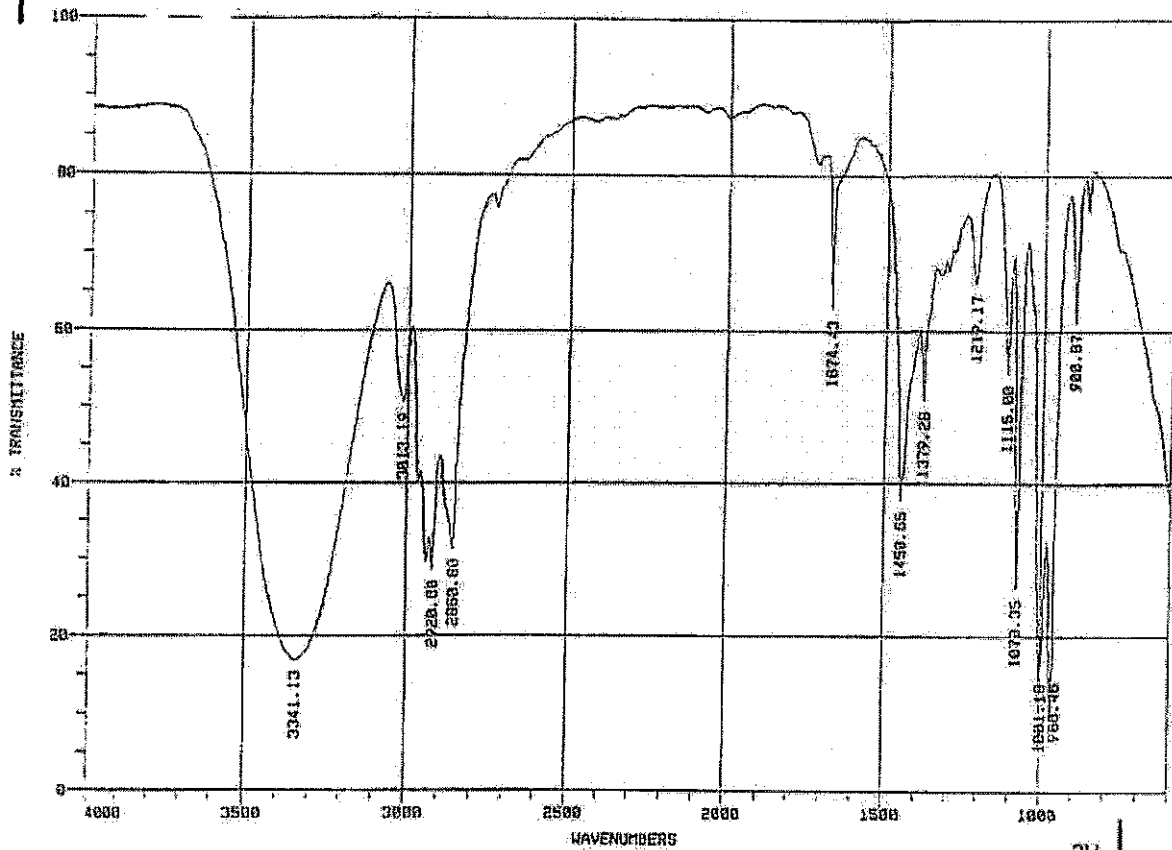


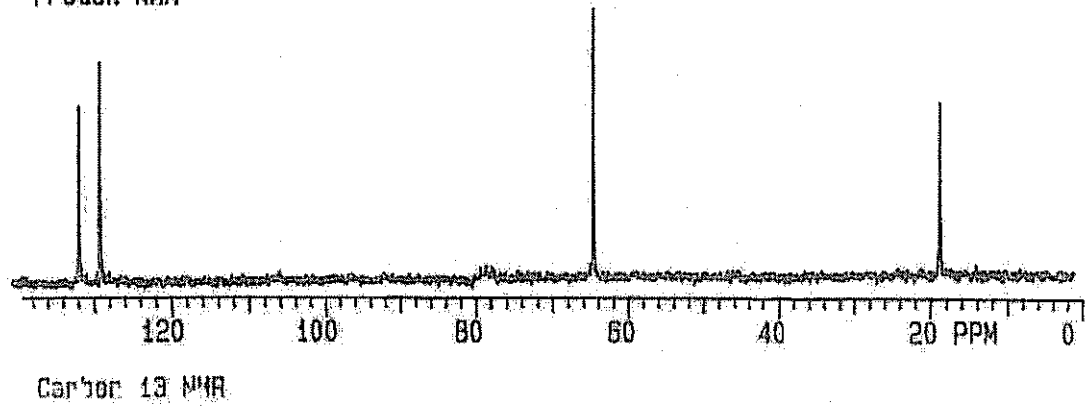
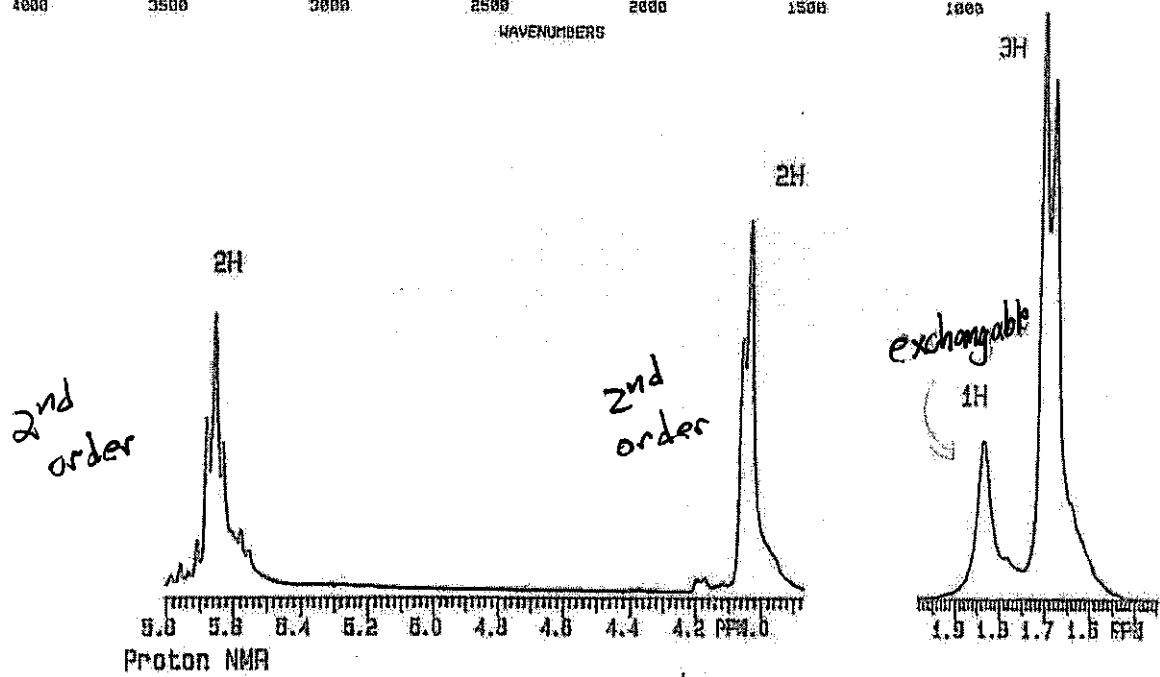
Handout 7: Combination Problem Set

Do problems 1-8 in Techniques in Organic Chemistry chapter 26 and problems 9-25 on the following pages.

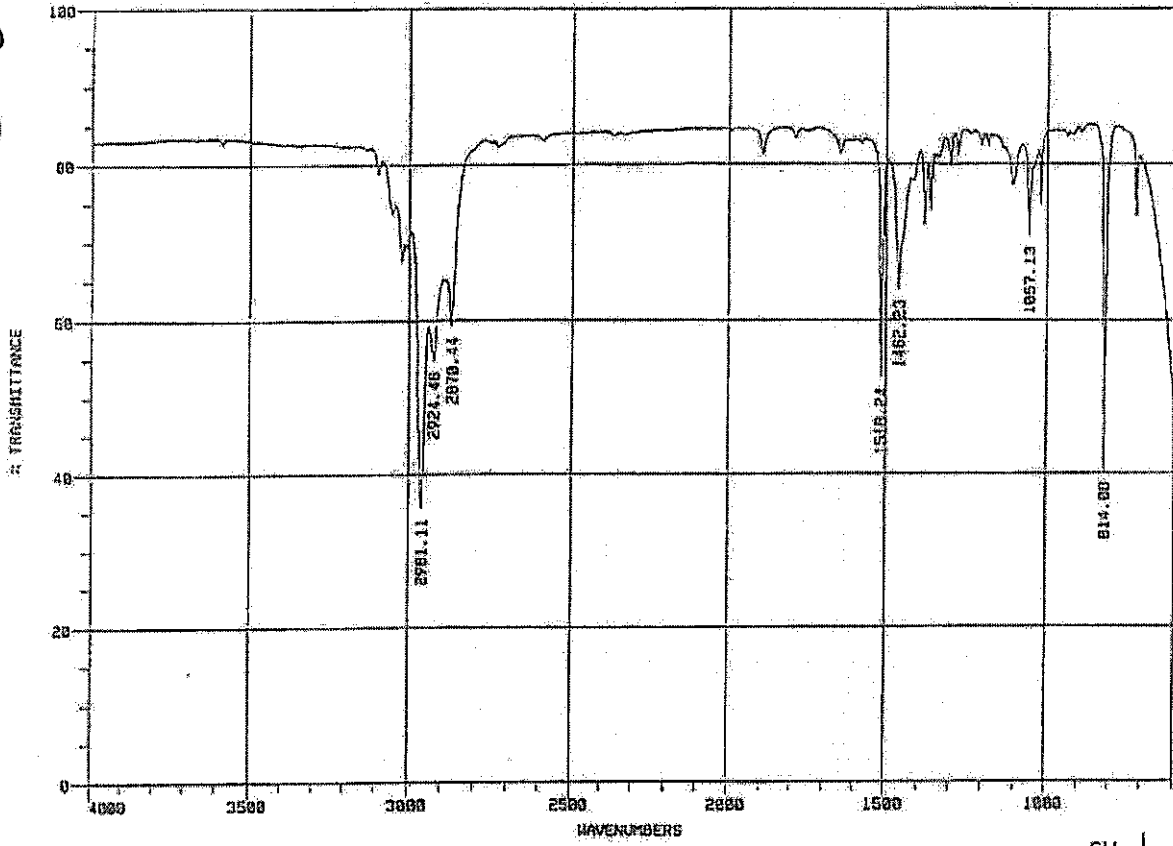
9



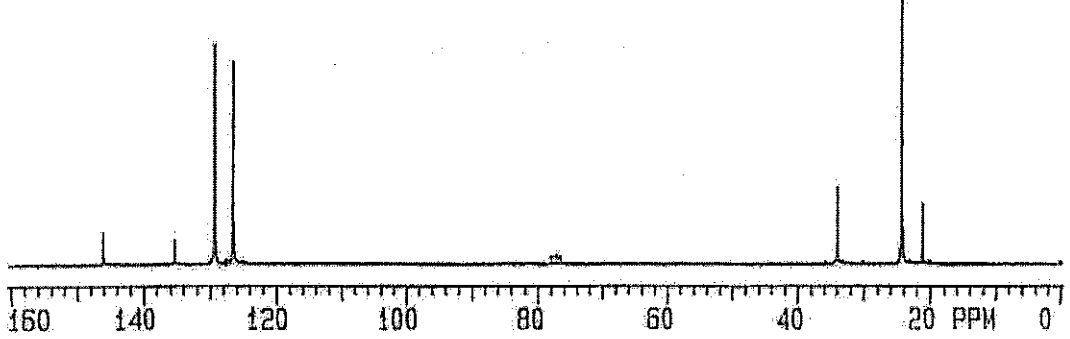
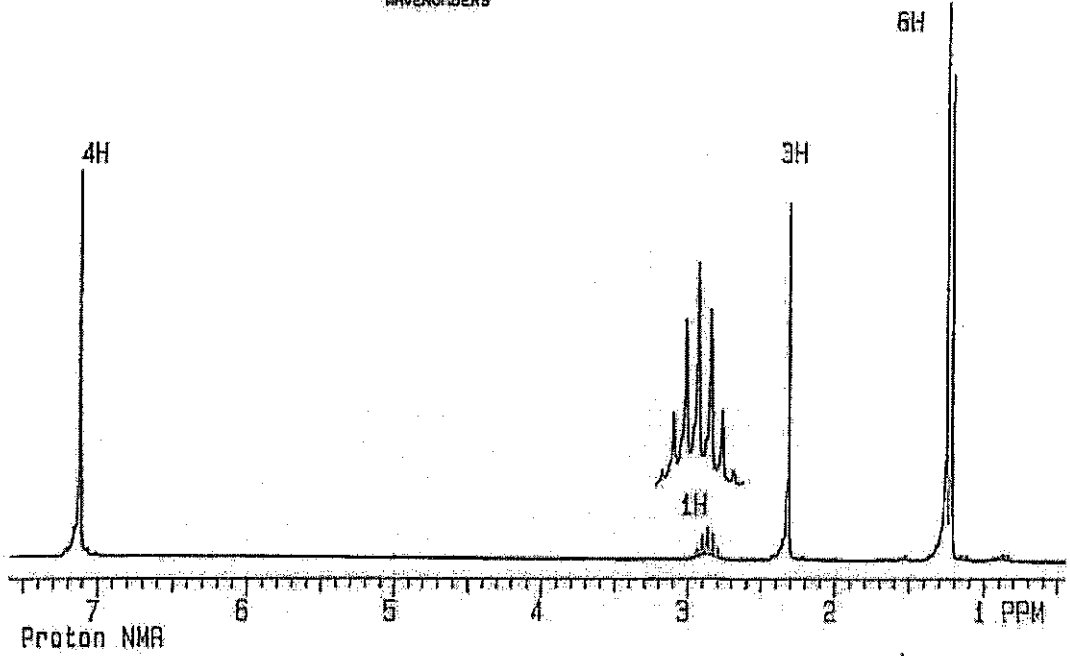
MW 72
%C 66.6
%H 11.2



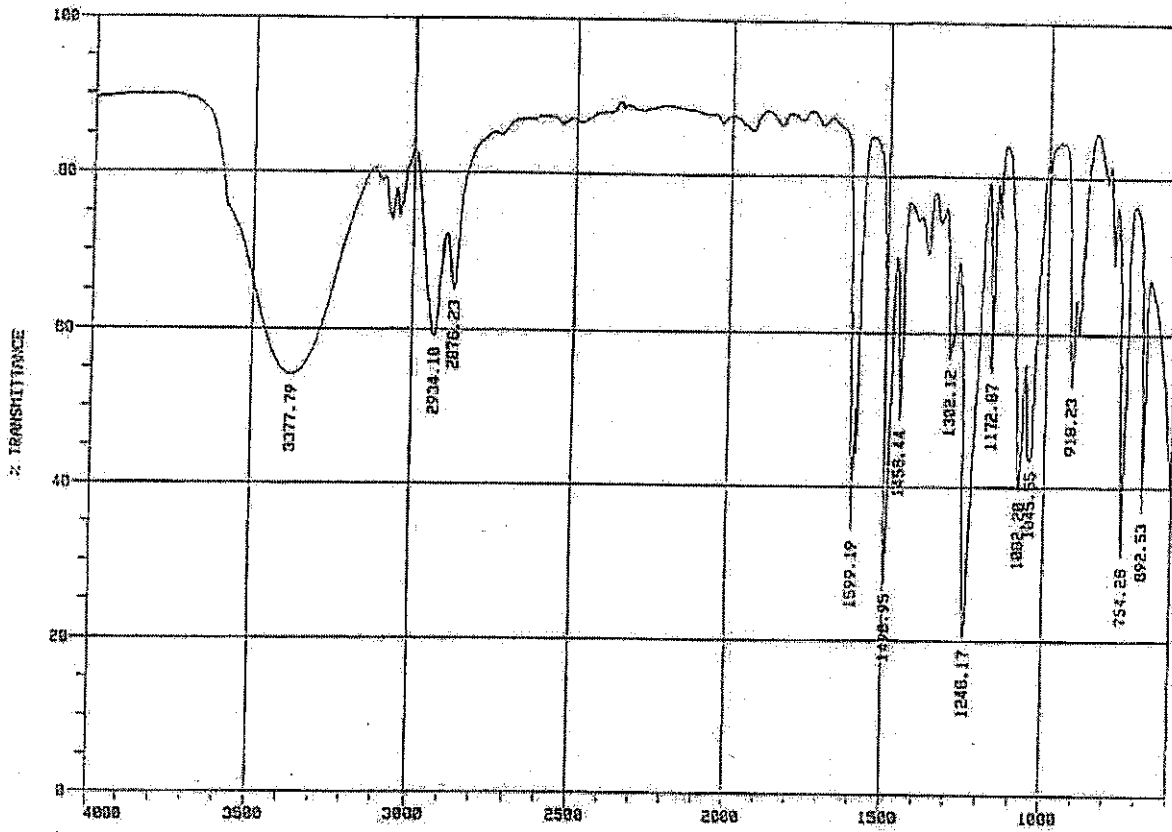
10



MW 134
%C 89.5
%H 10.5

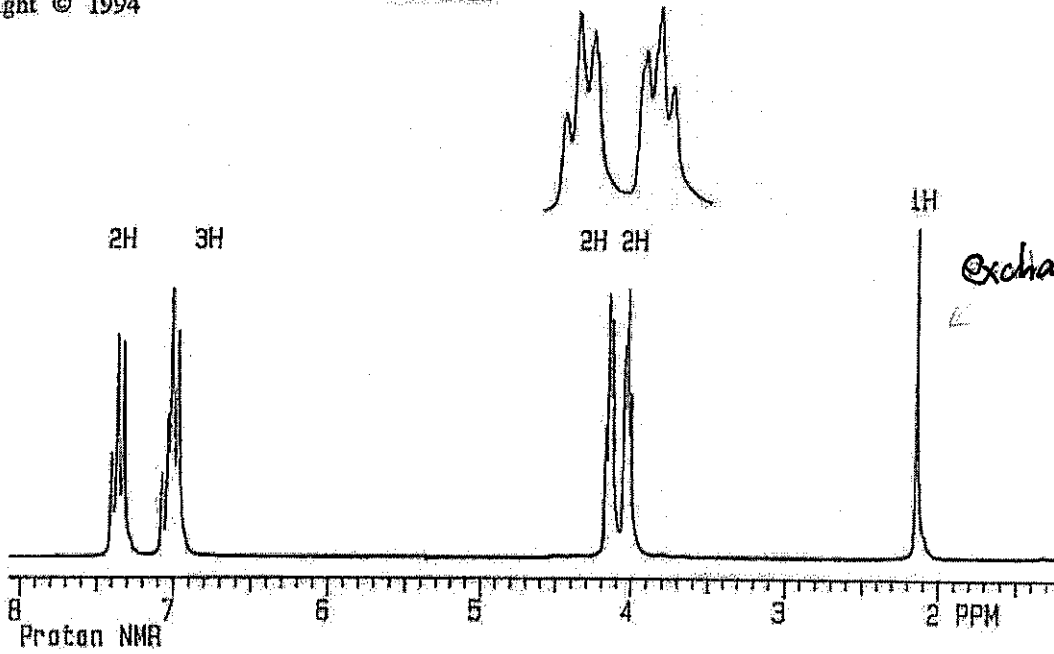


11

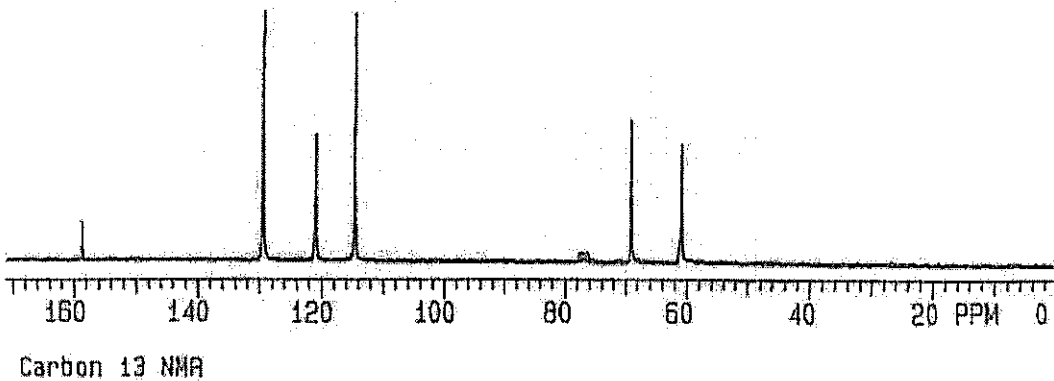


MW 138
%C 69.5
%H 7.4

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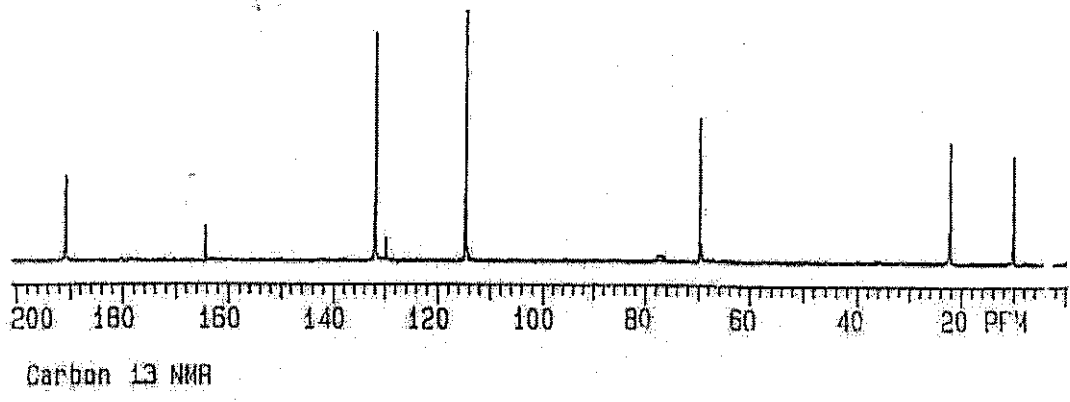
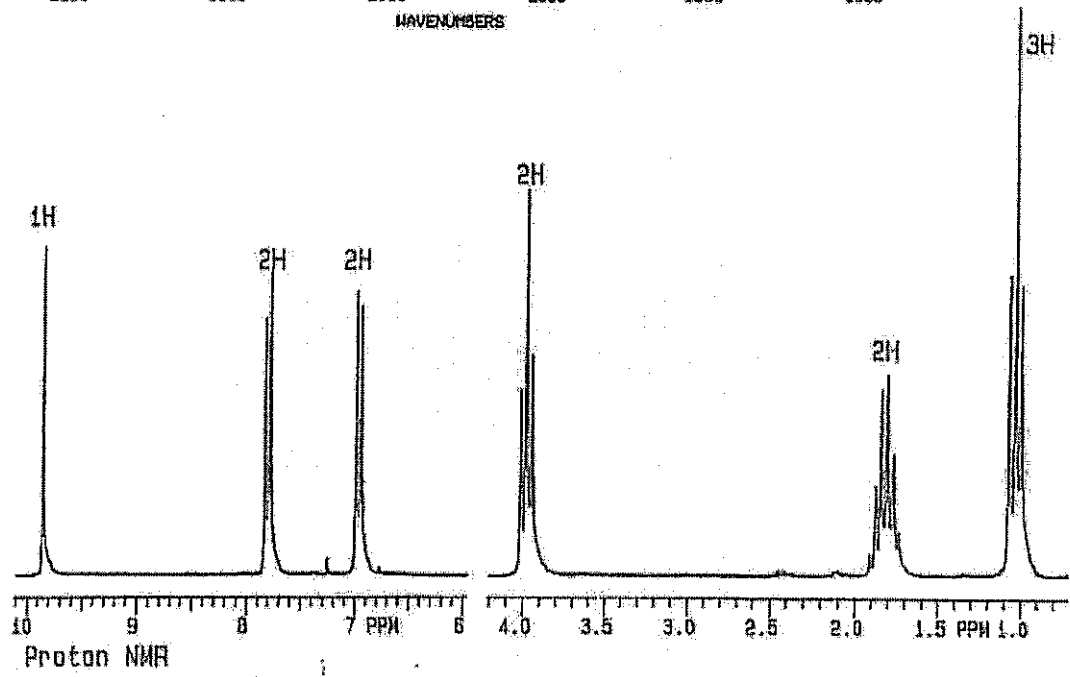
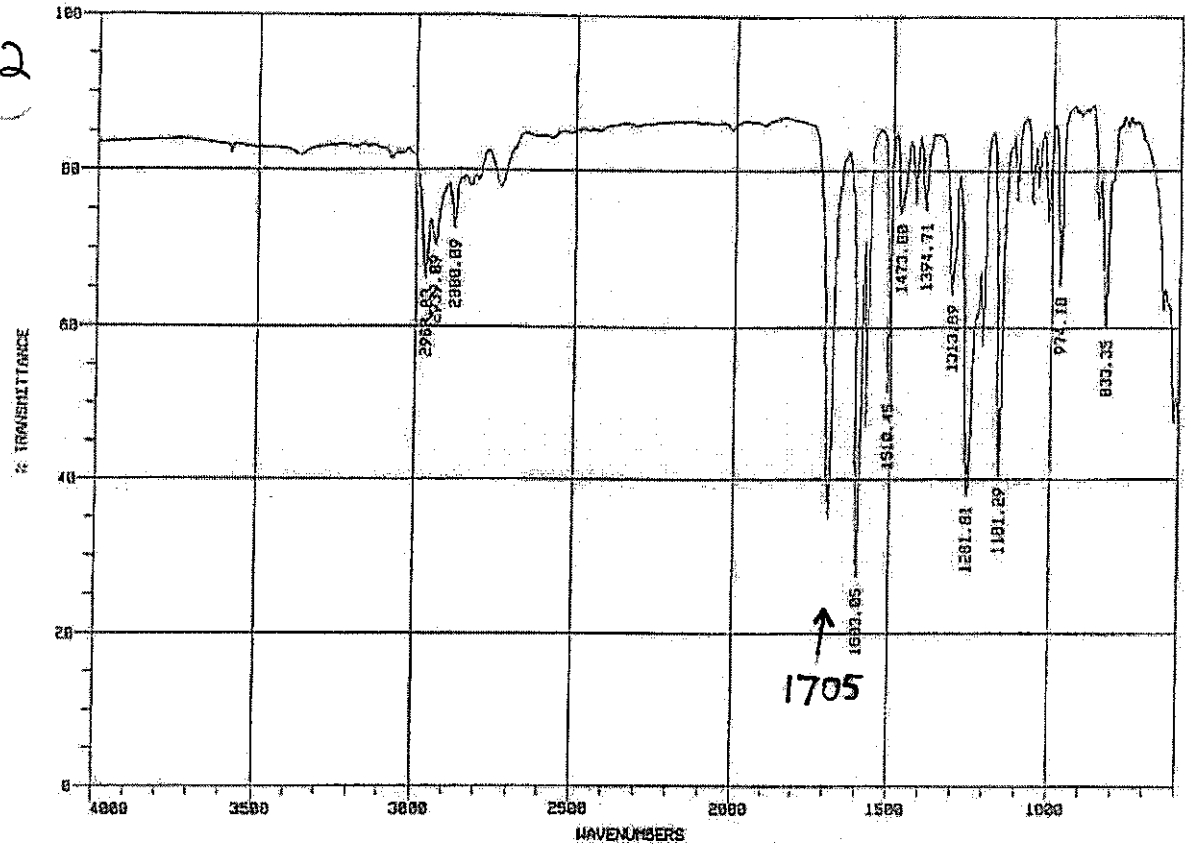


Exchangeable



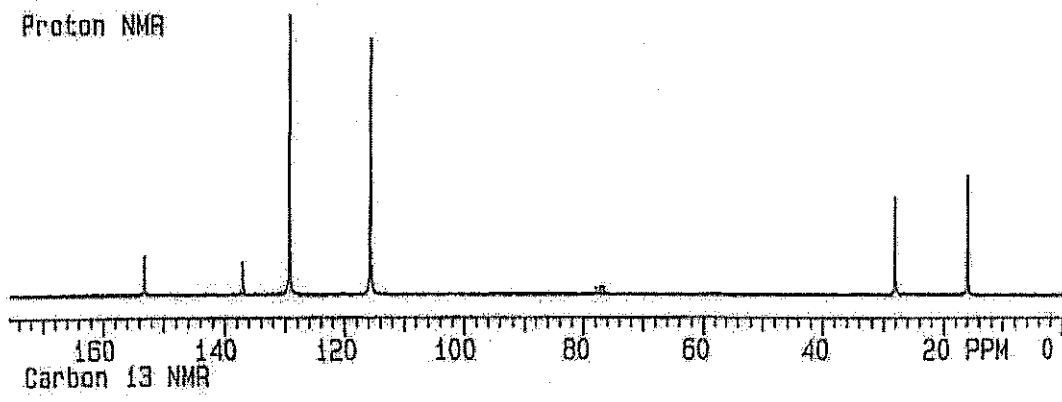
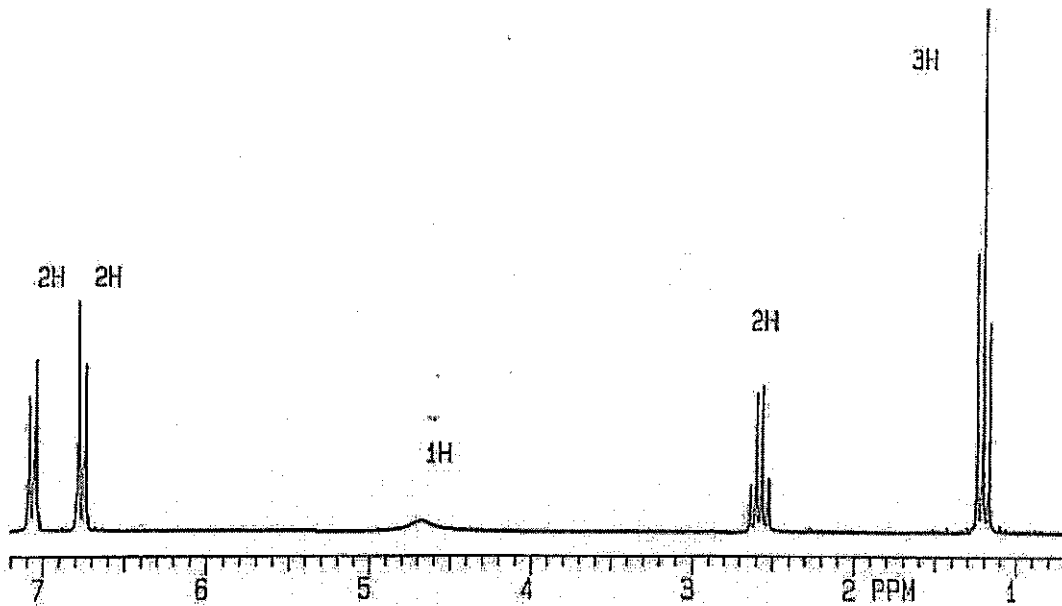
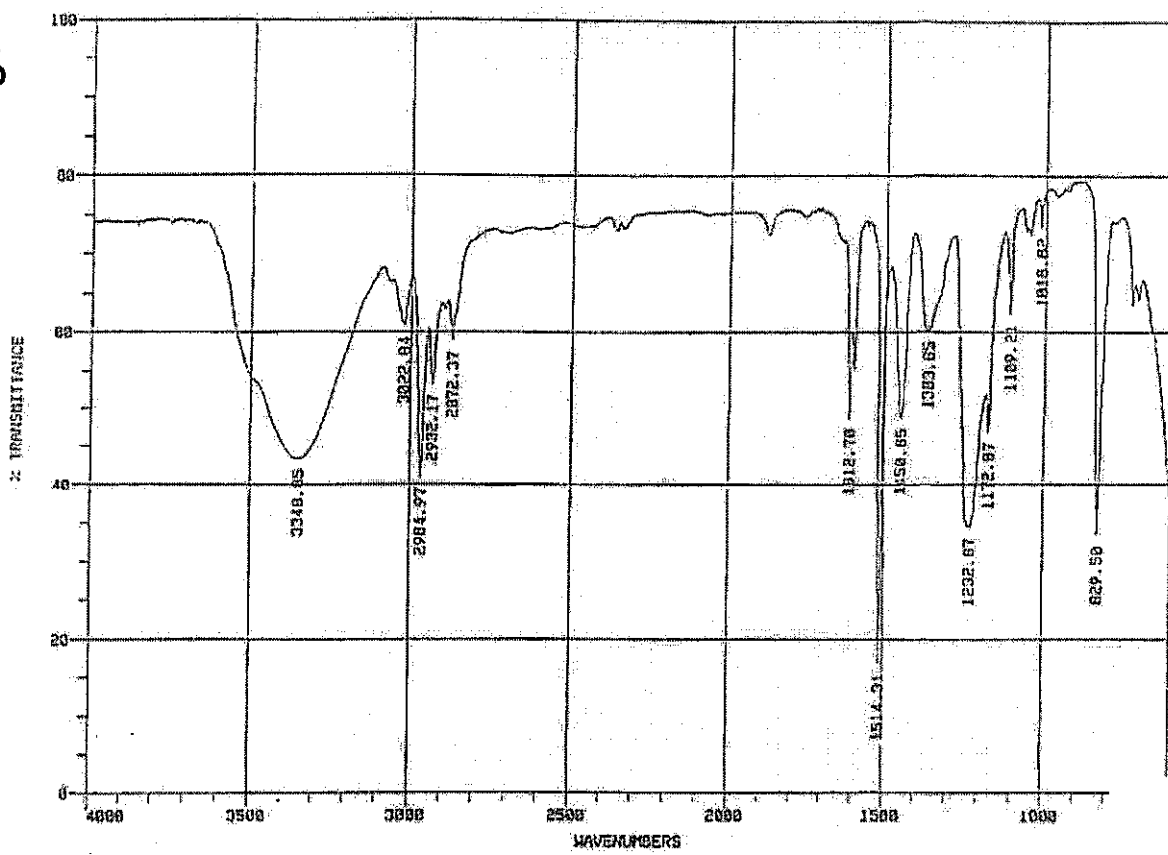
(2)

$M^+ = 164$

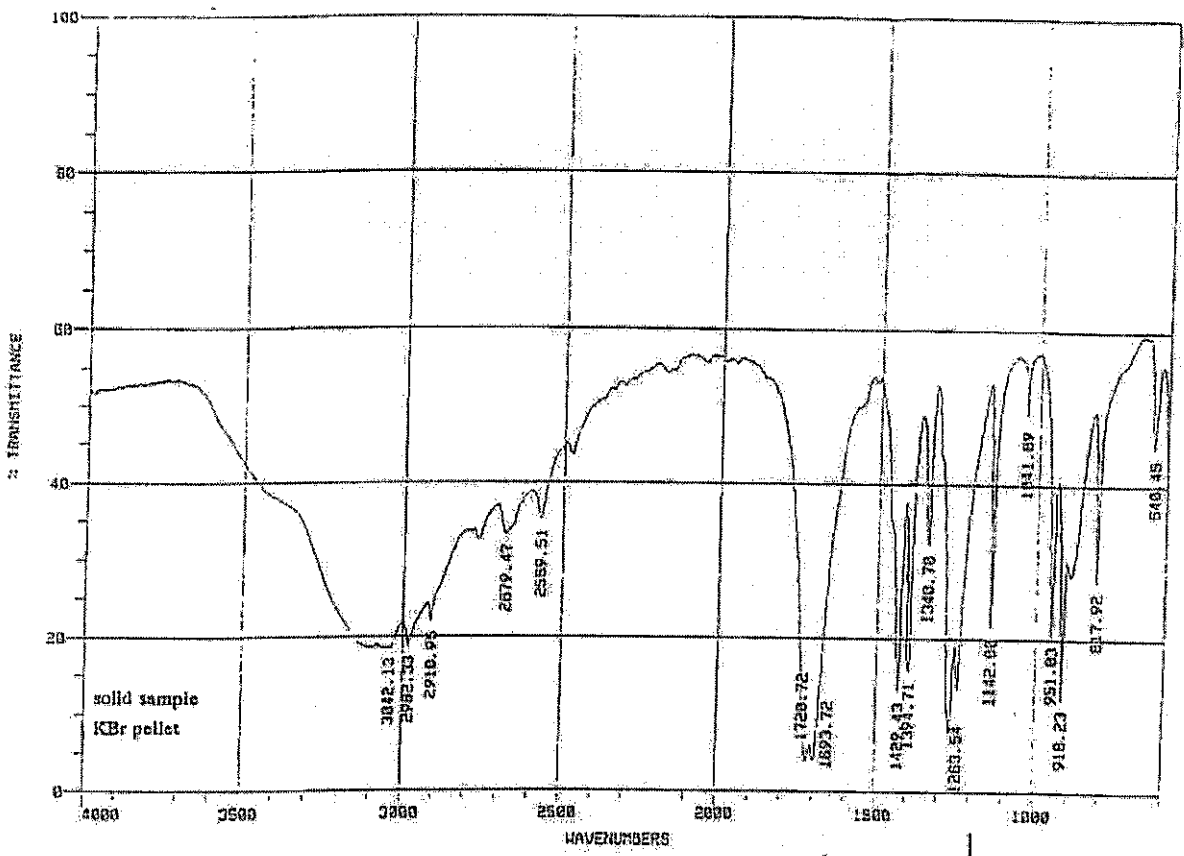


13

MW 122

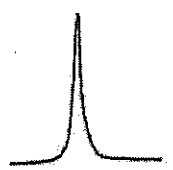


74



$M^+ = 152$
 $M^+ + 2 = 154$
same relative abundance

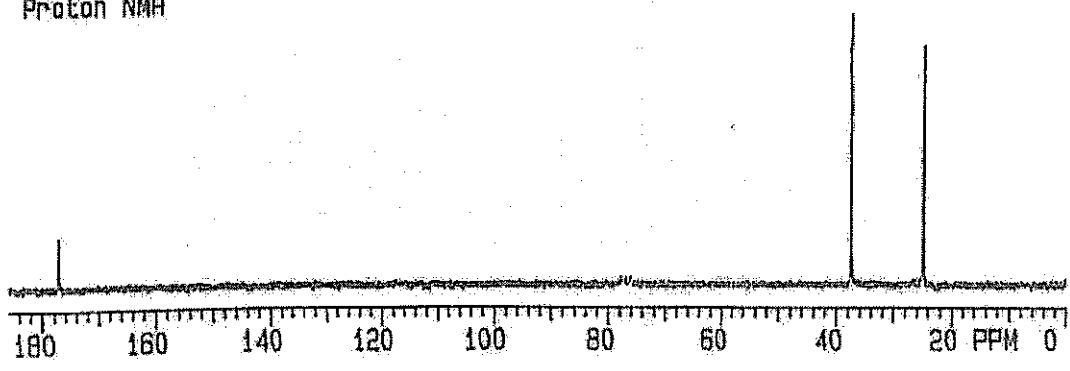
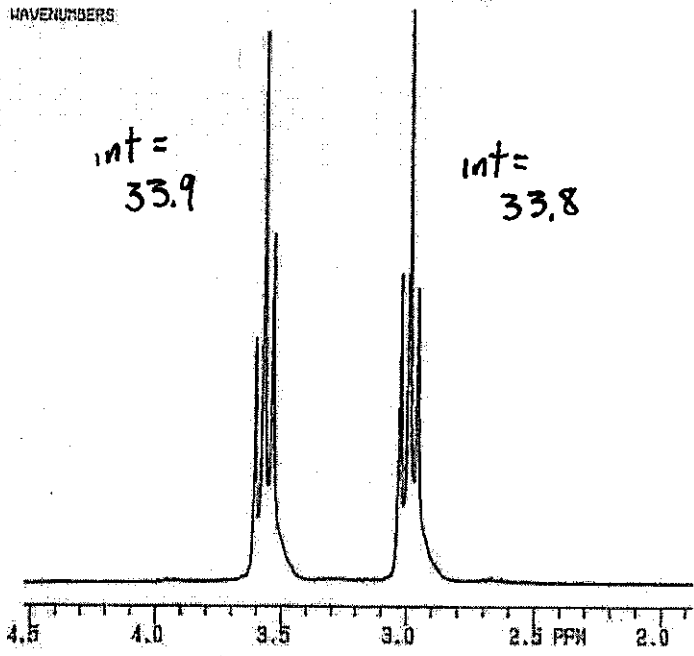
int = 17.1



11.6 PPM
Proton NMR

int = 33.9

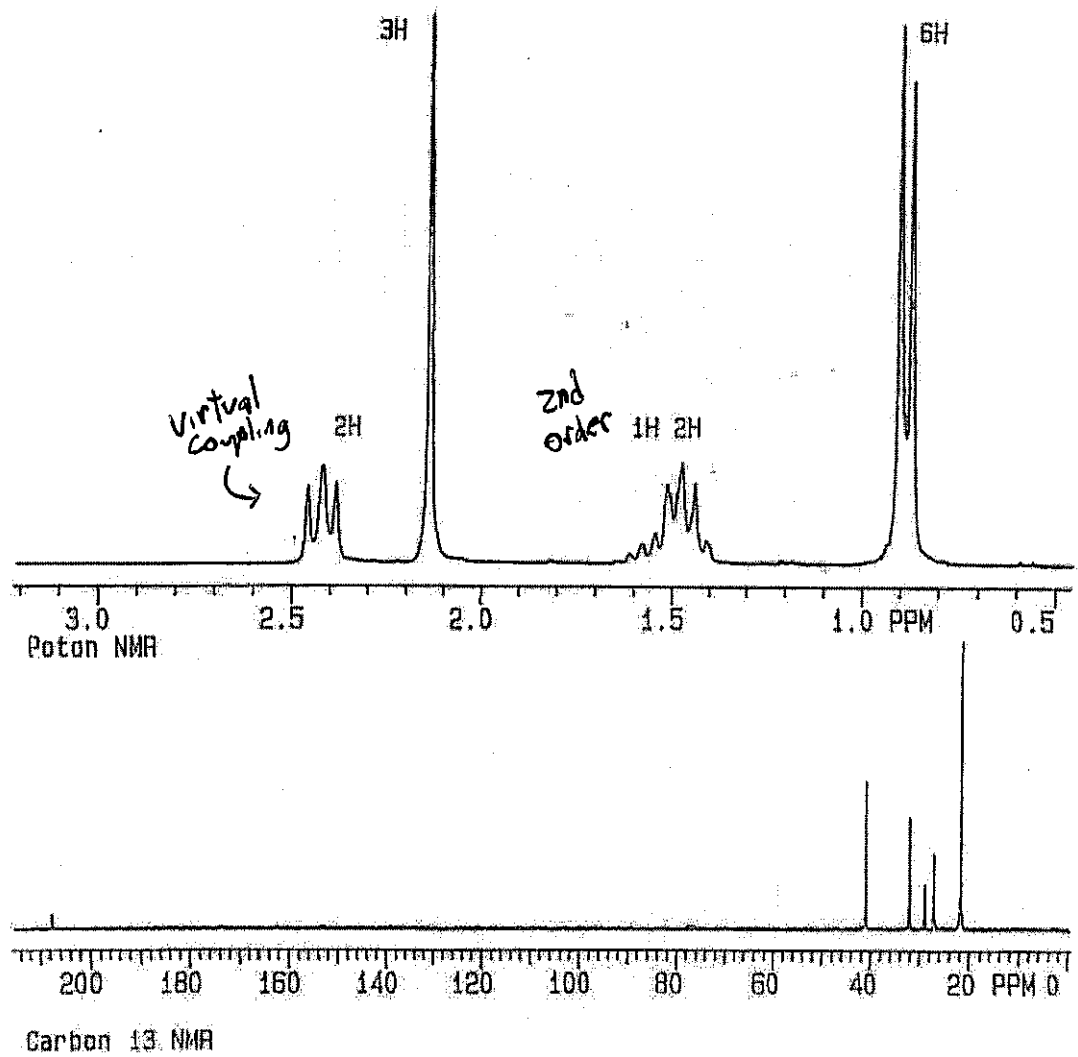
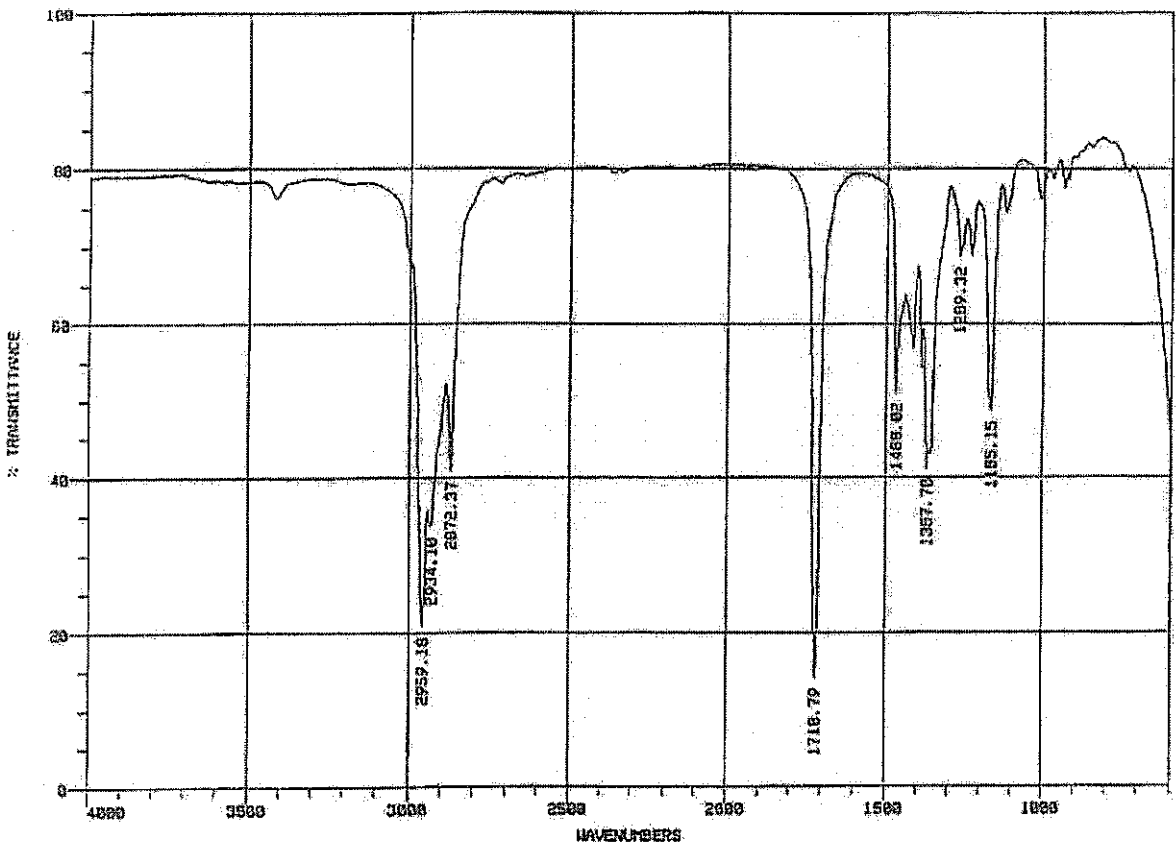
int = 33.8



Carbon 13 NMR

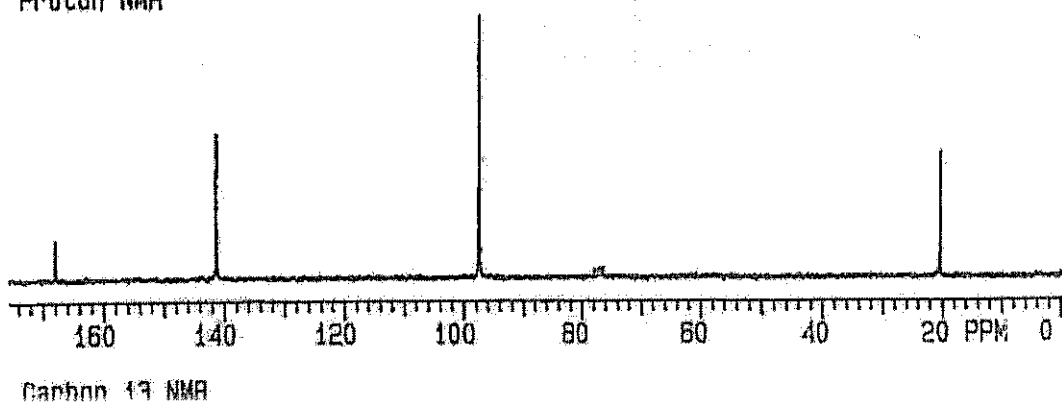
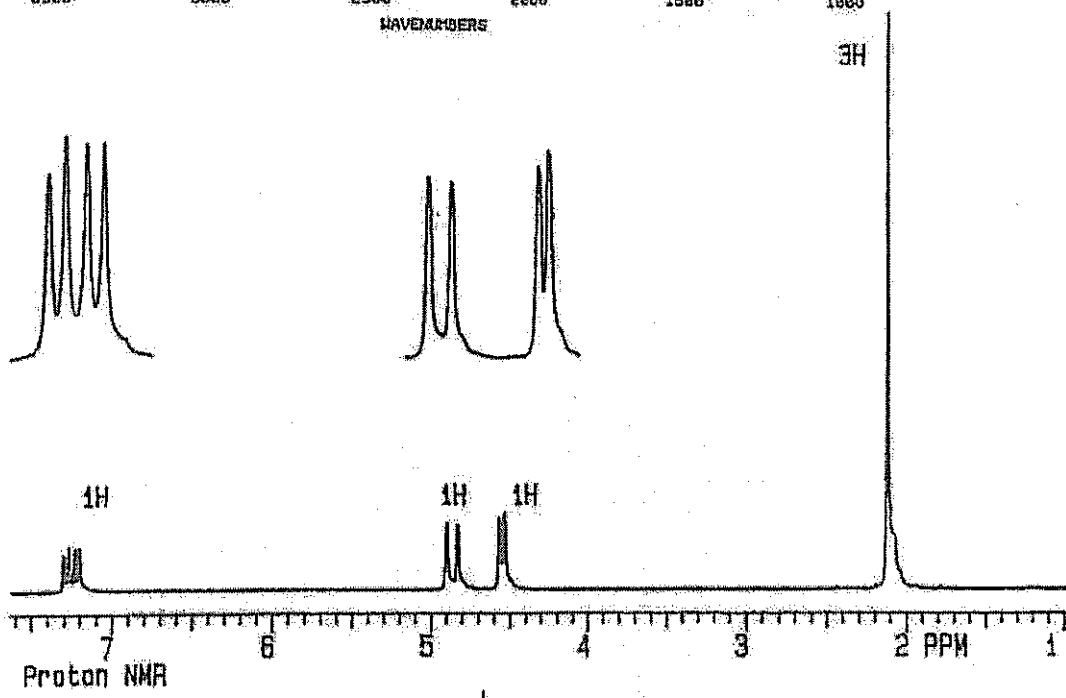
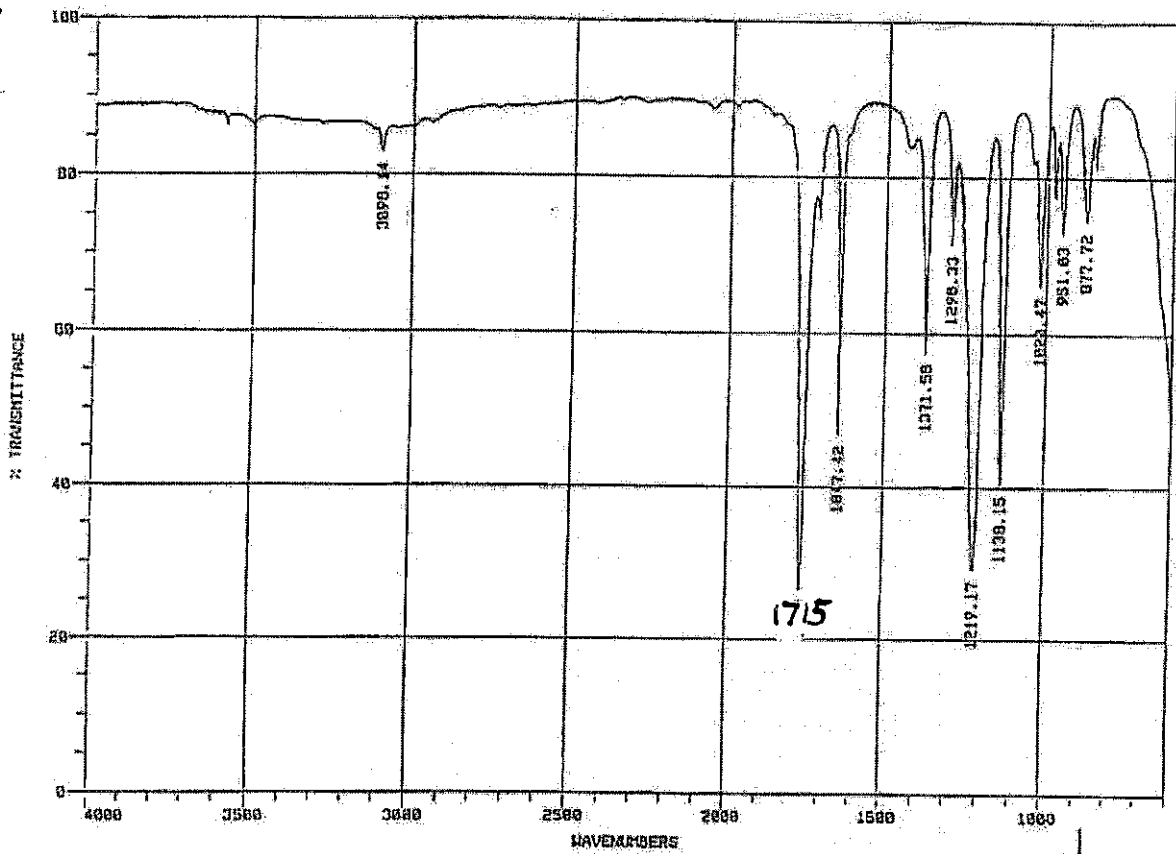
15

MW 114

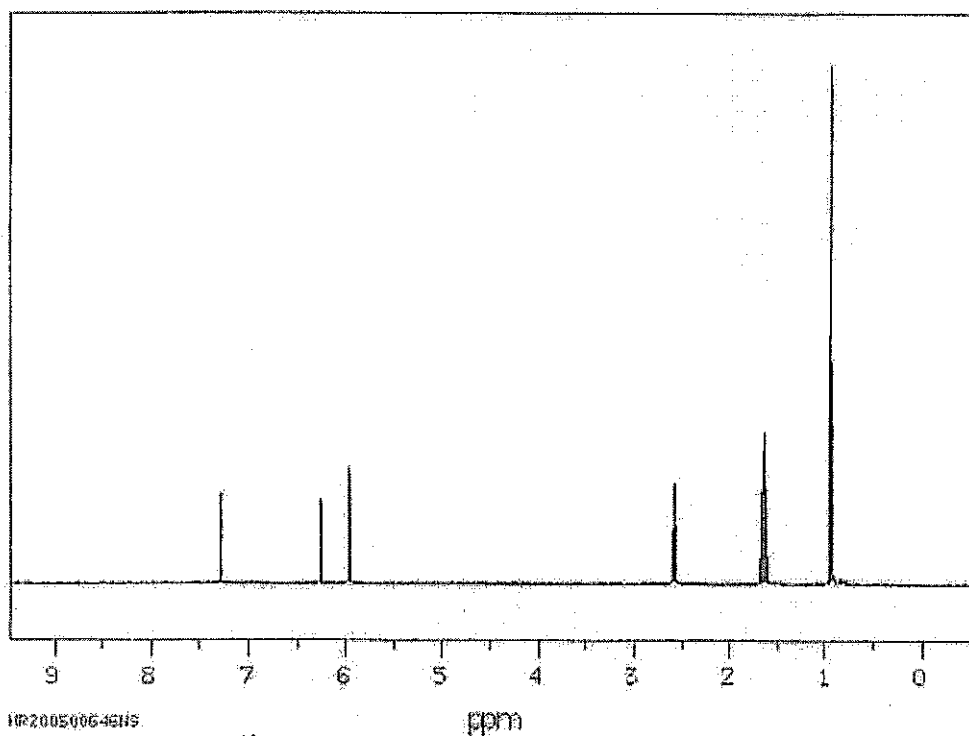


16

$M^+ = 86$
base peak = 43



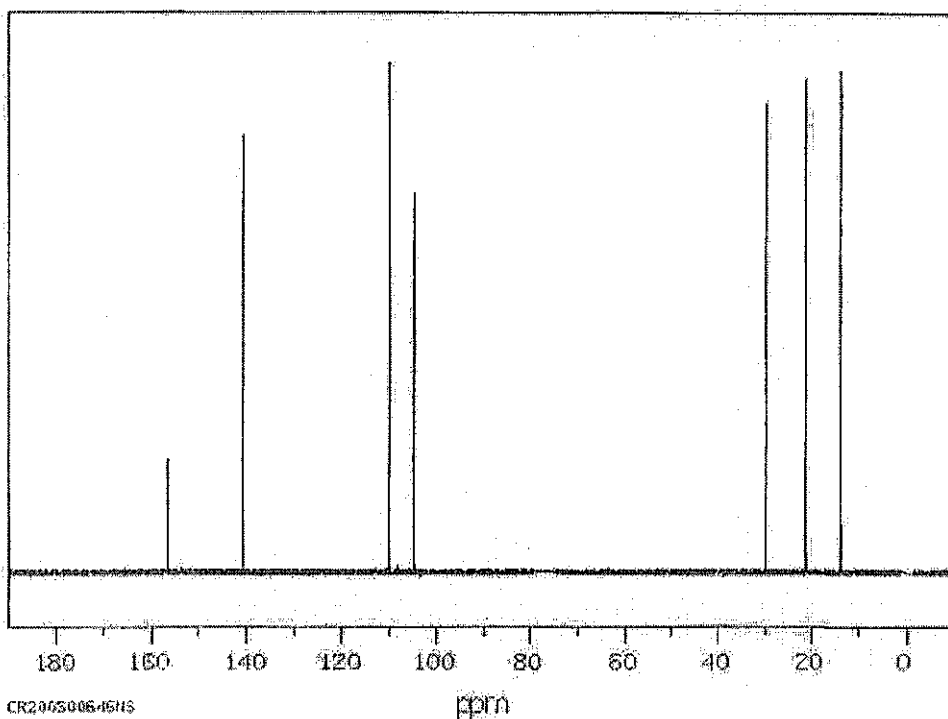
17



CR200500646HS

$J=10\text{ Hz}$

Data: shift 7.2 (1H, d), shift 6.2 (1H, t, $J=10\text{ Hz}$), shift 5.9 (1H, d, $J=10\text{ Hz}$), shift 2.6 (t, $J=7\text{ Hz}$, 2H), shift 1.6 (sx, $J=7\text{ Hz}$, 2H), shift 0.9 (t, $J=7\text{ Hz}$, 3H)

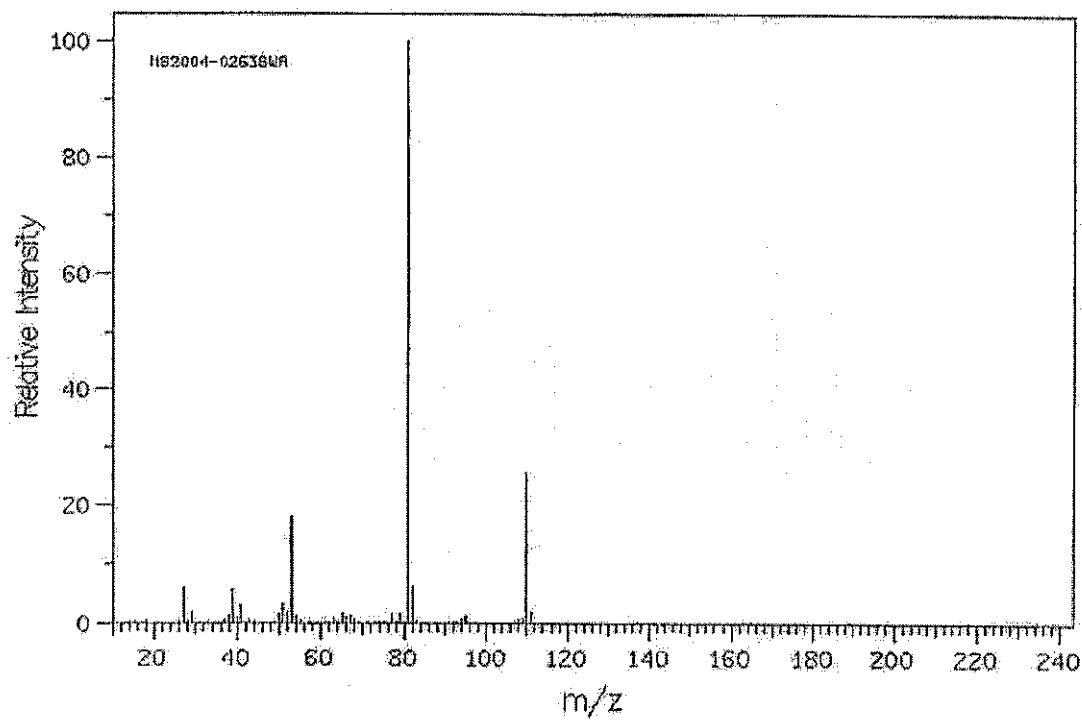
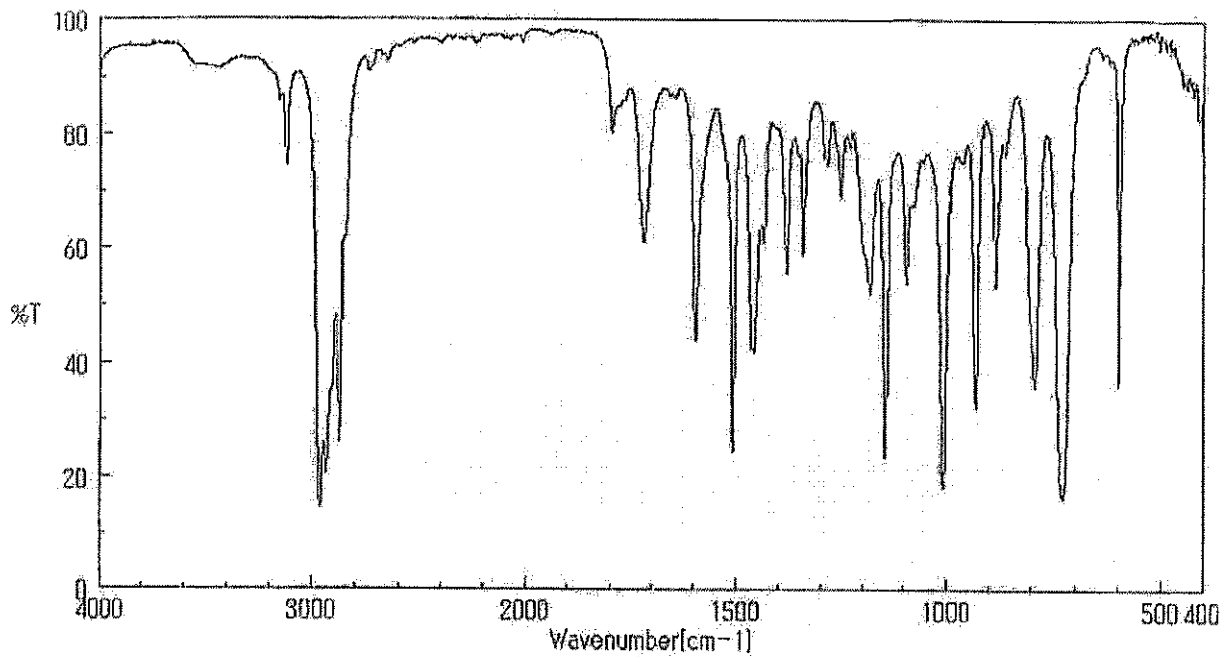


CR200500646HS

ppm

Shift: 156, 140, 110, 104, 30, 21, 14

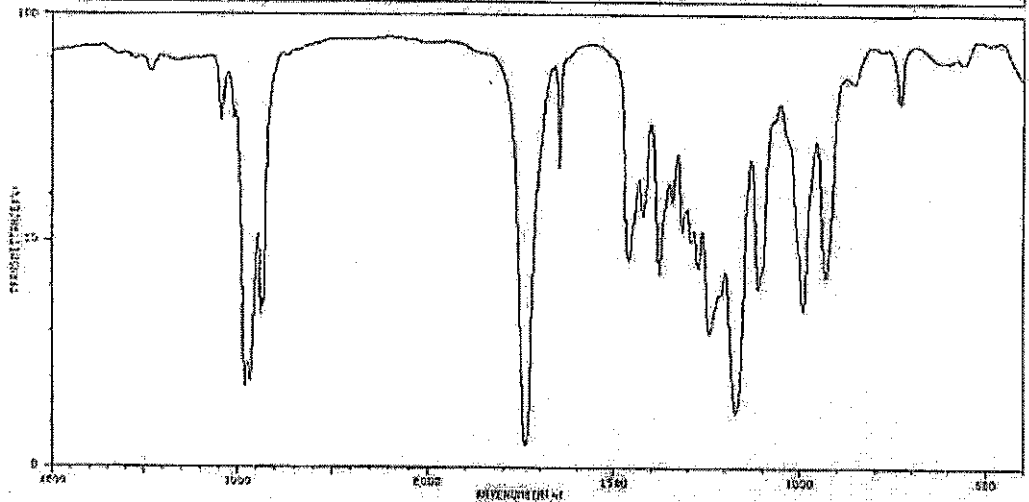
17 cont



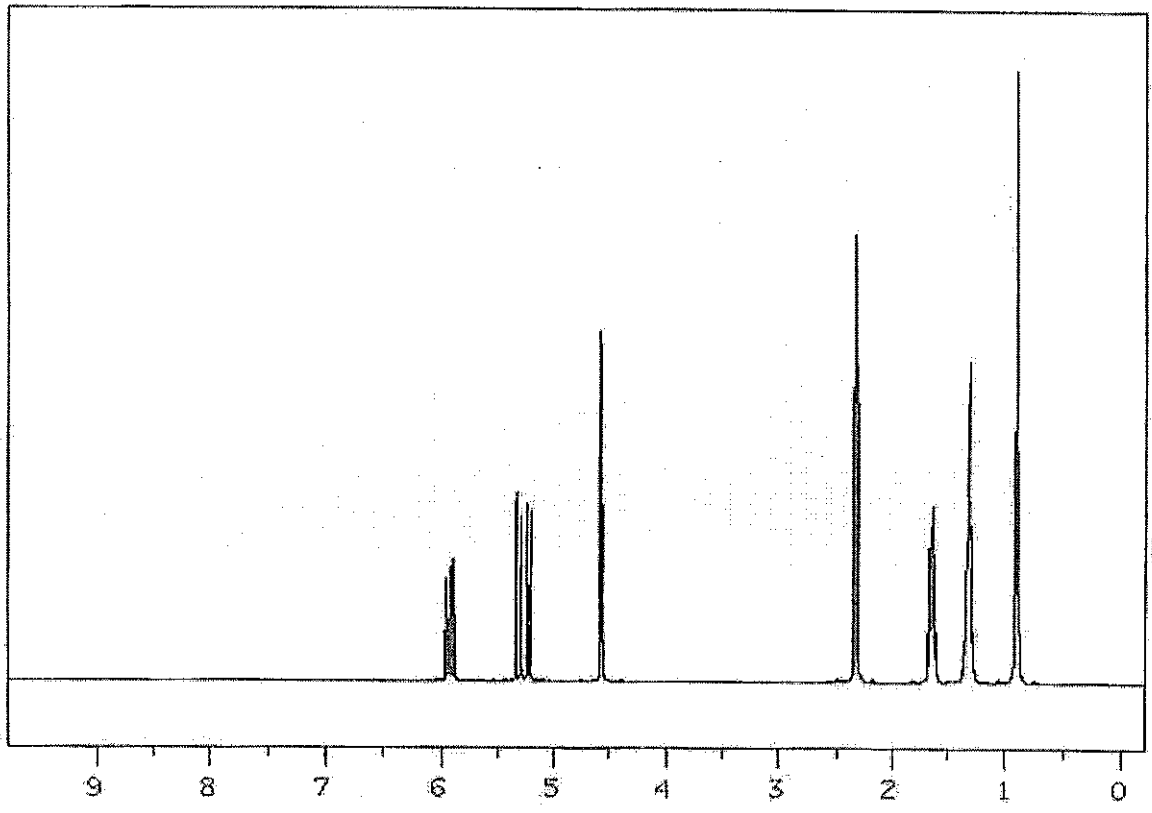
Peaks: 53, 81, M⁺ = 110

18

HIL-NO-1459 | SCORP- | 1 | 8065-NO-1472 | IR-NIDA-04367 : LIQUID FILM



3464	04	1741	4	1315	50	931	41
3057	74	1650	64	1283	47	867	81
3020	74	1468	48	1274	42	735	77
2959	17	1460	44	1243	20	661	00
2934	10	1422	53	1172	11		
2874	32	1380	41	1112	37		
2853	34	1341	57	991	13		

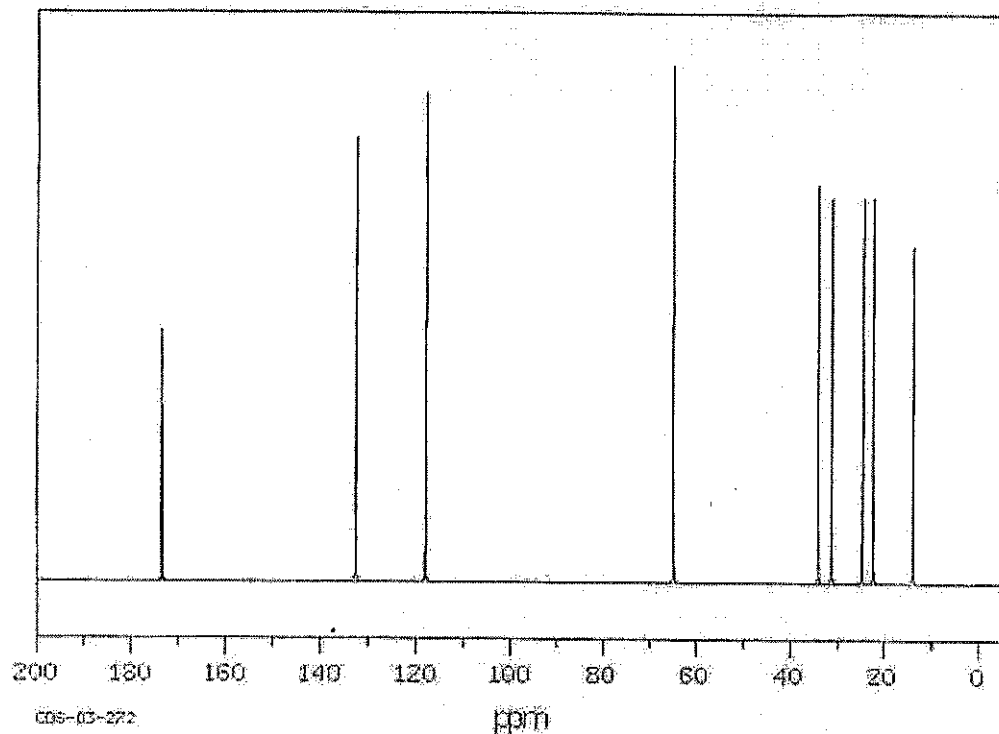


HSP-42-524

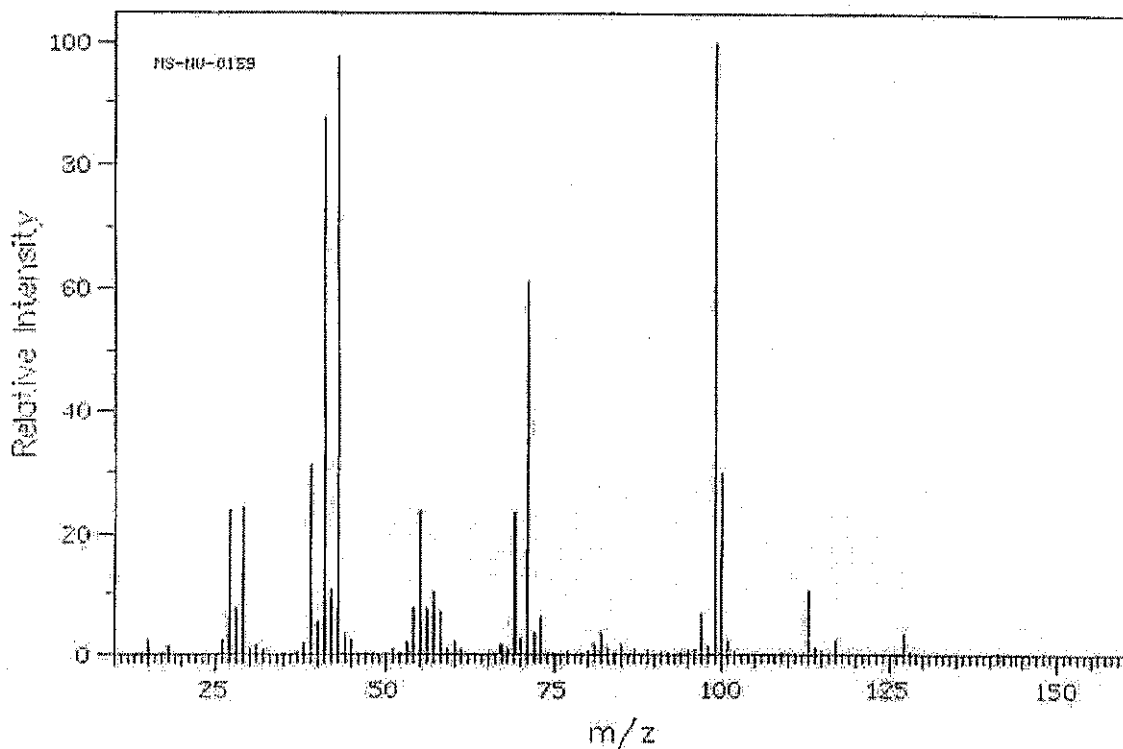
ppm

18 cont.

Data: shift 6.0 (ddt, $J=17, J=10, J=5$, 1H), shift 5.3 (d, $J=17$, 1H), shift 5.2 (d, $J=10$, 1H), shift 4.6 (d, $J=5$, 2H), shift 2.3 (t, $J=8\text{Hz}$, 2H), shift 1.7 (p, $J=8\text{Hz}$, 2H), shift 1.35 (p, $J=8\text{Hz}$, 2H), shift 1.25 (sx, $J=8\text{Hz}$, 2H), shift 0.9 (t, $J=8\text{Hz}$, 3H)



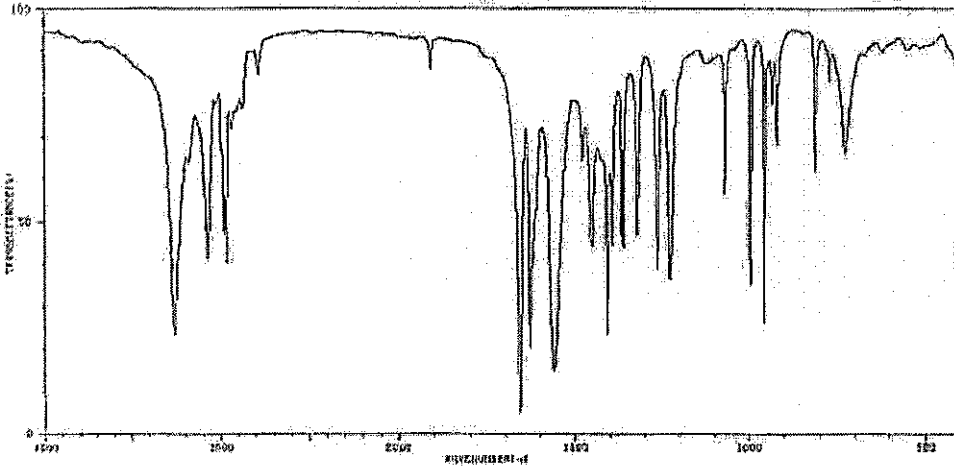
Peaks: 173, 133, 118, 65, 34, 31, 25, 22, 14 ppm



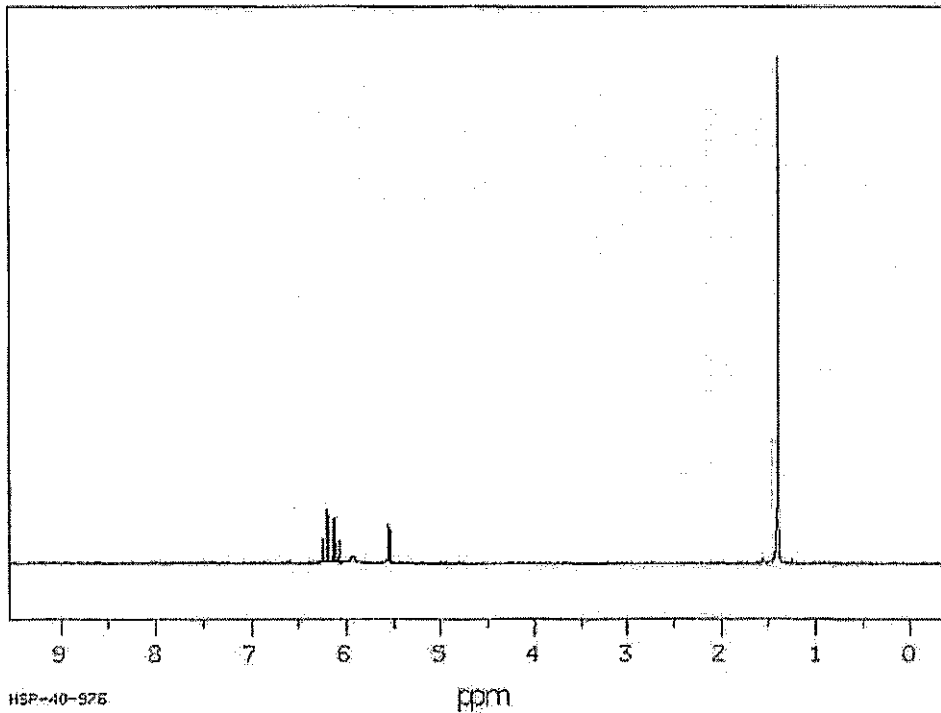
Peaks: 29, 41, 43, 71, 99, $M^+=156$

19

SDBS-NO-1558 IR-NIDA-37897 : RDR DISC

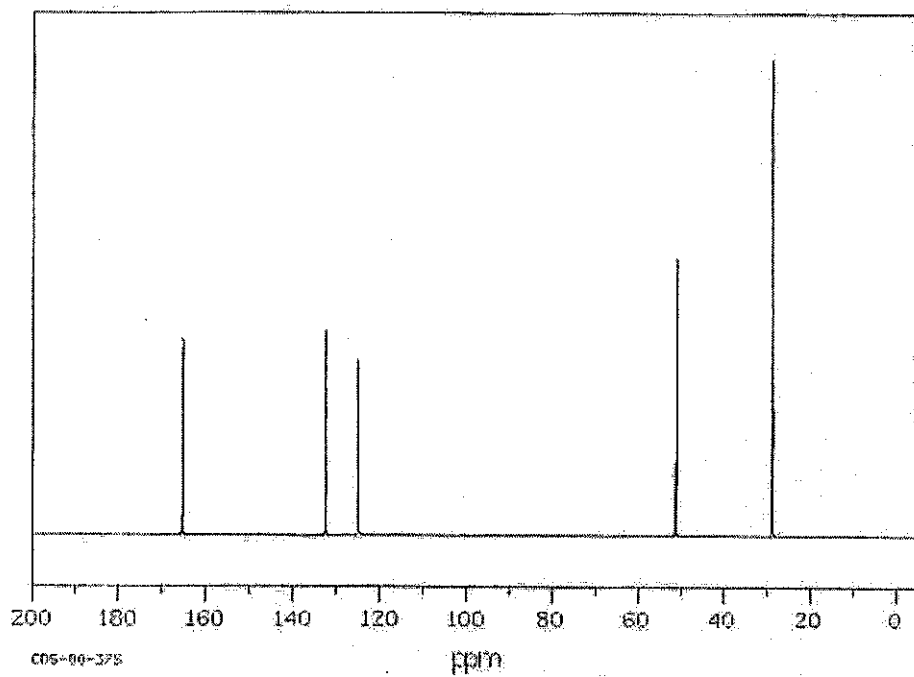


3268	28	2973	68	1479	67	1263	37	930	74
3179	62	2871	74	1452	42	1227	35	918	66
3075	57	2787	61	1407	22	1113	64	812	30
3073	39	1918	61	1394	42	1084	66	771	79
2986	64	1657	4	1387	43	894	34	726	64
2960	44	1627	20	1560	42	855	25	620	60
2753	38	1061	14	1328	44	647	61		

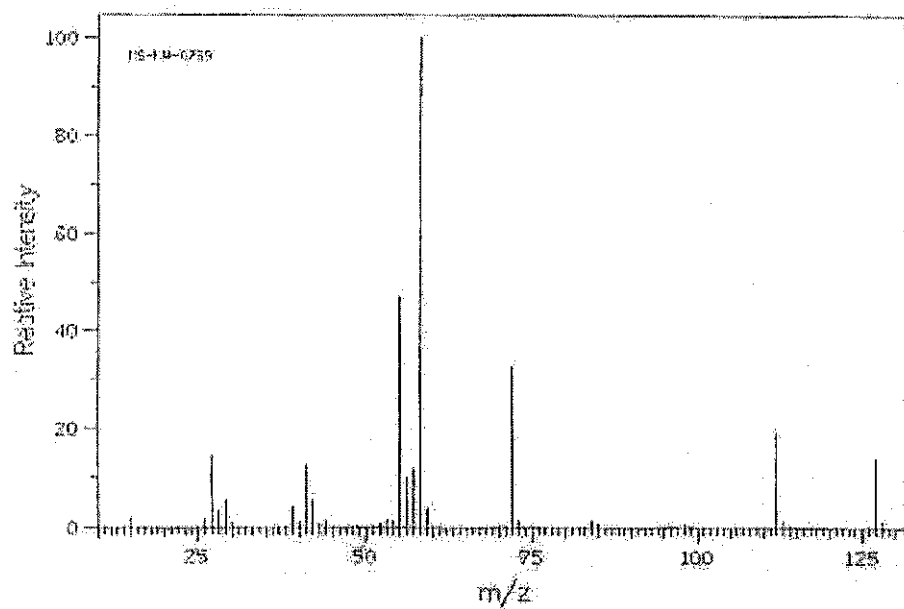


Data: shift 6.2 (d, J=18, 1H), shift 6.1 (dd, J=18, J=10, 1H), shift 5.9 (exch, 1H), shift 5.5 (d, J=10Hz, 1H), shift 1.4 (s, 9H)

19 cont.



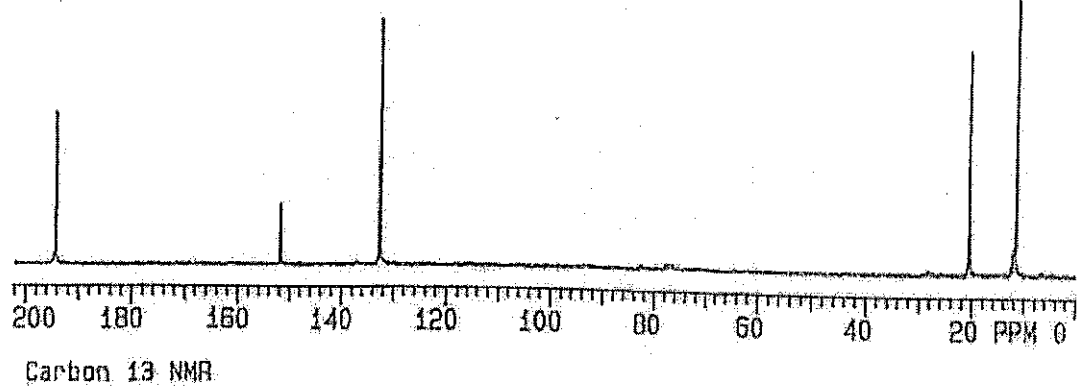
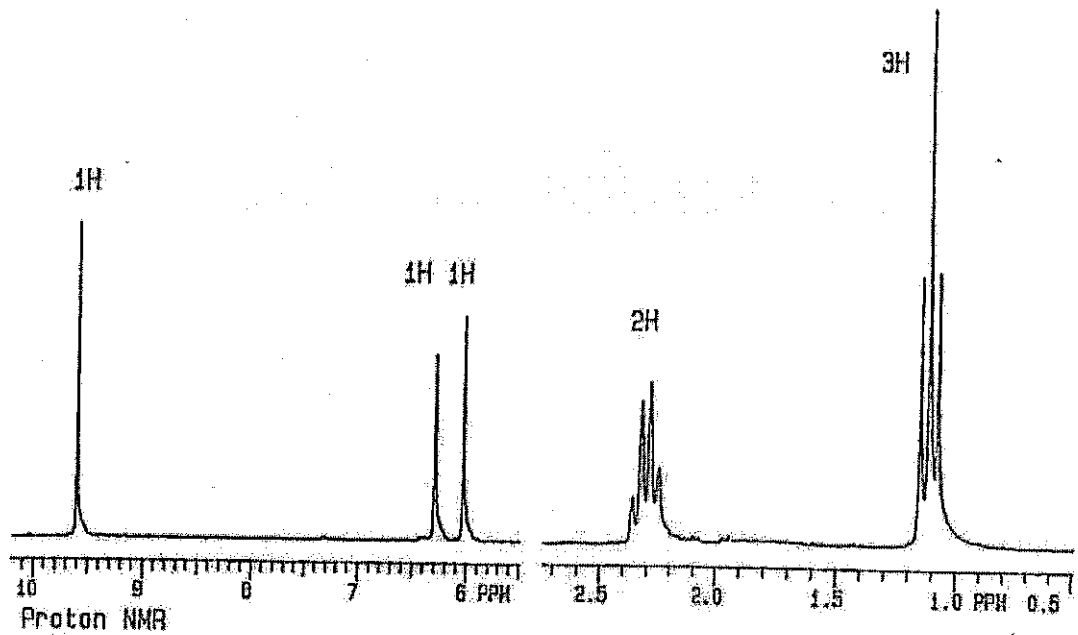
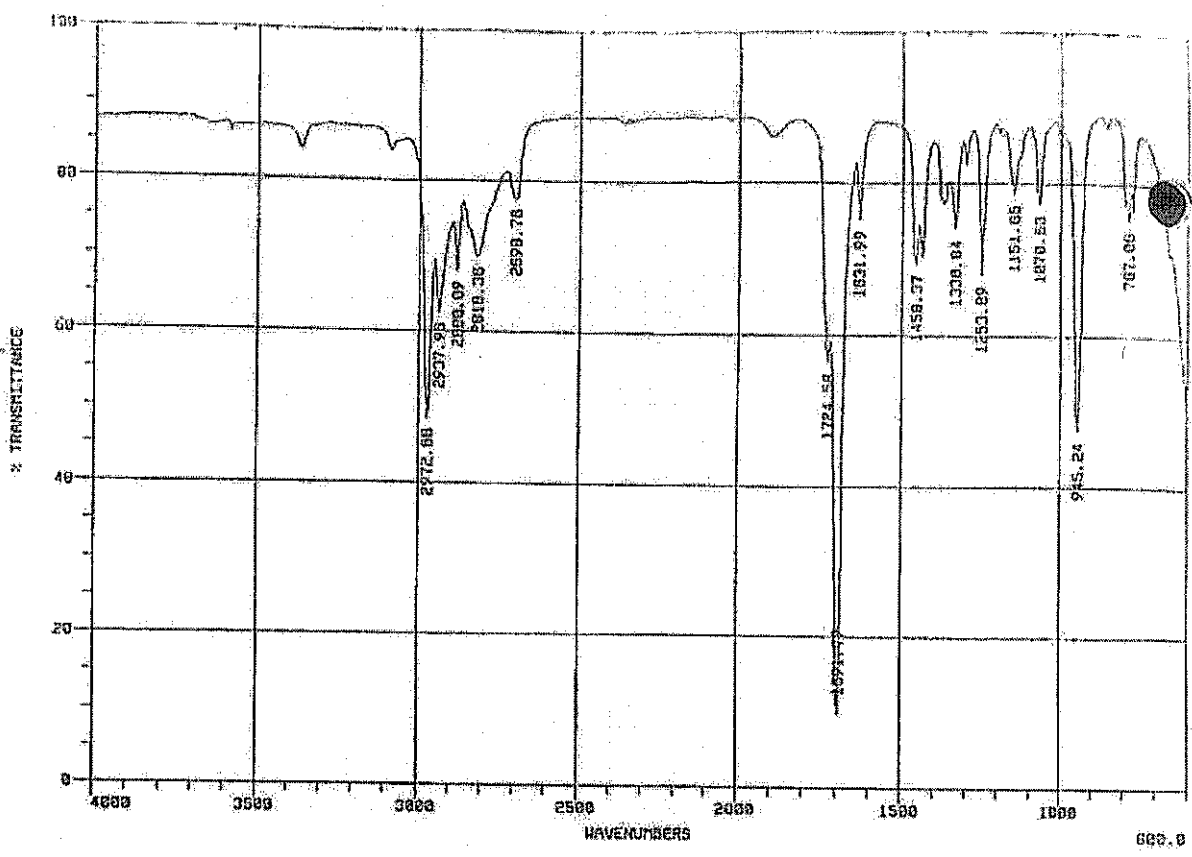
Peaks: 165, 132, 125, 51, 29



Peaks: 27, 41, 55, 58 (base), 72, 112, M⁺=127

20

MS
M_r = 84
base = 55

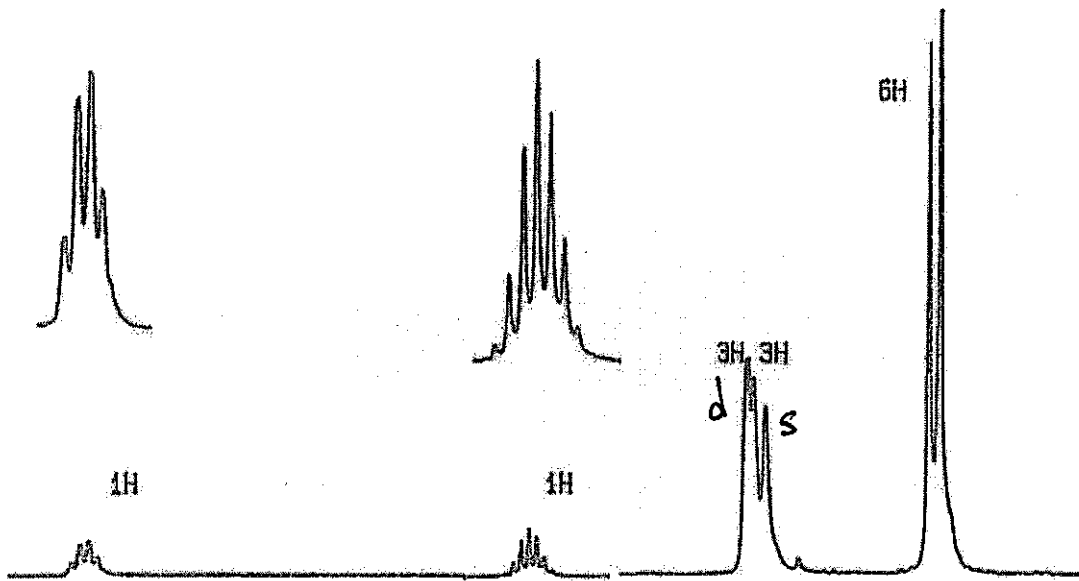
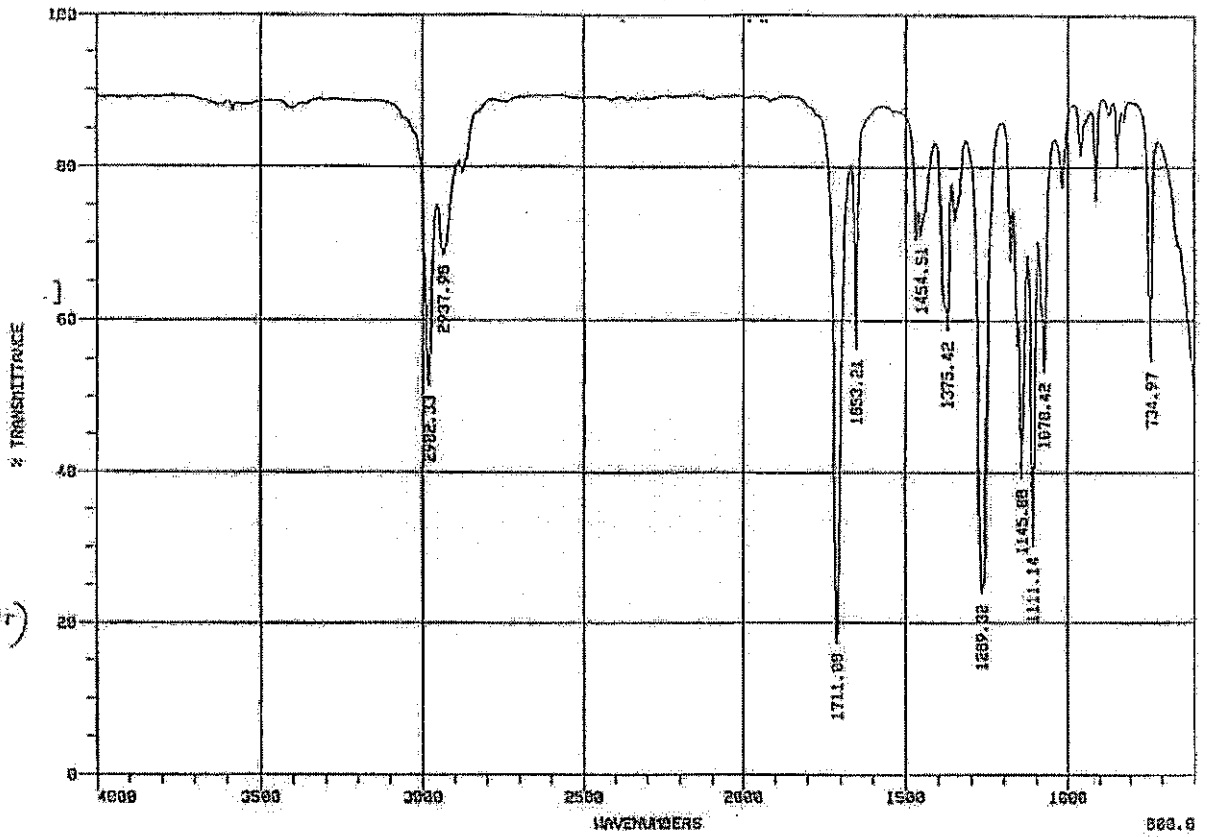


28

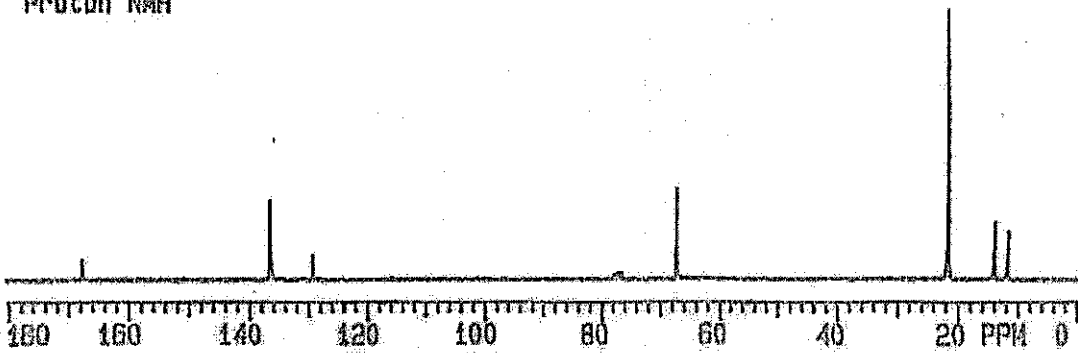
m/z

relative abundance

27	29
55	60
83	100
100	27
127	25
142	7 (M ⁺)

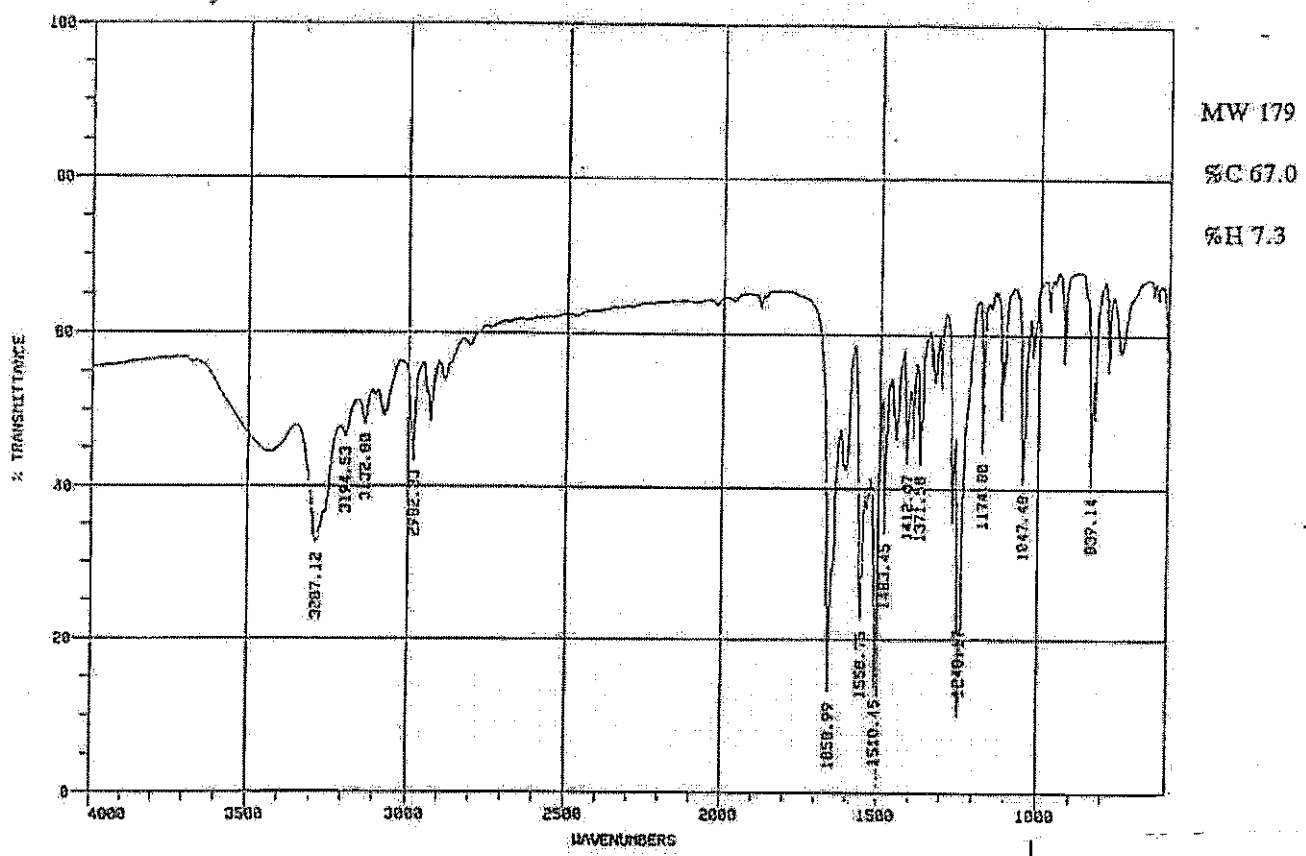


7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 2.2 2.0 1.8 1.6 1.4 1.2 PPM, δ
Proton NMR



Carbon 13 NMR

22



Integration:

237

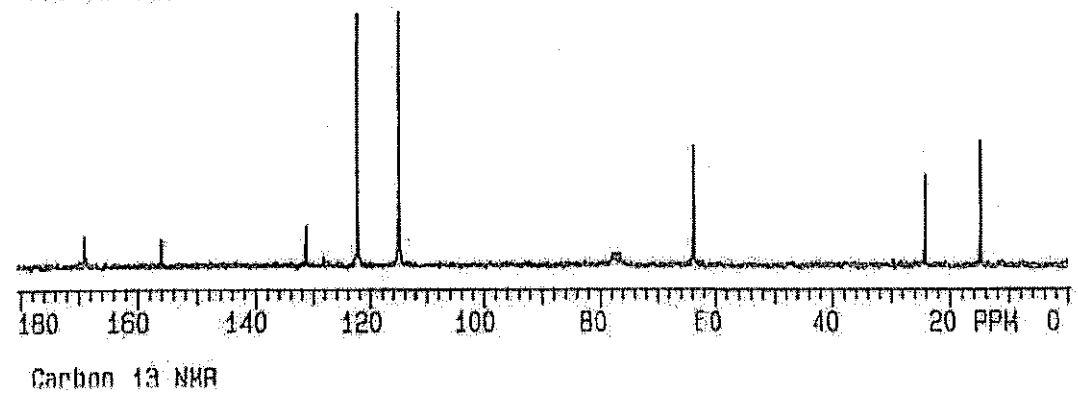
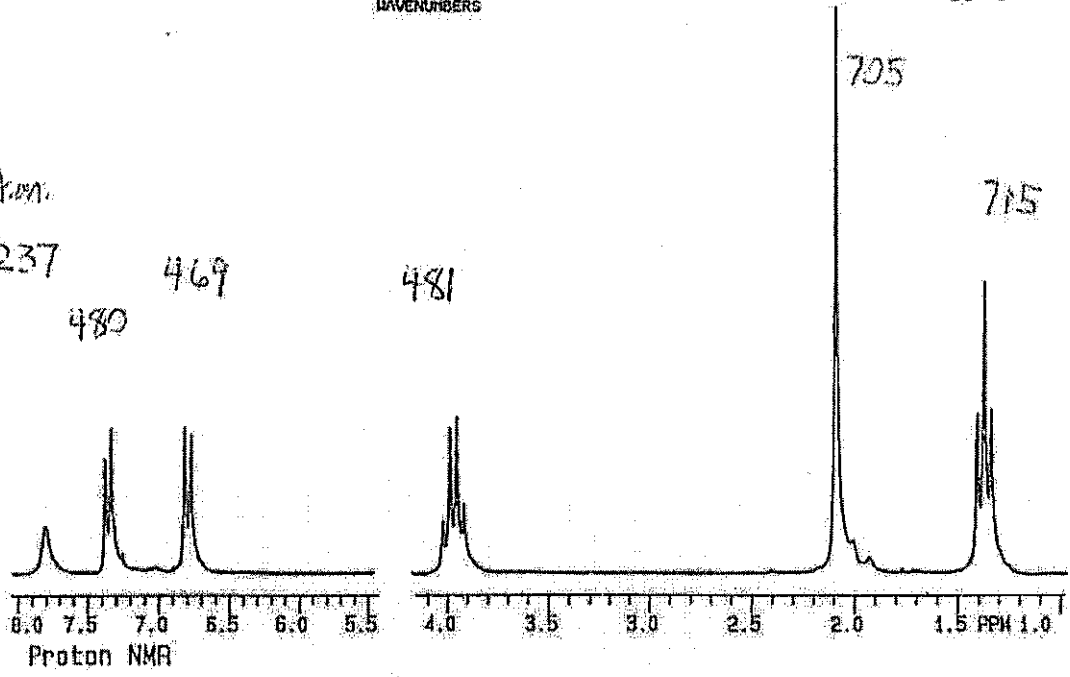
480

469

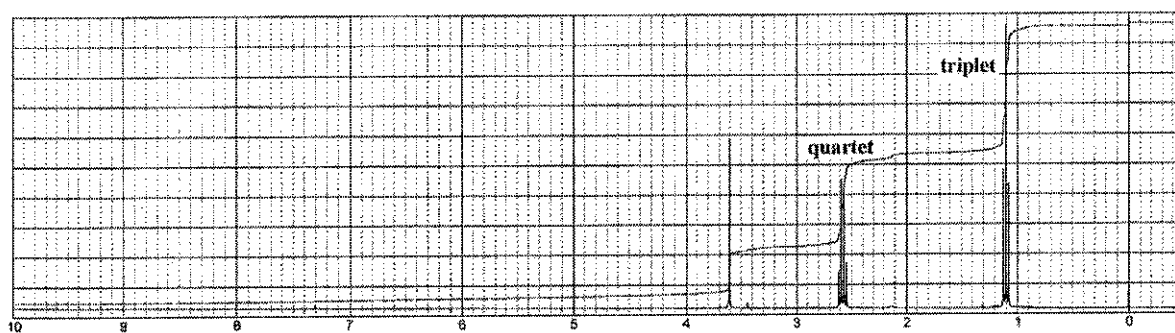
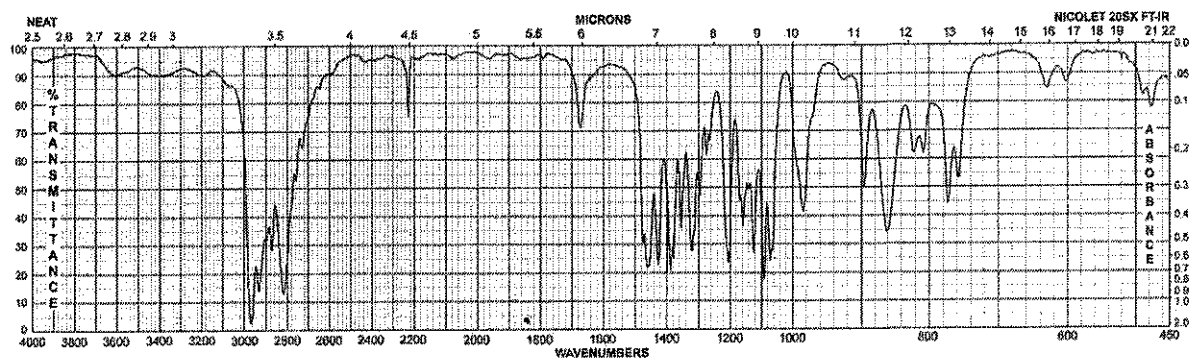
481

705

715



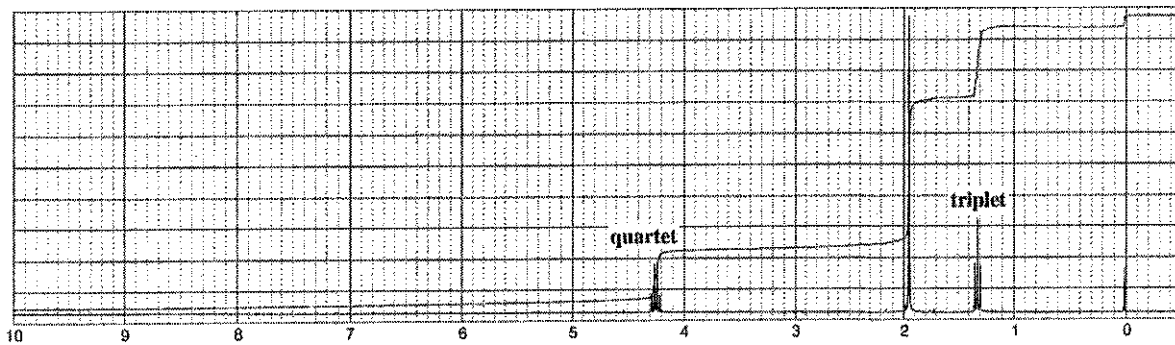
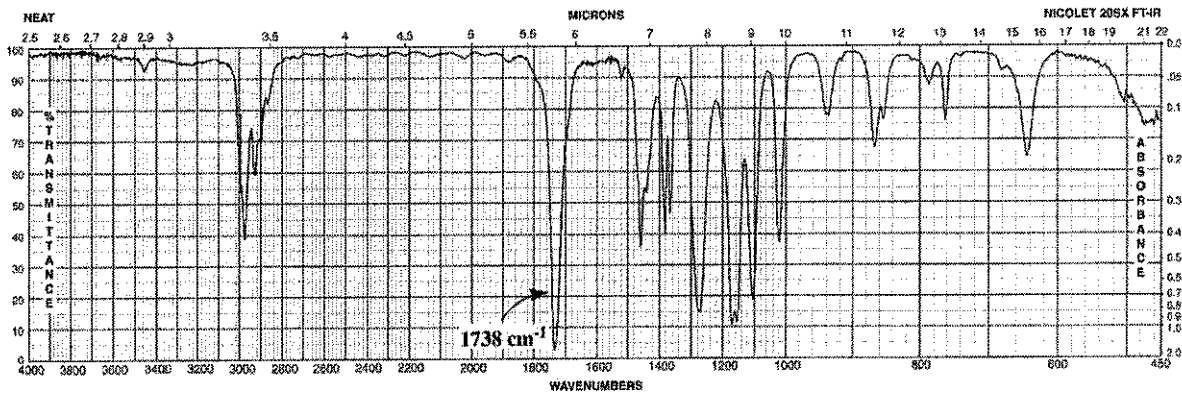
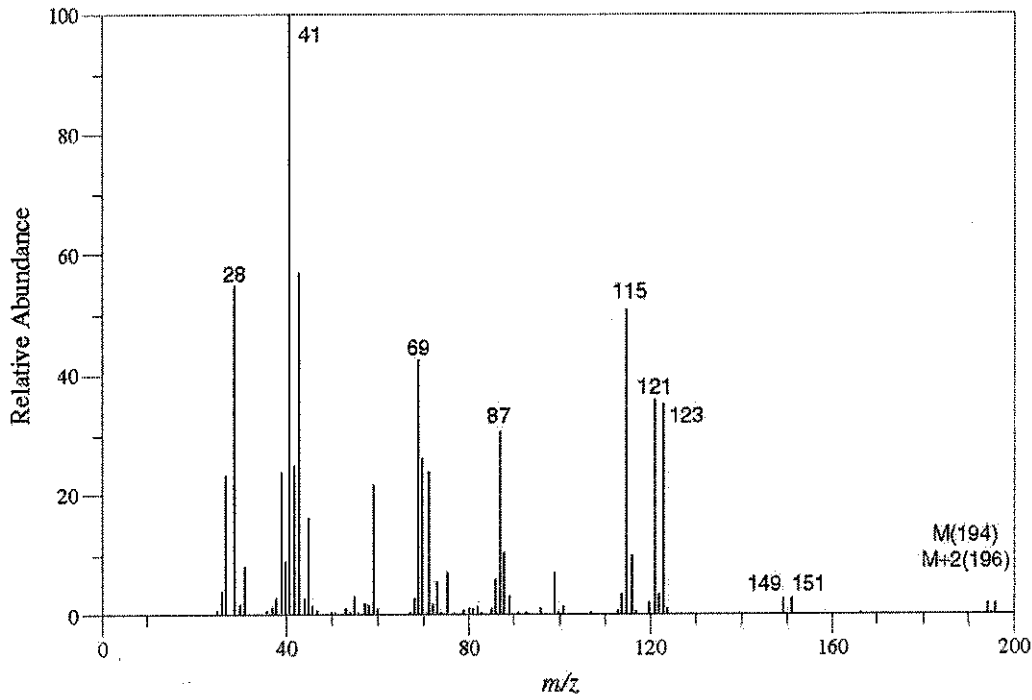
23

Molecular formula: $C_6H_{12}N_2$ 

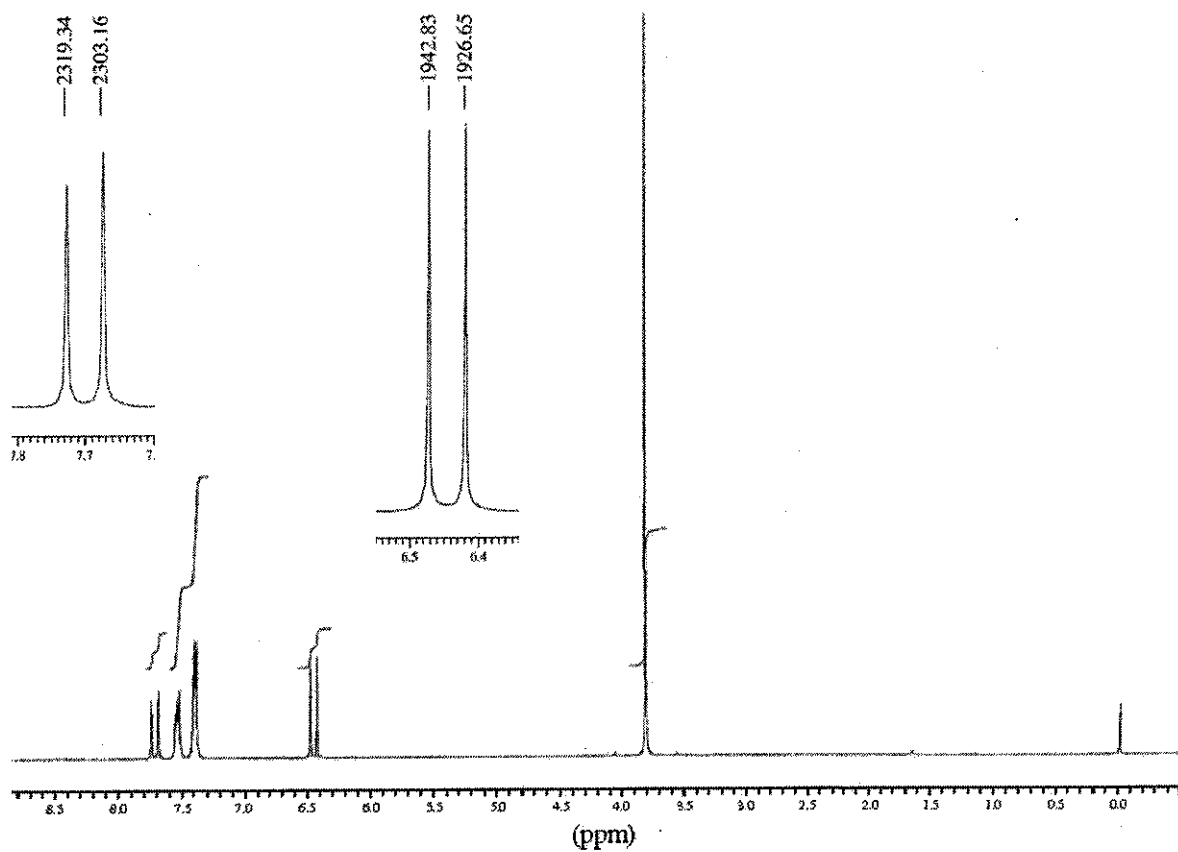
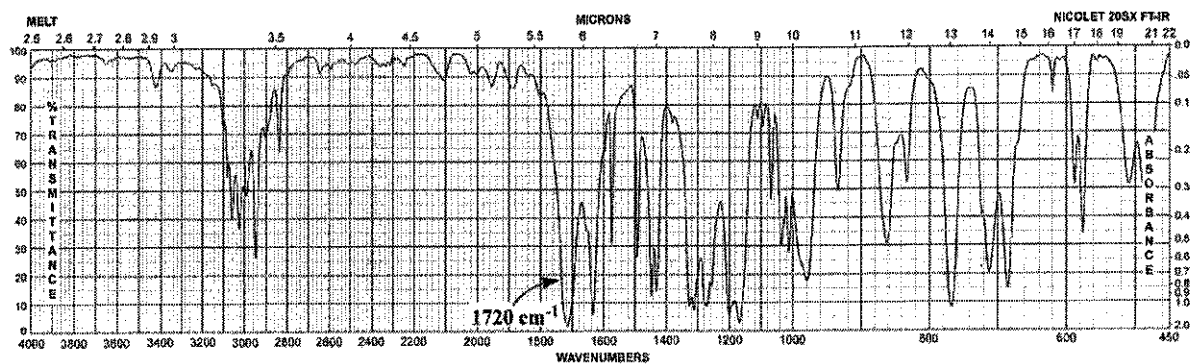
Normal C	DEPT-135	DEPT-90
13 ppm	+	No peak
41	-	No peak
48	-	No peak
113	No peak	No peak

24

Molecular formula: $C_6H_{11}BrO_2$



^{13}C NMR: δ 172, 62, 56, 31, 14

Molecular formula: $C_{10}H_{10}O_2$ ¹³C NMR: δ 167, 145, 134, 130, 129, 128, 118, 52