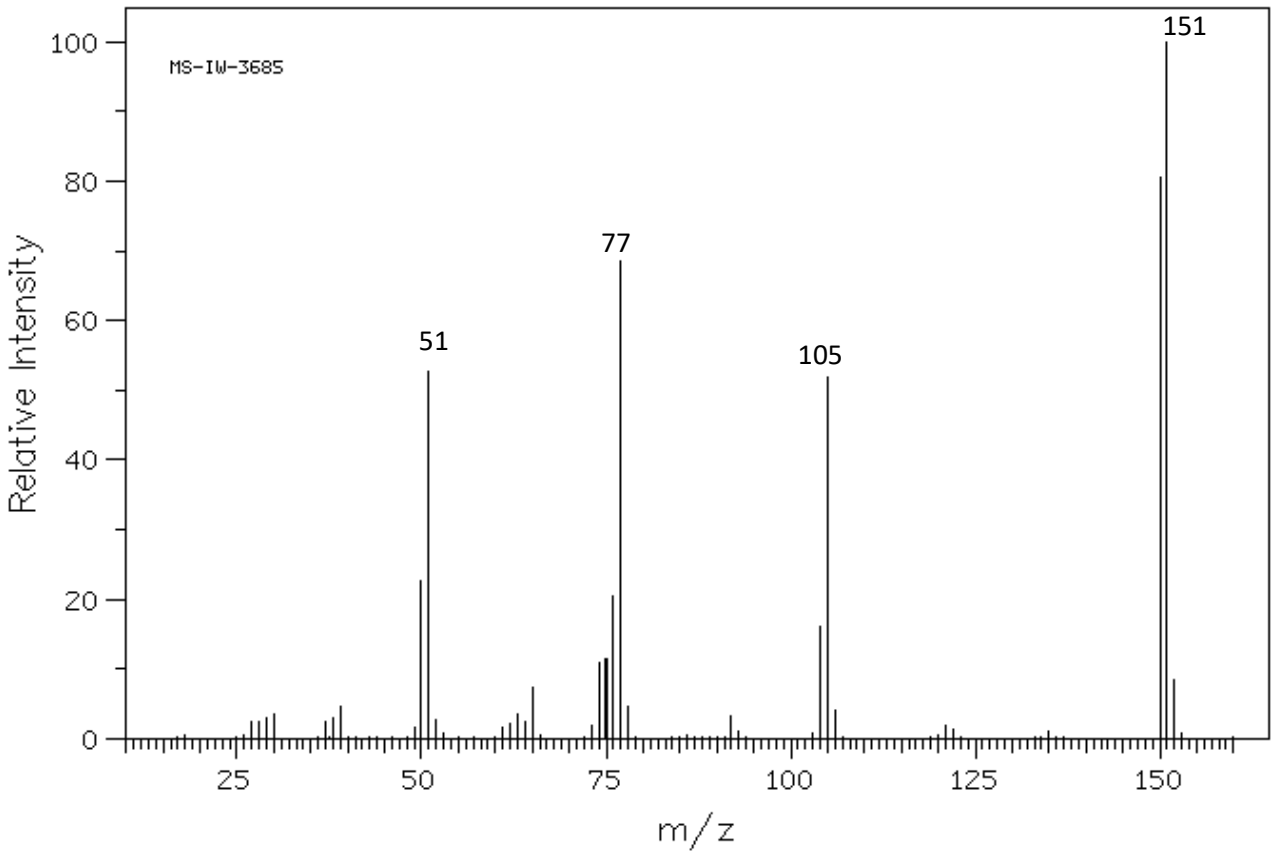
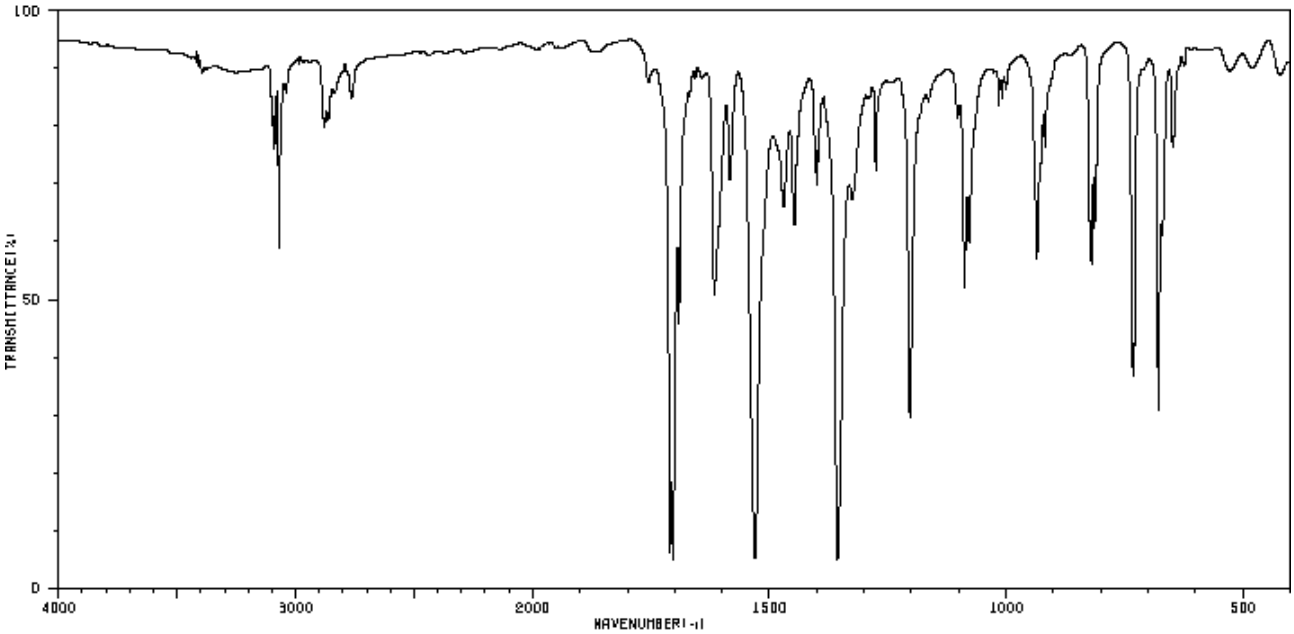
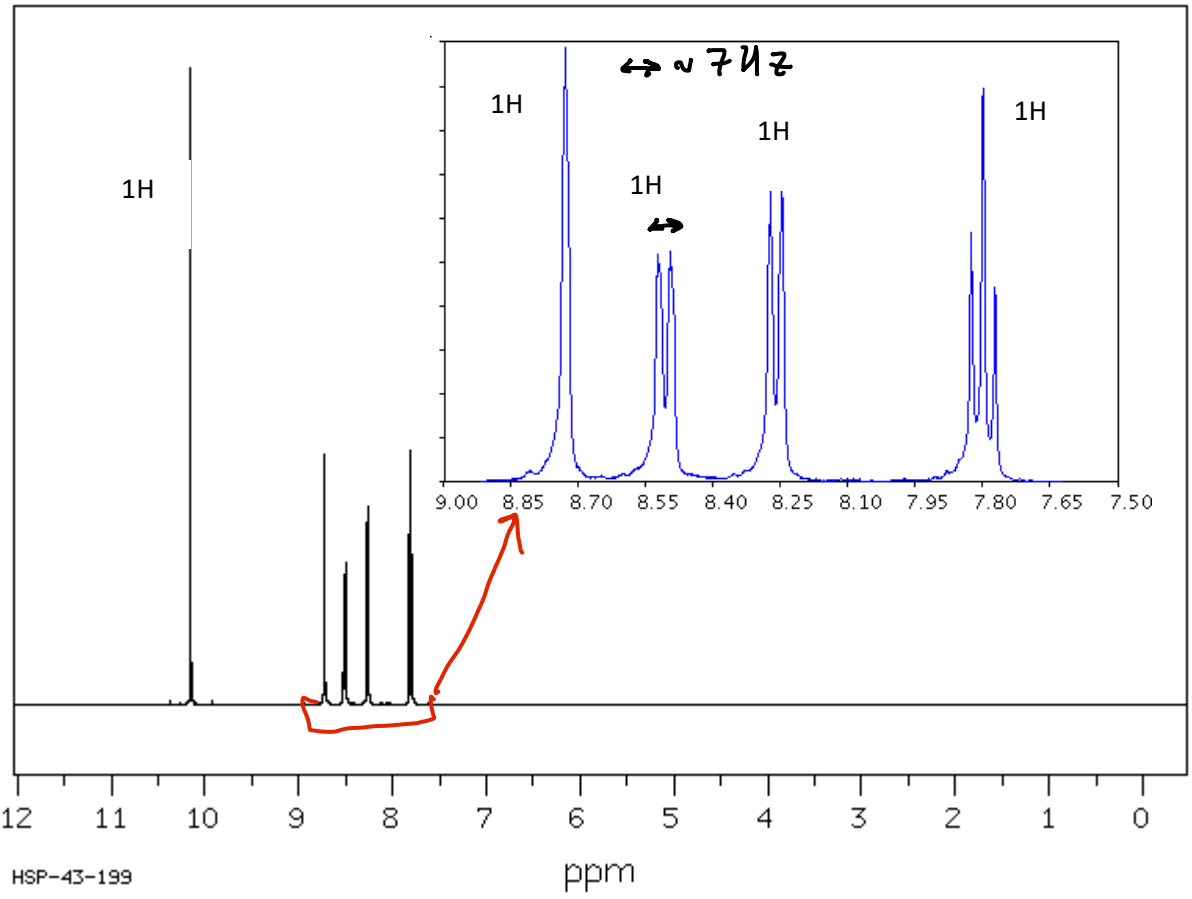
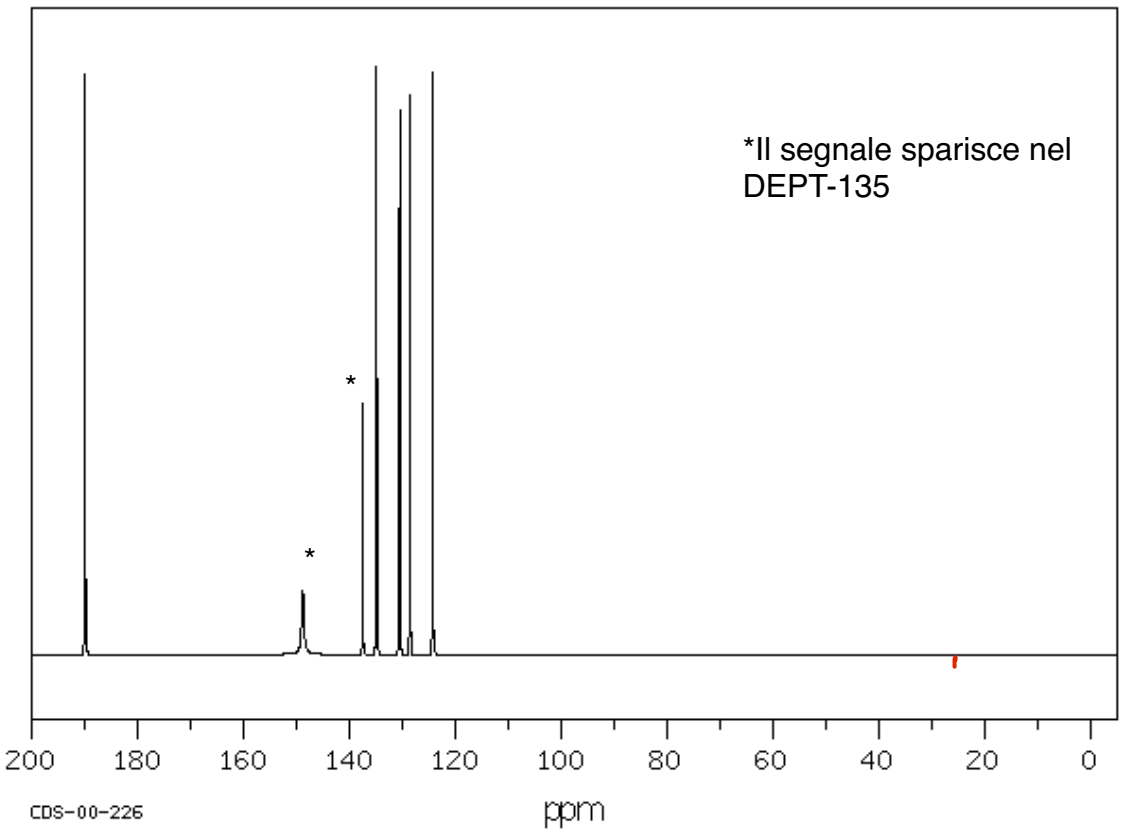
$C_7H_5NO_3$





3089	72	1710	6	1447	60	1103	79	918	74
3070	57	1703	4	1400	68	1088	50	820	53
3041	81	1691	45	1357	4	1079	57	813	60
2878	77	1616	49	1325	64	1016	79	739	36
2863	77	1584	68	1276	70	1007	81	679	29
2764	81	1531	5	1203	28	1000	84	672	56
1766	84	1470	64	1165	81	936	55	648	74





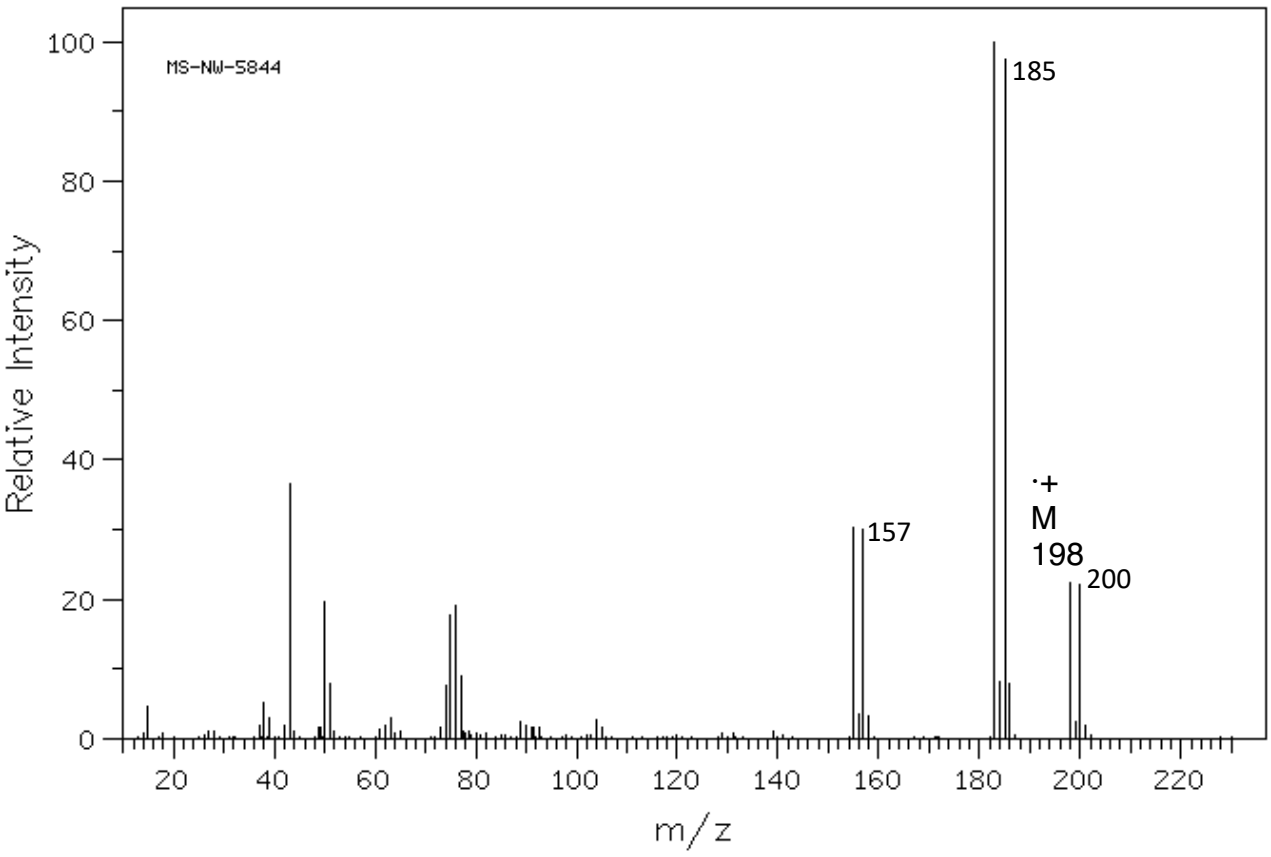
*Il segnale sparisce nel DEPT-135

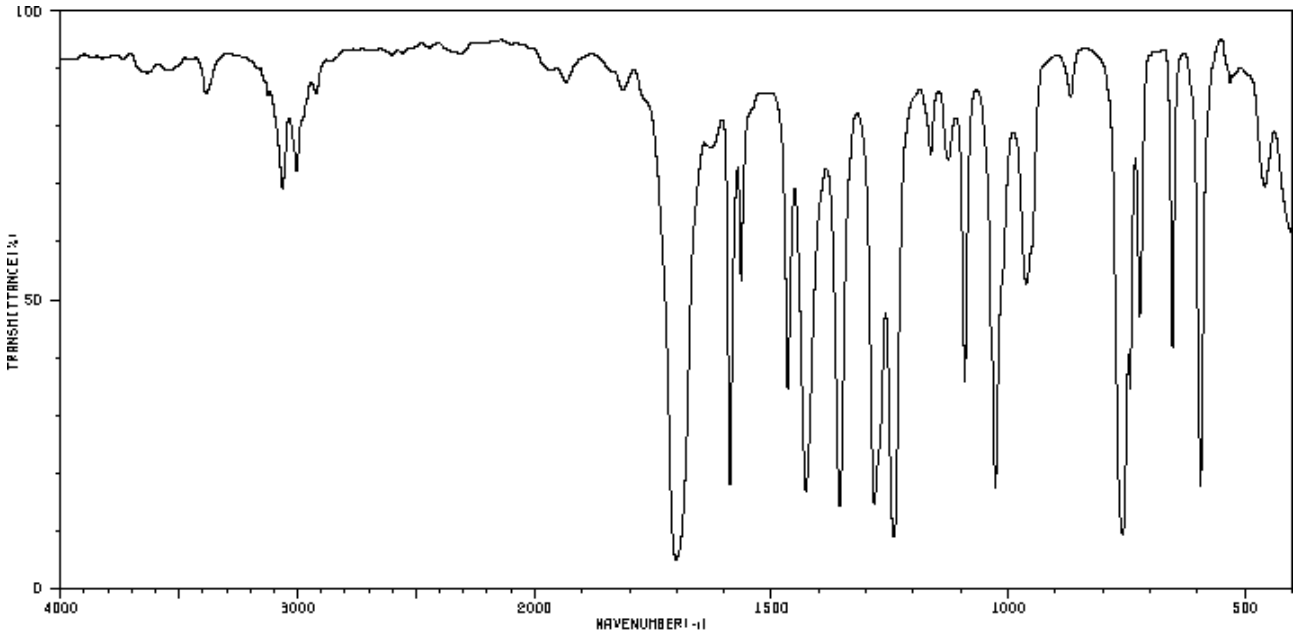
ESERCIZIO 2

Utilizzando i dati di NMR, IR e MS. Proporre una struttura per un composto che contiene carbonio, idrogeno e due eteroatomi diversi.

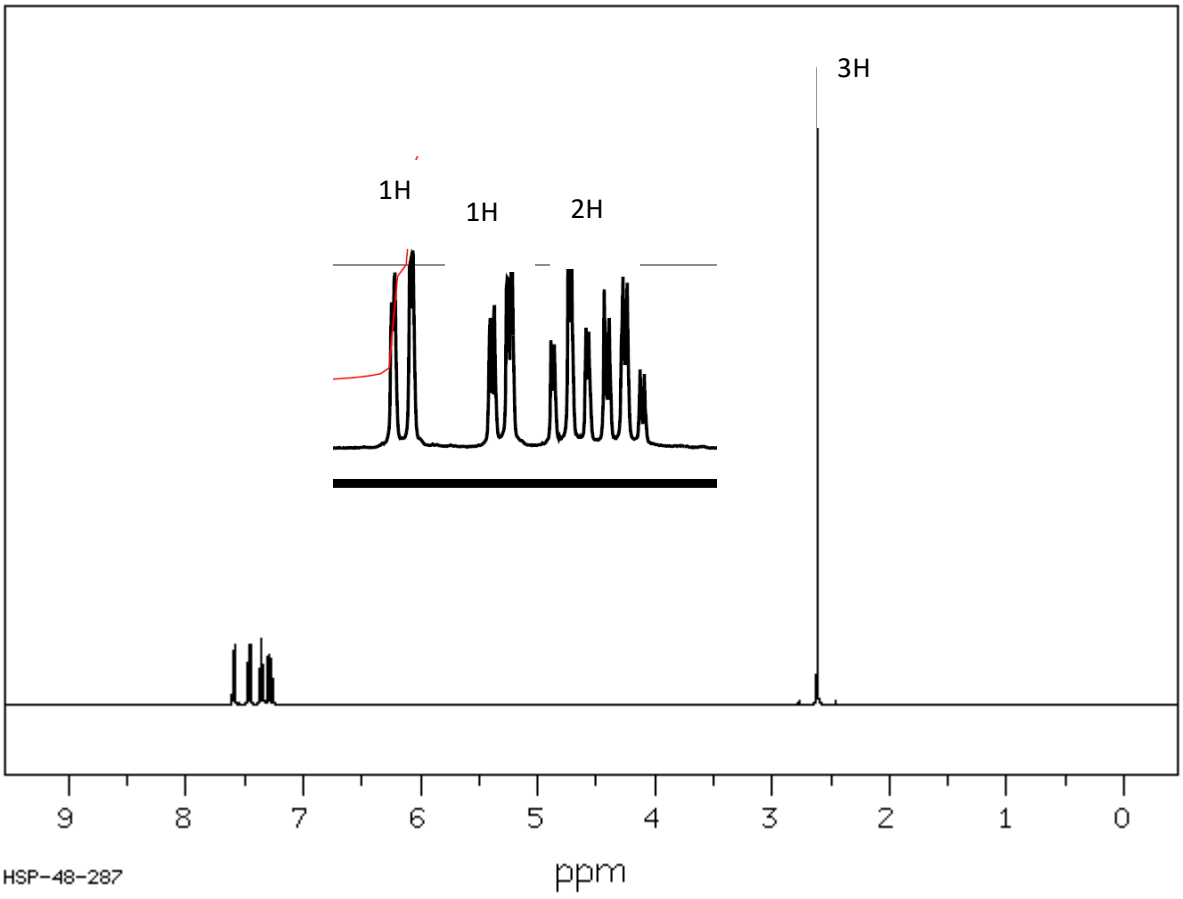
C8H7BrO

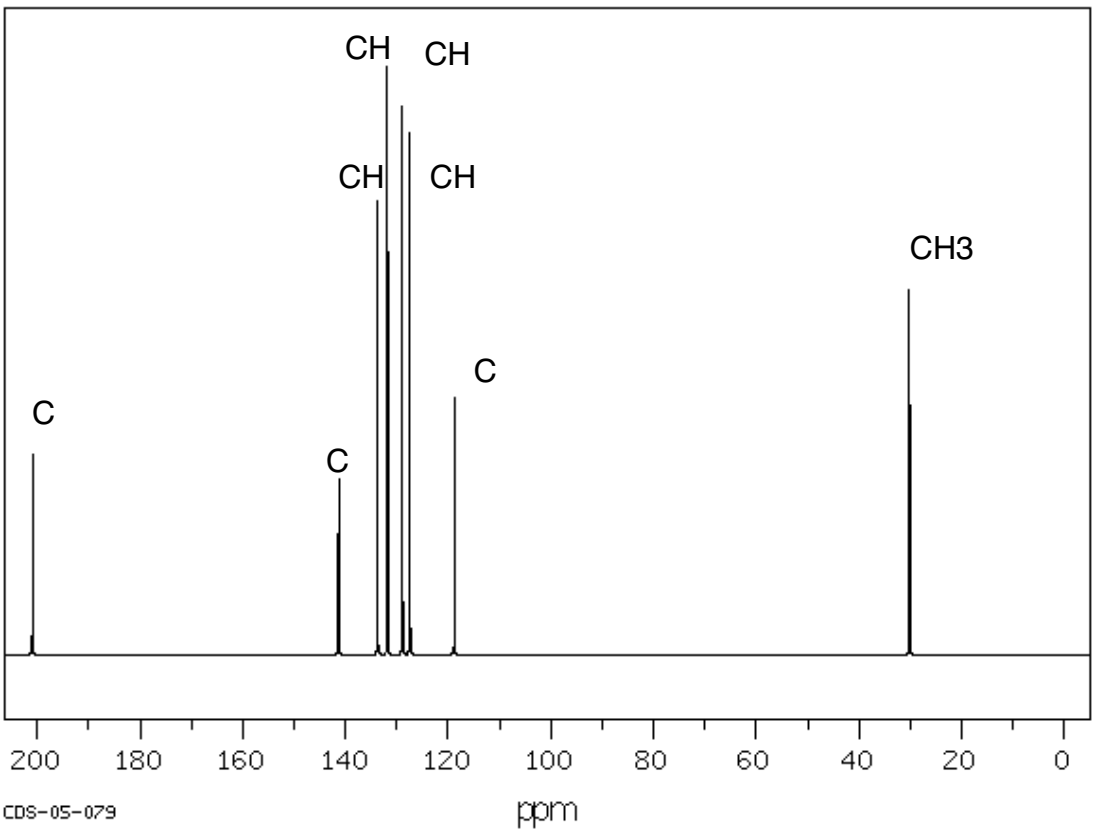
Digita qu





3646	86	2924	81	1428	16	1027	16	694	17
3635	86	1933	84	1356	13	961	50	533	84
3384	81	1813	84	1283	15	868	61	526	64
3368	84	1702	4	1242	8	768	8	469	66
3081	74	1588	17	1164	72	743	33		
3064	86	1564	50	1126	72	722	44		
3006	70	1466	39	1092	34	663	39		

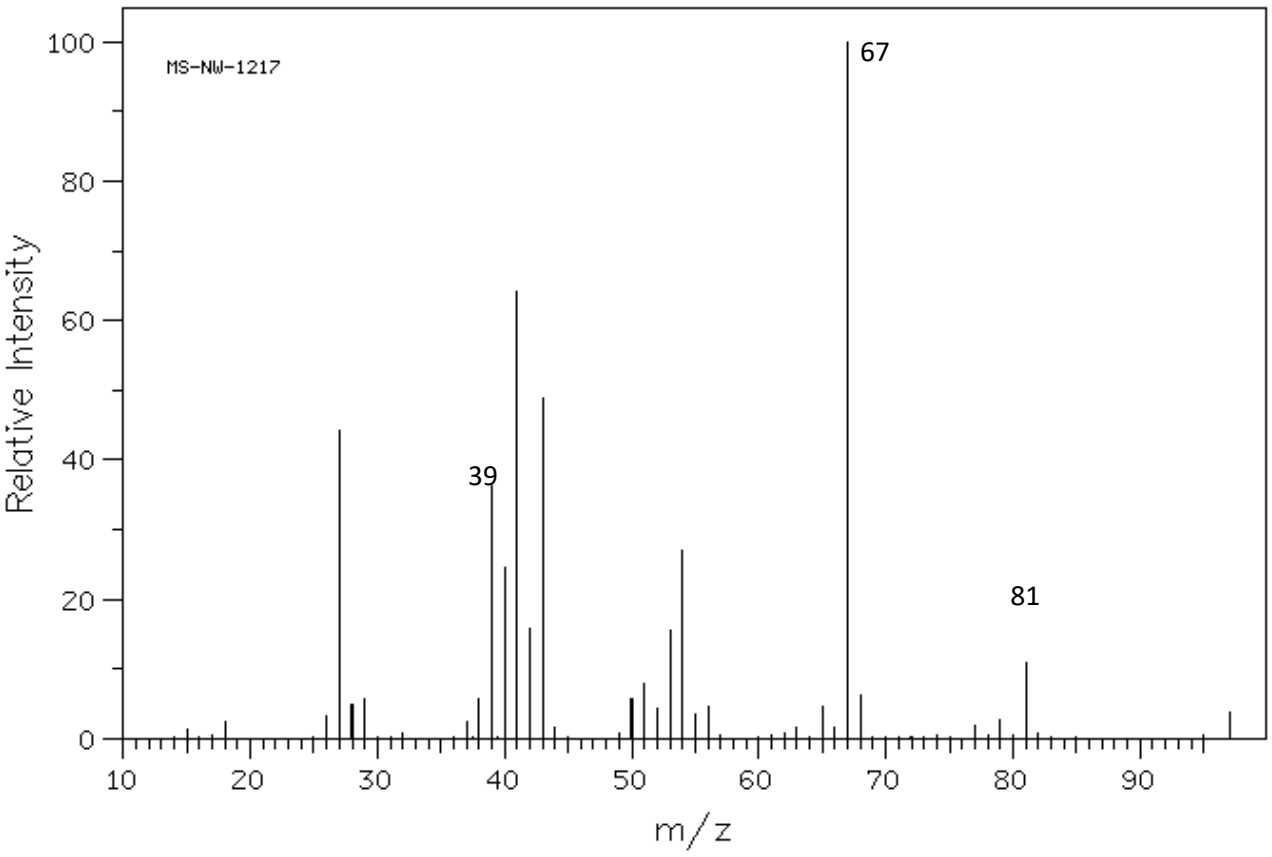

3H
1H
1H
2H
9
8
7
6
5
4
3
2
1
0
HSP-48-287
ppm

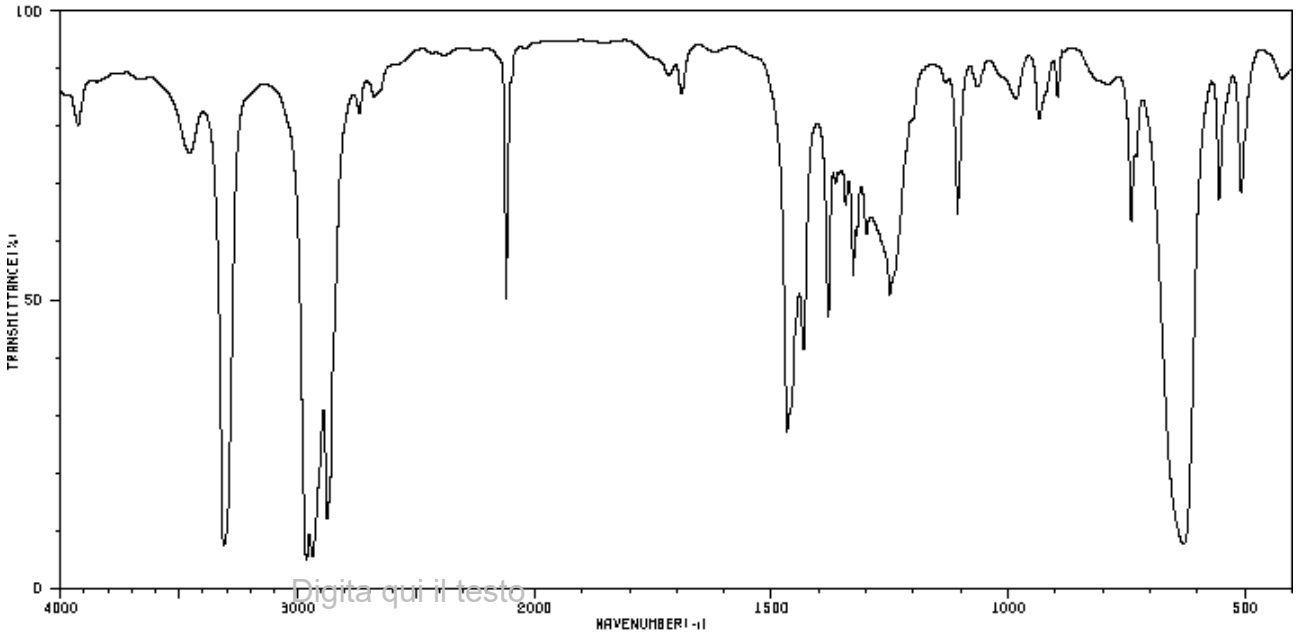

CH
CH
CH
CH
CH3
C
C
C
200
180
160
140
120
100
80
60
40
20
0
CDS-05-079
ppm

ESERCIZIO 3

Utilizzando i dati di NMR, IR e MS. Proporre una struttura per un composto di peso molecolare 82 che contiene un 87.73% di carbonio e un 12.27% d'idrogeno.

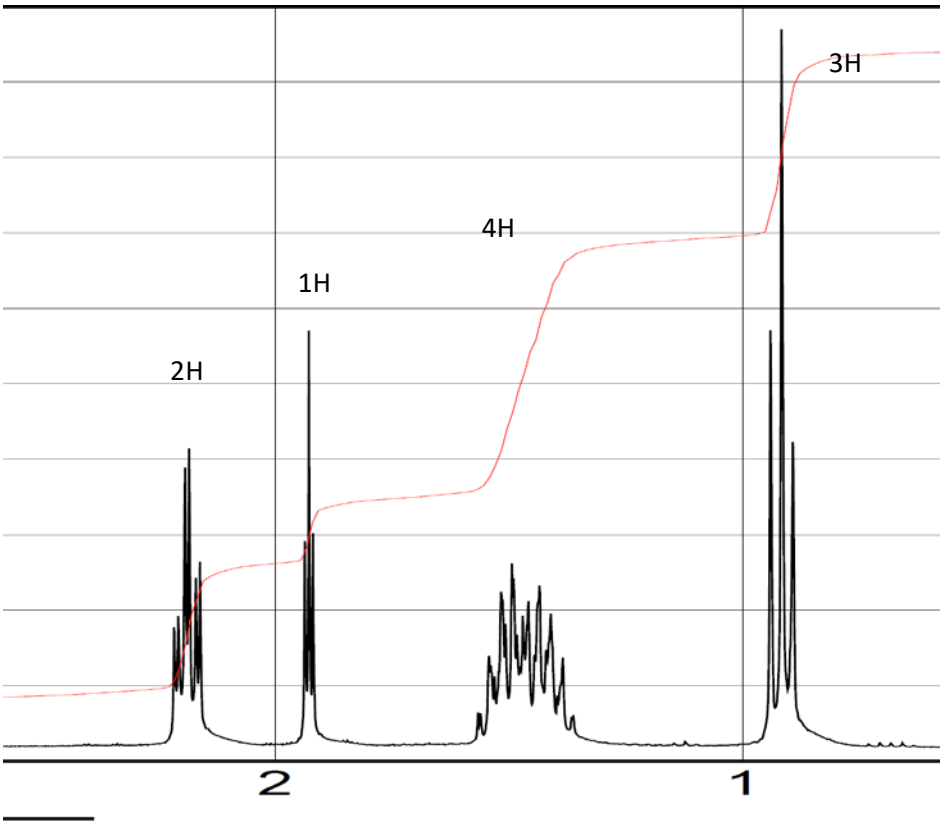
C6H10

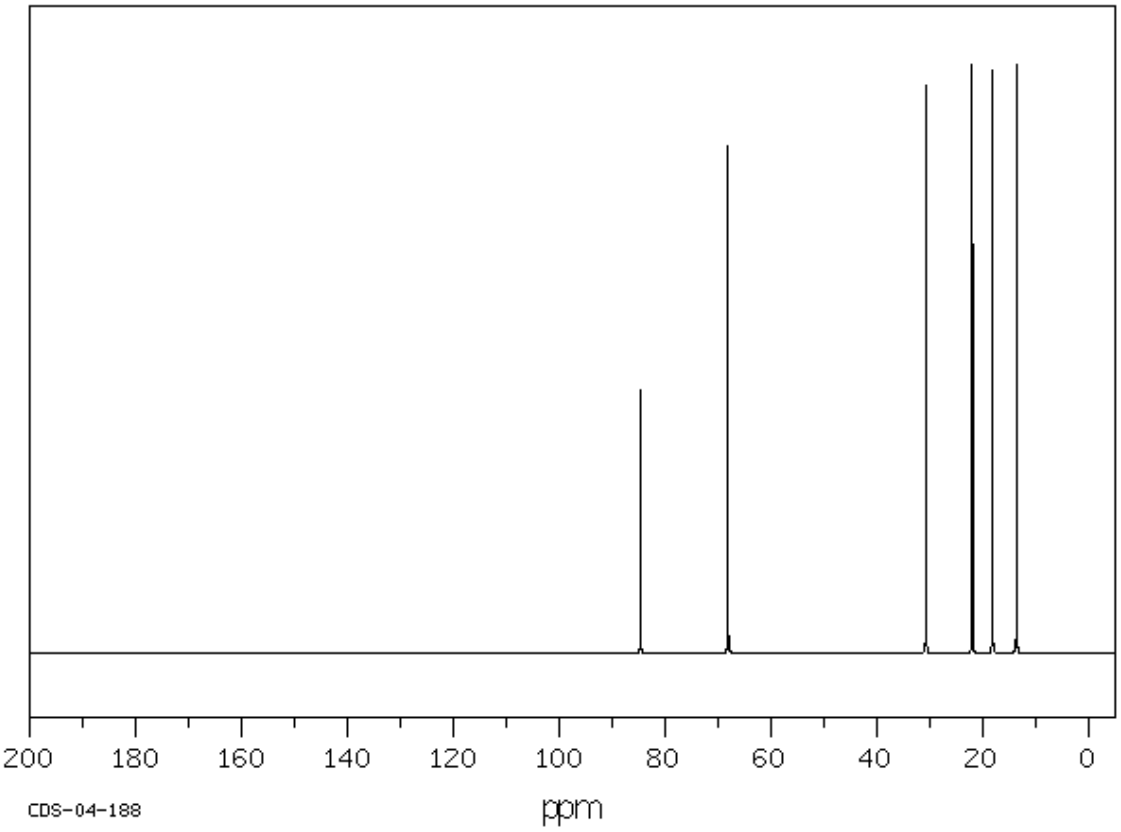




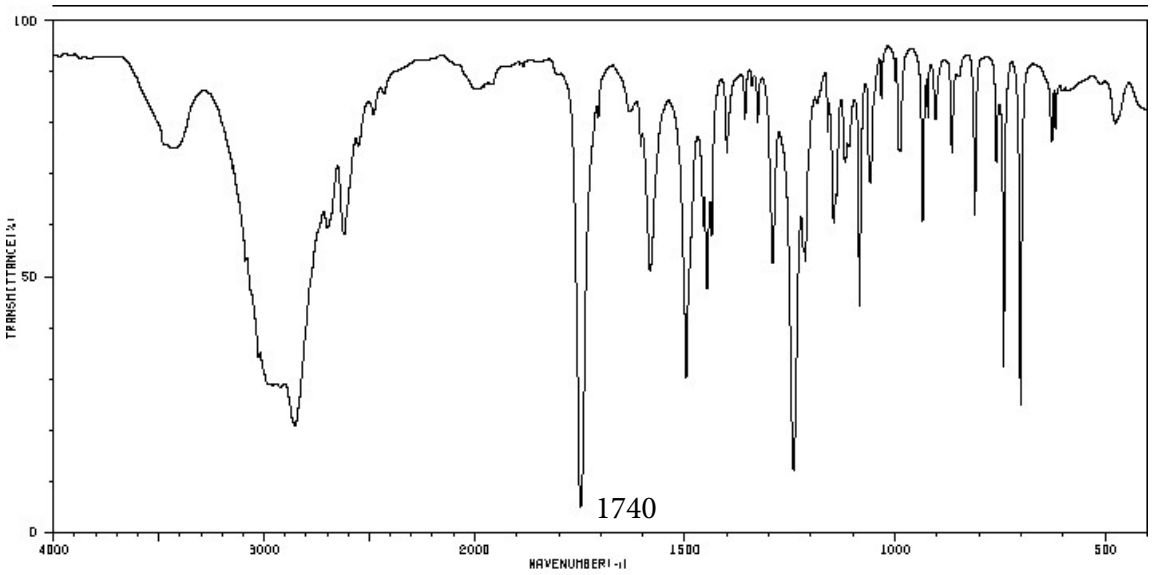
Digita qui il testo

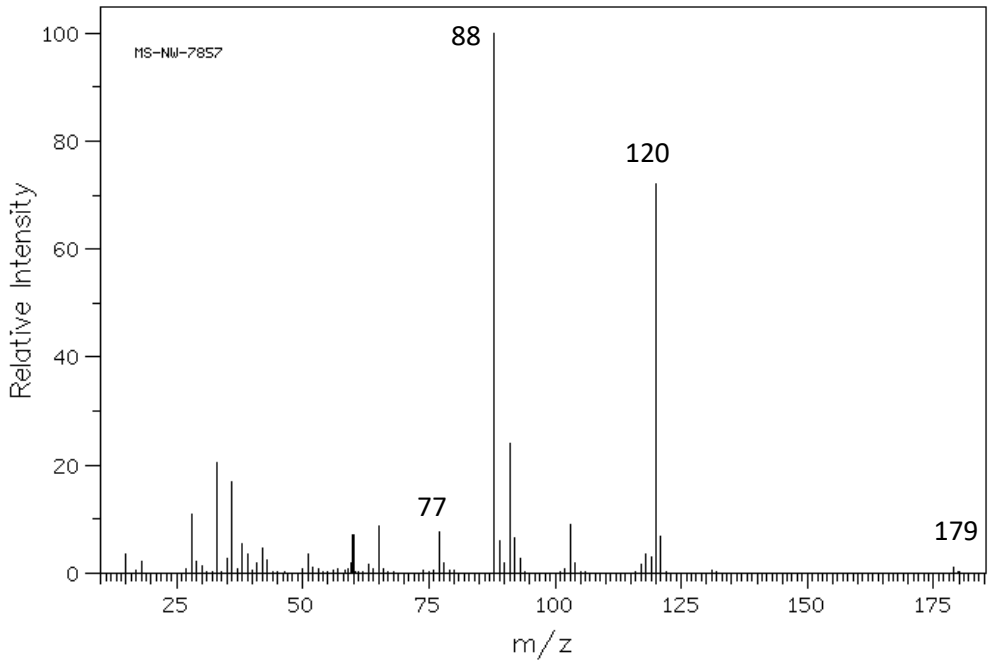
3926	77	2679	81	1432	39	1260	49	740	60
3455	72	2120	49	1380	46	1107	62	730	72
3311	7	2097	84	1366	88	1063	84	630	7
2962	4	1717	86	1344	64	983	81	555	64
2937	5	1690	81	1328	52	934	79	509	66
2876	11	1467	26	1320	58	895	81		
2738	79	1461	29	1300	58	793	84		


3H
4H
1H
2H
2
1

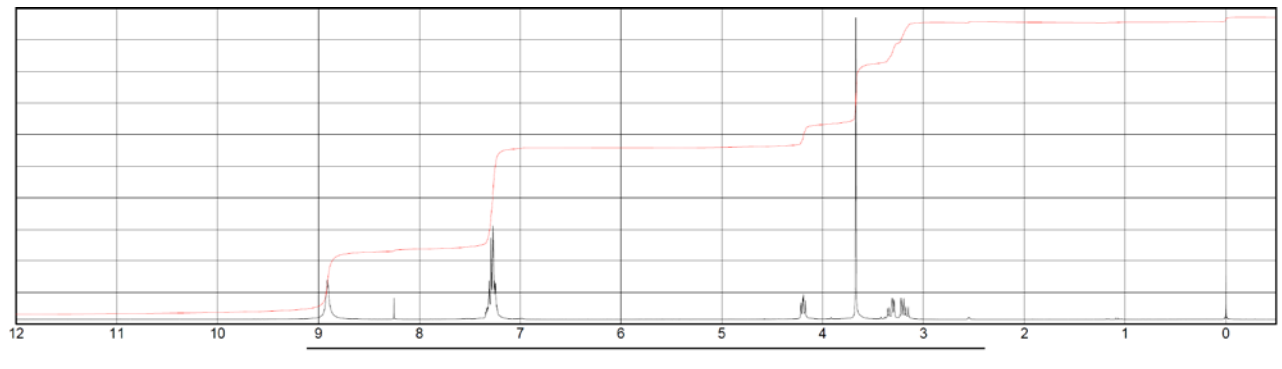

200
180
160
140
120
100
80
60
40
20
0
CDS-04-188
ppm

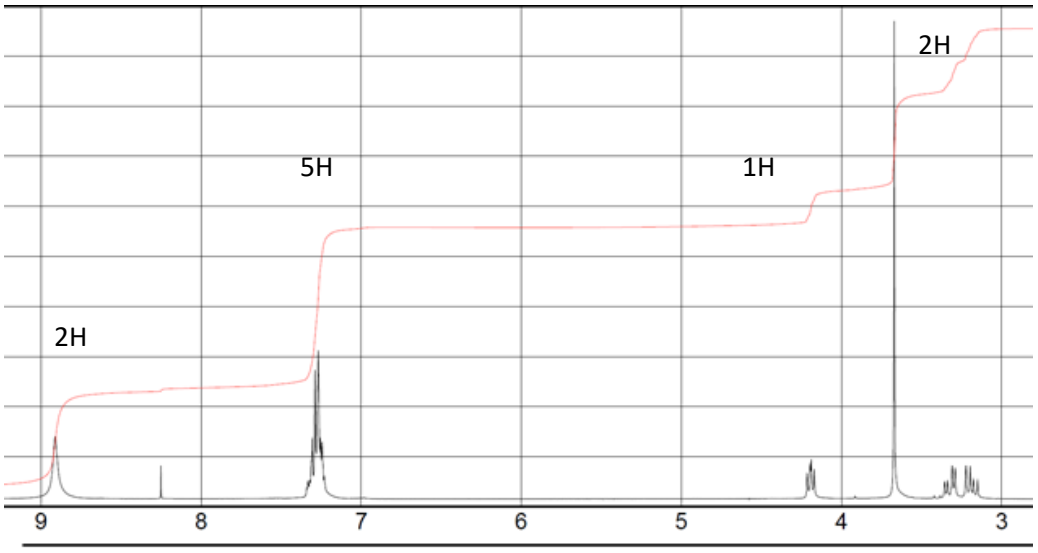
$C_{10}H_{13}NO_2$

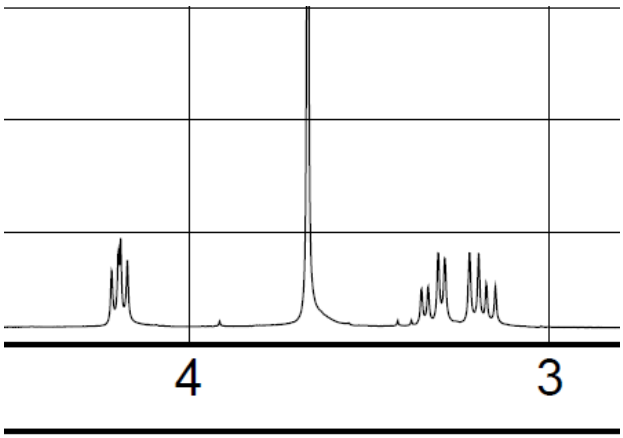


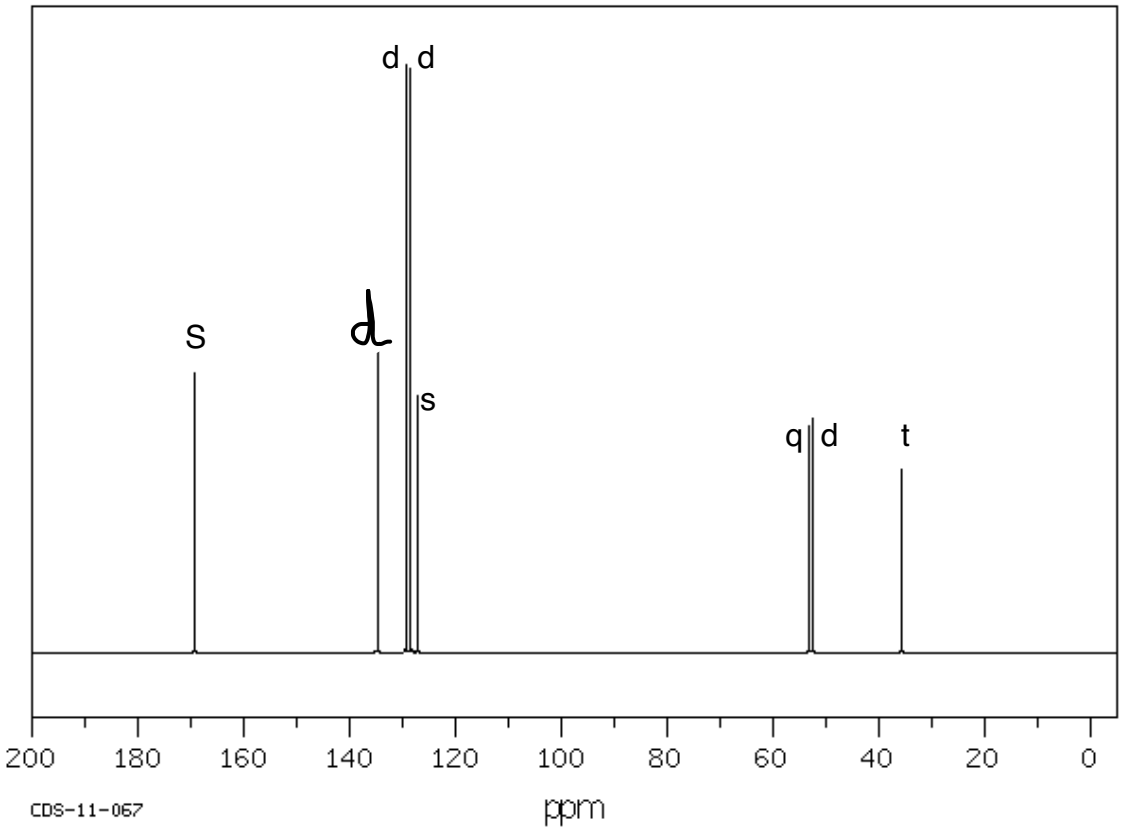


^{1}H-NMR e ^{13}C-NMR, $CDCl_3$+DMSO-d_6





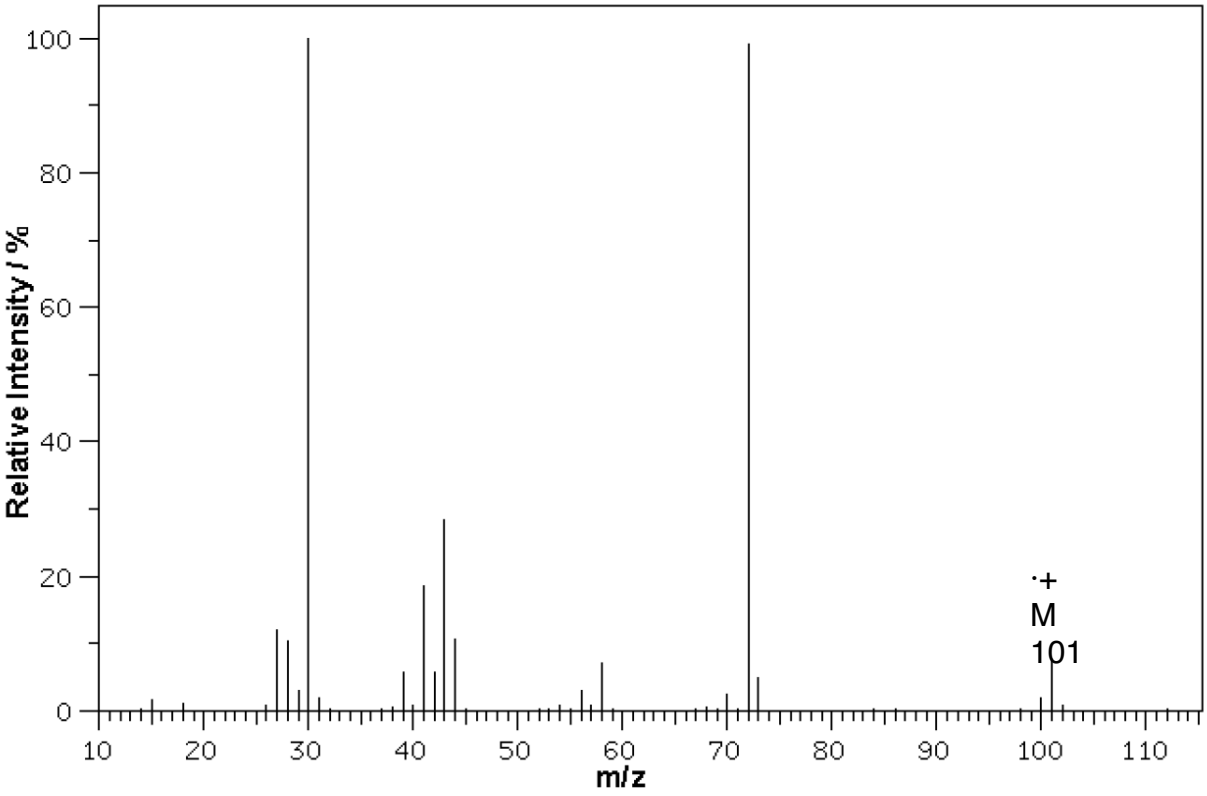


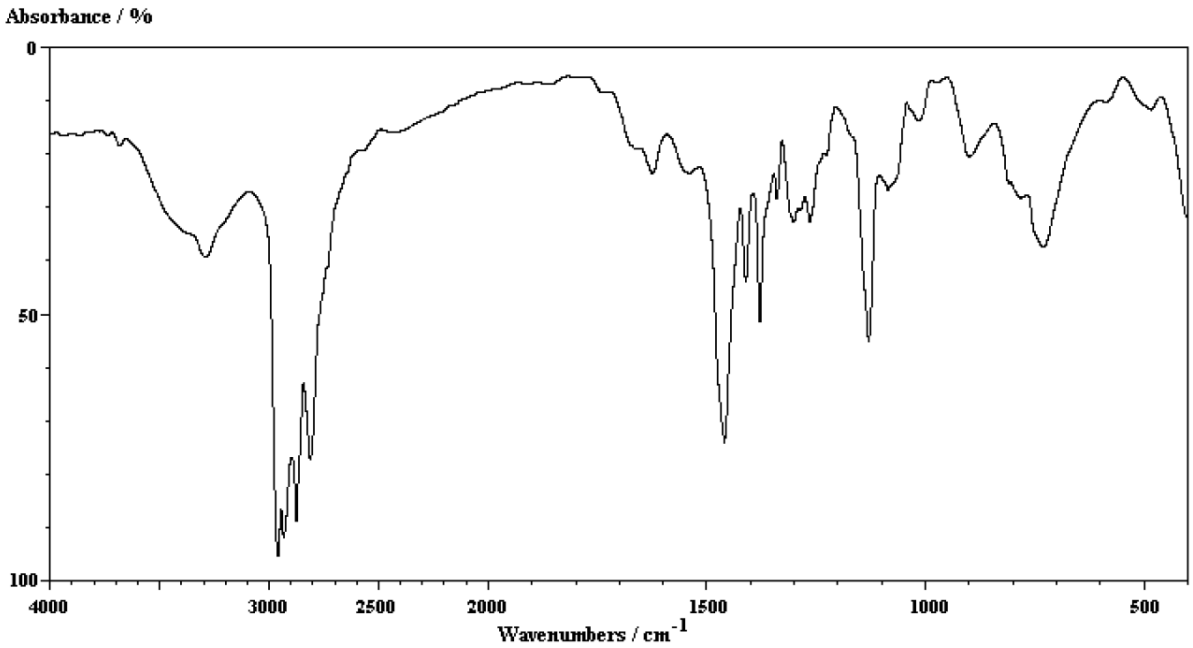


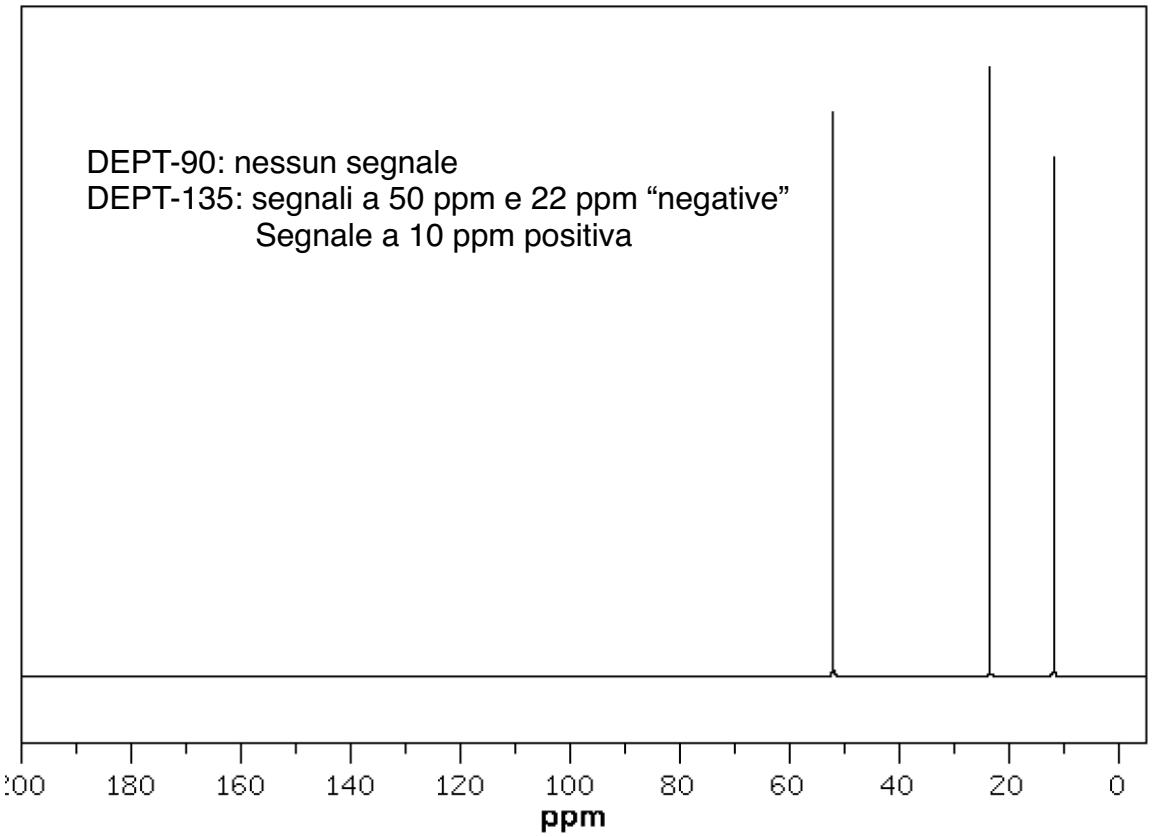
È indicata la molteplicità del carbonio nello spettro accoppiato al protone

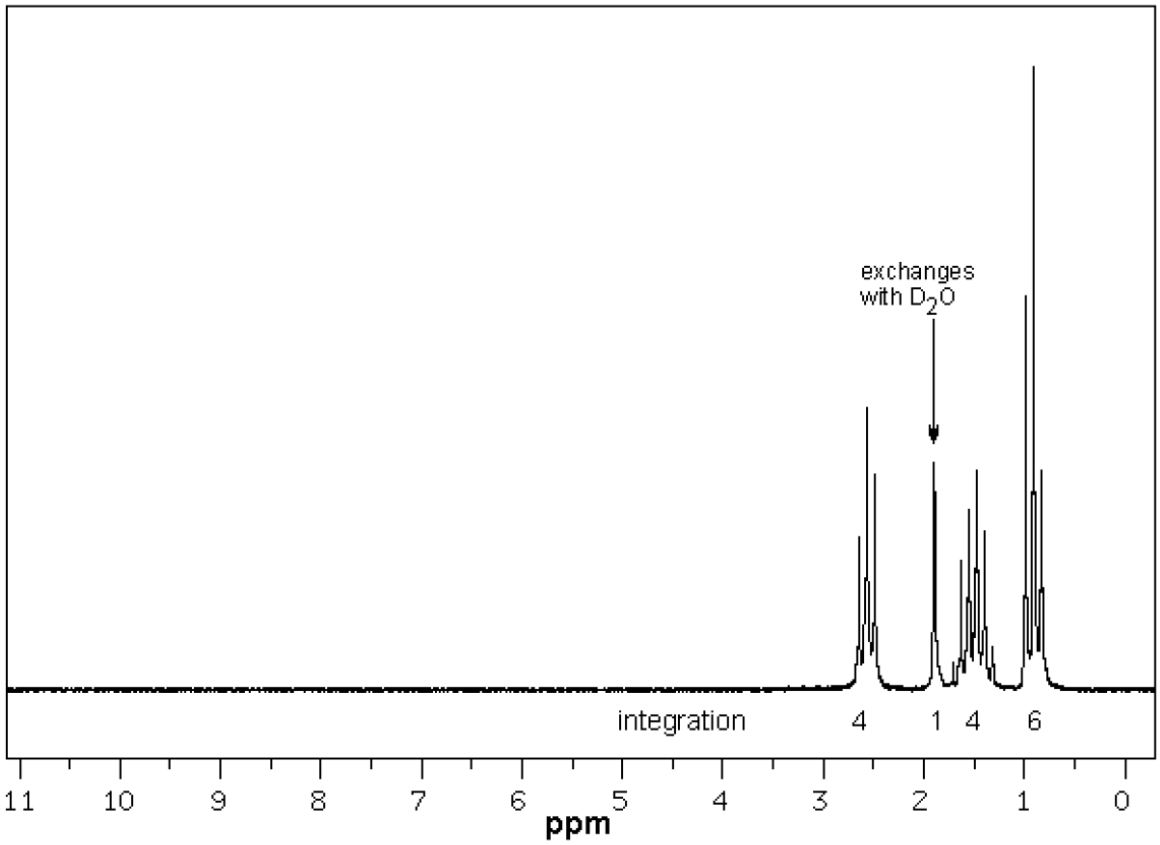
ESERCIZIO 5 Utilizzando i dati di NMR, IR e MS. Proporre una struttura per un composto di formula C6H15N, che contiene un 71.22% di carbonio, un 14.94% d'idrogeno e un 13.84% d'azoto.

~~C8H8O2~~



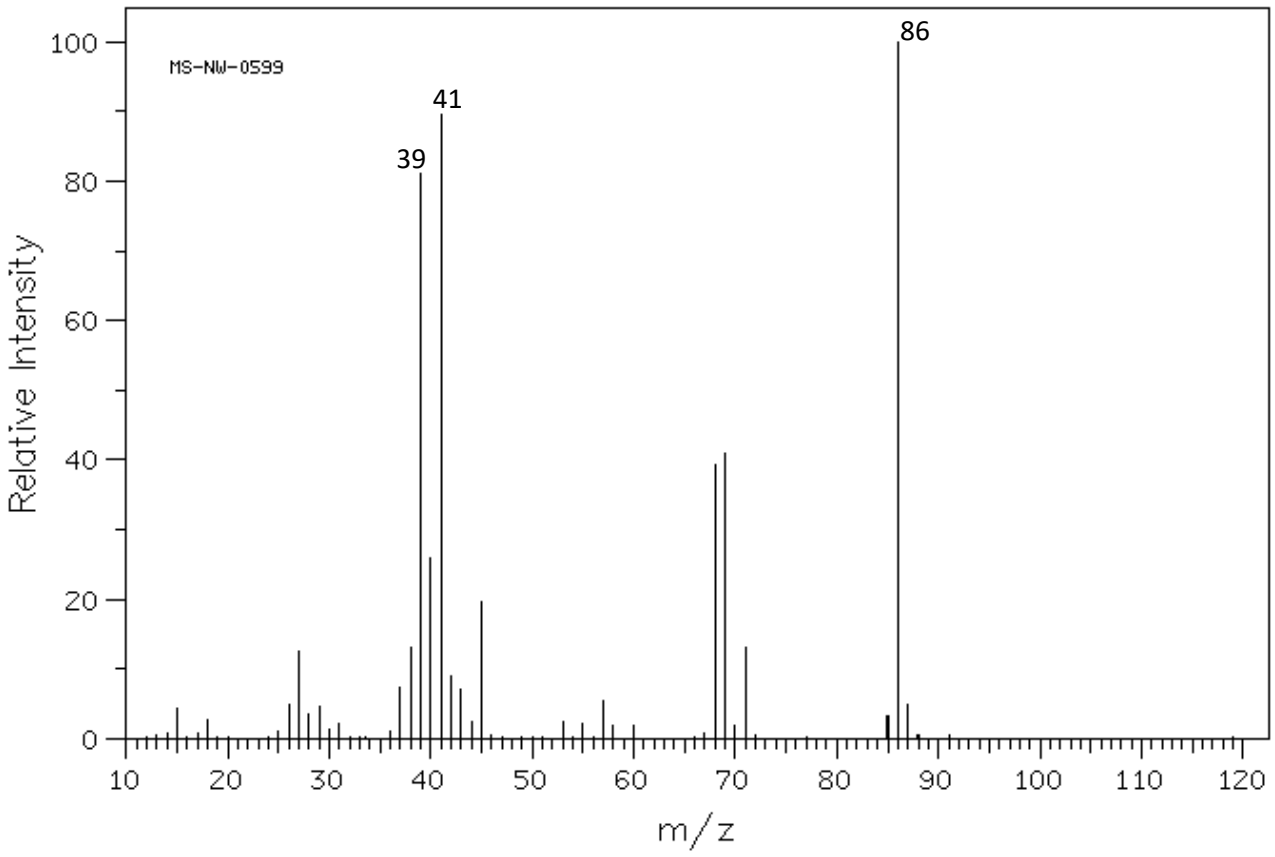


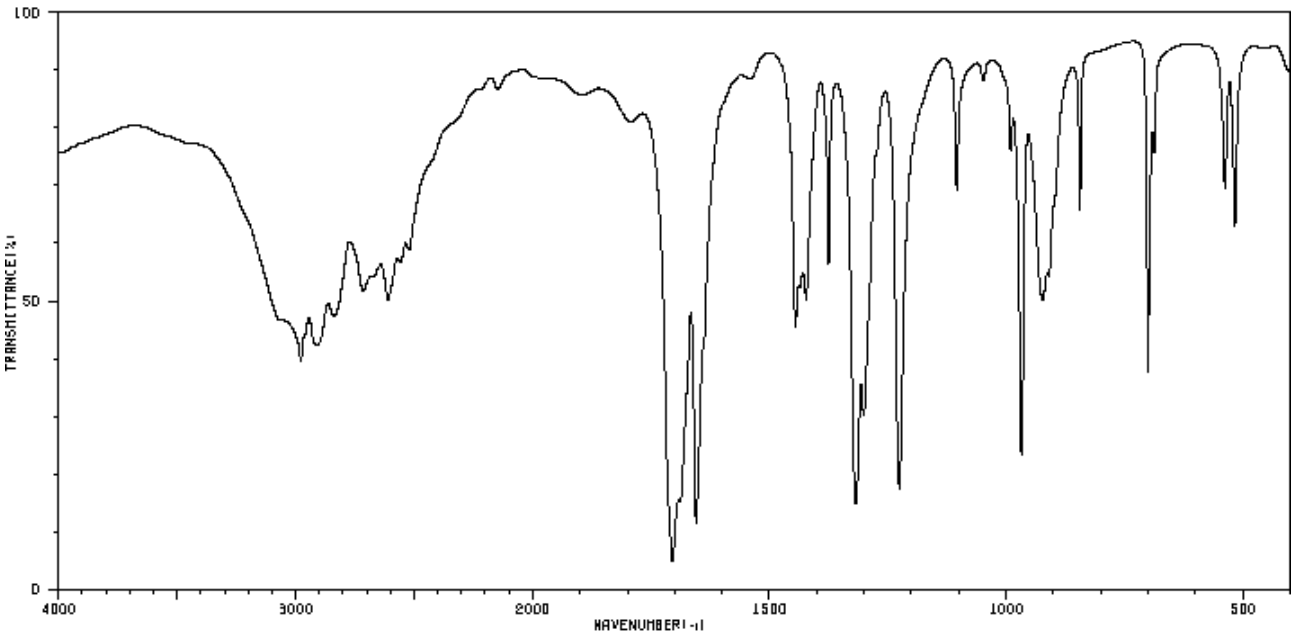

DEPT-90: nessun segnale
DEPT-135: segnali a 50 ppm e 22 ppm “negative”
Segnale a 10 ppm positiva
200
180
160
140
120
100
80
60
40
20
0
ppm


exchanges
with D2O
integration
4
1
4
6
11
10
9
8
7
6
5
4
3
2
1
0
ppm

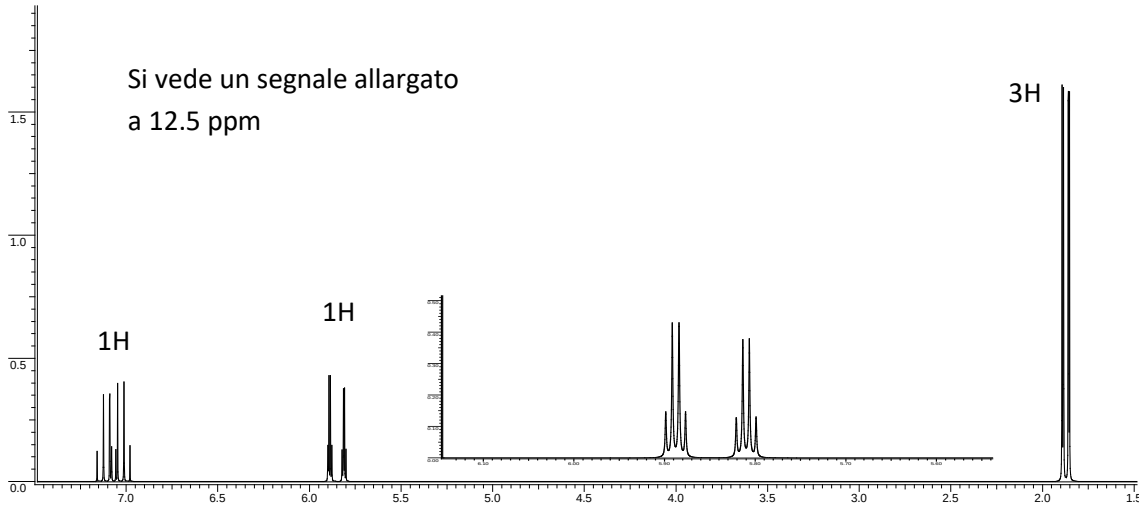
ESERCIZIO 6
Utilizzando i dati di NMR, IR e MS. Proporre una struttura per un composto di formula C4H6O2.

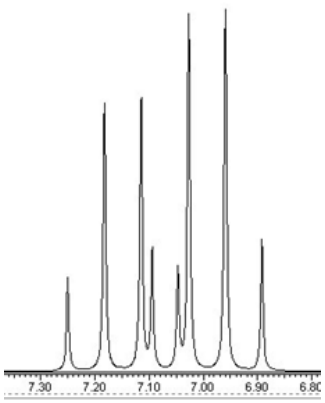
$C_4H_6O_2$



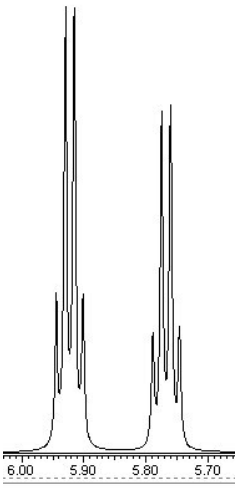


2977	37	2148	84	1436	60	1049	84	688	72
2922	41	1893	81	1423	49	991	72	538	66
2911	41	1792	77	1376	53	968	22	518	60
2836	46	1706	4	1318	14	924	47		
2715	49	1692	14	1302	29	910	52		
2810	47	1655	10	1226	16	844	64		
2621	67	1446	49	1104	66	701	36		

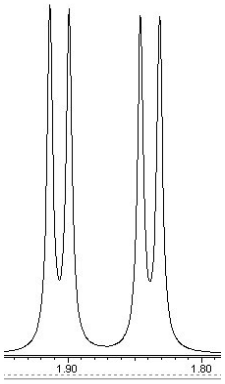




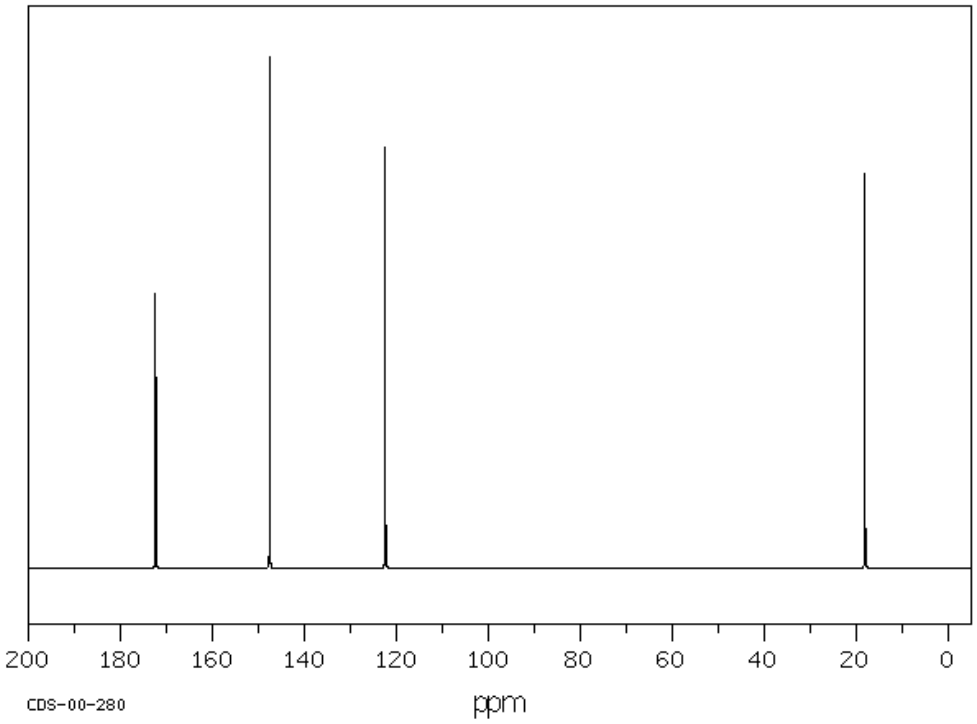
J = 15.5, 6.9 Hz



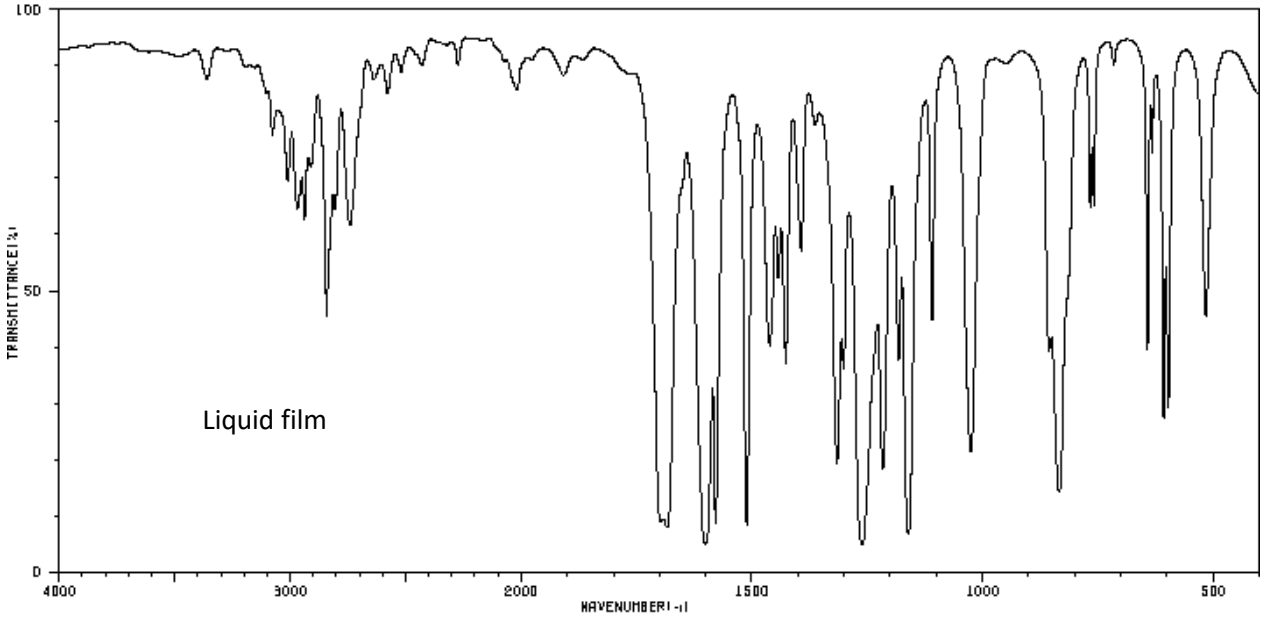
J = 15.5, 1.7 Hz

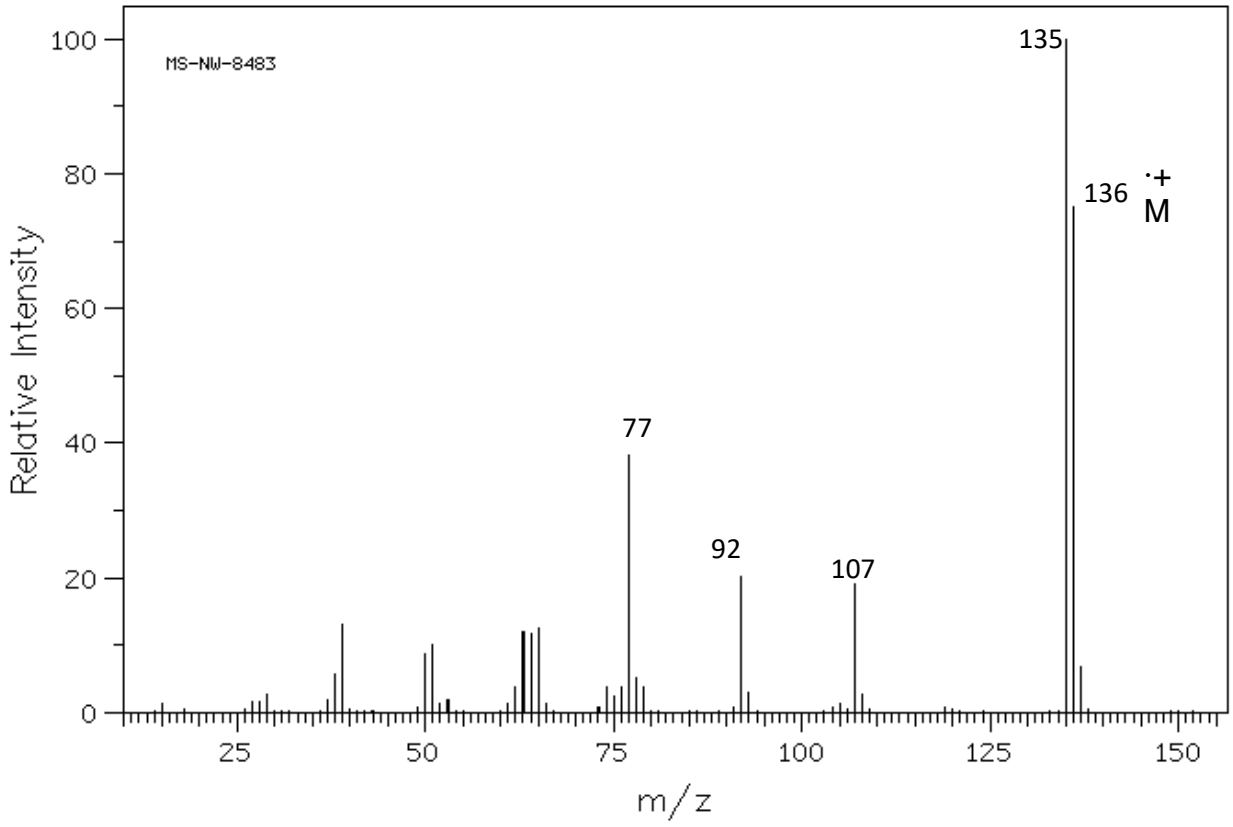


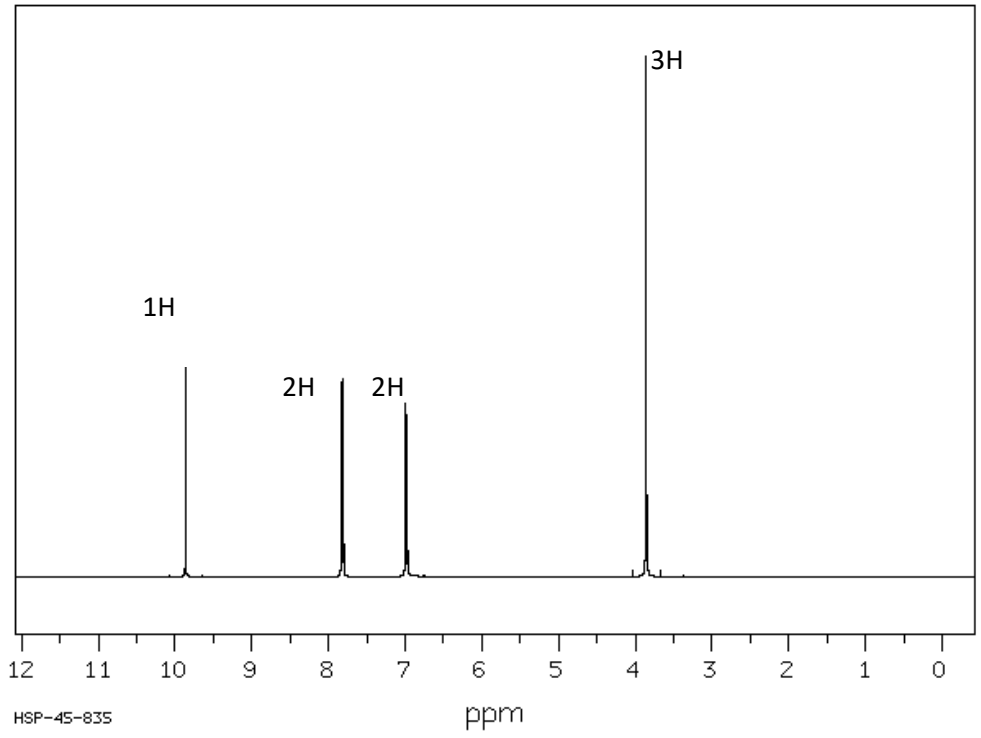
J = 6.9, 1.7 Hz

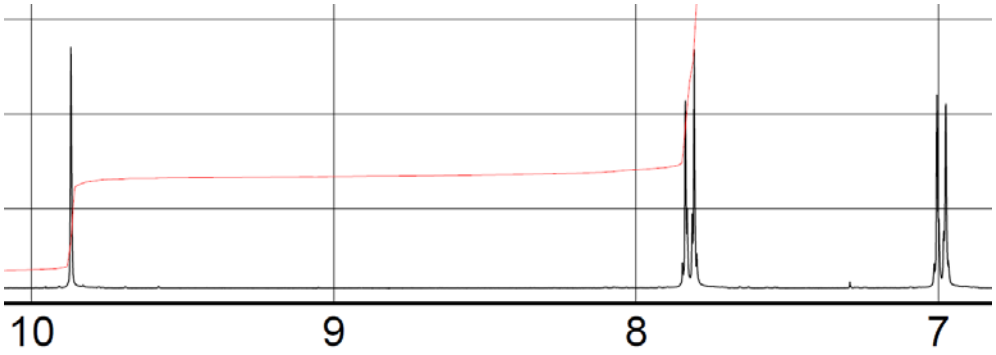


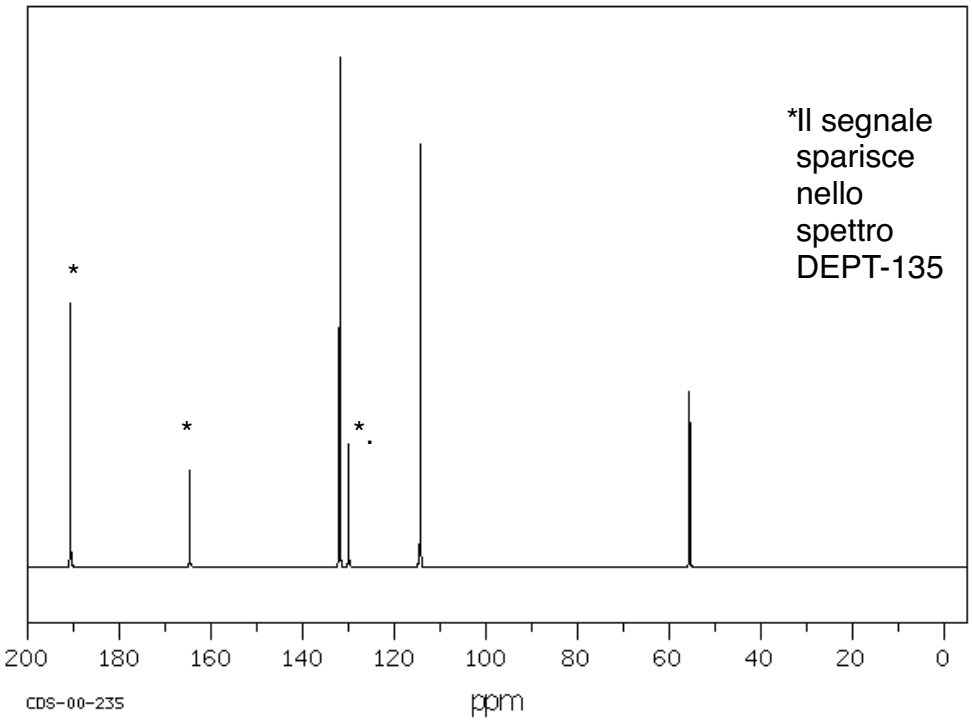
ESERCIZIO 7 Utilizzando i dati di NMR, IR e MS. Proporre una struttura per un composto di formula C8H8O2 (che contiene un 70.58% di carbonio, un 5.92% d'idrogeno e il resto è ossigeno).







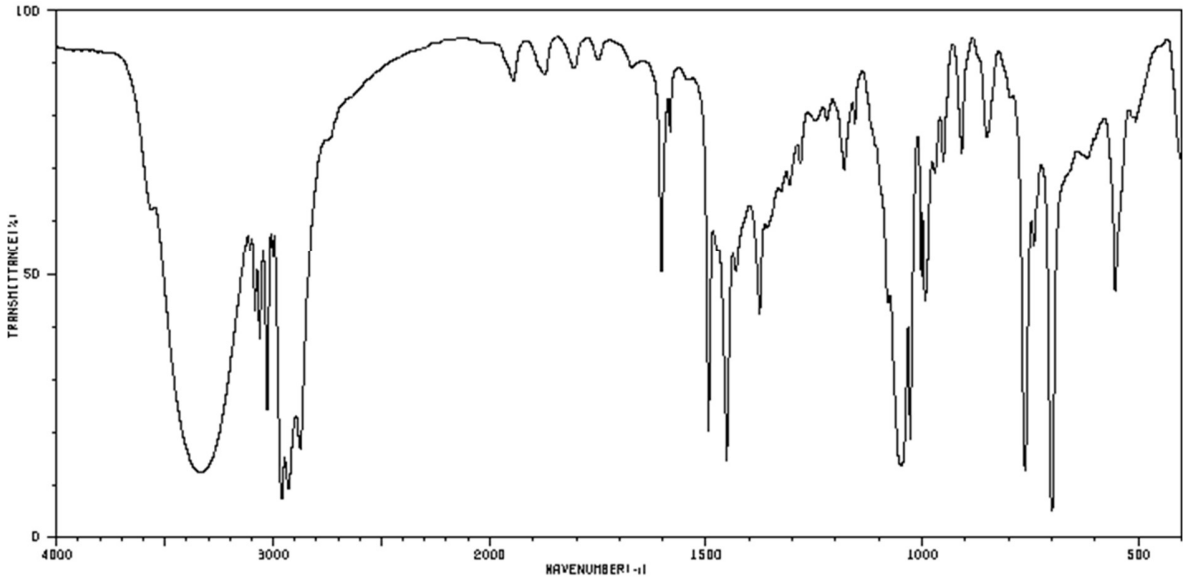




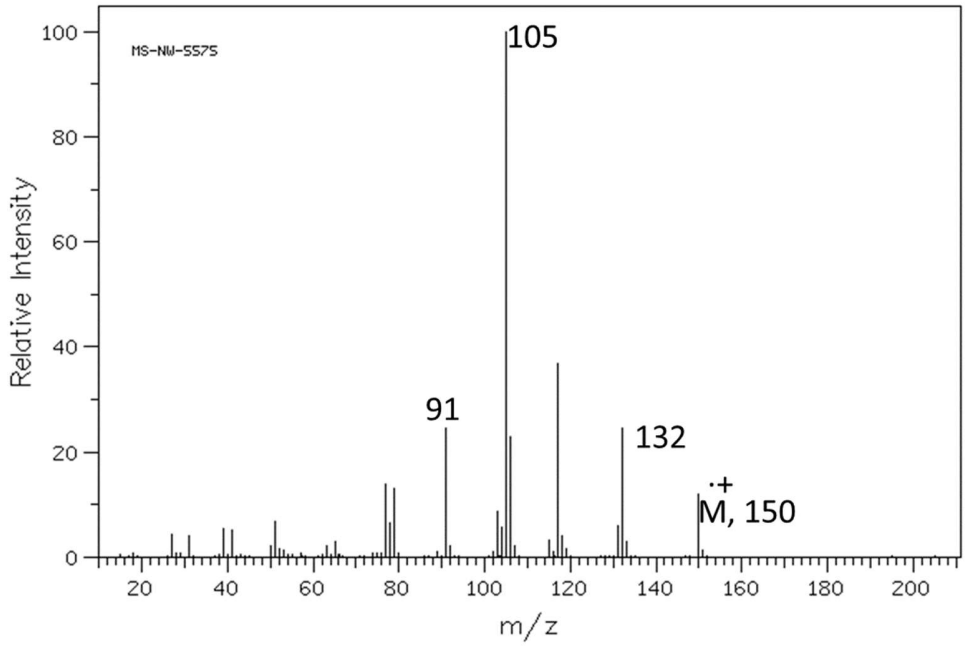
*Il segnale sparisce nello spettro DEPT-135

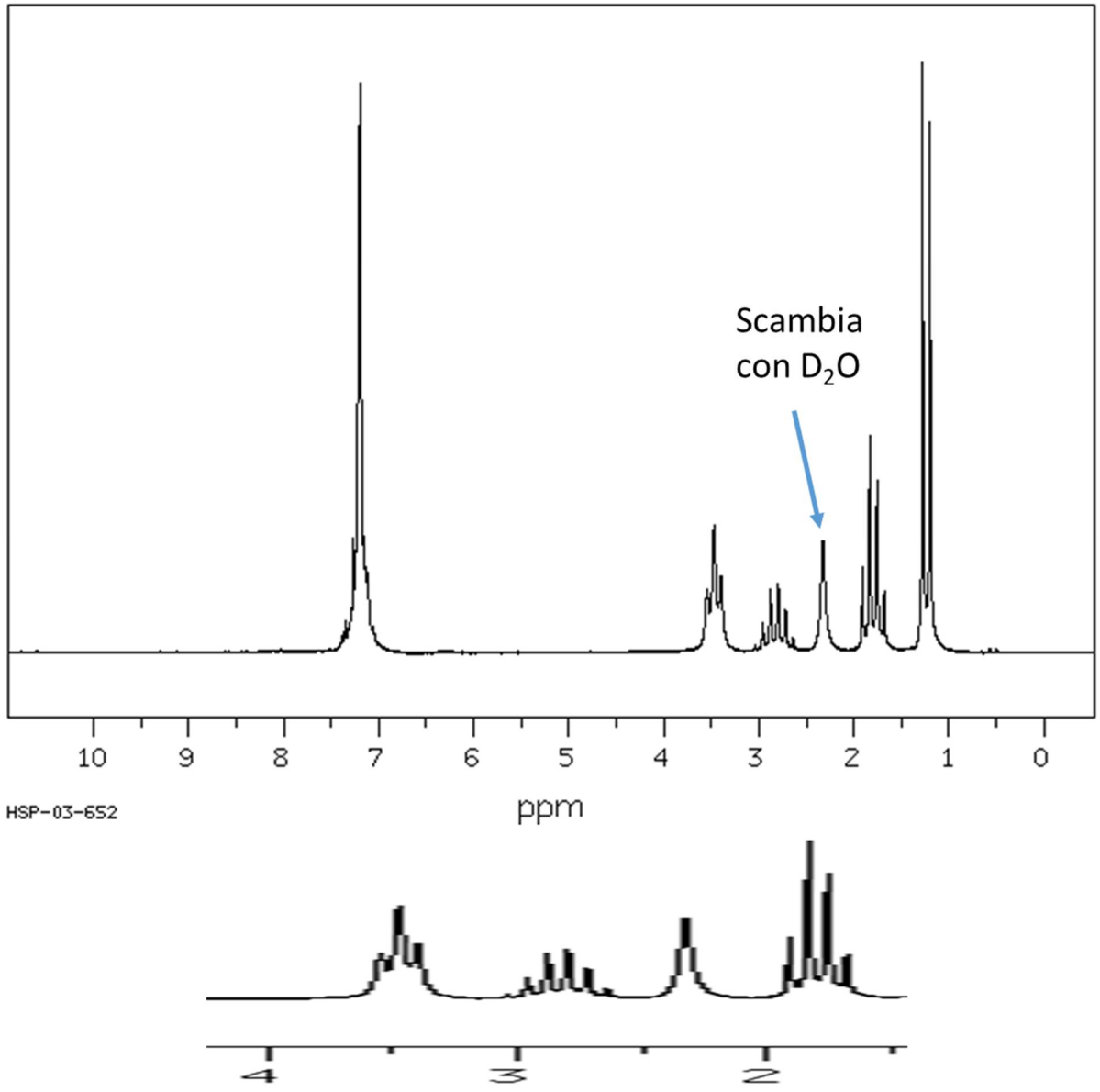
ESERCIZIO 8 C10H14O

Proporre una struttura a partire dei dati forniti. Calcolare la formula molecolare sapendo che l'analisi elementare è C: 79.96, H: 9.39, il resto è ossigeno. ~~Calcolare il grado d'insaturazione. Identificare i principali gruppi funzionali presenti nello spettro IR (film) e confermare con i dati degli altri spettri. Per lo spettro ^{1}H NMR ($CDCl_3$, 90 MHz) fare una tabella dando chemical shift, molteplicità, numero di protoni e valori di costanti di accoppiamento, assegnare i segnali. Assegnare i segnali di ^{13}C NMR~~.

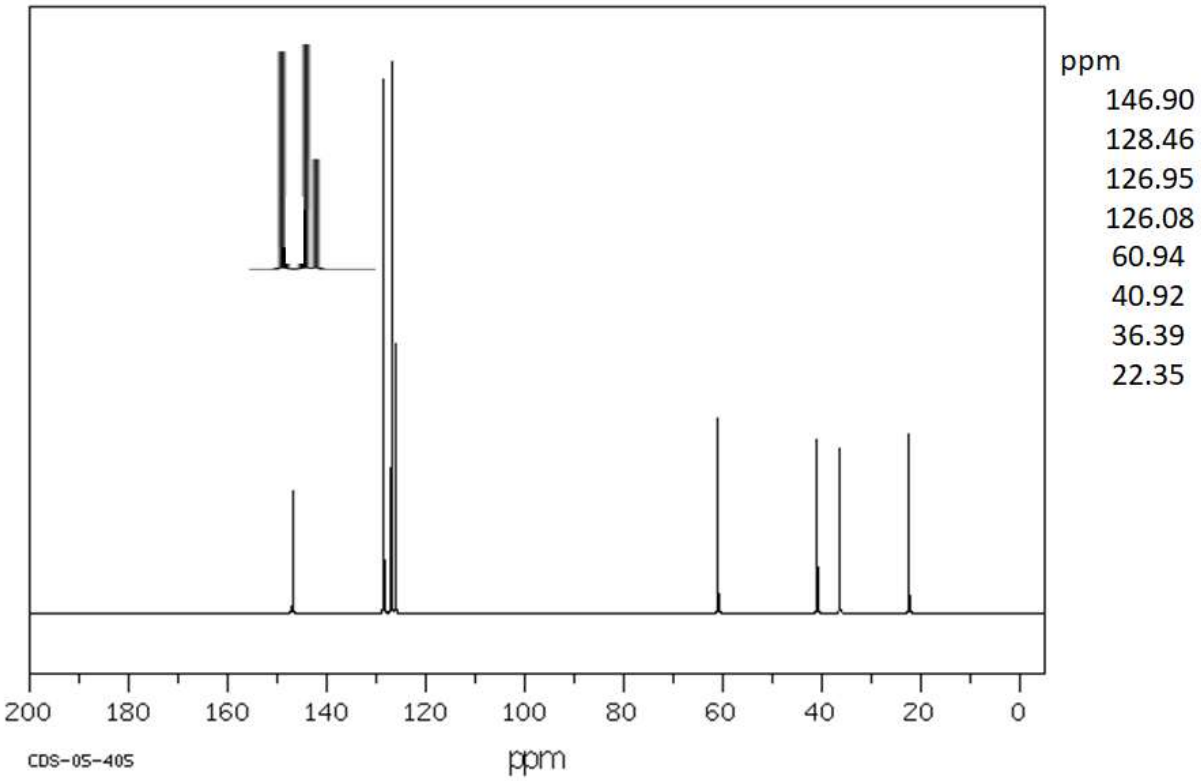


3344	12	2968	7	1431	49	1079	42	909	70		
3332	12	2929	8	1376	41	1048	13	850	72		
3107	52	2874	15	1307	84	1028	17	763	12		
3084	41	1603	49	1282	68	1002	47	742	63		
3062	36	1583	74	1247	77	993	43	700	4		
3028	23	1494	19	1181	86	971	66	618	70		
3002	62	1453	19	1156	74	951	68	554	44		

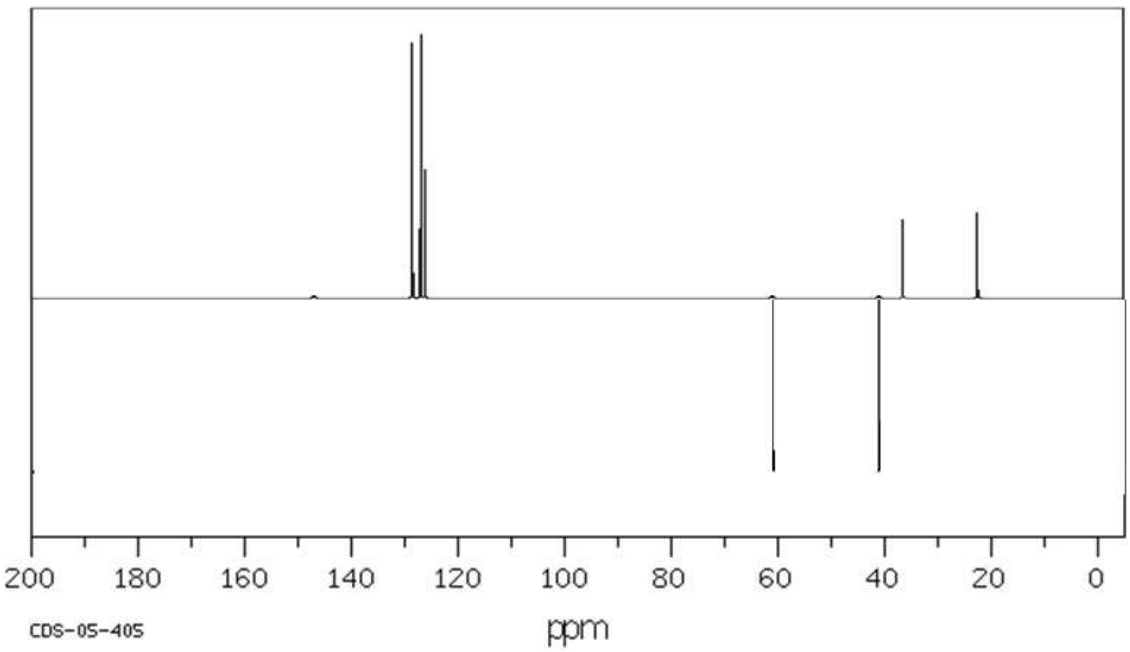



Scambia
con D_2O
10
9
8
7
6
5
4
3
2
1
0
ppm
HSP-03-652
4
3
2

Hz	ppm	Int.
658.44	7.352	53
655.94	7.325	41
655.13	7.315	44
653.19	7.294	75
650.38	7.262	194
648.00	7.236	242
645.94	7.213	894
644.19	7.193	966
642.13	7.170	266
640.63	7.154	199
638.56	7.130	145
638.13	7.126	143
637.00	7.113	134
632.63	7.064	41
631.69	7.054	45
630.13	7.036	32
317.31	3.543	107
315.00	3.518	69
310.88	3.472	218
307.06	3.429	75
304.31	3.398	130
304.13	3.396	130
264.88	2.958	51
257.69	2.878	106
250.50	2.798	118
243.38	2.718	73
208.06	2.324	189
170.81	1.908	144
164.25	1.834	369
160.50	1.793	45
157.00	1.754	293
152.63	1.705	32
152.25	1.700	32
150.19	1.677	105
114.25	1.276	1000
107.31	1.199	901

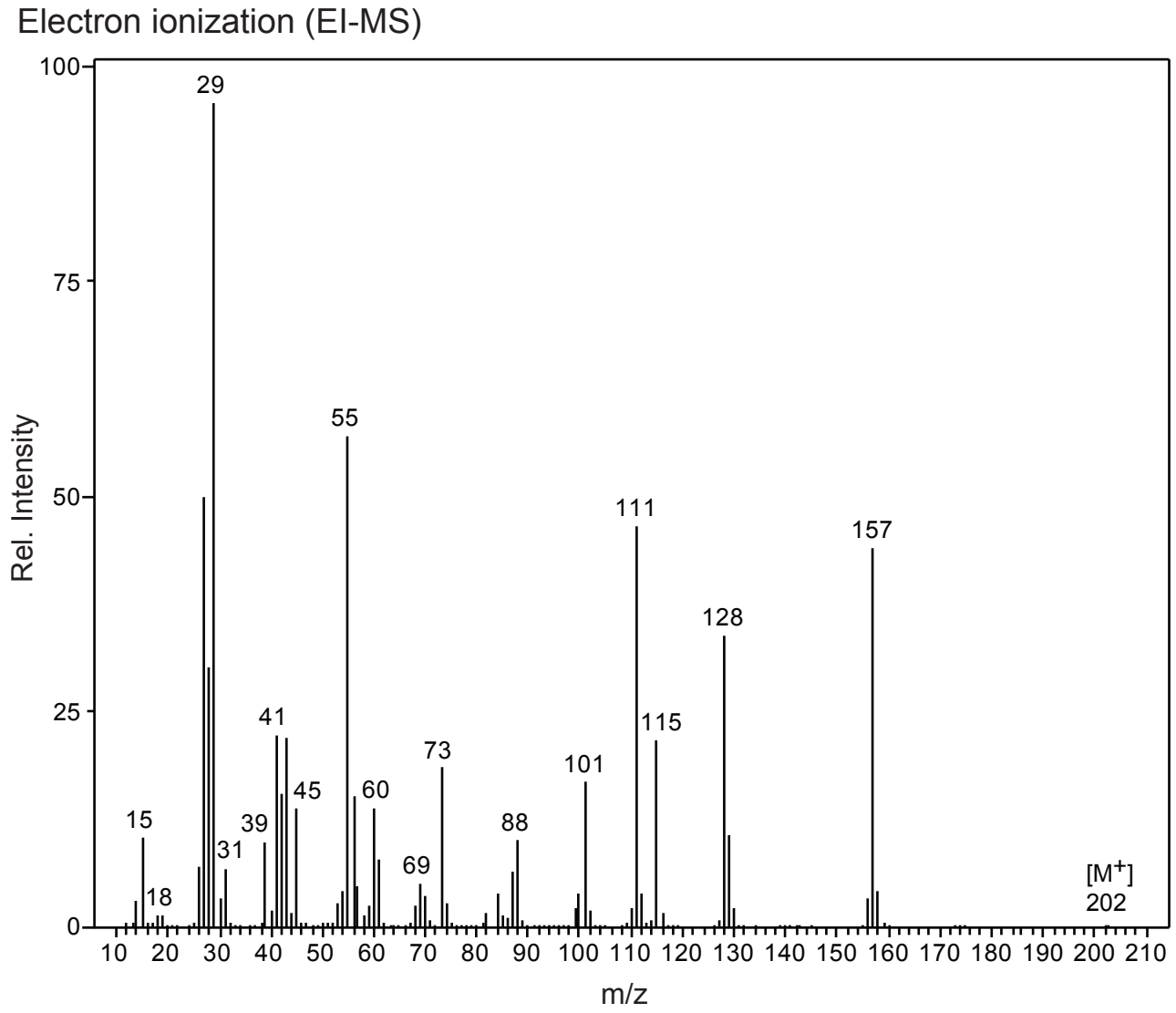

ppm
146.90
128.46
126.95
126.08
60.94
40.92
36.39
22.35
200
180
160
140
120
100
80
60
40
20
0
CDS-0S-40S
ppm

DEPT-135

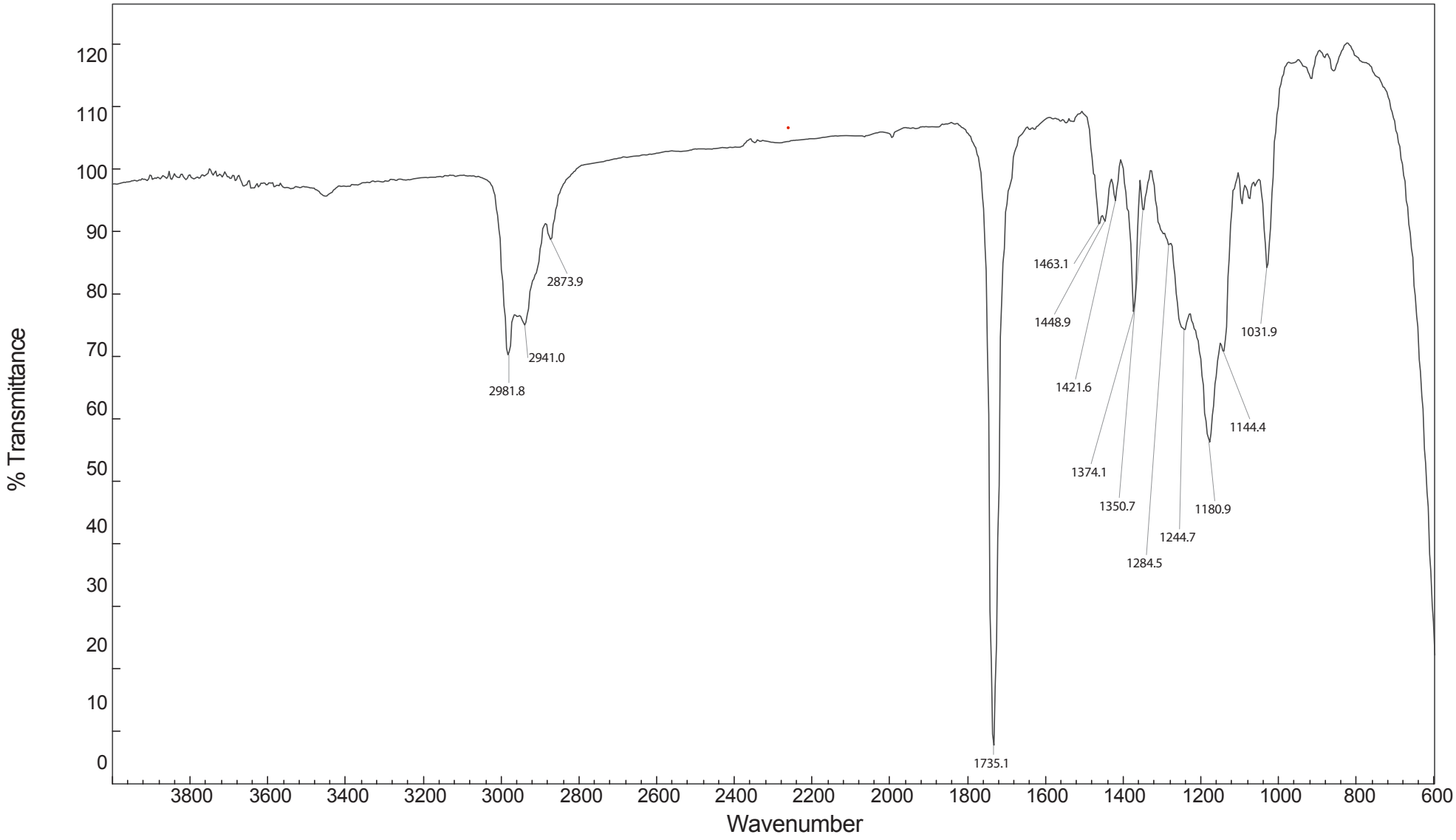

200
180
160
140
120
100
80
60
40
20
0
CDS-0S-40S
ppm

ESERCICIO 9

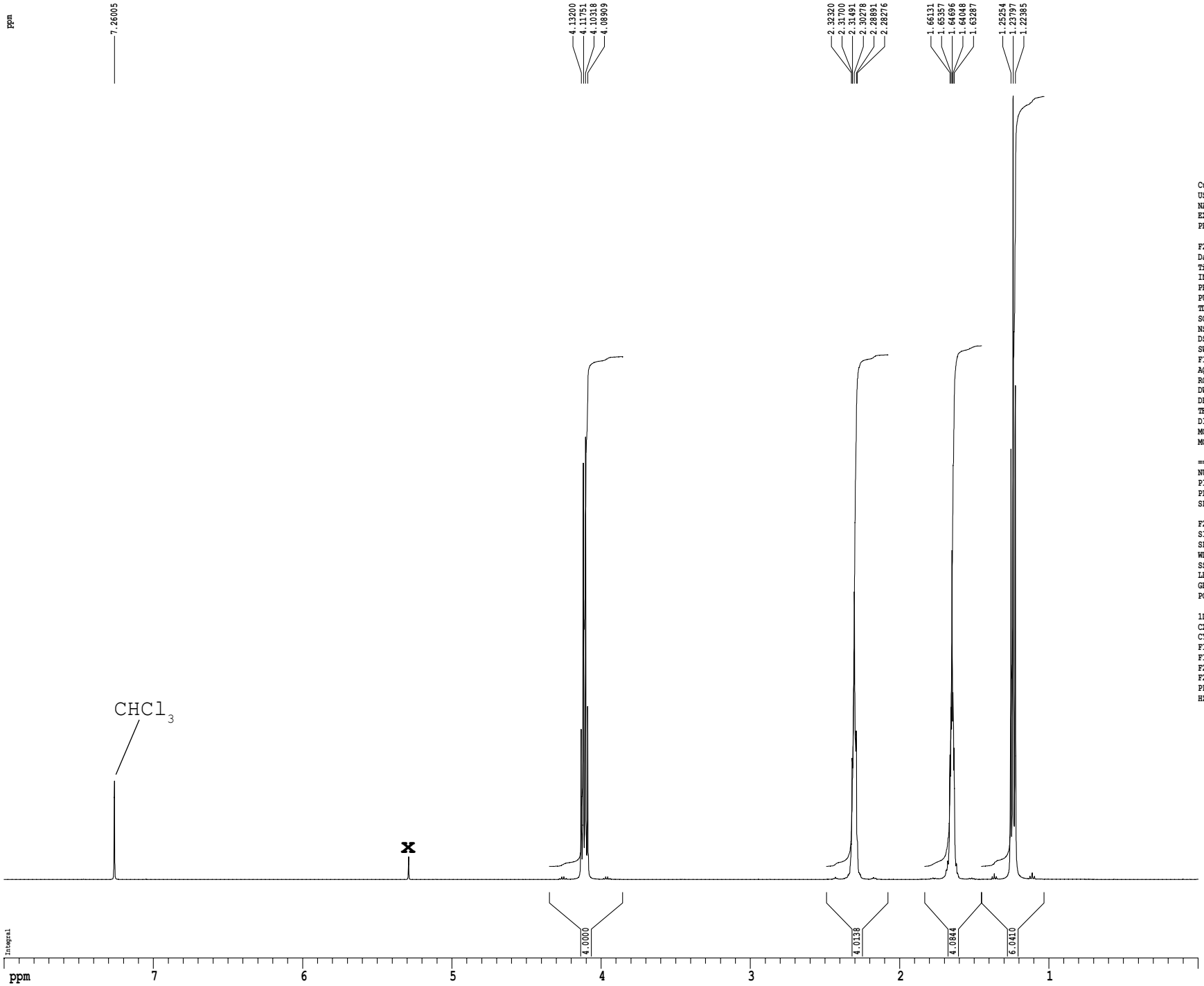
Proporre una struttura per un composto di formula C10H18O4.Si forniscono i dati di EI-MS, IR (film), 1H-NMR (500 MHz), 13C-NMR (125 MHz), DEPT 90, e DEPT 135 in CDCl3.



Varian Resolutions Pro

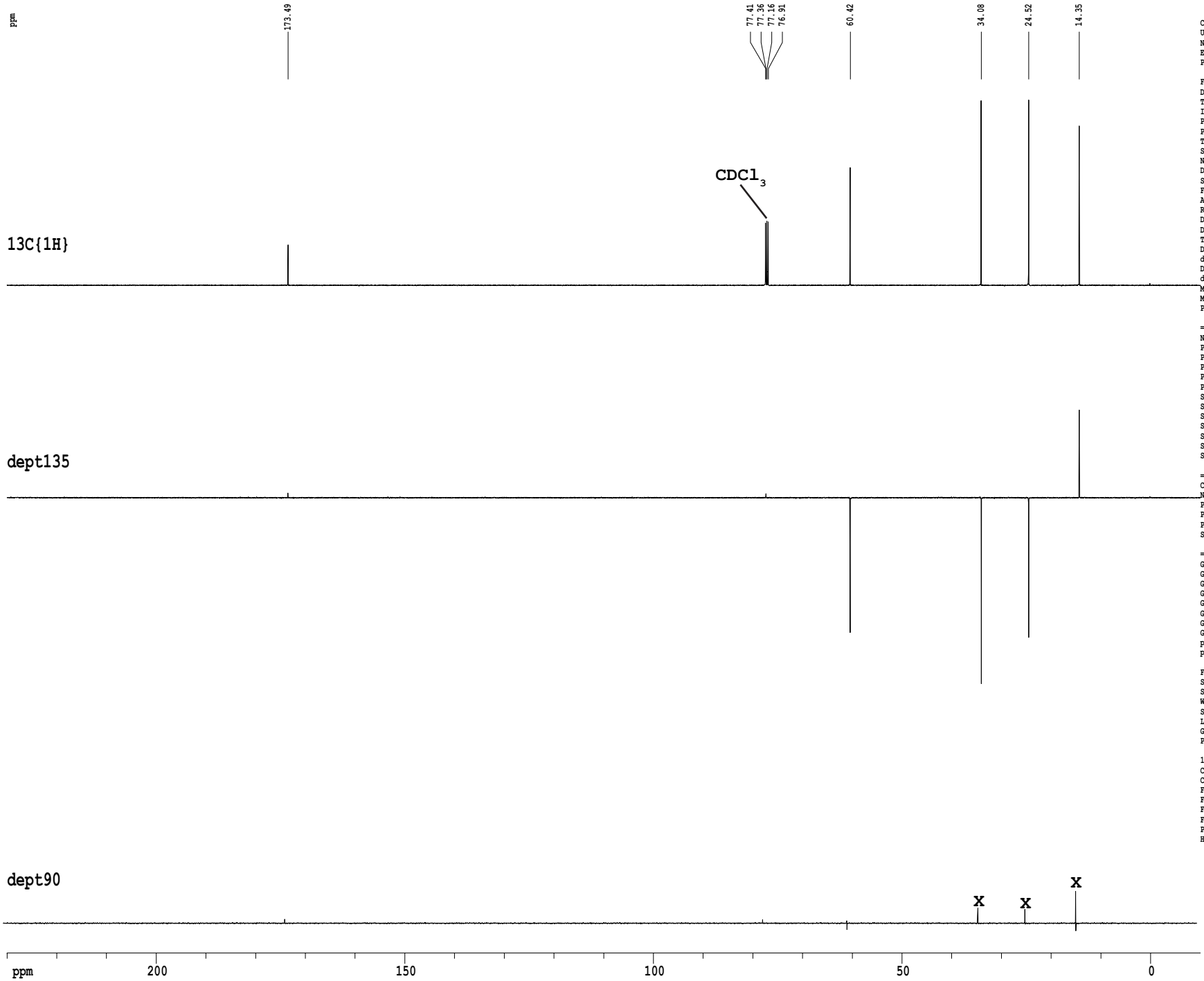


1H spectrum



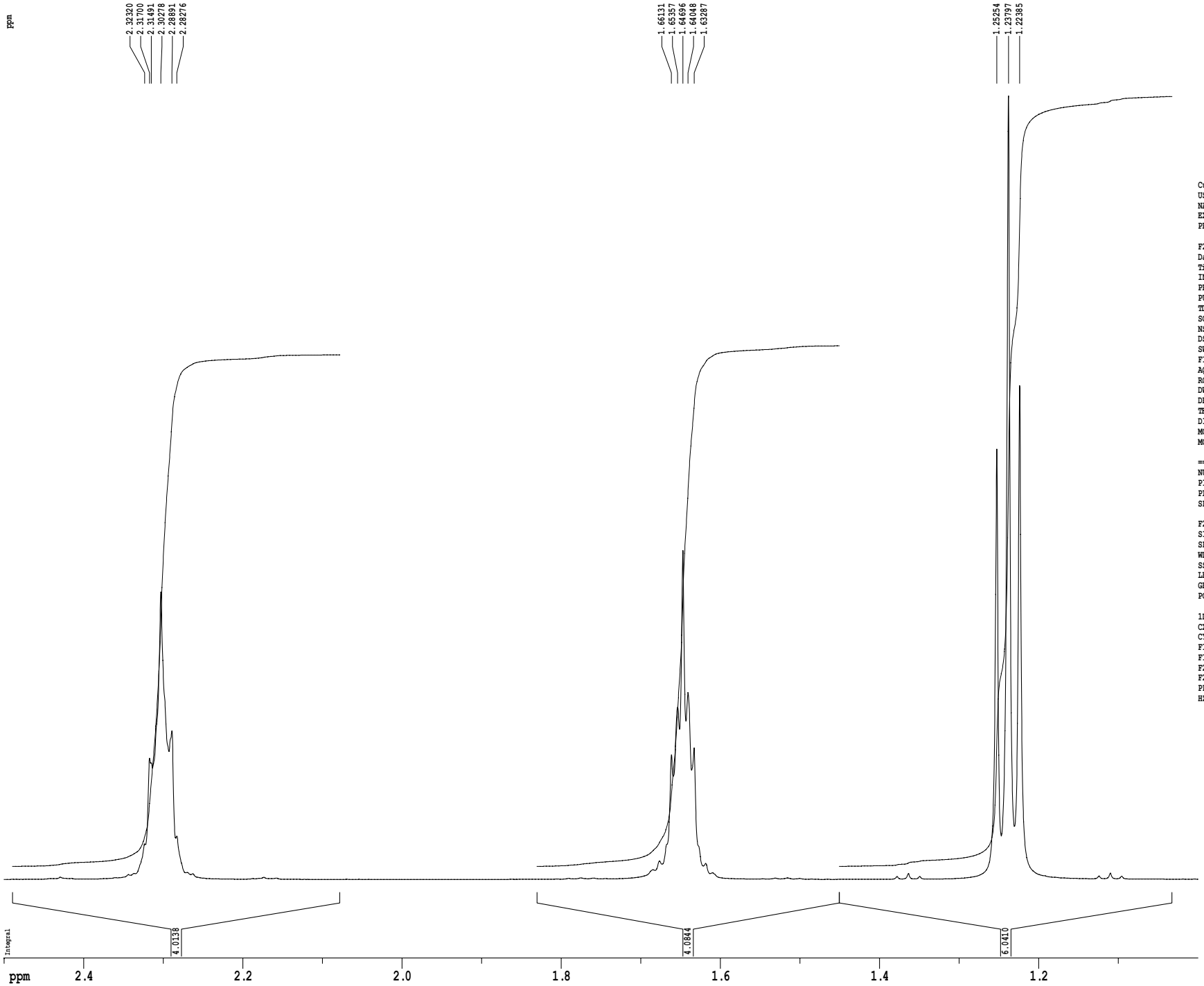

```
Current Data Parameter
USER              nmr14t
NAME      midterm I b
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20141030
Time              20.45
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG            zg30
TD                81728
SOLVENT           CDCl3
NS                   32
DS                    2
SWH            8012.820 Hz
FIDRES         0.098043 Hz
AQ             5.0998774 sec
RG                 6.3
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1           0.10000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                1H
P1                7.50 usec
PL1               1.60 dB
SFO1        500.2235015 MHz

F2 - Processing parameter
SI                65536
SF          500.2200312 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 4.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P               8.000 ppm
F1              4001.76 Hz
F2P               0.000 ppm
F2                 0.00 Hz
PPMCM          0.35088 ppm/cm
HZCM         175.51581 Hz/cm
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER              nmr14t
NAME         midterm I b
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141030
Time              20.59
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                65536
SOLVENT           CDCl3
NS                  648
DS                   16
SWH           30303.031 Hz
FIDRES        0.462388 Hz
AQ            1.0813940 sec
RG               7298.2
DW               16.500 usec
DE                6.00 usec
TE               298.0 K
D1           0.25000000 sec
d11          0.03000000 sec
D16          0.00020000 sec
d17          0.00019600 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec
P2                31.00 usec

======== CHANNEL f1 =======
NUC1                13C
P1                15.50 usec
P11              500.00 usec
P12             2000.00 usec
PL0              120.00 dB
PL1               -1.00 dB
SFO1         125.7942548 MHz
SP1               3.20 dB
SP2               3.20 dB
SPNAM1   Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1              0.00 Hz
SPOFF2              0.00 Hz

======== CHANNEL f2 =======
CPDPRG2         waltz16
NUC2                1H
PCPD2            100.00 usec
PL2               1.60 dB
PL12             24.60 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15              500.00 usec
p16             1000.00 usec

F2 - Processing parameters
SI                  65536
SF           125.7804094 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                 2.00

1D NMR plot parameters
CX                 22.80 cm
CY                  3.56 cm
F1P               230.000 ppm
F1              28929.49 Hz
F2P               -10.000 ppm
F2              -1257.80 Hz
PPMCM           10.52632 ppm/cm
HZCM          1324.00439 Hz/cm
```

1H spectrum



Current Data Parameter

USER	nmr14t
NAME	midterm I b
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20141030
Time	20.45
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	zg30
TD	81728
SOLVENT	CDCl3
NS	32
DS	2
SWH	8012.820 Hz
FIDRES	0.098043 Hz
AQ	5.0998774 sec
RG	6.3
DW	62.400 usec
DE	6.00 usec
TE	298.0 K
D1	0.10000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2235015 MHz

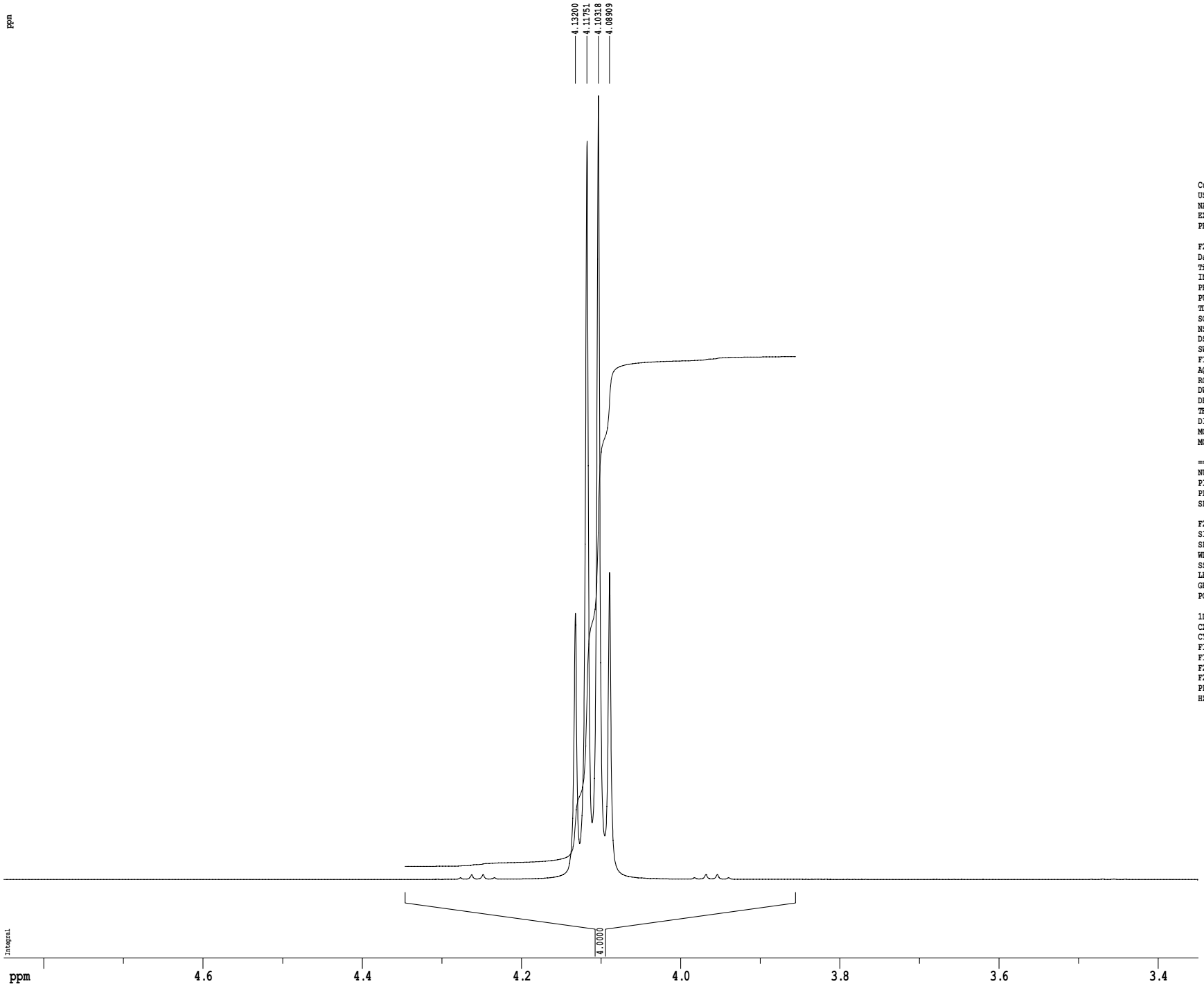
F2 - Processing parameter

SI	65536
SF	500.2200312 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00

1D NMR plot parameters

CX	22.80 cm
CY	15.00 cm
F1P	2.500 ppm
F1	1250.55 Hz
F2P	1.000 ppm
F2	500.22 Hz
PPMCM	0.06579 ppm/cm
HZCM	32.90921 Hz/cm

1H spectrum

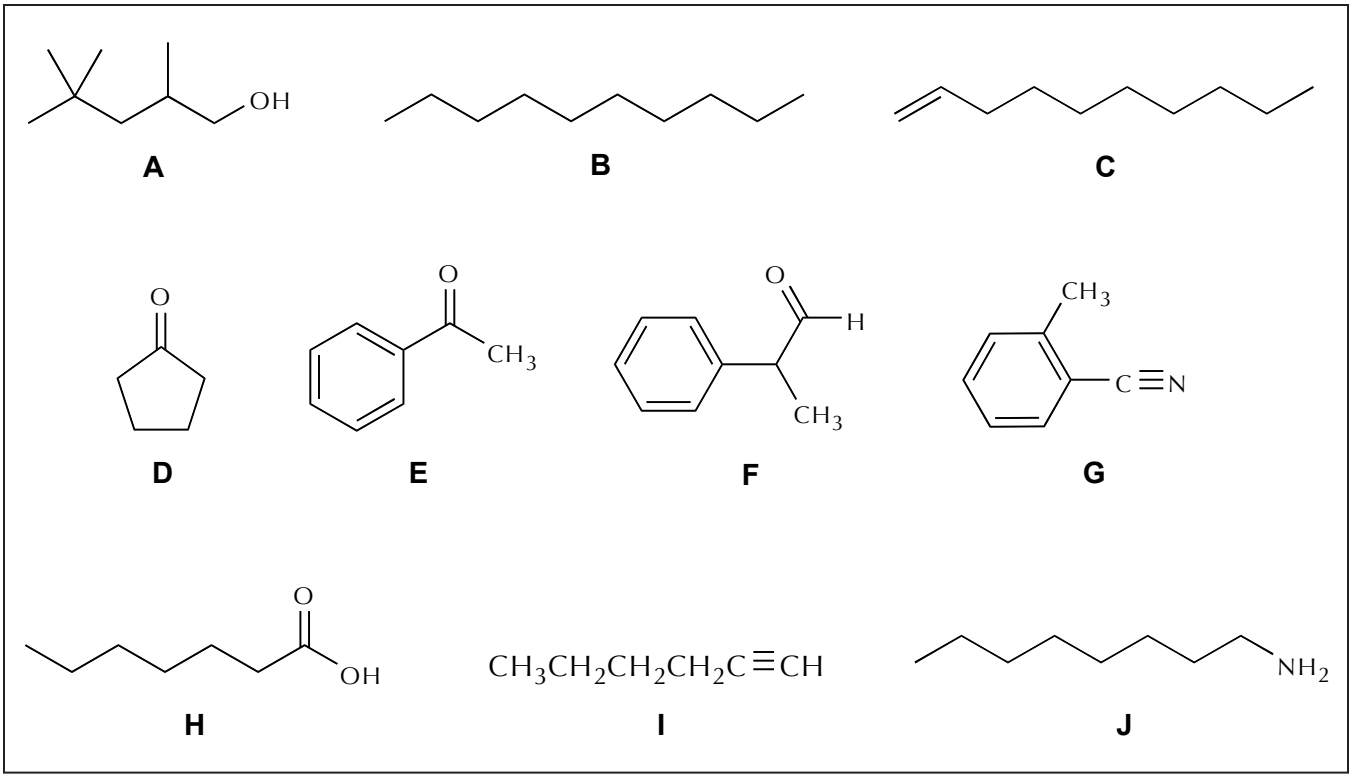



```
Current Data Parameter
USER                nmr14t
NAME           midterm I b
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20141030
Time                20.45
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG               zg30
TD                   81728
SOLVENT              CDCl3
NS                      32
DS                       2
SWH              8012.820 Hz
FIDRES           0.098043 Hz
AQ               5.0998774 sec
RG                     6.3
DW                62.400 usec
DE                 6.00 usec
TE                 298.0 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
PL1                  1.60 dB
SFO1          500.2235015 MHz

F2 - Processing parameter
SI                   65536
SF            500.2200312 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   4.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.00 cm
F1P                  4.850 ppm
F1                 2426.07 Hz
F2P                  3.350 ppm
F2                 1675.74 Hz
PPMCM             0.06579 ppm/cm
HZCM             32.90921 Hz/cm
```

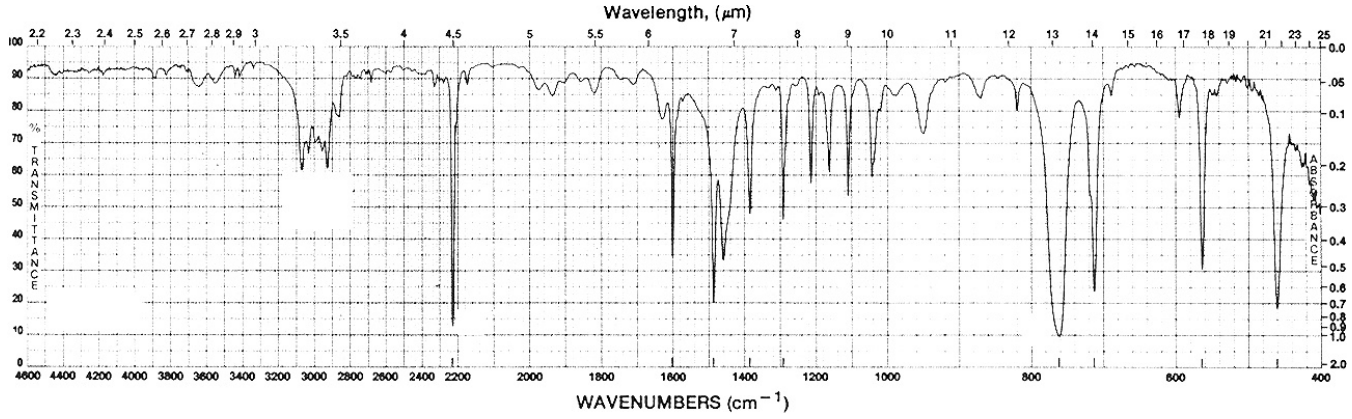
DU=/v, USER=nmr14t, NAME=midterm I b, EXPNO=1, PROCNO=1
F1=8.000ppm, F2=0.000ppm, MI=0.50cm, MAXI=10000.00cm, PC=4.000

#	ADDRESS	FREQUENCY [Hz]	FREQUENCY [PPM]	INTENSITY
1	31448.8	3631.621	7.260	1.88
2	44246.4	2066.911	4.1320	2.88
3	44305.7	2059.659	4.1175	7.97
4	44364.4	2052.490	4.1032	8.46
5	44422.0	2045.443	4.0891	3.31
6	51646.7	1162.111	2.3232	0.68
7	51672.0	1159.011	2.3170	2.32
8	51680.6	1157.965	2.3149	2.23
9	51730.2	1151.898	2.3028	5.50
10	51787.0	1144.957	2.2889	2.84
11	51812.1	1141.880	2.2828	0.83
12	54354.6	831.020	1.6613	2.39
13	54386.3	827.148	1.6536	3.30
14	54413.3	823.841	1.6470	6.29
15	54439.9	820.599	1.6405	3.57
16	54471.0	816.795	1.6329	2.51
17	56027.0	626.545	1.2525	8.22
18	56086.6	619.256	1.2380	15.00
19	56144.4	612.195	1.2239	9.46

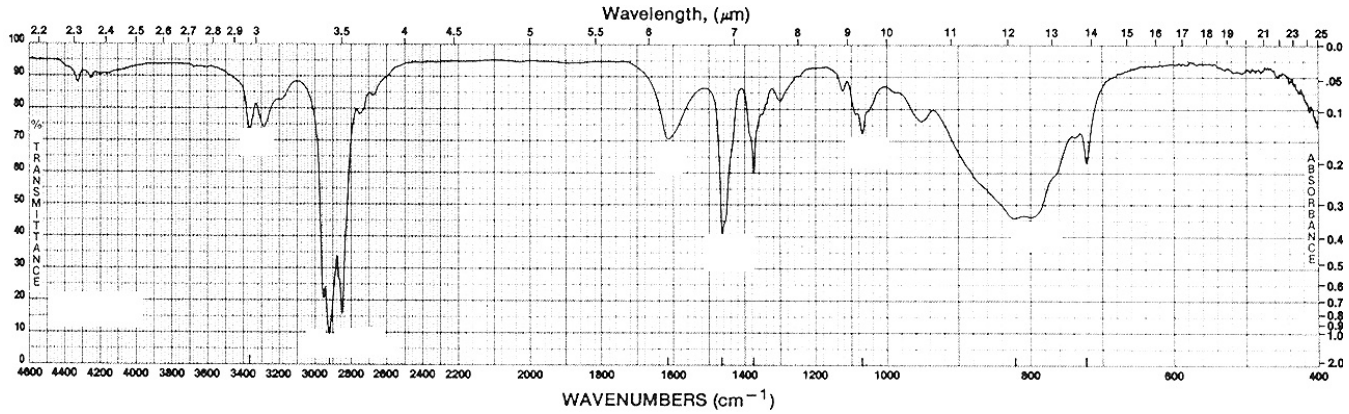
ASSEGNARE AD OGNI STRUTTURA UNO DEGLI SPETTRI IR



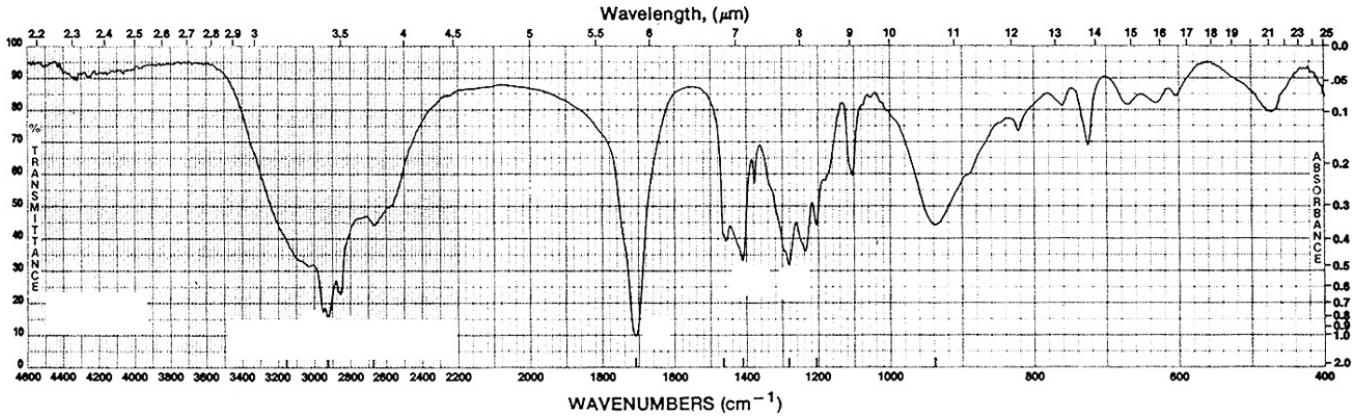
SPECTRUM 1



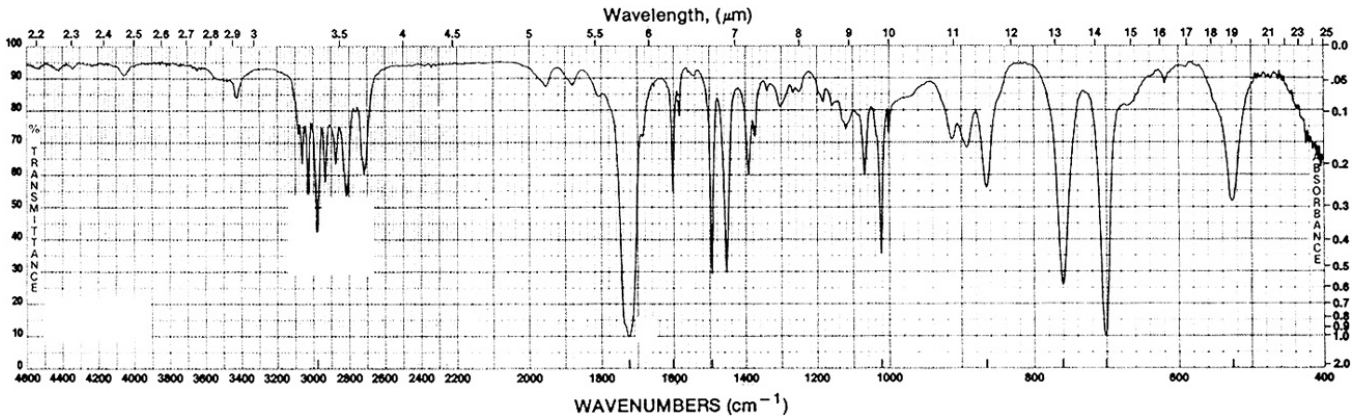
SPECTRUM 2



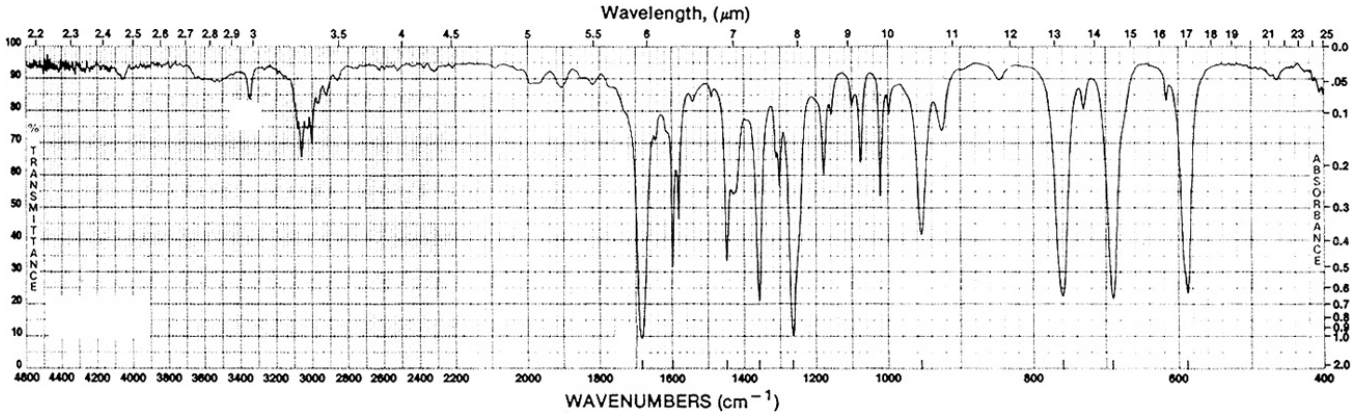
SPECTRUM 3



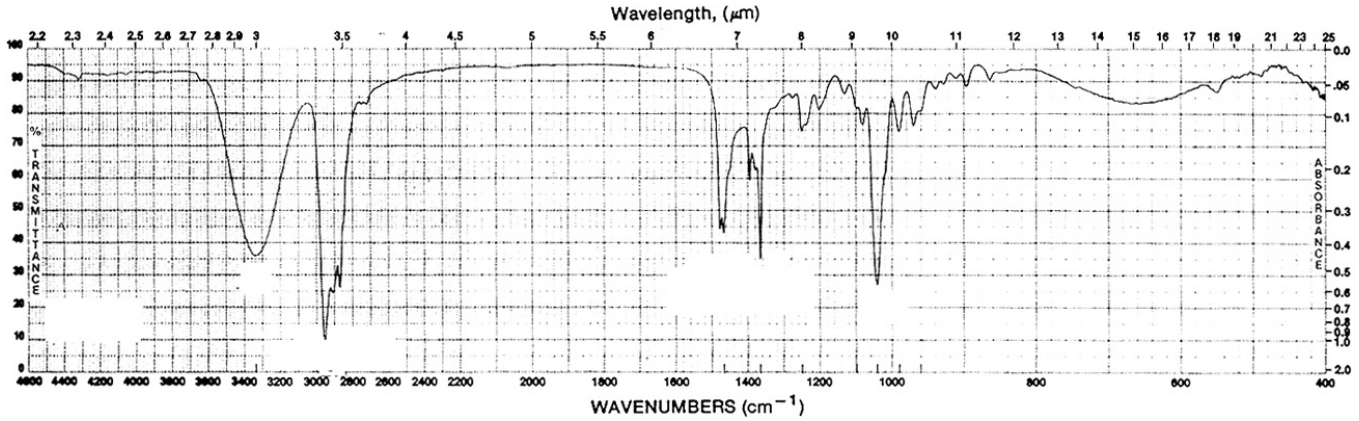
SPECTRUM 4



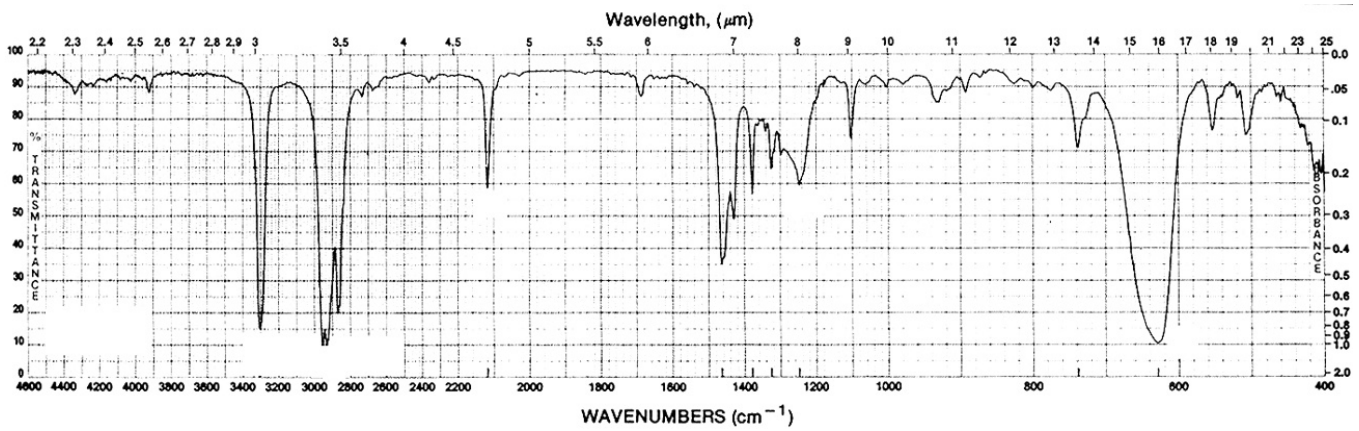
SPECTRUM 5



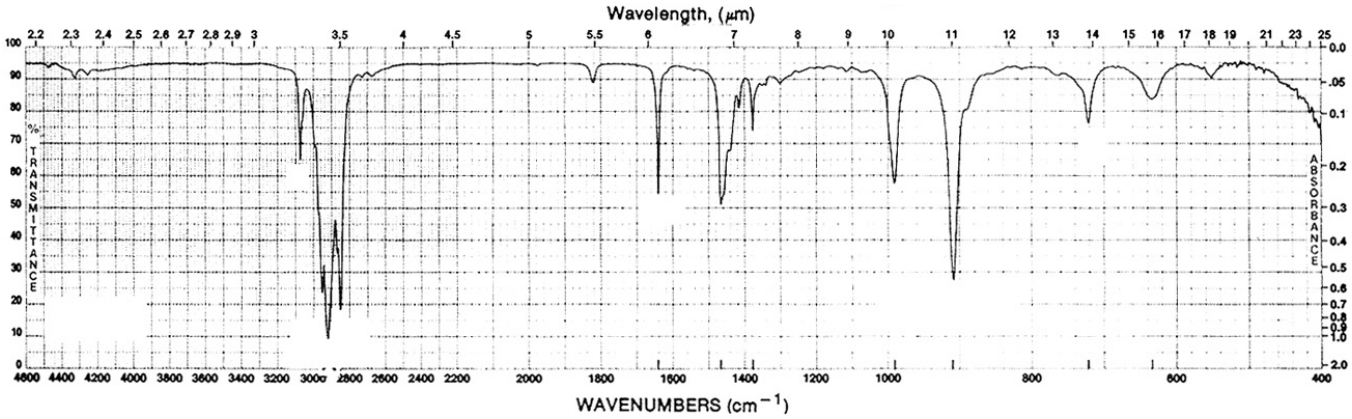
SPECTRUM 6



SPECTRUM 7



SPECTRUM 8



SPECTRUM 10