Supporting Informations

It is "2-imino-4-thiazolidinones" and not thiohydantoins as the reaction product of 1,3-disubstituted thioureas and chloroacetylchloride

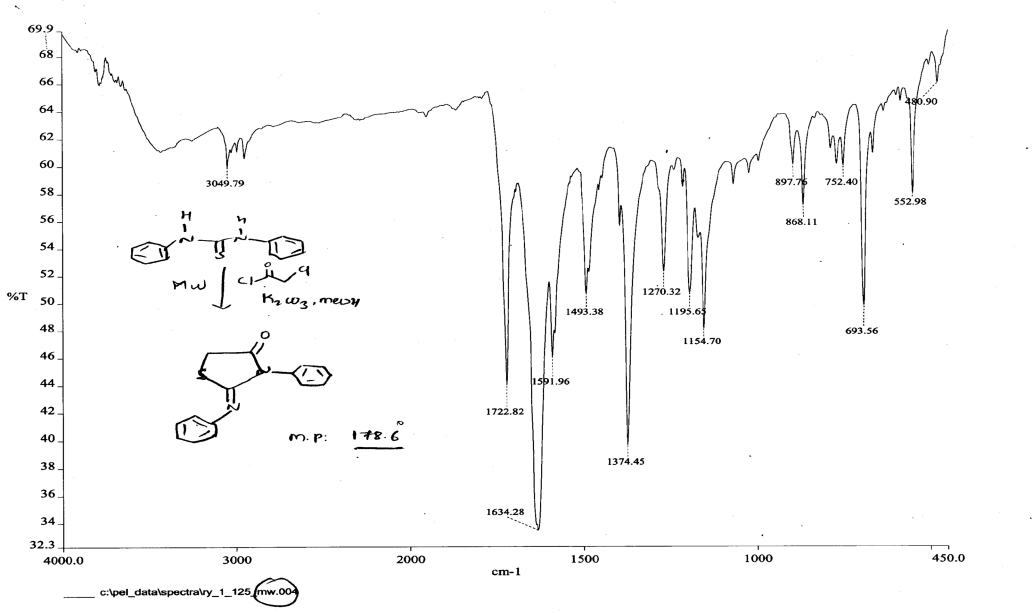
Ramesh Yella,[a] Harisadhan Ghosh,[a] and Bhisma K. Patel*[a]

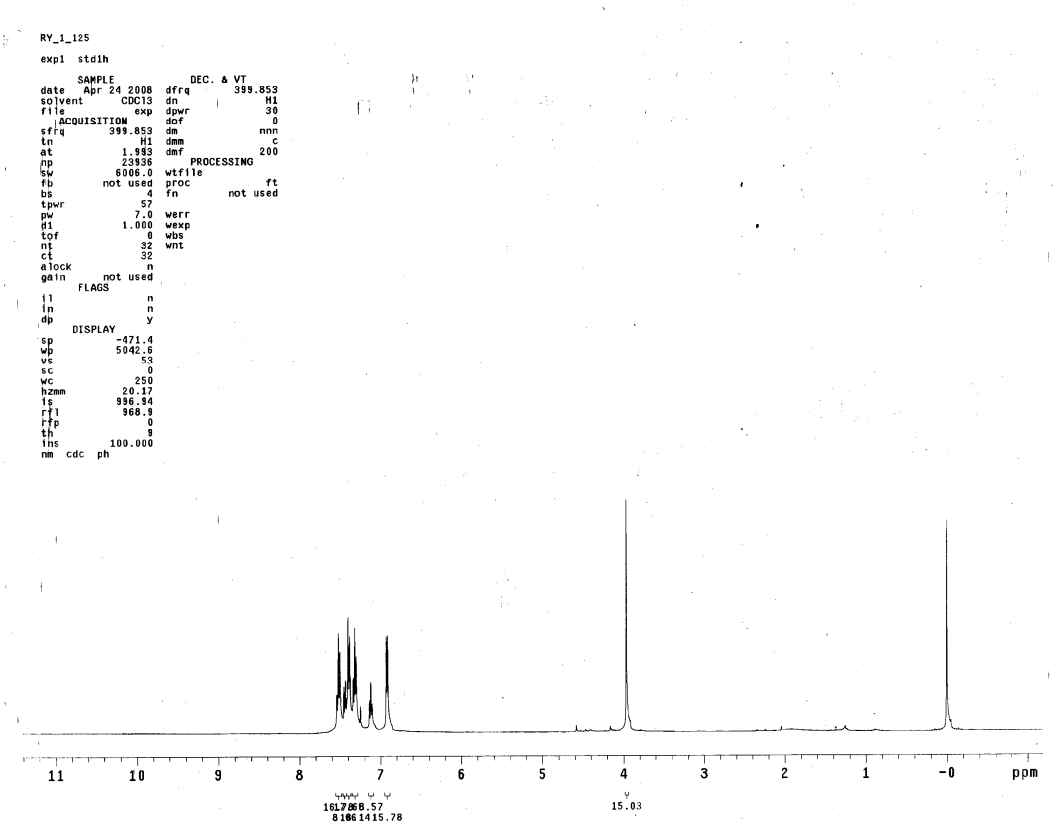
[a] *Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati -781 039, Assam, India.*
E-mail: patel@iitg.ernet.in.

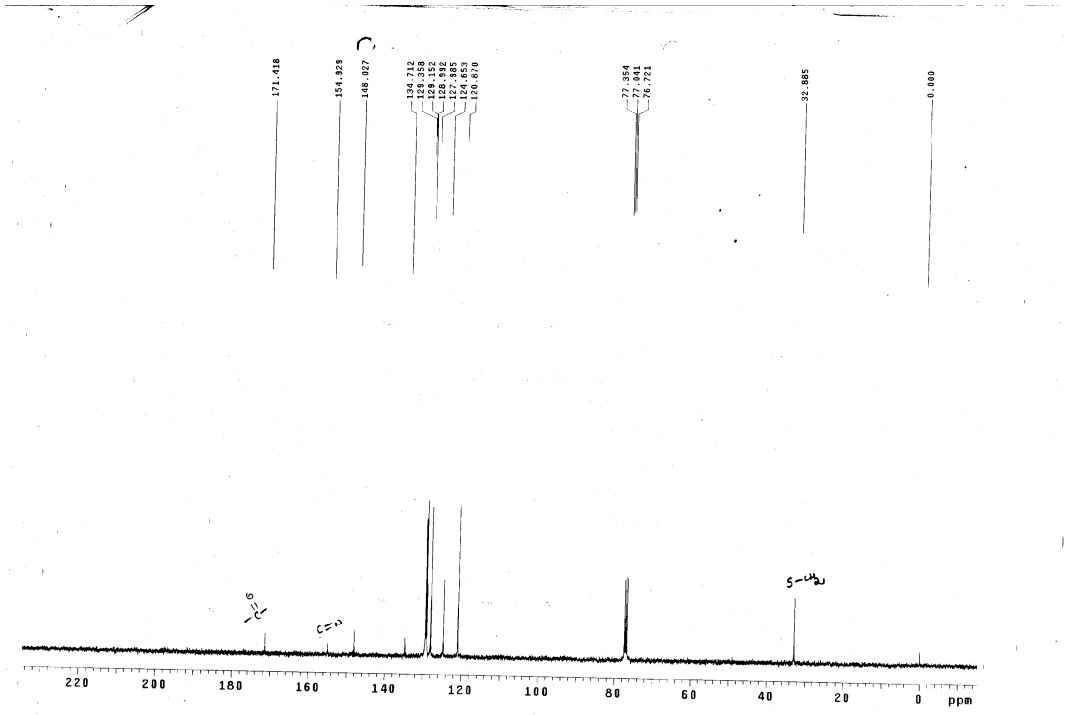
List of Contents

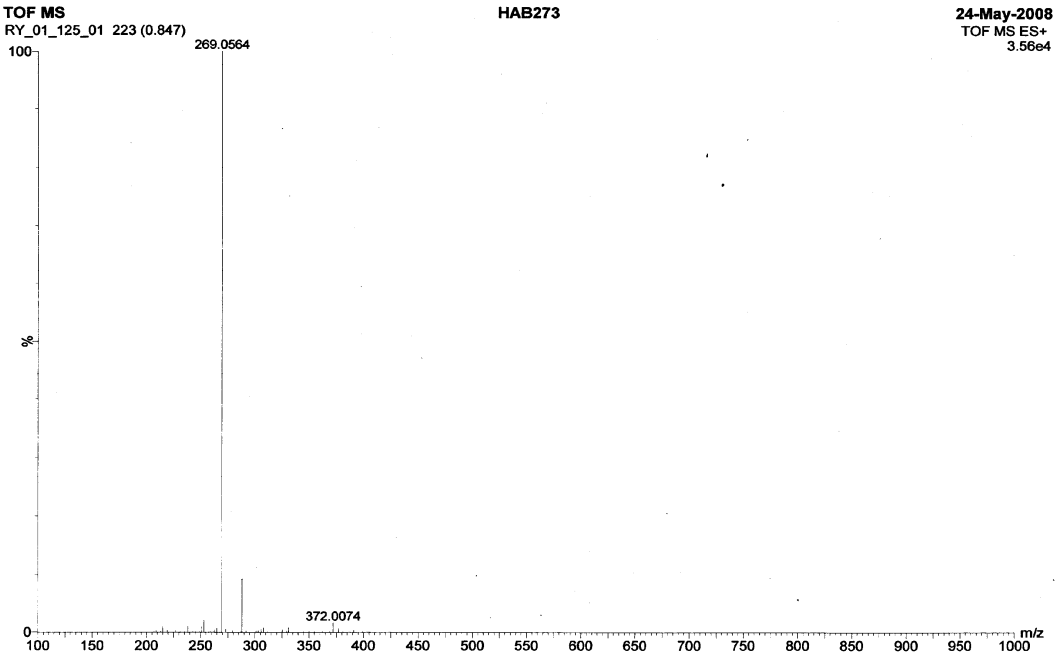
1. IR Spectra of 1a S3
2. ^{1}H NMR of 1a S4
3. ^{13}C NMR of 1a S5
4. MS of 1a S6
5. COSY of 1a S6
6. HETCOR of 1a S8
7. IR Spectra of 2a S9
8. ^{1}H NMR of 2a S10
9. ^{13}C NMR of 2a S11
10. HRMS of 2a S12
11. IR Spectra of 3a S13
12. ^{1}H NMR of 3a S14
13. ^{13}C NMR of 3a S15
14. MS of 3a S16
15. IR Spectra of 4a S17
16. ^{1}H NMR of 4a S18
17. ^{13}C NMR of 4a S19
18. MS of 4a S20
19. IR Spectra of 5a S21
20. ^{1}H NMR of 5a S21
21. H NMR of 5a (expanded) S23
22. ^{13}C NMR of 5a S24
23. MS of 5a S25

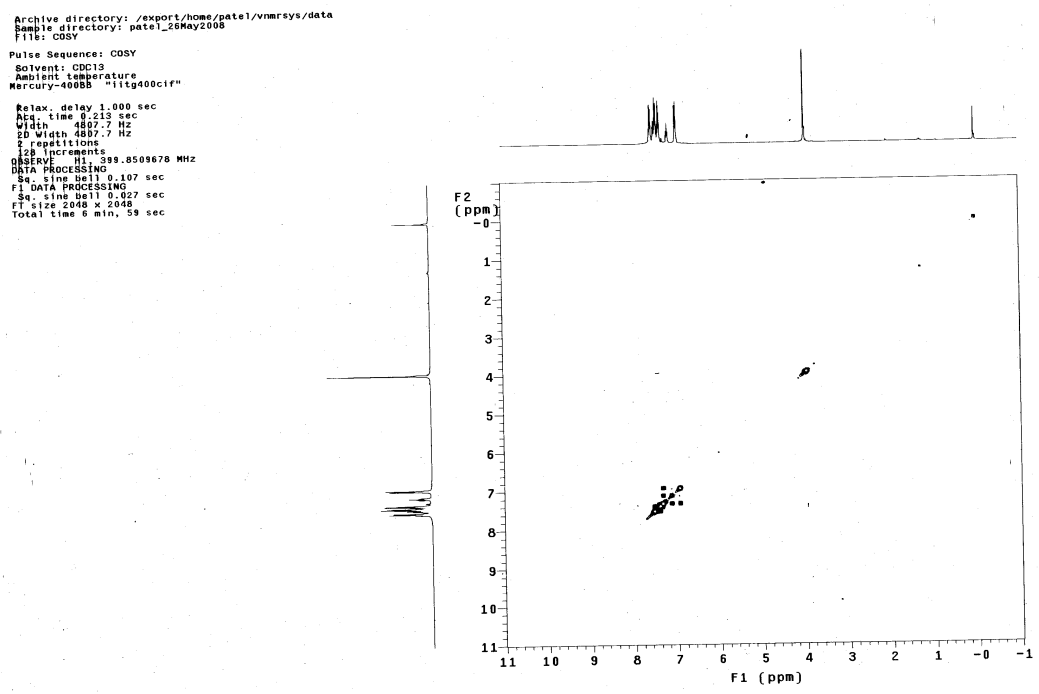
24. IR Spectra of 6a S26
25. ^{1}H NMR of 6a S27
26. ^{13}C NMR of 6a S28
27. MS of 6a S29
28. IR Spectra of 7a S30
29. ^{1}H NMR of 7a S31
30. ^{13}C NMR of 7a S32
31. MS of 7a S33
32. IR Spectra of 8a S34
33. ^{1}H NMR of 8a S35
34. ^{13}C NMR of 8a S36
35. IR Spectra of 9a S37
36. ^{1}H NMR of 9a S38
37. ^{13}C NMR of 9a S39
38. IR Spectra of 10a S40
39. ^{1}H NMR of 10a S41
40. ^{13}C NMR of 10a S42
41. MS of 10a S43
42. IR Spectra of 11a S44
43. ^{1}H NMR of 11a S45
44. ^{13}C NMR of 11a S46
45. MS of 11a S47
46. IR Spectra of 12a S48
47. ^{1}H NMR of 12a S49
48. ^{13}C NMR of 12a S50
49. MS of 12a S51

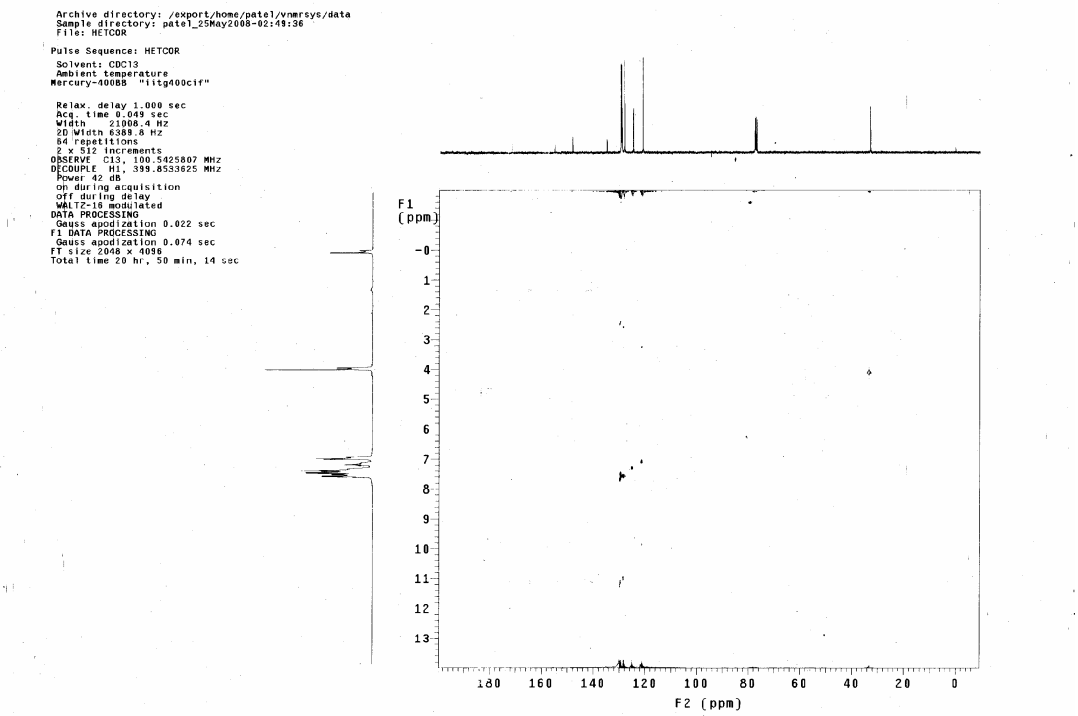

%T
cm-1
3049.79
1722.82
1634.28
1591.96
1493.38
1374.45
1270.32
1195.65
1154.70
897.76
868.11
752.40
693.56
552.98
480.90
MW
K2CO3, MeCN
m.p: 178.6°
c:\pel_data\spectra\vy_1_125_mw.004

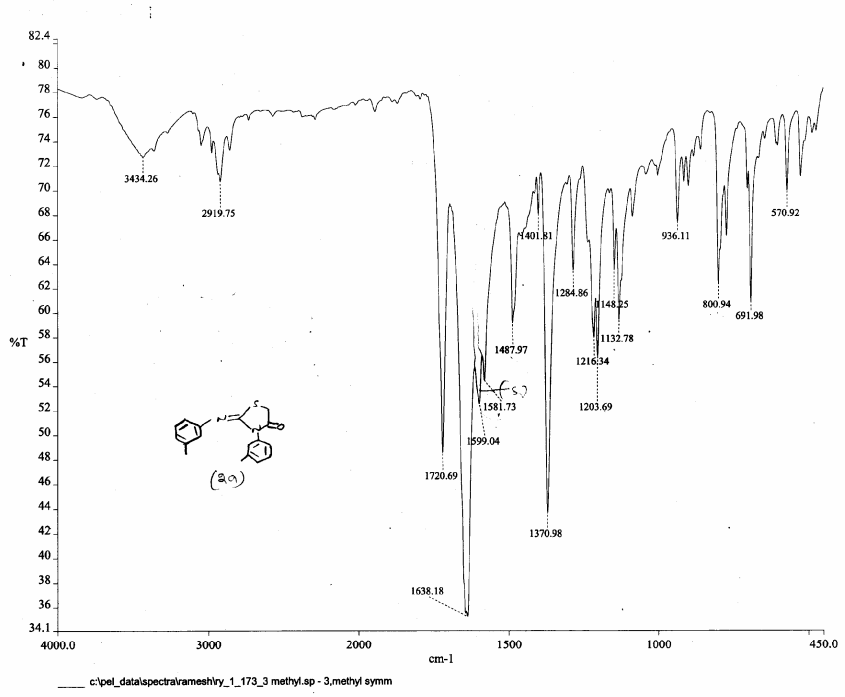

RY_1_125
exp1 stdih
SAMPLE
date Apr 24 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 399.853
tn H1
at 1.993
np 23936
sw 6006.0
fb not used
bs 4
tpwr 57
pw 7.0
d1 1.000
tof 0
nt 32
ct 32
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -471.4
wp 5042.6
vs 53
sc 0
wc 250
hzmm 20.17
is 996.94
rfl 968.9
rfp 0
th 9
ins 100.000
nm cdc ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
11
10
9
8
7
6
5
4
3
2
1
-0
ppm
15.03

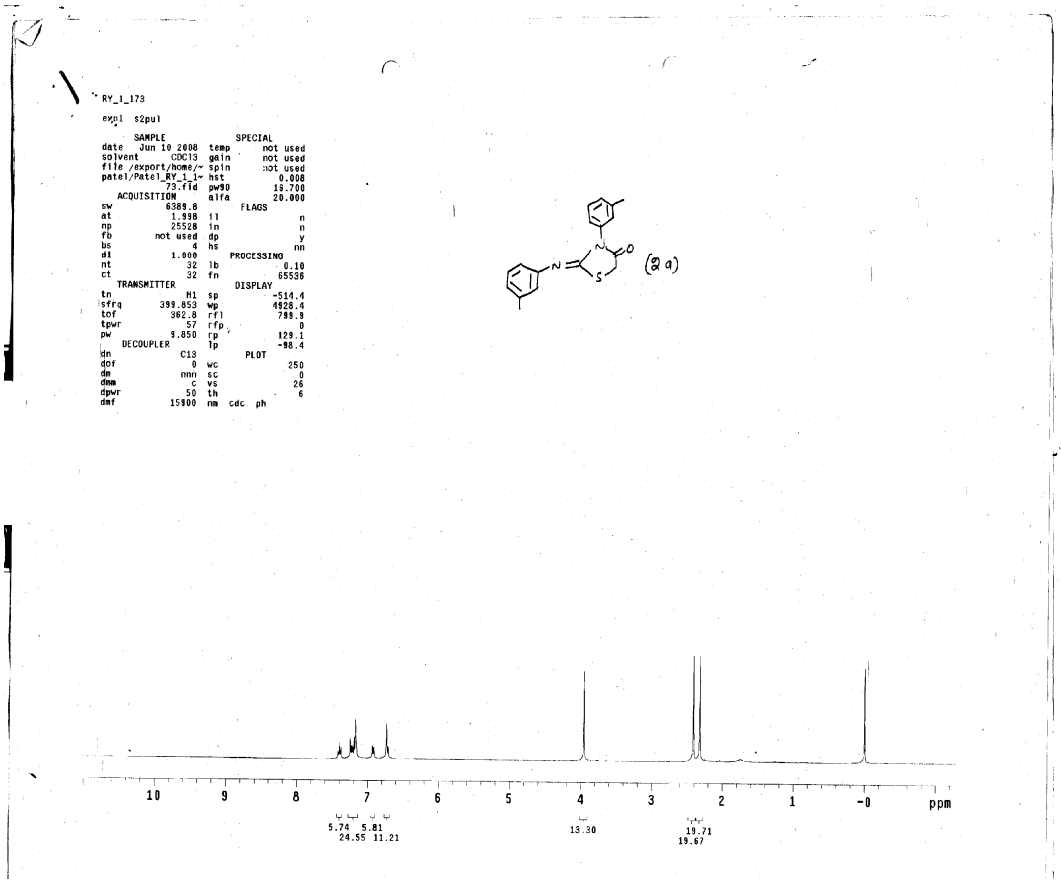

171.418
154.929
148.027
134.712
129.358
129.152
128.992
127.985
124.653
120.870
77.354
77.041
76.721
32.885
0.000
220
200
180
160
140
120
100
80
60
40
20
0
ppm

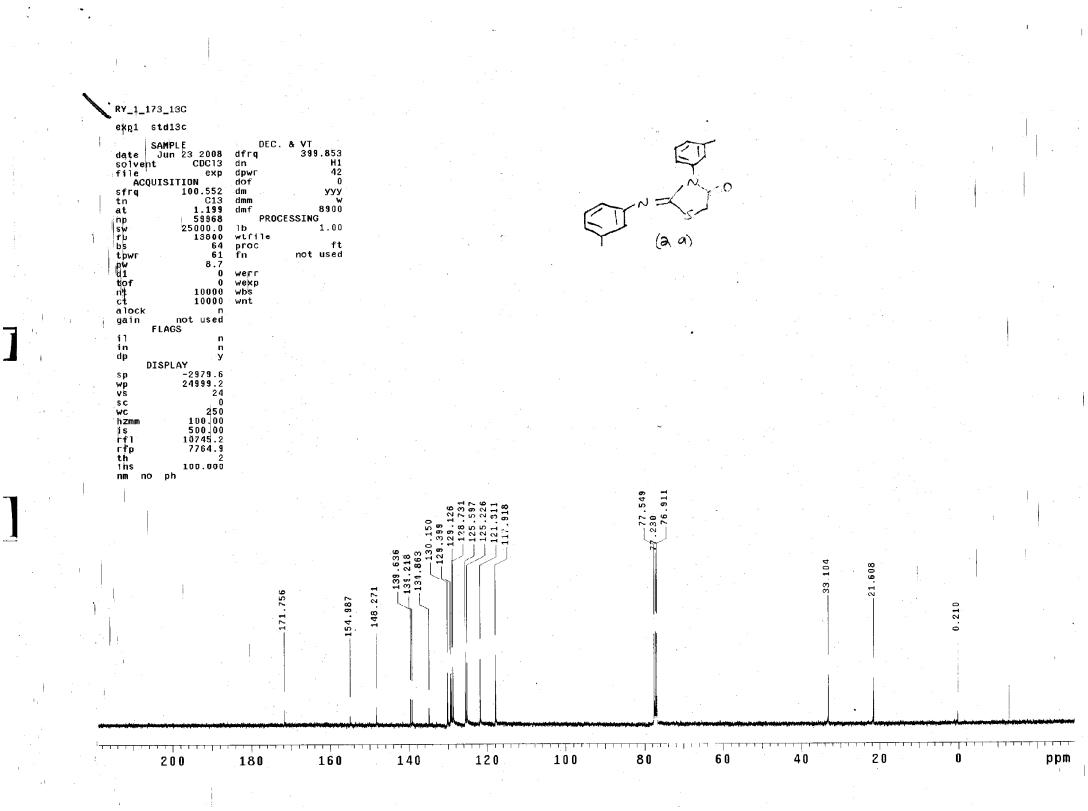

TOF MS
RY_01_125_01 223 (0.847)
HAB273
24-May-2008
TOF MS ES+
3.56e4
100
%
0
269.0564
372.0074
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z

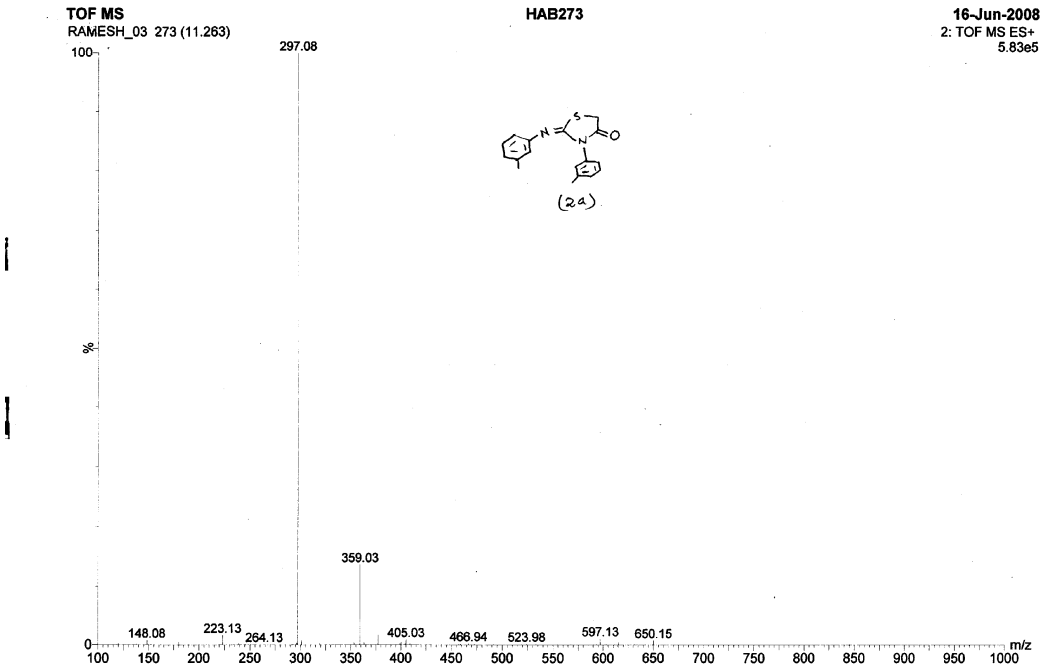

Archive directory: /export/home/patel/vnmrsys/data
Sample directory: patel_26May2008
File: COSY
Pulse Sequence: COSY
Solvent: CDCl3
Ambient temperature
Mercury-400BB "iitg400cif"
Relax. delay 1.000 sec
Acq. time 0.213 sec
Width 4807.7 Hz
2D Width 4807.7 Hz
2 repetitions
128 increments
OBSERVE H1, 399.8509678 MHz
DATA PROCESSING
Sq. sine bell 0.107 sec
F1 DATA PROCESSING
Sq. sine bell 0.027 sec
FT size 2048 x 2048
Total time 6 min, 59 sec
F2 (ppm)
F1 (ppm)

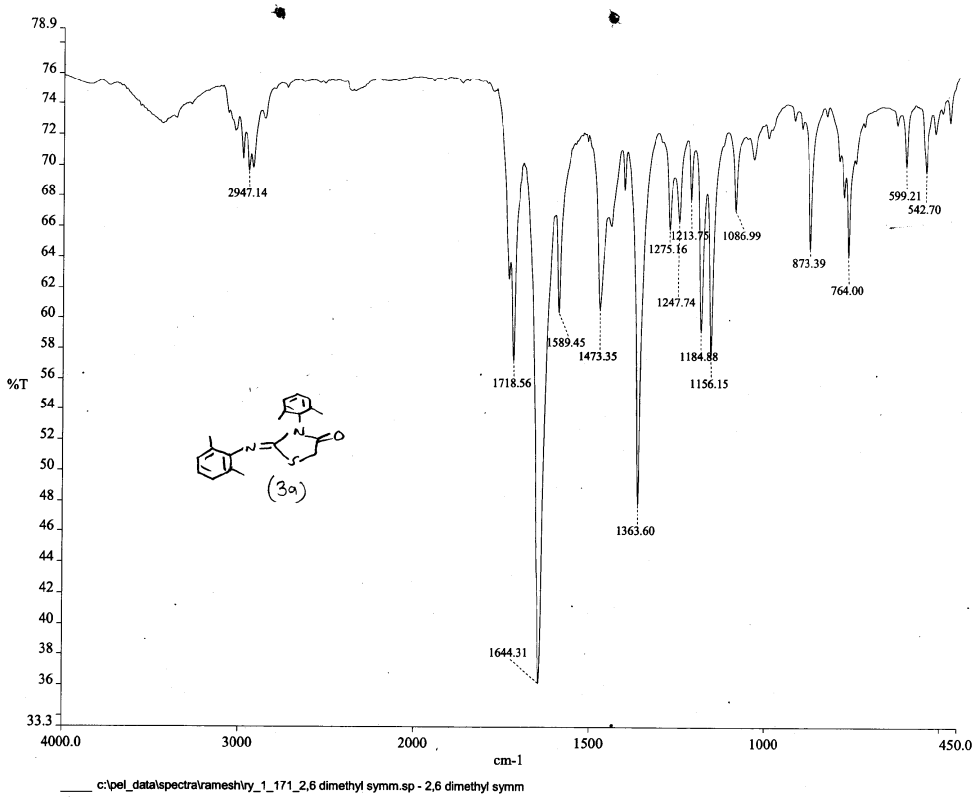

Archive directory: /export/home/patel/vnmrsys/data
Sample directory: patel_25May2008-02:49:36
File: HETCOR
Pulse Sequence: HETCOR
Solvent: CDCl3
Ambient temperature
Mercury-400BB "iitg400cif"
Relax. delay 1.000 sec
Acq. time 0.049 sec
Width 21008.4 HZ
2D Width 6389.8 Hz
64 repetitions
2 x 512 increments
OBSERVE C13, 100.5425807 MHz
DECOUPLE H1, 399.8533625 MHz
Power 42 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Gauss apodization 0.022 sec
F1 DATA PROCESSING
Gauss apodization 0.074 sec
FT size 2048 x 4096
Total time 20 hr, 50 min, 14 sec
F1 (ppm)
F2 (ppm)

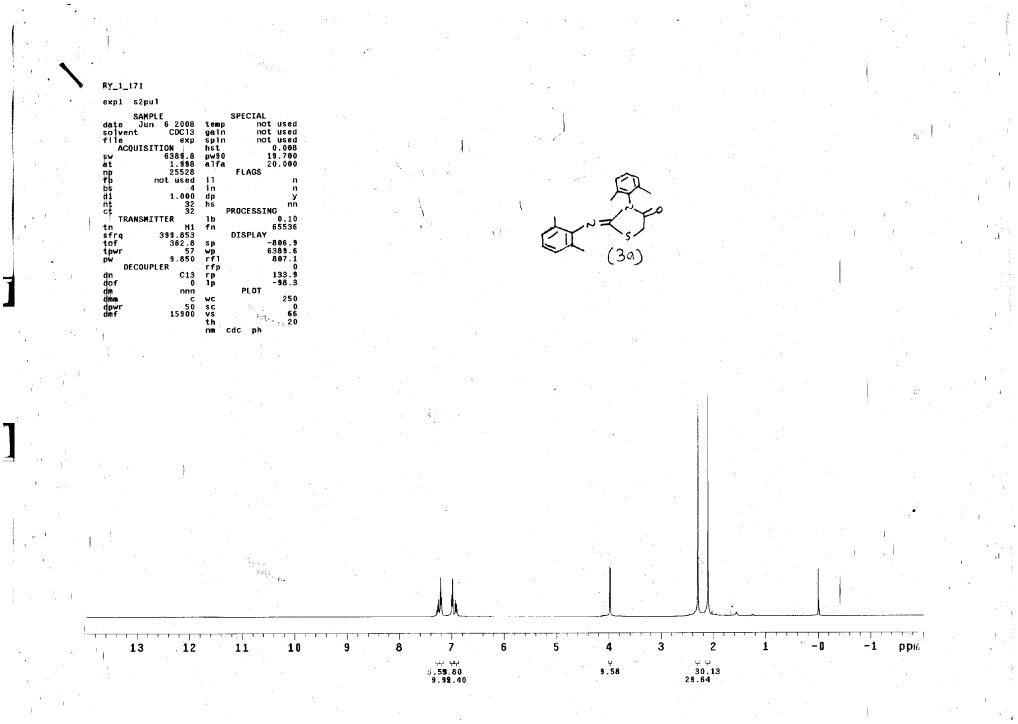

82.4
80
78
76
74
72
70
68
66
64
62
60
58
56
54
52
50
48
46
44
42
40
38
36
34.1
%T
3434.26
2919.75
1720.69
1638.18
1599.04
1581.73
1487.97
1401.81
1370.98
1284.86
1216.34
1203.69
1148.25
1132.78
936.11
800.94
691.98
570.92
4000.0
3000
2000
1500
1000
450.0
cm-1
c:\pel_data\spectra\ramesh\ry_1_173_3 methyl.sp - 3,methyl symm

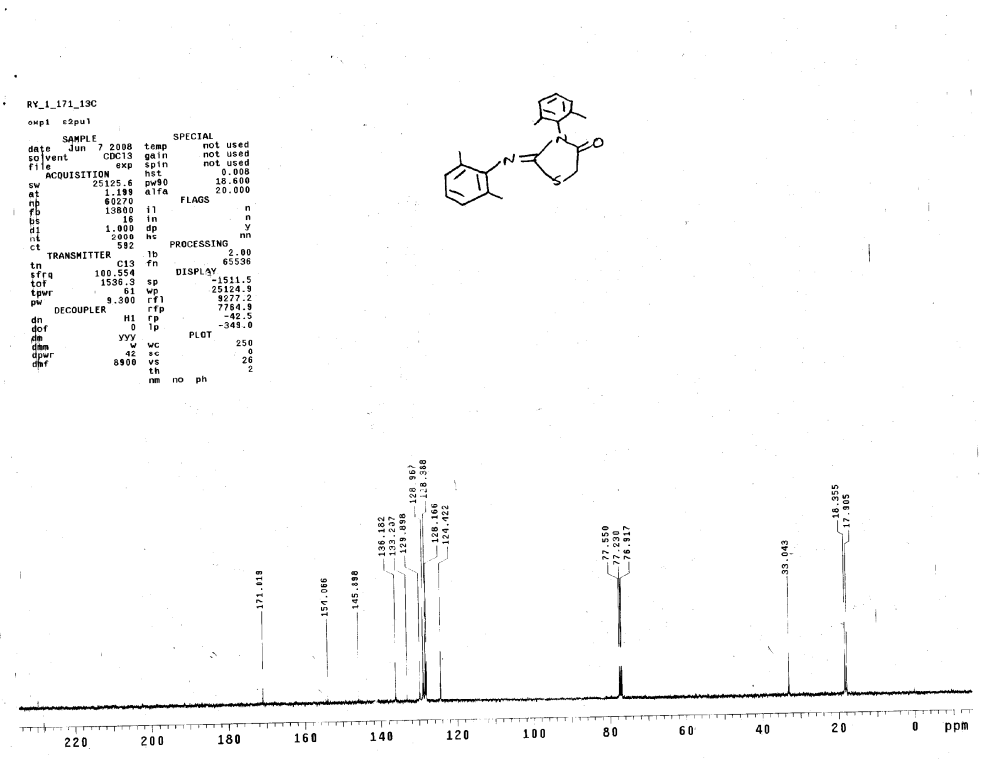

RY_1_173
expl s2pul
SAMPLE
date Jun 10 2008
solvent CDCl3
file /export/home/~
patel/Patel_RY_1_1~
73.fid
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
dt 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 59
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
fl n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -514.4
wp 4928.4
rfl 799.9
rfp 0
rp 129.1
lp -98.4
PLOT
wc 250
sc 0
vs 26
th 6
nm cdc ph
(3 a)
10
9
8
7
6
5
4
3
2
1
-0
ppm
5.74
24.55
5.81
11.21
13.30
19.71
19.67

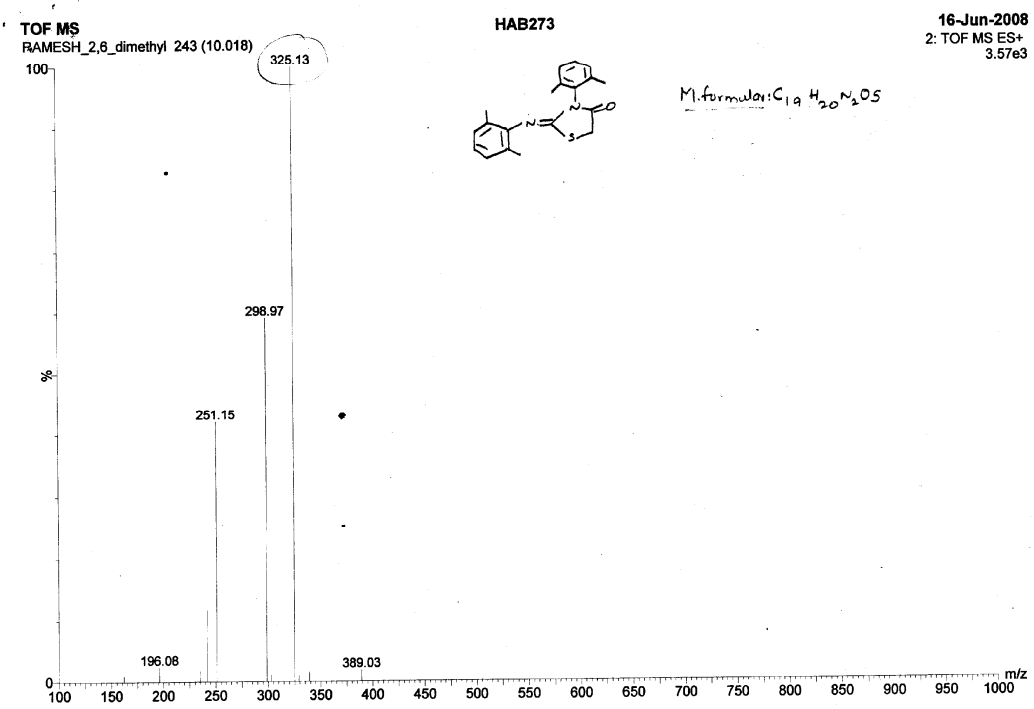

RY_1_173_13C
ekp1 std13c
SAMPLE
date Jun 23 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 100.552
tn C13
at 1.199
np 53868
sw 25000.0
fb 13000
bs 64
tpwr 61
pw 8.7
d1 0
tof 0
nt 10000
ct 10000
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -2979.6
wp 24999.2
vs 24
sc 0
wc 250
hzmm 100.00
is 500.00
rfl 10745.2
rfp 7764.9
th 2
lns 100.000
nm no ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 8900
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
(3a,a)
171.756
154.887
148.271
139.636
131.218
131.083
130.150
129.399
129.126
128.734
125.597
123.268
121.311
117.918
77.549
77.230
76.911
33.104
21.608
0.210
200
180
160
140
120
100
80
60
40
20
0
ppm

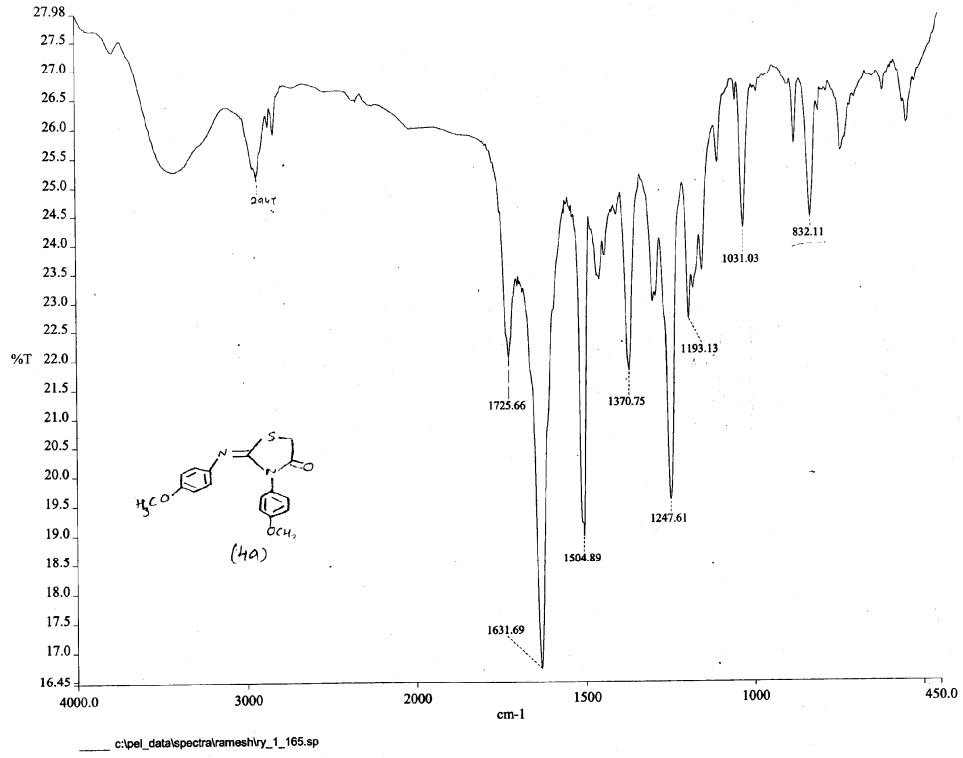

TOF MS
RAMESH_03 273 (11.263)
HAB273
16-Jun-2008
2: TOF MS ES+
5.83e5
100
%
0
297.08
359.03
148.08
223.13
264.13
405.03
466.94
523.98
597.13
650.15
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z
(2a)

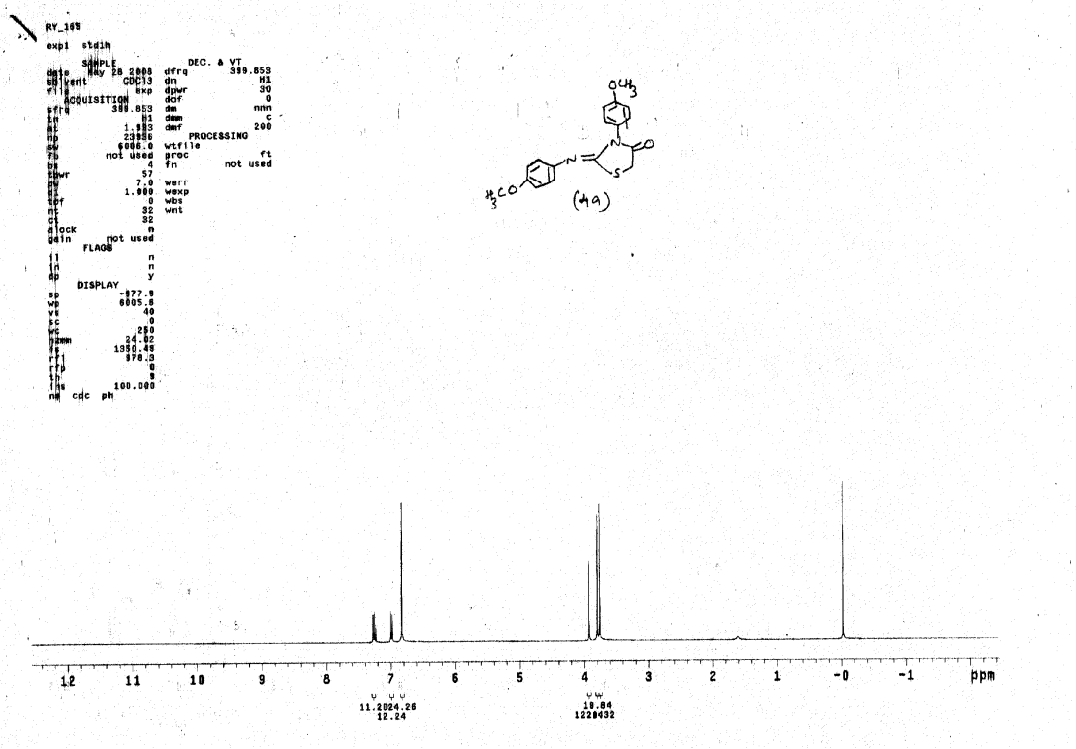

78.9
76
74
72
70
68
66
64
62
60
58
56
54
52
50
48
46
44
42
40
38
36
33.3
%T
2947.14
1718.56
1644.31
1589.45
1473.35
1363.60
1275.16
1247.74
1213.75
1184.88
1156.15
1086.99
873.39
764.00
599.21
542.70
4000.0
3000
2000
1500
1000
450.0
cm-1
(3a)
c:\pel_data\spectra\vamesh\ry_1_171_2,6 dimethyl symm.sp - 2,6 dimethyl symm

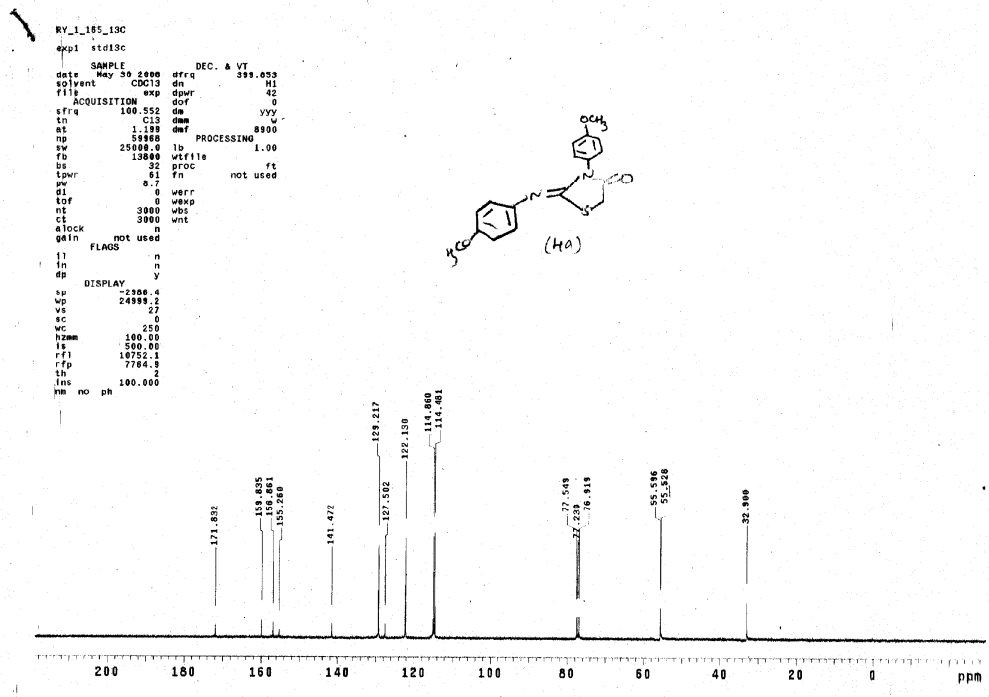

RY_1_171
expl s2pul
SAMPLE
date Jun 6 2008
solvent CDCl3
file exp
ACQUISITION
sw 6388.8
at 1.986
np 25528
fb not used
bs 4
dl 1.000
ns 32
cf 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
at1fa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -806.9
wp 6389.6
rf1 807.1
rfp 0
rp 133.8
lp -98.3
PLOT
wc 250
sc 0
vs 66
th 20
nm cdc ph
(3a)
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
0.59.80
9.98.40
9.58
30.13
28.64

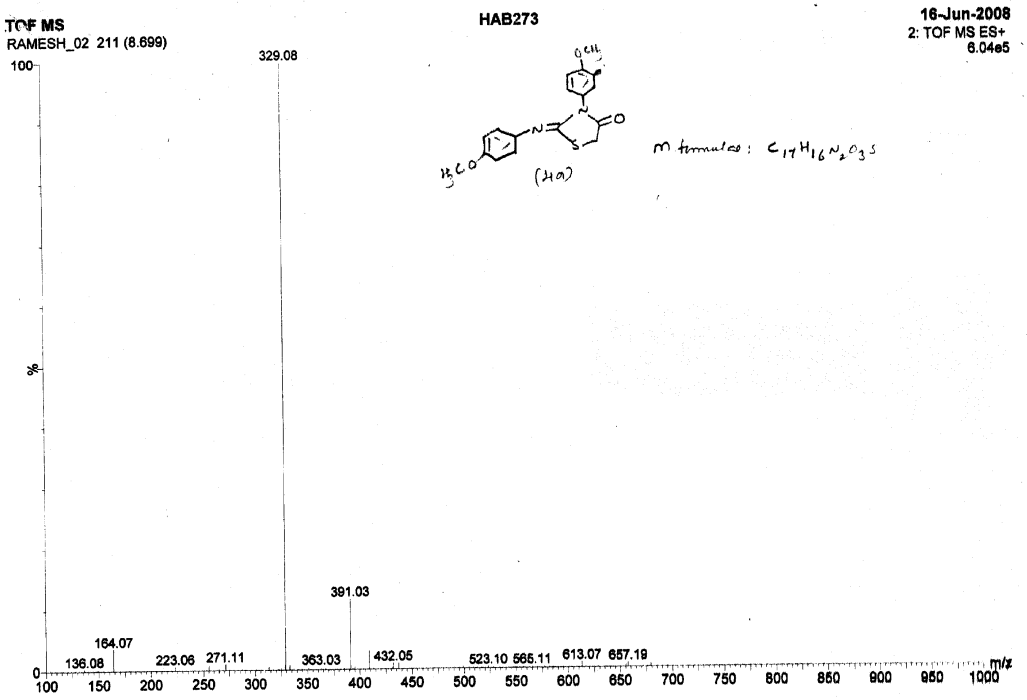

RY_1_171_13C
owp1 c2pul
SAMPLE
date Jun 7 2008
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
dl 1.000
nt 2000
ct 582
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm y
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 16.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1511.5
wp 25124.9
rfl 9277.2
rfp 7764.9
rp -42.5
lp -348.0
PLOT
wc 250
sc 0
vs 26
th 2
nm no ph
171.619
154.066
145.498
136.182
133.247
129.858
128.967
128.388
126.166
124.422
77.550
77.230
76.917
33.043
18.955
17.905
220
200
180
160
140
120
100
80
60
40
20
0
ppm

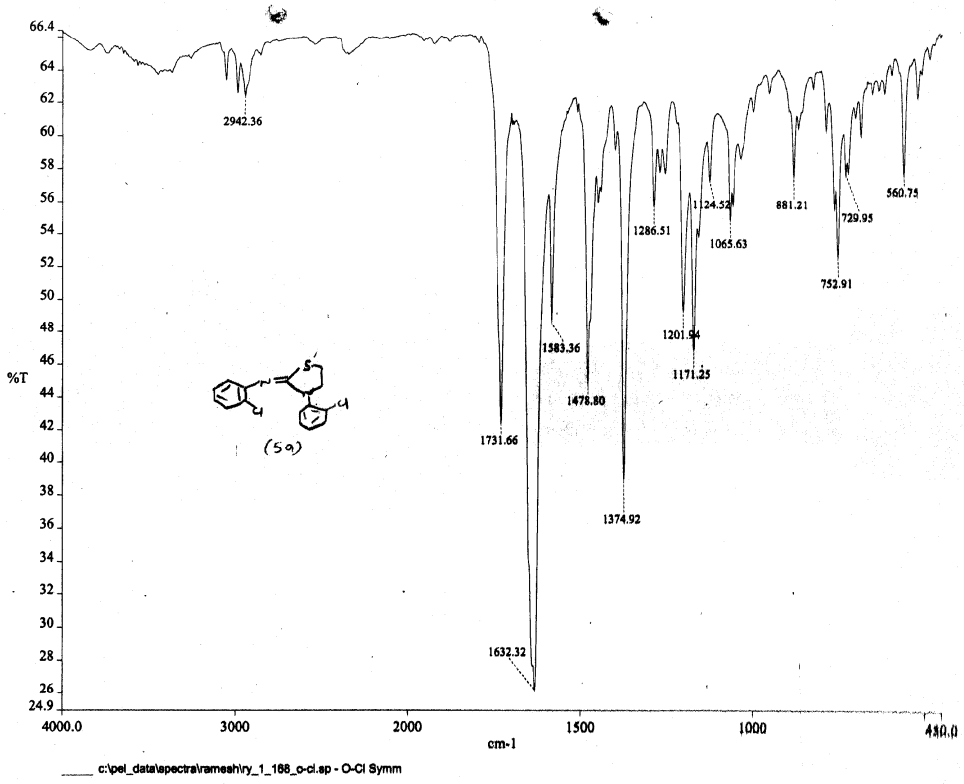

TOF MS
RAMESH_2,6_dimethyl 243 (10.018)
HAB273
16-Jun-2008
2: TOF MS ES+
3.57e3
M.formula: C19 H20 N2 O5
325.13
298.97
251.15
196.08
389.03
%
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000


%T
cm-1
4000.0
3000
2000
1500
1000
450.0
1725.66
1631.69
1504.89
1370.75
1247.61
1193.13
1031.03
832.11
(4a)
c:\pel_data\spectra\ramesh\ry_1_165.sp


RY_165
exp1 stdin
SAMPLE
date May 28 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 399.853
tn H1
at 1.993
np 23936
sw 6006.0
fb not used
bs 4
tpwr 57
pw 7.0
pl 1.000
tof 0
nt 32
ct 32
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -977.9
wp 6005.6
vs 40
sc 0
wc 250
hzmm 24.02
fs 1350.45
rfl 978.3
rfp 0
th 9
ins 100.000
nm cdc ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
OCH3
H3CO
N
S
O
(4a)
12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
11.20 24.26
12.24
19.84
1220432


RY_1_165_13C
exp1 std13c
SAMPLE
date May 30 2000
solvent CDCl3
file exp
ACQUISITION
sfrq 100.552
tn C13
at 1.199
np 59968
sw 25000.0
fb 13800
bs 32
tpwr 61
pw 8.7
d1 0
tof 0
nt 3000
ct 3000
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -2986.4
wp 24999.2
vs 27
sc 0
wc 250
hzmm 100.00
is 500.00
rfl 10752.1
rfp 7764.9
th 2
ins 100.000
nm no ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 8900
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
(Ha)
171.832
159.835
158.861
155.260
141.472
129.217
127.502
122.130
114.860
114.481
77.549
77.230
76.919
55.596
55.528
32.900
200
180
160
140
120
100
80
60
40
20
0
ppm

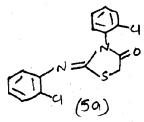

TOF MS
RAMESH_02 211 (8.699)
HAB273
16-Jun-2008
2: TOF MS ES+
6.04e5
100
%
0
329.08
391.03
164.07
136.08
223.06
271.11
363.03
432.05
523.10
565.11
613.07
657.19
m/z
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
(4a)
m formula: C17H16N2O3S


66.4
64
62
60
58
56
54
52
50
48
46
44
42
40
38
36
34
32
30
28
26
24.9
%T
4000.0
3000
2000
1500
1000
cm-1
2942.36
1731.66
1632.32
1583.36
1478.80
1374.92
1286.51
1201.94
1171.25
1124.52
1065.63
881.21
752.91
729.95
560.75
(5a)
c:\pel_data\spectra\rameshlry_1_168_o-cl.sp - O-Cl Symm

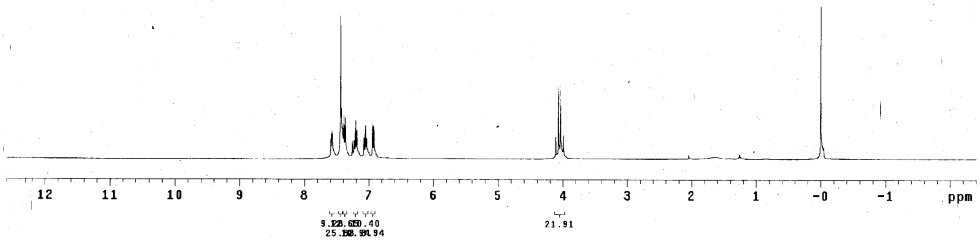
RY_1_168

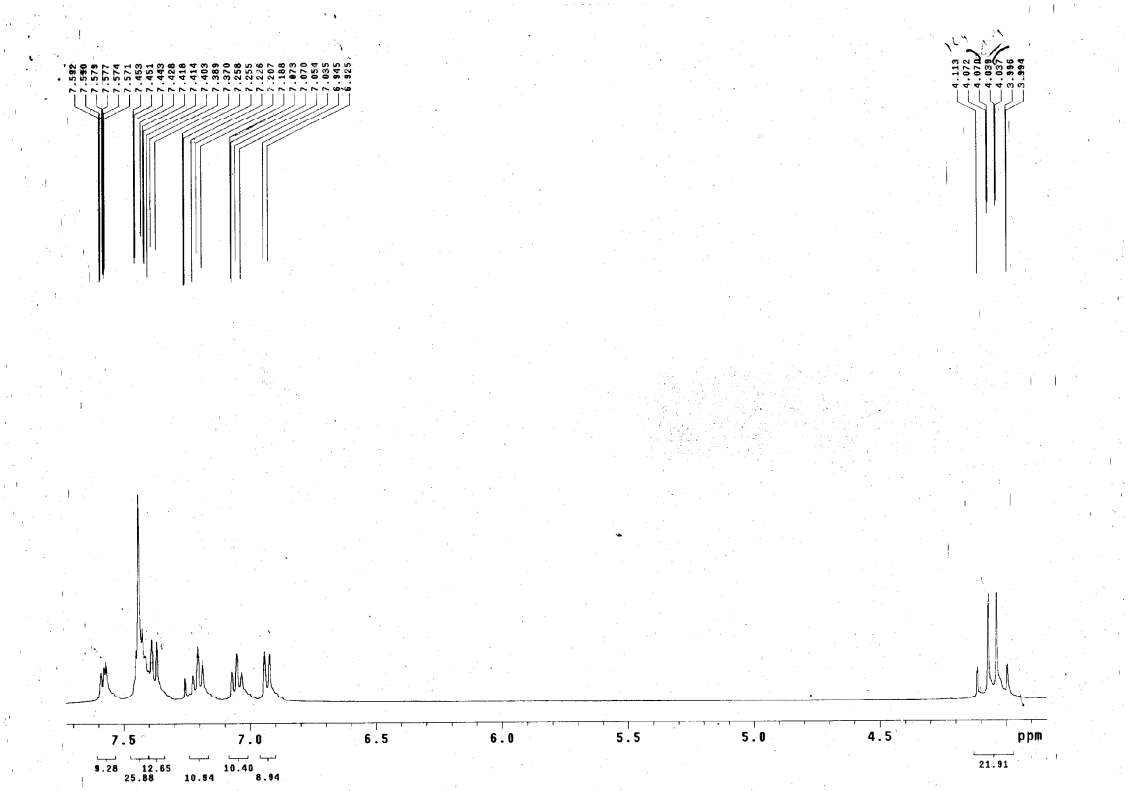
exp1 std1h

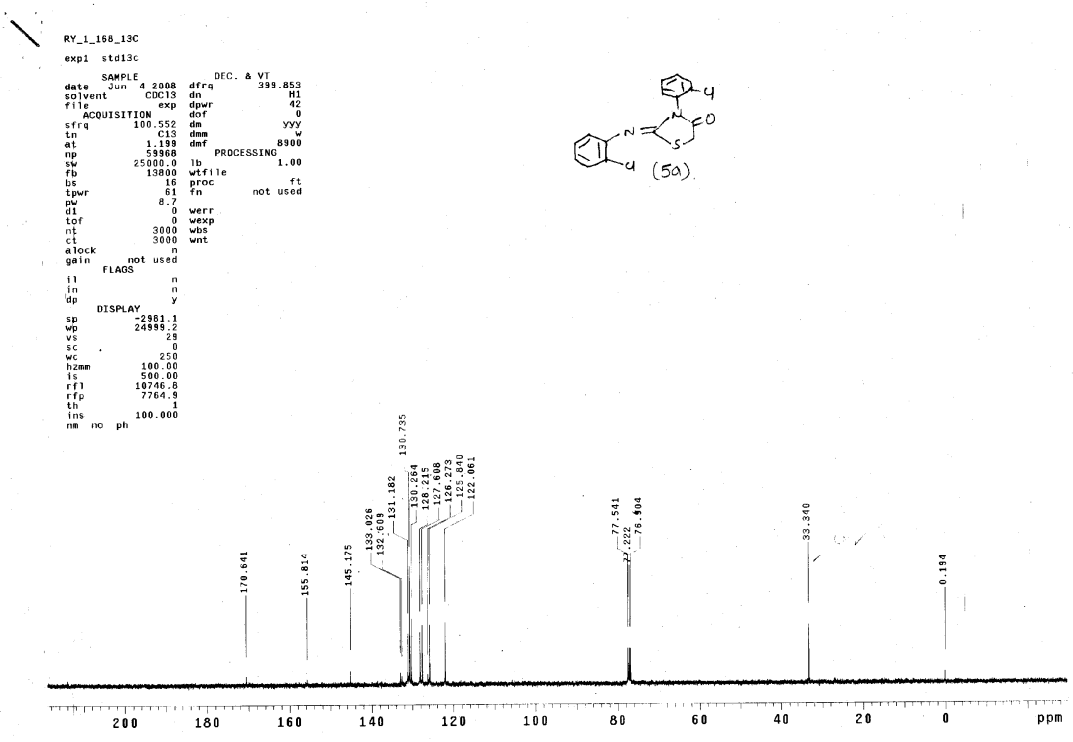
SAMPLE		DEC. & VT	
date	Jun 4 2008	dfrq	399.853
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	399.853	dm	nnn
tn	H1	dmm	c
at	1.993	dmf	200
np	23936	PROCESSING	
sw	6006.0	wtfile	
fb	not used	proc	ft
bs	4	fn	not used
tpwr	57		
pw	7.0	werr	
d1	1.000	wexp	
tof	0	wbs	
nt	32	wnt	
ct	32		
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-966.3		
wp	6005.6		
vs	39		
sc	0		
wc	250		
hzmm	24.02		
is	1290.19		
rfl	966.7		
rfp	0		
th	20		
ins	100.000		
nm cdc ph			

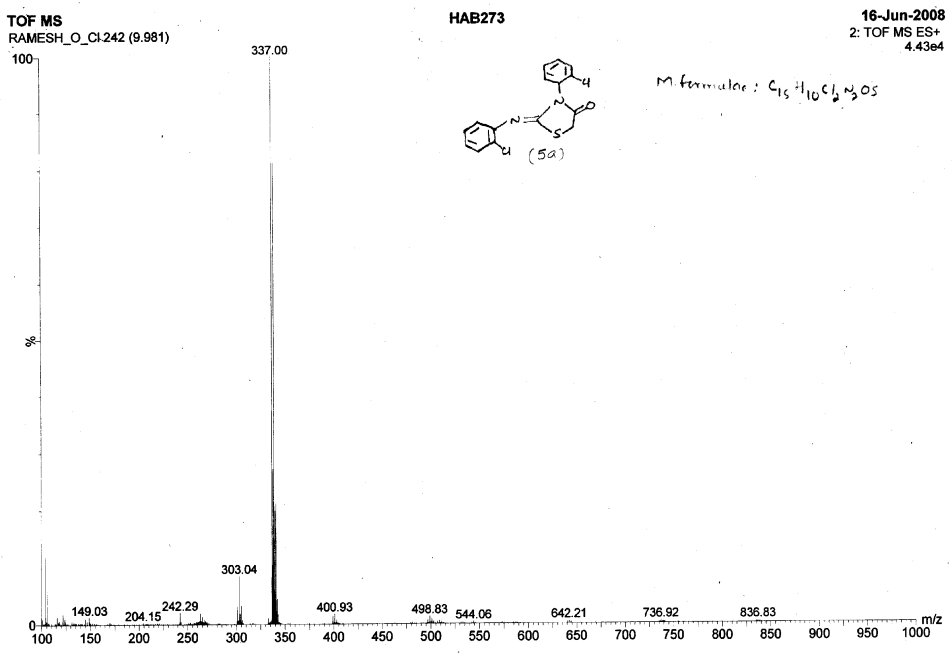


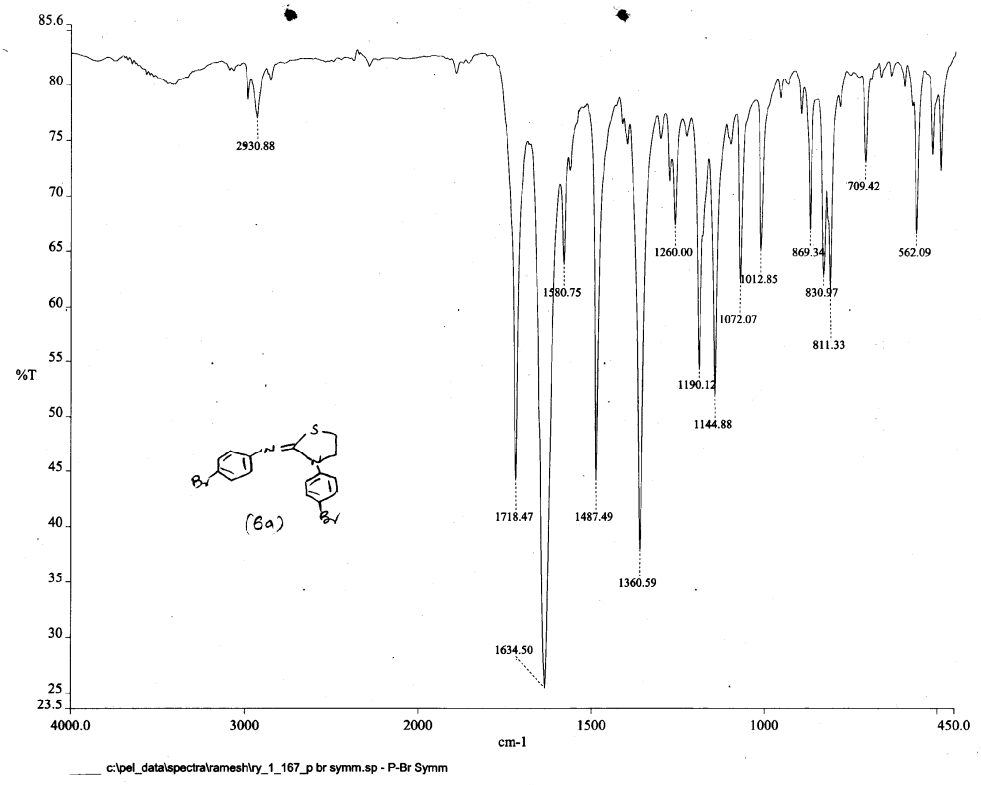
(5a)

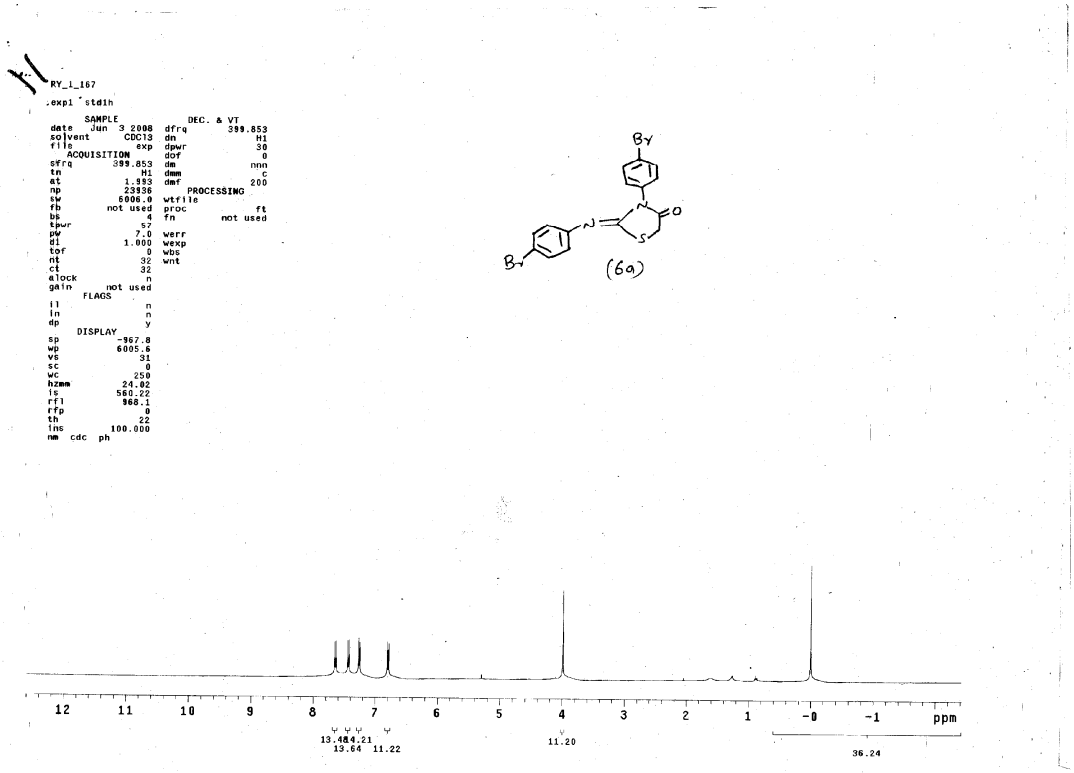


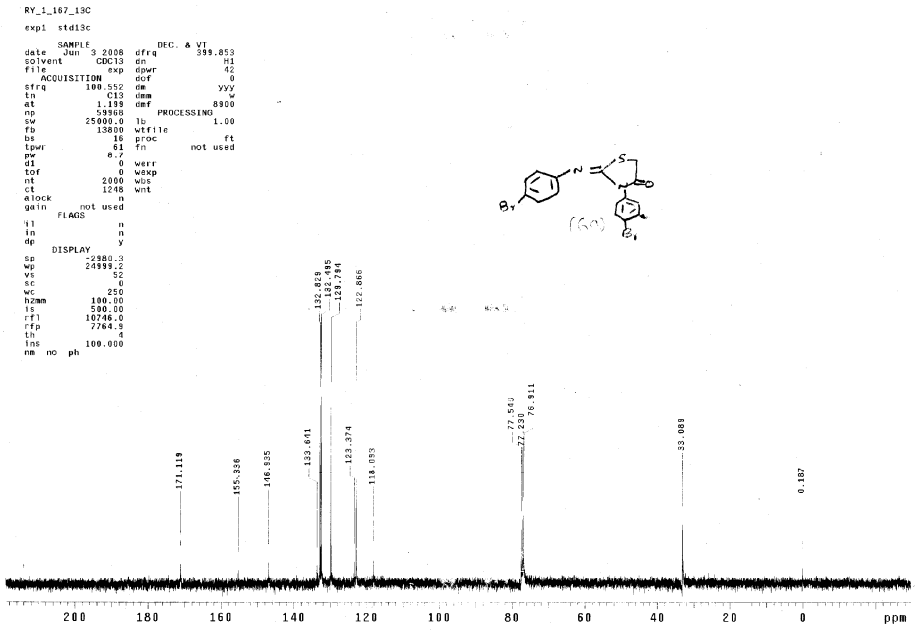

7.592
7.590
7.579
7.577
7.574
7.571
7.453
7.451
7.448
7.446
7.418
7.414
7.403
7.398
7.390
7.258
7.255
7.226
7.207
7.188
7.073
7.070
7.054
7.035
6.945
6.925
4.113
4.072
4.070
4.059
4.057
3.986
3.984
7.5
7.0
6.5
6.0
5.5
5.0
4.5
ppm
9.28
12.65
25.88
10.84
10.40
8.94
21.91

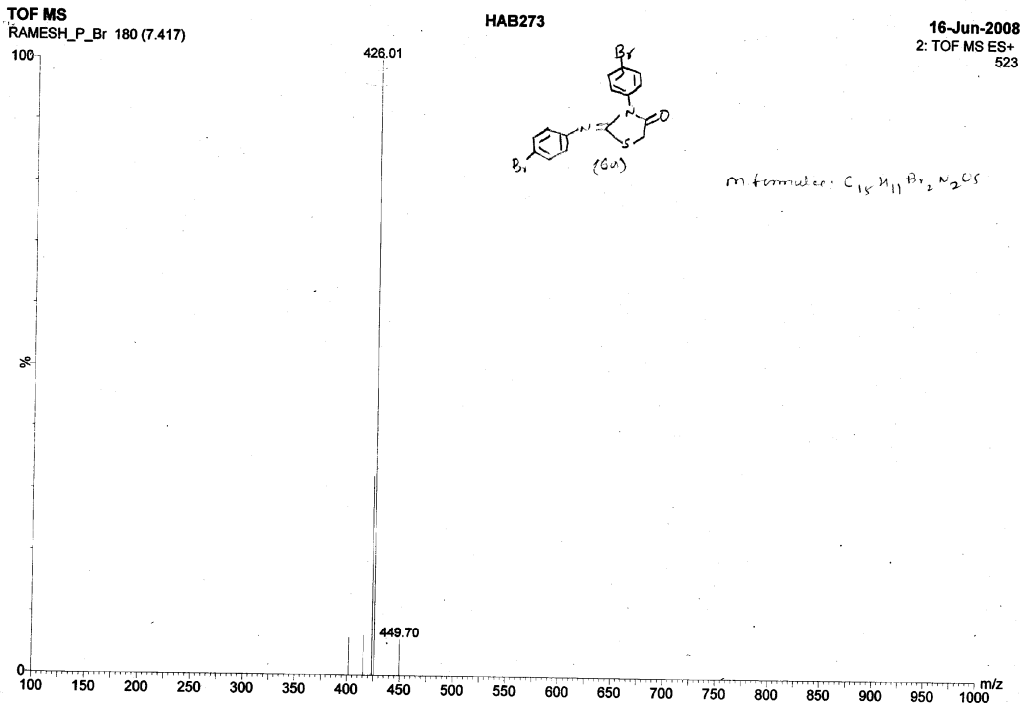

RY_1_168_13C
exp1 std13c
SAMPLE
date Jun 4 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 100.552
tn C13
at 1.199
np 59968
sw 25000.0
fb 13800
bs 16
tpwr 61
pw 8.7
d1 0
tof 0
nt 3000
ct 3000
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -2981.1
wp 24999.2
vs 28
sc 0
wc 250
hzmm 100.00
is 500.00
rfl 10746.8
rfp 7764.9
th 1
ins 100.000
nm no ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 8900
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
(5a)
170.641
155.814
145.175
133.026
132.609
131.182
130.735
130.264
128.215
127.608
126.273
125.840
122.061
77.541
77.222
76.904
33.340
0.184
200
180
160
140
120
100
80
60
40
20
0
ppm

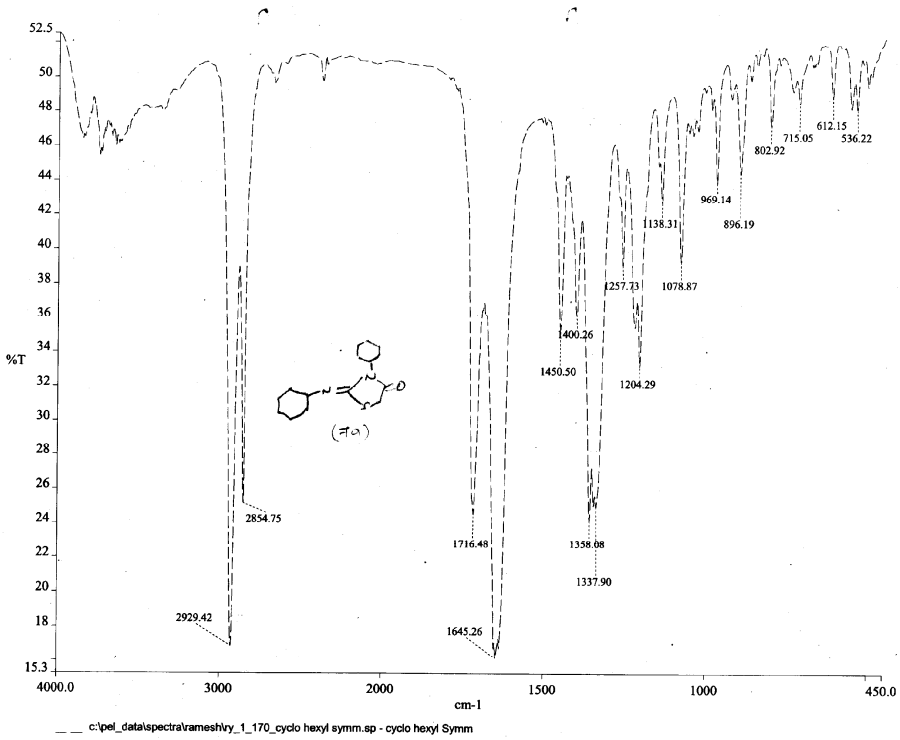

TOF MS
RAMESH_O_CI-242 (9.981)
HAB273
16-Jun-2008
2: TOF MS ES+
4.43e4
M.formula : C15H10Cl2N2O5
(5a)
337.00
303.04
149.03
204.15
242.29
400.93
498.83
544.06
642.21
736.92
836.83
%
m/z

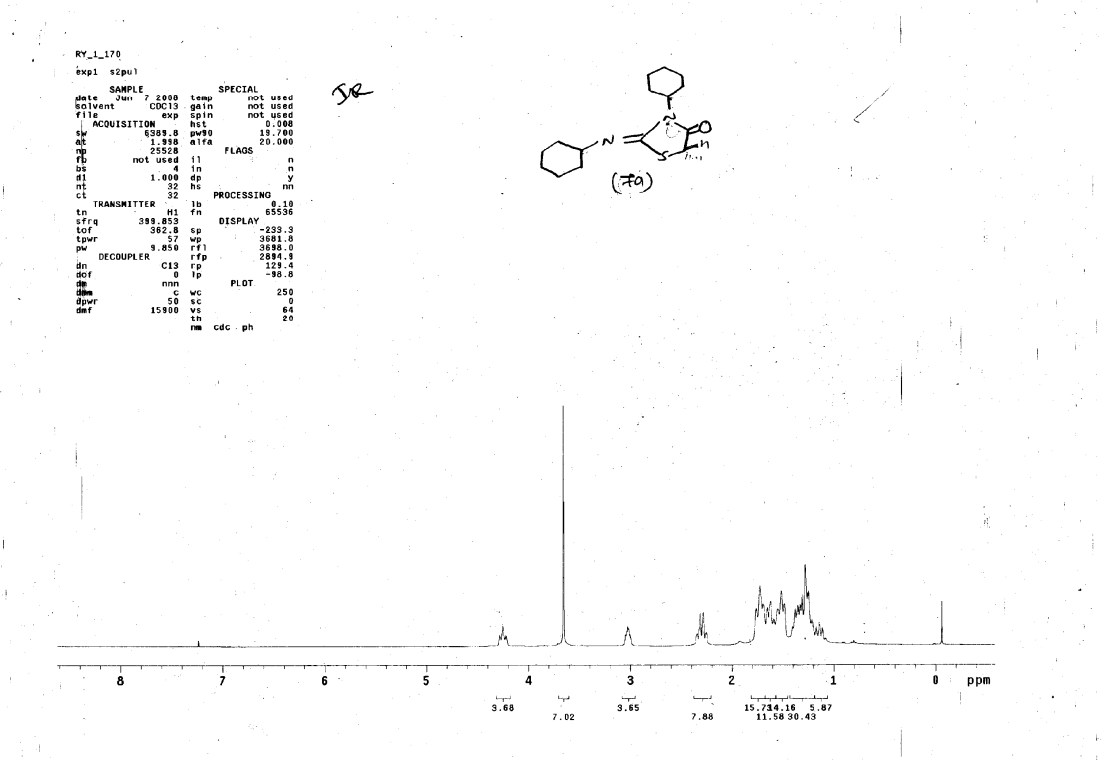

85.6
80
75
70
65
60
55
50
45
40
35
30
25
23.5
%T
4000.0
3000
2000
1500
1000
450.0
cm-1
2930.88
1718.47
1634.50
1580.75
1487.49
1360.59
1260.00
1190.12
1144.88
1072.07
1012.85
869.34
830.97
811.33
709.42
562.09
(6a)
c:\pel_data\spectra\ramesh\ry_1_167_p br symm.sp - P-Br Symm

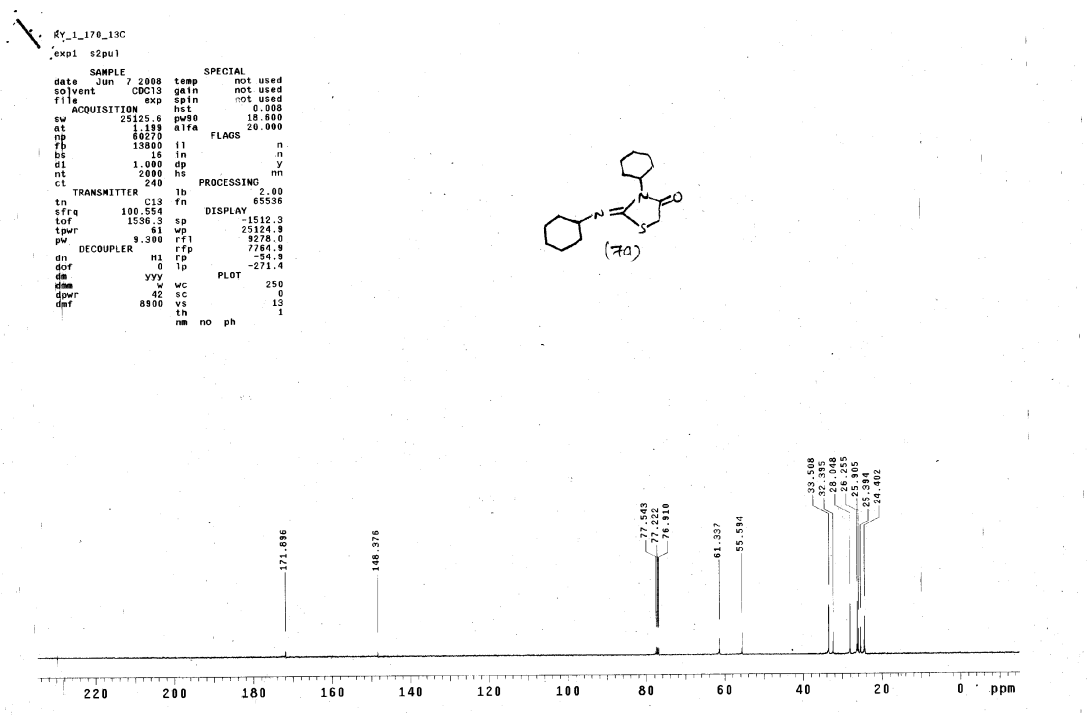

RY_1_167
.exp1 stdih
SAMPLE
date Jun 3 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 399.853
tn H1
at 1.993
np 23936
sw 6006.0
fb not used
bs 4
tpwr 57
pw 7.0
d1 1.000
tof 0
nt 32
ct 32
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -967.8
wp 6005.6
vs 31
sc 0
wc 250
hzmm 24.02
is 560.22
rfl 968.1
rfp 0
th 22
ins 100.000
nm cdc ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
Br
N
O
S
Br
(6a)
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
13.48
4.21
13.64
11.22
11.20
36.24

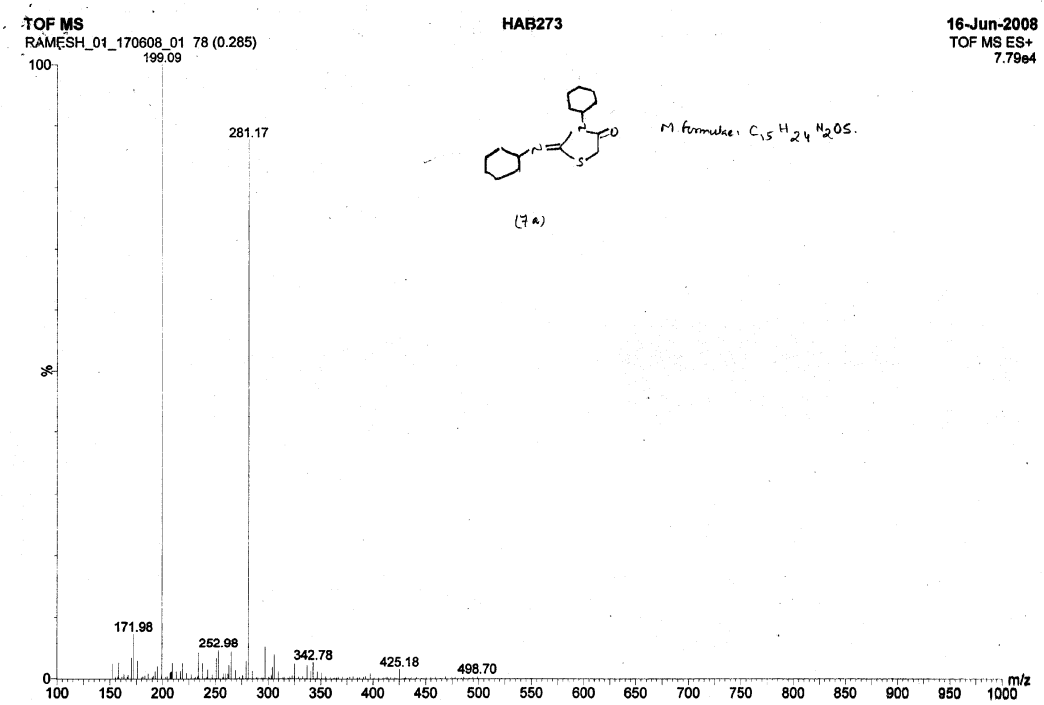

RY_1_167_13C
exp1 std13c
SAMPLE
date Jun 3 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 100.552
tn C13
at 1.199
np 59968
sw 25000.0
fb 13800
bs 16
tpwr 61
pw 8.7
dl 0
tof 0
nt 2000
ct 1248
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -2980.3
wp 24999.2
vs 52
sc 0
wc 250
hzmm 100.00
is 500.00
rfl 10746.0
rfp 7764.8
th 4
ins 100.000
nm no ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 8900
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
171.119
155.386
146.835
133.661
132.858
131.495
128.794
123.374
122.866
118.053
77.540
77.230
76.911
53.088
0.187
200
180
160
140
120
100
80
60
40
20
0
ppm

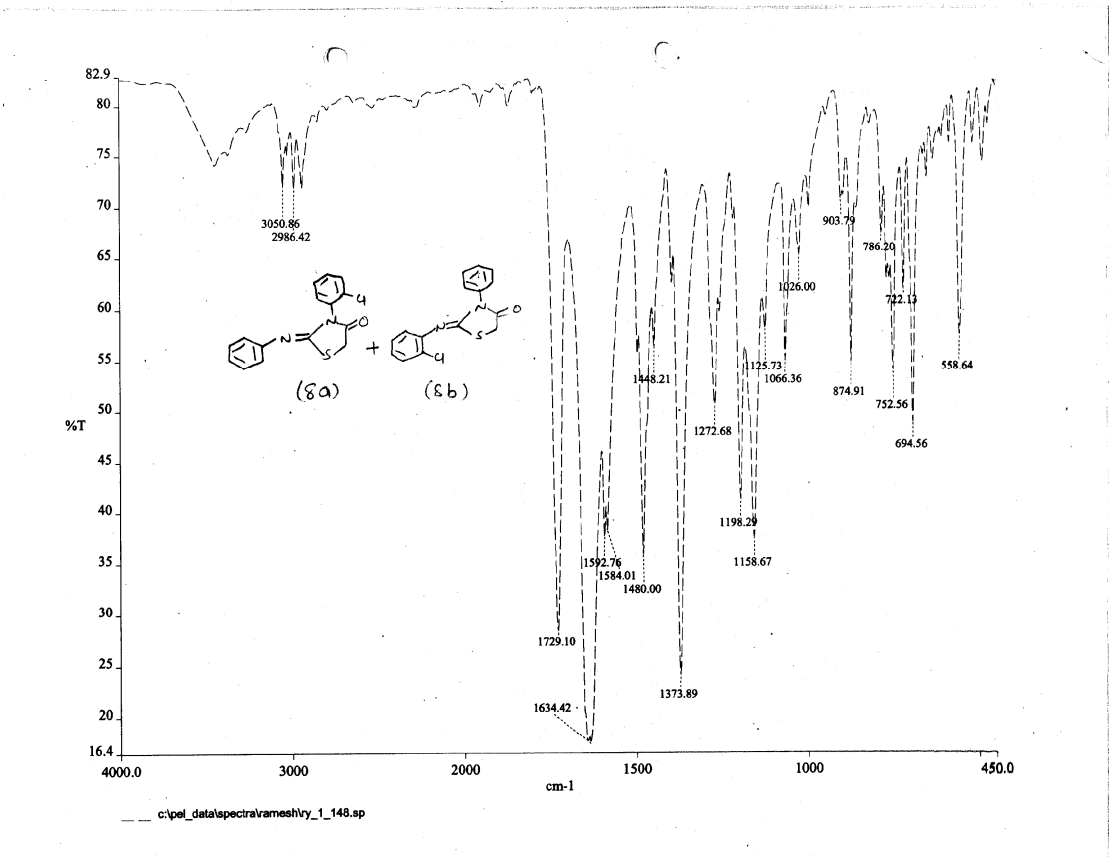

TOF MS
RAMESH_P_Br 180 (7.417)
100
%
0
426.01
449.70
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z
HAB273
16-Jun-2008
2: TOF MS ES+
523
(6u)
m formula: C15 H11 Br2 N2 O S

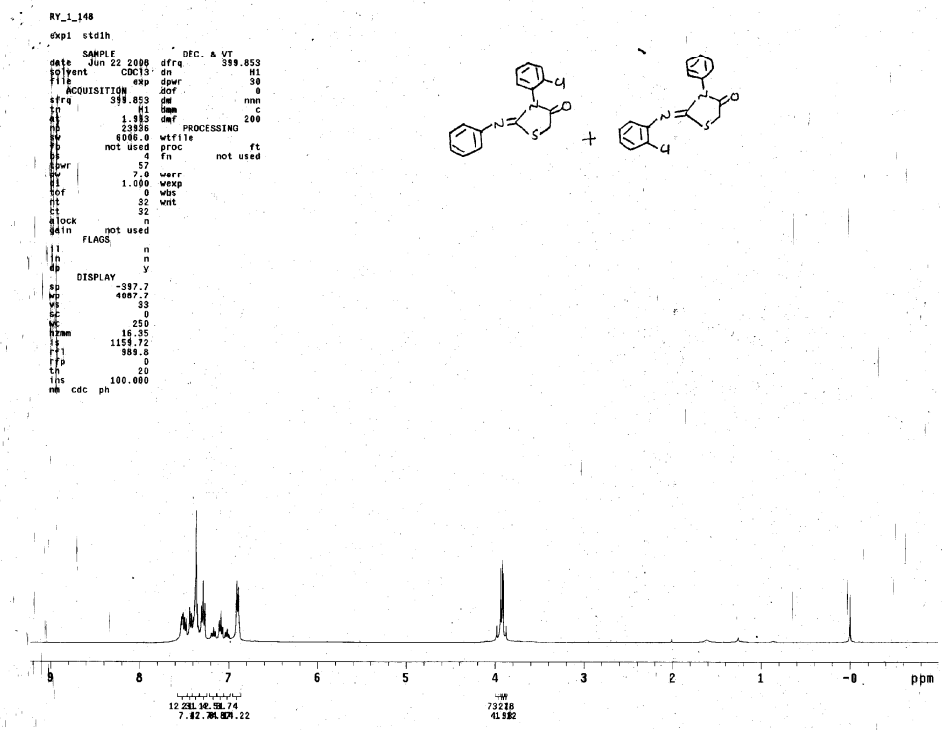

52.5
50
48
46
44
42
40
38
36
34
32
30
28
26
24
22
20
18
15.3
%T
4000.0
3000
2000
1500
1000
450.0
cm-1
2929.42
2854.75
1716.48
1645.26
1450.50
1400.26
1358.08
1337.90
1257.73
1204.29
1138.31
1078.87
969.14
896.19
802.92
715.05
612.15
536.22
(7a)
c:\pel_data\spectra\ramesh\ry_1_170_cyclo hexyl symm.sp - cyclo hexyl Symm

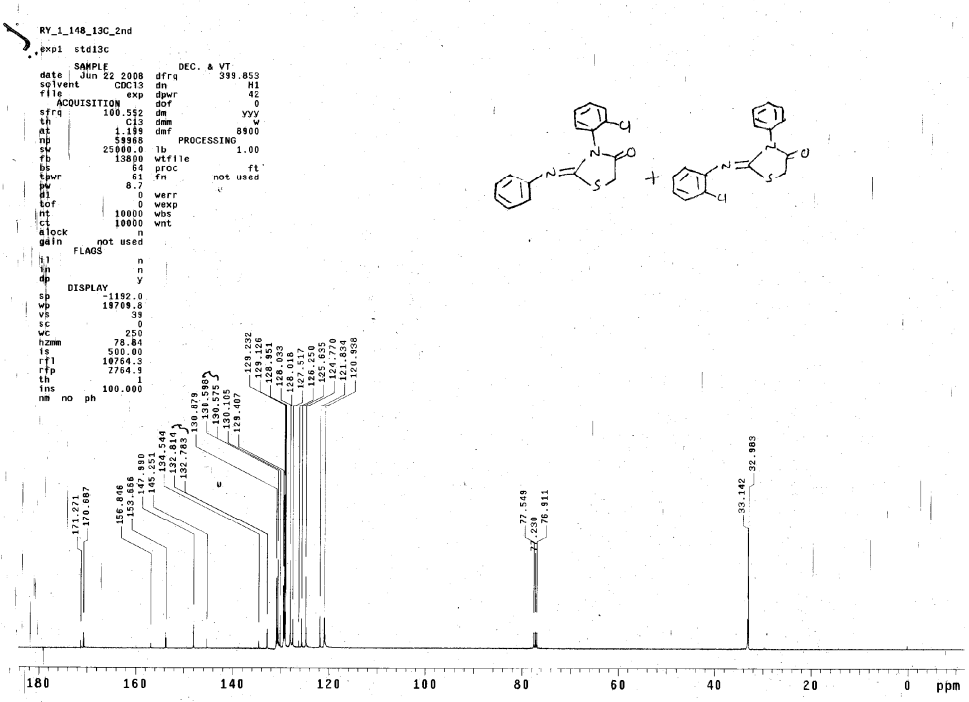

RY_1_170
expl s2pul
SAMPLE
date Jun 7 2008
solvent CDCl3
file exp
ACQUISITION
sw 6381.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.000
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -233.3
wp 3681.8
rfl 3698.0
rfp 2884.9
rp 129.4
lp -98.8
PLOT
wc 250
sc 0
vs 64
th 26
nm cdc - ph
JR
(7a)
8
7
6
5
4
3
2
1
0
ppm
3.68
7.02
3.65
7.88
15.73
14.16
11.58
5.87
30.43

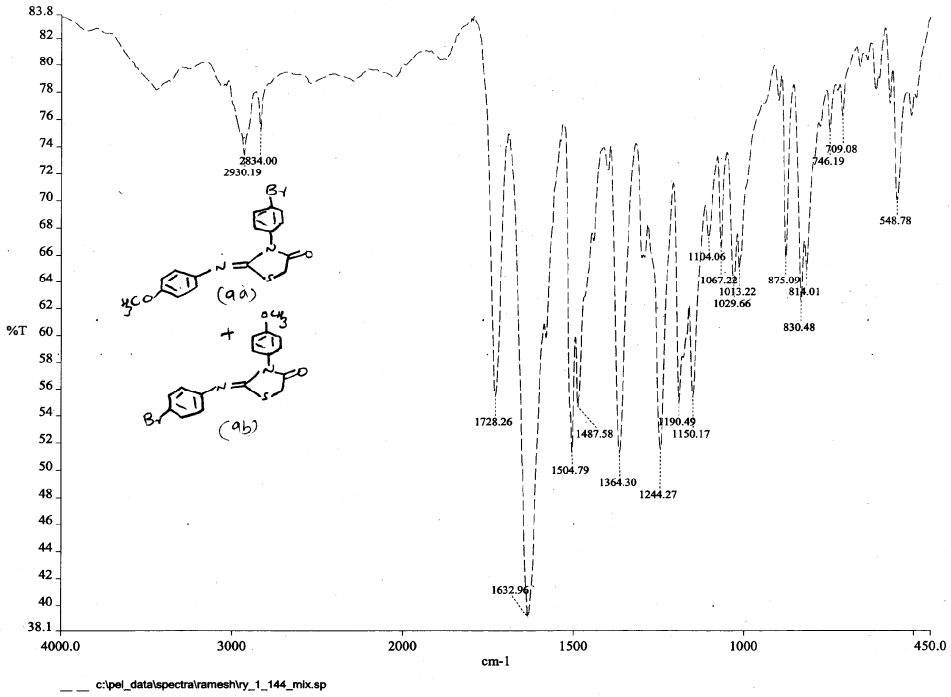

SY_1_170_13C
exp1 s2pul
SAMPLE
date Jun 7 2008
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.189
np 60270
fb 13800
bs 16
d1 1.000
nt 2000
ct 240
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1512.3
wp 25124.9
rfl 9278.0
rfp 7764.9
rp -54.9
lp -271.4
PLOT
wc 250
sc 0
vs 13
th 1
nm no ph
(7a)
171.886
148.376
77.543
77.222
76.910
61.337
55.594
33.508
32.385
28.048
26.255
25.905
25.548
24.402
220
200
180
160
140
120
100
80
60
40
20
0
ppm


TOF MS
RAMESH_01_170608_01 78 (0.285)
HAB273
16-Jun-2008
TOF MS ES+
7.79e4
199.09
281.17
171.98
252.98
342.78
425.18
498.70
%
m/z
M formula: C15 H24 N2 O S.
(7a)


82.9
80
75
70
65
60
55
50
45
40
35
30
25
20
16.4
%T
4000.0
3000
2000
1500
1000
450.0
cm-1
3050.86
2986.42
1729.10
1634.42
1592.76
1584.01
1480.00
1448.21
1373.89
1272.68
1198.29
1158.67
1125.73
1066.36
1026.00
903.79
874.91
786.20
752.56
722.13
694.56
558.64
(8a)
(8b)
c:\pel_data\spectra\ramesh\ry_1_148.sp


RY_1_148
exp1 std1h
SAMPLE
date Jun 22 2006
solvent CDCl3
file exp
ACQUISITION
sfrq 399.853
tn H1
at 1.913
nb 23936
sw 6006.0
fb not used
bs 4
bpwr 57
pw 7.0
pl 1.000
tof 0
nt 32
ct 32
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -397.7
wp 4087.7
vs 33
sc 0
wc 250
hzmm 16.35
is 1159.72
rfl 989.8
rfp 0
th 20
ins 100.000
nm cdc ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
9
8
7
6
5
4
3
2
1
-0
ppm

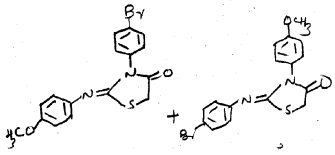

RY_1_148_13C_2nd
exp1 std13c
SAMPLE
date Jun 22 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 100.552
th C13
at 1.199
np 59968
sw 25000.0
fb 13800
bs 64
tpwr 61
pw 8.7
d1 0
tof 0
nt 10000
ct 10000
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1192.0
wp 19709.8
vs 39
sc 0
wc 250
hzmm 78.84
is 500.00
rfl 10764.3
rfp 2764.9
th 1
ins 100.000
nm no ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 8900
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
171.271
170.687
156.846
153.666
147.990
145.251
134.544
132.814
132.783
130.879
130.598
130.575
130.105
129.407
129.232
129.126
128.951
128.033
128.018
127.517
126.250
125.635
124.770
121.834
120.938
77.549
77.230
76.911
33.142
32.983
180
160
140
120
100
80
60
40
20
0
ppm


83.8
82
80
78
76
74
72
70
68
66
64
62
60
58
56
54
52
50
48
46
44
42
40
38.1
%T
4000.0
3000
2000
1500
1000
450.0
cm-1
2834.00
2930.19
1728.26
1632.96
1504.79
1487.58
1364.30
1244.27
1190.49
1150.17
1104.06
1067.22
1029.66
1013.22
875.09
830.48
814.01
746.19
709.08
548.78
(aa)
(ab)
c:\pel_data\spectra\ramesh\ry_1_144_mix.sp

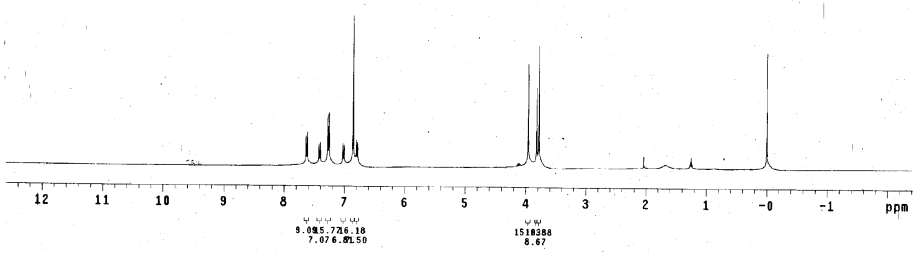
RY_1_144_mix

exp1 ,std1h

SAMPLE		DEC. & VT	
date	Jun 3 2008	dfrq	399.053
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	399.853	dm	nnn
tn	H1	dmm	c
at	1.993	dmf	200
np	23936	PROCESSING	
sw	6006.0	wtfile	
fb	not used	proc	ft
bs	4	fn	not used
tpwr	57		
pw	7.0	werr	
d1	1.000	wexp	
tof	0	wbs	
nt	32	wnt	
ct	32		
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-968.1		
wp	6005.6		
vs	39		
sc	0		
wc	250		
hzmm	24.02		
is	1130.60		
rfl	968.5		
rfp	0		
th	20		
ins	100.000		
nm cdc ph			



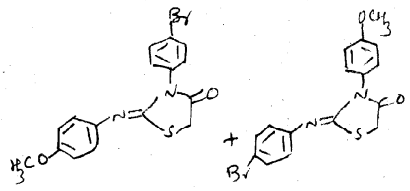
(9a) (9b)

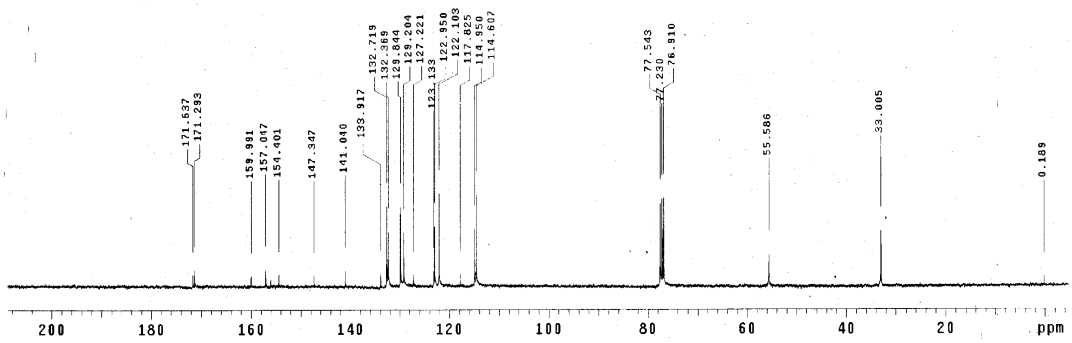


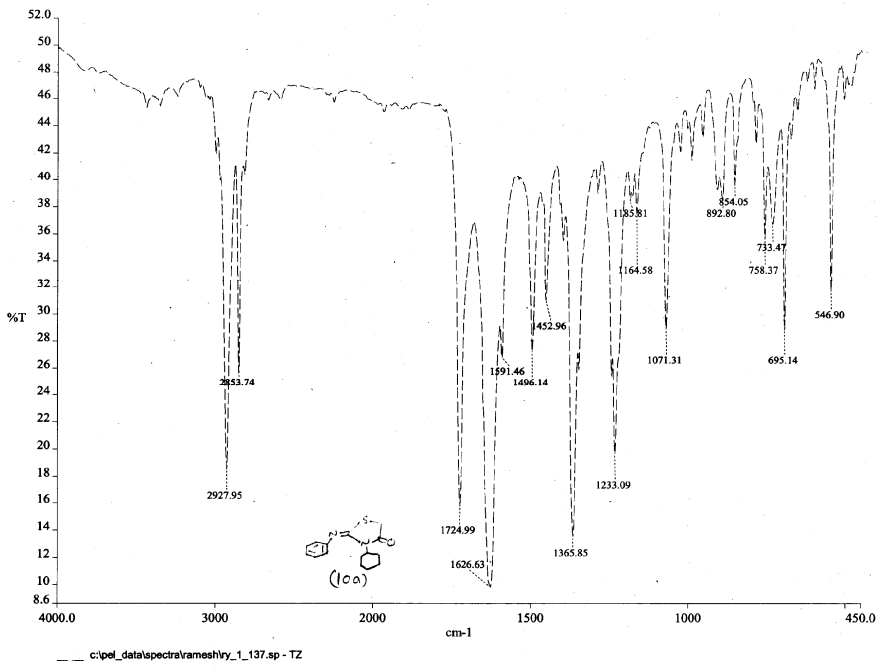
Ry-144-mix-13c

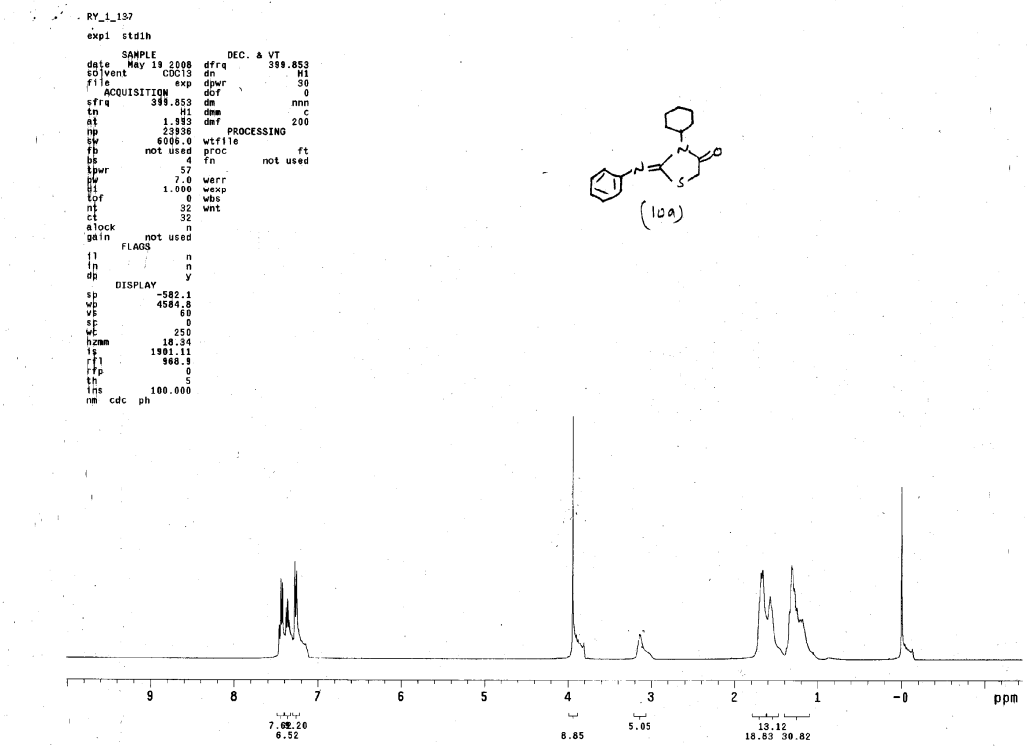
exp1 s2pul

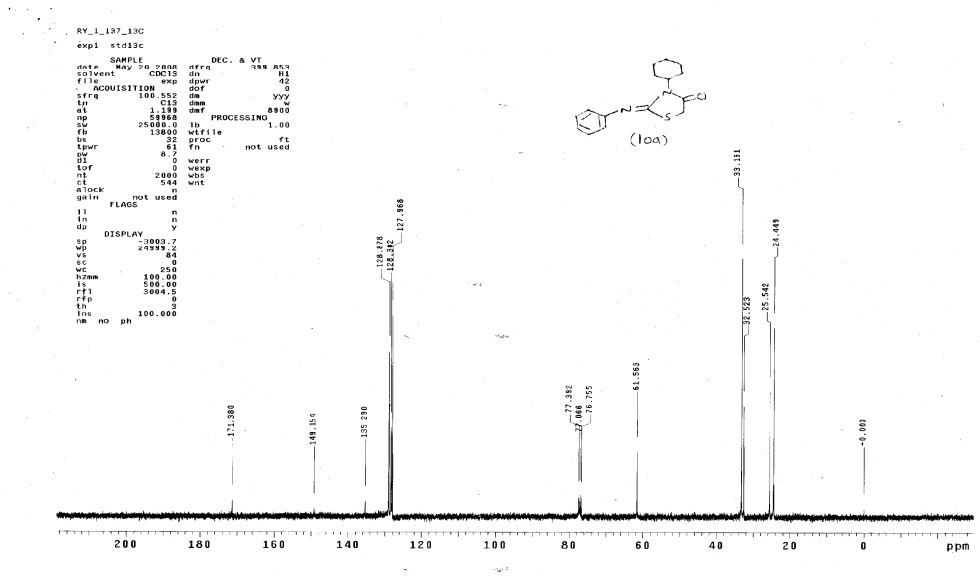
SAMPLE		SPECIAL	
date	Jun 4 2008	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	25125.6	pw90	18.600
at	1.199	alfa	20.000
np	60270	FLAGS	
fb	13800	il	n
bs	10	in	n
d1	1.000	dp	y
nt	6000	hs	nn
ct	6000	PROCESSING	
TRANSMITTER		lb	2.00
tn	C13	fn	65536
sfrq	100.554	DISPLAY	
tof	1536.3	sp	-486.3
tpwr	61	wp	21492.7
pw	9.300	rfl	9274.9
DECOUPLER		rfp	7764.9
dn	H1	rp	-37.7
dof	0	lp	-397.2
dm	yyy	PLOT	
dmm	w	wc	250
dpwr	42	sc	0
dmf	8900	vs	19
		th	2
		nm	no ph

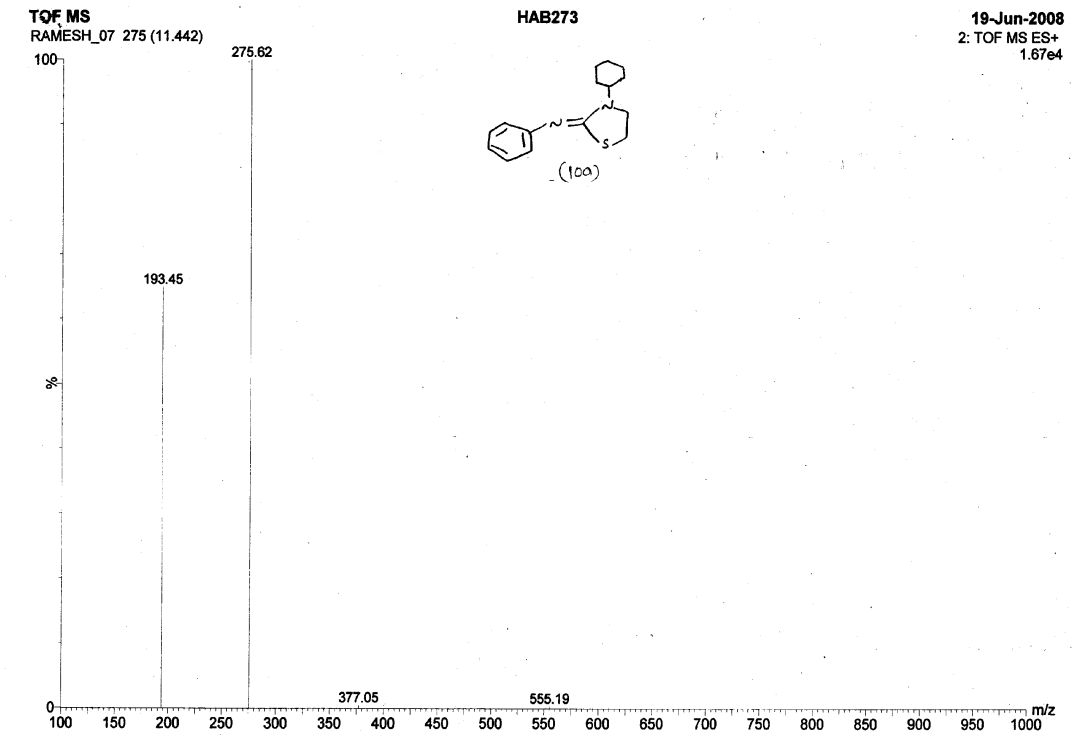


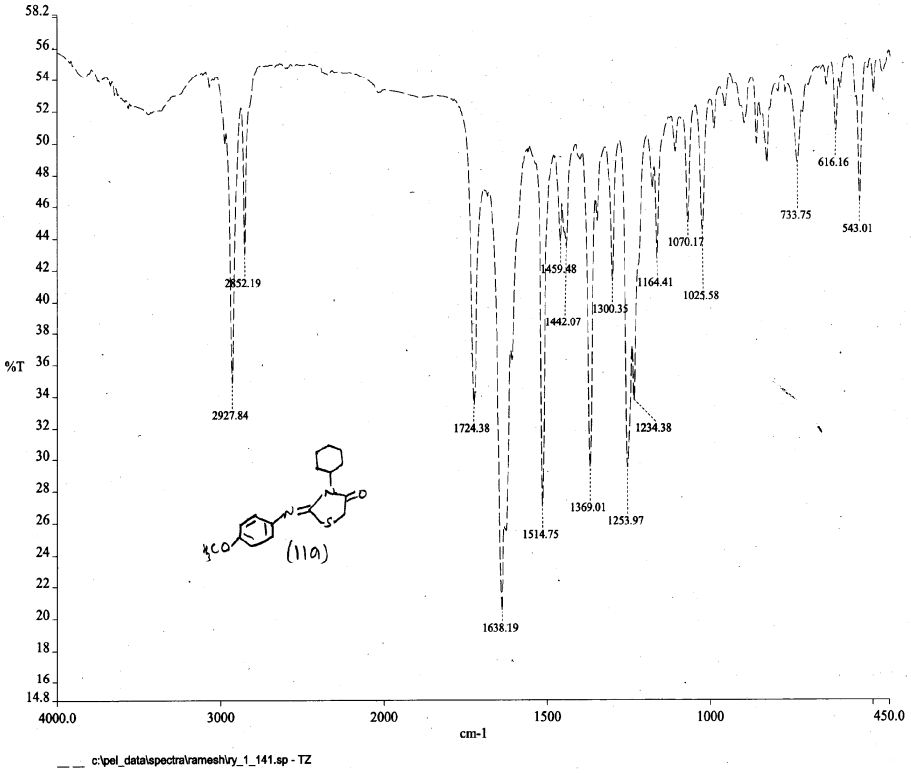


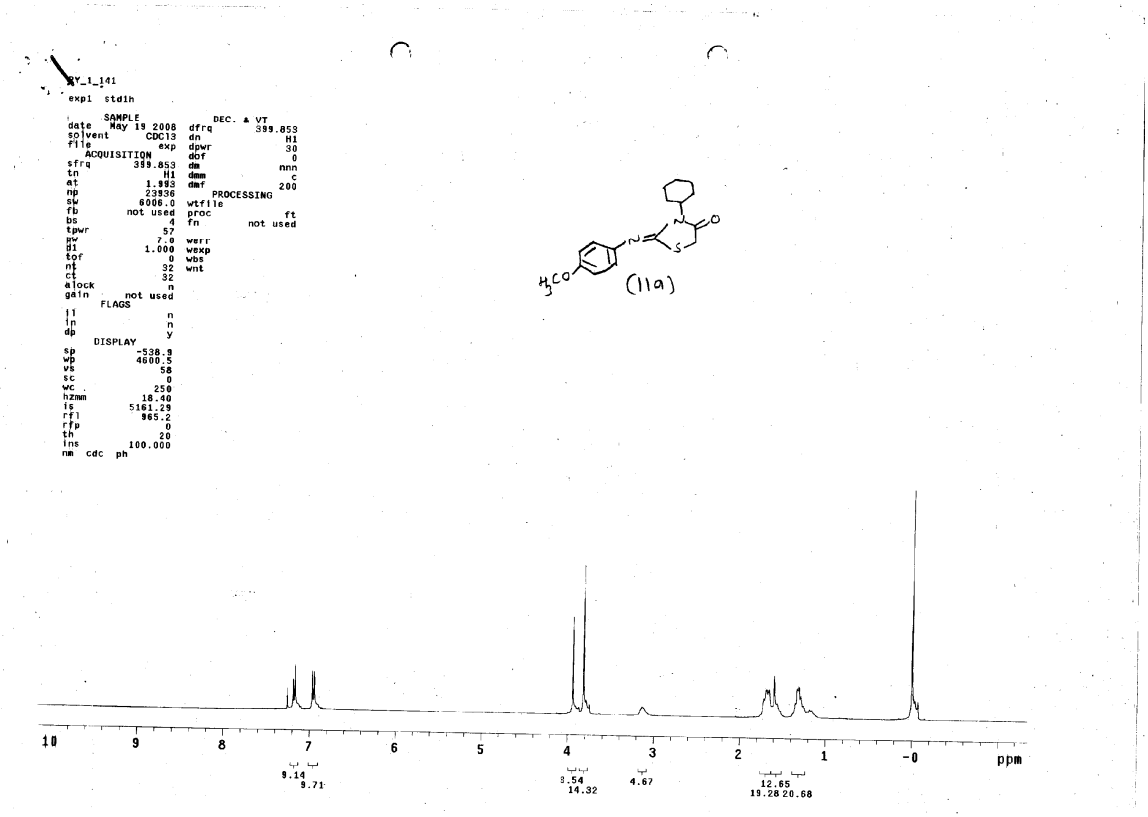

%T
cm-1
4000.0
3000
2000
1500
1000
450.0
2927.95
2853.74
1724.99
1626.63
1591.46
1496.14
1452.96
1365.85
1233.09
1185.81
1164.58
1071.31
892.80
854.05
758.37
733.47
695.14
546.90
(10a)
c:\pel_data\spectra\ramesh\ry_1_137.sp - TZ

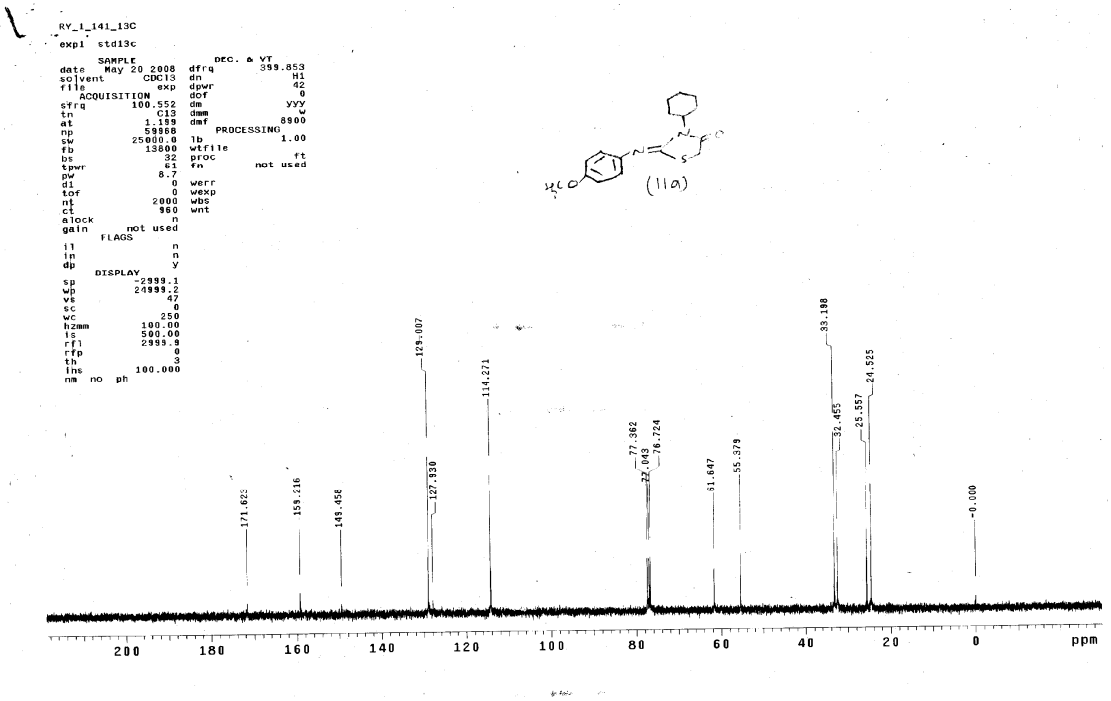

RY_1_137
expl stdlh
SAMPLE
date May 19 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 399.853
tn H1
at 1.993
np 23936
sw 6006.0
fb not used
bs 4
tpwr 57
pw 7.0
d1 1.000
tof 0
nt 32
ct 32
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -582.1
wp 4584.8
vs 60
sf 0
wc 250
hzmm 18.34
is 1901.11
rfl 968.9
rfp 0
th 5
ins 100.000
nm cdc ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
(10a)
9
8
7
6
5
4
3
2
1
-0
ppm
7.62
7.20
6.52
8.85
5.05
13.12
18.83
30.82

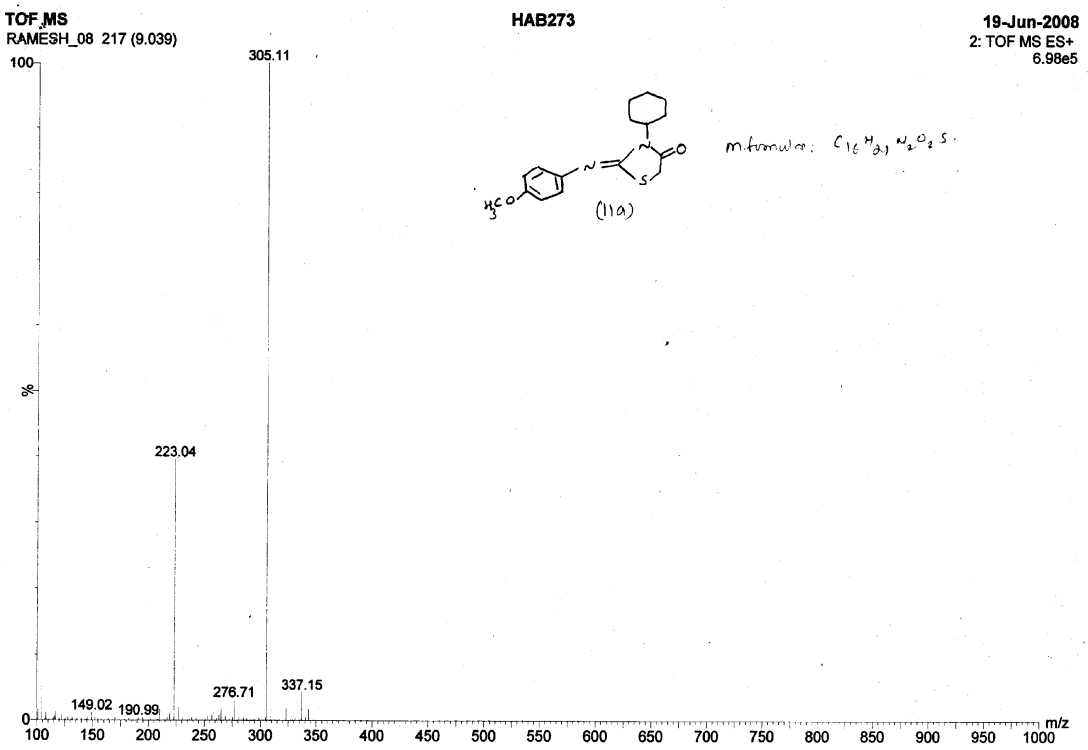

RY_1_137_13C
exp1 std13c
SAMPLE
date May 20 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 100.552
tn C13
at 1.199
np 59968
sw 25000.0
fb 13800
bs 32
tpwr 61
pw 8.7
pl 0
tof 0
nt 2000
ct 544
alock n
gain not used
FLAGS
il n
in n
dp Y
DISPLAY
sp -3003.7
wp 24999.2
vs 84
sc 0
wc 250
hzmm 100.00
hs 500.00
rfl 3004.5
rfp 0
th 3
ins 100.000
nm no ph
DEC. & VT
sfrq 399.859
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 8900
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
(10a)
171.880
149.154
135.230
128.878
128.342
127.988
77.392
77.066
76.755
61.583
33.151
32.523
25.542
24.449
0.000
200
180
160
140
120
100
80
60
40
20
0
ppm

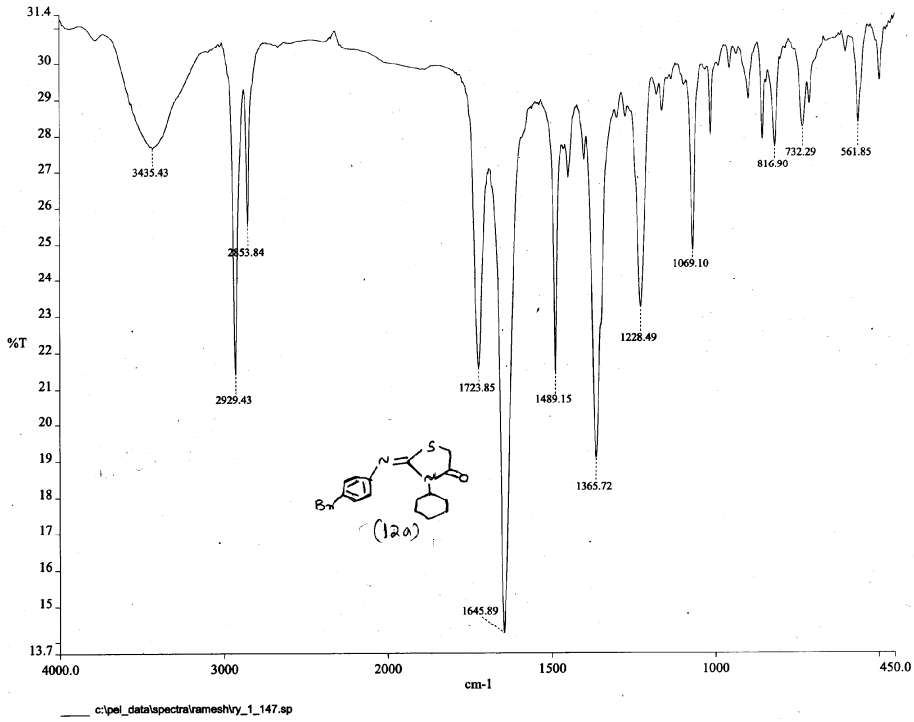

TOF MS
RAMESH_07 275 (11.442)
HAB273
19-Jun-2008
2: TOF MS ES+
1.67e4
100
%
0
275.62
193.45
377.05
555.19
(100)
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z

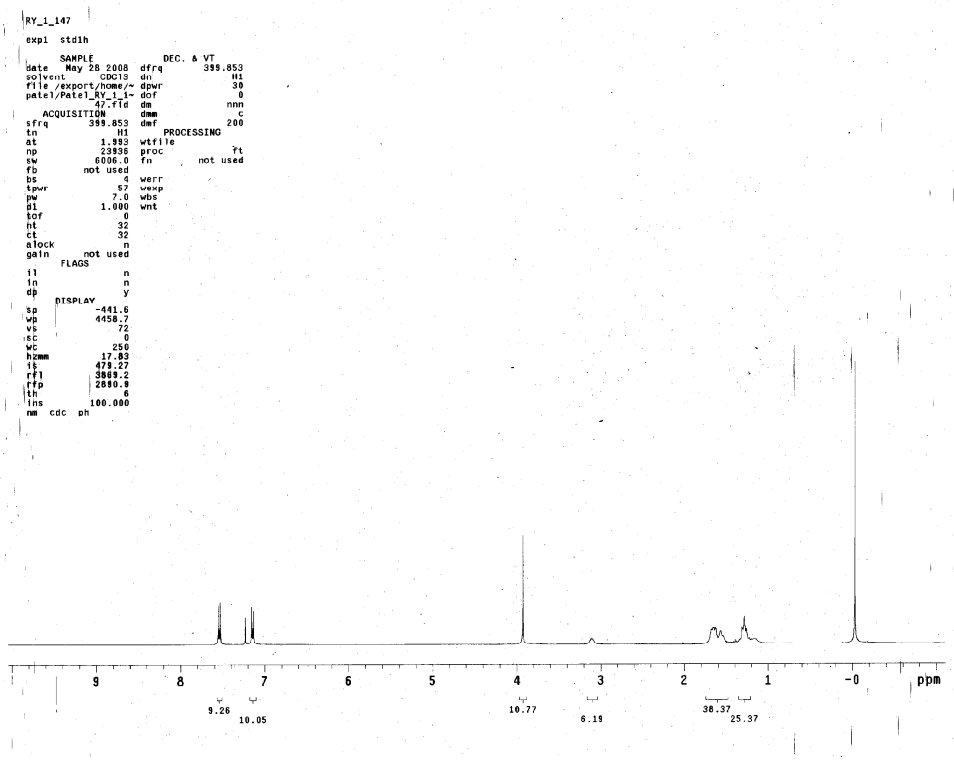

58.2
56
54
52
50
48
46
44
42
40
38
%T 36
34
32
30
28
26
24
22
20
18
16
14.8
4000.0
3000
2000
1500
1000
450.0
cm-1
2927.84
2852.19
1724.38
1638.19
1514.75
1459.48
1442.07
1369.01
1300.35
1253.97
1234.38
1164.41
1070.17
1025.58
733.75
616.16
543.01
H3CO
(11a)
c:\pel_data\spectra\ramesh\ry_1_141.sp - TZ

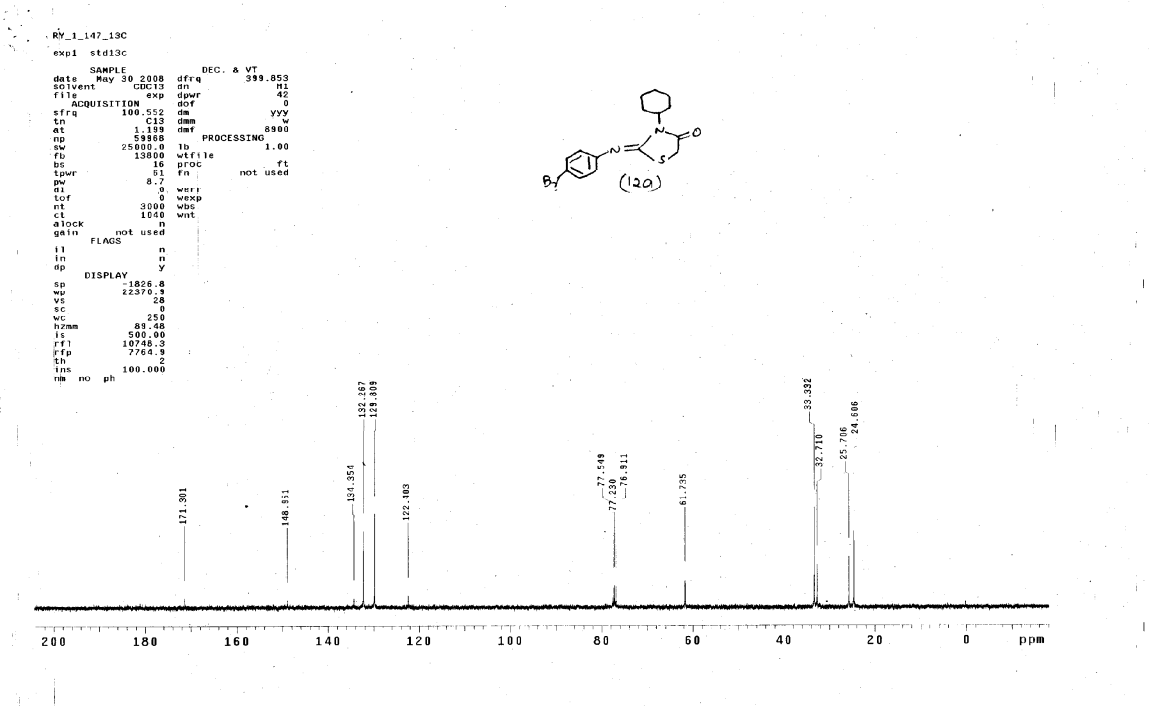

MY_1_141
expl stdin
SAMPLE
date May 19 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 399.853
tn H1
at 1.998
np 23936
sw 6006.0
fb not used
bs 4
tpwr 57
pw 7.0
d1 1.000
tof 0
nt 32
ct 32
alock n
gain not used
FLAGS
ii n
in n
dp y
DISPLAY
sp -538.9
wp 4600.5
vs 58
sc 0
wc 250
hzmm 18.40
is 5161.29
rfl 965.2
rfp 0
th 20
ins 100.000
nm cdc ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
(11a)
10
9
8
7
6
5
4
3
2
1
-0
ppm
9.14
9.71
3.54
14.32
4.67
12.65
19.28 20.68

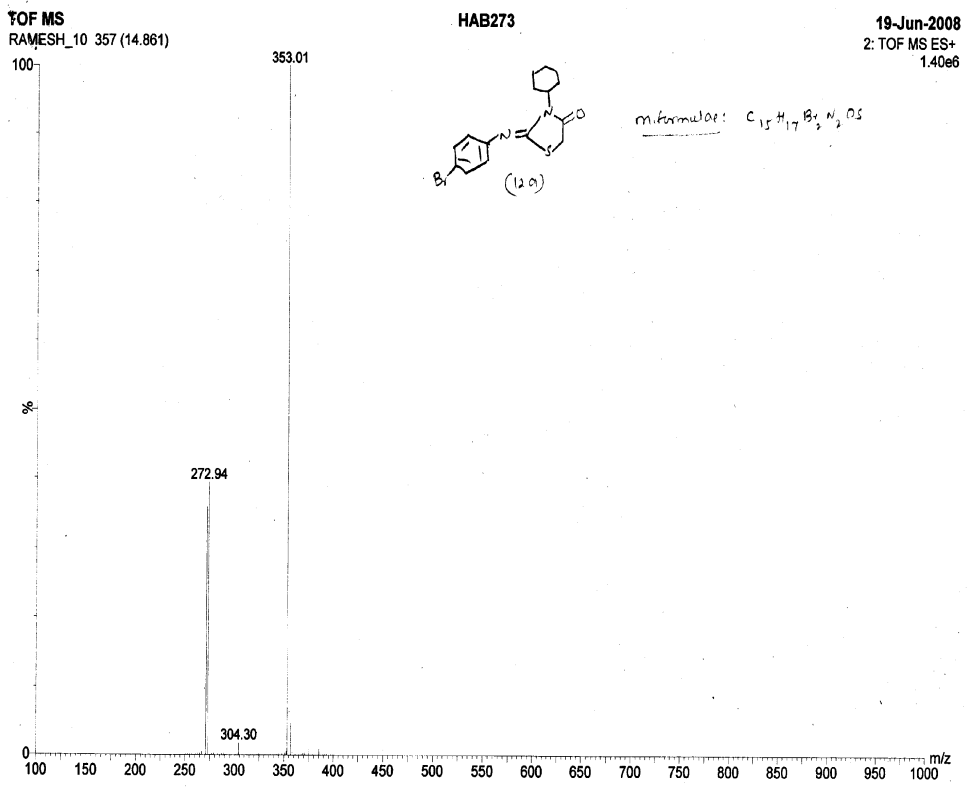

RY_I_141_13C
expl std13c
SAMPLE
date May 20 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 100.552
tn C13
at 1.189
np 59868
sw 25000.0
fb 13800
bs 32
tpwr 61
pw 8.7
d1 0
tof 0
nt 2000
ct 960
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -2999.1
wp 24999.2
vs 47
sc 0
wc 250
hzmm 100.00
is 500.00
rfl 2999.9
rfp 0
th 3
ins 100.000
nm no ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 8900
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
(11a)
171.625
159.216
149.458
129.007
127.330
114.271
77.362
77.043
76.724
61.647
55.379
33.198
32.455
25.557
24.525
0.000
200
180
160
140
120
100
80
60
40
20
0
ppm


TOF MS
RAMESH_08 217 (9.039)
HAB273
19-Jun-2008
2: TOF MS ES+
6.98e5
100
%
0
305.11
223.04
149.02
190.99
276.71
337.15
m/z
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
(11a)
molecular formula: C16H20N2O2S


%T
cm-1
3435.43
2853.84
2929.43
1723.85
1645.89
1489.15
1365.72
1228.49
1069.10
816.90
732.29
561.85
(12a)
c:\pel_data\spectra\rameshlry_1_147.sp


RY_1_147
expl stdih
SAMPLE
date May 28 2008
solvent CDCl3
file /export/home/~
pate1/Pate1_RY_1_1~
47.fid
ACQUISITION
sfrq 399.853
tn H1
at 1.993
np 23936
sw 6006.0
fb not used
bs 4
tpwr 57
pw 7.0
d1 1.000
tof 0
nt 32
ct 32
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -441.6
wp 4458.7
vs 72
sc 0
wc 250
hzmm 17.83
fb 479.27
rfl 3869.2
rfp 2880.8
th 6
ins 100.000
nm cdc ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
ppm
9.26
10.05
10.77
6.19
38.37
25.37


RY_1_147_13C
exp1 std13c
SAMPLE
date May 30 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 100.552
tn C13
at 1.199
np 59968
sw 25000.0
fb 13800
bs 16
tpwr 51
pw 8.7
d1 0
tof 0
nt 3000
ct 1040
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1826.8
wp 22370.3
vs 28
sc 0
wc 250
hzmm 88.48
is 500.00
rfl 10748.3
rfp 7764.9
th 2
ins 100.000
nm no ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 8900
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
wexp
wbs
wnt
Br
(120)
171.301
148.851
134.354
132.167
129.309
122.103
77.549
77.230
76.911
61.735
33.332
32.710
25.706
24.606
200
180
160
140
120
100
80
60
40
20
0
ppm


TOF MS
RAMESH_10 357 (14.861)
HAB273
19-Jun-2008
2: TOF MS ES+
1.40e6
353.01
272.94
304.30
%
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
(12a)
m.formula: C15H17Br2N2OS