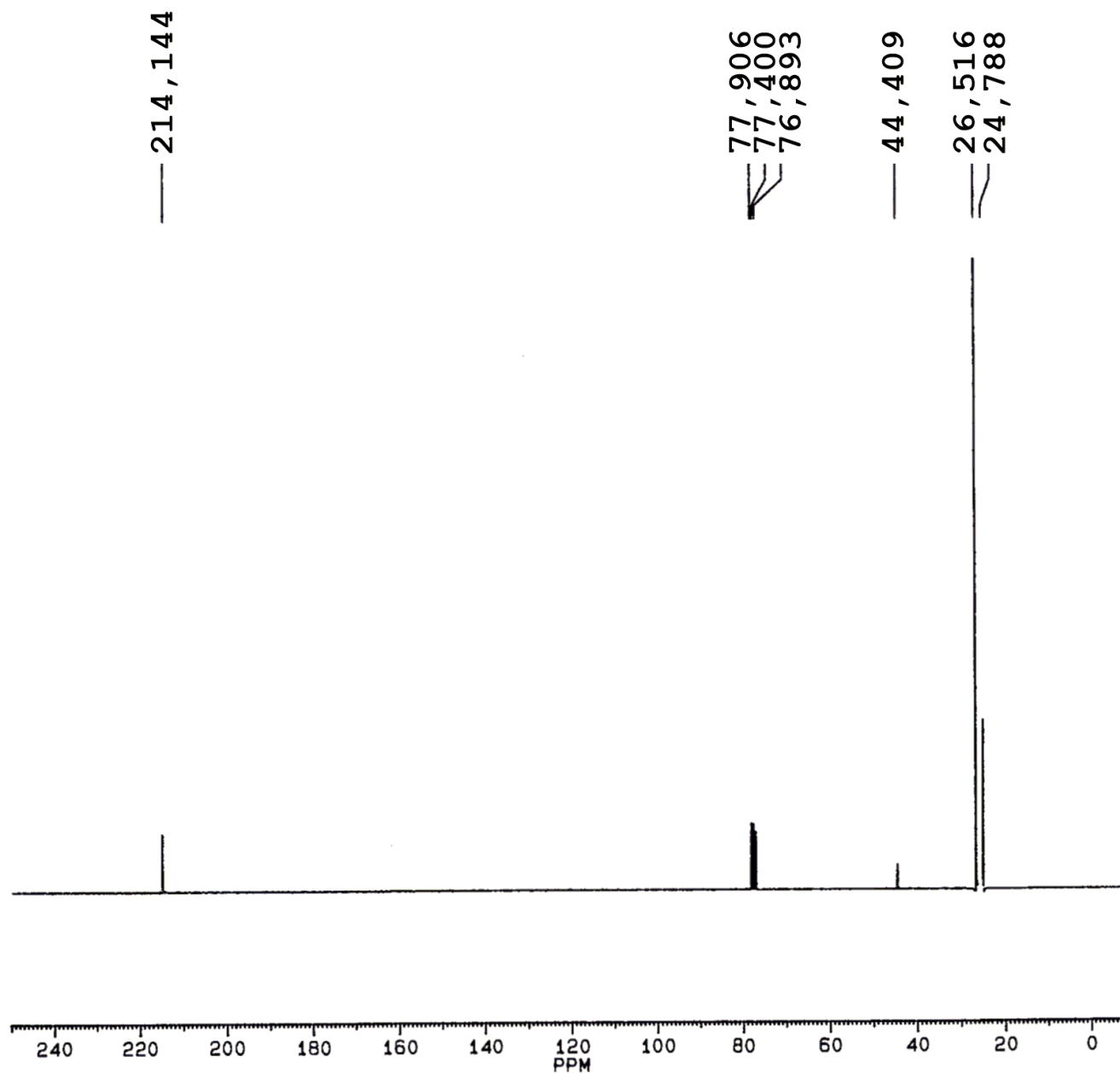
^1H NMR spektar analiziranog spoja snimljen u CDCl_3 uz uvećani prikaz signala pri 1,763 ppm

$\delta(^1\text{H})/\text{ppm}$	Integral	Multipletnost	H-atom
0,91	6,0	d	$-\text{CH}_3$
1,75	0,8	m (nonet)	$\begin{array}{c} \diagup \\ \text{---} \text{CH} \\ \diagdown \end{array}$
1,98	0,9	t	$-\text{OH}$
3,40	1,9	t	$-\text{CH}_2-$

rješenje:



16. Identificirajte spoj molekulske formule $C_6H_{12}O$ čiji je ^{13}C NMR spektar prikazan na slici. Otkuda potječu signali pri 76,9; 77,4 i 77,9 ppm?

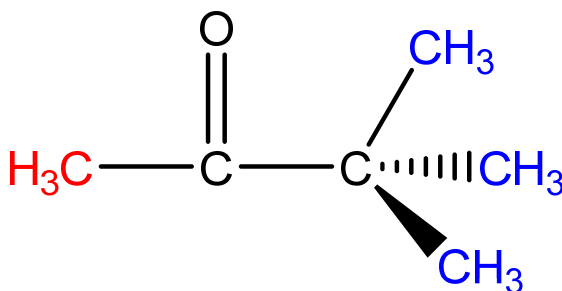


^{13}C NMR spektar
analiziranog spoja

$$\text{IHD} = [2 \cdot 6 + 2 - 12] / 2 = 1$$

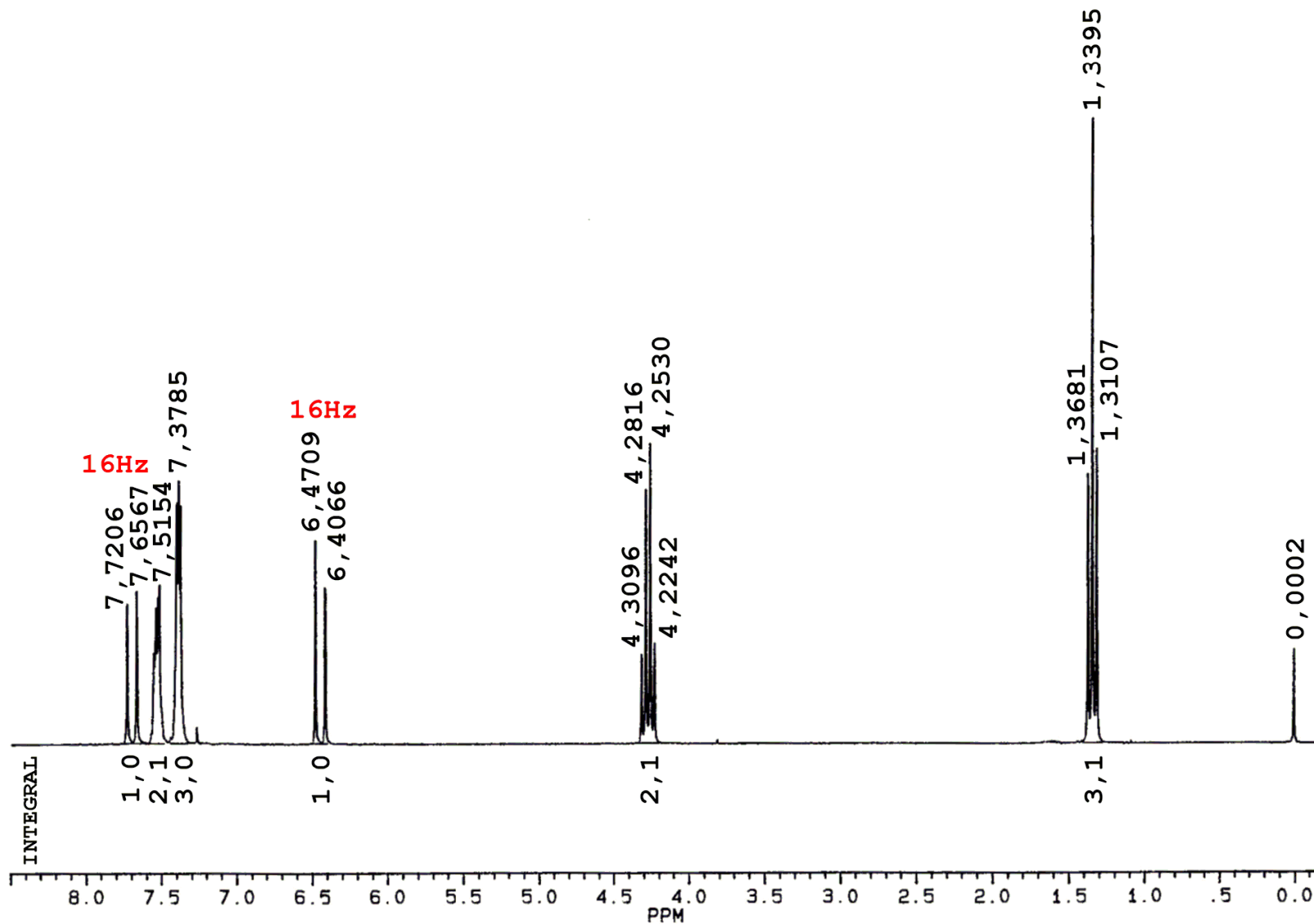
$\delta(^{13}\text{C})/\text{ppm}$	C-atom
24,7	-CH ₃
26,5	-CH ₃
44,4	
214,1	

rješenje:



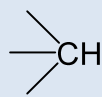
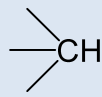
- signali pri 76,9 ppm, 77,4 ppm i 77,9 ppm potječu od rezonancije deuteriranog kloroforma

17. Prikazani ^1H NMR spektar pripada spoju molekulske formule $\text{C}_{11}\text{H}_{12}\text{O}_2$. ^{13}C NMR spektar sadrži signal pri 170 ppm. Identificirajte spoj.

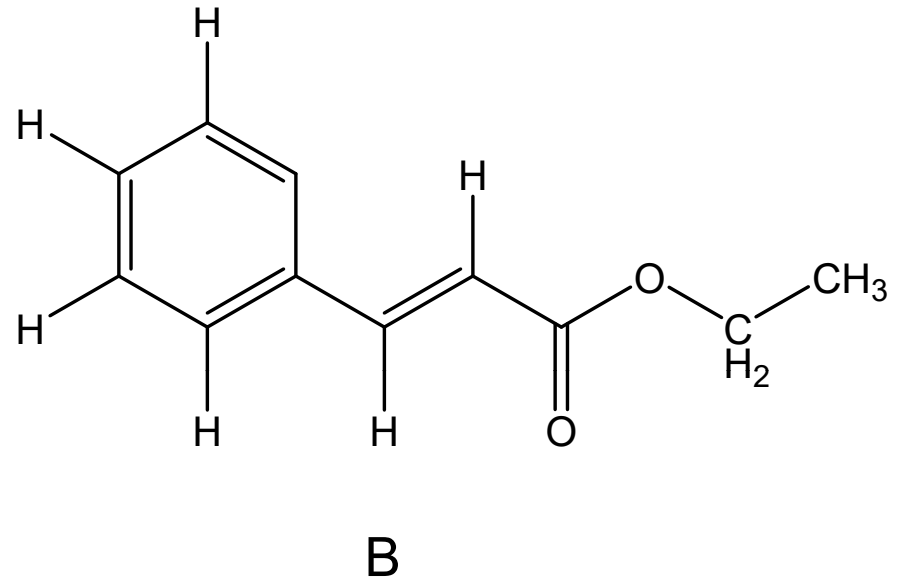
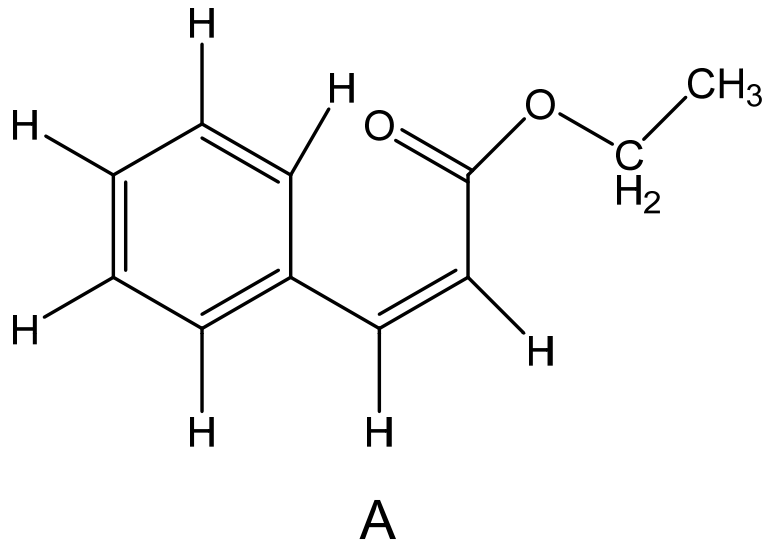


^1H NMR spektar analiziranog spoja snimljen u CDCl_3

$$\text{IHD} = [2 \cdot 11 + 2 - 12] / 2 = 6$$

$\delta(^1\text{H})/\text{ppm}$	Integral	Multipletnost	H-atom
1,34	3,1	t	$-\text{CH}_3$
4,27	2,1	q	$-\text{CH}_2-$
6,44	1,0	d	$=\text{CH}-$
7,37	3,0	m	aromatski 
7,51	2,0	m	aromatski 
7,68	1,0	d	$=\text{CH}-$

- moguće strukture:



$J=16$ Hz

cis-sprega: 10–12 Hz

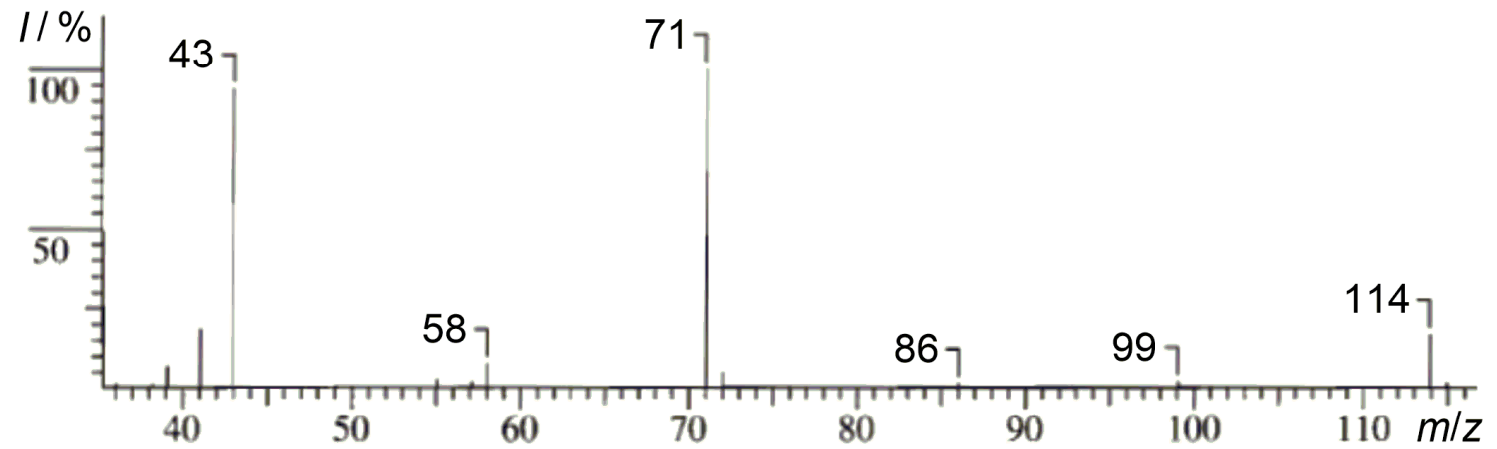
trans-sprega: 16–18 Hz

rješenje:

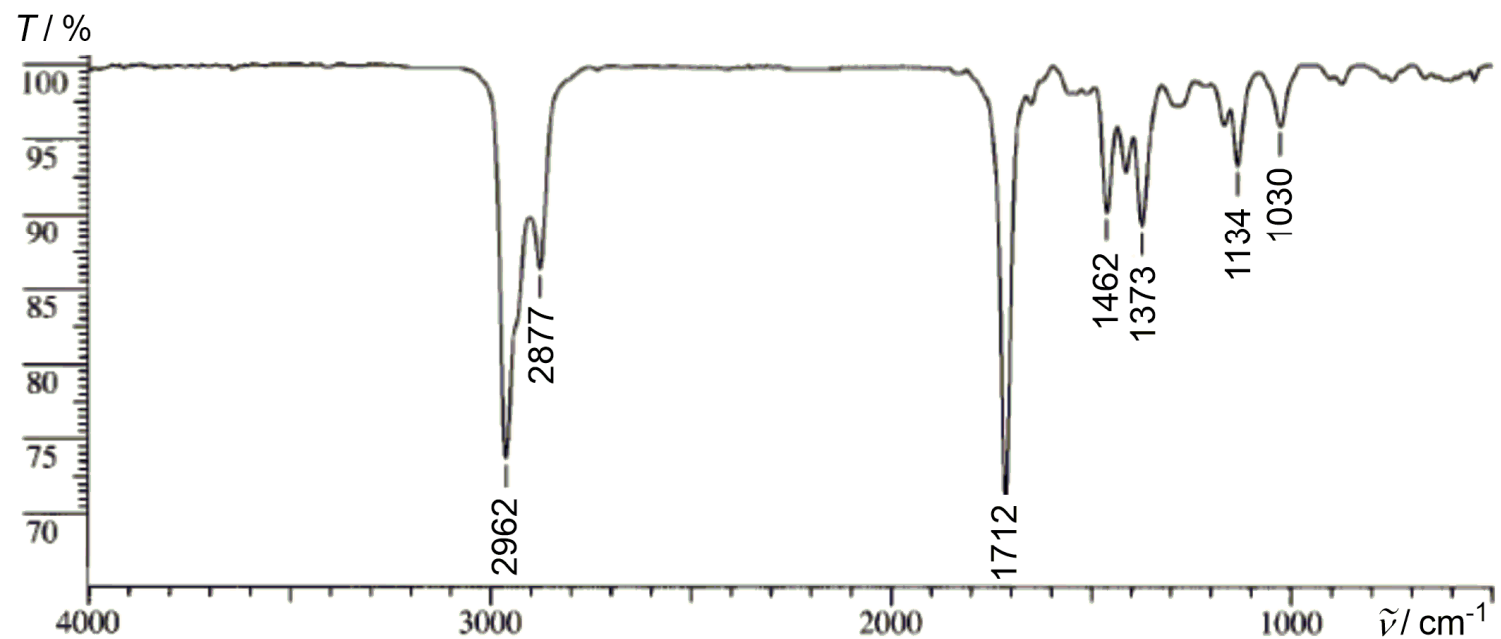
izomer B (*trans*-izomer)

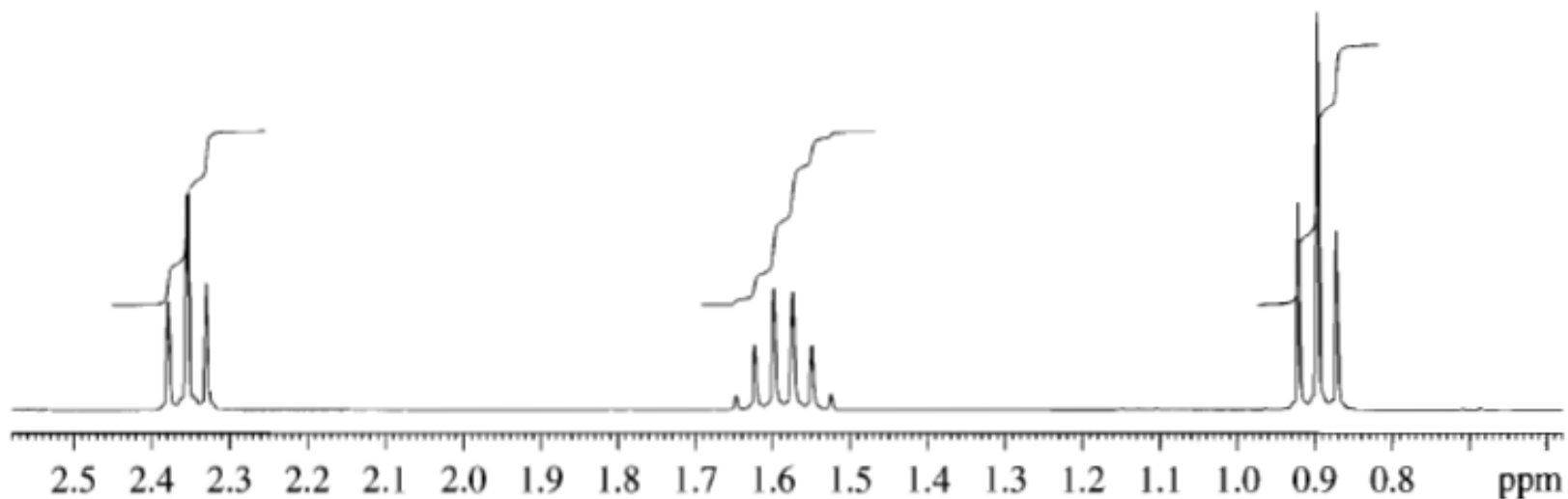
18. Identificirajte spoj na temelju njegovih MS, IR i ^1H NMR spektara

MS spektar



IR spektar





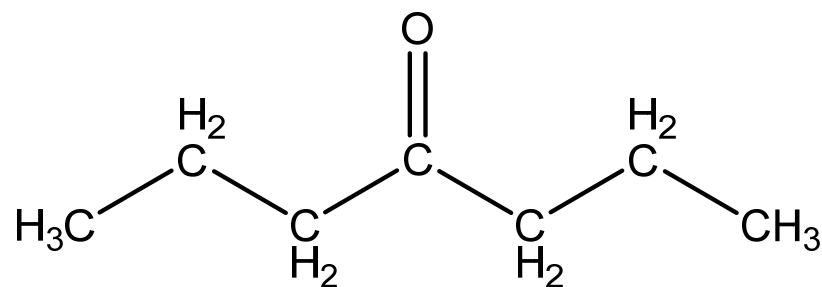
^1H NMR spektar

- informacije iz MS:
 $M^+ = 114$
bazni pik: $m/z = 71$
- informacije iz IR:
 1712 cm^{-1} C=O
 2877 cm^{-1} C–H istežanje
 2962 cm^{-1} C–H istežanje

- informacije iz ^1H NMR:

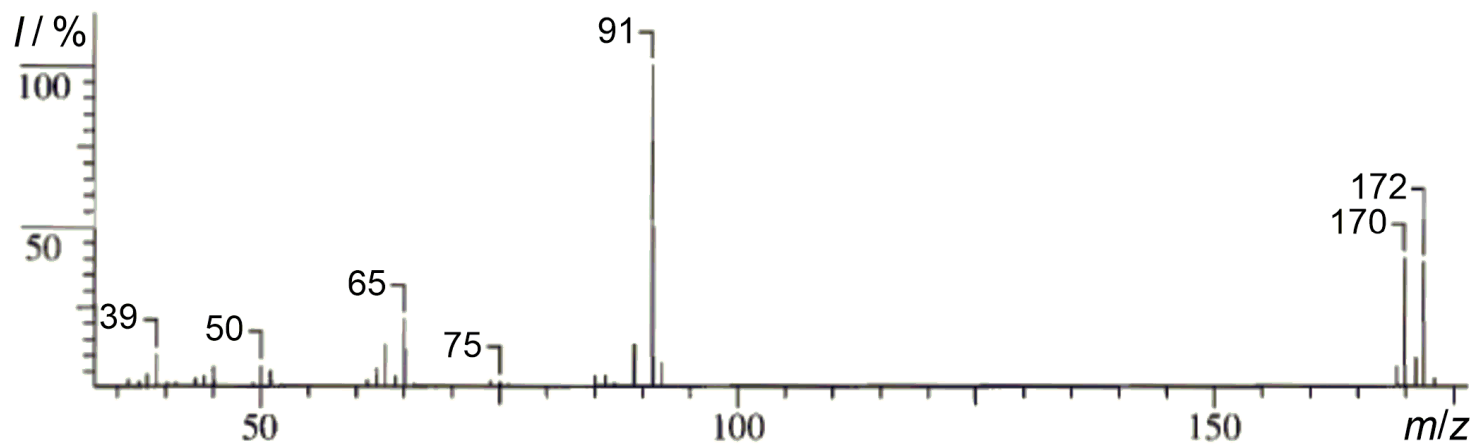
$\delta(^1\text{H})/\text{ppm}$	Integral	Multipletnost	H-atom
0,90	3	t	$-\text{CH}_3$
1,57	2	m	$-\text{CH}_2-$
2,35	2	t	$-\text{CH}_2-$

- rješenje:

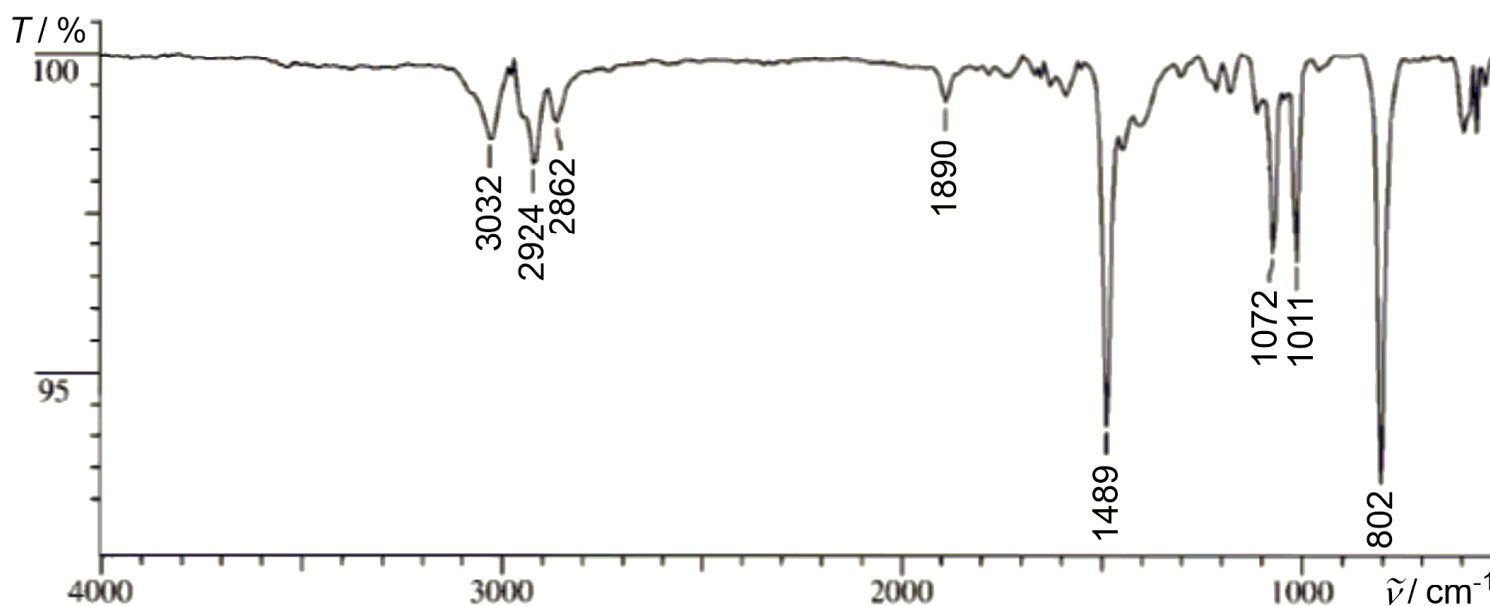


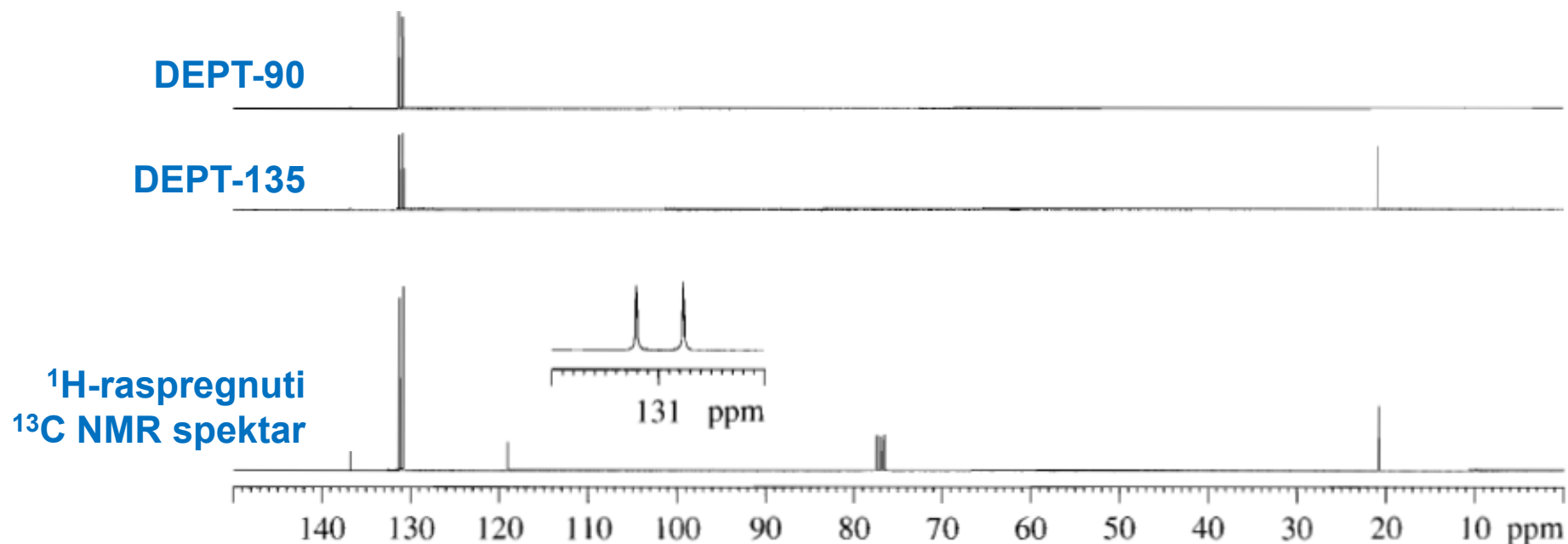
19. Identificirajte spoj na temelju njegovih MS, IR i ^{13}C NMR spektara

MS spektar



IR spektar





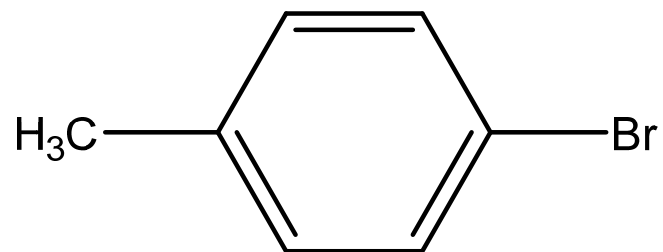
- informacije iz MS:
 $M^+ = 170$
 $(M+2)^+ = 172$
 bazni pik: $m/z = 91$
 sadrži 1 Br!

- informacije iz IR:
 3032 cm^{-1} C–H aromatsko istezanje
 2862 cm^{-1} C–H alifatsko istezanje
 2924 cm^{-1} C–H alifatsko istezanje
 $< 2862\text{ cm}^{-1}$ vrpce karakteristične za aromatski sustav

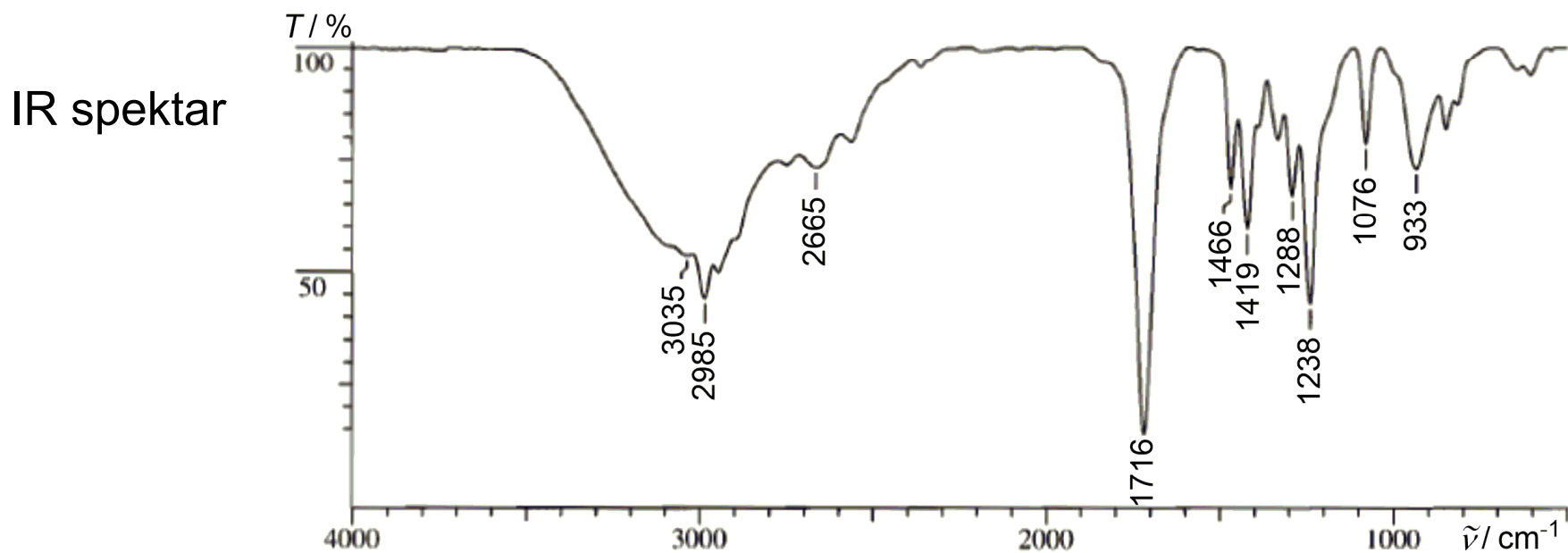
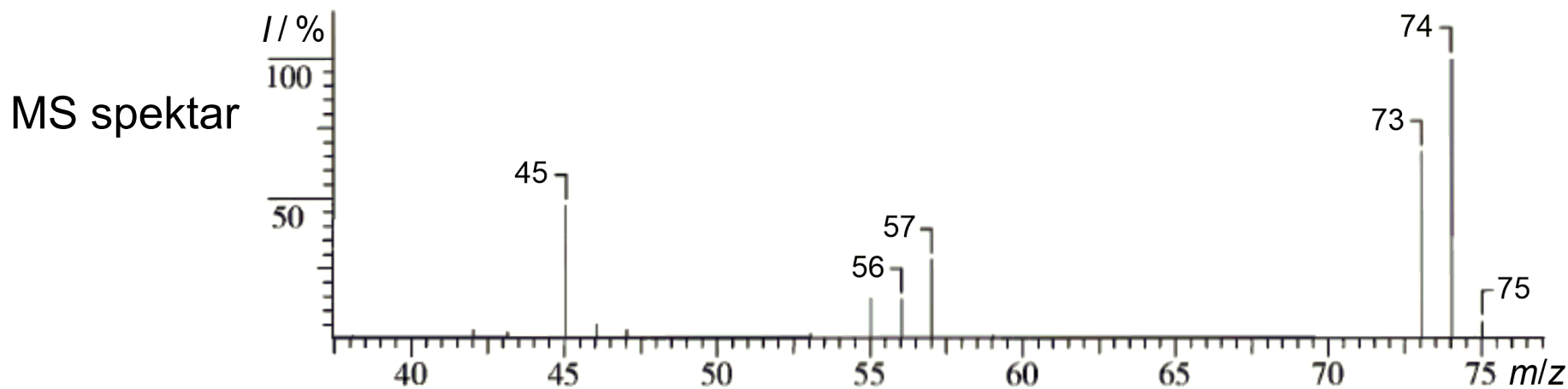
- informacije iz ^{13}C NMR:

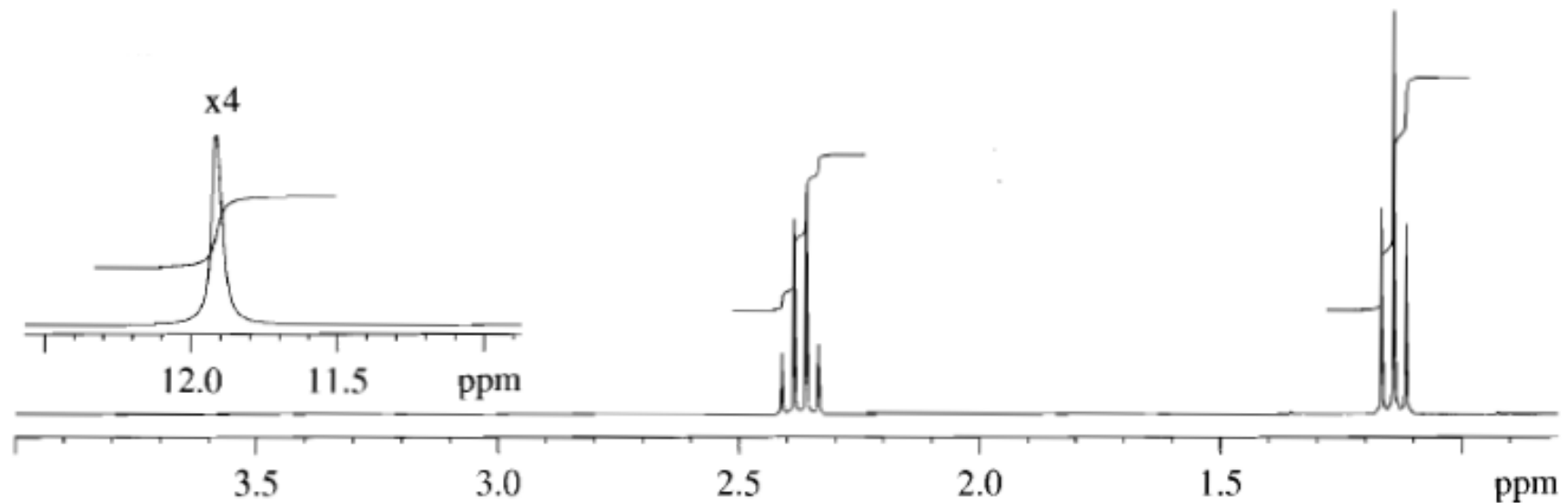
$\delta(^{13}\text{C})/\text{ppm}$	C-atom
21,0	$-\text{CH}_3$
118,0	aromatski 
130,8	aromatski 
131,2	aromatski 
137,0	aromatski 

- rješenje:



20. Identificirajte spoj na temelju njegovih MS, IR i ^1H NMR spektara





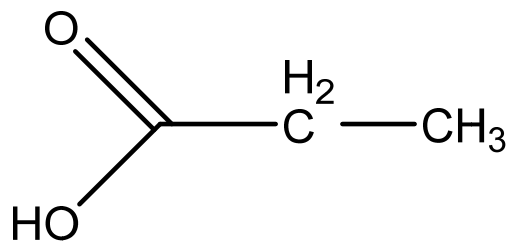
^1H NMR spektar

- informacije iz MS:
 - $M^+ = 74$
 - $(M+1)^+ = 75$
 - bazni pik: $m/z = 74$
- informacije iz IR:
 - $3500\text{--}2500\text{ cm}^{-1}$ O–H istežanje
 - 1716 cm^{-1} C=O istežanje
 - 2985 cm^{-1} C–H alifatsko istežanje

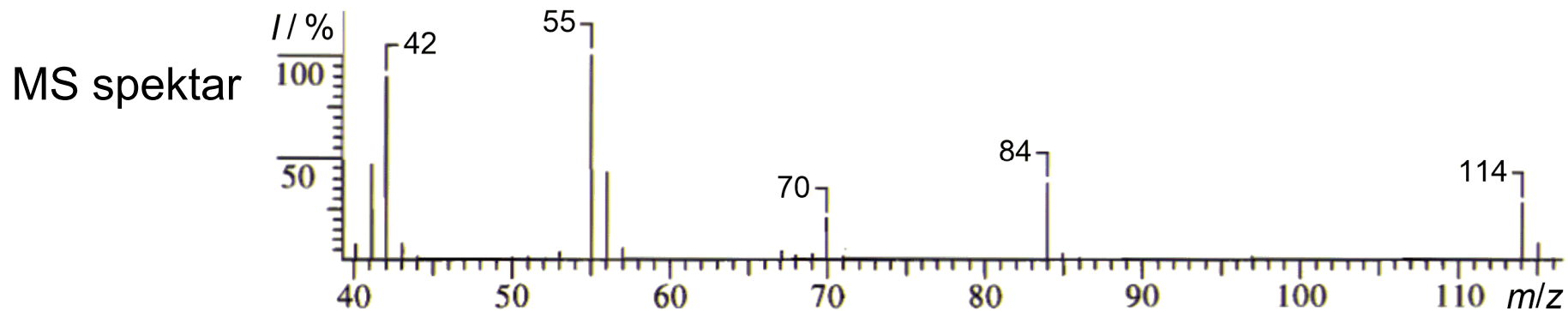
- informacije iz ^1H NMR:

$\delta(^1\text{H})/\text{ppm}$	Integral	Multipletnost	H-atom
1,15	3	t	$-\text{CH}_3$
2,35	2	q	$-\text{CH}_2-$
11,90	1	s	$-\text{OH}$

- rješenje:



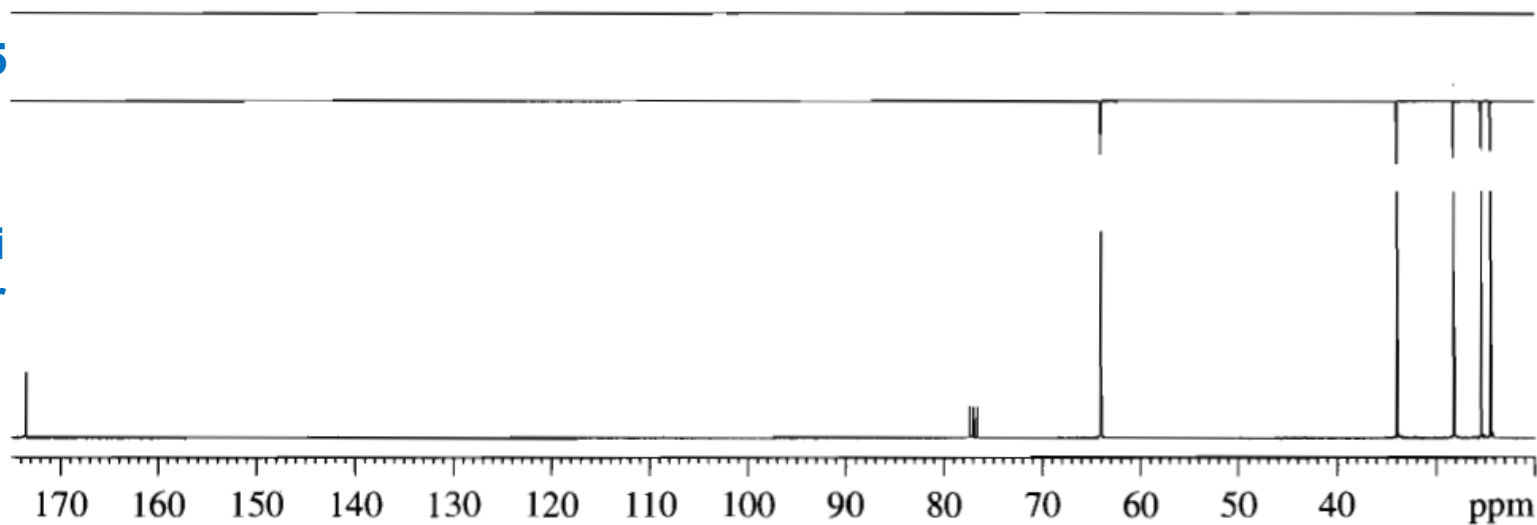
21. Odredite strukturu spoja na temelju njegovih MS, ^{13}C NMR, COSY i HETCOR spektara

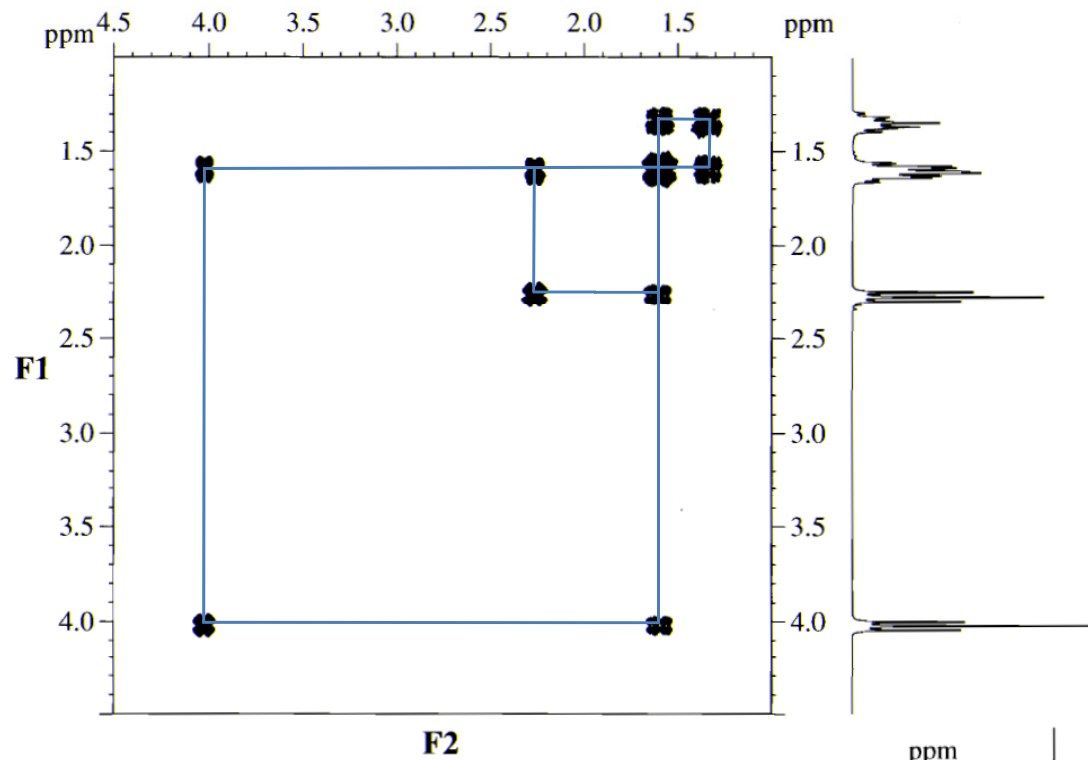


DEPT-90

DEPT-135

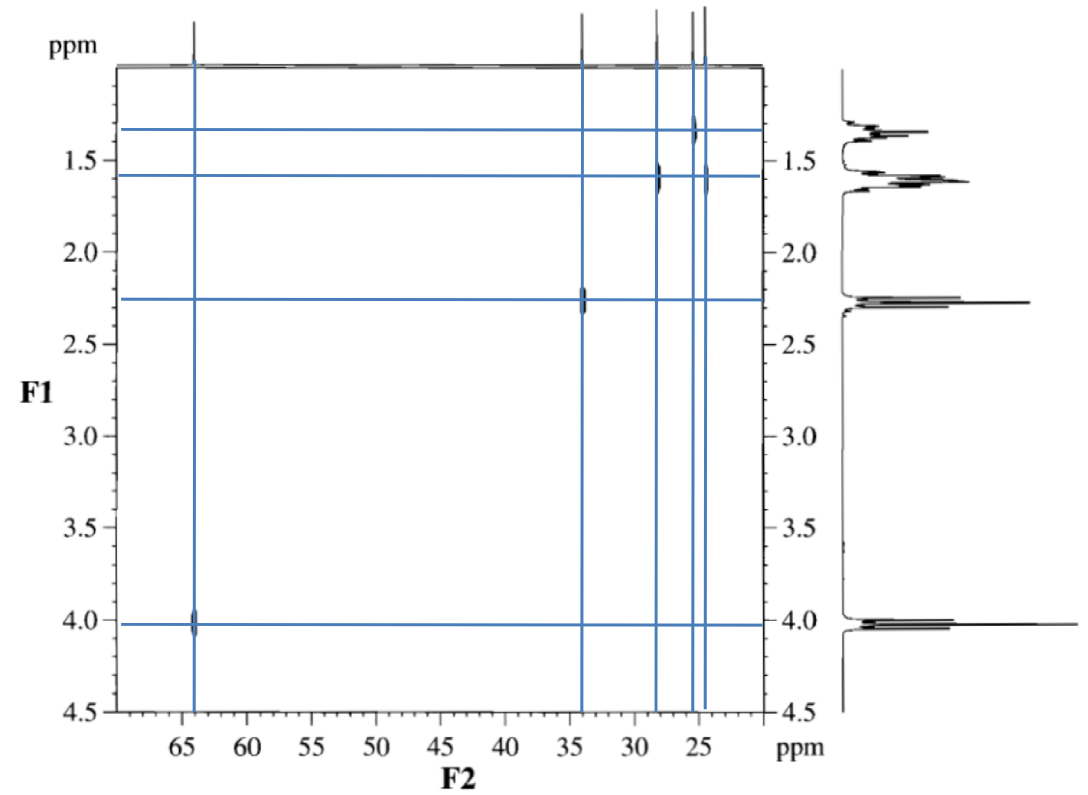
^1H -raspregnuti
 ^{13}C NMR spektar





COSY spektar

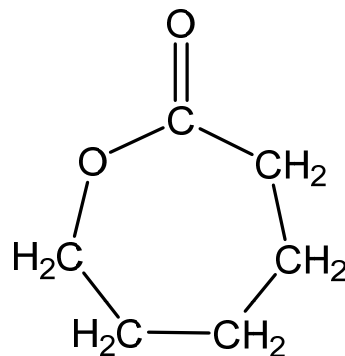
HETCOR spektar



- informacije iz MS:
 $M^+ = 114$
 bazni pik: $m/z = 55$
- informacije iz ^{13}C NMR:

$\delta(^{13}\text{C})/\text{ppm}$	C-atom
24	$-\text{CH}_2-$
26	$-\text{CH}_2-$
28	$-\text{CH}_2-$
34	$-\text{CH}_2-$
63	$-\text{CH}_2-$
173	$\text{C}=\text{O}$

- rješenje:

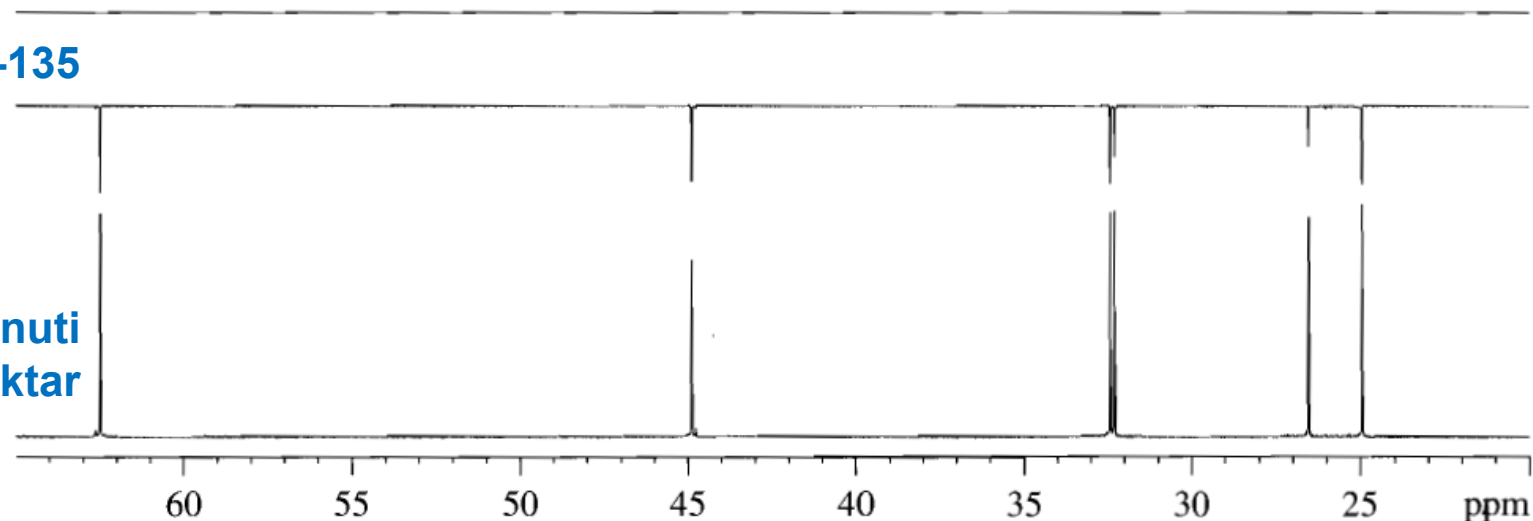


22. Odredite strukturu spoja molarne mase 136 g/mol, a koji sadrži 1 atom klora na temelju njegovih ^{13}C NMR, COSY i HMQC spektara

DEPT-90

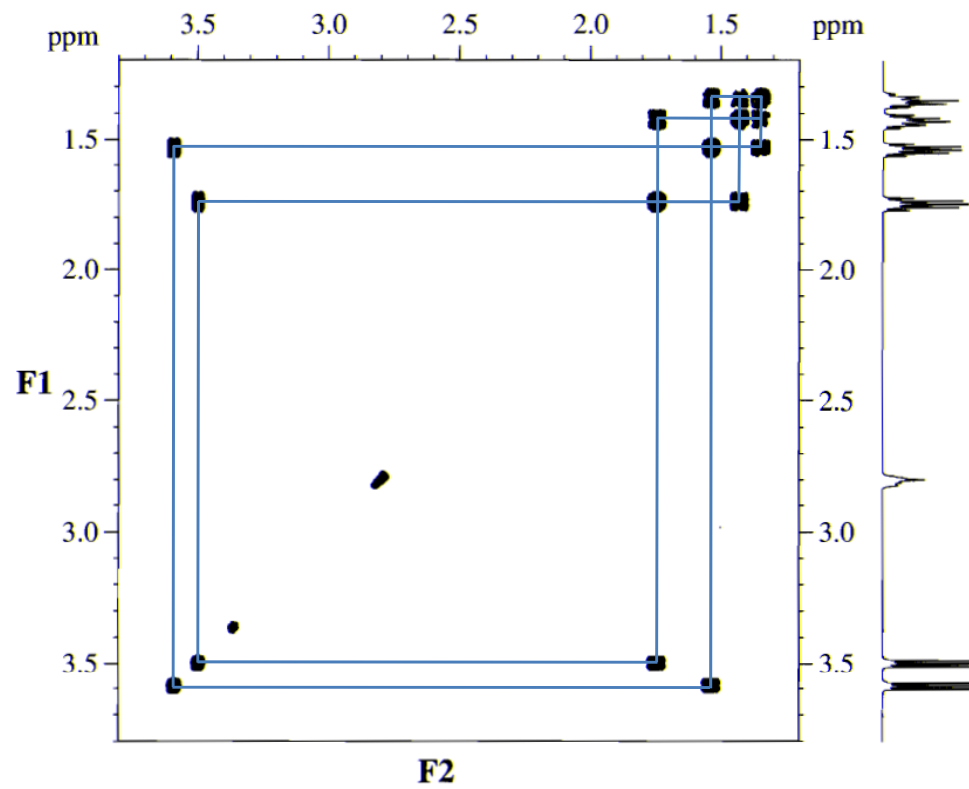
DEPT-135

^1H -raspregnuti
 ^{13}C NMR spektar

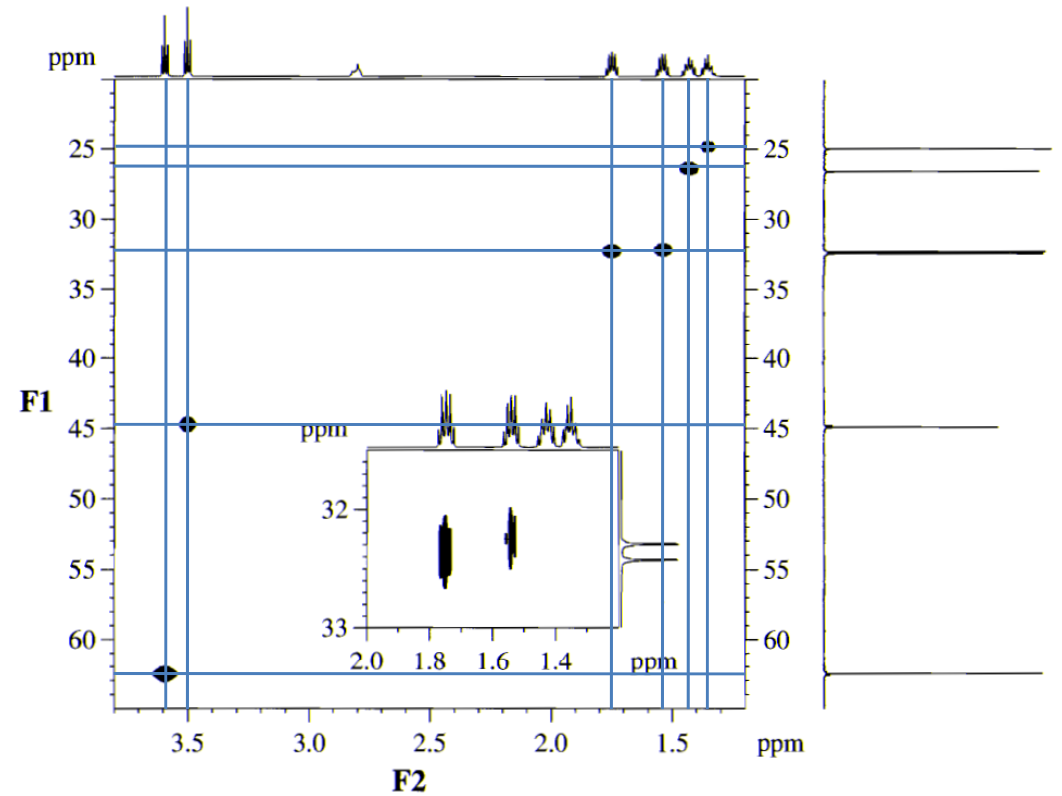


- informacije iz ^{13}C NMR:

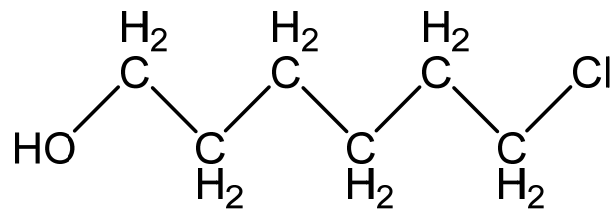
$\delta(^{13}\text{C})/\text{ppm}$	C-atom
25,0	$-\text{CH}_2-$
26,5	$-\text{CH}_2-$
32,2	$-\text{CH}_2-$
32,5	$-\text{CH}_2-$
45,0	$-\text{CH}_2-$
62,5	$-\text{CH}_2-$



HMQC spektar

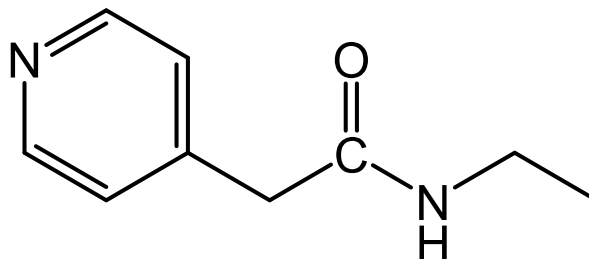


- rješenje:



DODATNI ZADACI I PITANJA

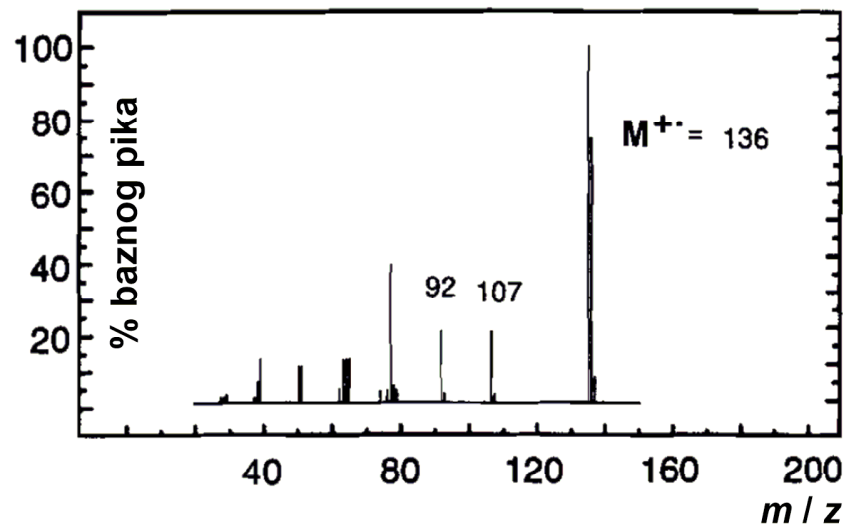
23. Skicirajte ^1H i potpuno raspregnuti ^{13}C NMR spektar spoja na slici:



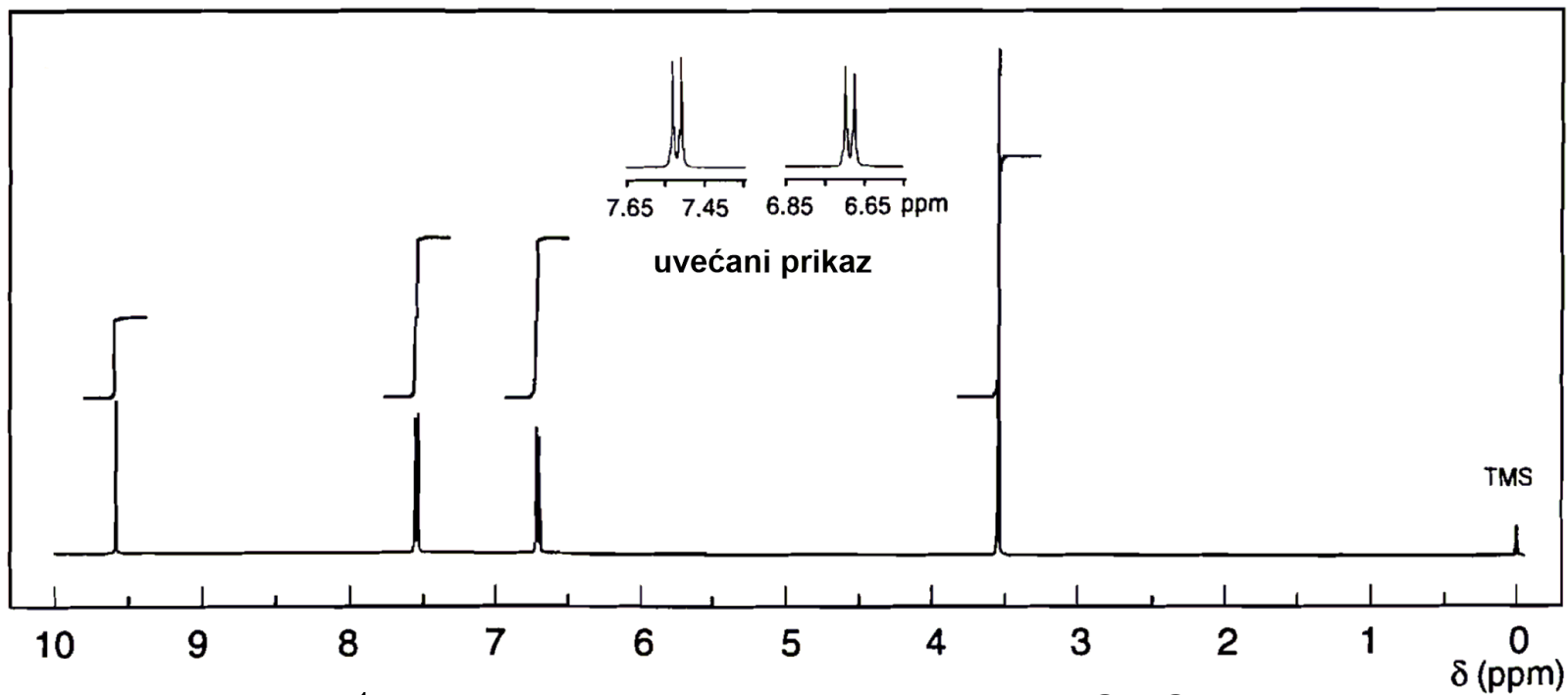
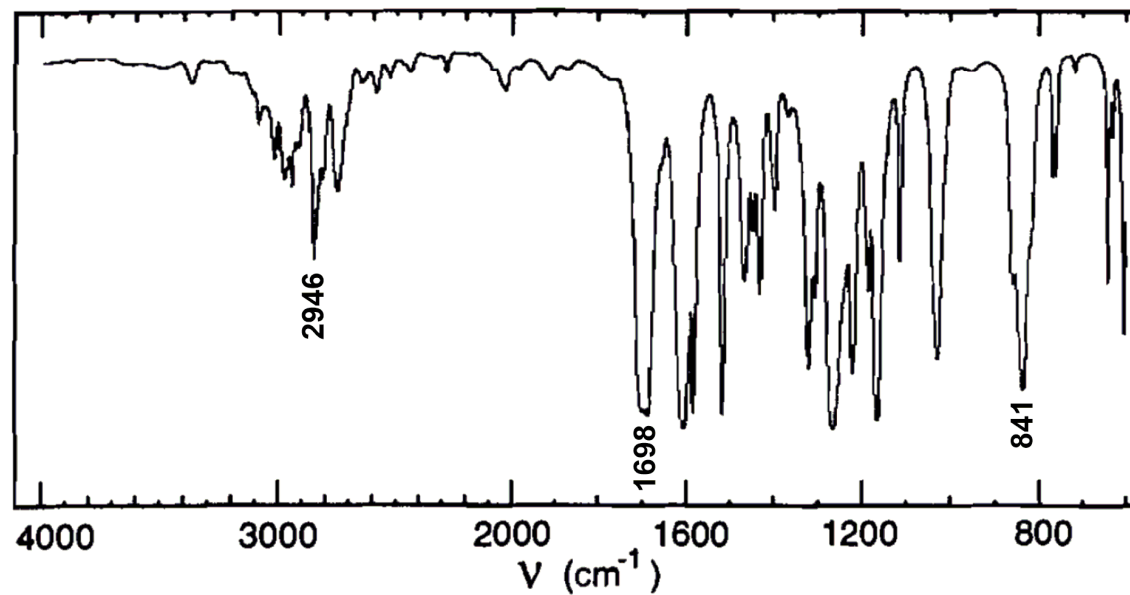
24. Razmotrimo spinski sustav A_2M_2X , gdje je $I_A=I_M=I_X=1/2$. Skicirajte signale spinova A, M i X u spektru NMR, ako je $J_{AM} > J_{MX} = J_{AX}$.

25. Odredite strukturu spoja na temelju njegovih MS, IR, ^1H i ^{13}C NMR spektara

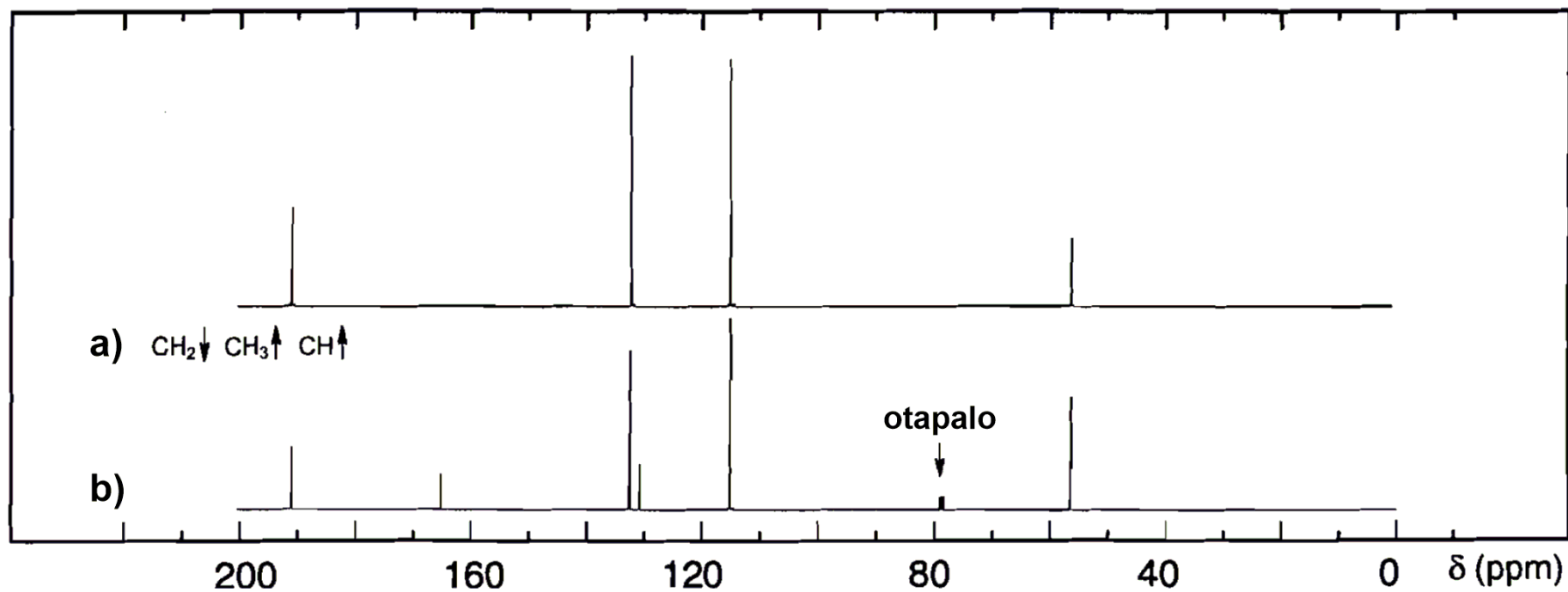
Spektar MS spoja
dobiven ionizacijom
brzim elektronima (EI)



Spektar IR spoja
snimljen tehnikom
KBr pastile

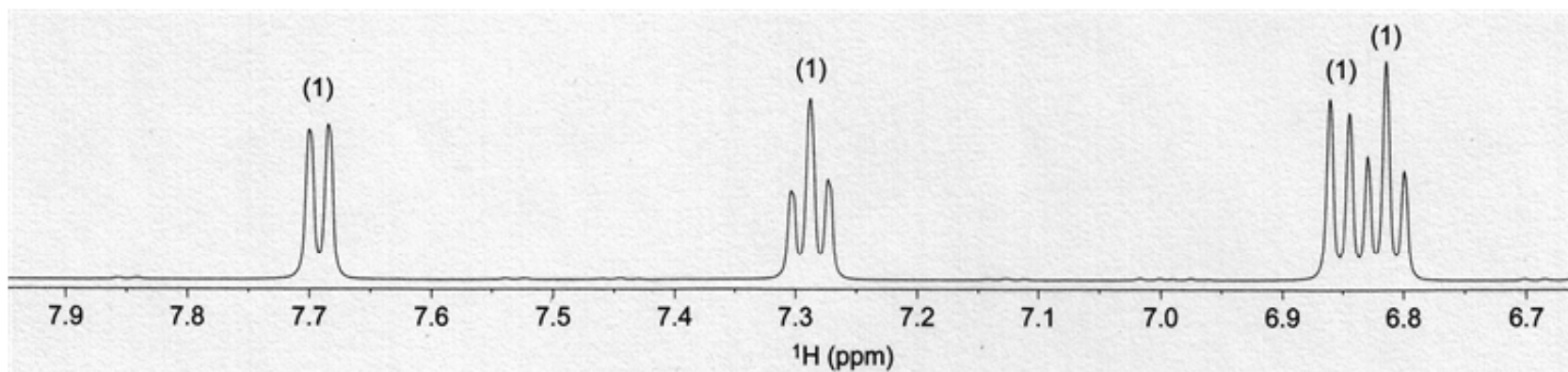


^1H NMR spektar spoja snimljen u CDCl_3

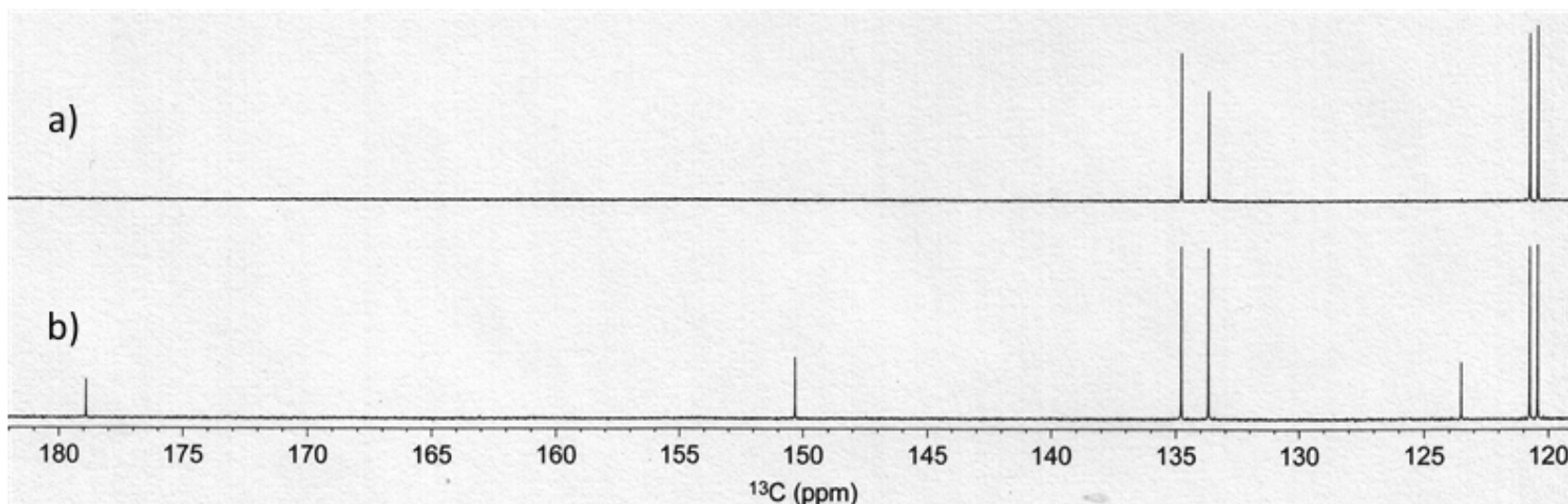


a) APT i b) potpuno raspregnuti ^{13}C NMR spektar spoja snimljen u CDCl_3

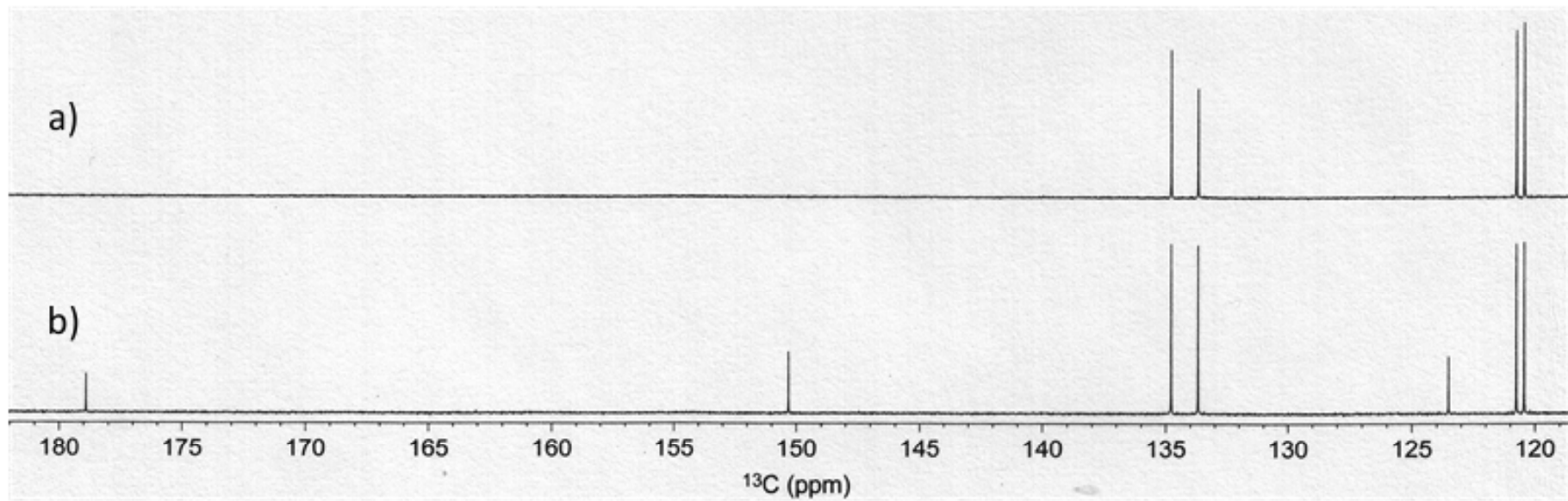
26. Odredite strukturu spoja molekulske formule $C_7H_7NO_2$ na temelju njegovih 1H NMR, ^{13}C NMR, COSY, HSQC i HMBC spektara.



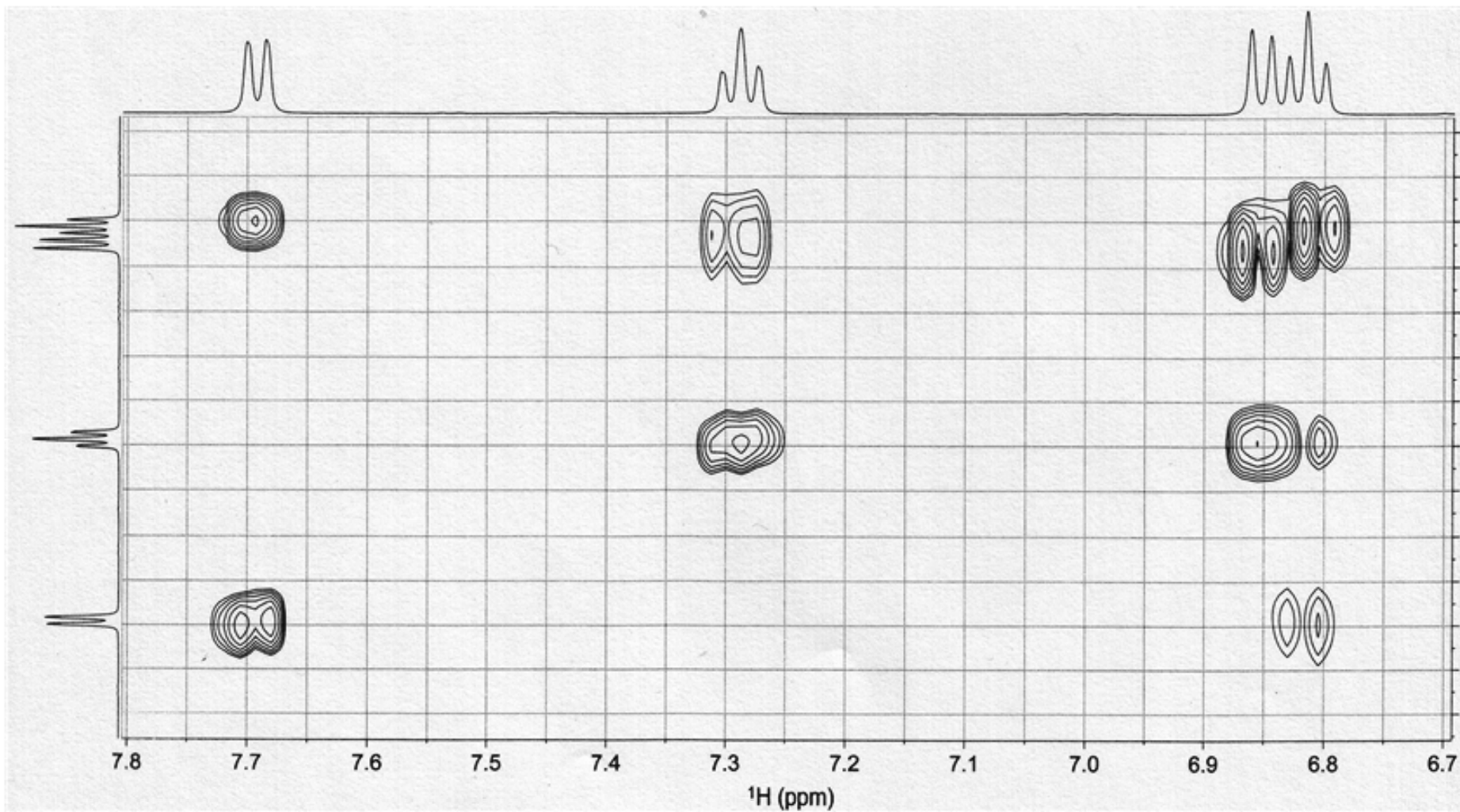
1H NMR spektar spoja snimljen u D_2O . Integrali su označeni brojevima. Spoj sadrži i protone koji se izmijene u D_2O .



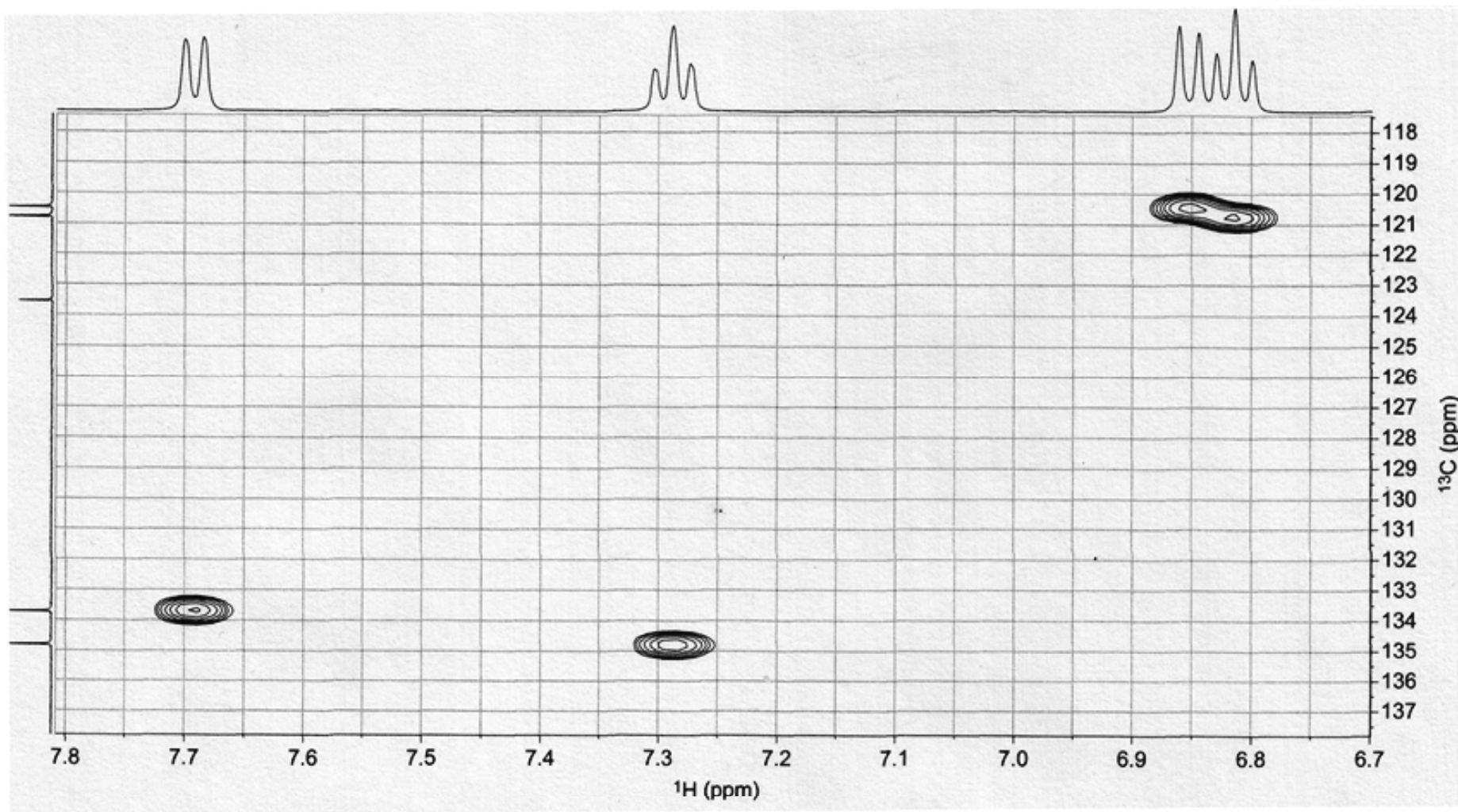
a) DEPT-135; b) potpuno raspregnuti ^{13}C NMR spektar spoja snimljen u D_2O



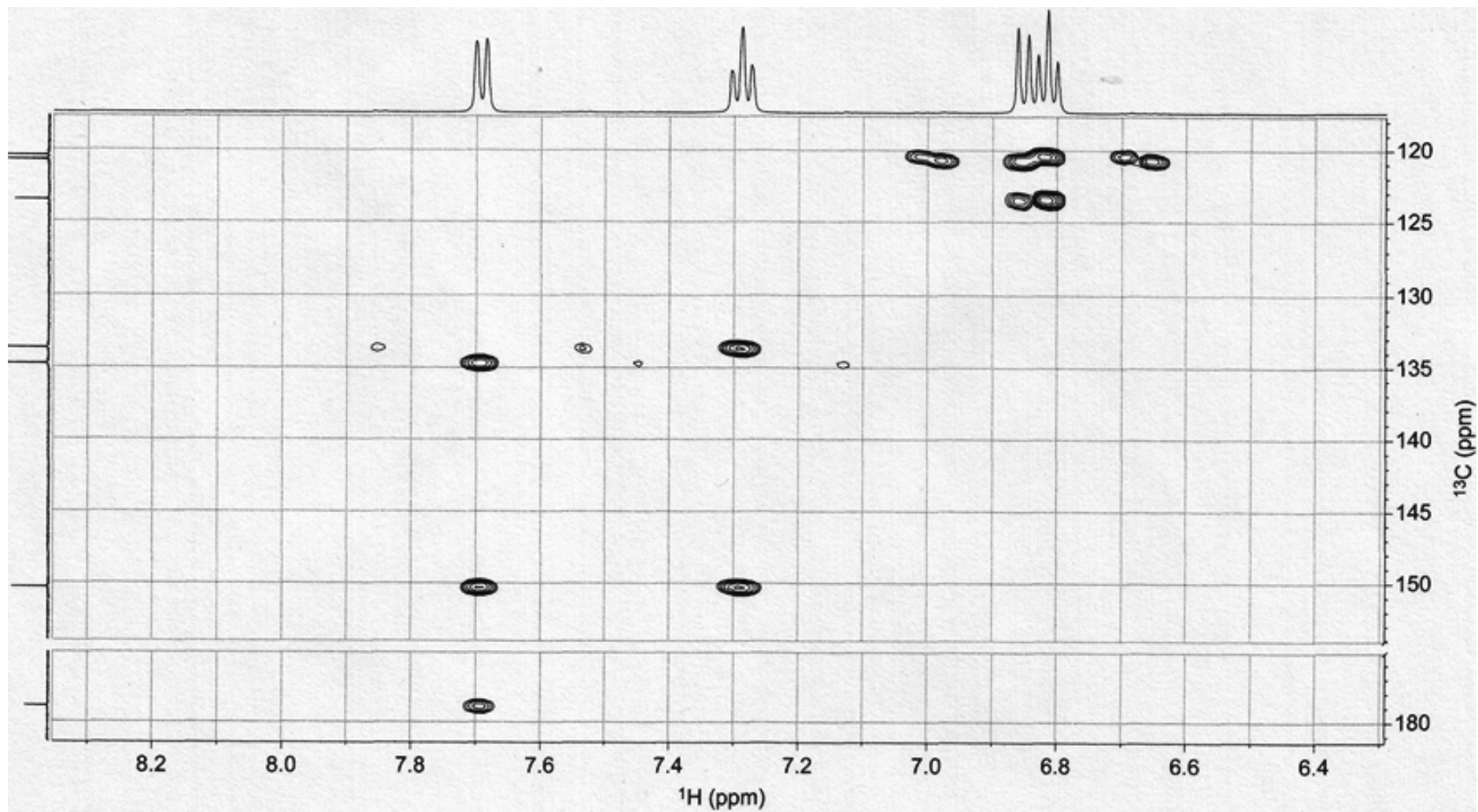
a) DEPT-135; b) potpuno raspregnuti ^{13}C NMR spektar spoja snimljen u D_2O



COSY spektar spoja snimljen u D₂O



HSQC spektar spoja snimljen u D_2O



HMBC spektar spoja snimljen u D_2O