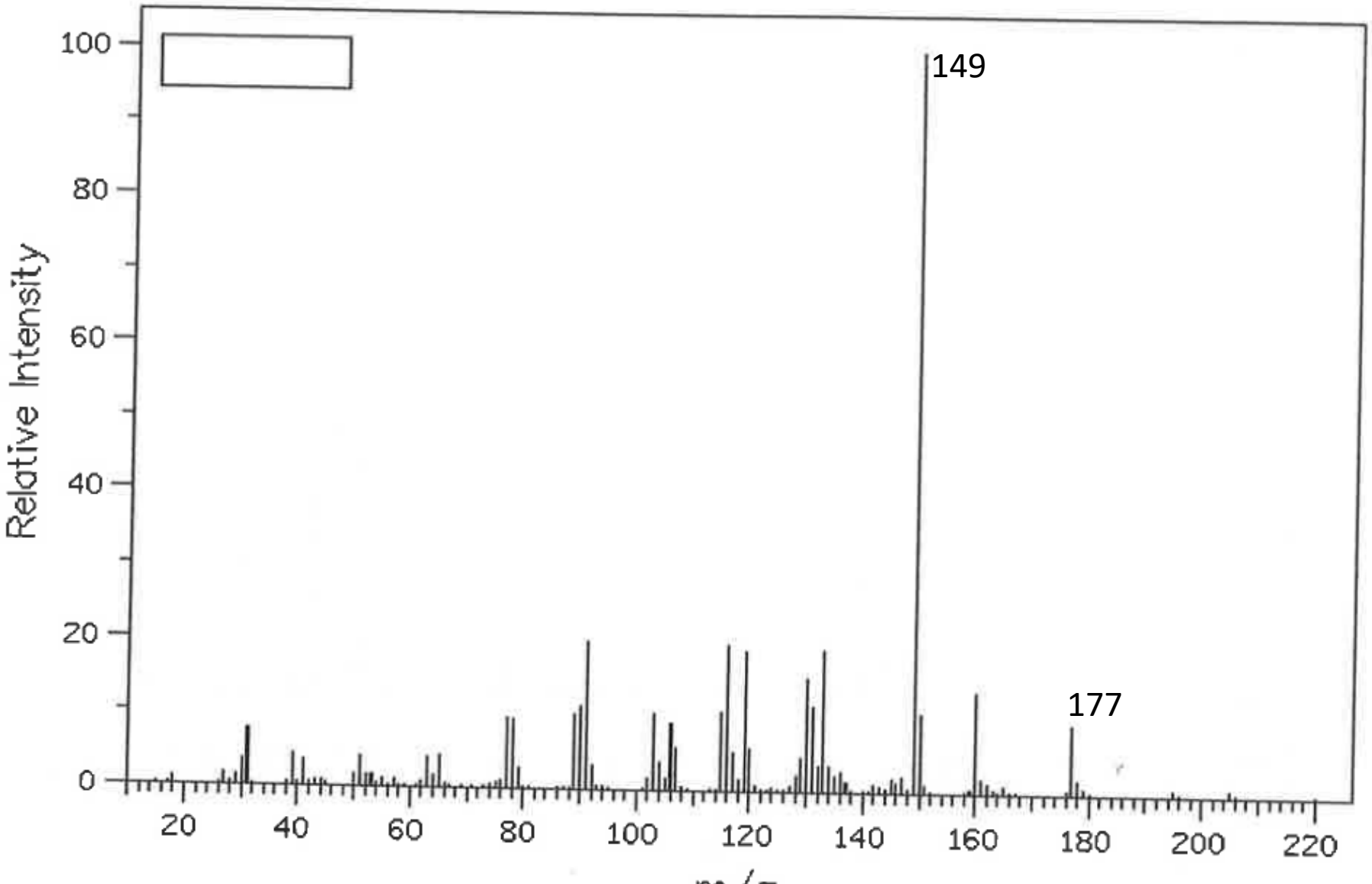
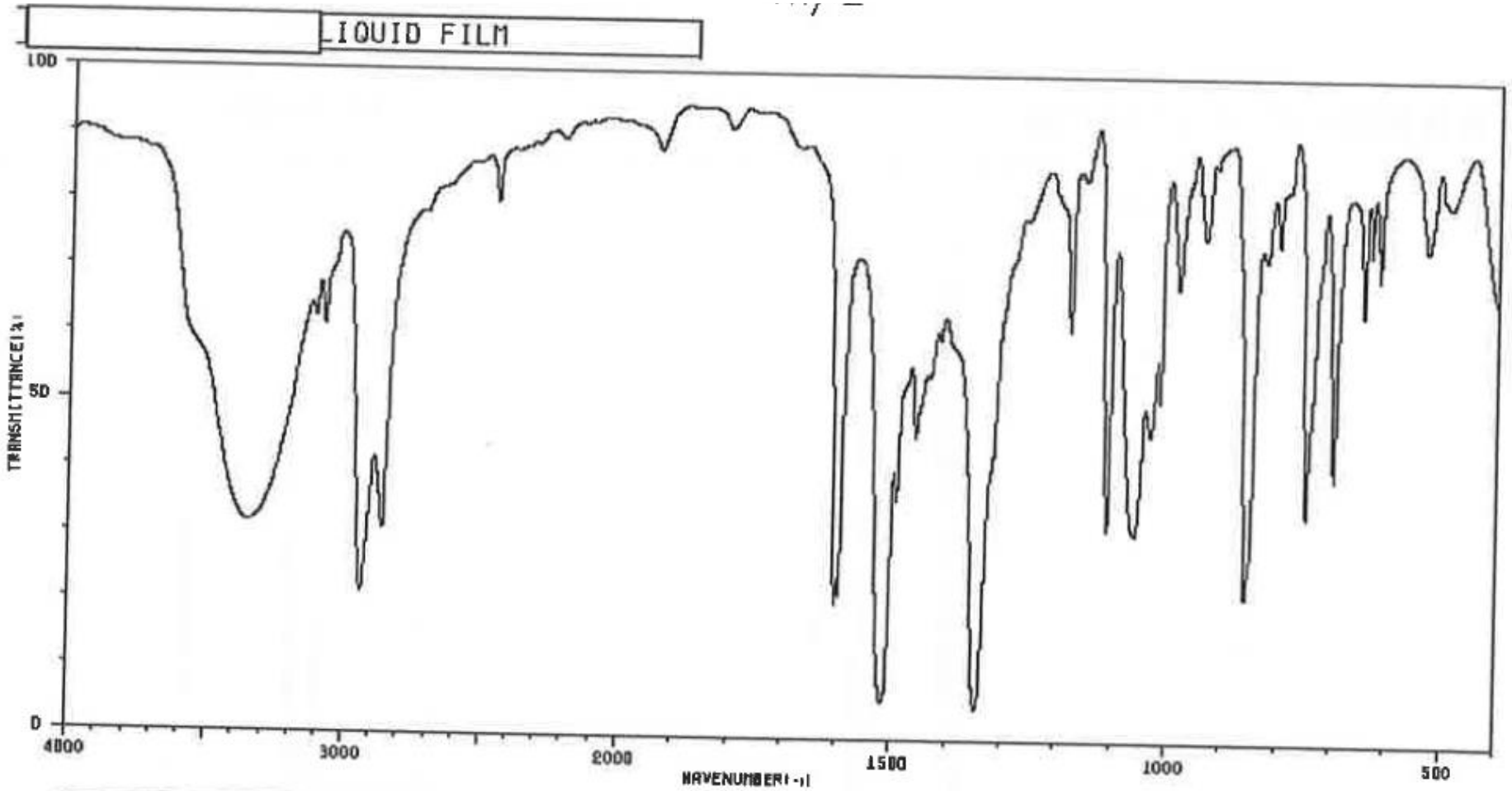
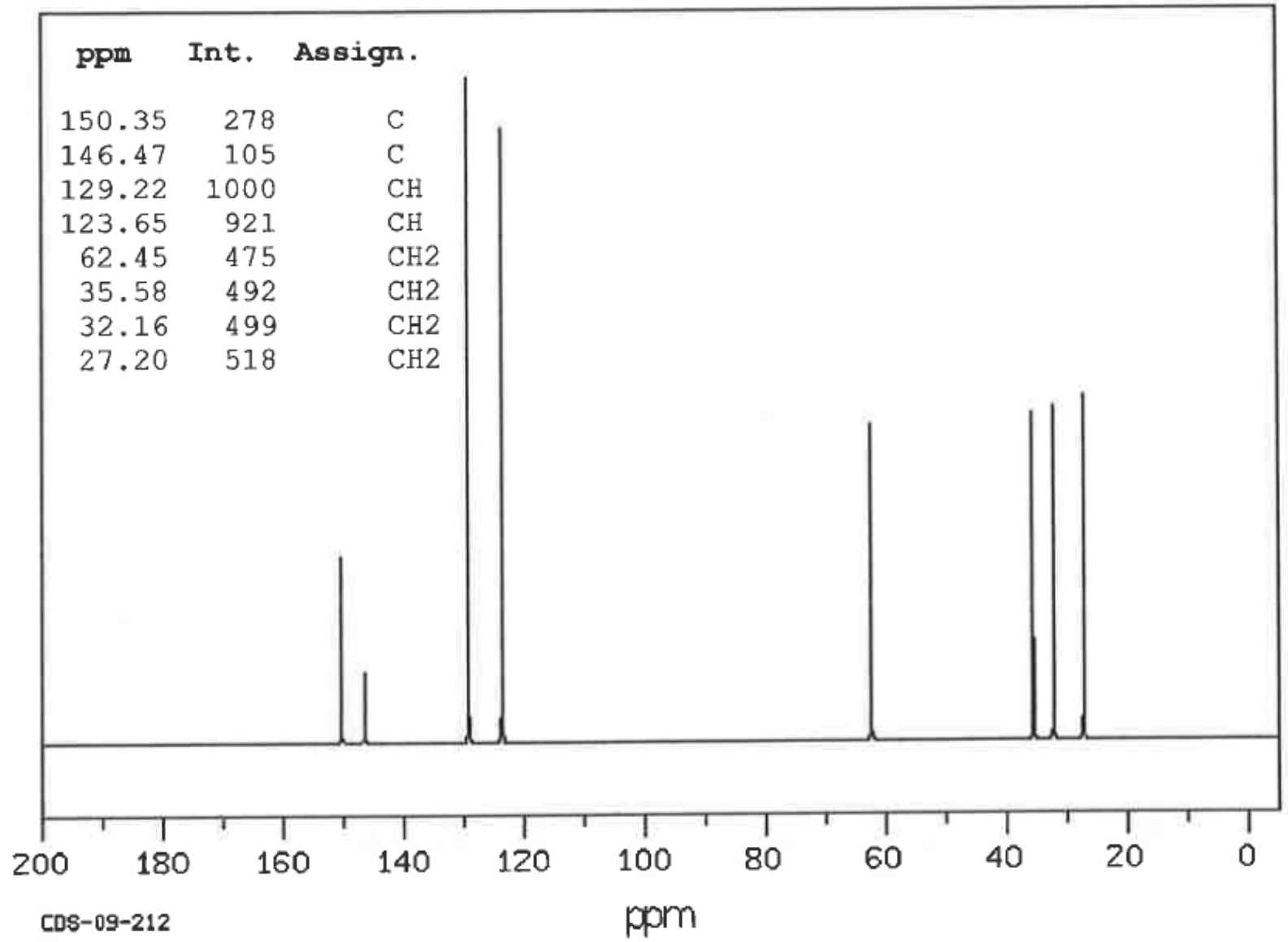
C10H13NO3 (Mass of molecular ion: 195)





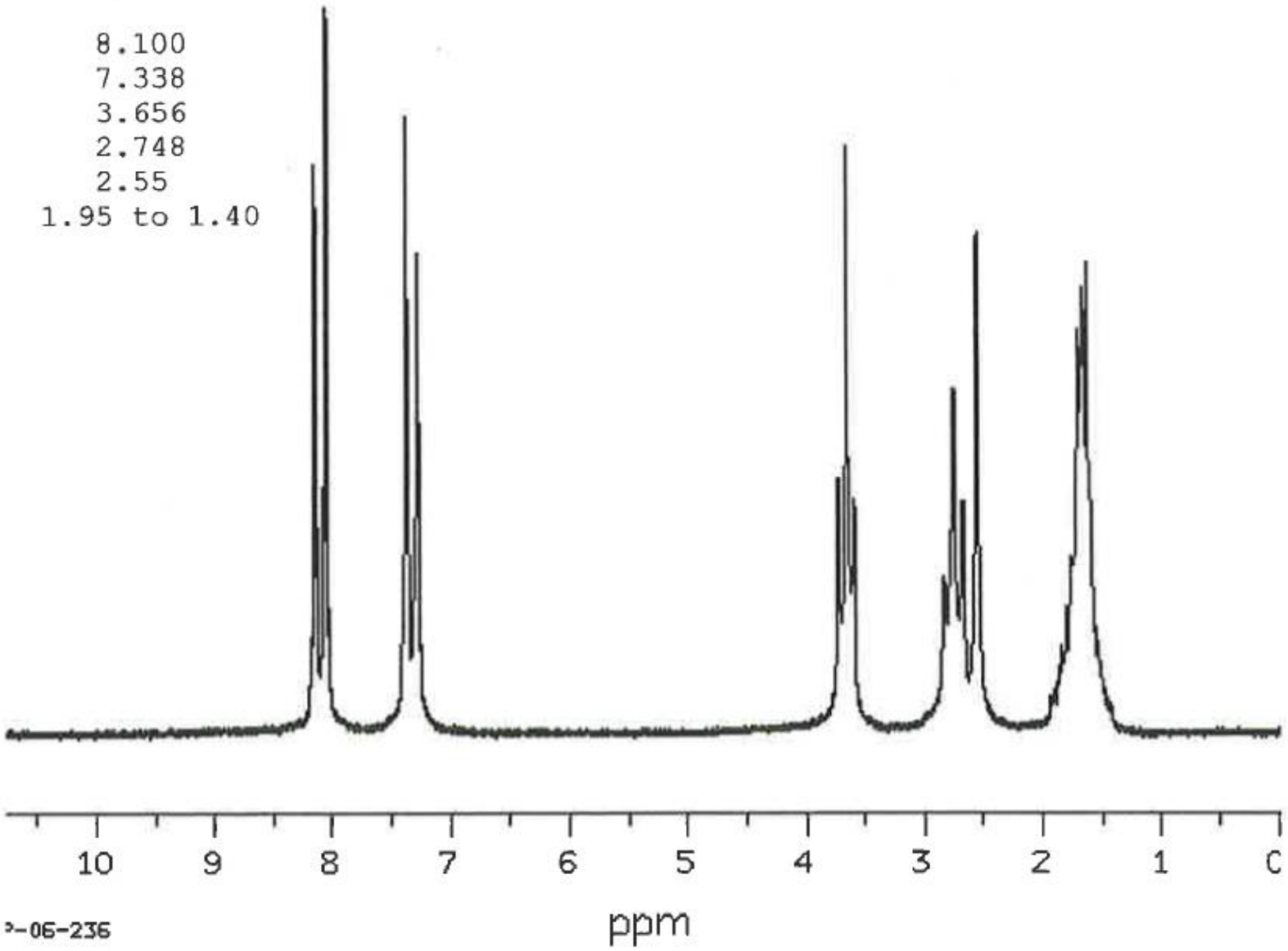
3364	31	1929	84	1345	4	1075	49	698	36
3111	60	1605	20	1193	77	983	66	645	62
3078	66	1598	21	1180	80	935	72	632	70
2938	20	1616	5	1154	81	868	21	617	68
2863	30	1495	35	1110	31	824	70	530	72
2462	77	1450	44	1061	30	800	72	486	79
2212	86	1417	68	1033	44	748	39		

^{13}C NMR 0.05 ml : 0.5 ml $CDCl_3$ 22.53 MHz



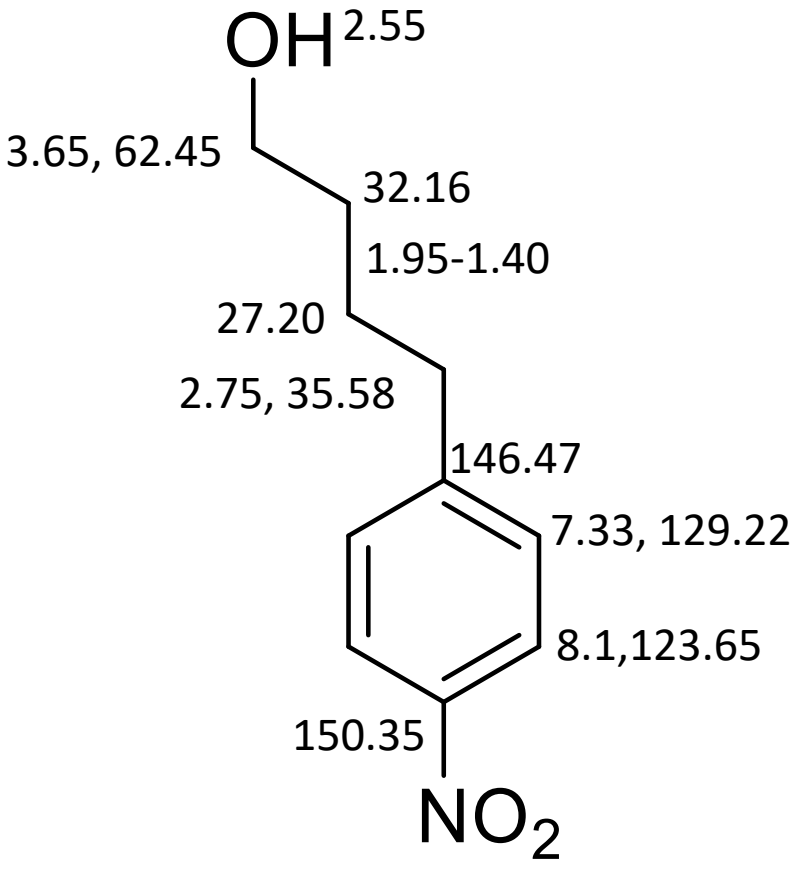
^{1}H NMR 0.05 ml : 0.5 ml $CDCl_3$ 89.56 MHz

Assign.		Shift (ppm)
A	2H	8.100
B	2H	7.338
C	2H	3.656
D	2H	2.748
E	1H	2.55
F	4H	1.95 to 1.40



-06-236

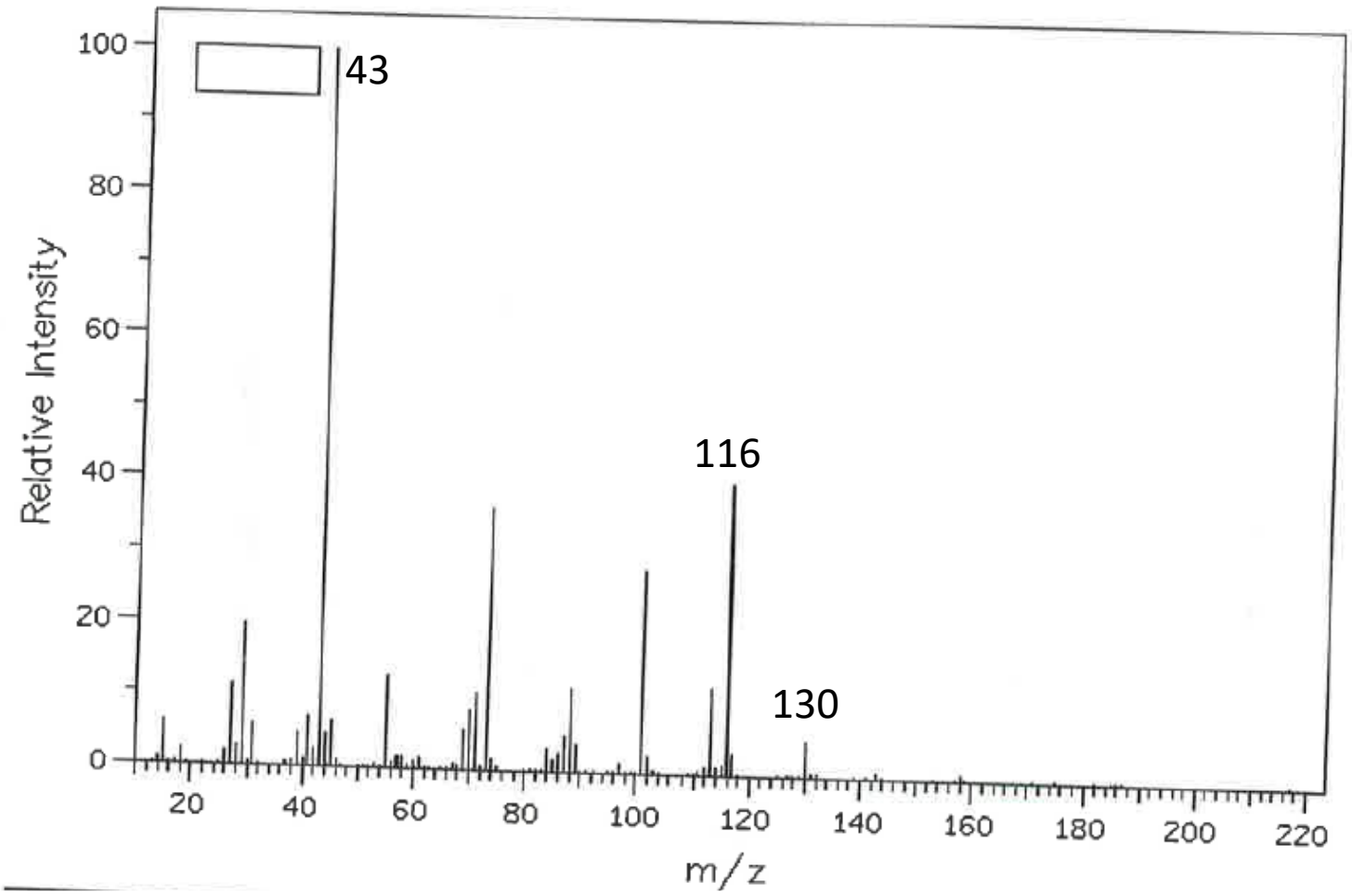
Soluzione
$C_{10}H_{13}NO_3$

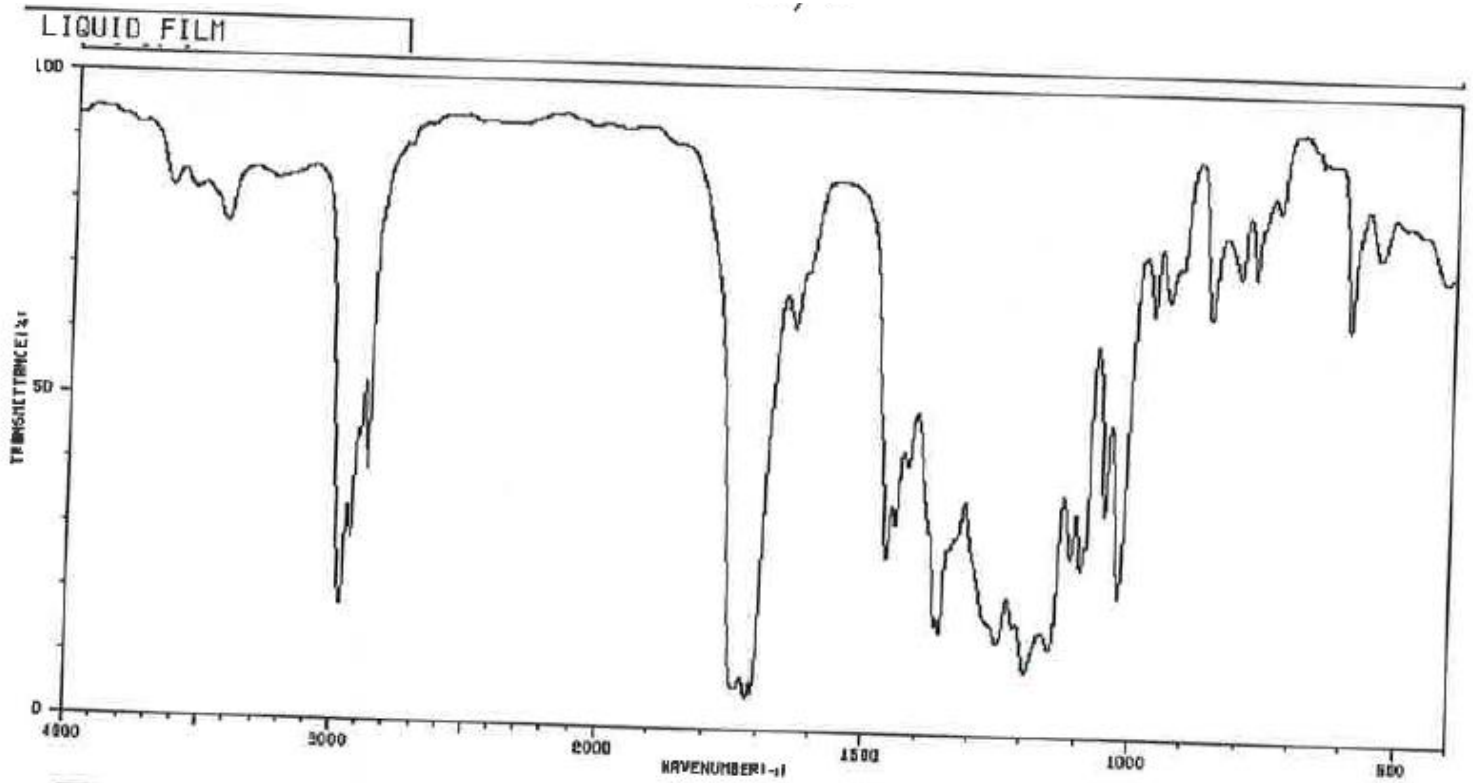


IR (cm^{-1}) : 3354 stretching O-H, 1605, 1598 stretching C=C aromatico, tra 2000 e 1600 bande armoniche e di combinazione, 1516 stretching asimmetrico e 1354 stretching simmetrico del gruppo NO_2 coniugato con l'anello aromatico

MS: picco intenso a m/z 149 (195 $-NO_2$) e picco a m/z 177 (195- H_2O) altri picchi diagnostici?

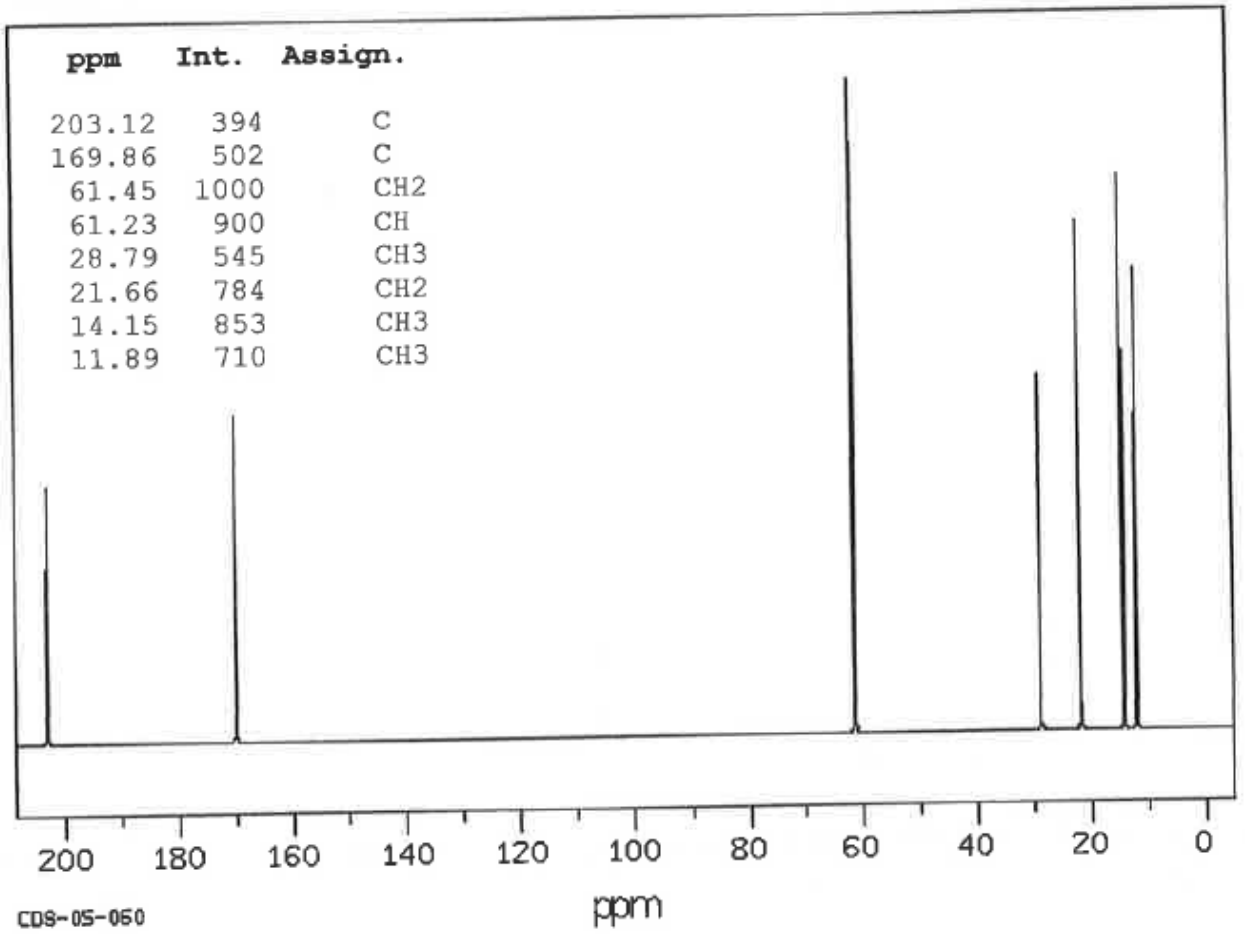
Mass C8H14O3 (Mass of molecular ion: 158)





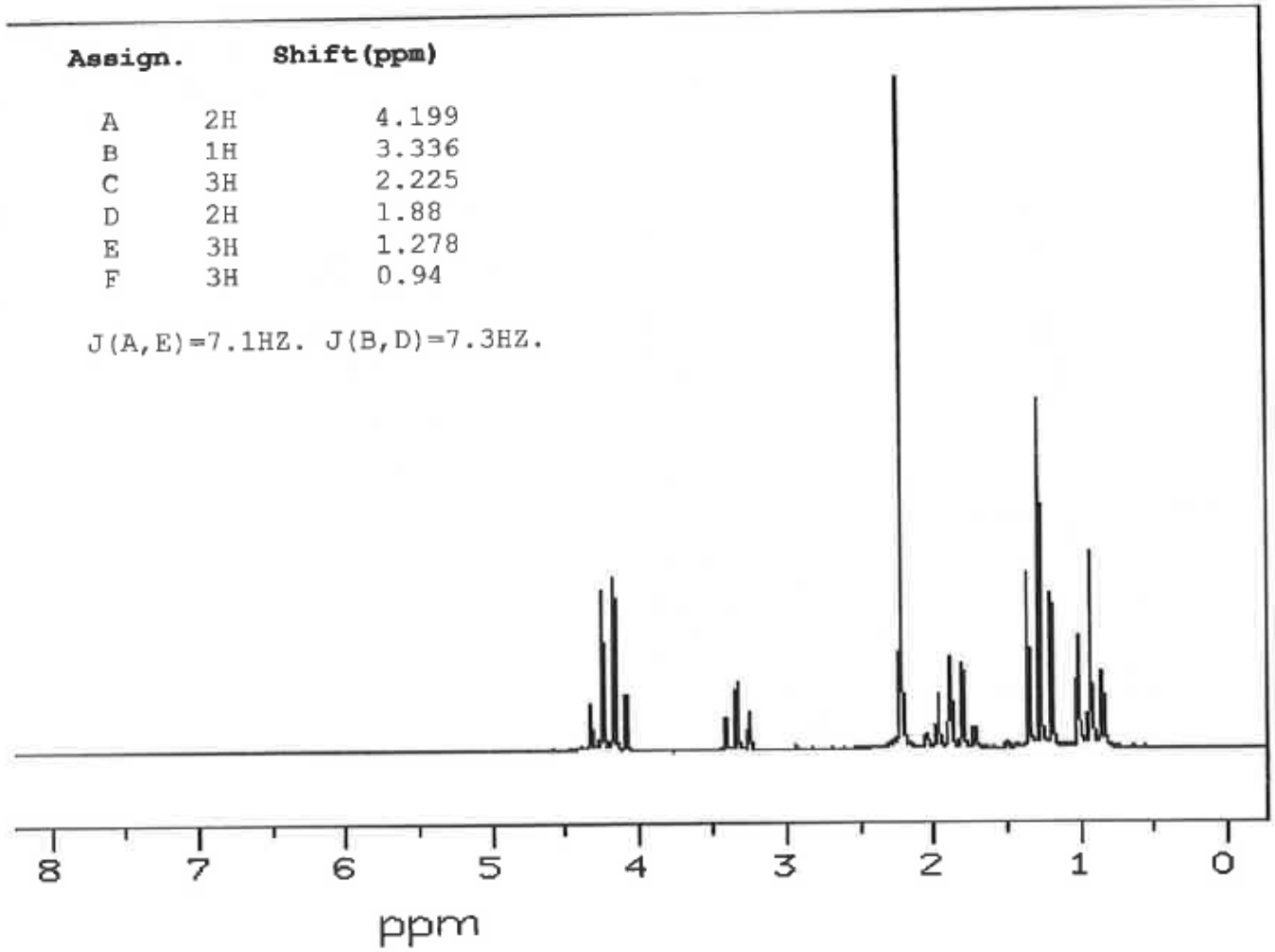
3638	79	1717	4	1252	13	1026	21	698	60
3431	74	1643	60	1197	9	968	62	544	72
2973	17	1464	25	1153	13	940	65		
2939	26	1447	31	1116	26	860	62		
2881	37	1424	39	1096	25	807	58		
1739	6	1368	16	1087	28	778	68		
1732	7	1380	16	1063	33	736	79		

^{13}C NMR 0.5 ml : 1.5 ml $CDCl_3$ 25.16 MHz

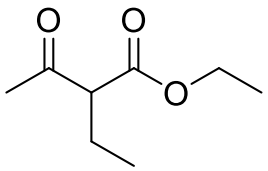


^{1}H NMR 0.04 ml : 0.5 ml $CDCl_3$

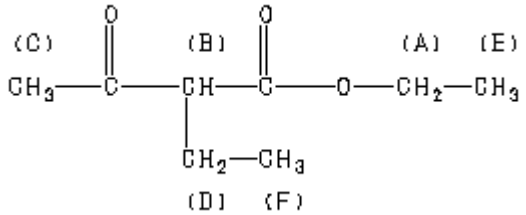
89.56 MHz

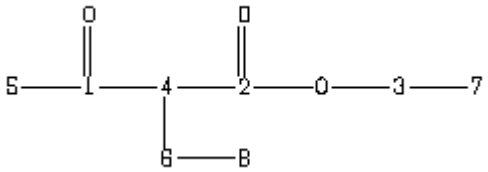


SOLUZIONE compito B



Chemical Formula: $C_8H_{14}O_3$
Molecular Weight: 158,19700

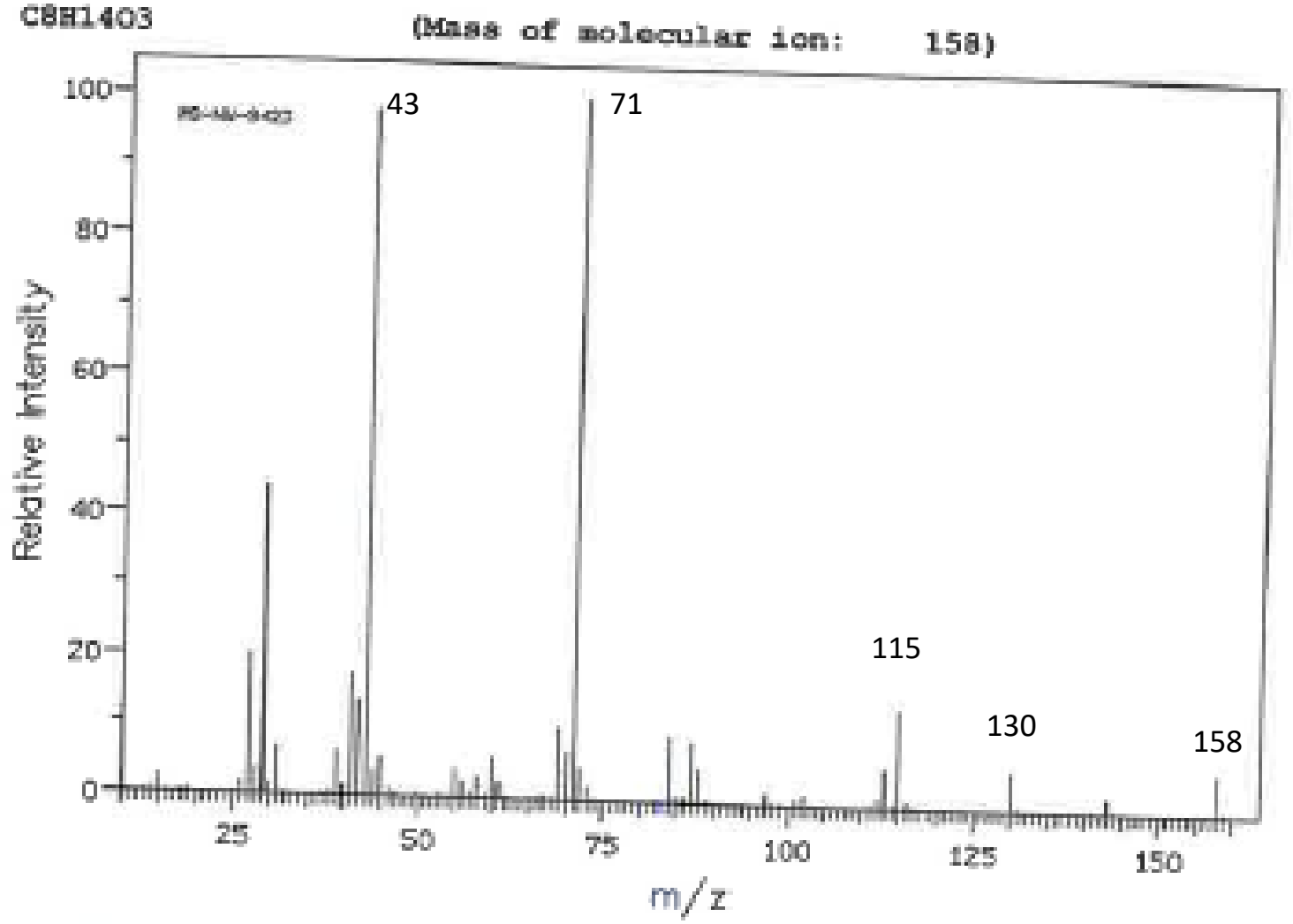


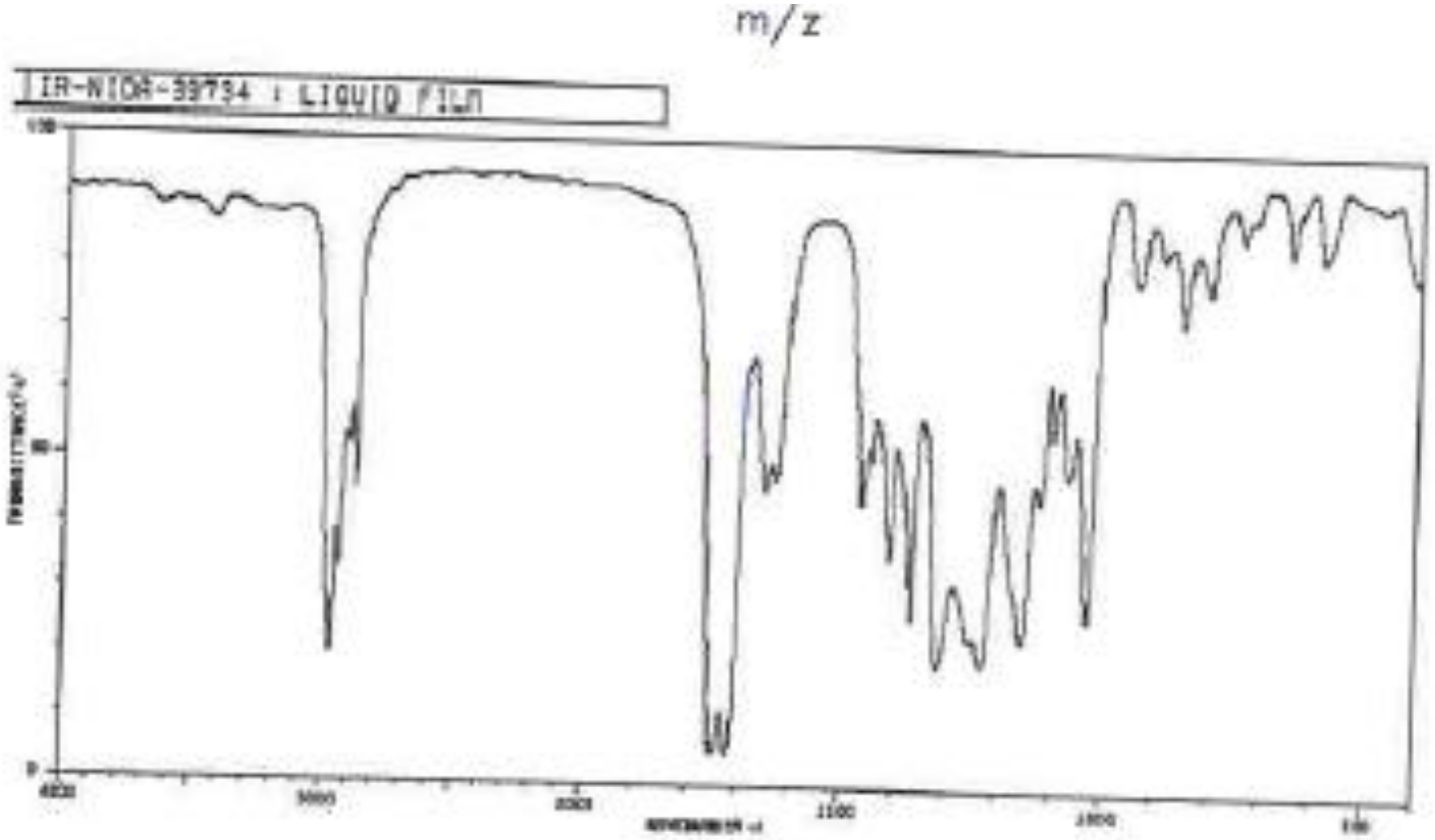


Assign. Shift(ppm)

A 4.199
B 3.336
C 2.225
D 1.88
E 1.278
F 0.94
J(A,E)=7.1HZ.
J(B,D)=7.3HZ.
J(B,C)=0.3HZ.

ppm	Int.	Assign.
203.12	394	1
169.86	502	2
61.45	1000	3
61.23	900	4
28.79	545	5
21.66	784	6
14.15	853	7
11.89	710	8


C8H14O3
(Mass of molecular ion: 158)
Relative Intensity
m/z
43
71
115
130
158
100
80
60
40
20
0
25
50
75
100
125
150

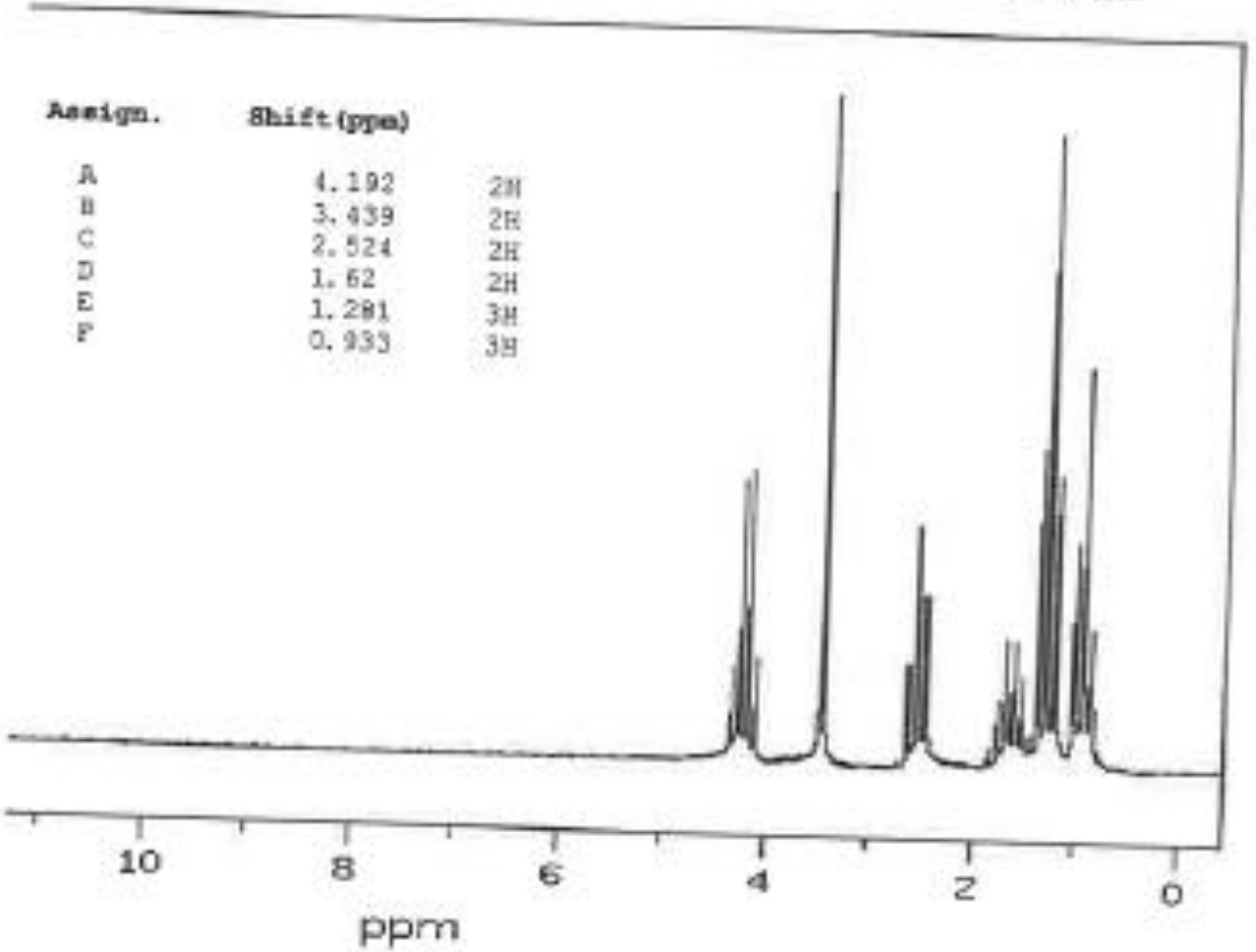


3428	84	1648	44
2967	19	1620	46
2956	32	1457	42
2908	60	1447	49
2878	43	1412	34
1745	5	1358	25
1718	4	1317	10

^{1}H NMR 0.05 ml : 0.5 ml $CDCl_3$

89.56 MHz

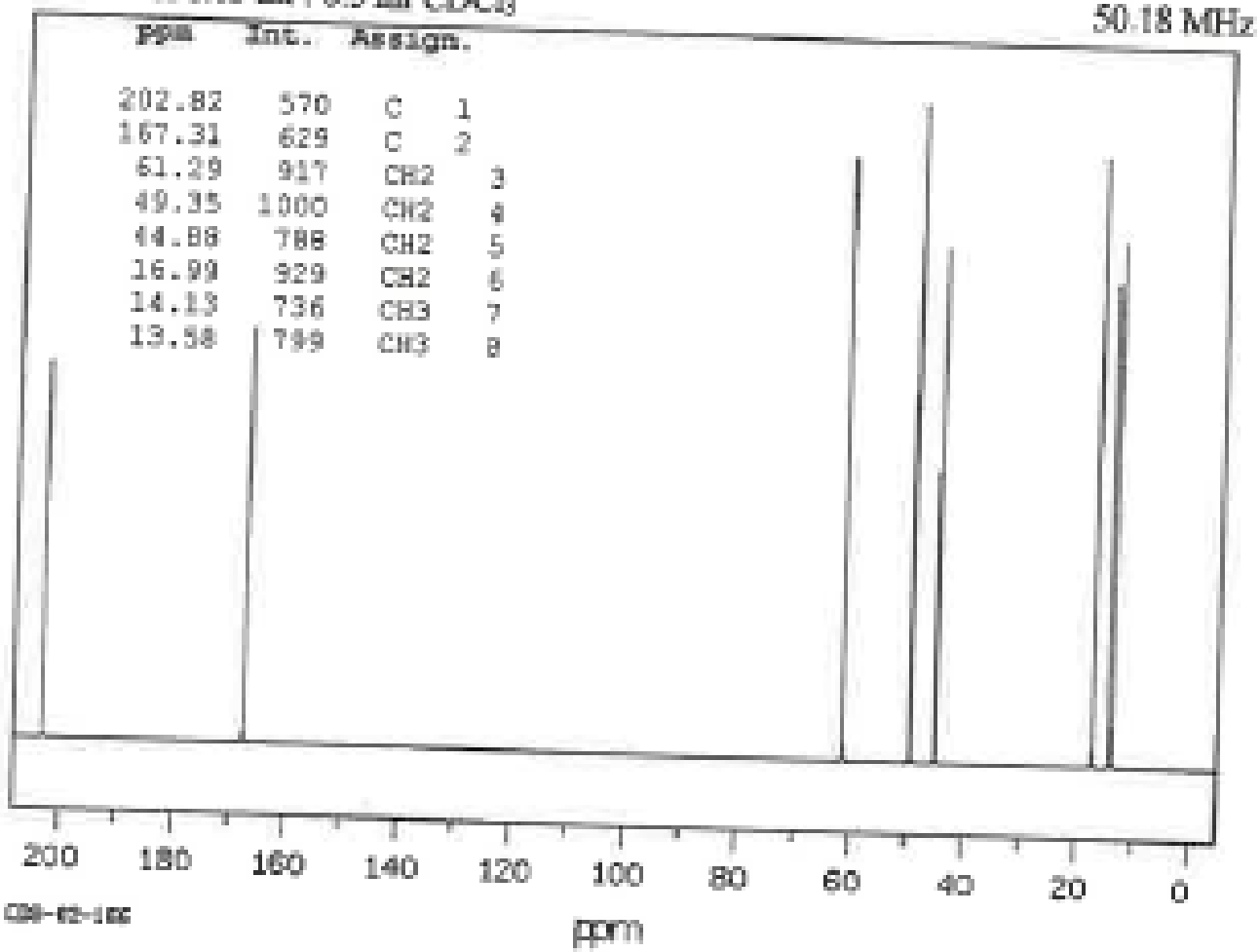
Assign.	δshift (ppm)	
A	4.192	2H
B	3.439	2H
C	2.524	2H
D	1.62	2H
E	1.281	3H
F	0.933	3H



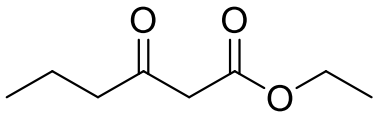
^{13}C NMR 0.05 ml : 0.5 ml $CDCl_3$

50.18 MHz

ppm	Int.	Assign.	
202.82	570	C	1
167.31	629	C	2
61.29	917	CH2	3
49.35	1000	CH2	4
44.88	788	CH2	5
16.99	929	CH2	6
14.13	736	CH3	7
13.58	799	CH3	8

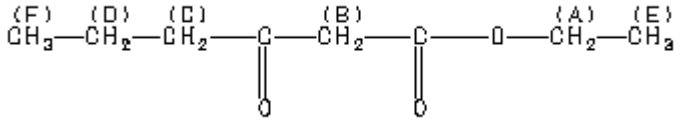


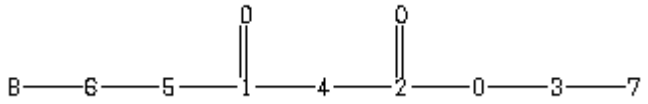
Compito C



Chemical Formula: $C_8H_{14}O_3$
Molecular Weight: 158,19700

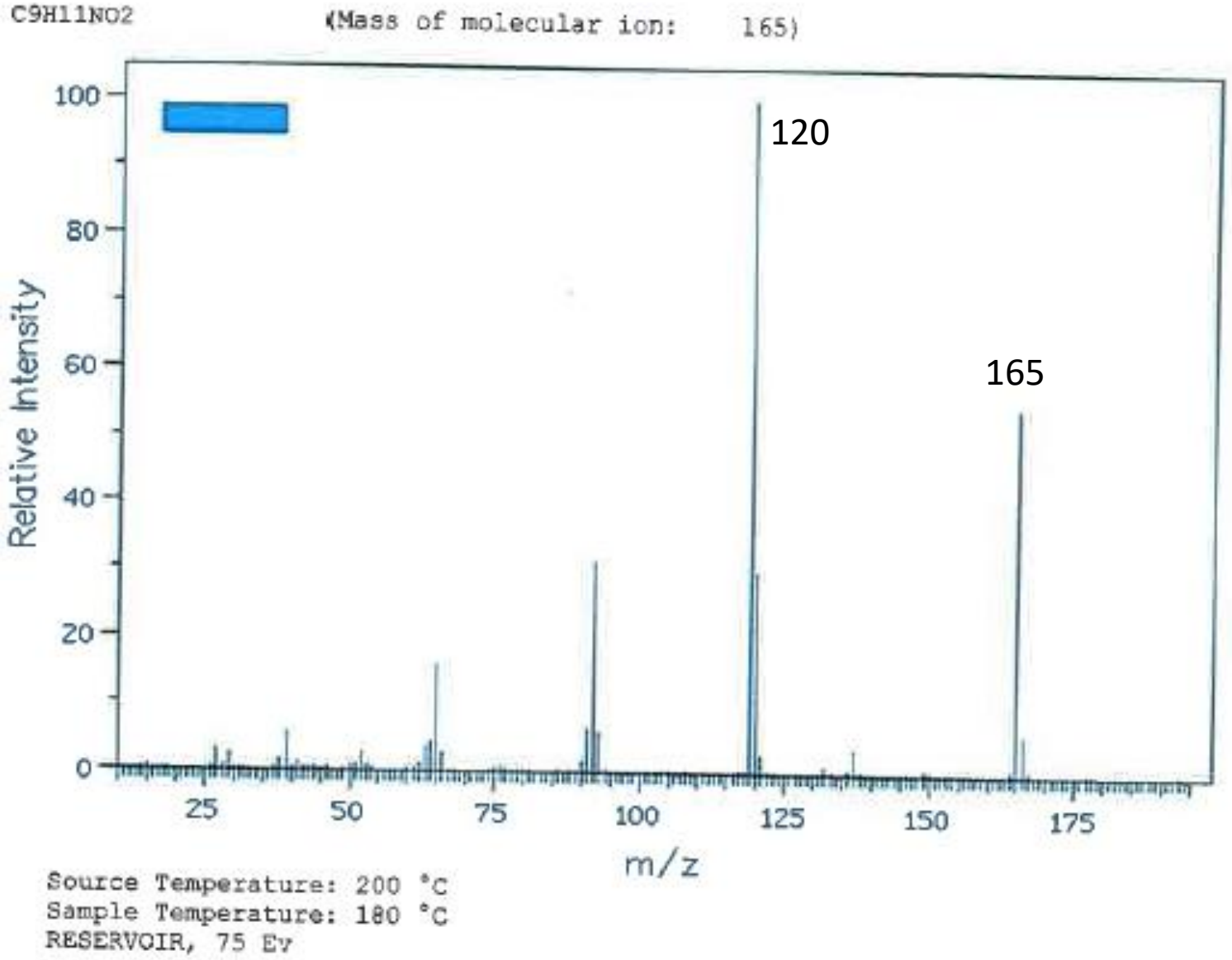
MS: 158 $M^{+\cdot}$, 130 (M-etilene: McLafferty),
115 (M-43, C_3H_7) , 71 $[CH_3CH_2CH_2CO]^+$, 43 $[C_3H_7]^+$
IR: 1745 cm^{-1} carbonile estereo
1718 cm^{-1} carbonile chetonico





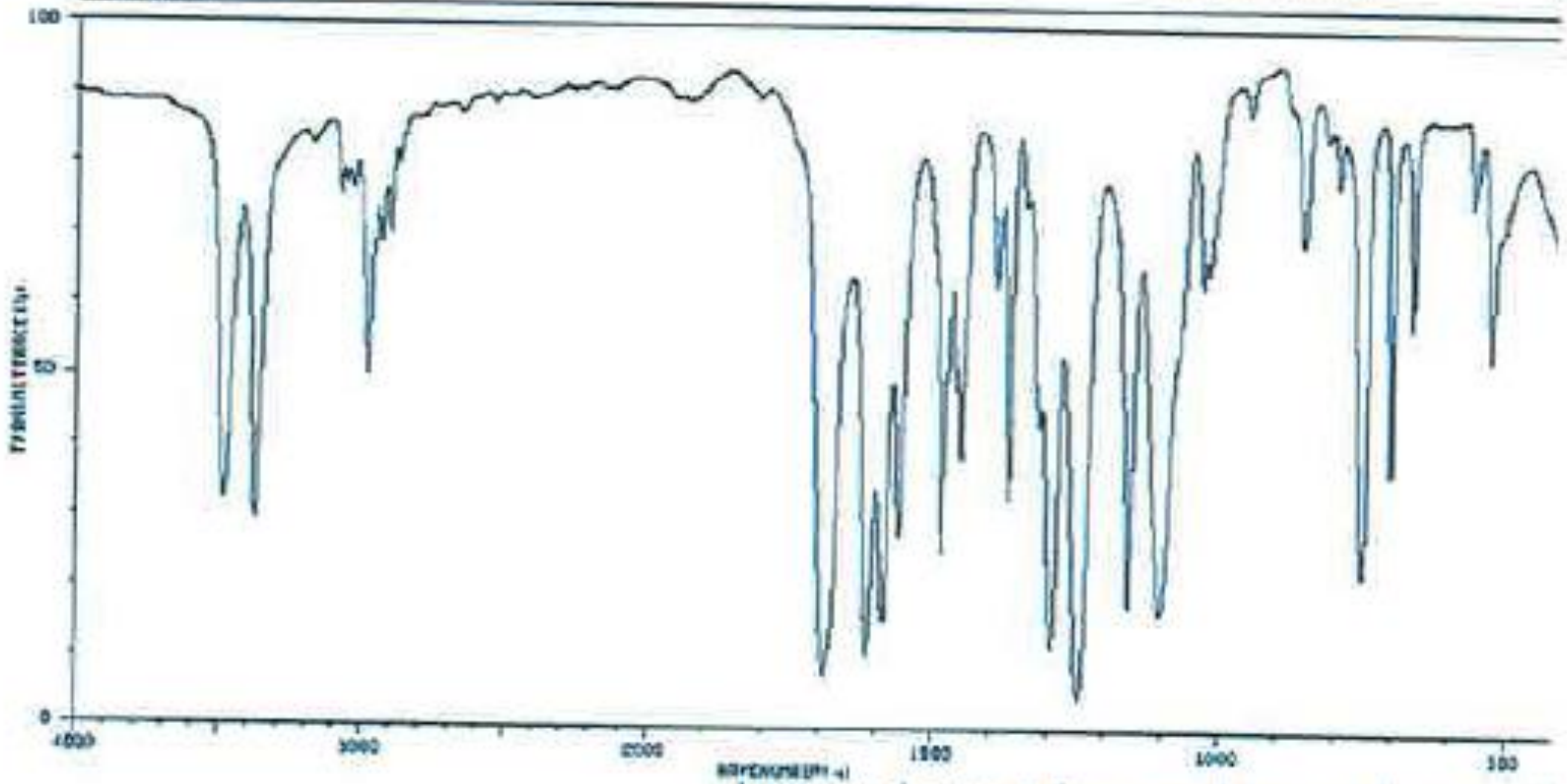
Assign.	Shift(ppm)
A	4.192
B	3.439
C	2.524
D	1.62
E	1.281
F	0.933

ppm	Int.	Assign.
202.82	570	1
167.31	629	2
61.29	917	3
49.35	1000	4
44.88	788	5
16.99	929	6
14.13	736	7
13.58	799	8


C9H11NO2
(Mass of molecular ion: 165)
120
165
Relative Intensity
100
80
60
40
20
0
25
50
75
100
125
150
175
m/z
Source Temperature: 200 °C
Sample Temperature: 180 °C
RESERVOIR, 75 Ev

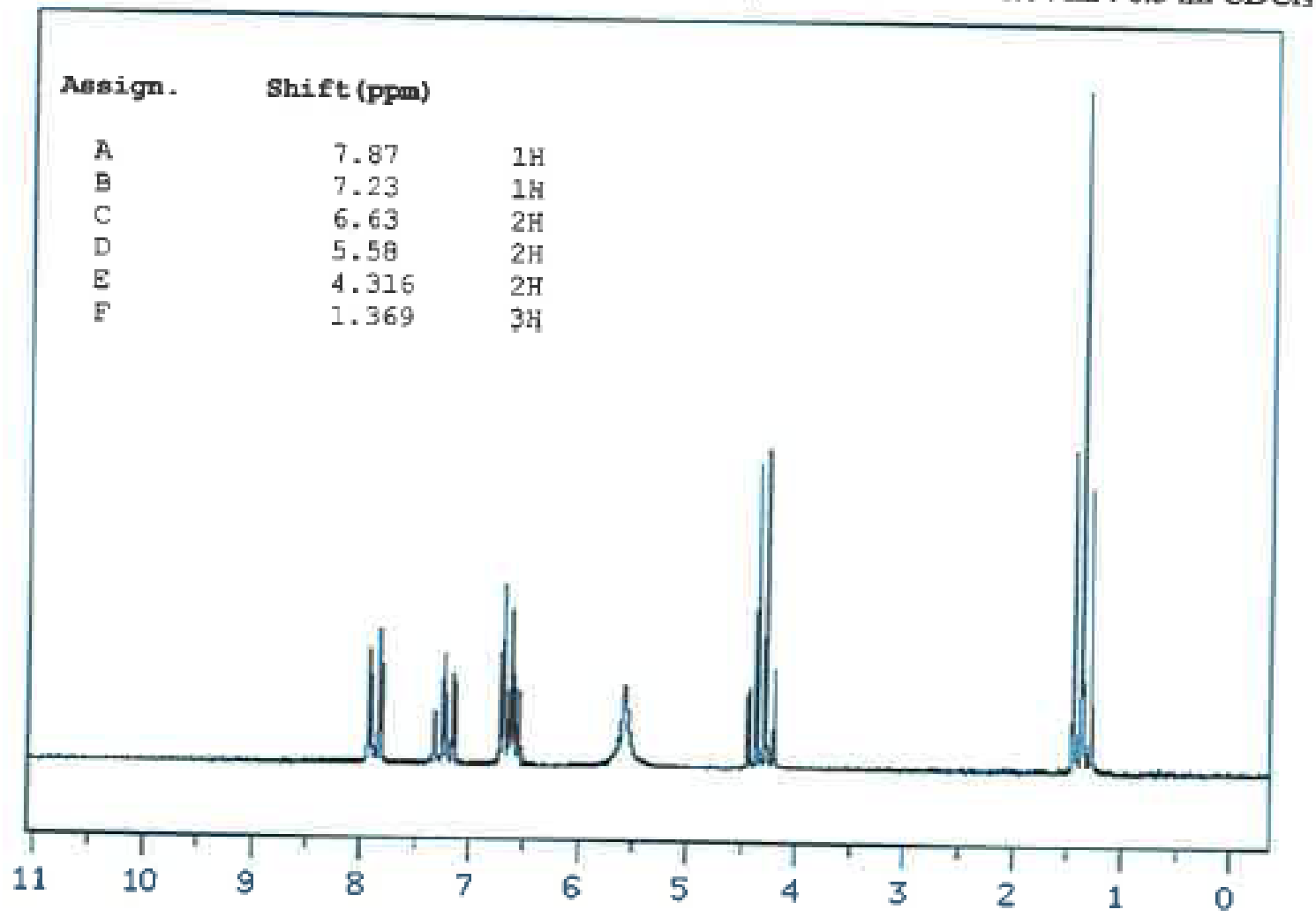
$C_9H_{11}NO_2$

LIQUID FILM

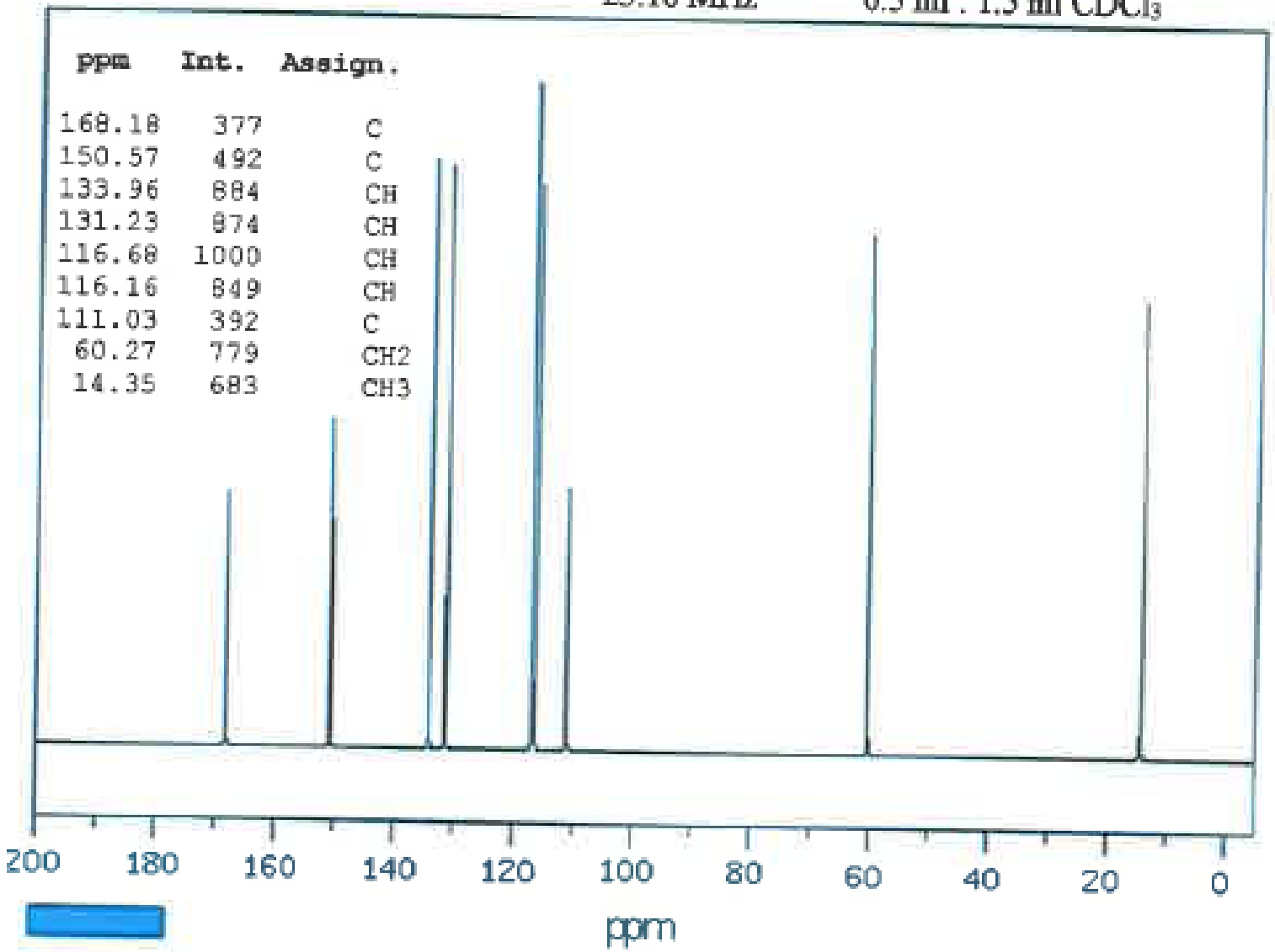


3482	32	2986	69	1479	49	1296	12	797	74
3372	29	2878	77	1463	47	1246	4	752	22
3077	72	1698	7	1455	37	1162	17	705	36
3060	74	1617	10	1392	62	1104	15	666	67
3033	74	1589	15	1369	32	1032	62	563	72
2985	49	1552	27	1341	72	1021	64	529	52
2938	66	1488	28	1316	42	867	68	613	68

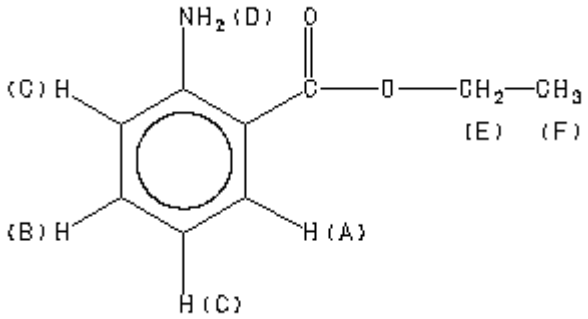
$C_9 H_{11} N O_2$ 89.56 MHz 0.04 ml : 0.5 ml $CDCl_3$

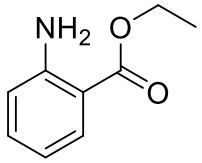


$C_9 H_{11} N O_2$ 25.16 MHz 0.5 ml : 1.5 ml $CDCl_3$

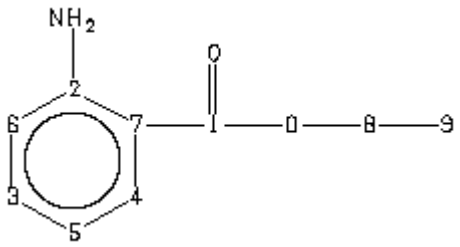


Compito E





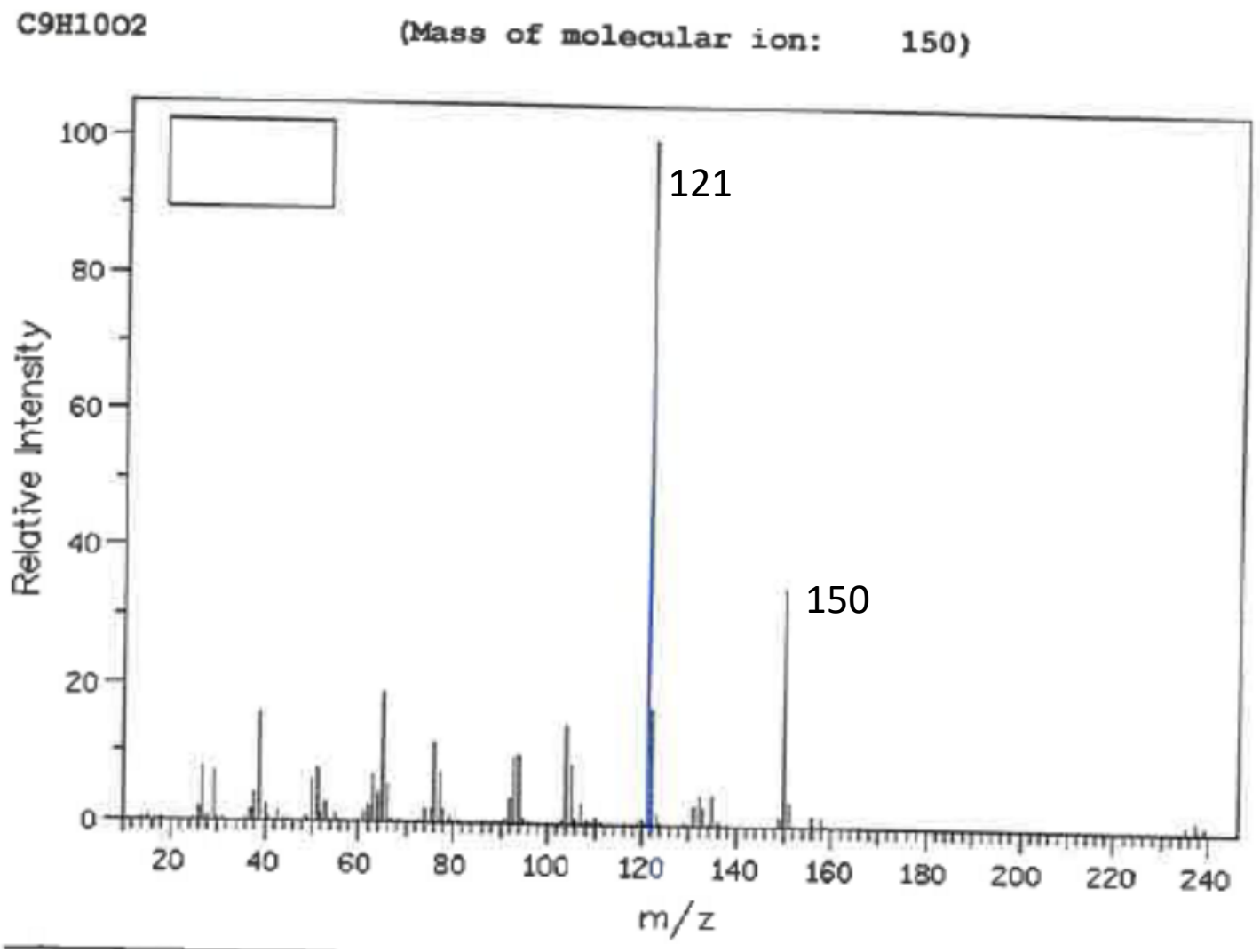
Chemical Formula:
$C_9H_{11}NO_2$
Molecular Weight:
165,19



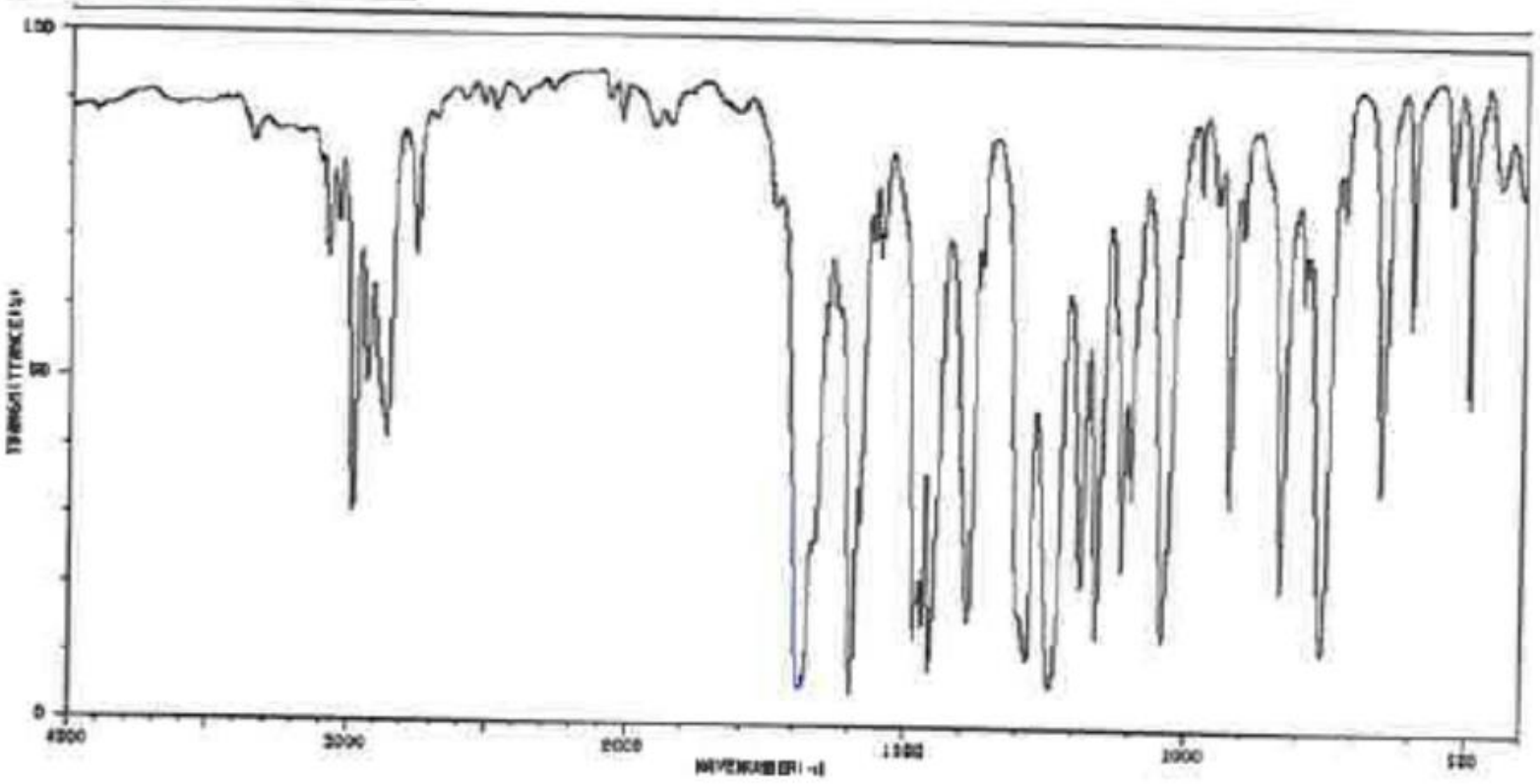
Assign.
Shift(ppm)

A 7.87
B 7.23
C 6.63
D 5.58
E 4.316
F 1.369

ppm	Int.	Assign.
168.18	377	1
150.57	492	2
133.96	884	3
131.23	874	4
116.68	1000	5
116.16	849	6
111.03	392	7
60.27	779	8
14.35	683	9

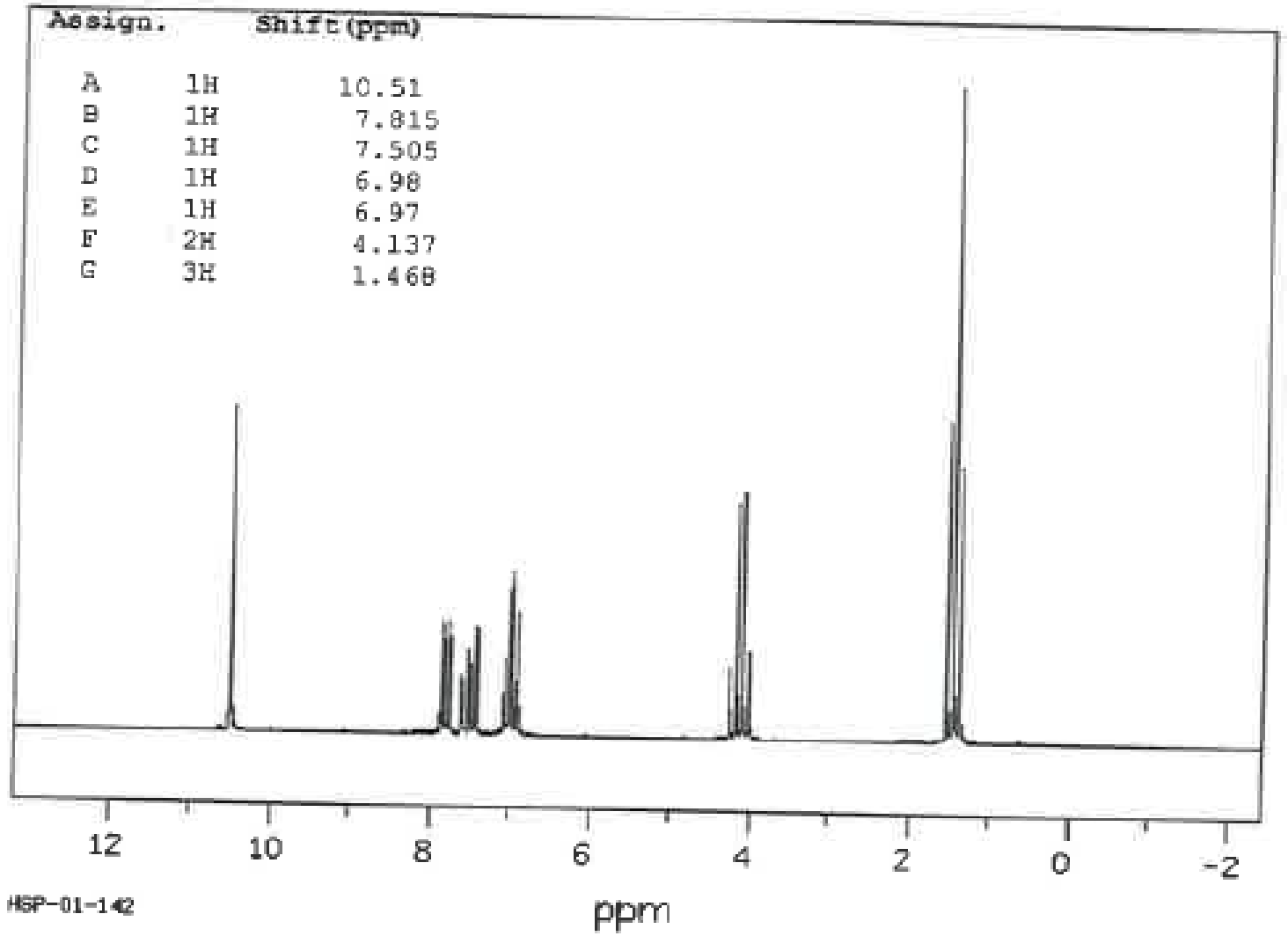

C9H10O2
(Mass of molecular ion: 150)
Relative Intensity
100
80
60
40
20
0
121
150
20
40
60
80
100
120
140
160
180
200
220
240
m/z

LIQUID FILM



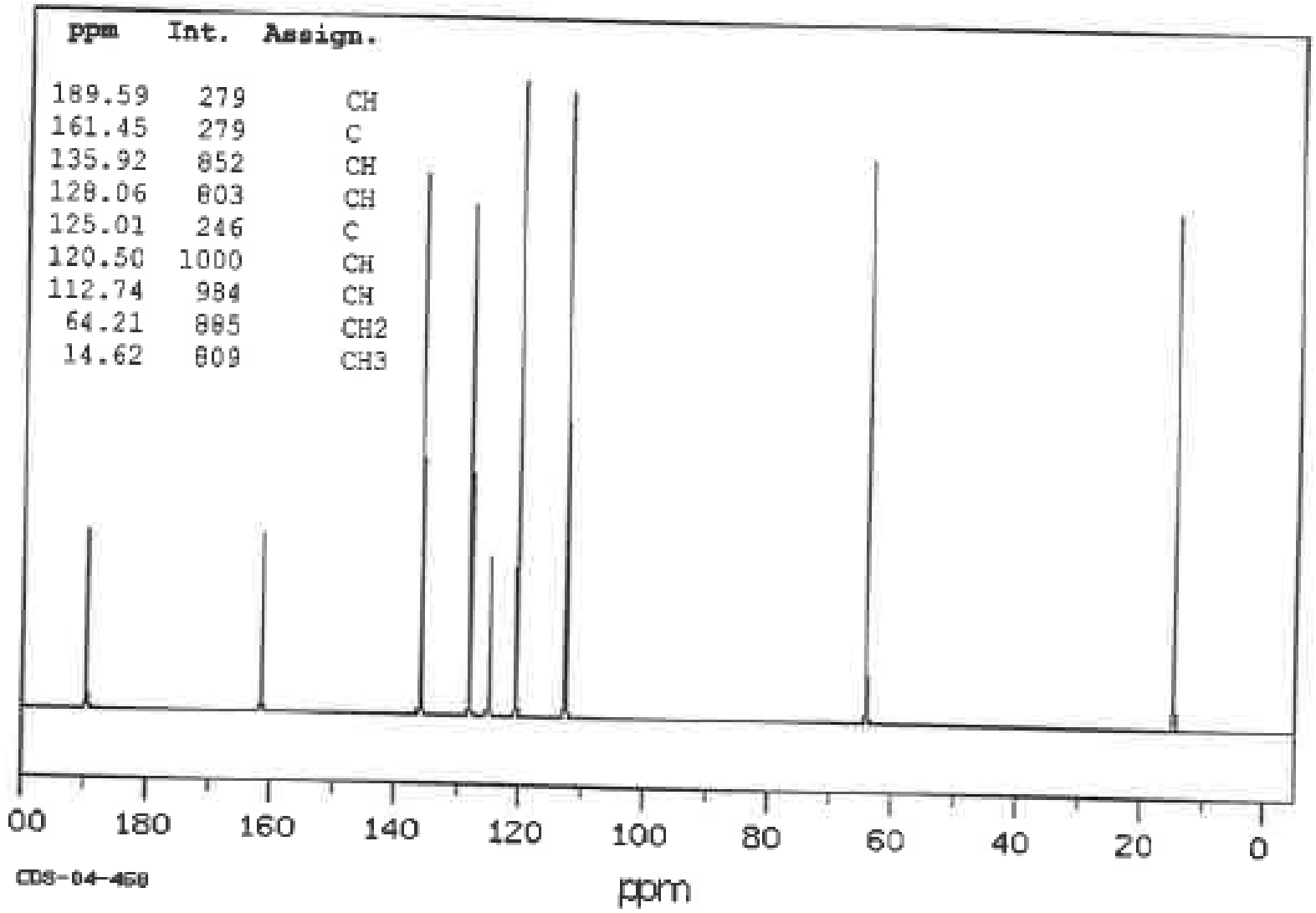
3077	64	1608	4	1474	14	1180	20	833	19
3042	70	1594	28	1460	7	1162	12	793	60
2983	29	1554	68	1390	14	1117	22	759	10
2939	47	1552	68	1366	84	1069	32	729	72
2851	39	1546	68	1289	16	1042	12	554	33
2760	66	1488	12	1265	9	925	31	501	57
1890	5	1482	17	1243	5	905	79	497	46

^{1}H NMR 0.04 ml : 0.5 ml $CDCl_3$ 89.56 MHz

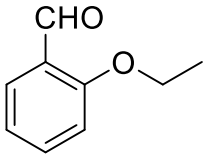


^{13}C NMR 0.25 ml : 0.8 ml $CDCl_3$

15.09 MHz

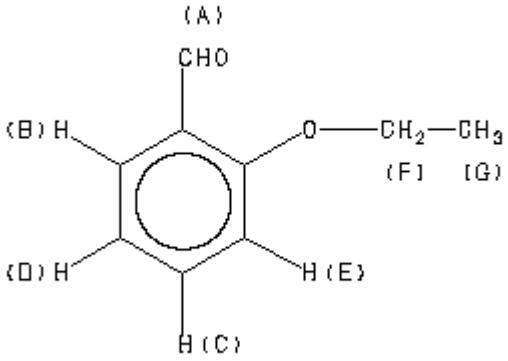


Compito D

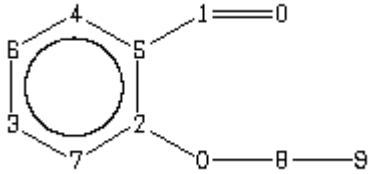


Chemical Formula: $C_9H_{10}O_2$
Molecular Weight: 150,17700

Massa: m/z 121 : perdita di 29 (CH_3CH_2)
IR: 1690 cm^{-1} carbonile coniugato
1600 cm^{-1} anello aromatico

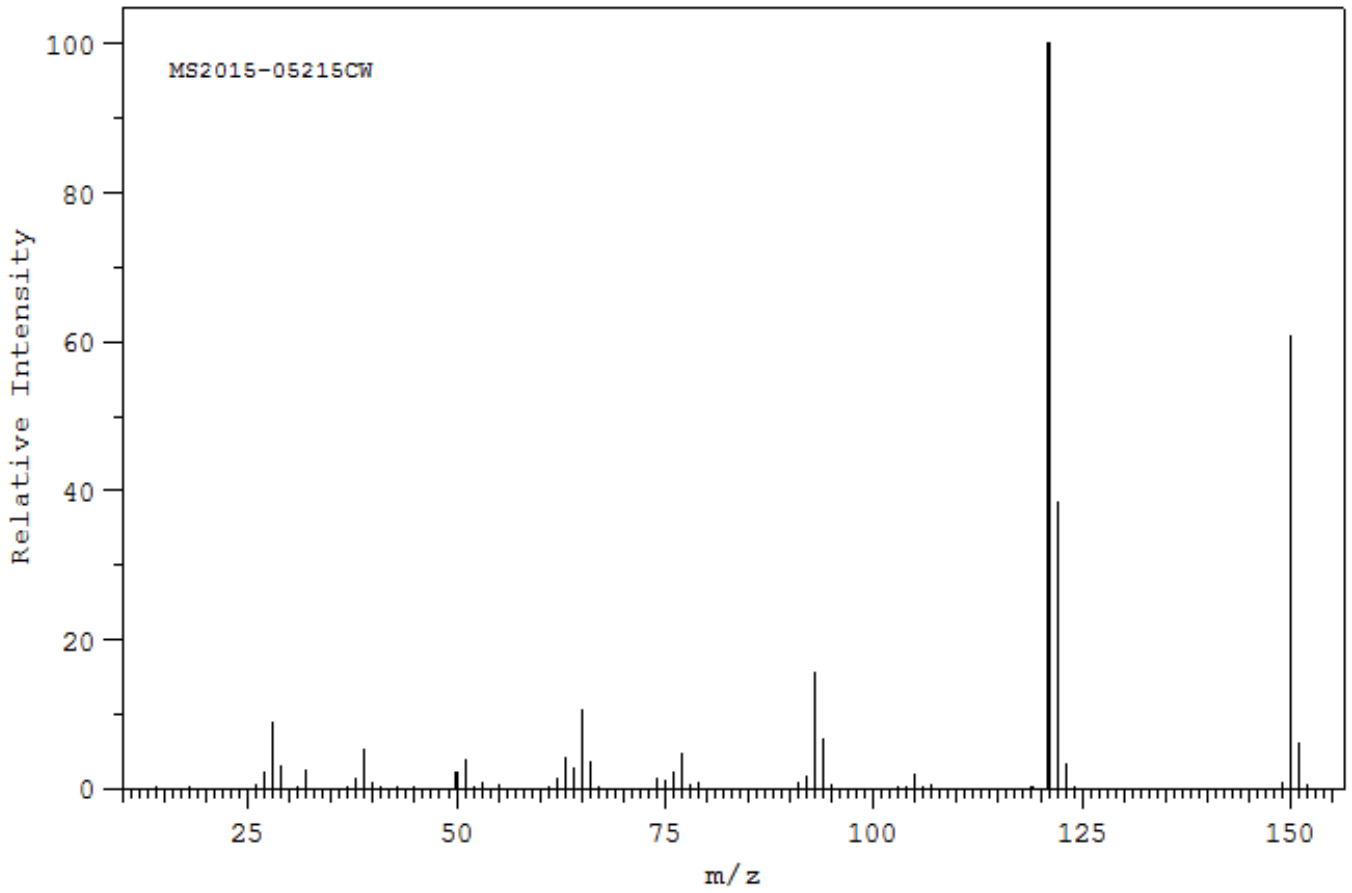


Assign.	Shift(ppm)
A	10.51
B	7.815
C	7.505
D	6.98
E	6.97
F	4.137
G	1.468



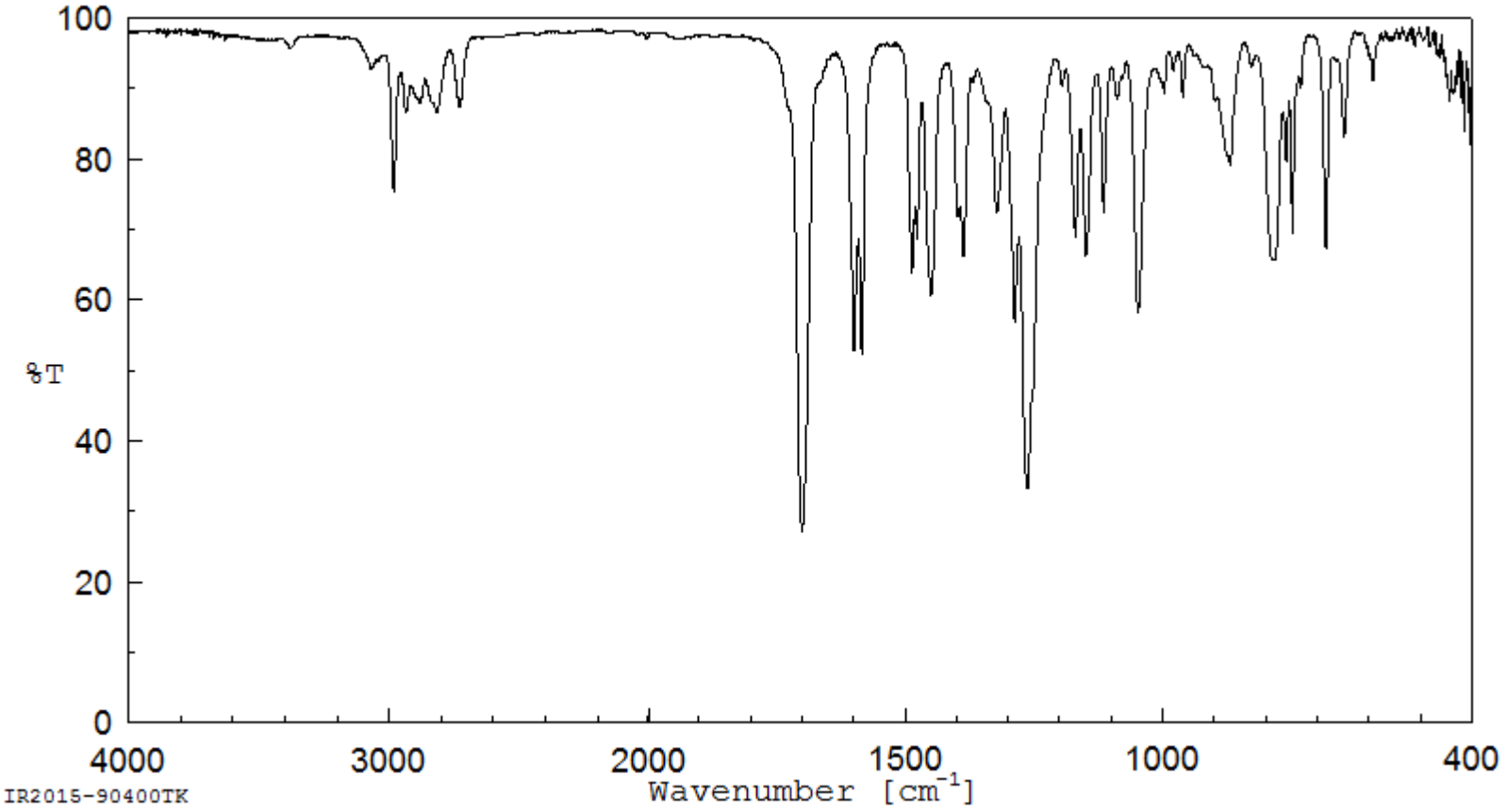
ppm	Int.	Assign.
189.59	279	1
161.45	279	2
135.92	852	3
128.06	803	4
125.01	246	5
120.50	1000	6
112.74	984	7
64.21	885	8
14.62	809	9

$C_9H_{10}O_2$ m-etossibenzaldeide



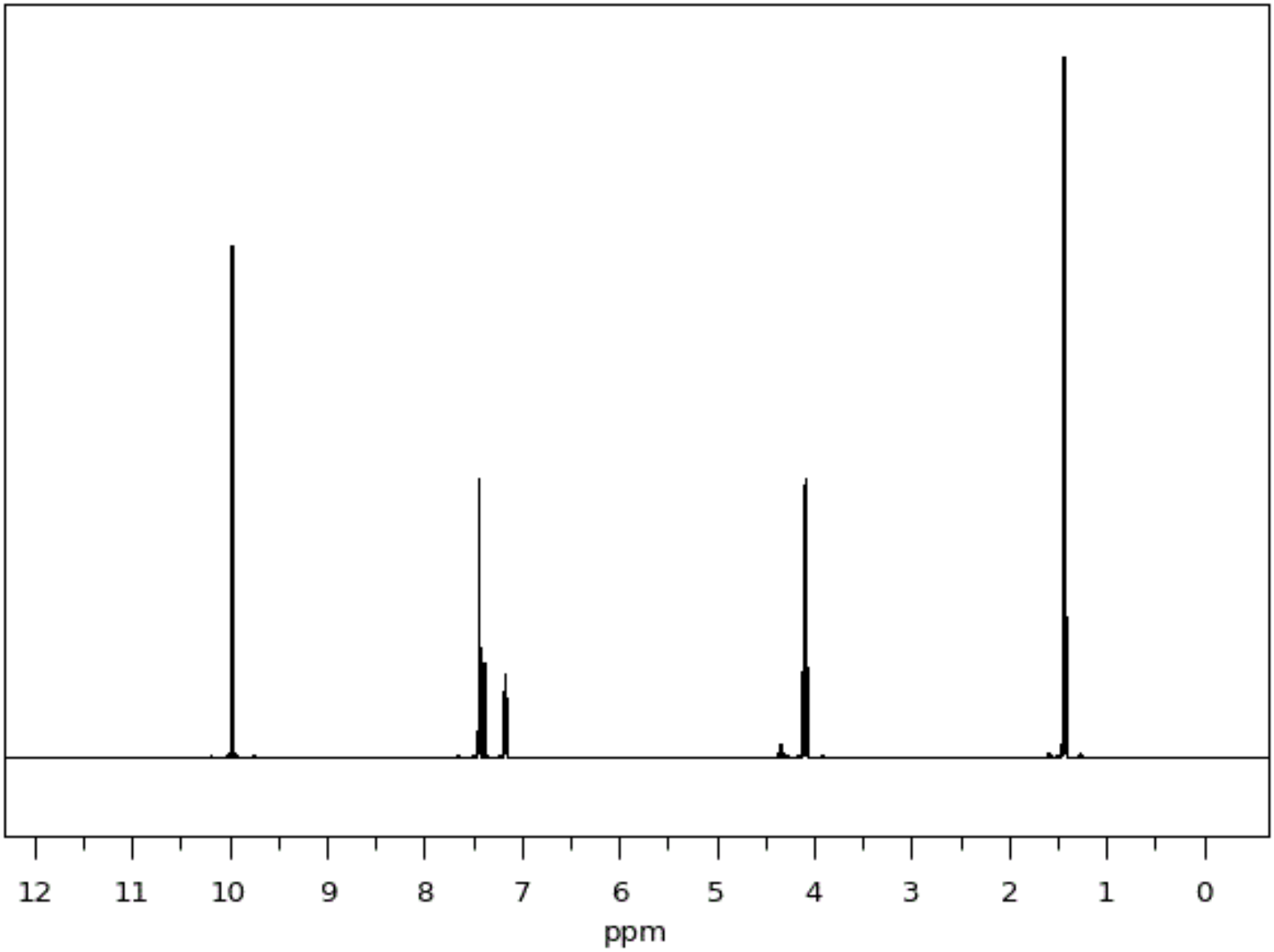
m/z	int%
65.0	10.6
93.0	15.7
121.0	100.0
122.0	38.4
150.0	60.7

$C_9H_{10}O_2$ m-etossibenzaldeide



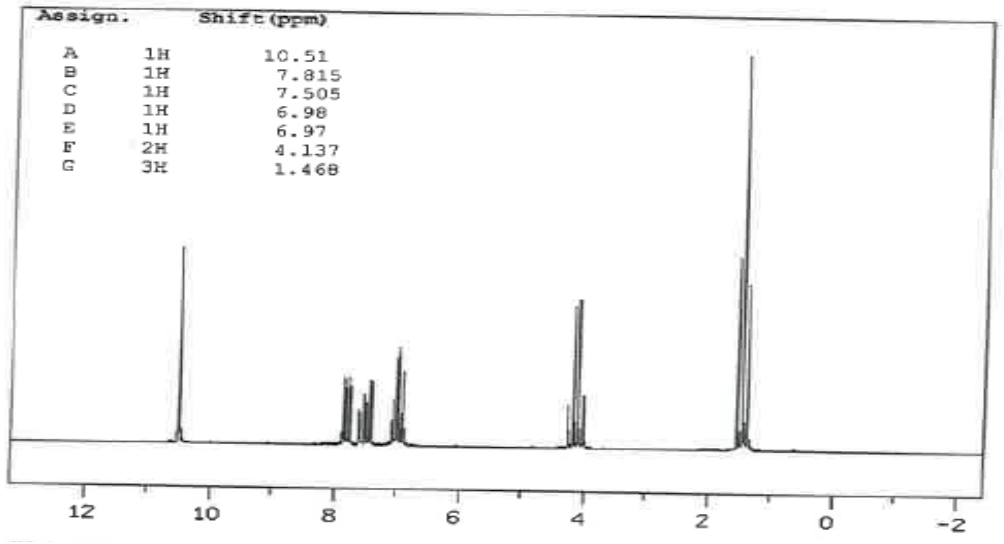
3069	93	1700	27
2982	76	1599	53
2936	87	1584	52
2817	87	1486	64
2728	88	1477	69

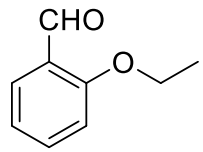
$C_9H_{10}O_2$ m-etossibenzaldeide

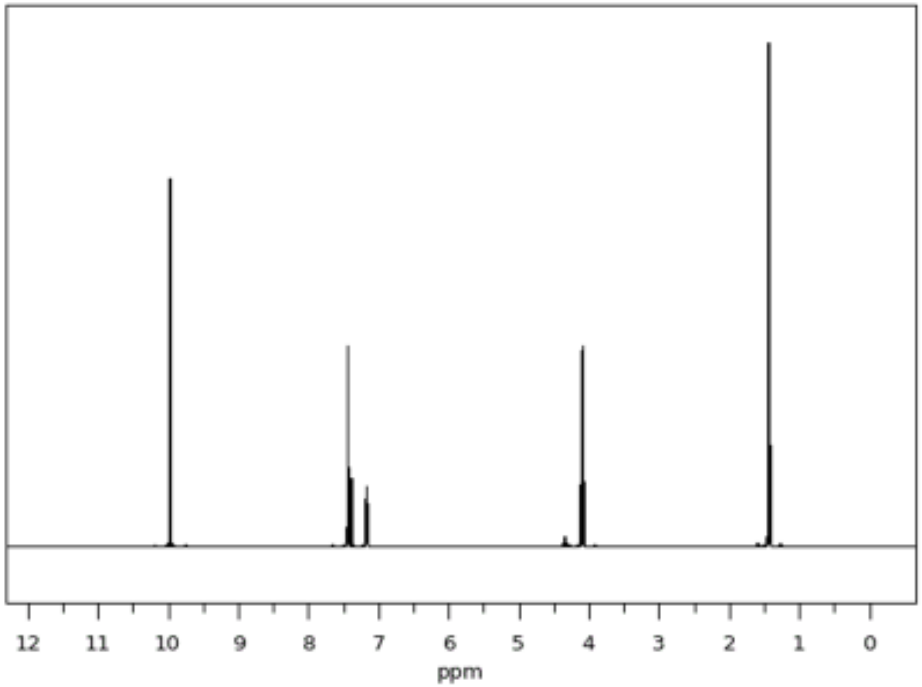


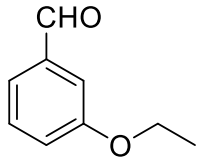
HR201603312NS

^{1}H NMR 0.04 ml : 0.5 ml $CDCl_3$ 89.56 MHz



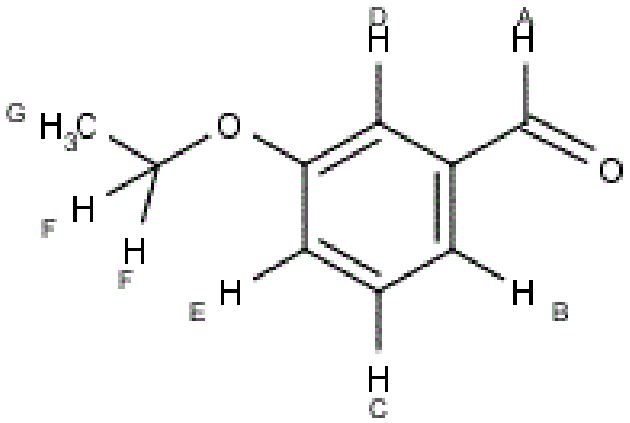




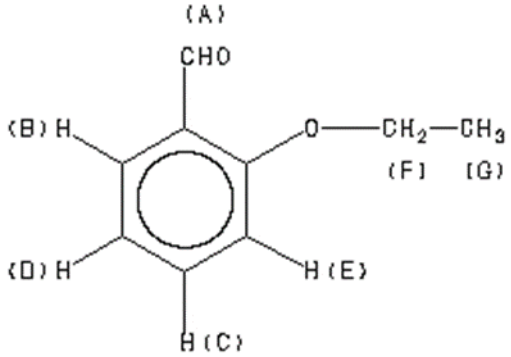


HR201603312N5

^{1}HNMR



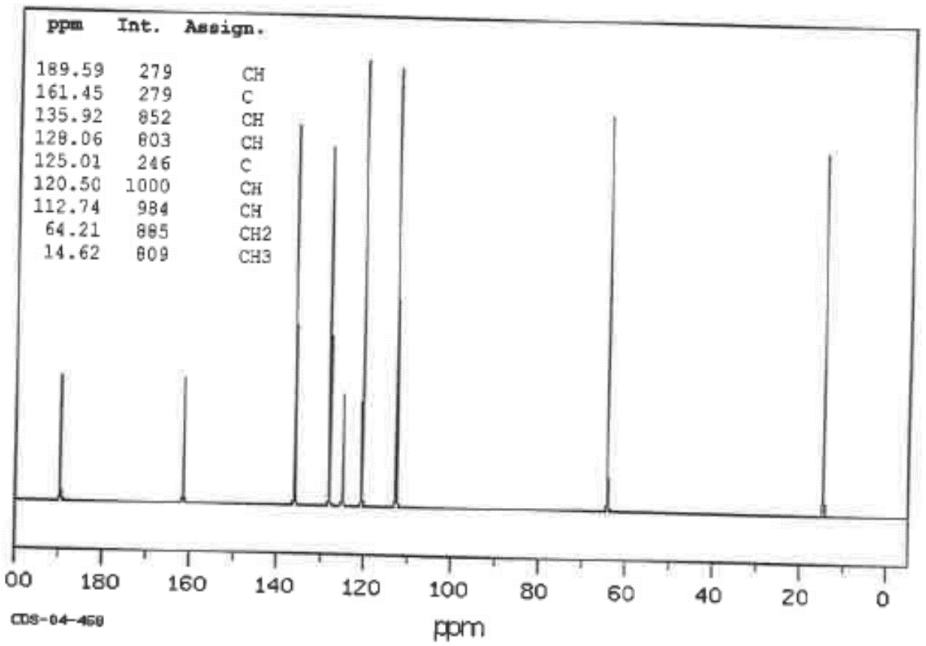
Assign.	Shift(ppm)
A	9.968
B	7.44
C	7.43
D	7.378
E	7.166
F	4.095
G	1.439

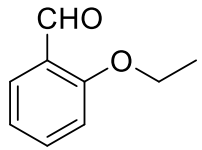


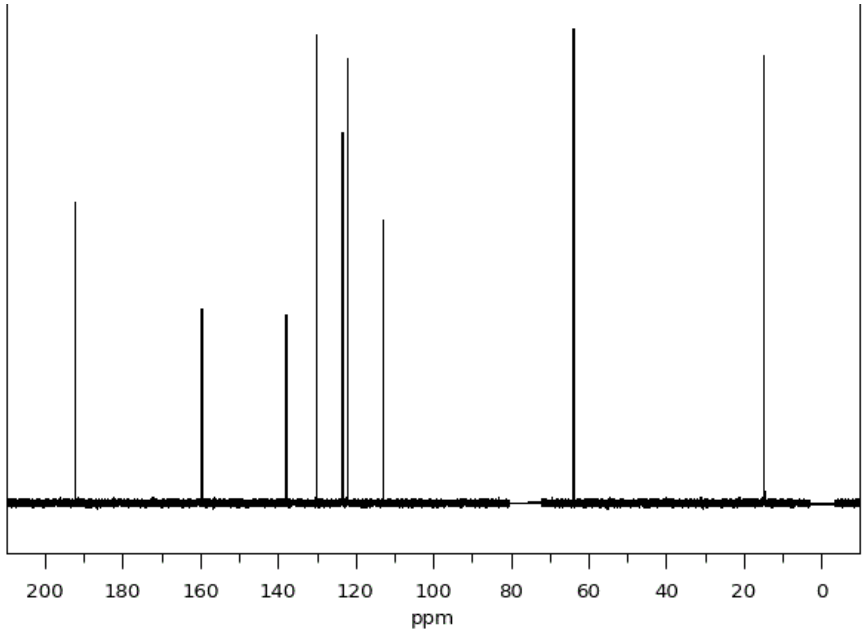
Assign.	Shift(ppm)
A	10.51
B	7.815
C	7.505
D	6.98
E	6.97
F	4.137
G	1.468

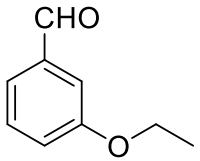
^{13}C NMR 0.25 ml : 0.8 ml $CDCl_3$ 15.09 MHz

ppm	Int.	Assign.
189.59	279	CH
161.45	279	C
135.92	852	CH
128.06	803	CH
125.01	246	C
120.50	1000	CH
112.74	984	CH
64.21	885	CH2
14.62	809	CH3



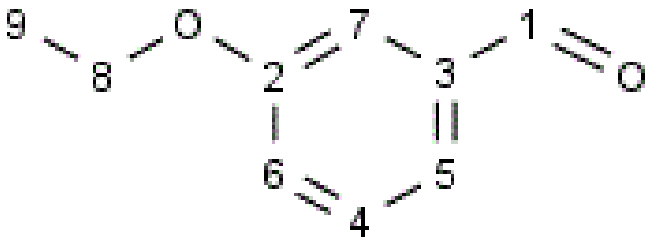






CR201603312NS

ppm	Int.	Assign.
192.16	632	1
159.58	407	2
137.86	397	3
130.03	988	4
123.31	780	5
121.95	937	6
112.87	598	7
63.80	1000	8
14.71	942	9



ppm	Int.	Assign.
189.59	279	1
161.45	279	2
135.92	852	3
128.06	803	4
125.01	246	5
120.50	1000	6
112.74	984	7
64.21	885	8
14.62	809	9