Electronic supplementally information

The facile and efficient stereoselective synthesis of novel monocyclic cis-β-lactam conjugates having a 1-methyl-1*H*-imidazole-2-thio nucleus

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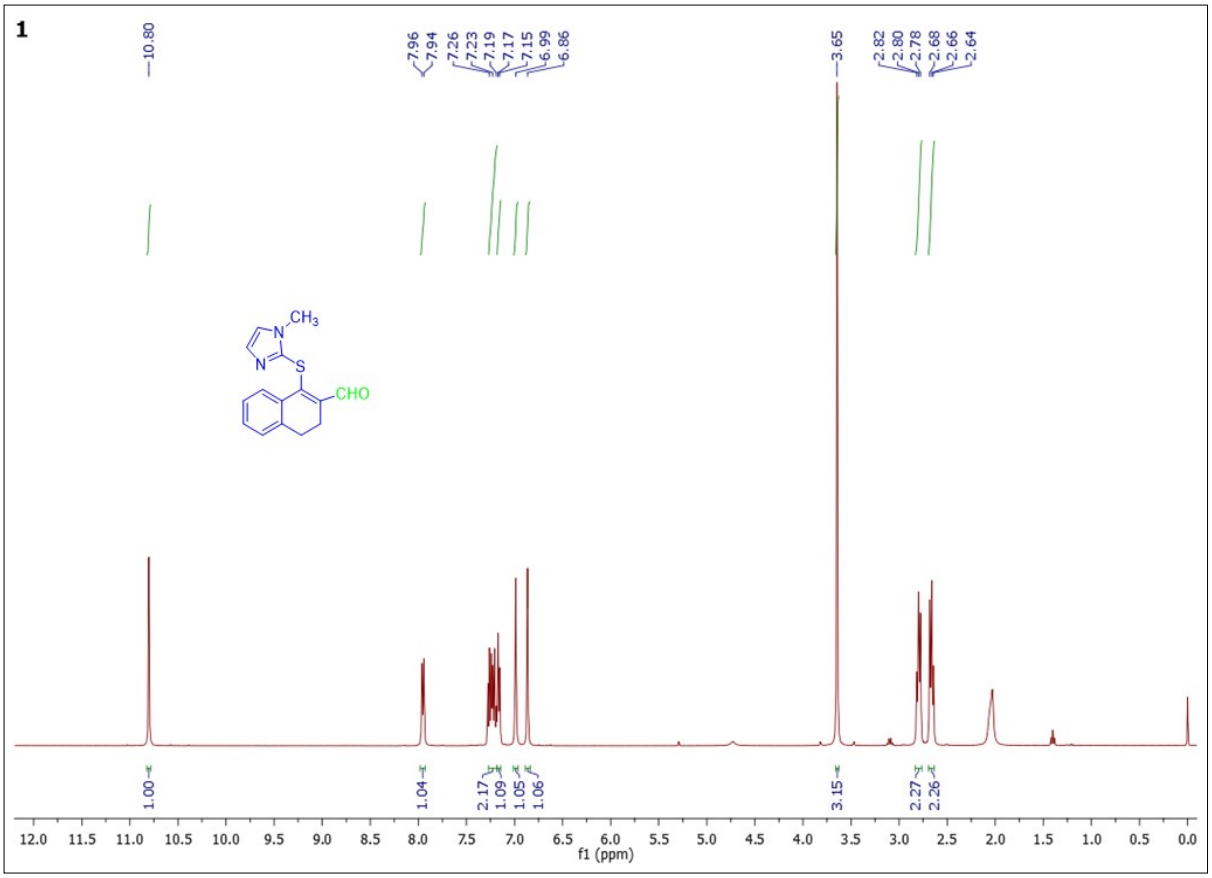
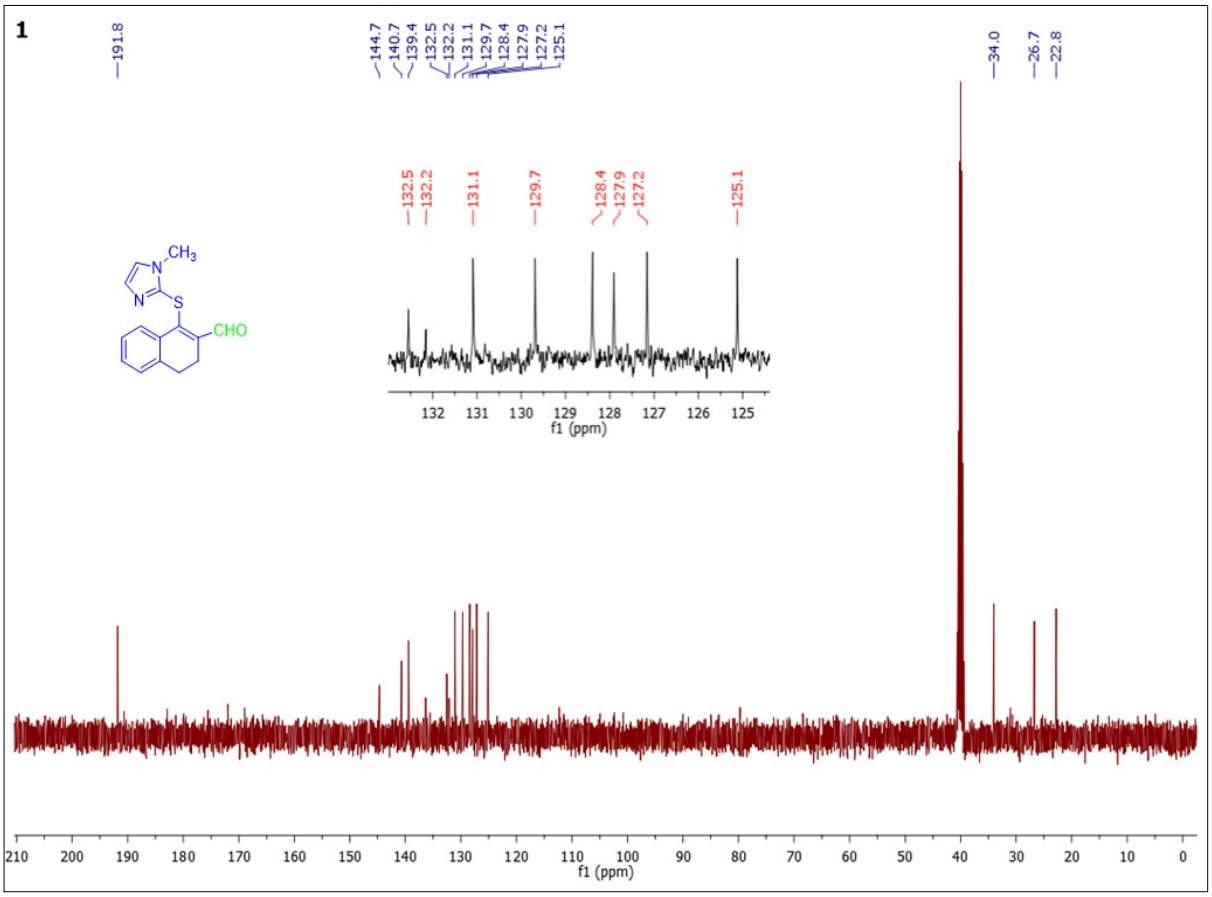
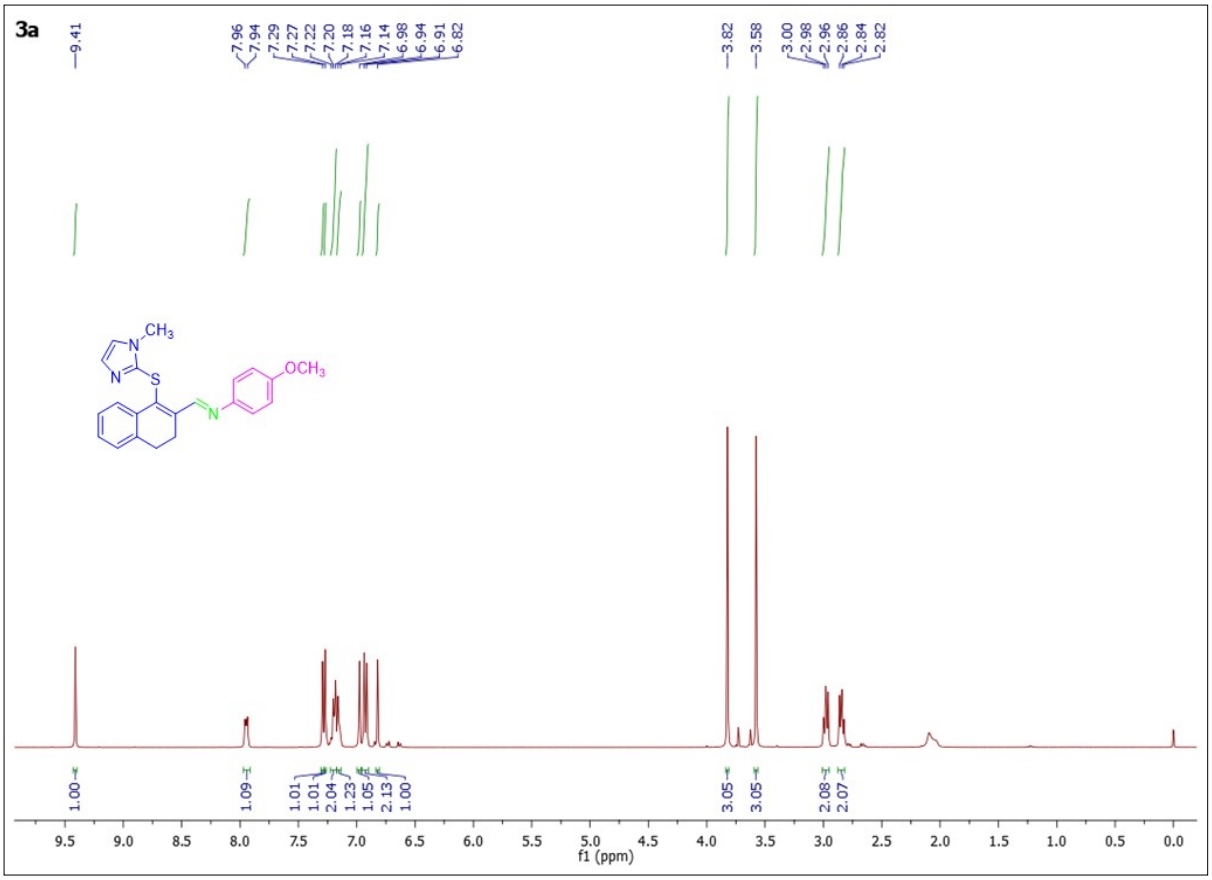
^{1}H NMR spectra and ^{13}C NMR spectra of compound (1)

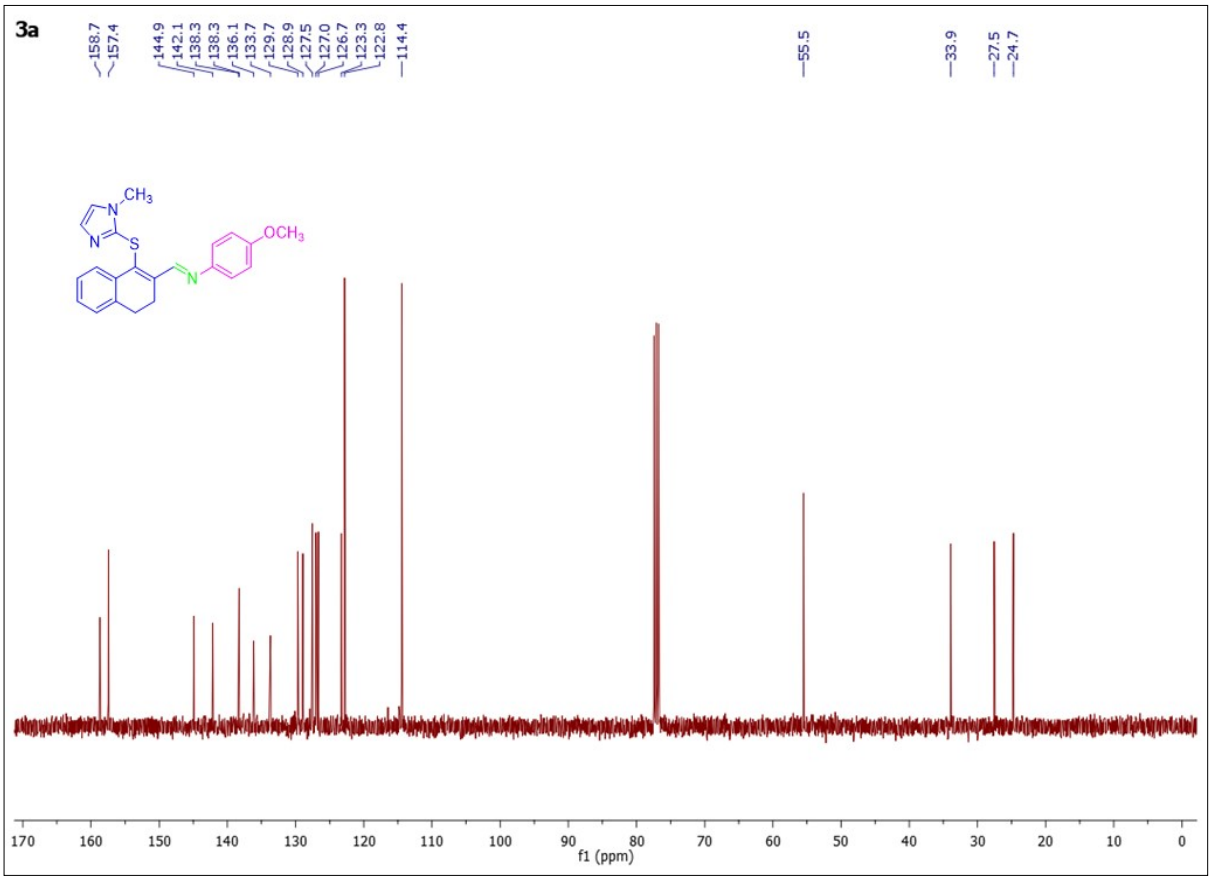




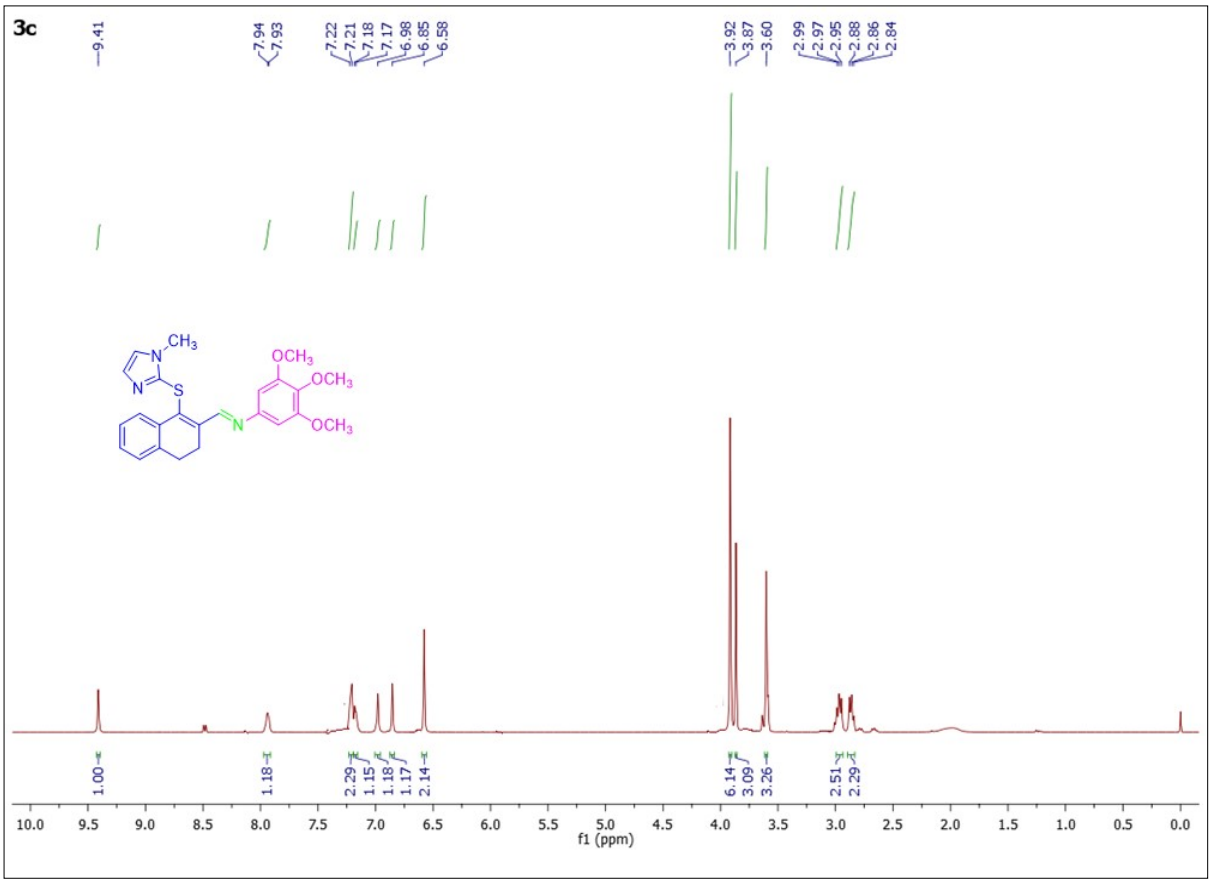
2. The copy of ^{1}H NMR spectra and ^{13}C NMR spectra of compounds 3a-3i

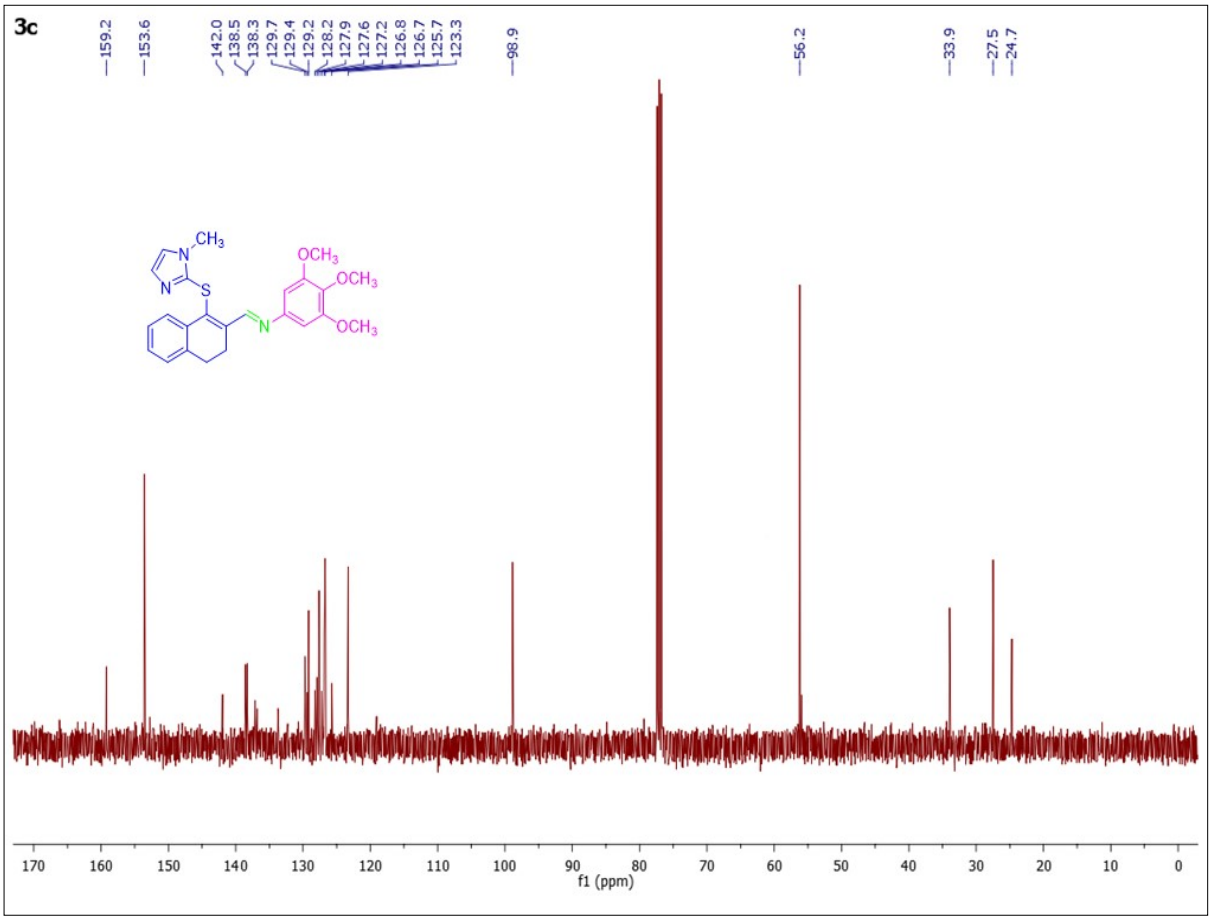
^{1}H NMR spectra and ^{13}C NMR spectra of compound (3a)



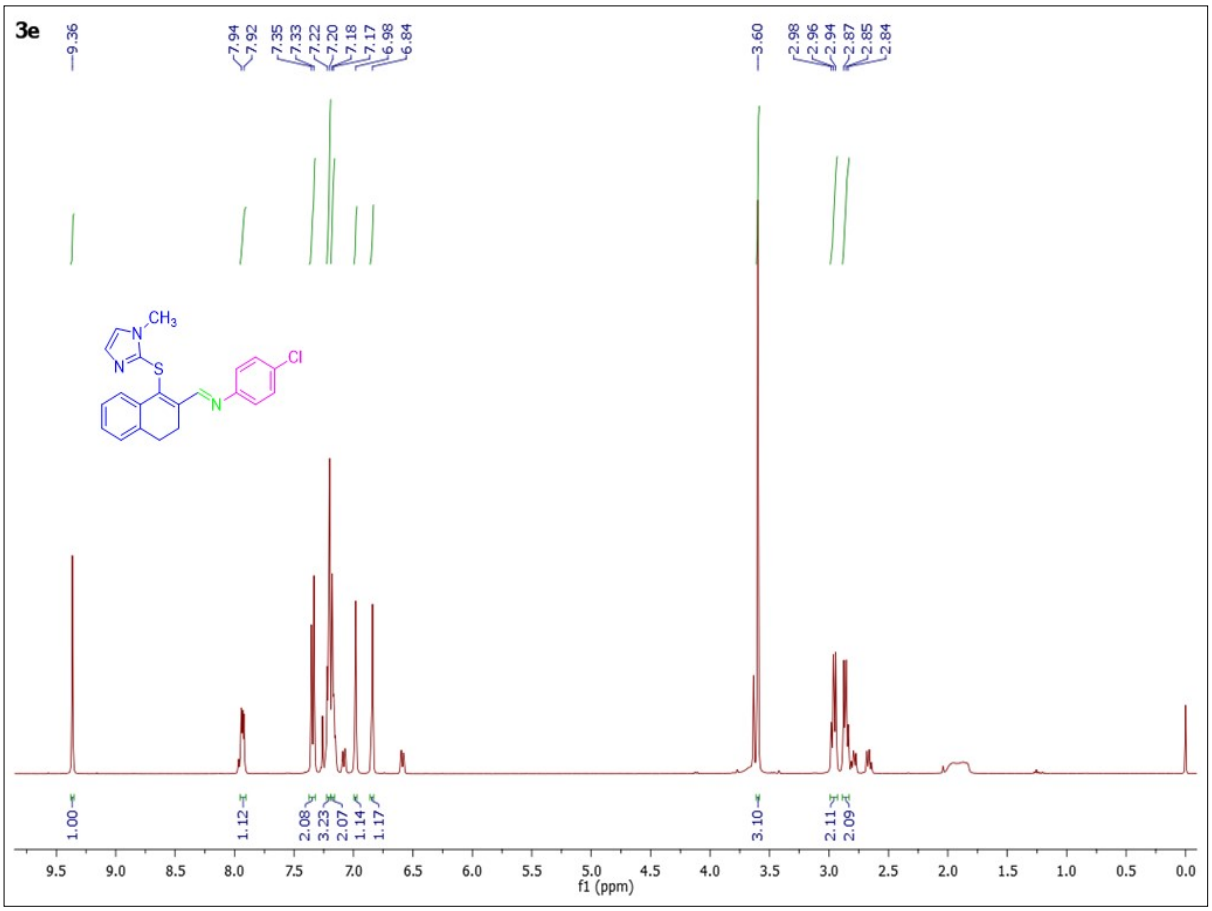


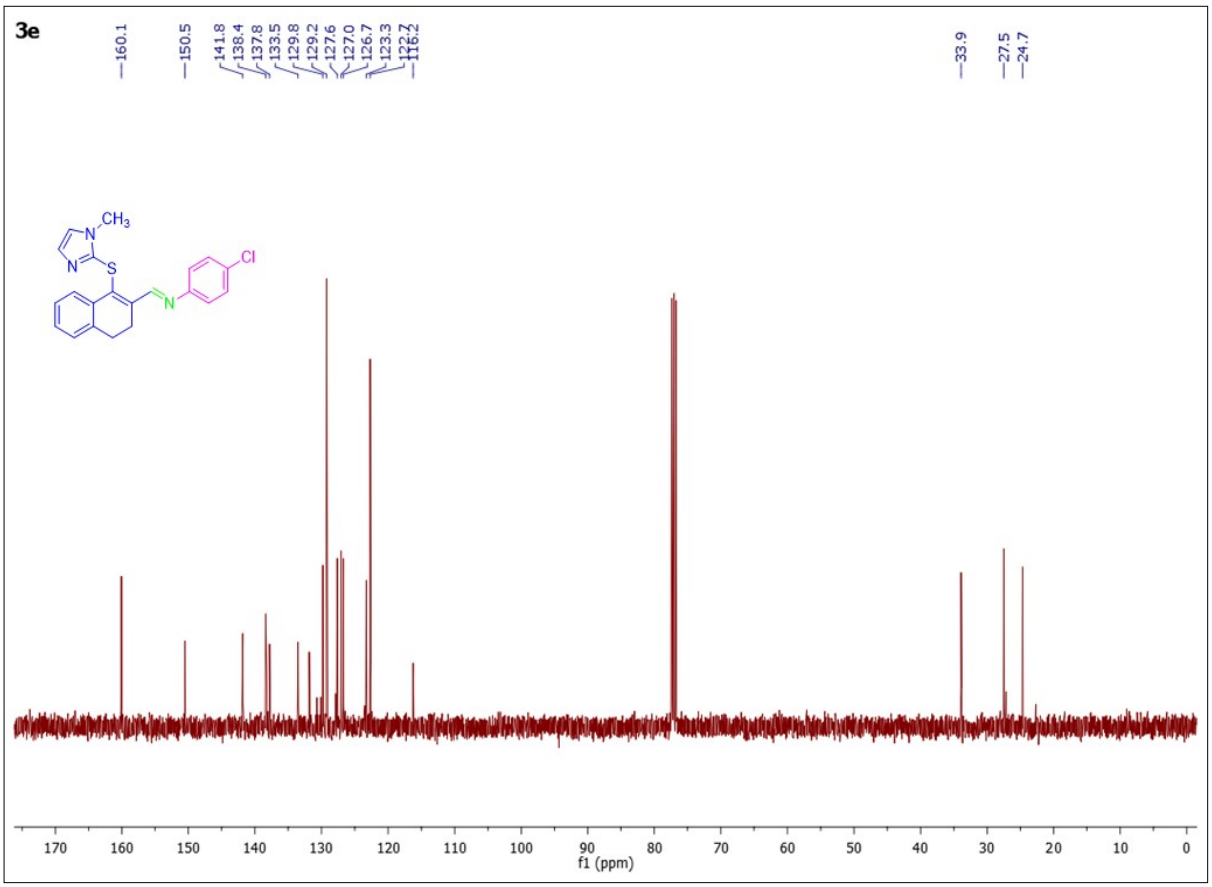
^{1}H NMR spectra and ^{13}C NMR spectra of compound (3c)



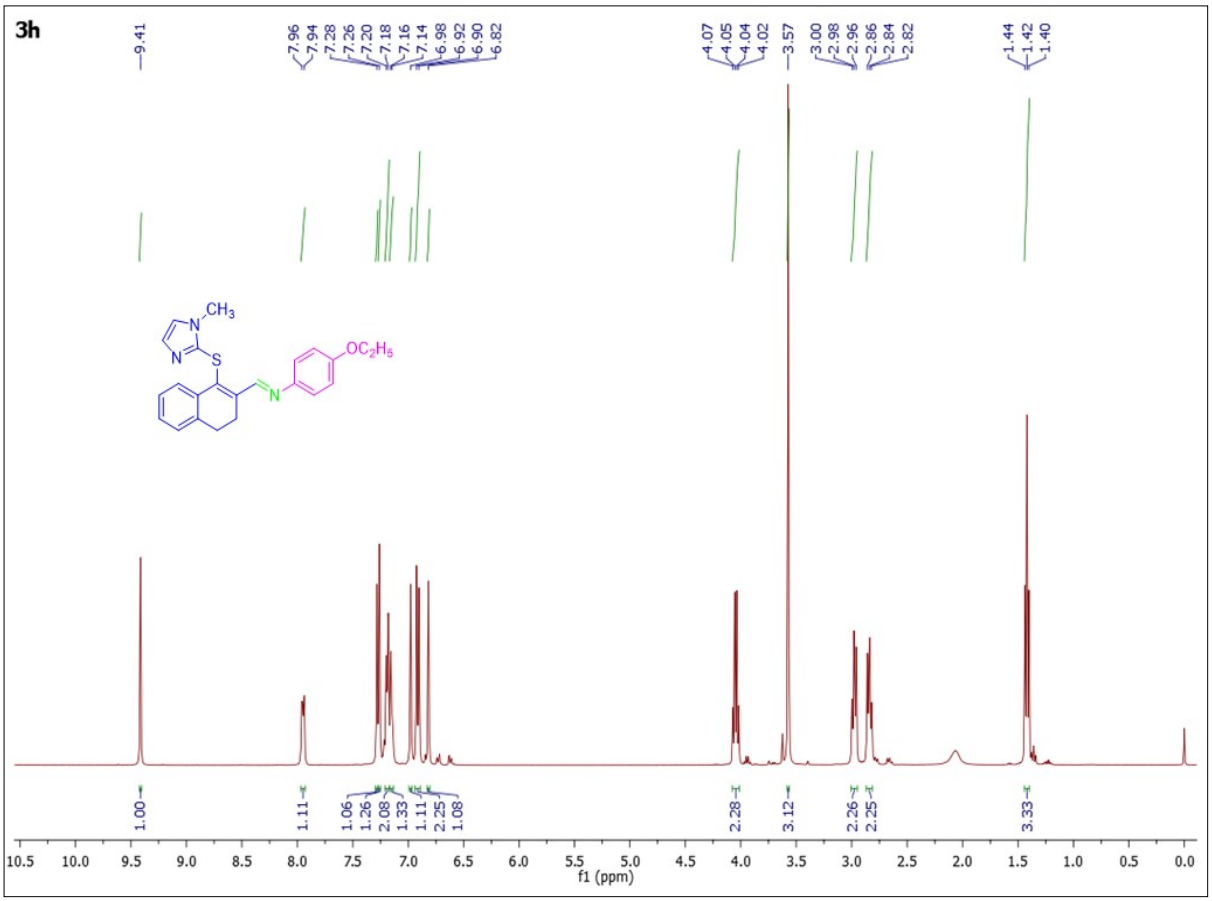


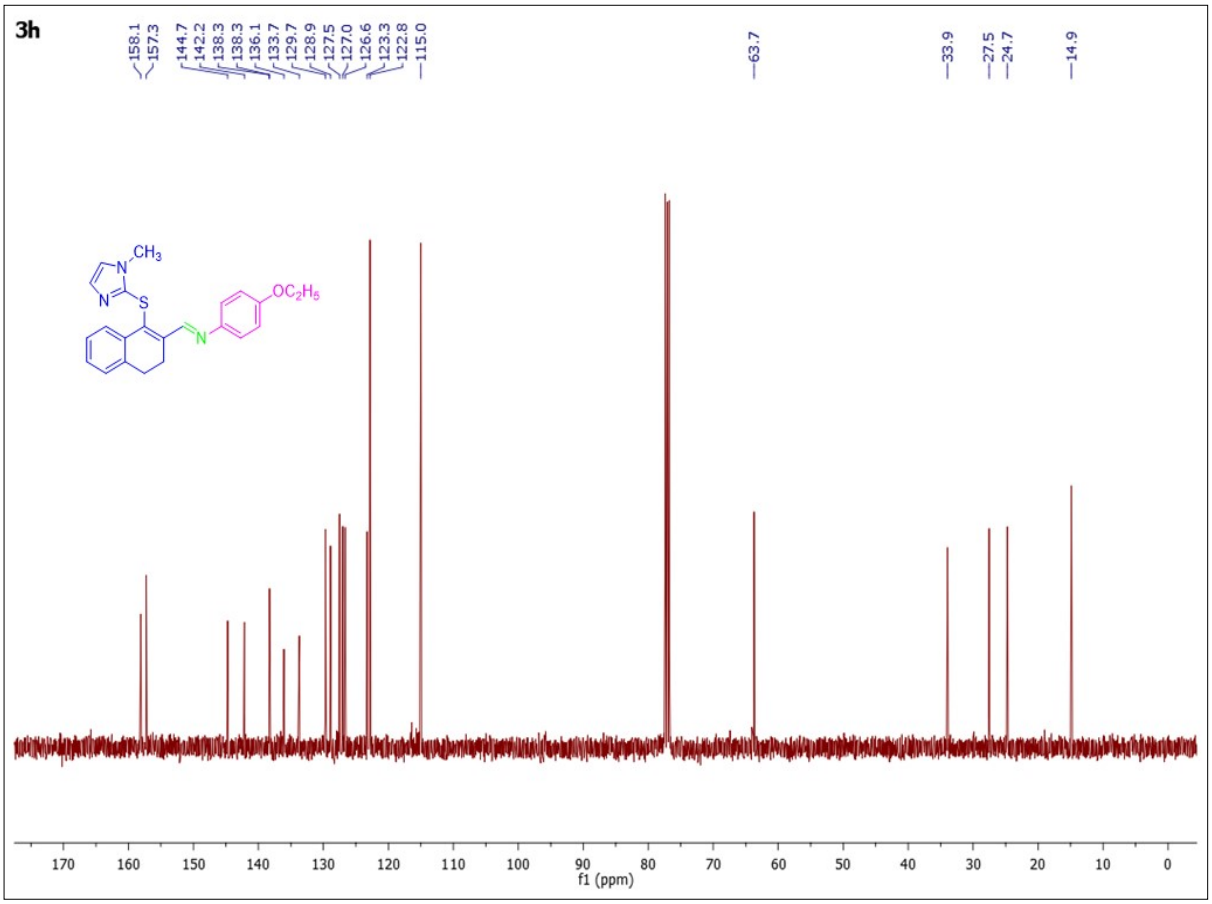
^{1}H NMR spectra and ^{13}C NMR spectra of compound (3e)



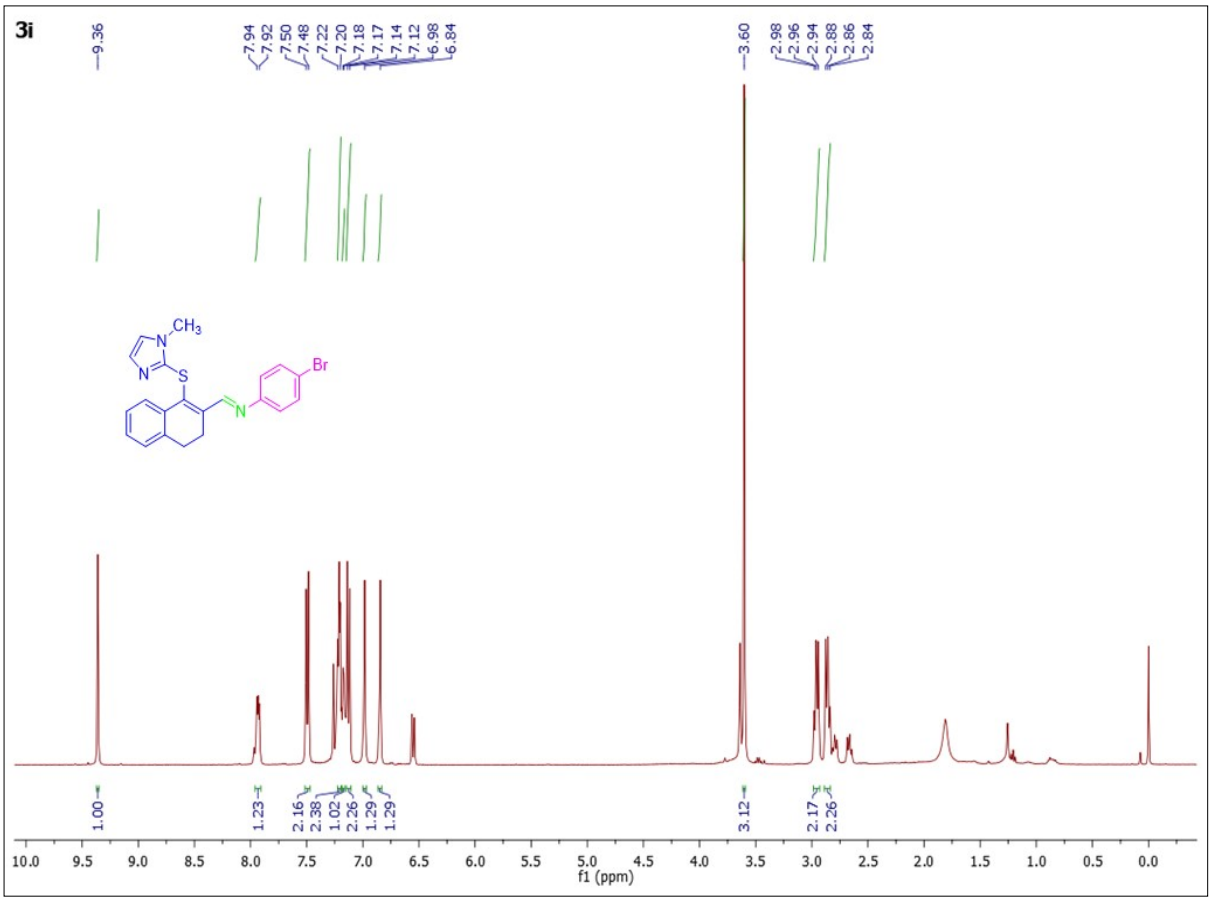


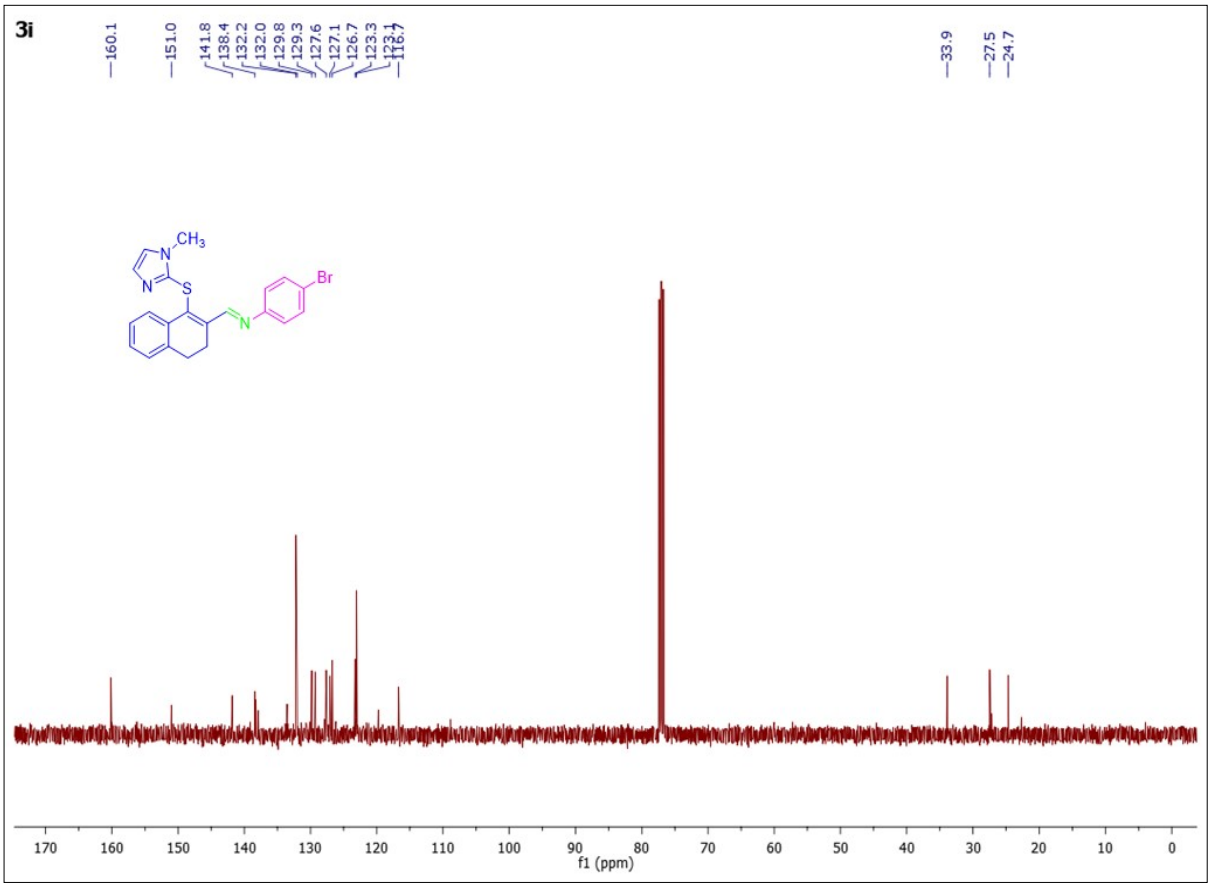
^{1}H NMR spectra and ^{13}C NMR spectra of compound (3h)





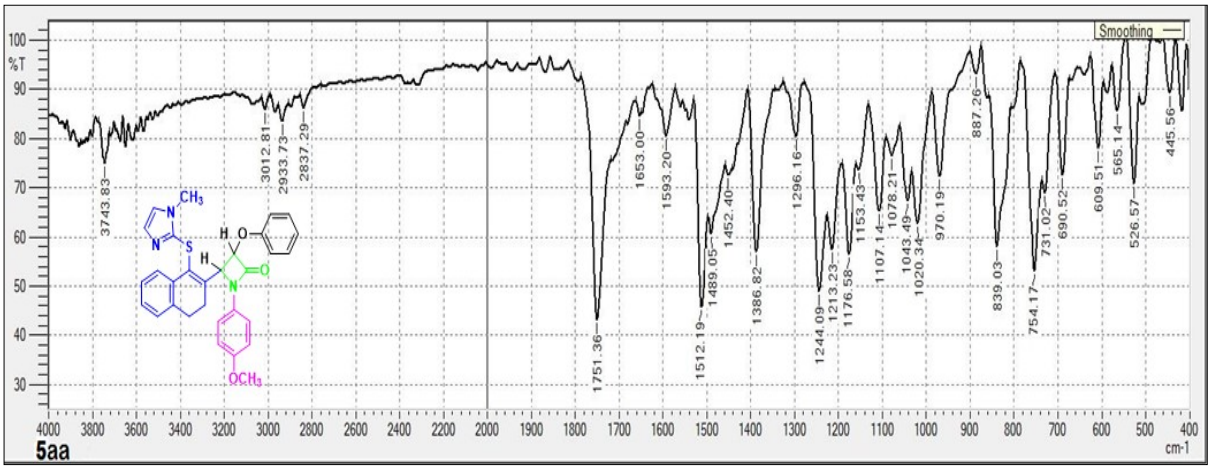
^{1}H NMR spectra and ^{13}C NMR spectra of compound (3i)

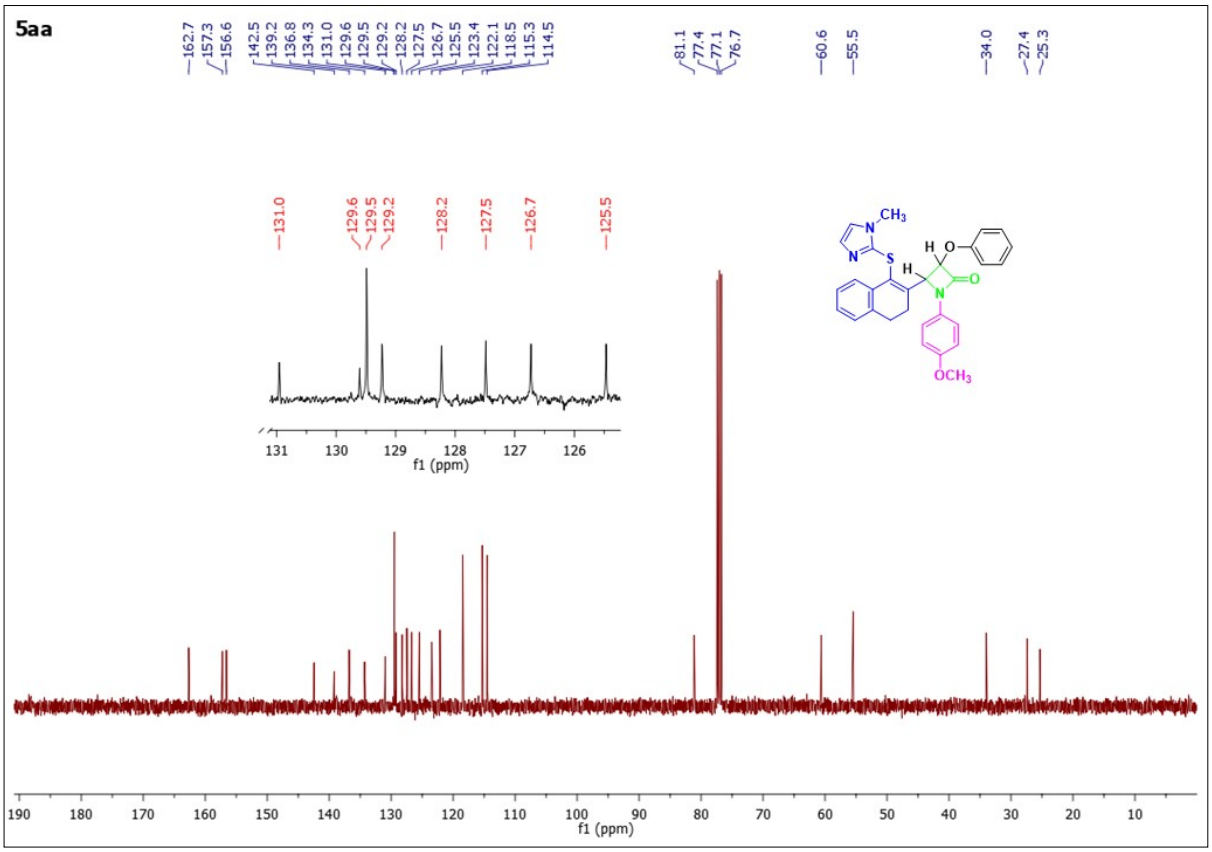


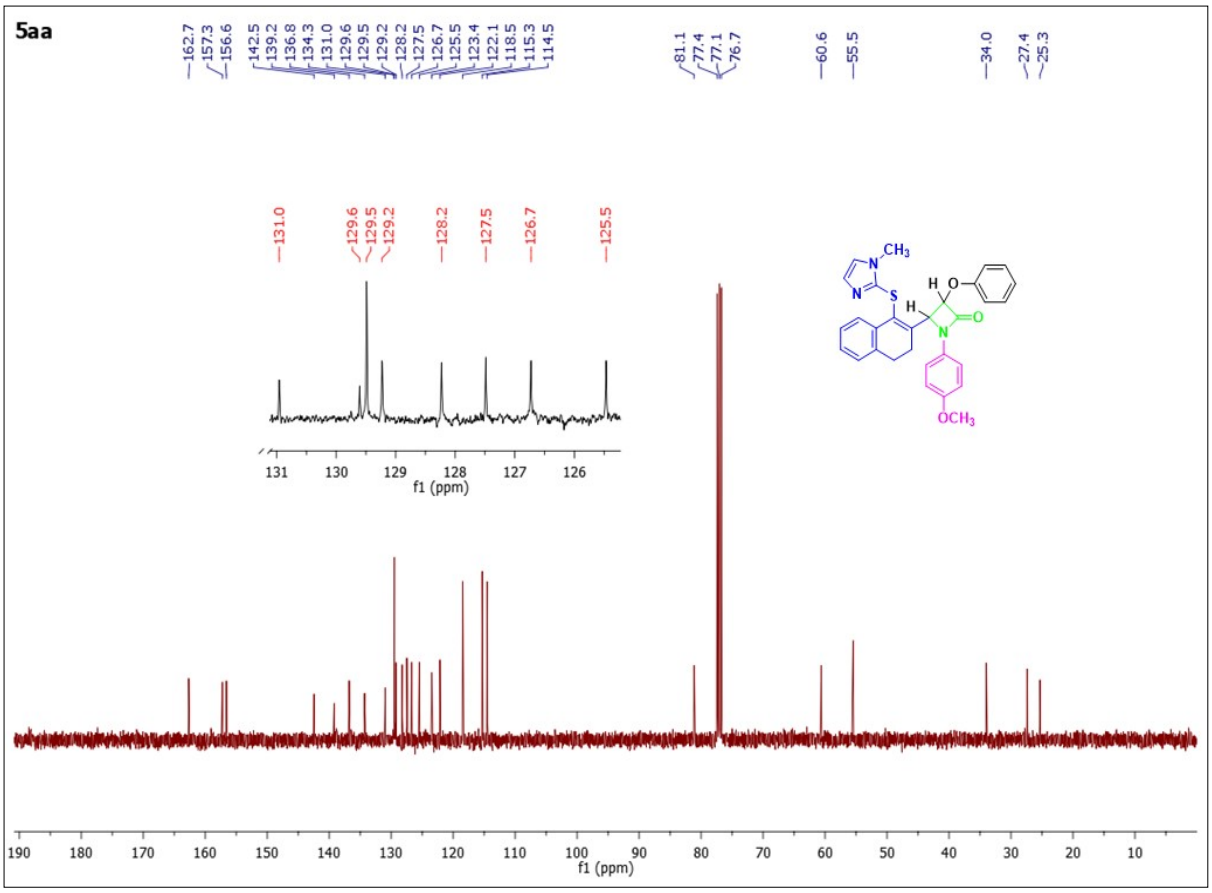


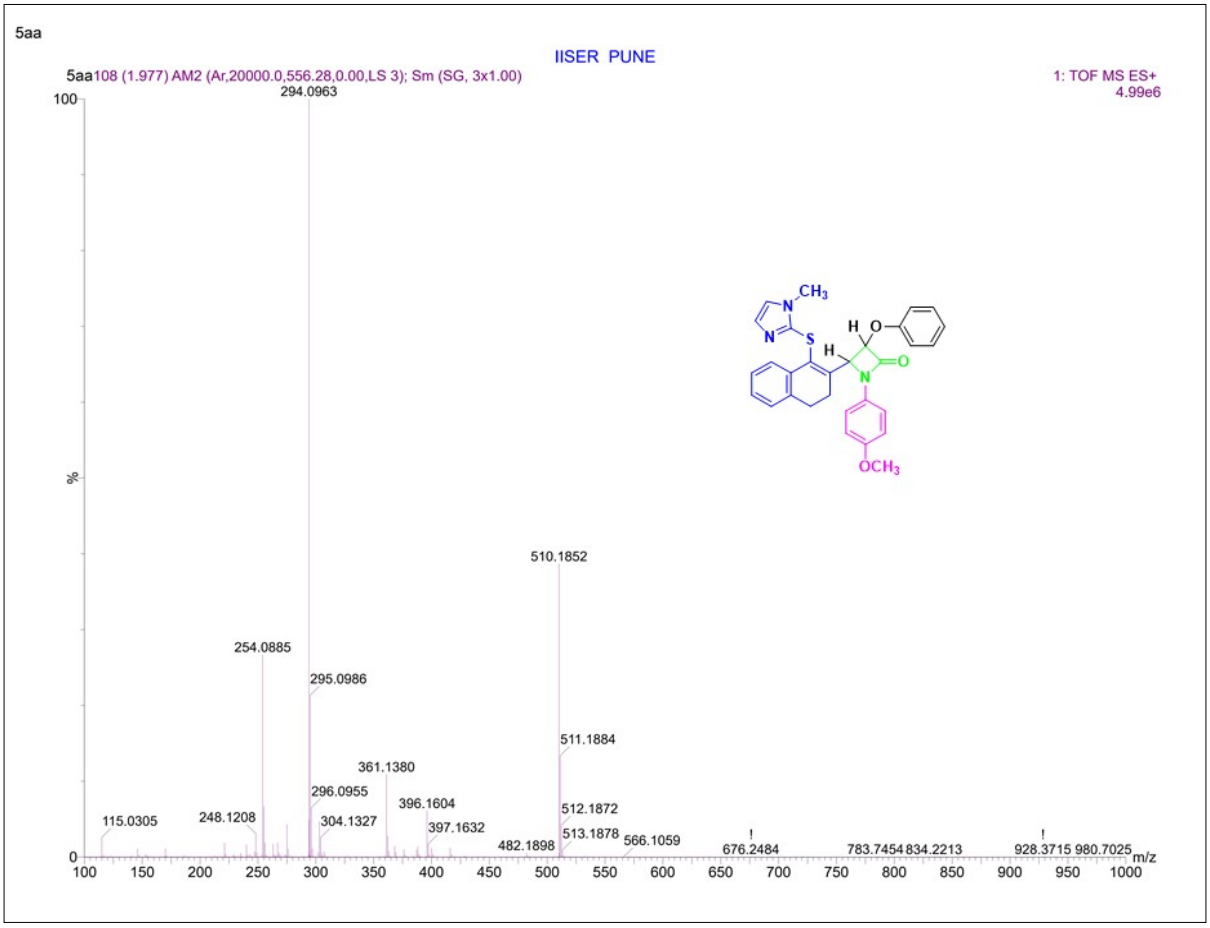
3. The copy of IR, ^{1}H NMR spectra, ^{13}C NMR spectra, and HRMS data of compounds (5aa-5ai) and (5ba-5bi)

FT-IR, ^{1}H NMR spectra, ^{13}C NMR spectra, and HRMS data of compound (5aa)

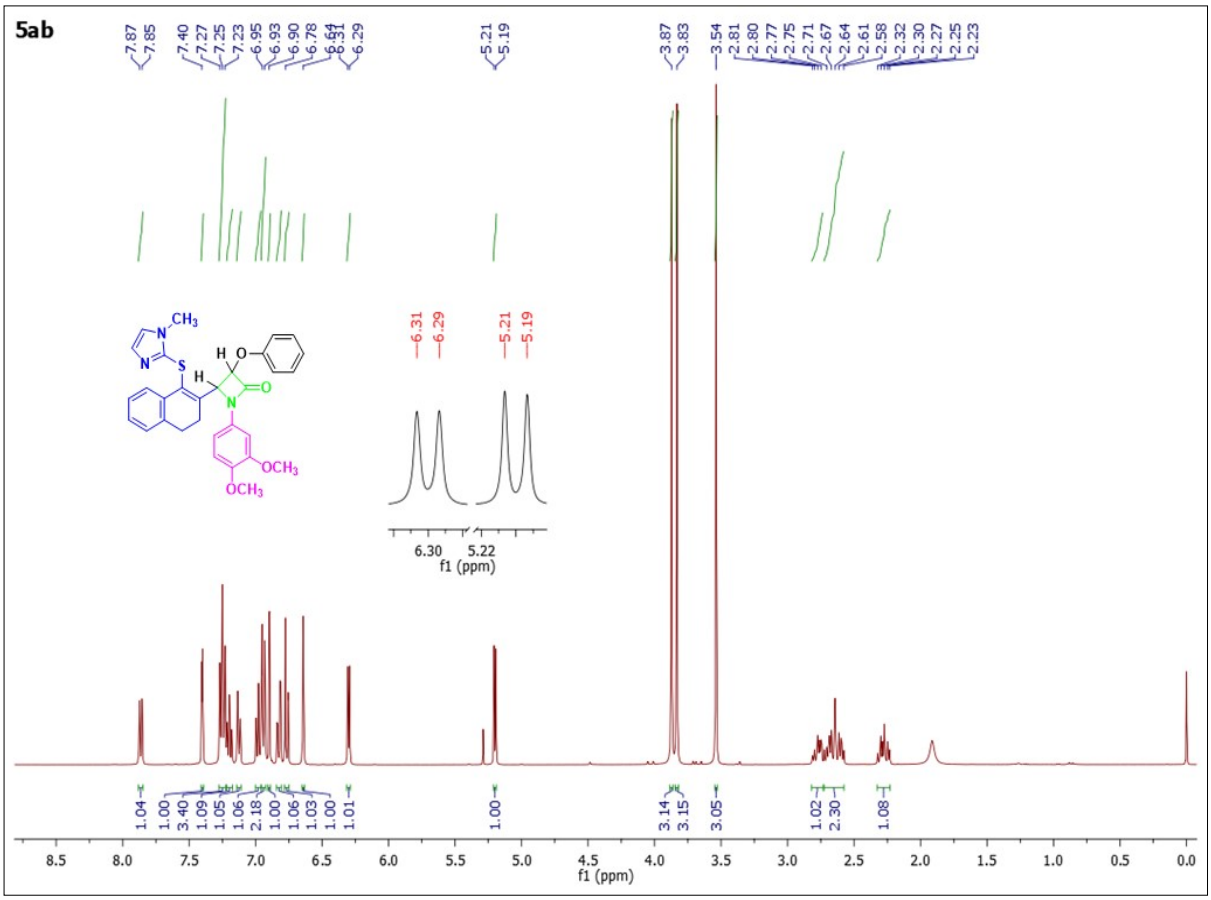


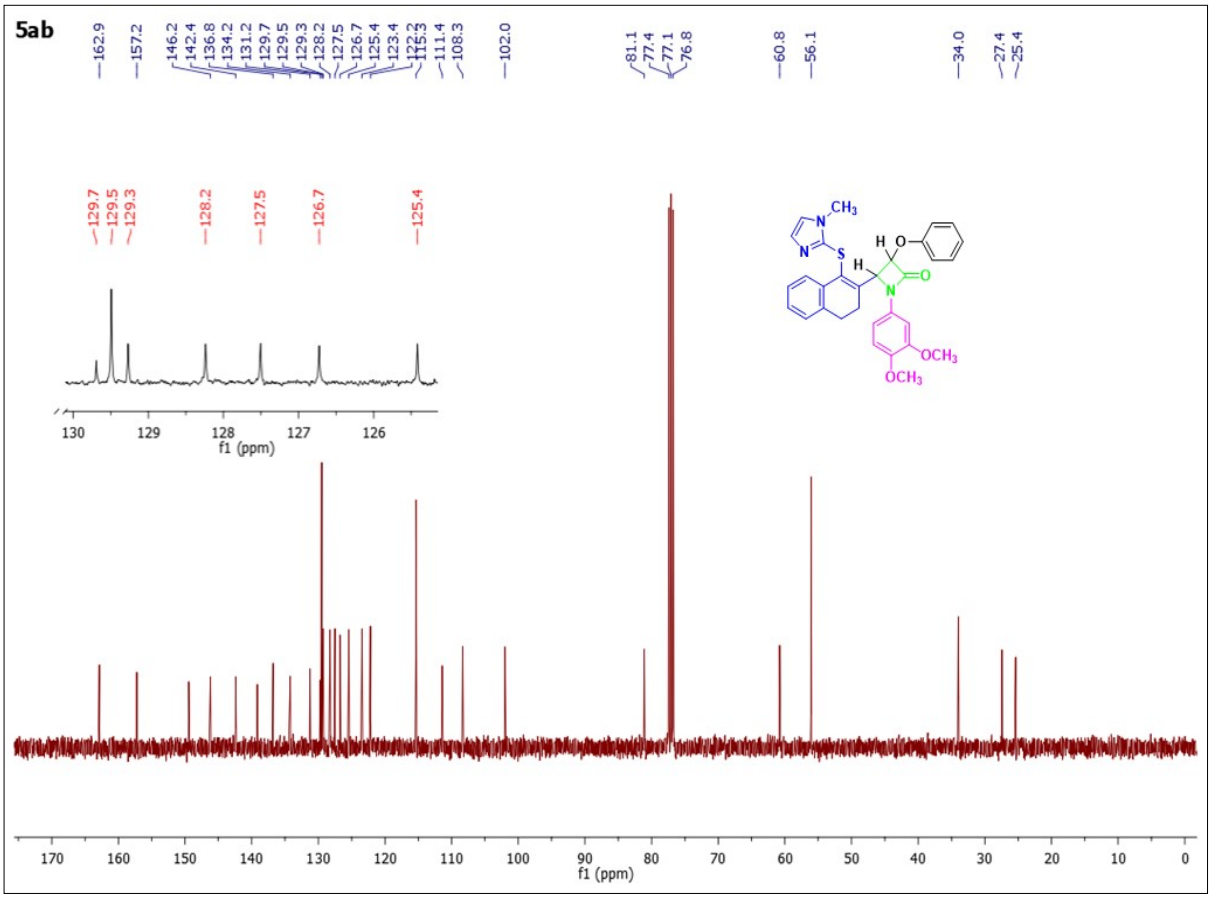


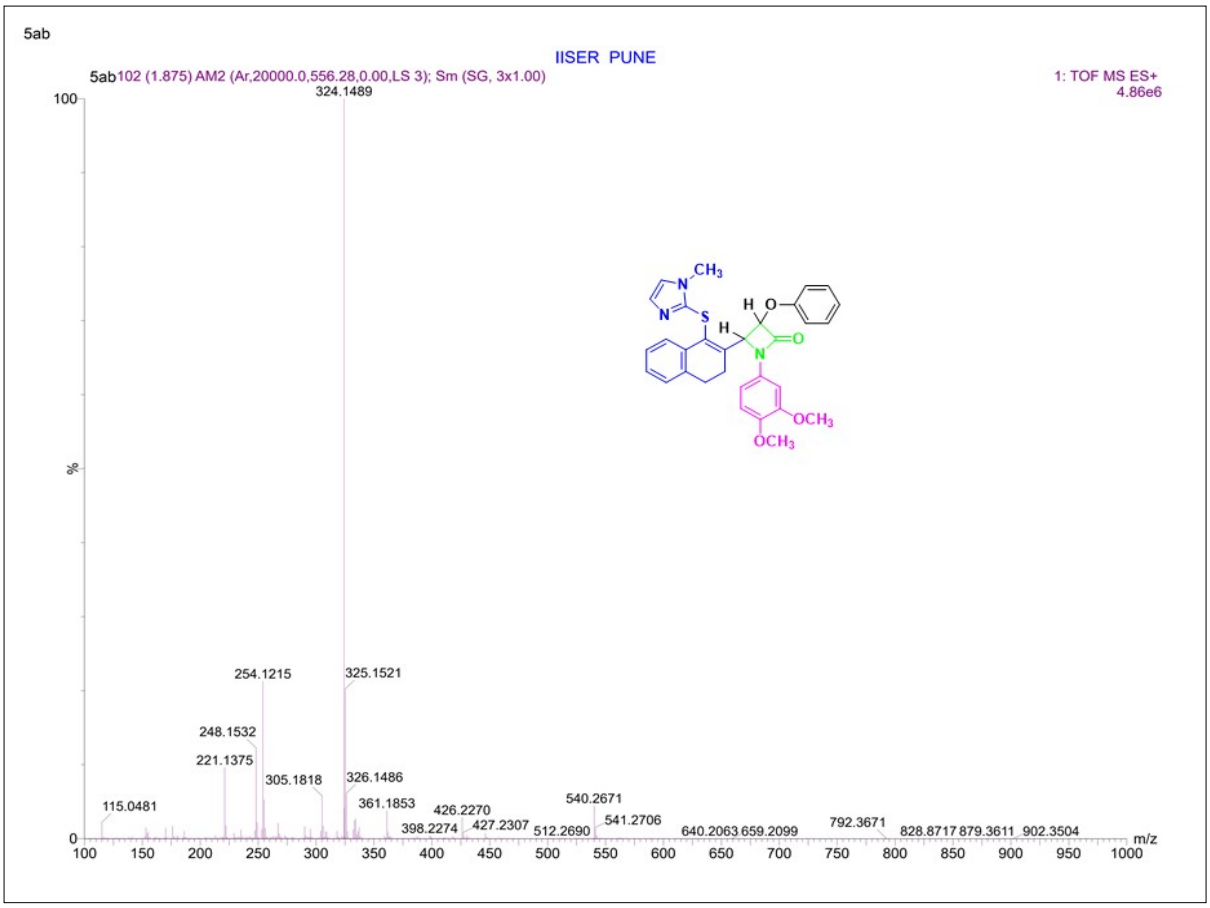

5aa
162.7
157.3
156.6
142.5
139.2
136.8
134.3
131.0
129.6
129.5
129.2
128.2
127.5
126.7
125.5
123.4
122.1
118.5
115.3
114.5
81.1
77.4
77.1
76.7
60.6
55.5
34.0
27.4
25.3
131.0
129.6
129.5
129.2
128.2
127.5
126.7
125.5
131 130 129 128 127 126
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


5aa
IISER PUNE
5aa108 (1.977) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00)
1: TOF MS ES+
4.99e6
294.0963
510.1852
254.0885
295.0986
511.1884
361.1380
296.0955
396.1604
512.1872
115.0305
248.1208
304.1327
397.1632
513.1878
482.1898
566.1059
676.2484
783.7454 834.2213
928.3715 980.7025
m/z
%
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000

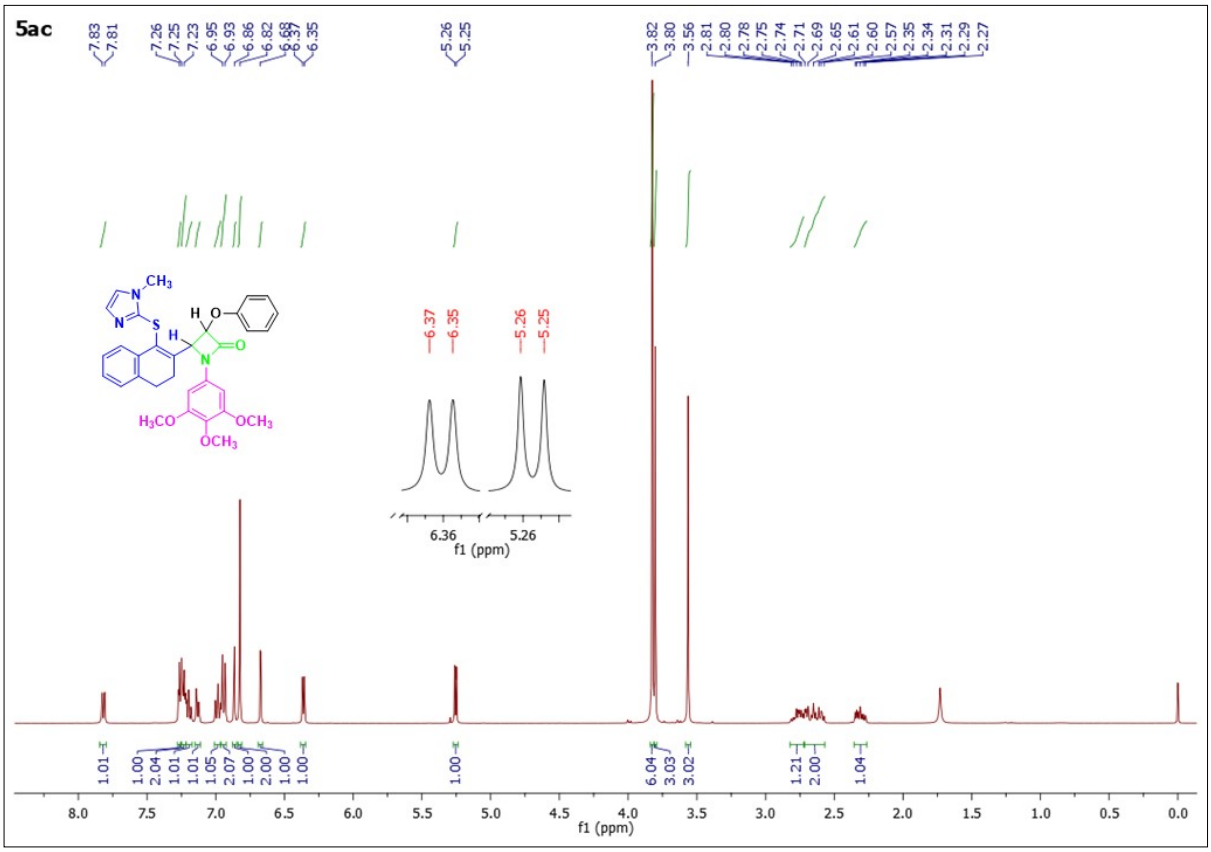
^{1}H NMR spectra, ^{13}C NMR spectra, and HRMS data of compound (5ab)

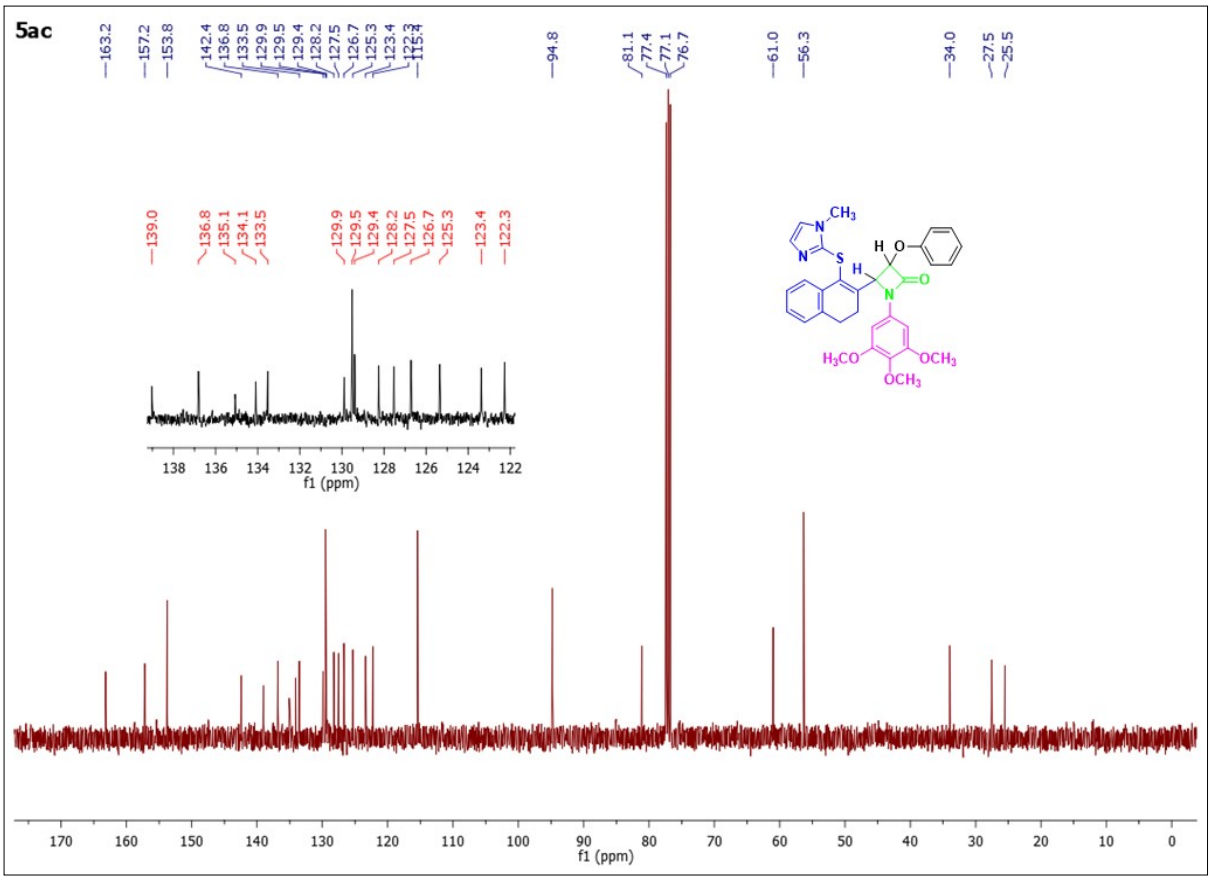


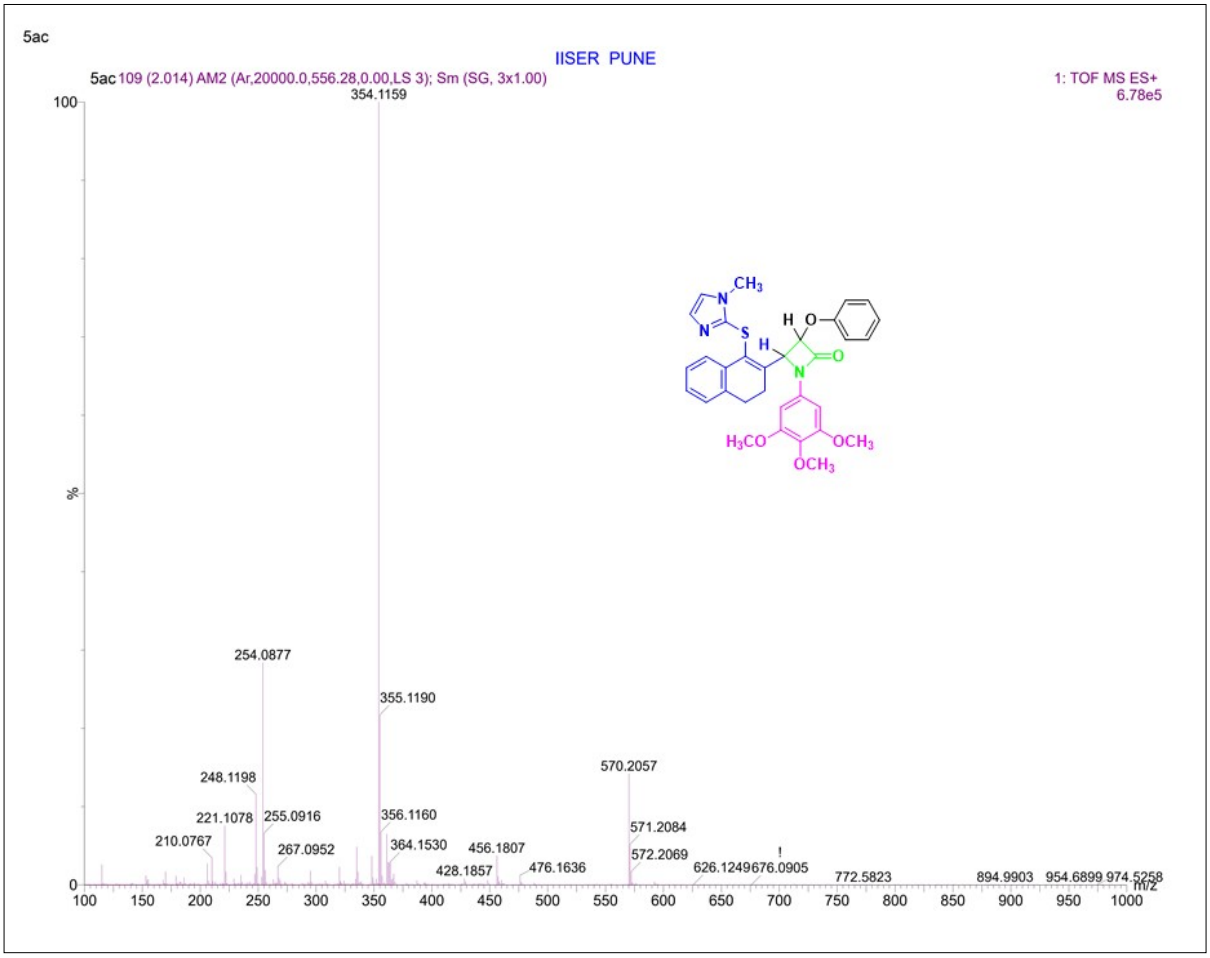




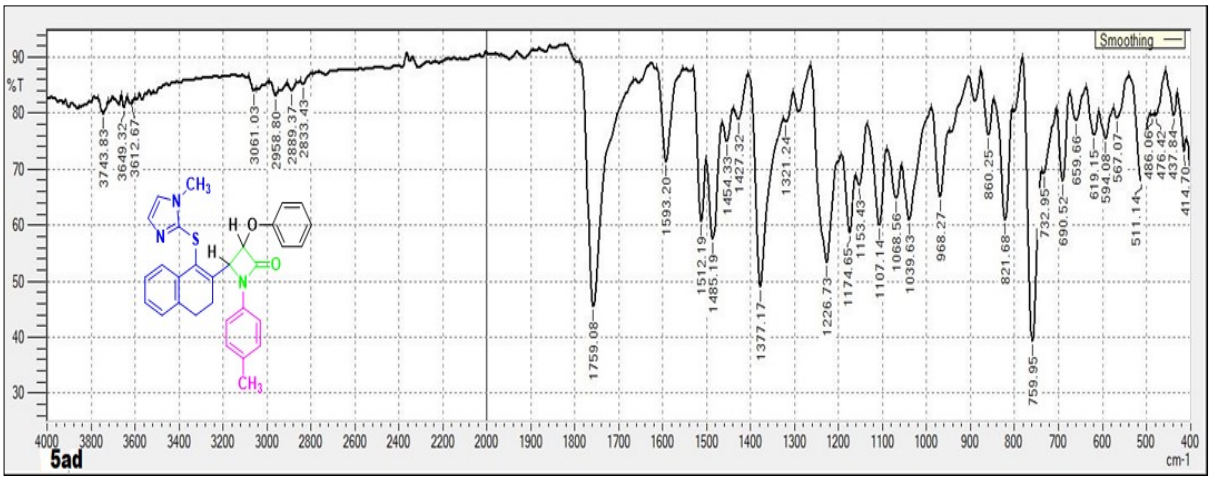
^{1}H NMR spectra, ^{13}C NMR spectra, and HRMS data of compound (5ac)

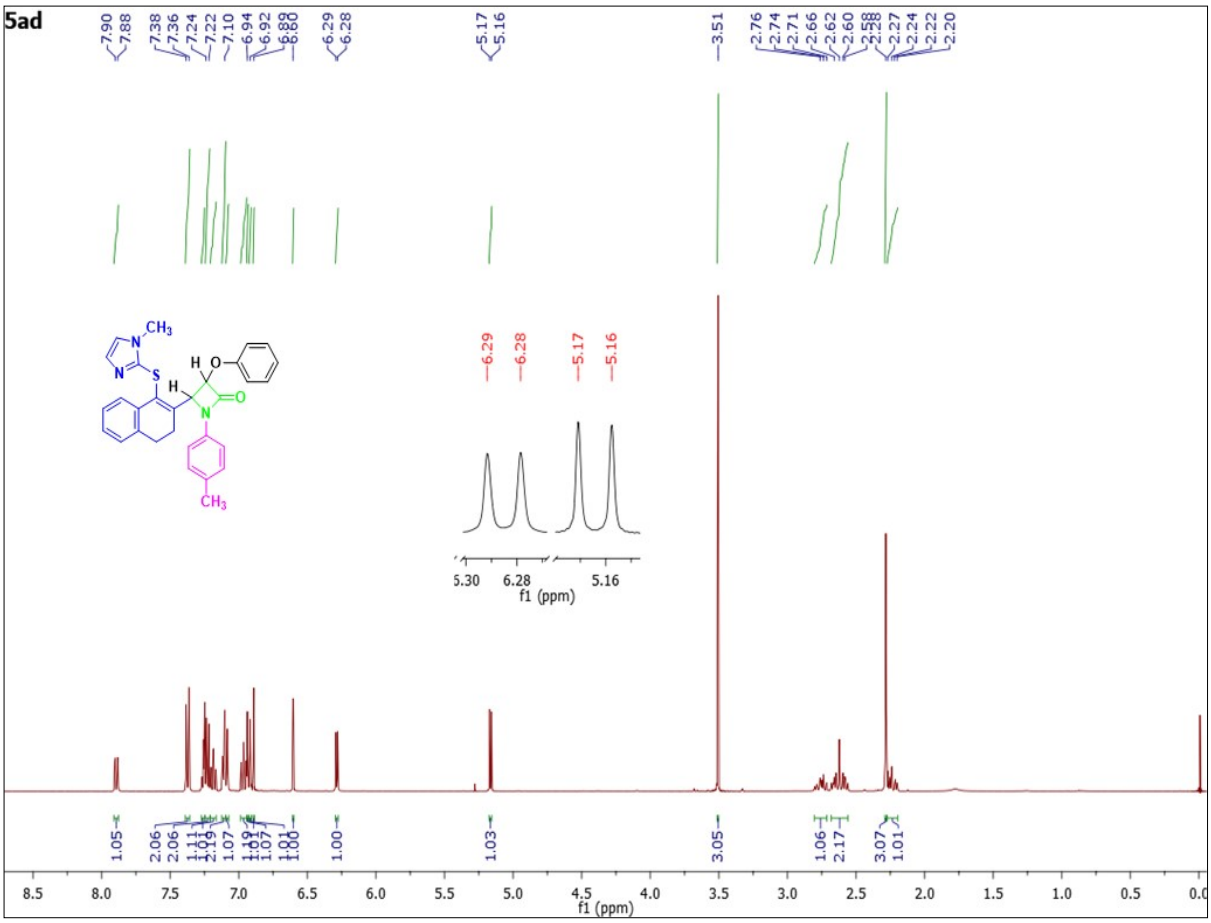


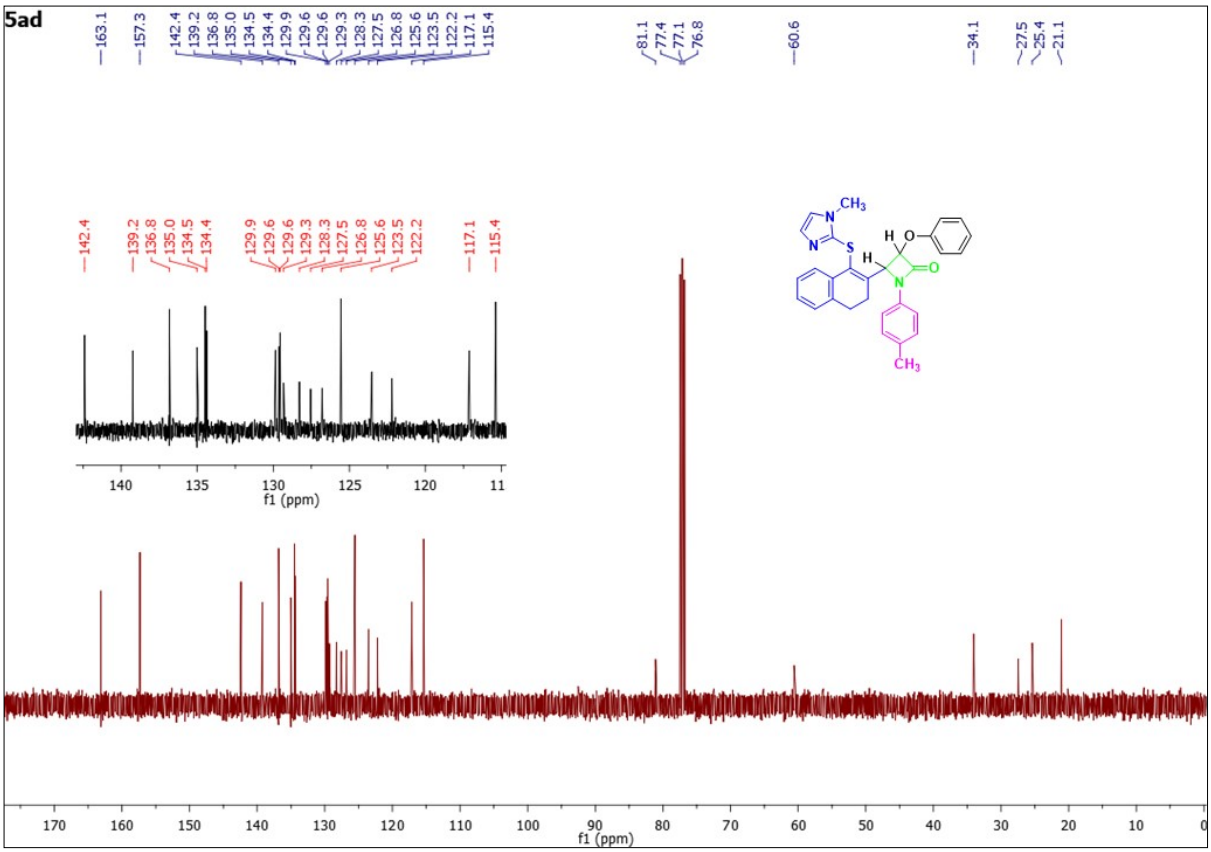

5ac
163.2
157.2
153.8
142.4
136.8
133.5
129.9
129.5
129.4
128.2
127.5
126.7
125.3
123.4
122.3
94.8
81.1
77.4
77.1
76.7
61.0
56.3
34.0
27.5
25.5
139.0
136.8
135.1
134.1
133.5
129.9
129.5
129.4
128.2
127.5
126.7
125.3
123.4
122.3
f1 (ppm)
f1 (ppm)

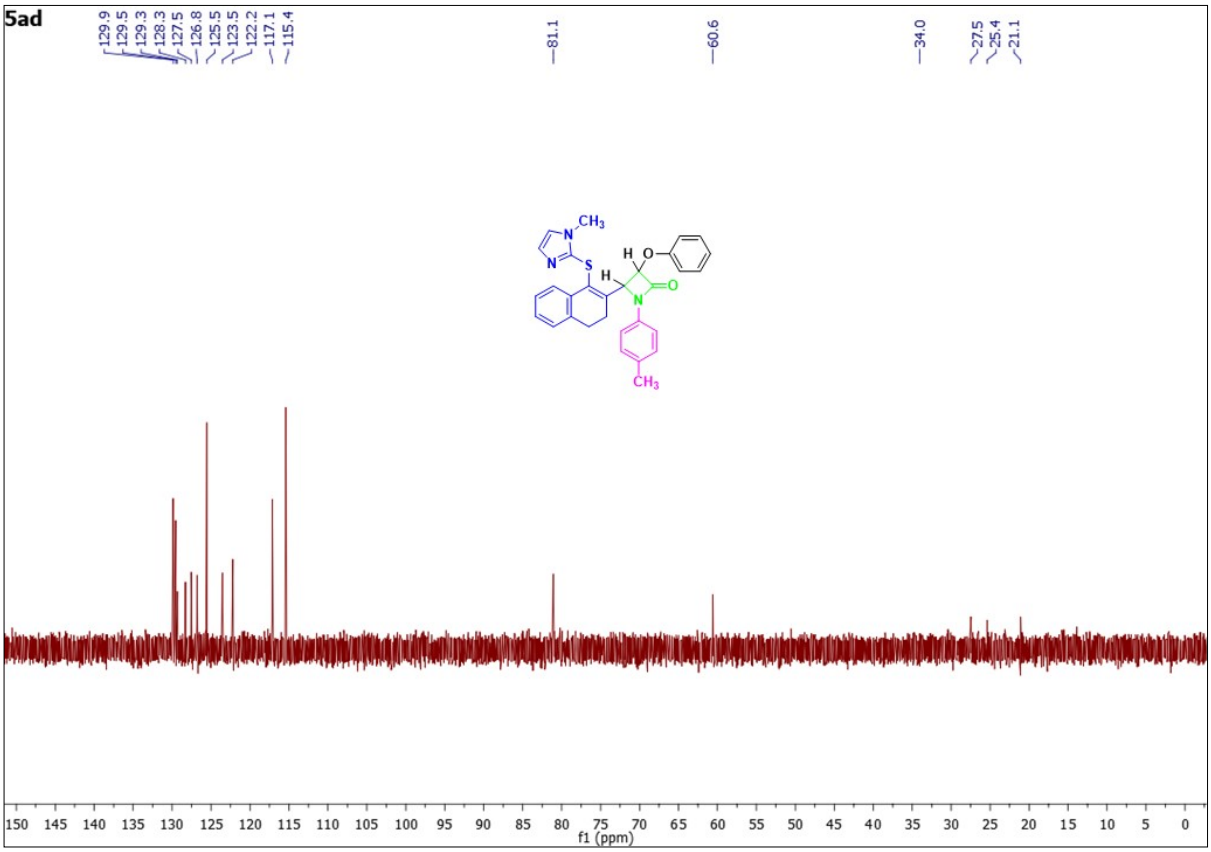

5ac
IISER PUNE
5ac 109 (2.014) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00)
1: TOF MS ES+
6.78e5
354.1159
254.0877
355.1190
248.1198
570.2057
221.1078
255.0916
356.1160
571.2084
210.0767
267.0952
364.1530
456.1807
572.2069
428.1857
476.1636
626.1249676.0905
772.5823
894.9903
954.6899
974.5258
%
m/z

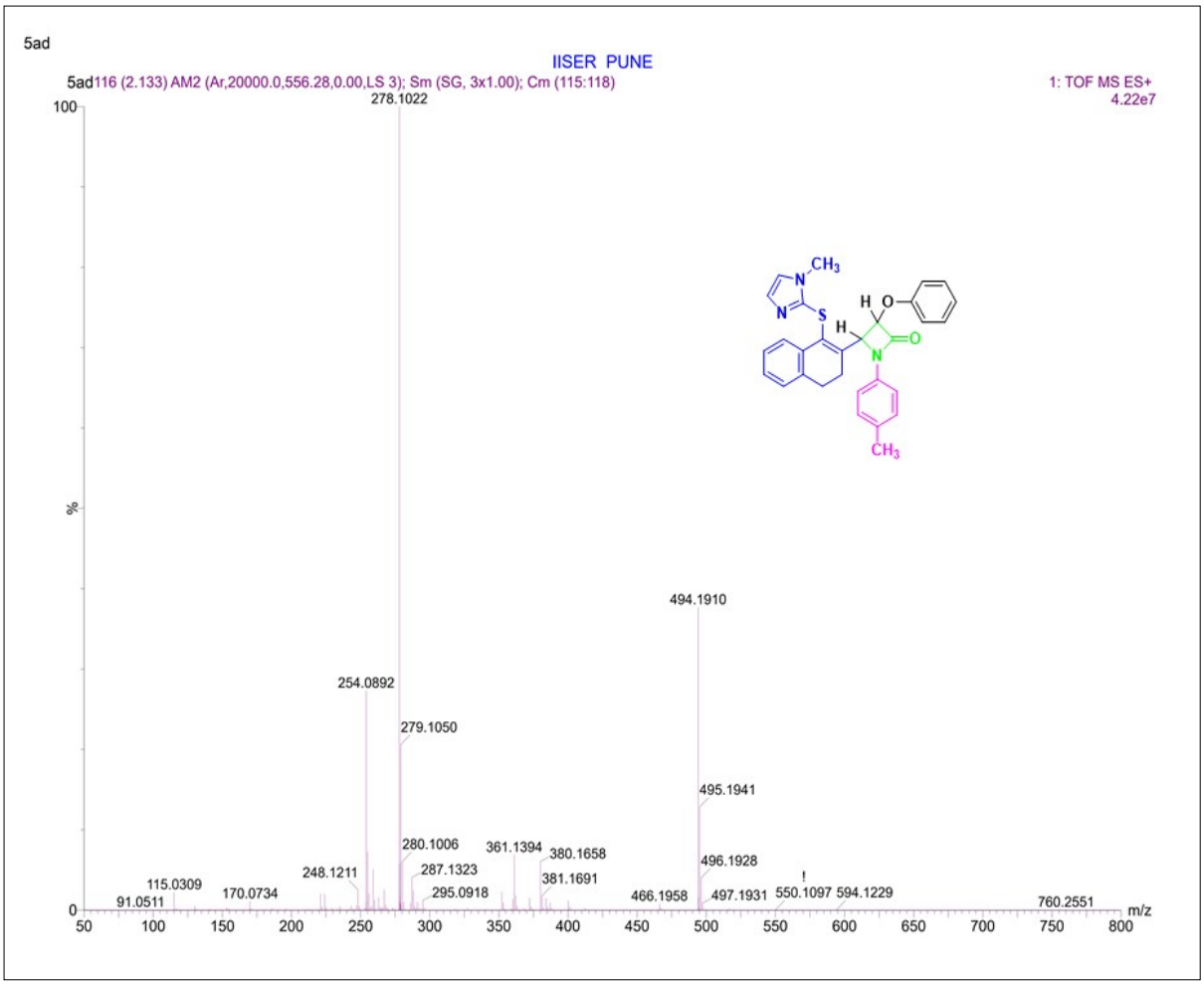
FT-IR, ^{1}H NMR spectra, ^{13}C NMR spectra, DEPT-135 spectra, and HRMS data of compound (5ad)



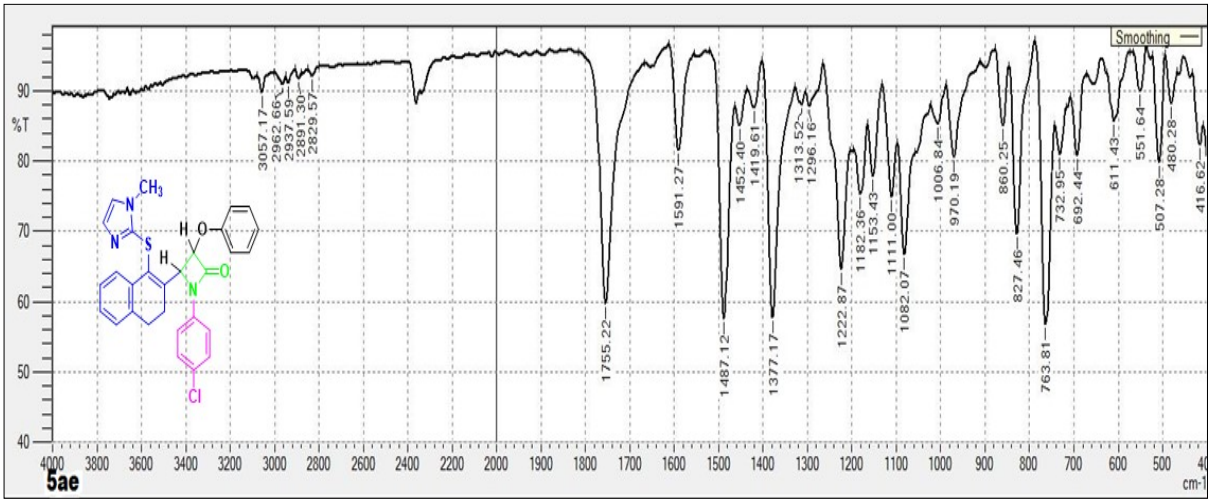


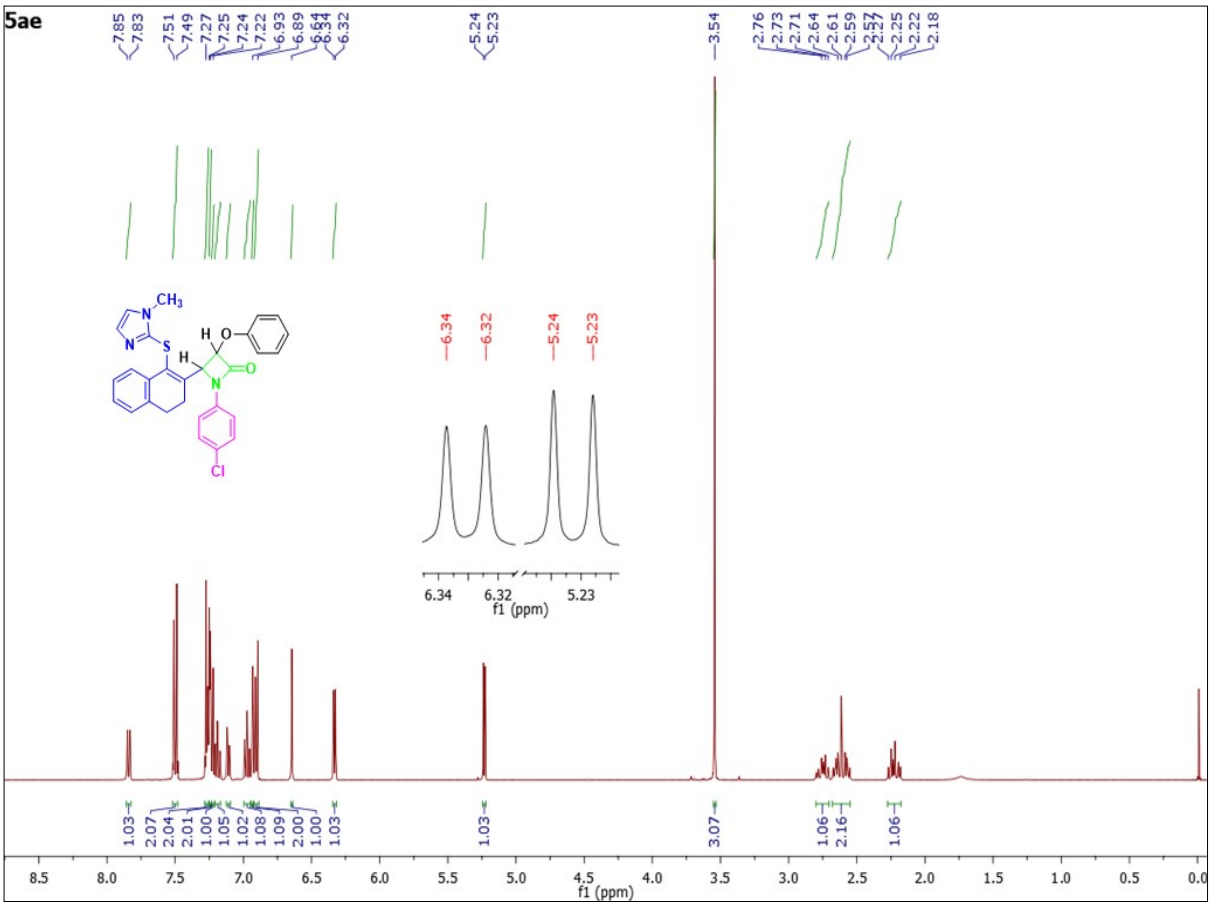

5ad
163.1
157.3
142.4
139.2
136.8
135.0
134.5
134.4
129.9
129.6
129.6
129.3
128.3
127.5
126.8
125.6
123.5
122.2
117.1
115.4
81.1
77.4
77.1
76.8
60.6
34.1
27.5
25.4
21.1
f1 (ppm)

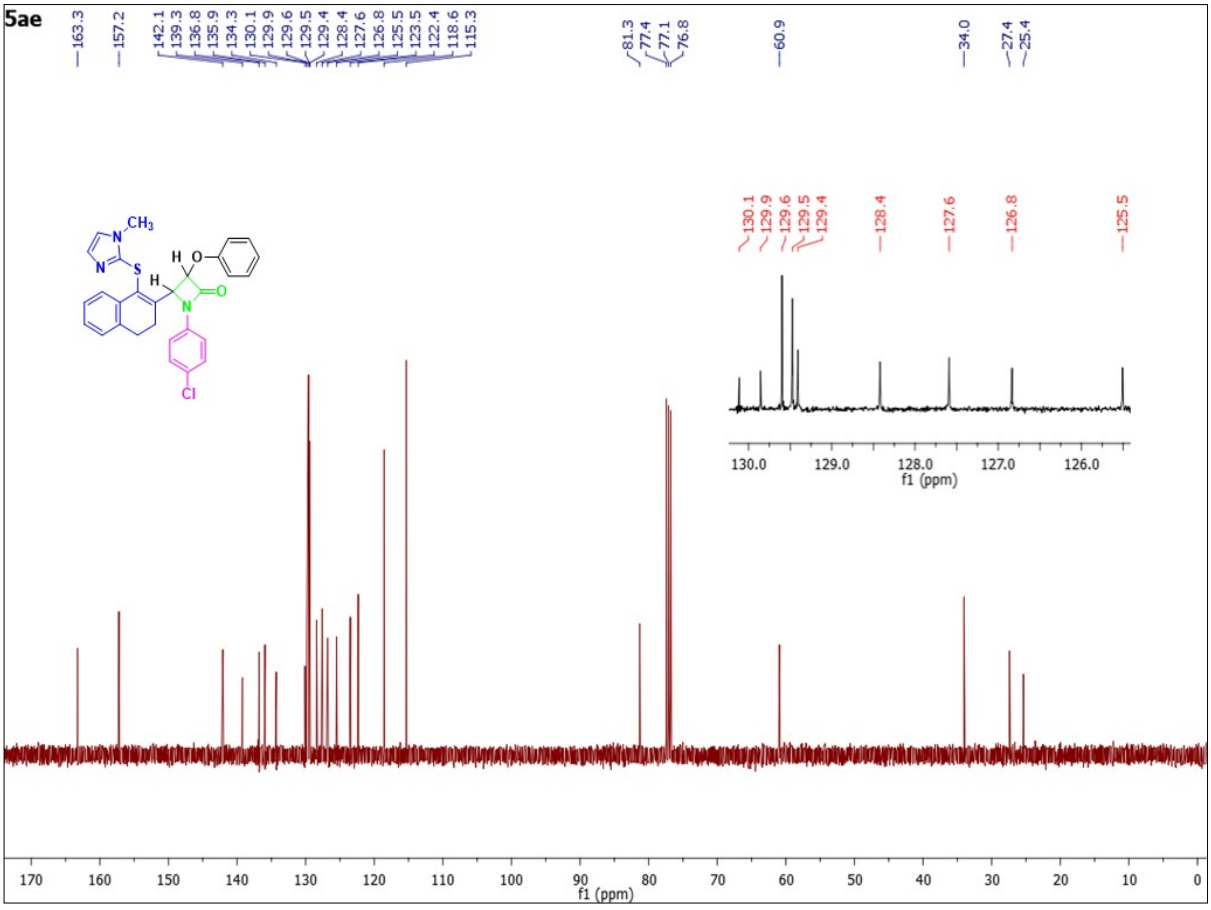

5ad
129.9
129.5
129.3
128.3
127.5
126.8
125.5
123.5
122.2
117.1
115.4
81.1
60.6
34.0
27.5
25.4
21.1
f1 (ppm)

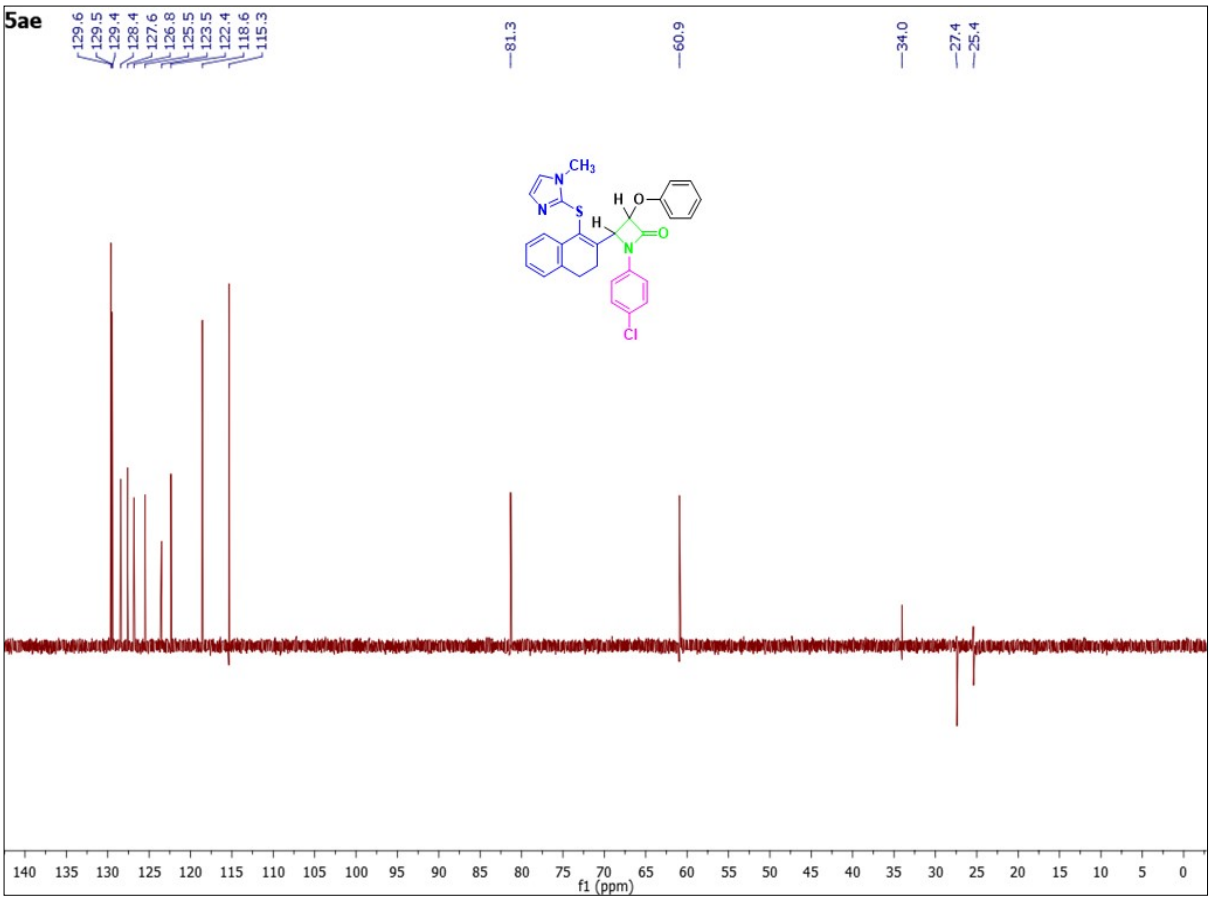


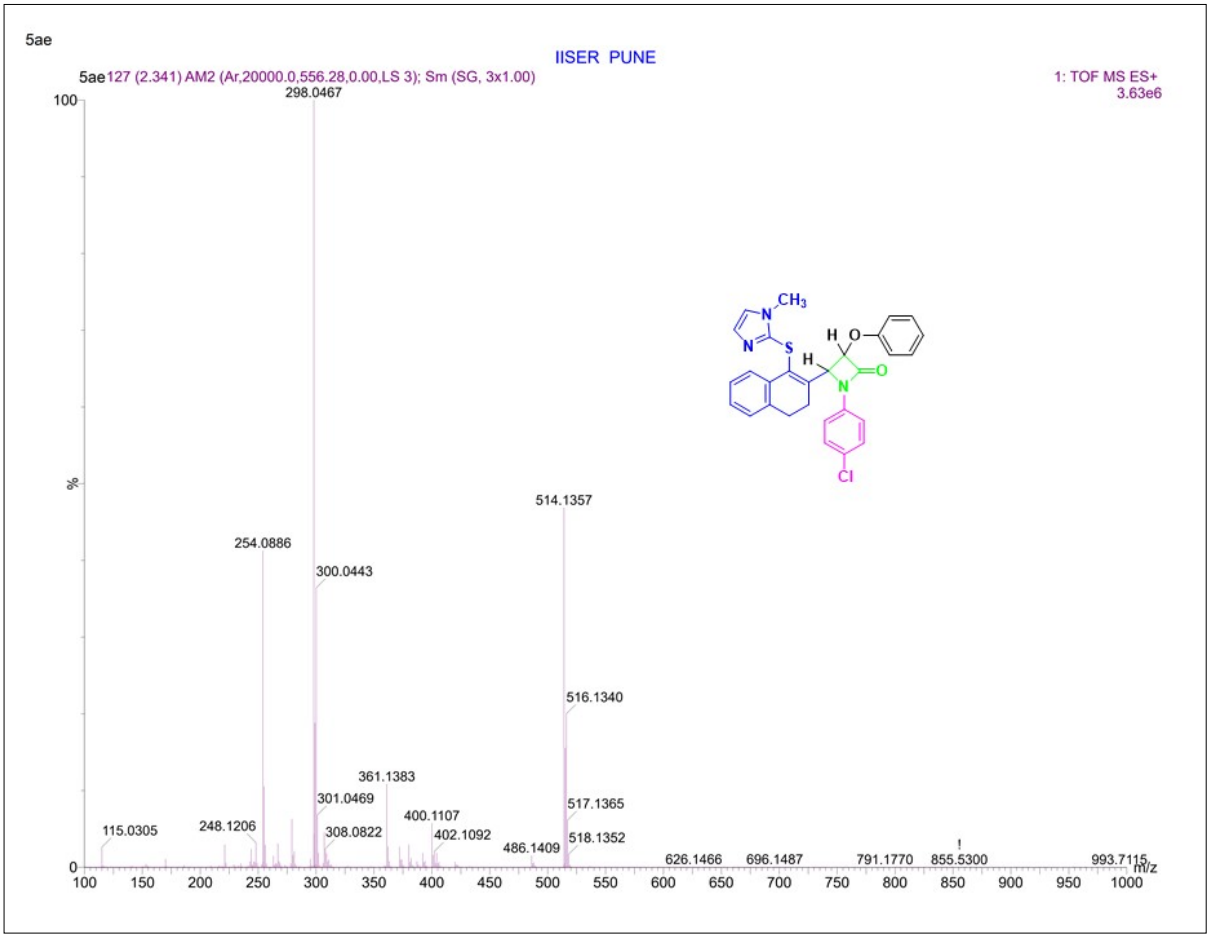
FT-IR, ^{1}H NMR spectra, ^{13}C NMR spectra, DEPT-135 spectra, and HRMS data of compound (5ae)



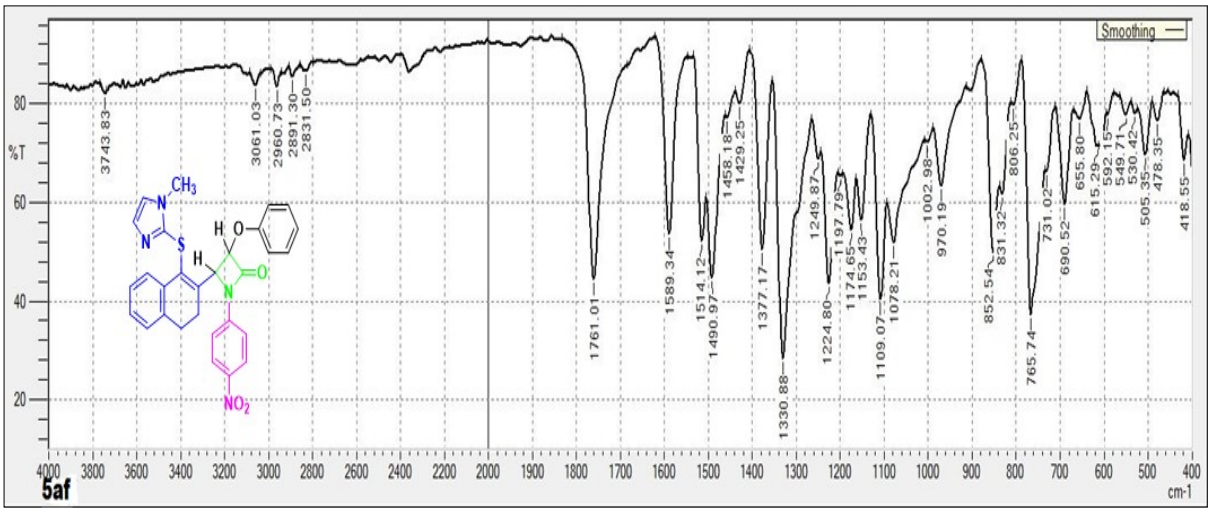

5ae
7.85
7.83
7.51
7.49
7.27
7.25
7.24
7.22
6.93
6.89
6.34
6.32
5.24
5.23
3.54
2.76
2.73
2.71
2.64
2.61
2.59
2.57
2.25
2.22
2.18
6.34
6.32
5.24
5.23
6.34
6.32
5.23
f1 (ppm)
1.03
2.07
2.04
2.01
1.00
1.05
1.02
1.08
1.09
2.00
1.00
1.03
1.03
3.07
1.06
2.16
1.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

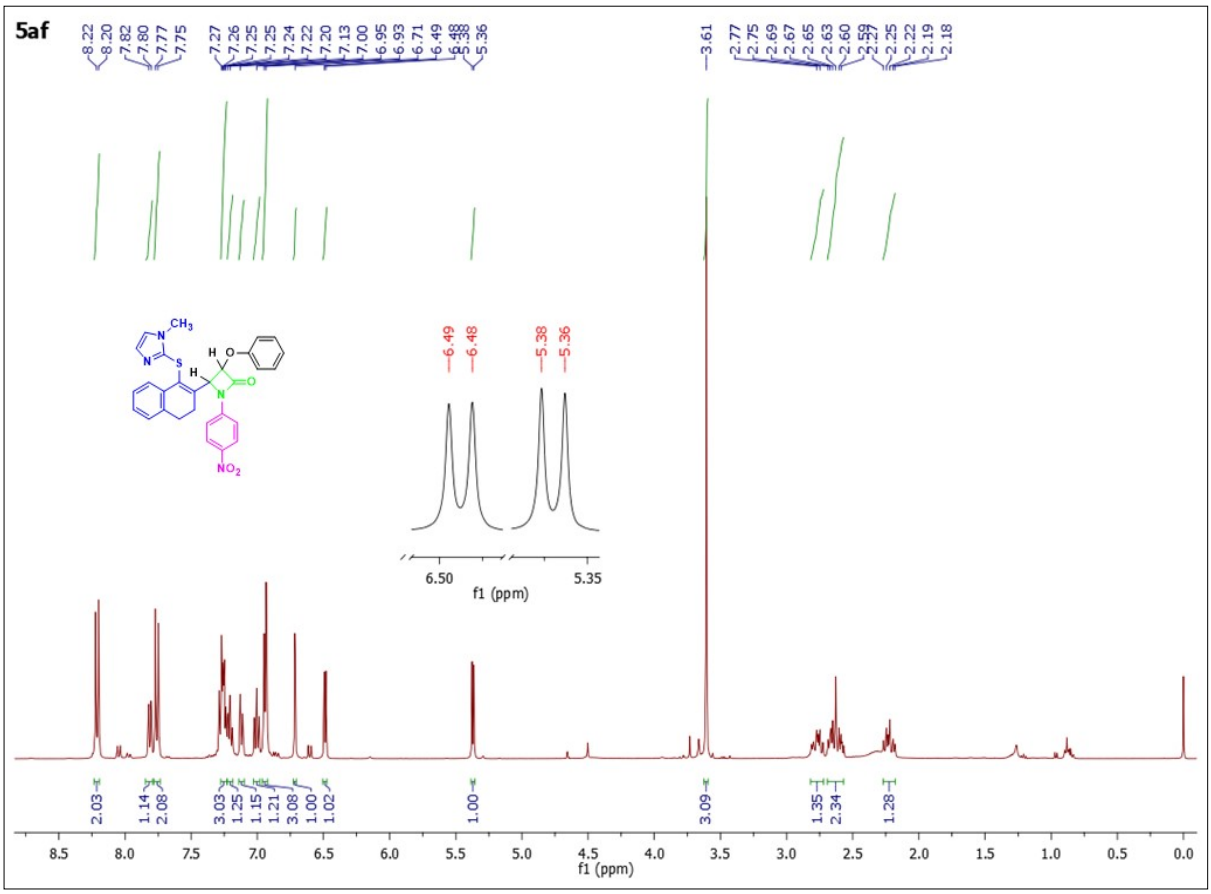

5ae
163.3
157.2
142.1
139.3
136.8
135.9
134.3
130.1
129.9
129.6
129.5
129.4
128.4
127.6
126.8
125.5
123.5
122.4
118.6
115.3
81.3
77.4
77.1
76.8
60.9
34.0
27.4
25.4
130.1
129.9
129.6
129.5
129.4
128.4
127.6
126.8
125.5
130.0
129.0
128.0
127.0
126.0
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

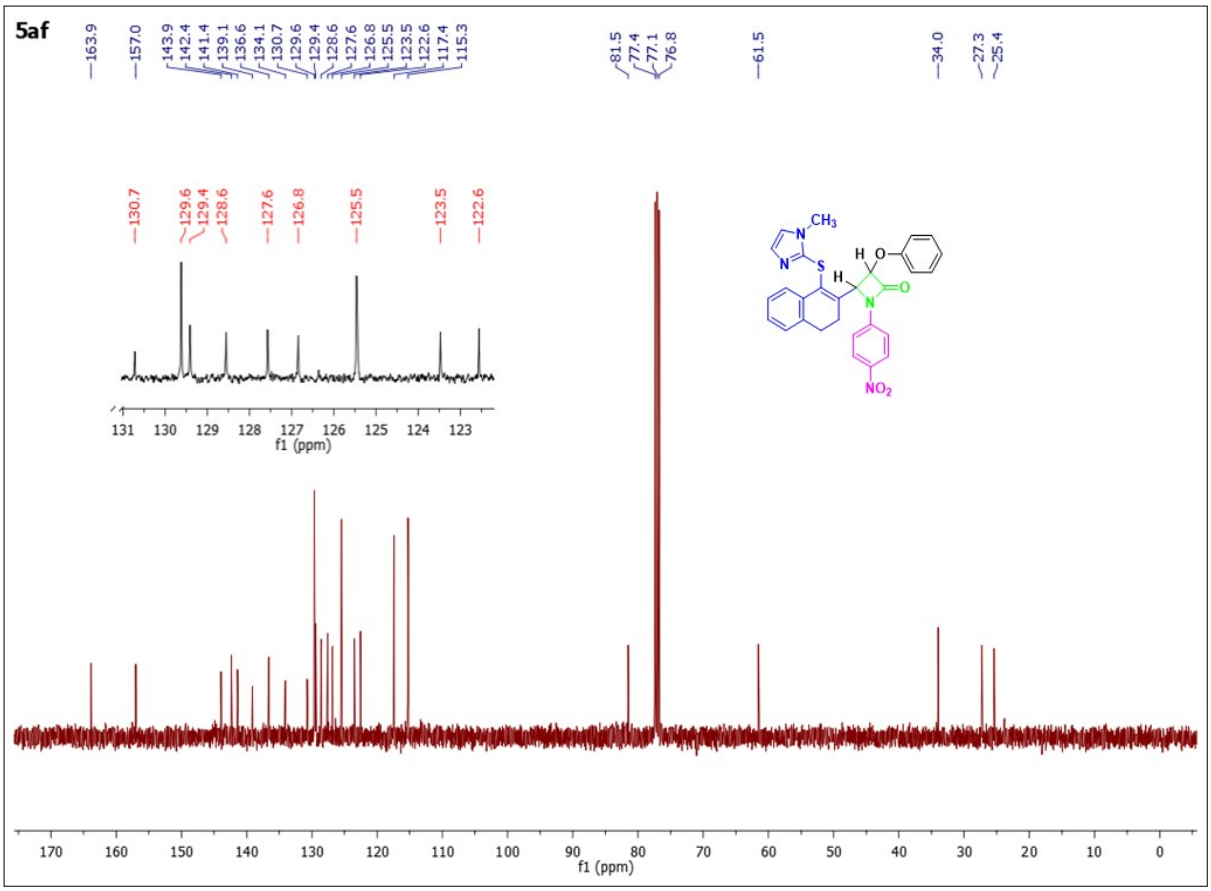

5ae
129.6
129.5
129.4
128.4
127.6
126.8
125.5
123.5
122.4
118.6
115.3
81.3
60.9
34.0
27.4
25.4
f1 (ppm)

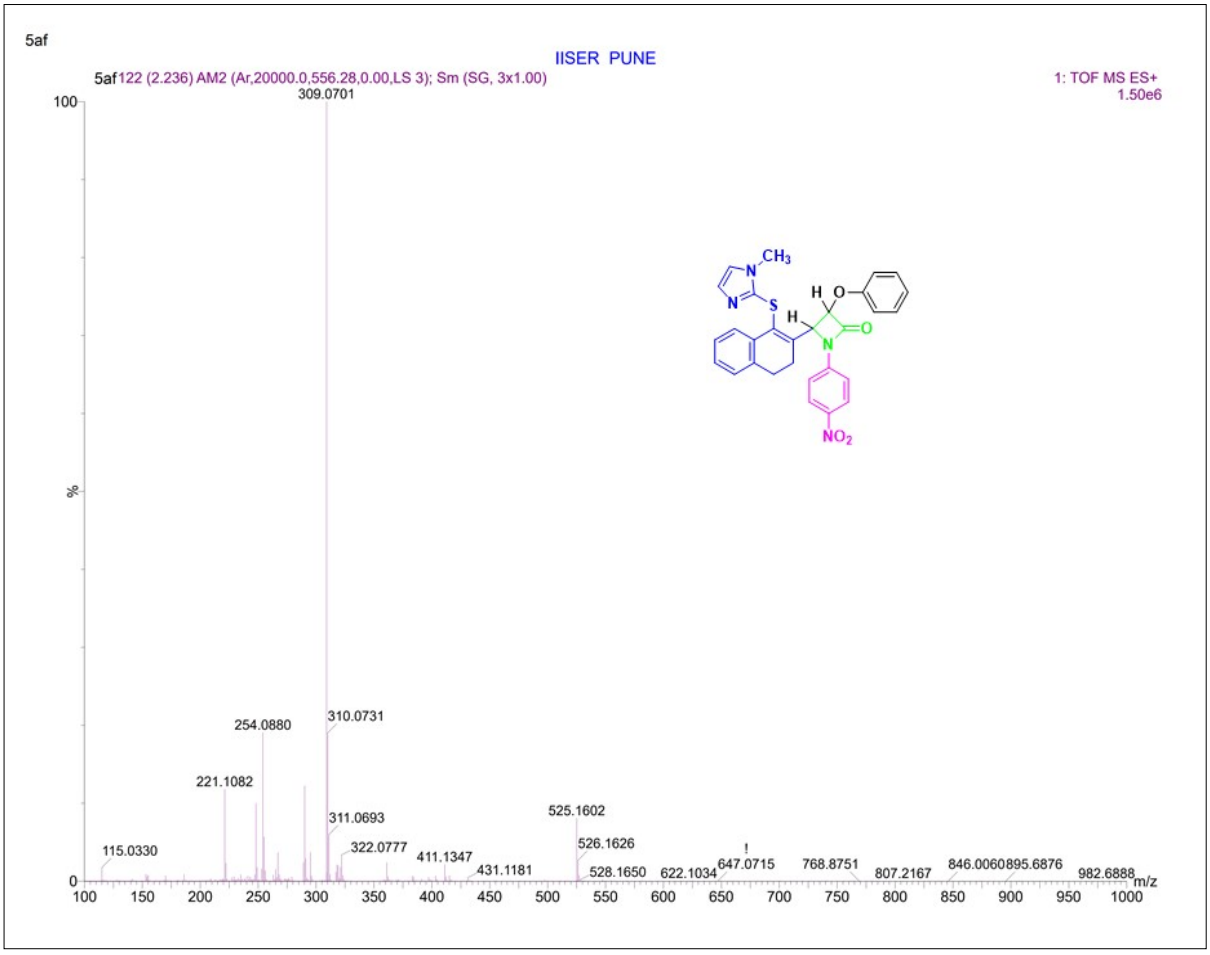

5ae
IISER PUNE
5ae127 (2.341) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00)
1: TOF MS ES+
3.63e6
298.0467
514.1357
254.0886
300.0443
516.1340
361.1383
301.0469
517.1365
400.1107
115.0305
248.1206
308.0822
402.1092
518.1352
486.1409
626.1466
696.1487
791.1770
855.5300
993.7115
%
m/z

FT-IR, ^{1}H NMR spectra, ^{13}C NMR spectra, and HRMS data of compound (5af)

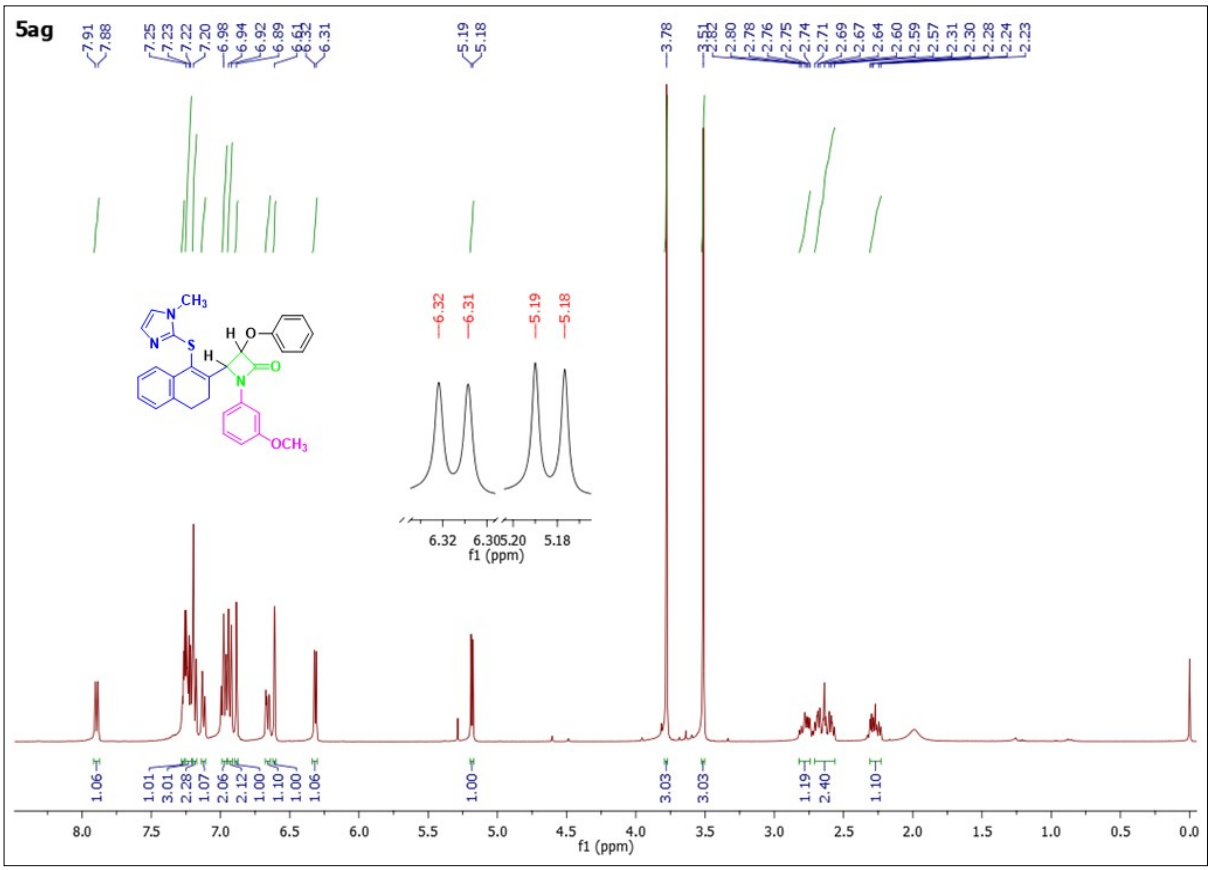


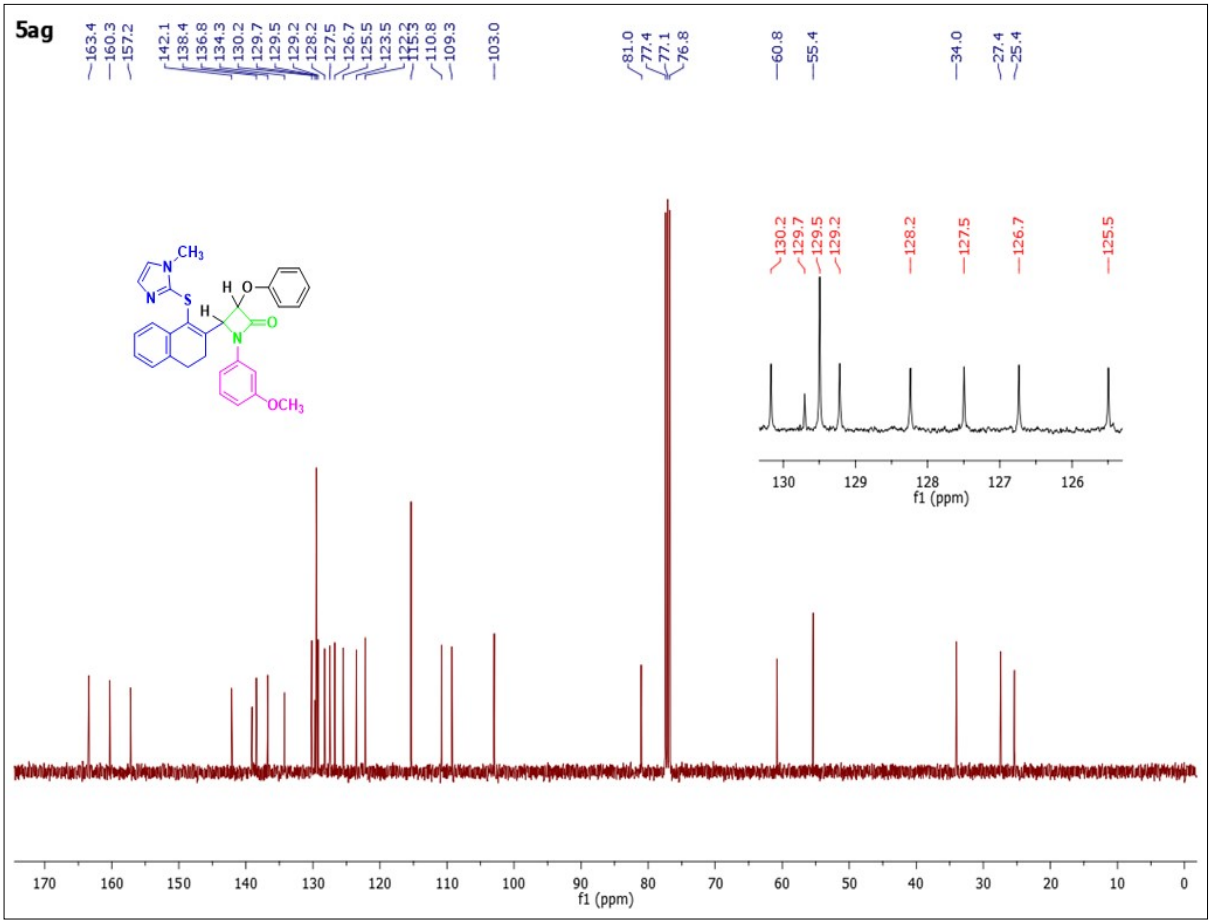


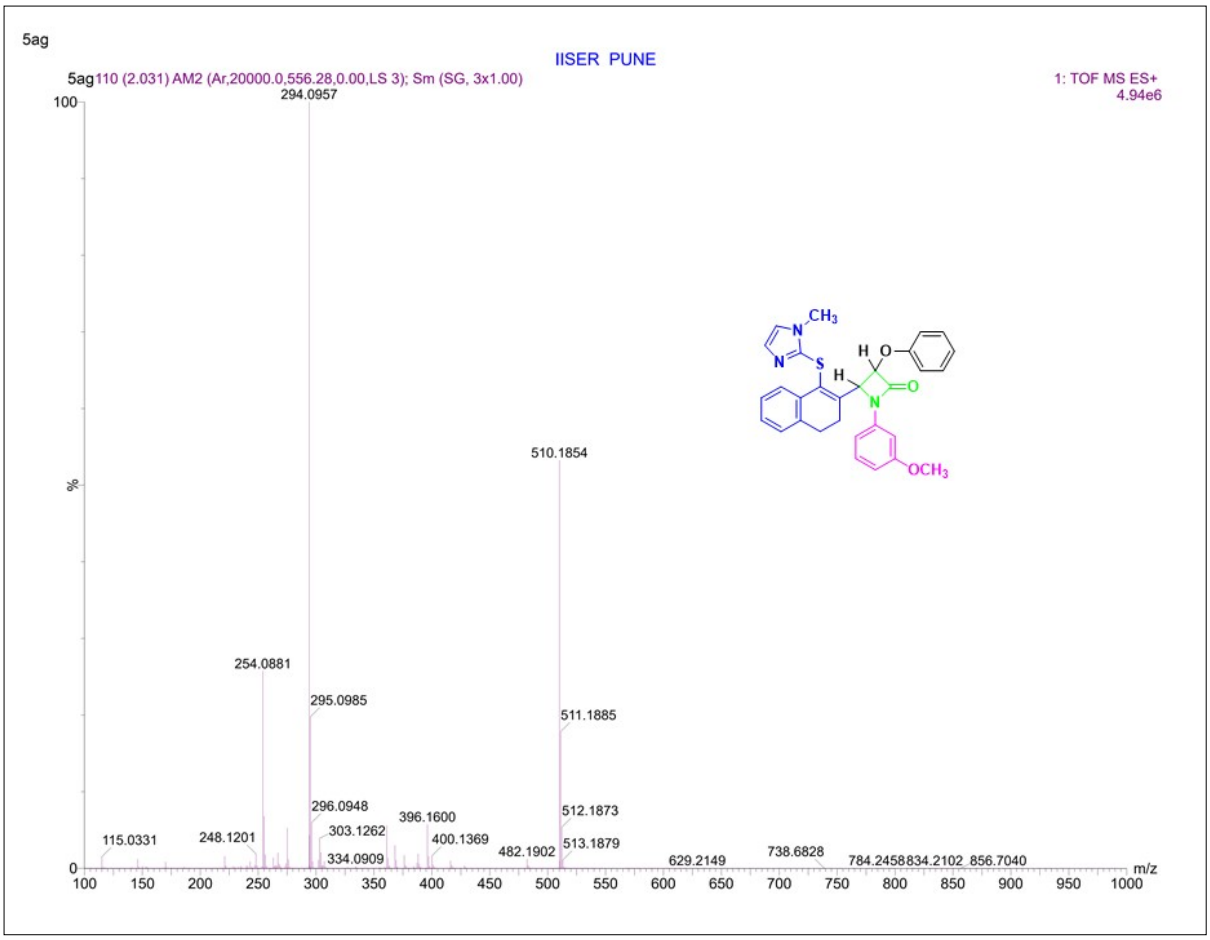

5af
163.9
157.0
143.9
142.4
141.4
139.1
136.6
134.1
130.7
129.6
129.4
128.6
127.6
126.8
125.5
123.5
122.6
117.4
115.3
81.5
77.4
77.1
76.8
61.5
34.0
27.3
25.4
f1 (ppm)


5af
IISER PUNE
5af122 (2.236) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00)
1: TOF MS ES+
1.50e6
309.0701
310.0731
254.0880
221.1082
311.0693
322.0777
115.0330
411.1347
431.1181
525.1602
526.1626
528.1650
622.1034
647.0715
768.8751
807.2167
846.0060895.6876
982.6888
m/z

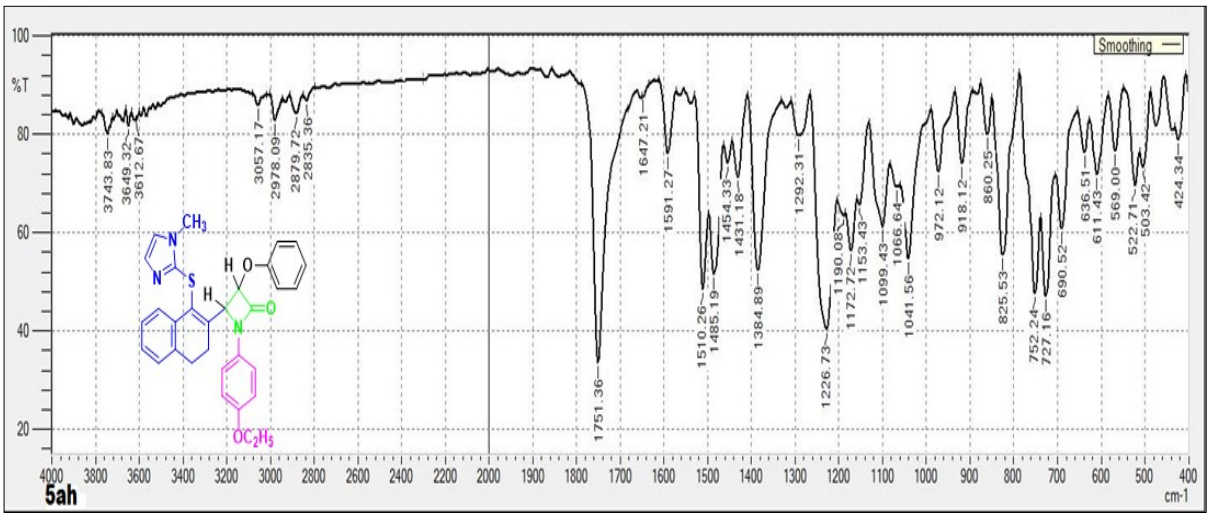
^{1}H NMR spectra, ^{13}C NMR spectra, and HRMS data of compound (5ag)

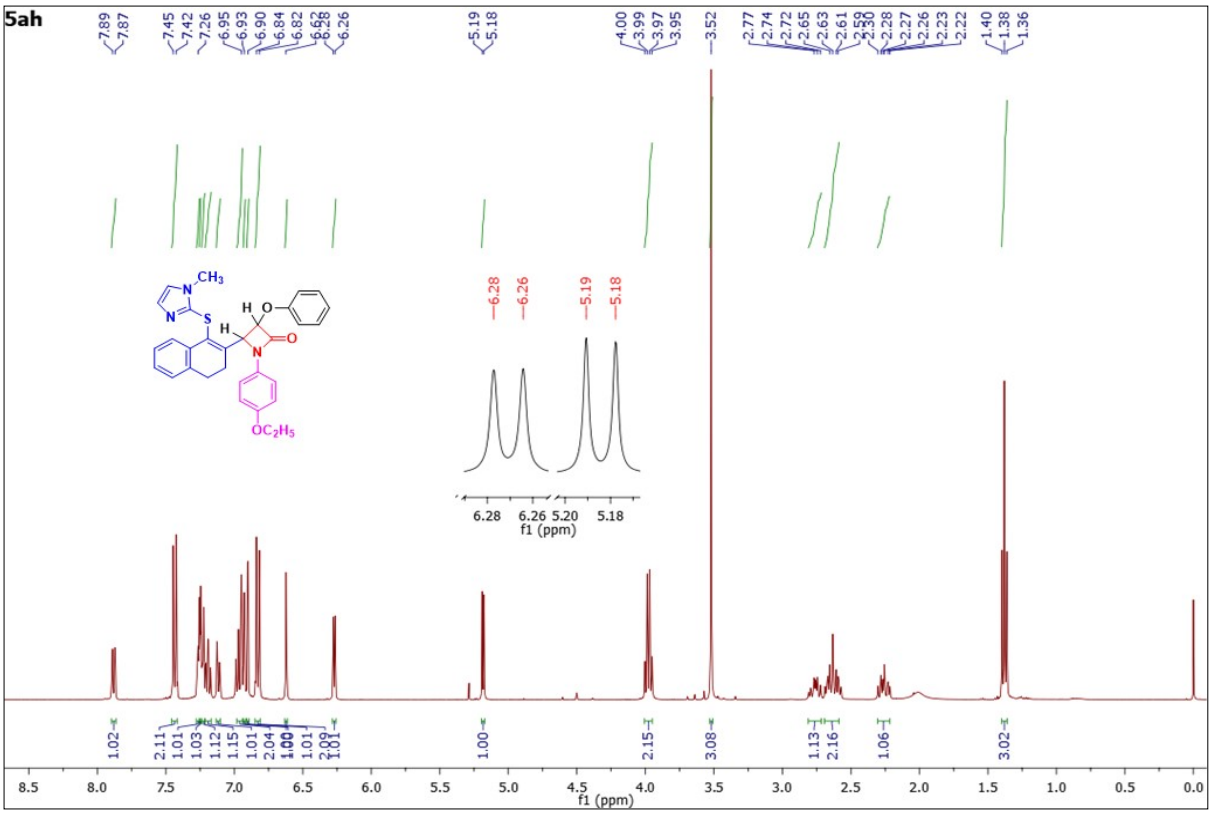


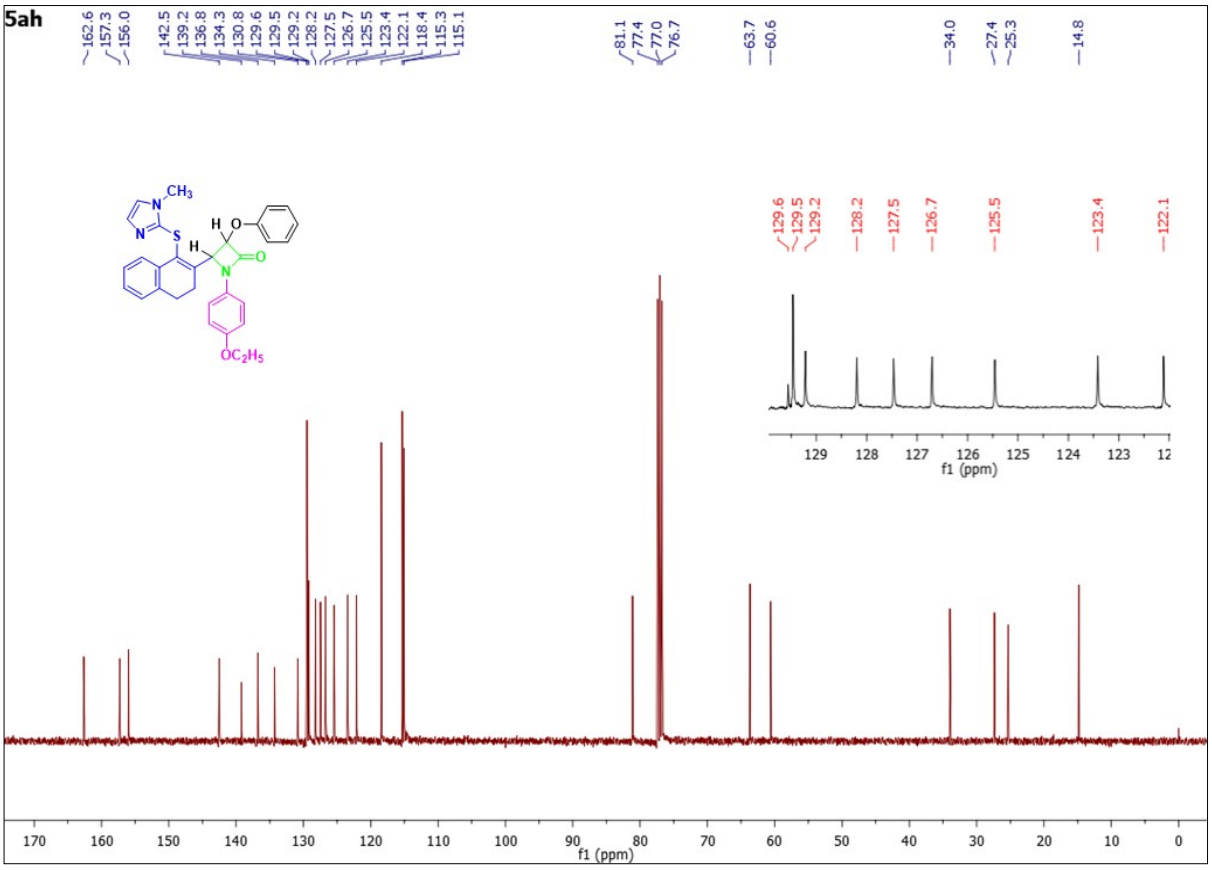


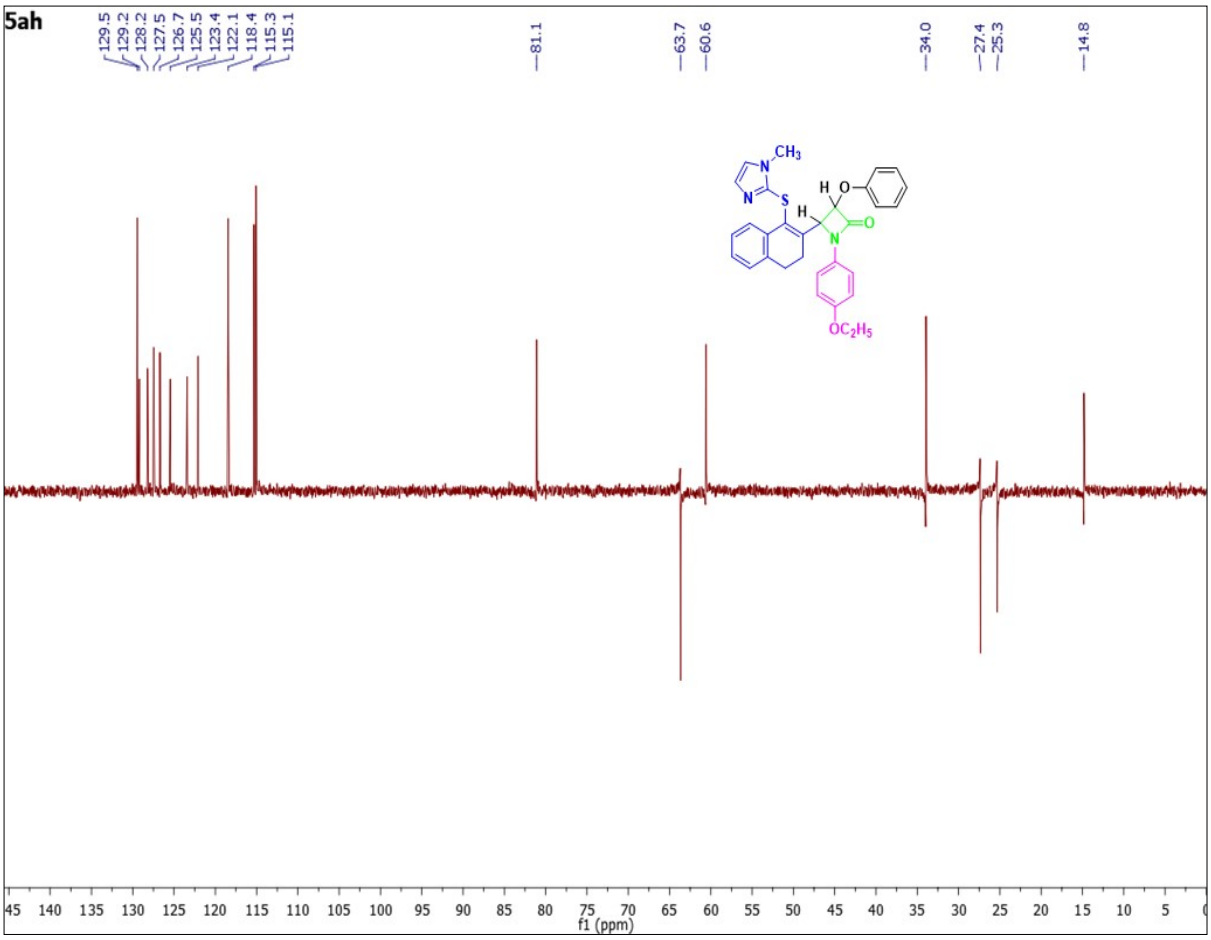


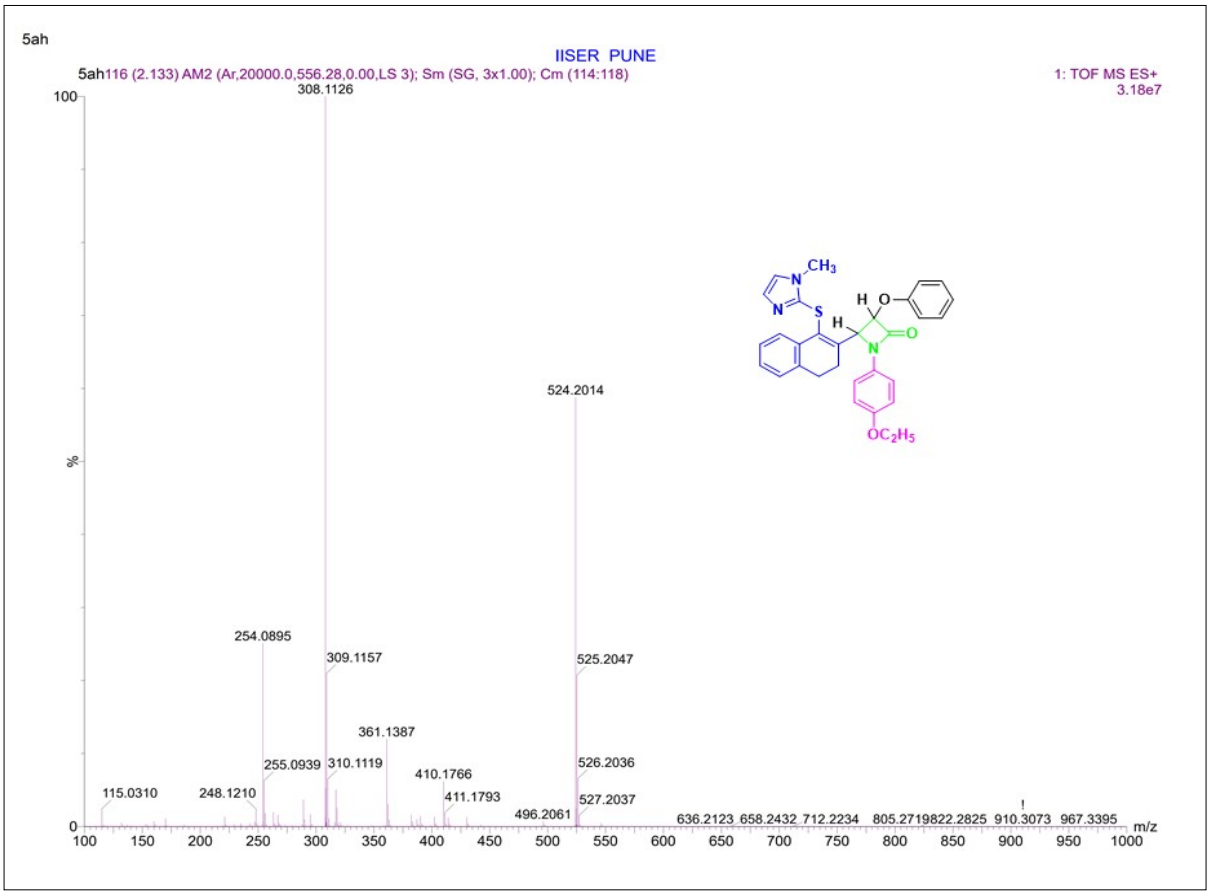
FT-IR, ^{1}H NMR spectra, ^{13}C NMR spectra, DEPT-135 spectra, and HRMS data of compound (5ah)



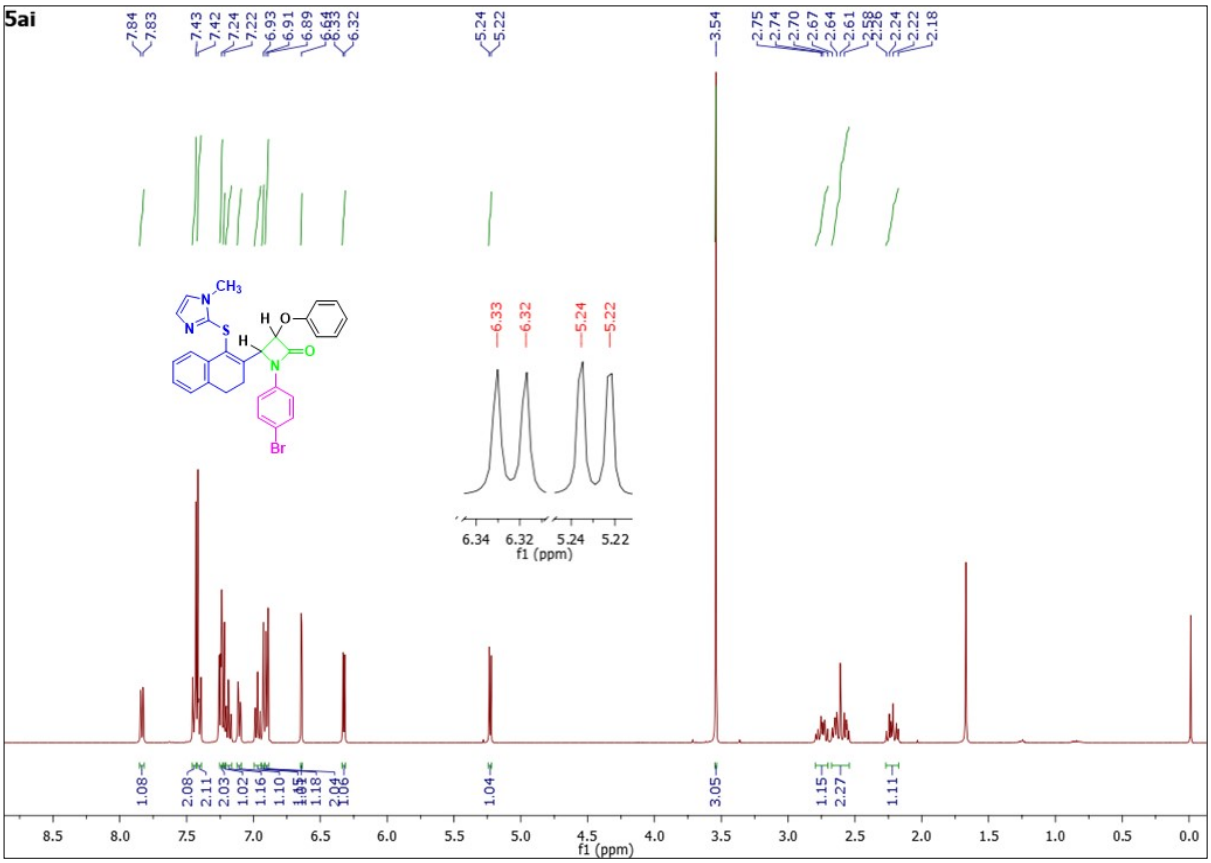

5ah
7.89
7.87
7.45
7.42
7.26
6.95
6.93
6.90
6.84
6.82
6.68
6.66
6.28
6.26
5.19
5.18
4.00
3.99
3.97
3.95
3.52
2.77
2.74
2.72
2.65
2.63
2.61
2.50
2.28
2.27
2.26
2.23
2.22
1.40
1.38
1.36
6.28 6.26 5.20 5.18
f1 (ppm)
1.02
2.11
1.01
1.03
1.12
1.15
1.01
2.04
1.00
1.01
2.09
1.01
1.00
2.15
3.08
1.13
2.16
1.06
3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

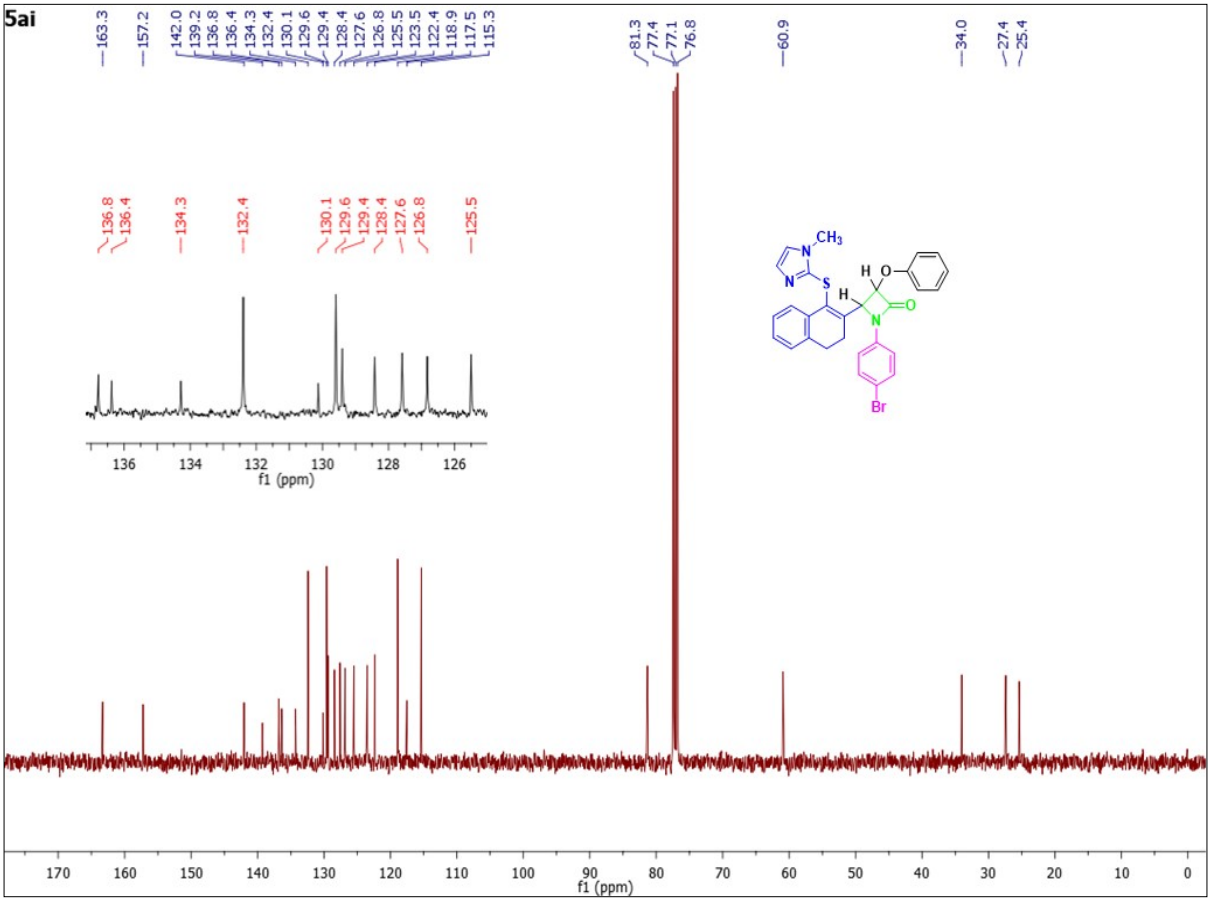

5ah
162.6
157.3
156.0
142.5
139.2
136.8
134.3
130.8
129.6
129.5
129.2
128.2
127.5
126.7
125.5
123.4
122.1
118.4
115.3
115.1
81.1
77.4
77.0
76.7
63.7
60.6
34.0
27.4
25.3
14.8
129.6
129.5
129.2
128.2
127.5
126.7
125.5
123.4
122.1
129 128 127 126 125 124 123 12
f1 (ppm)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

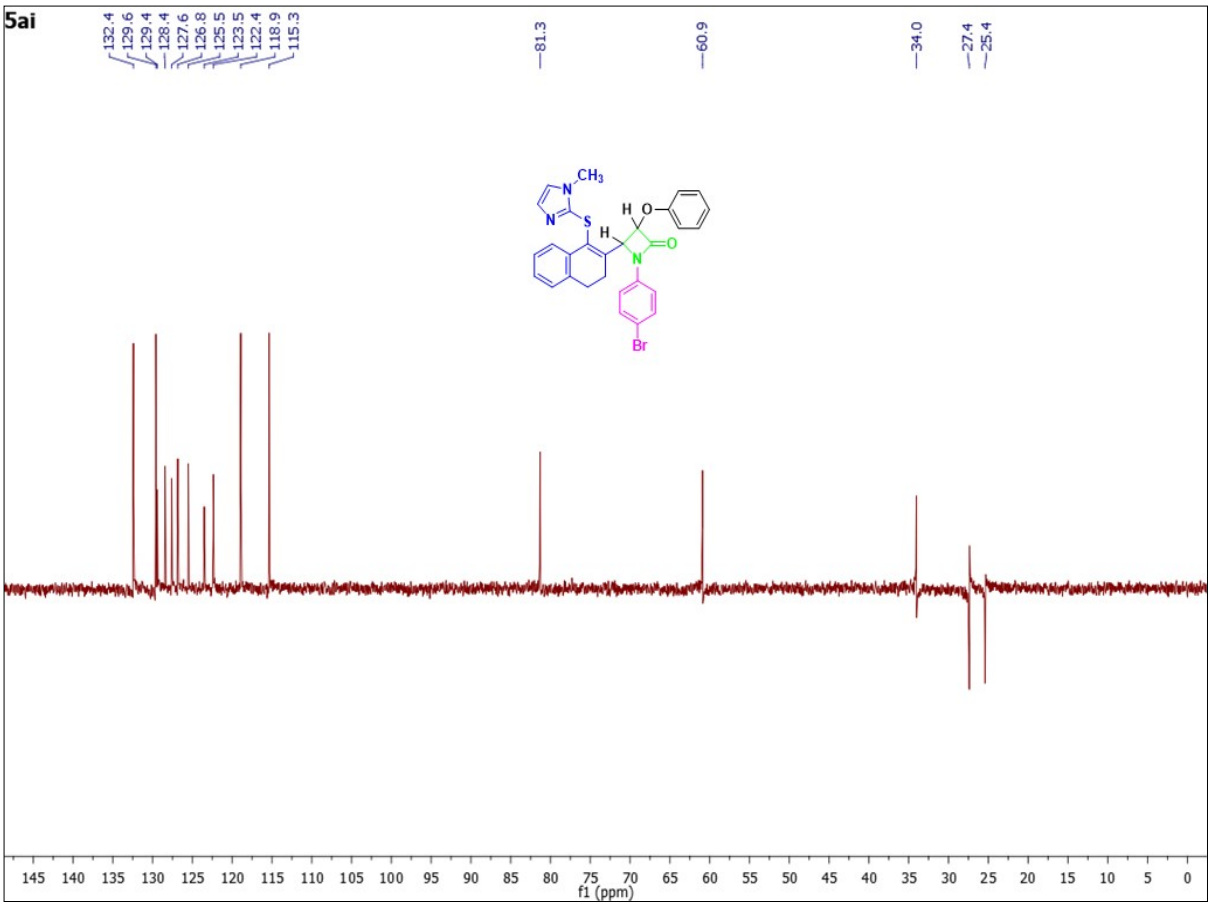

5ah
129.5
129.2
128.2
127.5
126.7
125.5
123.4
122.1
118.4
115.3
115.1
81.1
63.7
60.6
34.0
27.4
25.3
14.8
f1 (ppm)

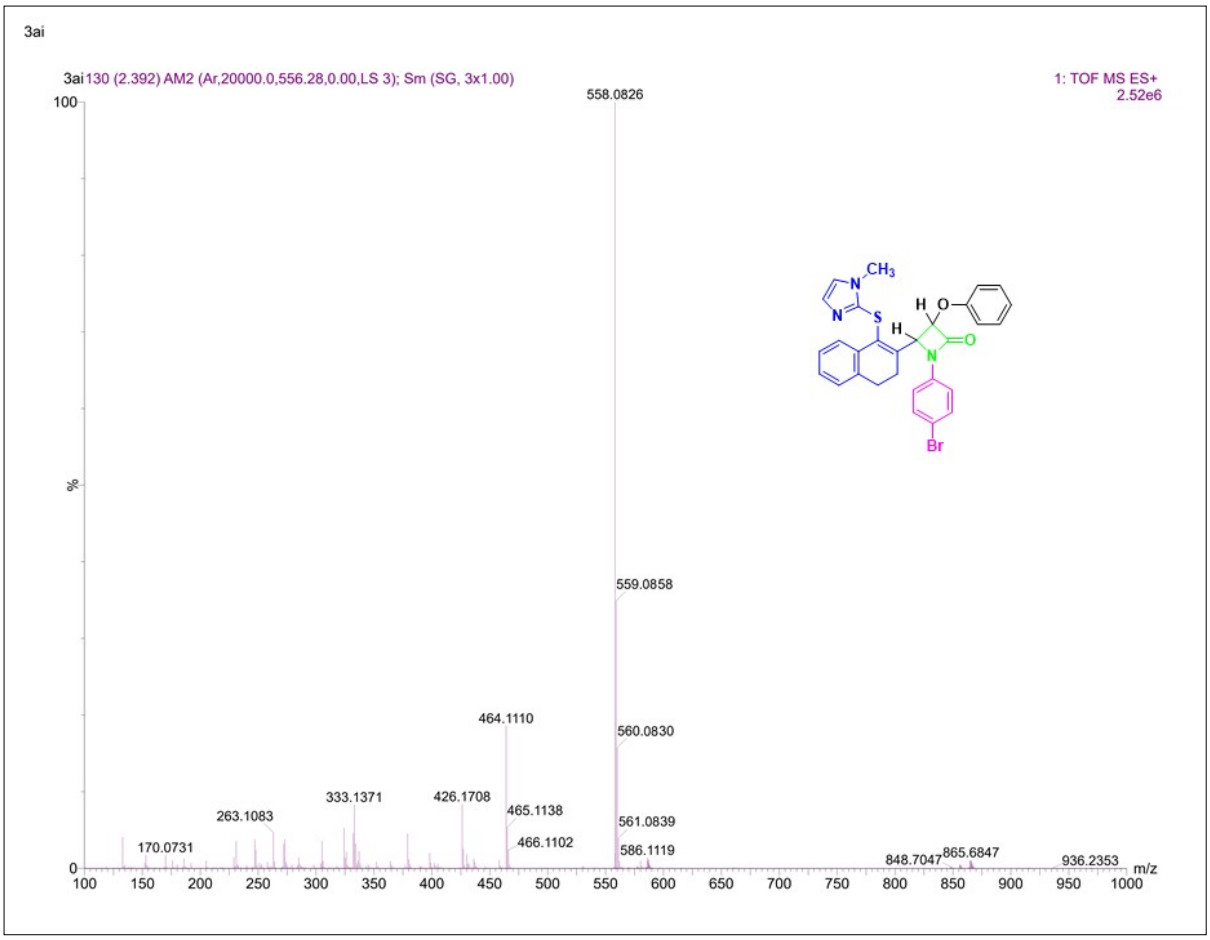

5ah
IISER PUNE
5ah116 (2.133) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00); Cm (114:118)
1: TOF MS ES+
3.18e7
308.1126
524.2014
254.0895
309.1157
525.2047
361.1387
255.0939
310.1119
526.2036
410.1766
115.0310
248.1210
411.1793
527.2037
496.2061
636.2123
658.2432
712.2234
805.2719
822.2825
910.3073
967.3395
%
m/z

^{1}H NMR spectra, ^{13}C NMR spectra, DEPT-135 spectra, and HRMS data of compound (5ai)

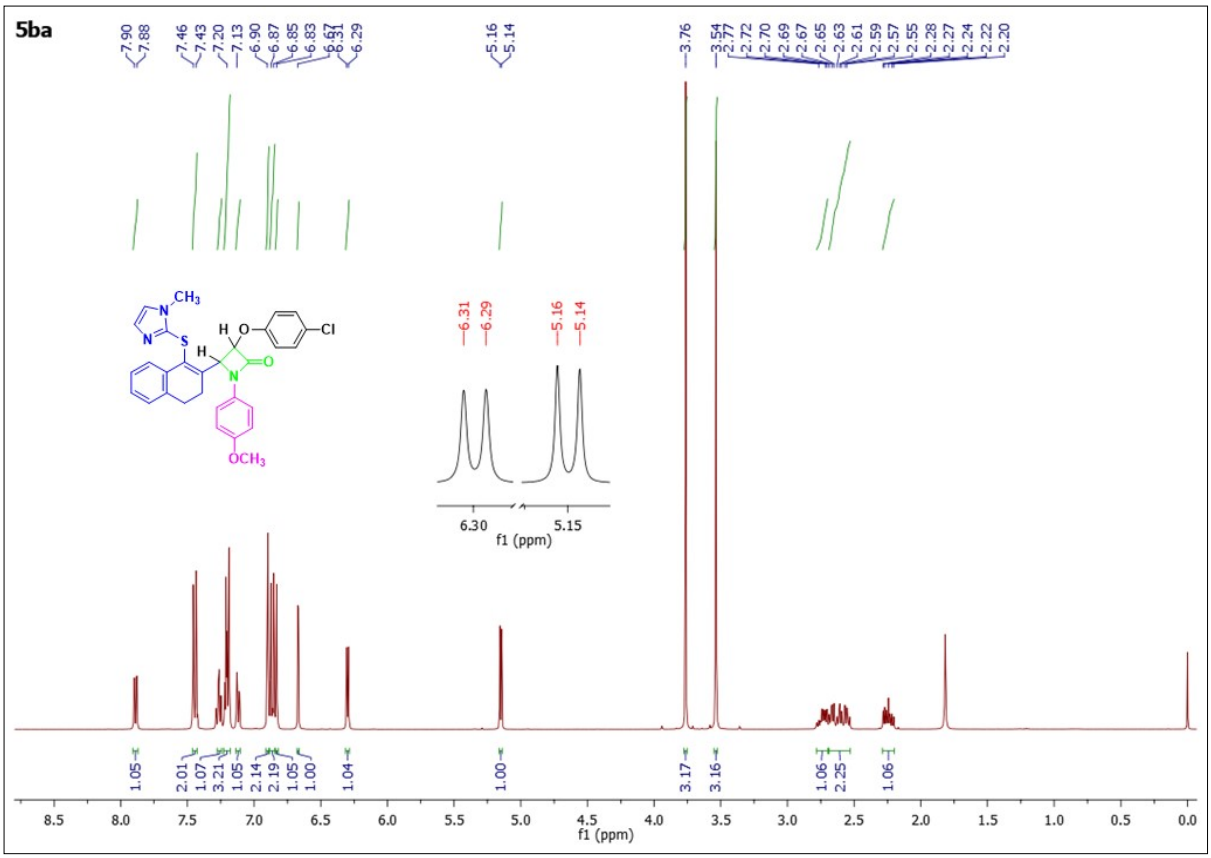


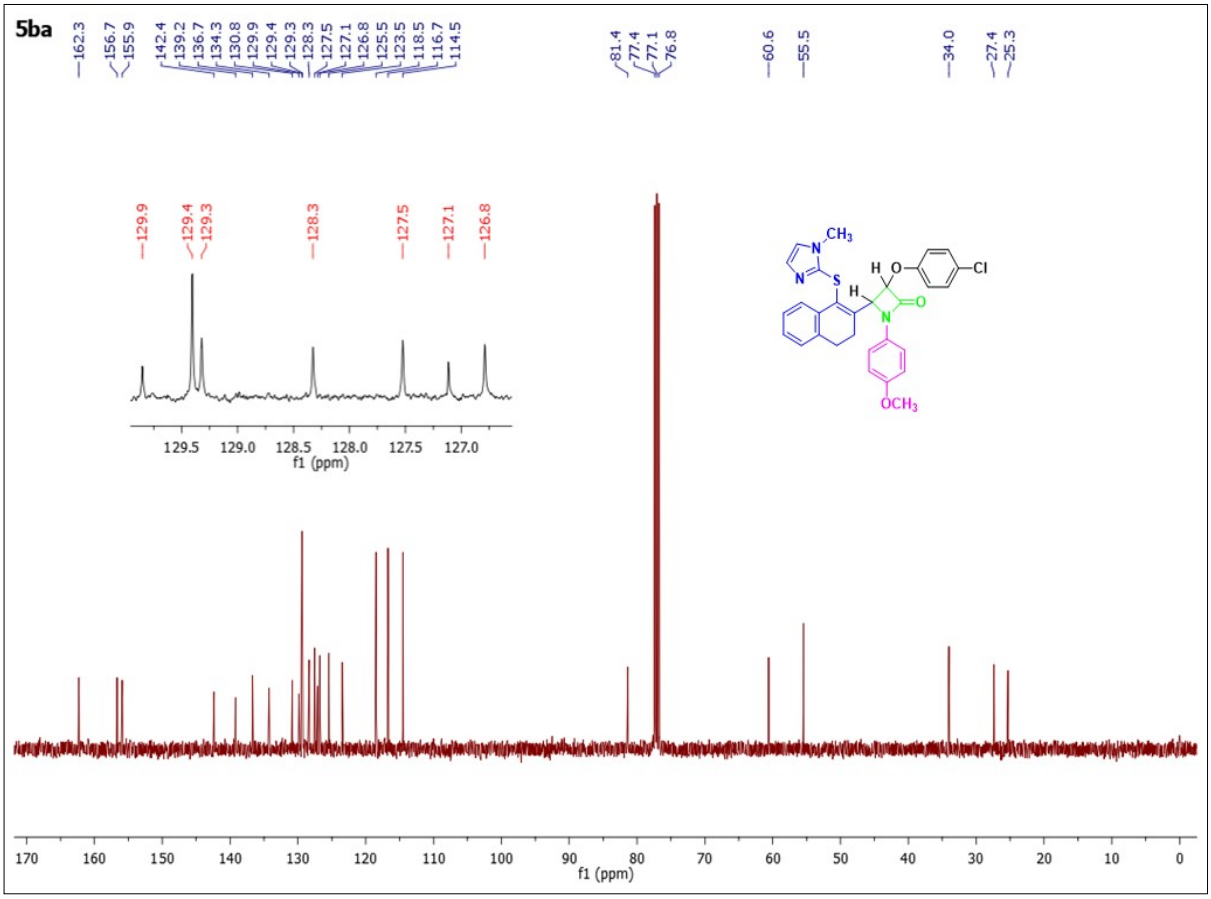


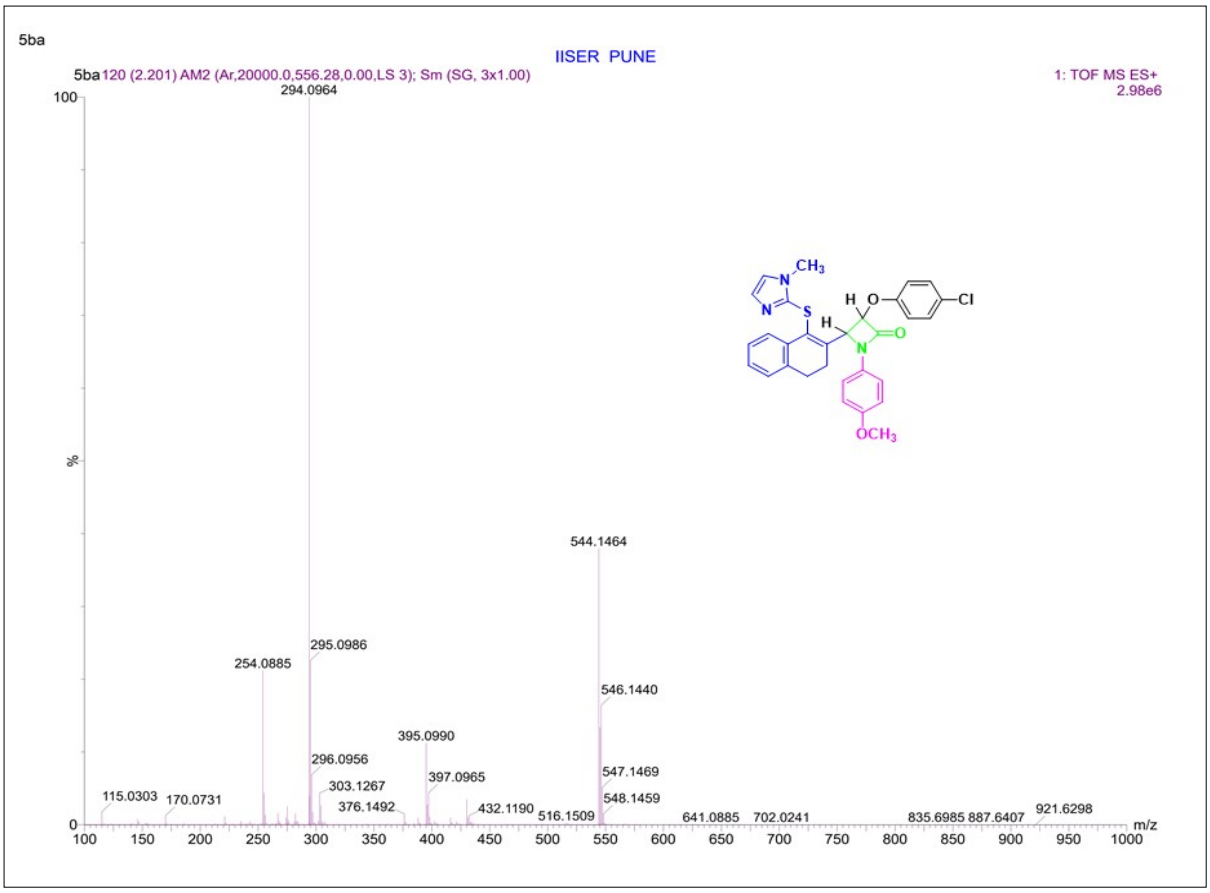

5ai
132.4
129.6
129.4
128.4
127.6
126.8
125.5
123.5
122.4
118.9
115.3
81.3
60.9
34.0
27.4
25.4
CH3
N
N
S
H
H
O
O
N
Br
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)



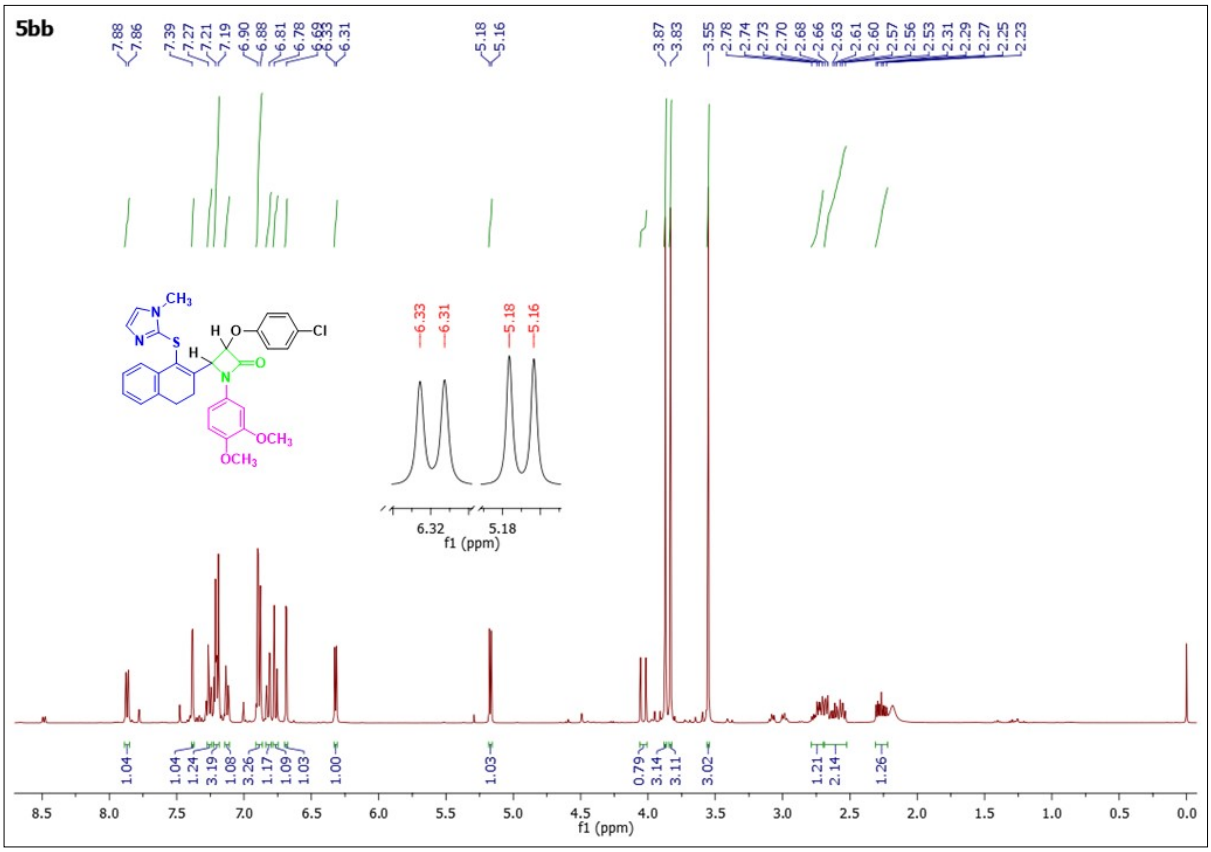
^{1}H NMR spectra, ^{13}C NMR spectra, and HRMS data of compound (5ba)

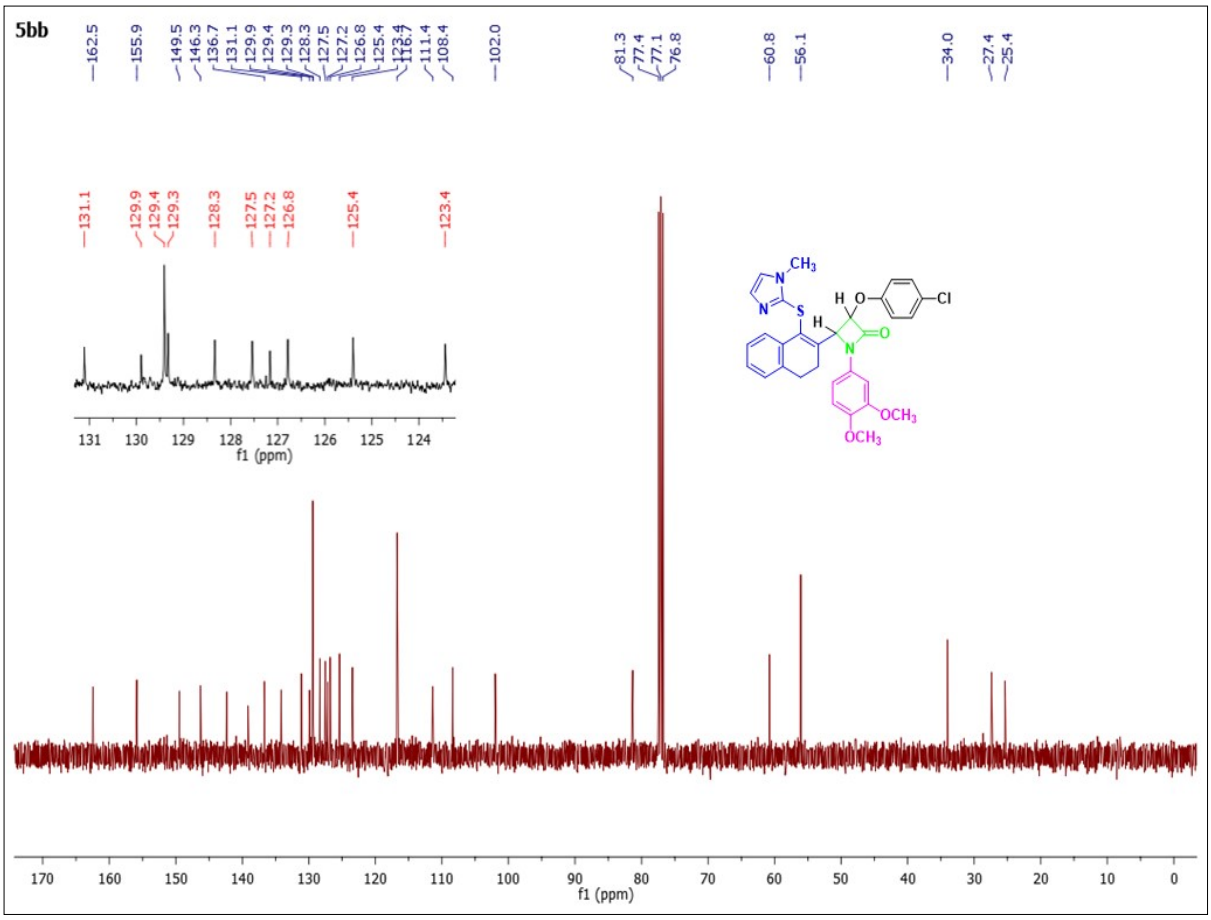

5ba
7.90
7.88
7.46
7.43
7.20
7.13
6.90
6.87
6.85
6.83
6.31
6.29
5.16
5.14
3.76
3.54
2.77
2.72
2.70
2.69
2.67
2.65
2.63
2.61
2.59
2.57
2.55
2.28
2.27
2.24
2.22
2.20
CH3
N
S
H
O
Cl
O
H
N
OCH3
6.31
6.29
5.16
5.14
6.30
5.15
f1 (ppm)
1.05
2.01
1.07
3.21
1.05
2.14
2.19
1.05
1.00
1.04
1.00
3.17
3.16
1.06
2.25
1.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

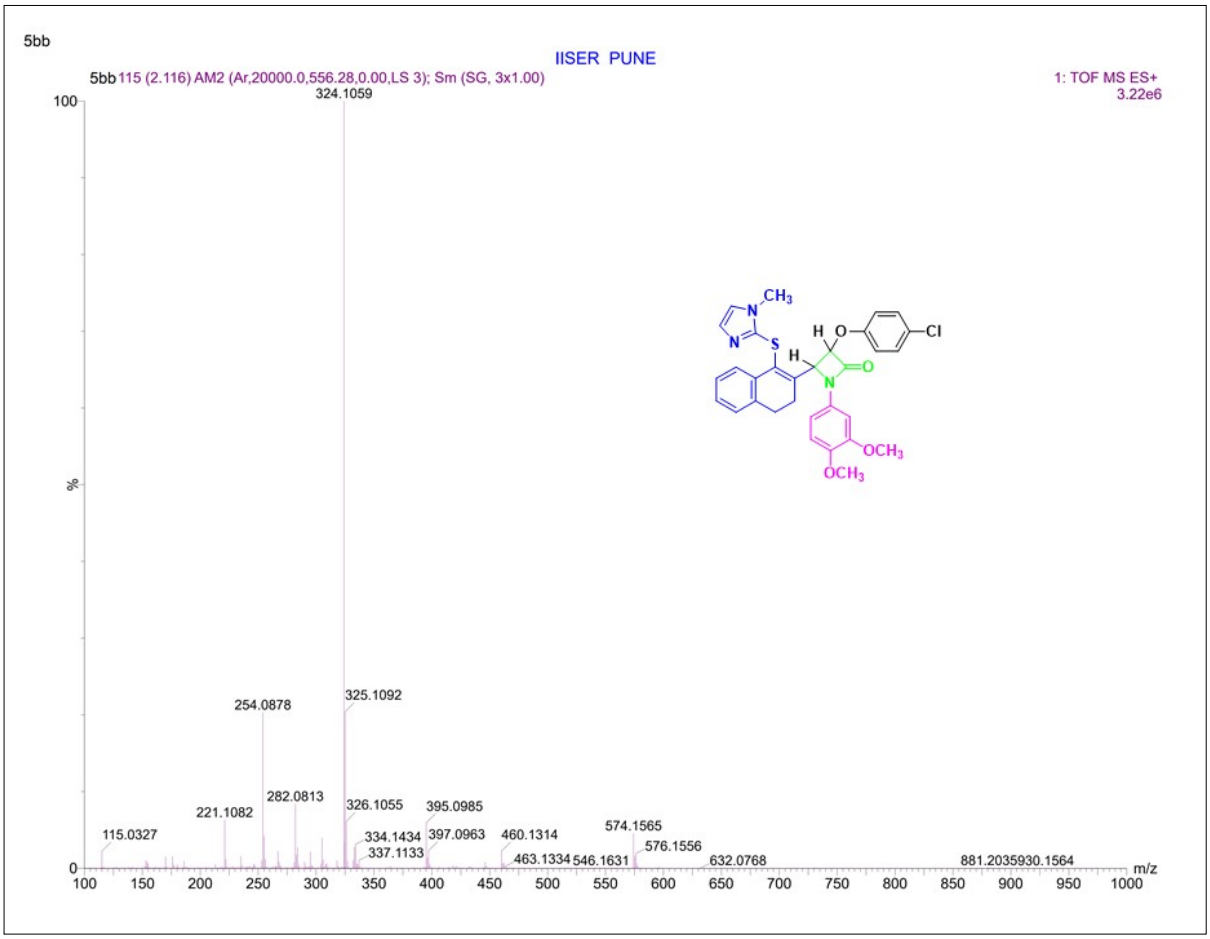

5ba
162.3
156.7
155.9
142.4
139.2
136.7
134.3
130.8
129.9
129.4
129.3
128.3
127.5
127.1
126.8
125.5
123.5
118.5
116.7
114.5
81.4
77.4
77.1
76.8
60.6
55.5
34.0
27.4
25.3
129.9
129.4
129.3
128.3
127.5
127.1
126.8
129.5
129.0
128.5
128.0
127.5
127.0
f1 (ppm)
CH3
N
S
H
O
Cl
O
H
N
OCH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



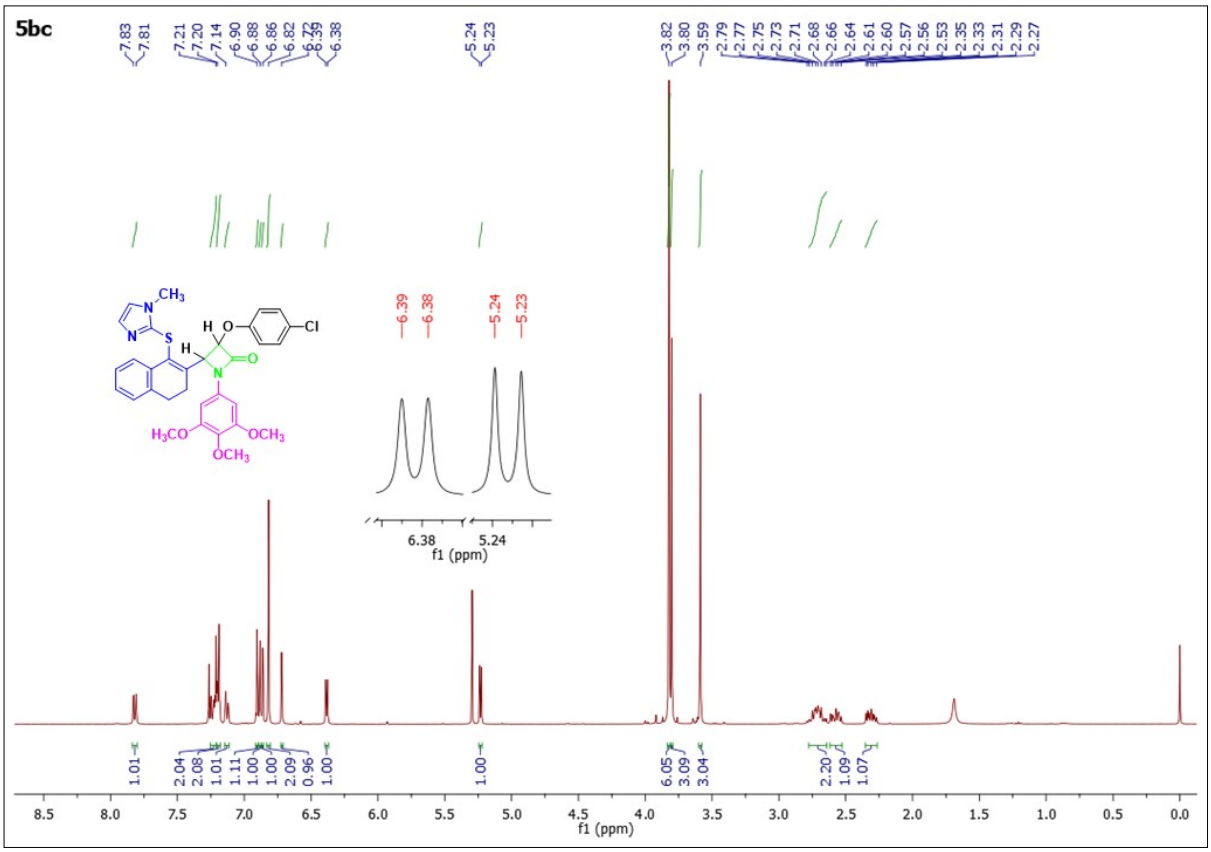
^{1}H NMR spectra, ^{13}C NMR spectra, and HRMS data of compound (5bb)

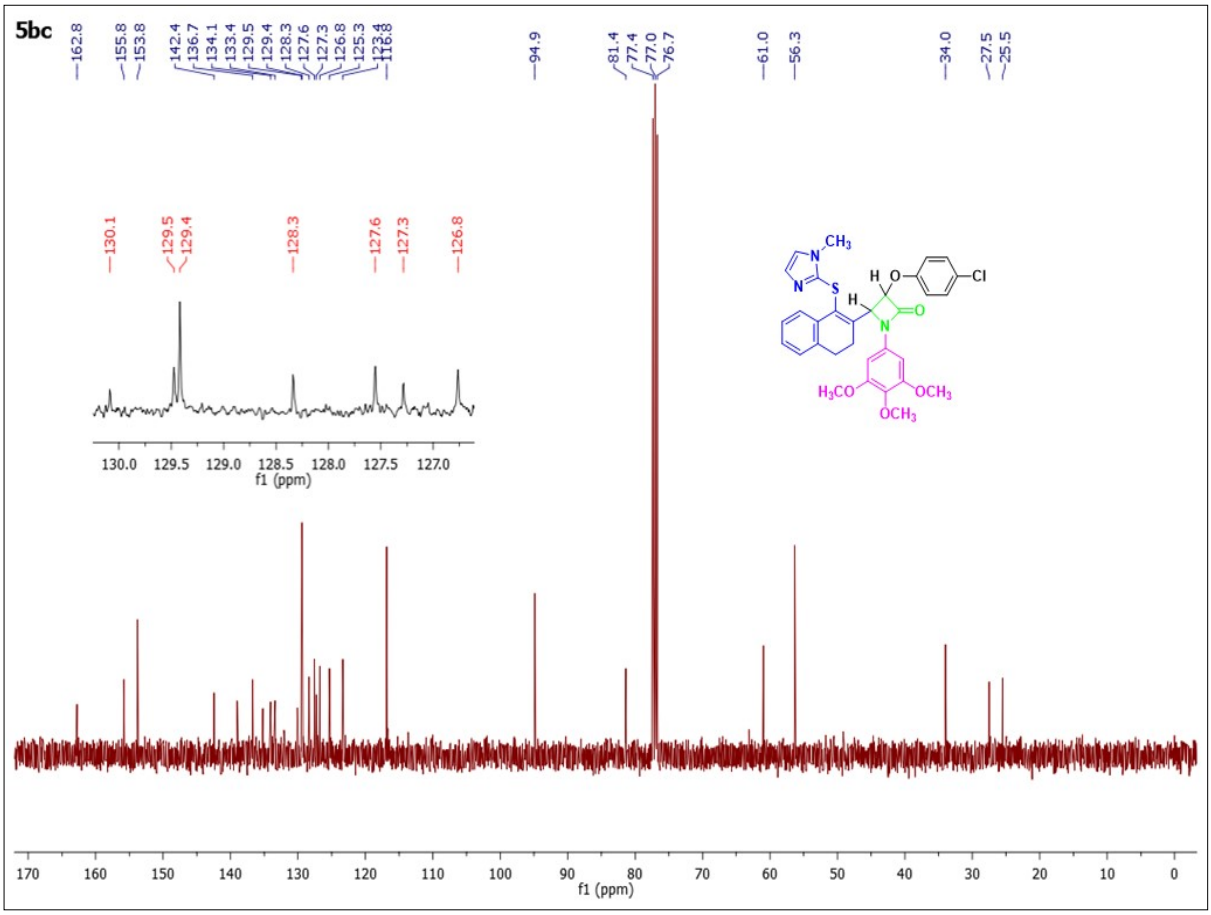


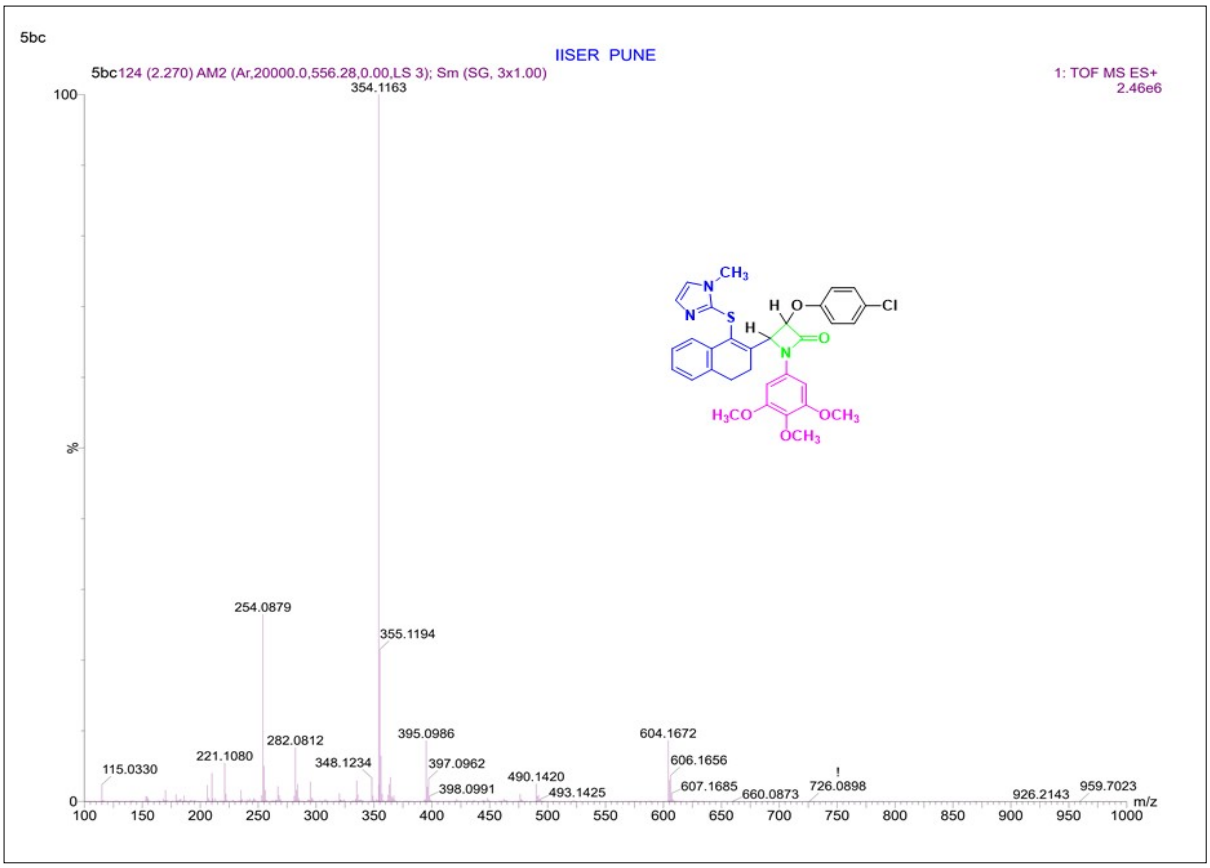

5bb
162.5
155.9
149.5
146.3
136.7
131.1
129.9
129.4
129.3
128.3
127.5
127.2
126.8
125.4
123.4
111.4
108.4
102.0
81.3
77.4
77.1
76.8
60.8
56.1
34.0
27.4
25.4
131.1
129.9
129.4
129.3
128.3
127.5
127.2
126.8
125.4
123.4
131 130 129 128 127 126 125 124
f1 (ppm)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


5bb
IISER PUNE
5bb 115 (2.116) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00)
1: TOF MS ES+
3.22e6
100
%
0
324.1059
325.1092
254.0878
282.0813
221.1082
326.1055
395.0985
115.0327
334.1434
397.0963
460.1314
337.1133
463.1334
546.1631
574.1565
576.1556
632.0768
881.2035930.1564
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z

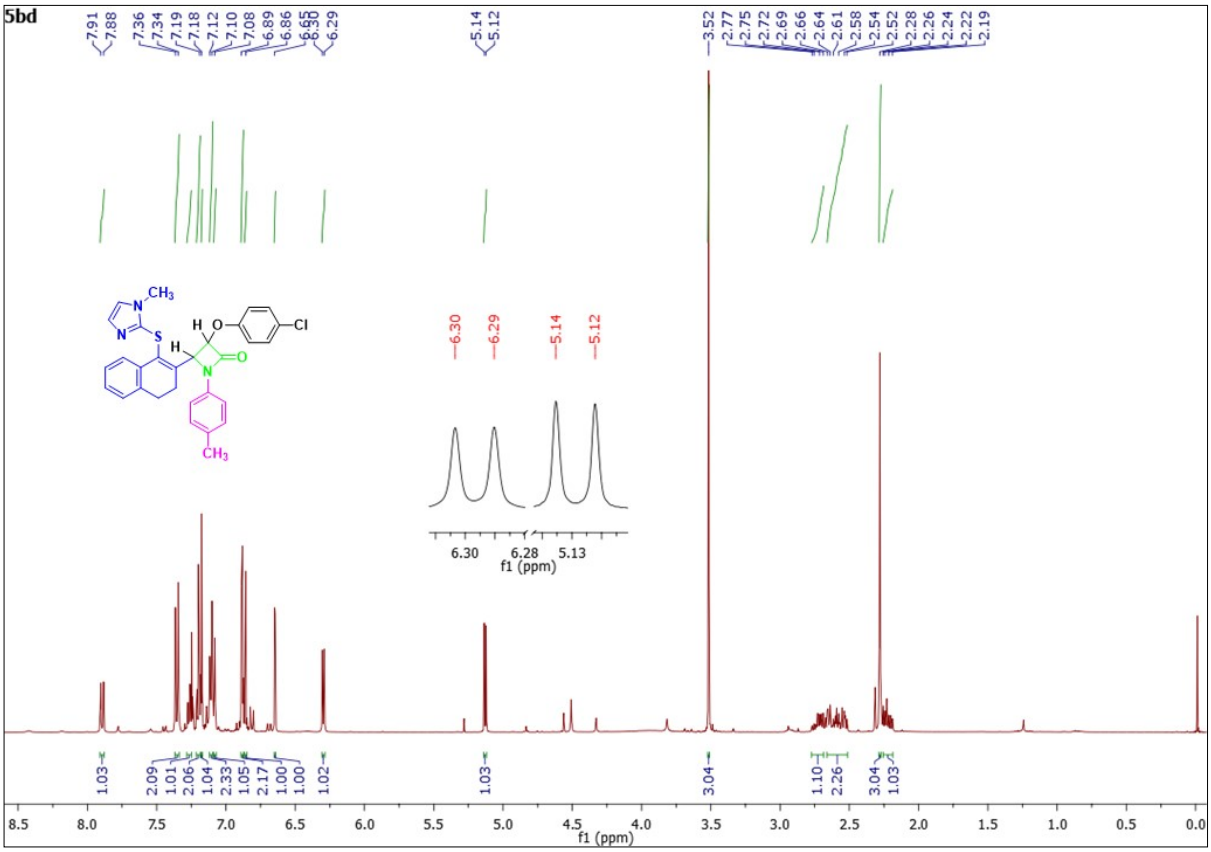
^{1}H NMR spectra, ^{13}C NMR spectra, and HRMS data of compound (5bc)

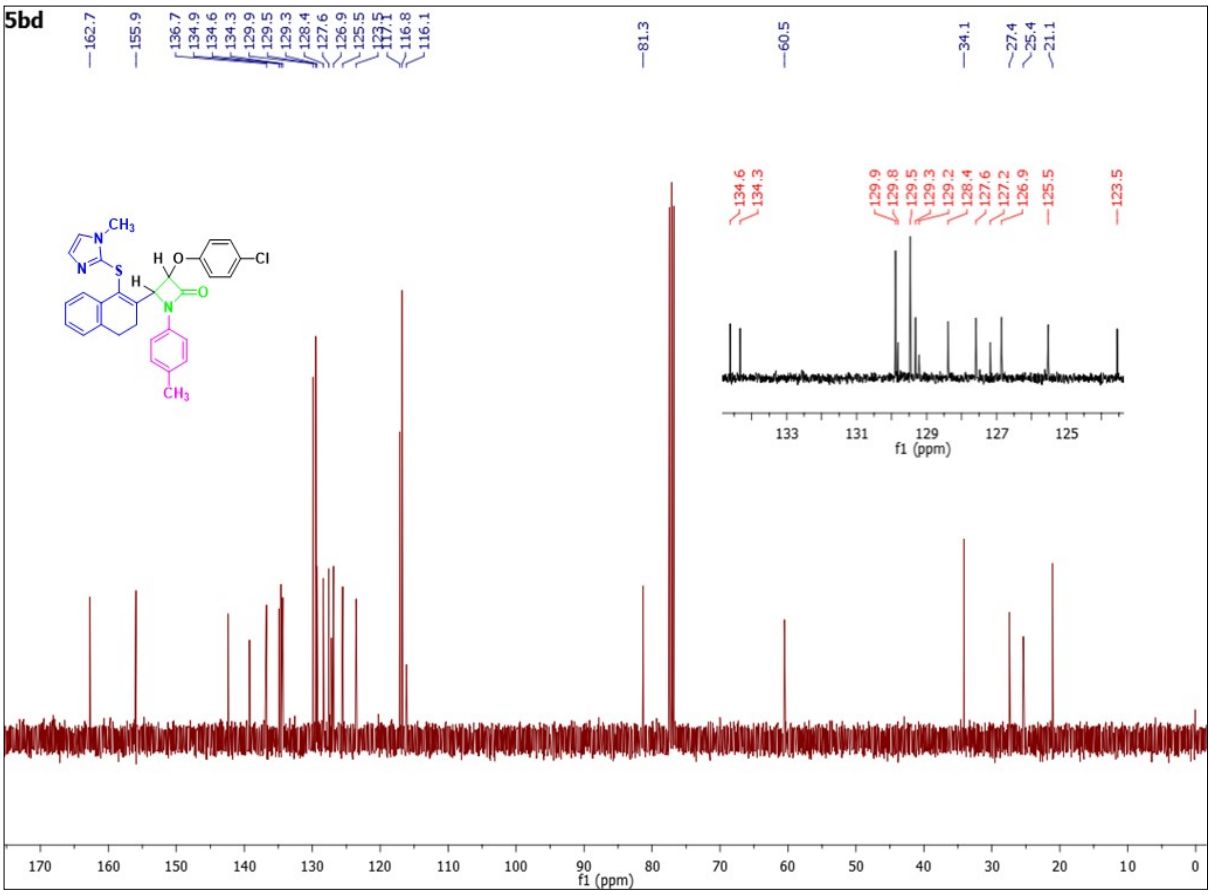


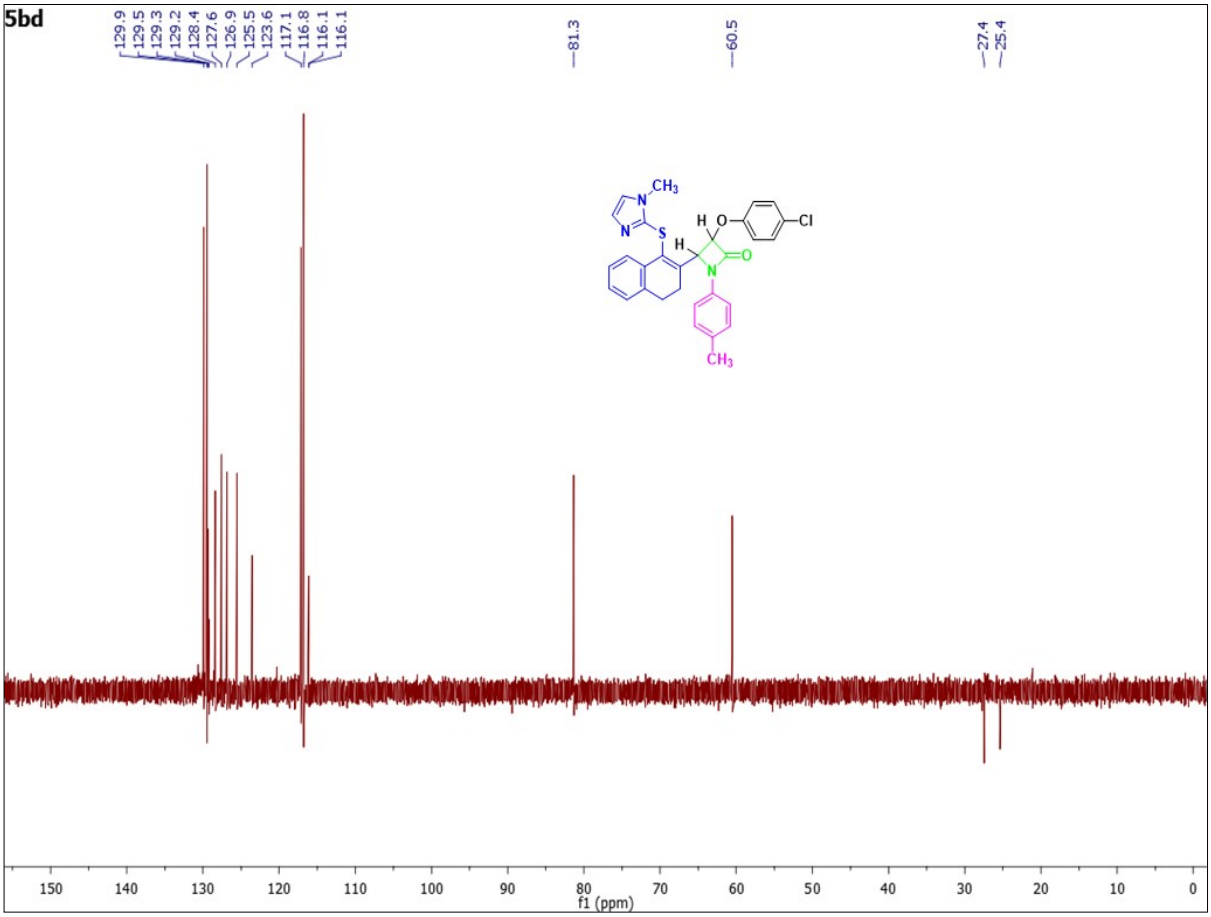


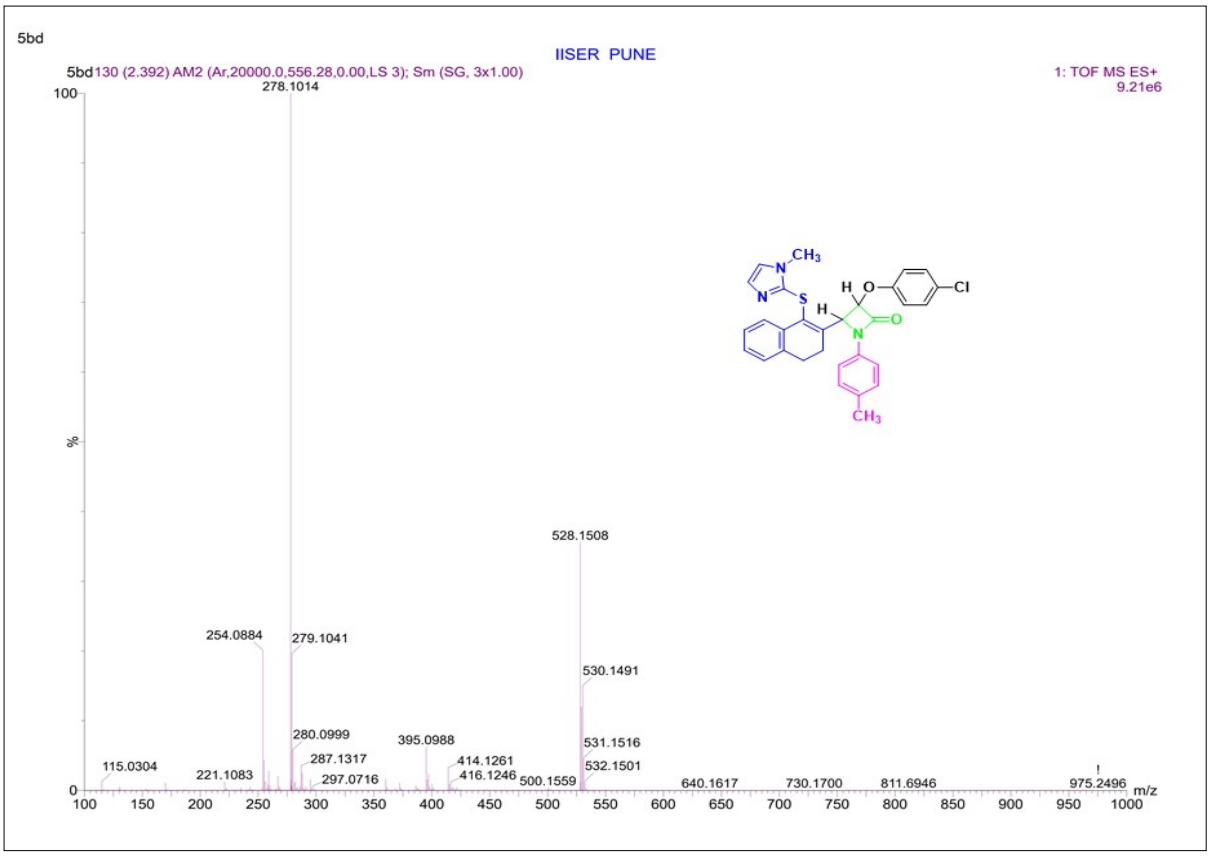


^{1}H NMR spectra, ^{13}C NMR spectra, DEPT-135 spectra, and HRMS data of compound (5bd)

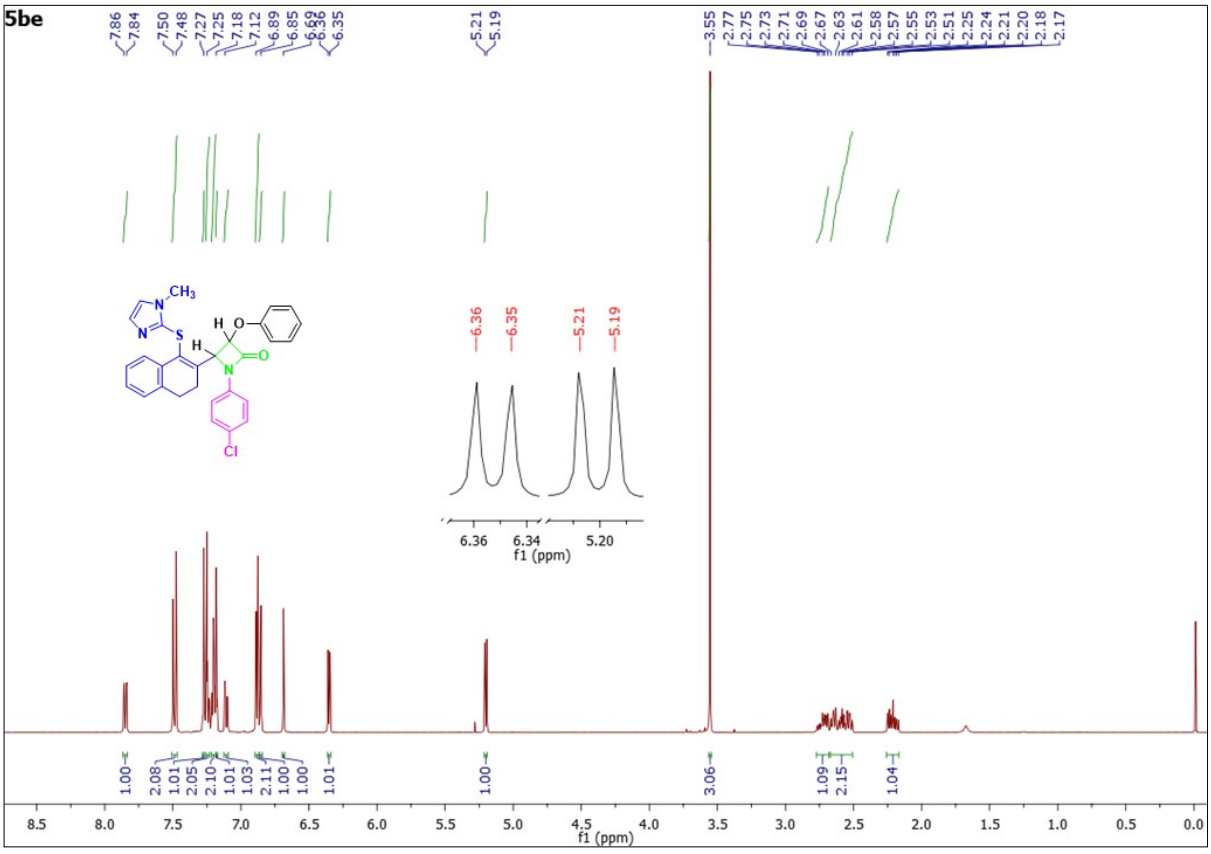


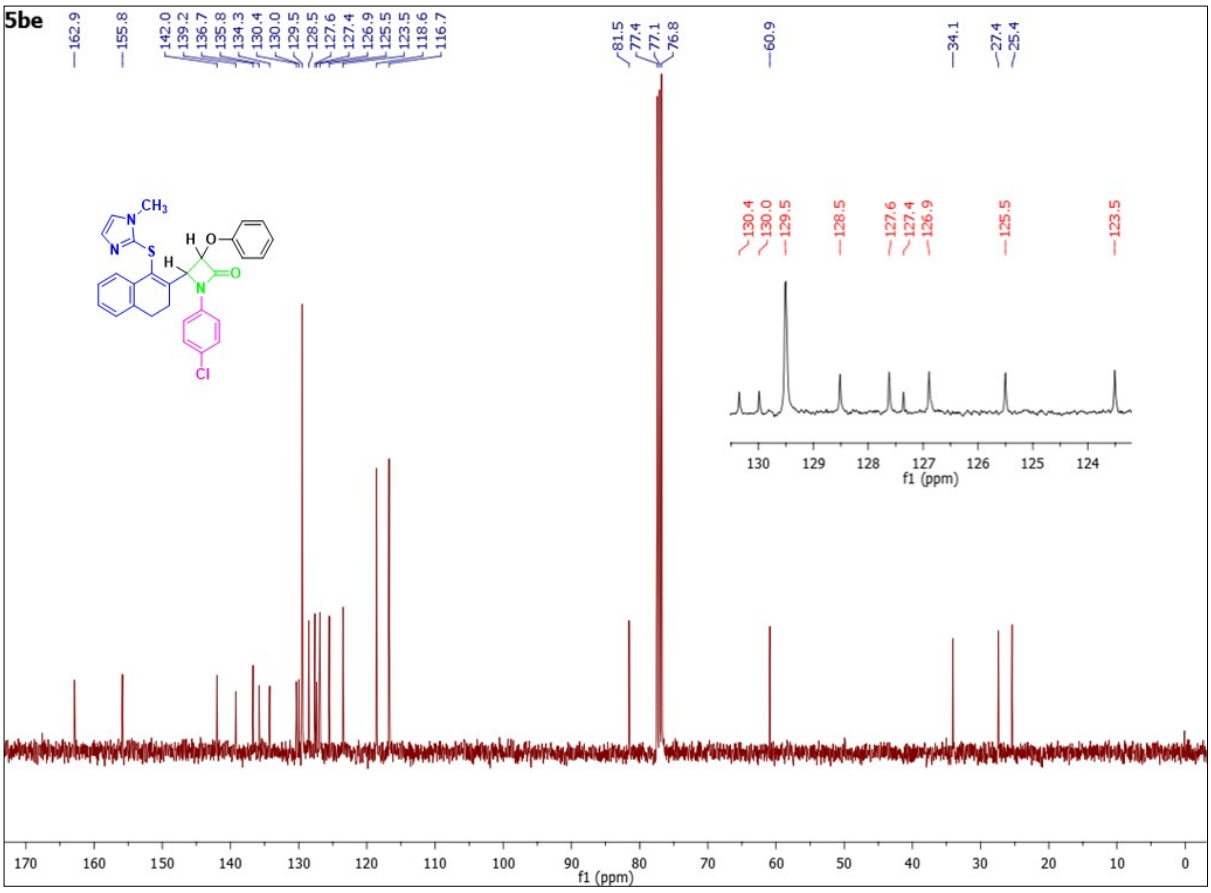

5bd
162.7
155.9
136.7
134.9
134.6
134.3
129.9
129.5
129.3
128.4
127.6
126.9
125.5
123.5
117.1
116.8
116.1
81.3
60.5
34.1
27.4
25.4
21.1
134.6
134.3
129.9
129.8
129.5
129.3
129.2
128.4
127.6
127.2
126.9
125.5
123.5
133
131
129
127
125
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

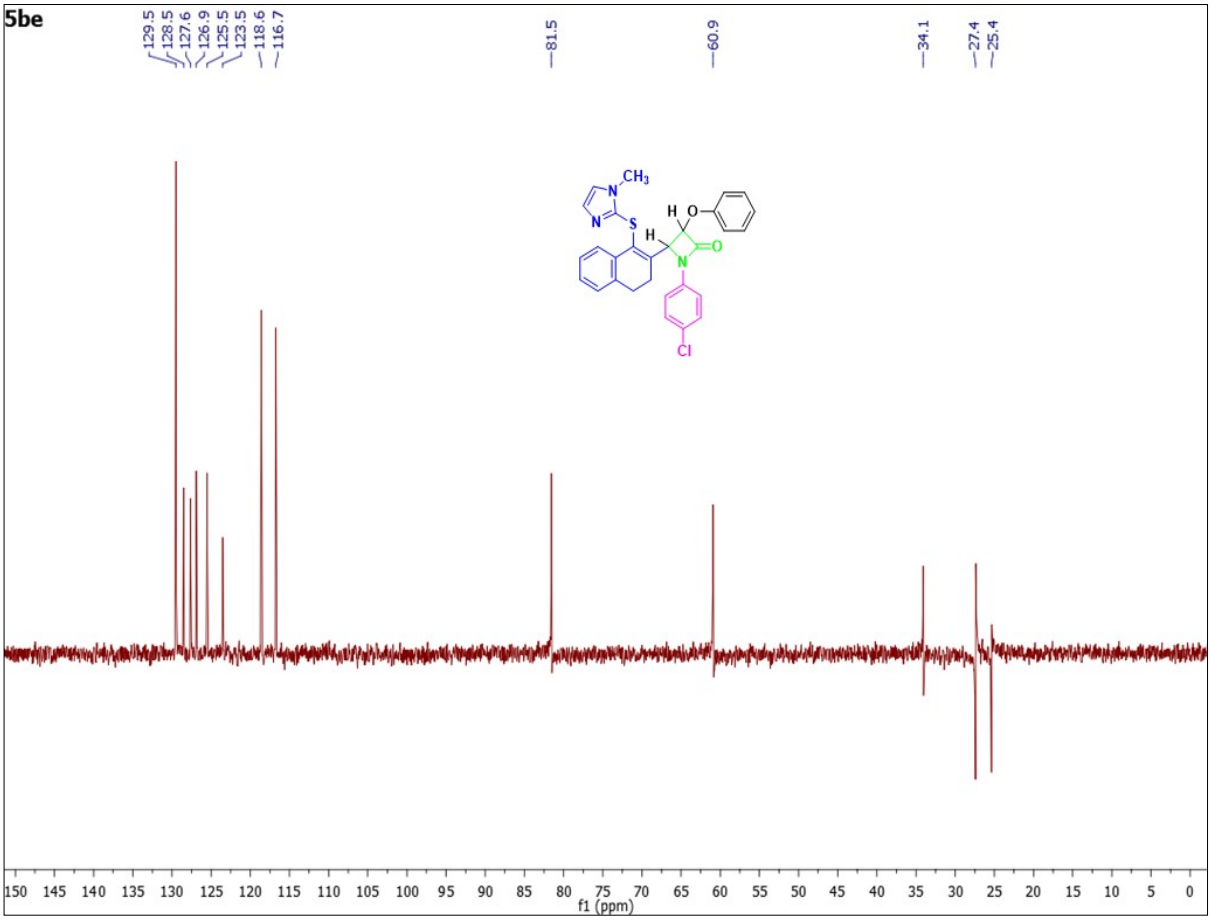

5bd
129.9
129.5
129.3
129.2
128.4
127.6
126.9
125.5
123.6
117.1
116.8
116.1
116.1
81.3
60.5
27.4
25.4
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

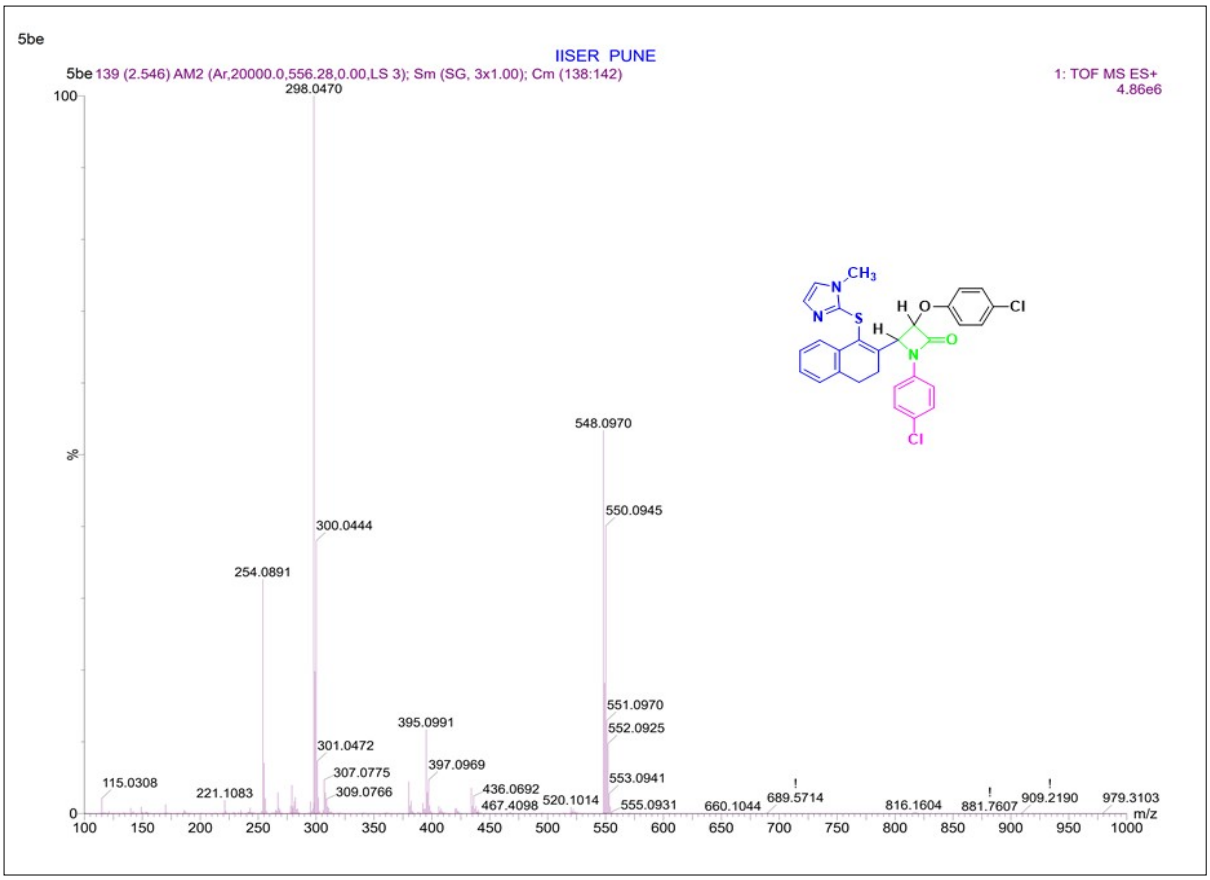


^{1}H NMR spectra, ^{13}C NMR spectra, DEPT-135 spectra, and HRMS data of compound (5be)

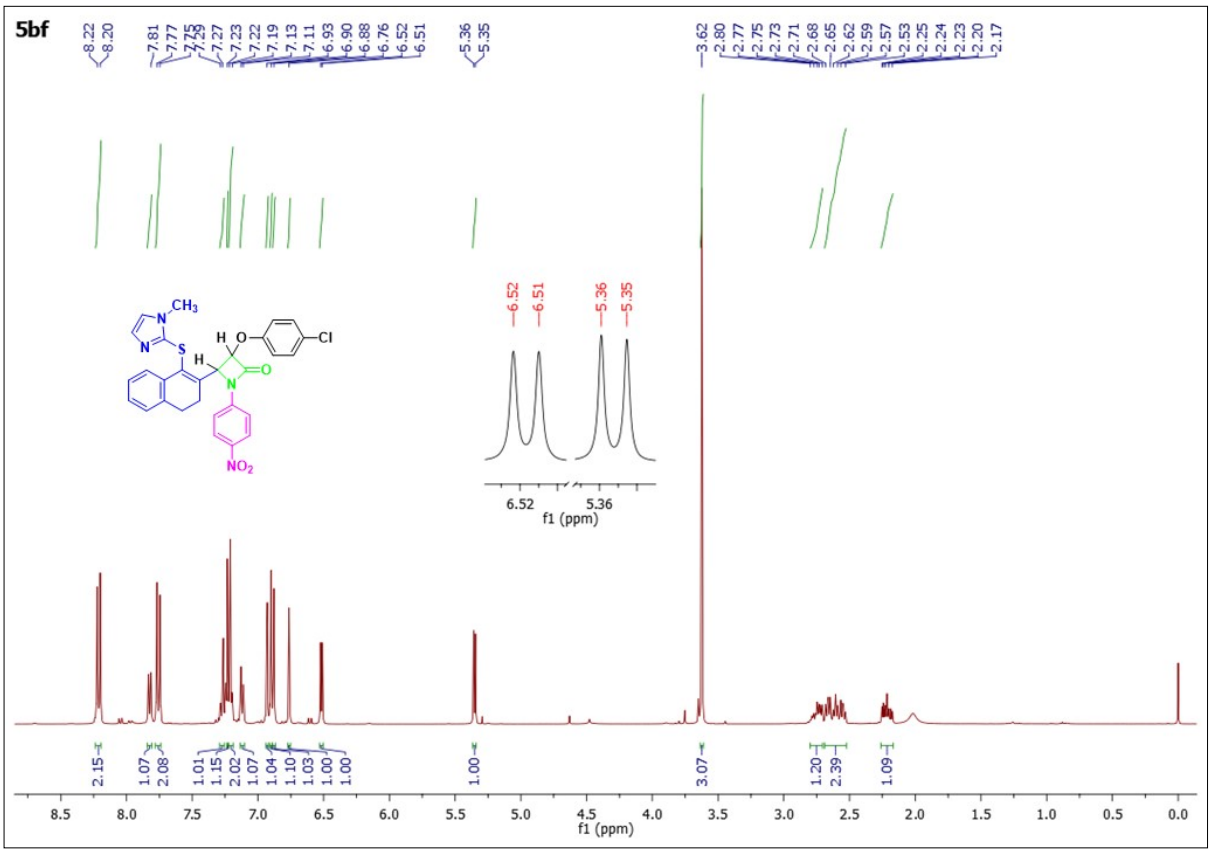


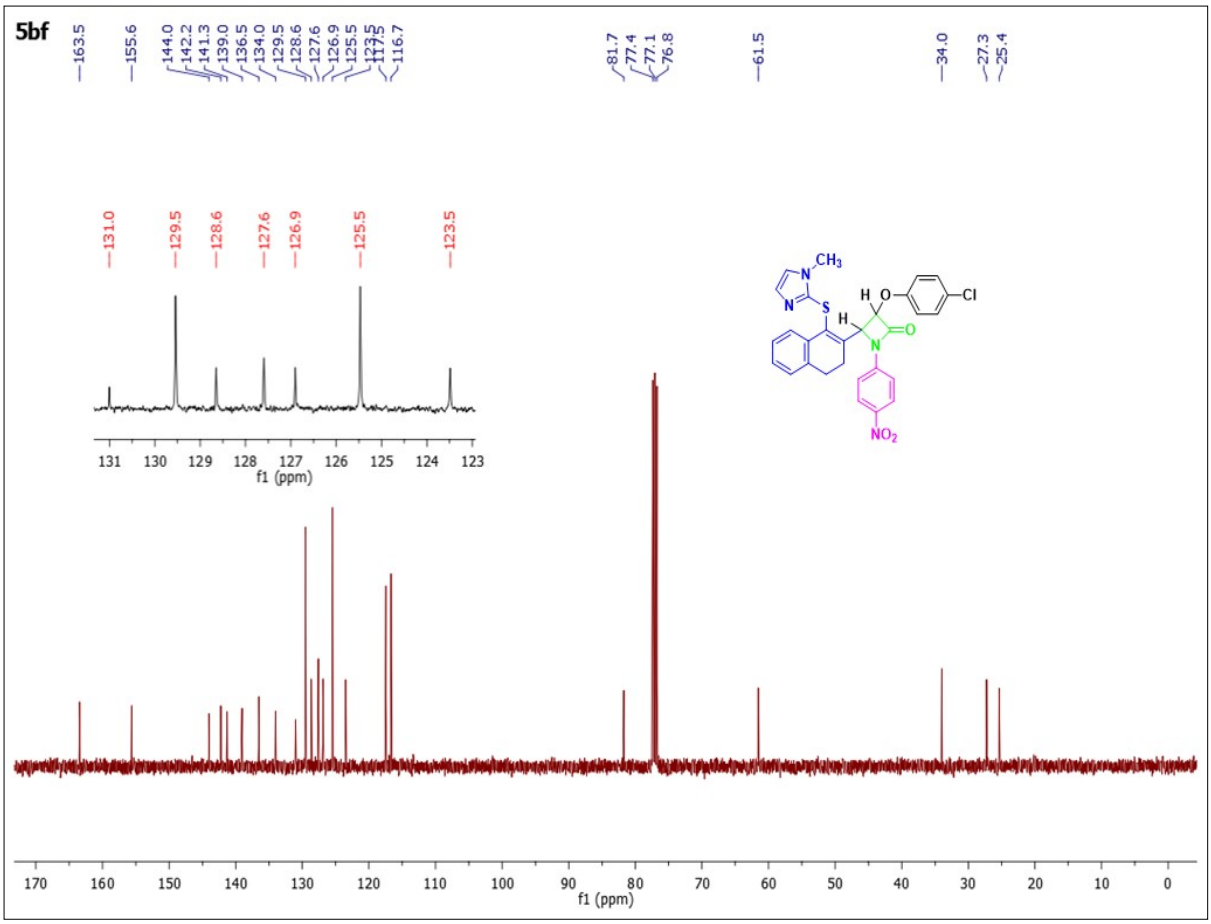

5be
162.9
155.8
142.0
139.2
136.7
135.8
134.3
130.4
130.0
129.5
128.5
127.6
127.4
126.9
125.5
123.5
118.6
116.7
81.5
77.4
77.1
76.8
60.9
34.1
27.4
25.4
130.4
130.0
129.5
128.5
127.6
127.4
126.9
125.5
123.5
130 129 128 127 126 125 124
f1 (ppm)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

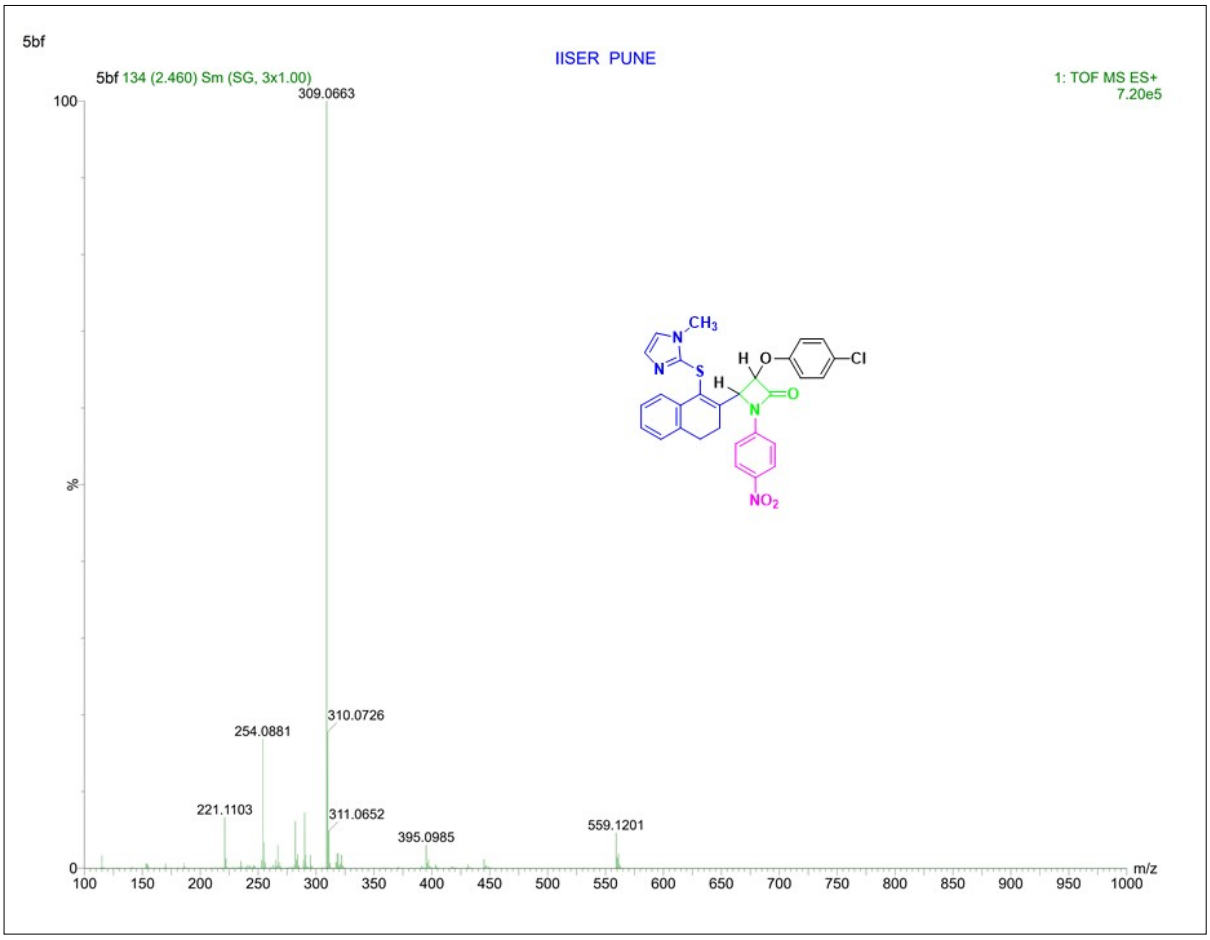

5be
129.5
128.5
127.6
126.9
125.5
123.5
118.6
116.7
81.5
60.9
34.1
27.4
25.4
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)



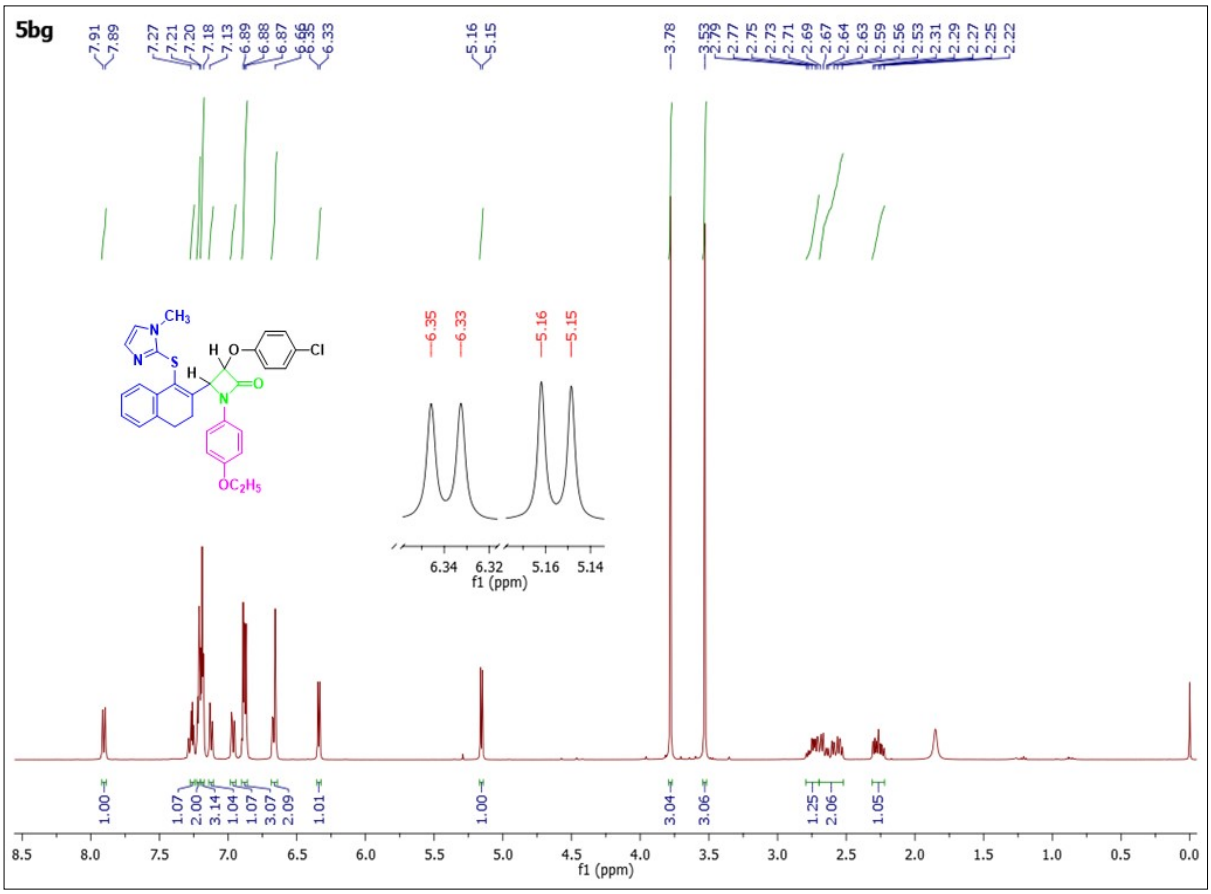
^{1}H NMR spectra, ^{13}C NMR spectra, and HRMS data of compound (5bf)

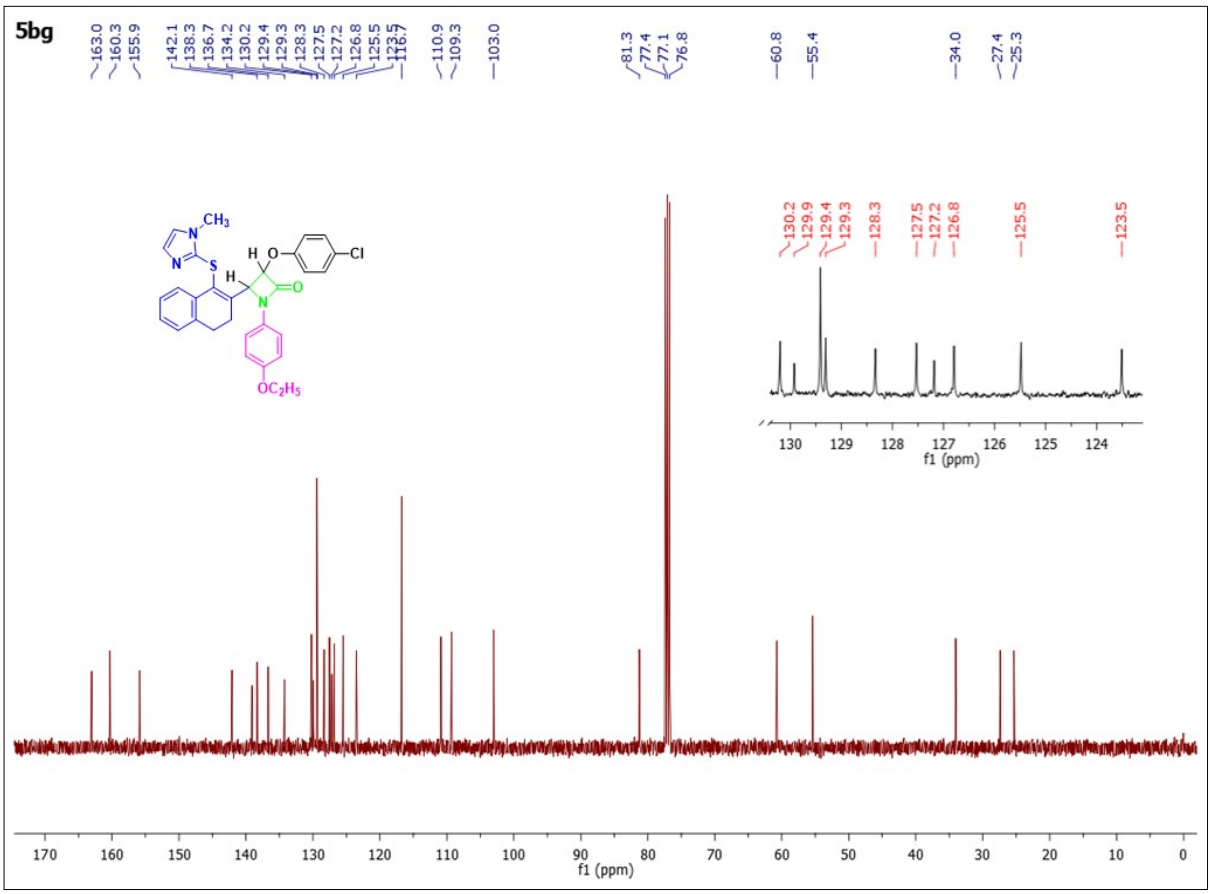


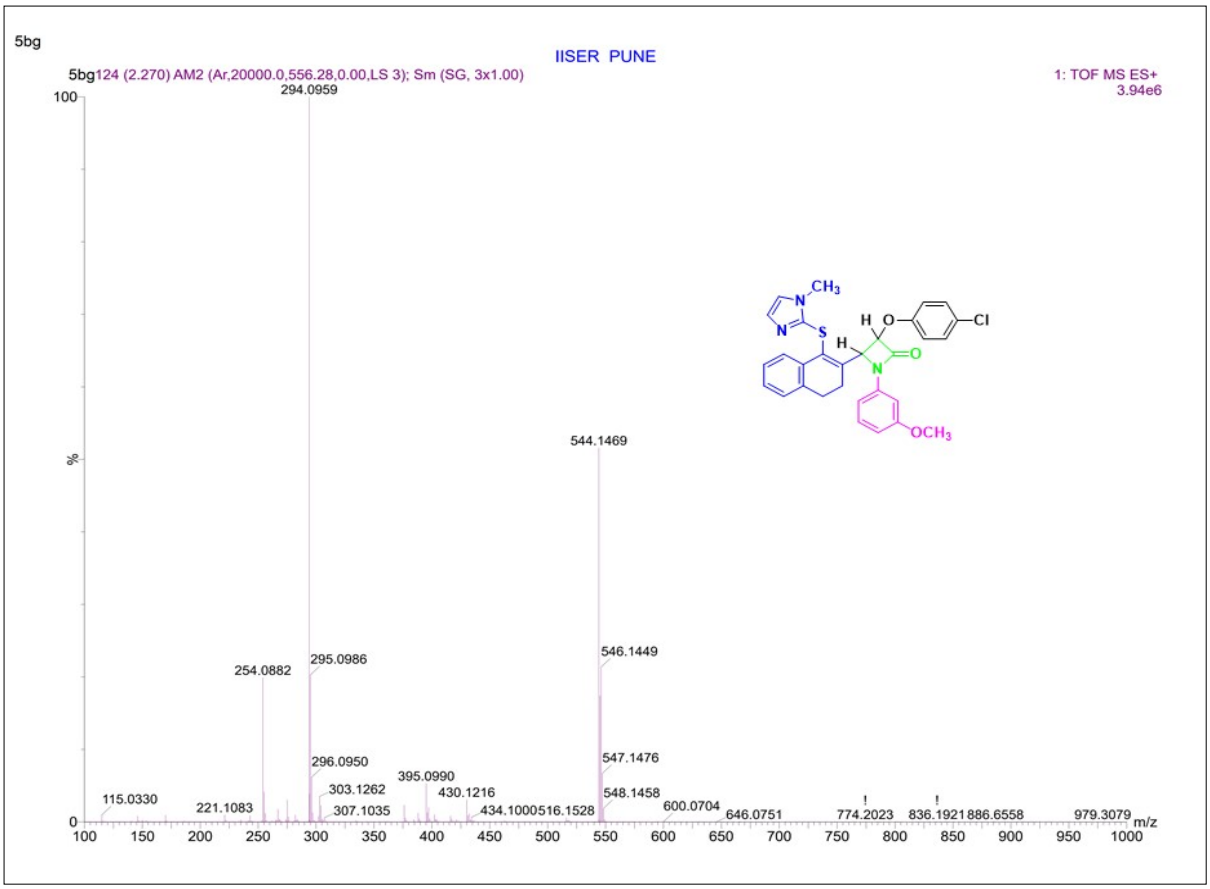

5bf
163.5
155.6
144.0
142.2
141.3
139.0
136.5
134.0
129.5
128.6
127.6
126.9
125.5
123.5
116.7
81.7
77.4
77.1
76.8
61.5
34.0
27.3
25.4
131.0
129.5
128.6
127.6
126.9
125.5
123.5
131 130 129 128 127 126 125 124 123
f1 (ppm)
CH3
N
S
H
O
Cl
O
N
NO2
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


5bf
IISER PUNE
5bf 134 (2.460) Sm (SG, 3x1.00)
1: TOF MS ES+
7.20e5
100
%
0
309.0663
310.0726
254.0881
221.1103
311.0652
395.0985
559.1201
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z
CH3
N
S
H
O
Cl
O
N
NO2

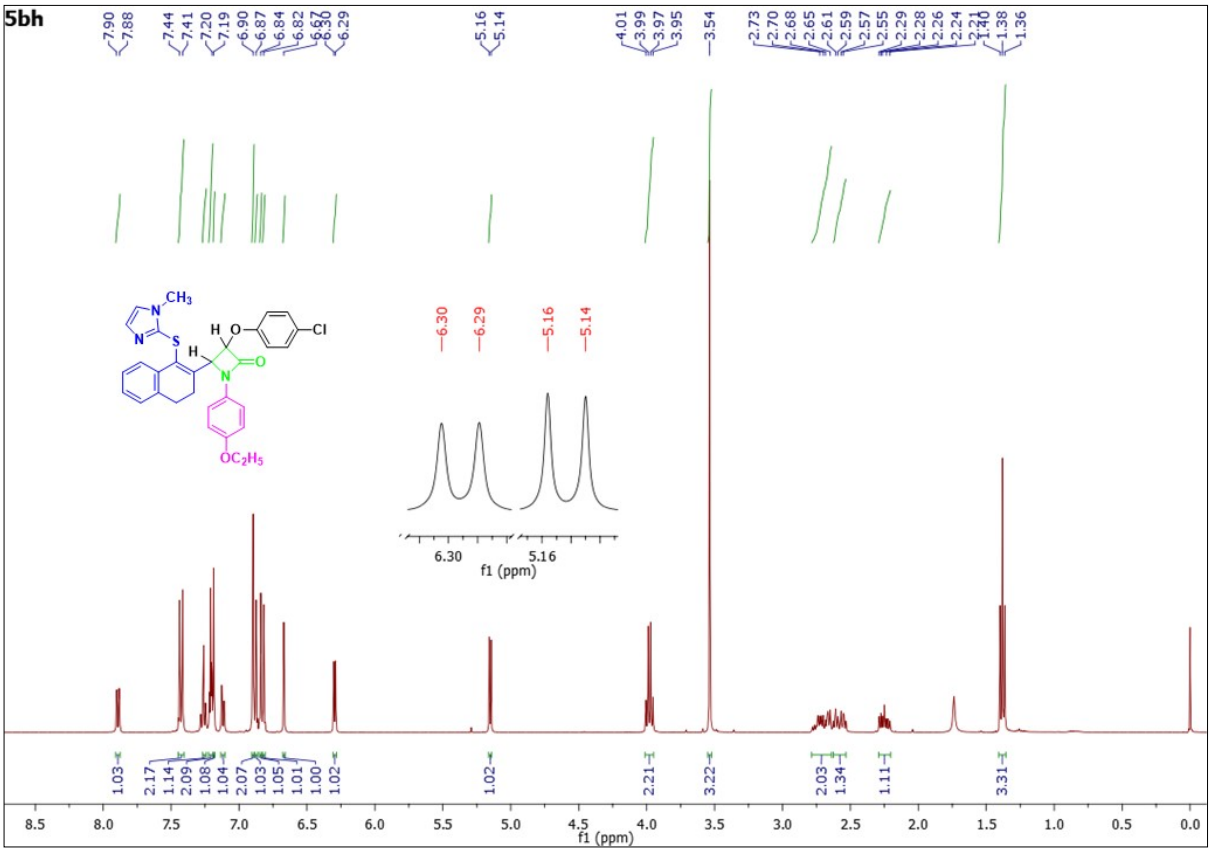
^{1}H NMR spectra, ^{13}C NMR spectra, and HRMS data of compound (5bg)

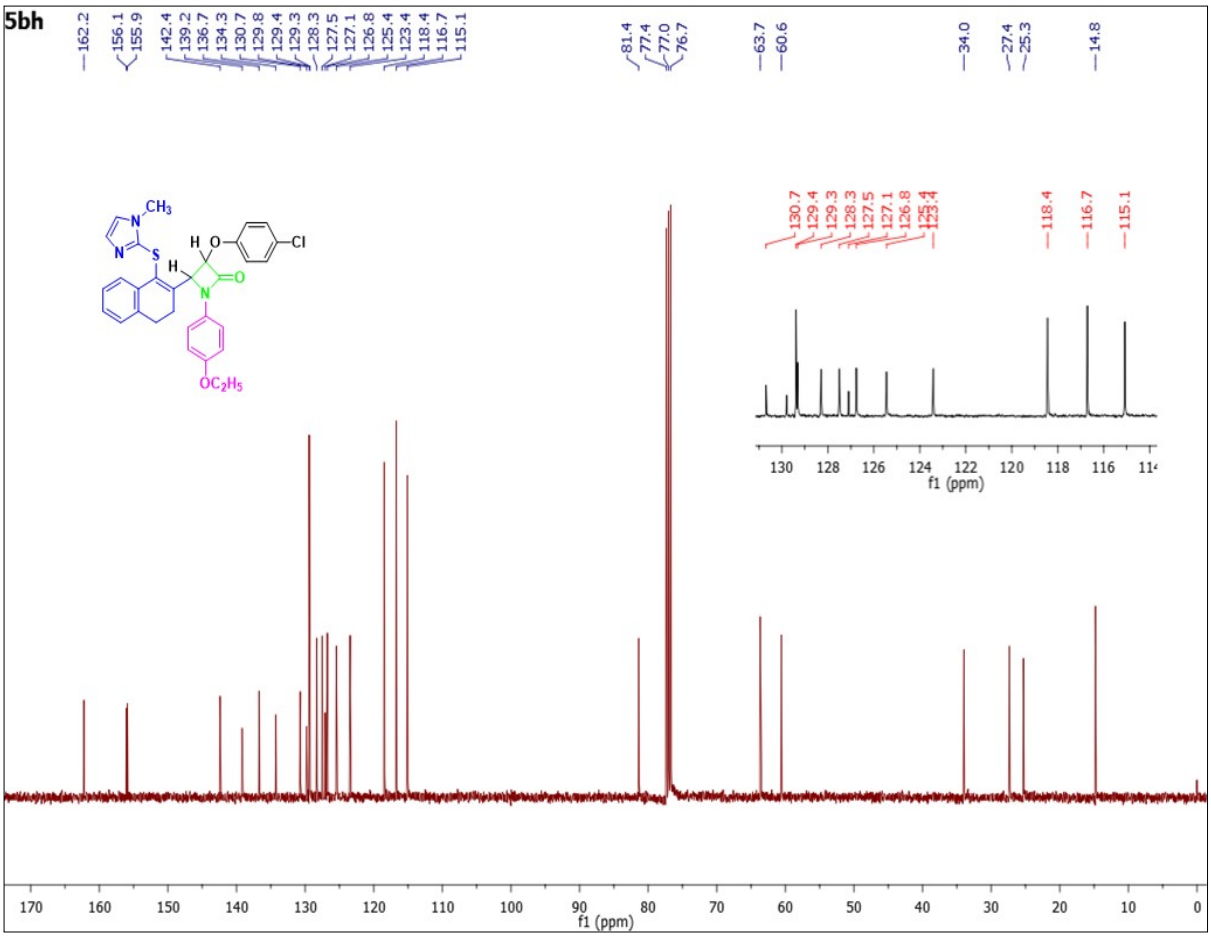


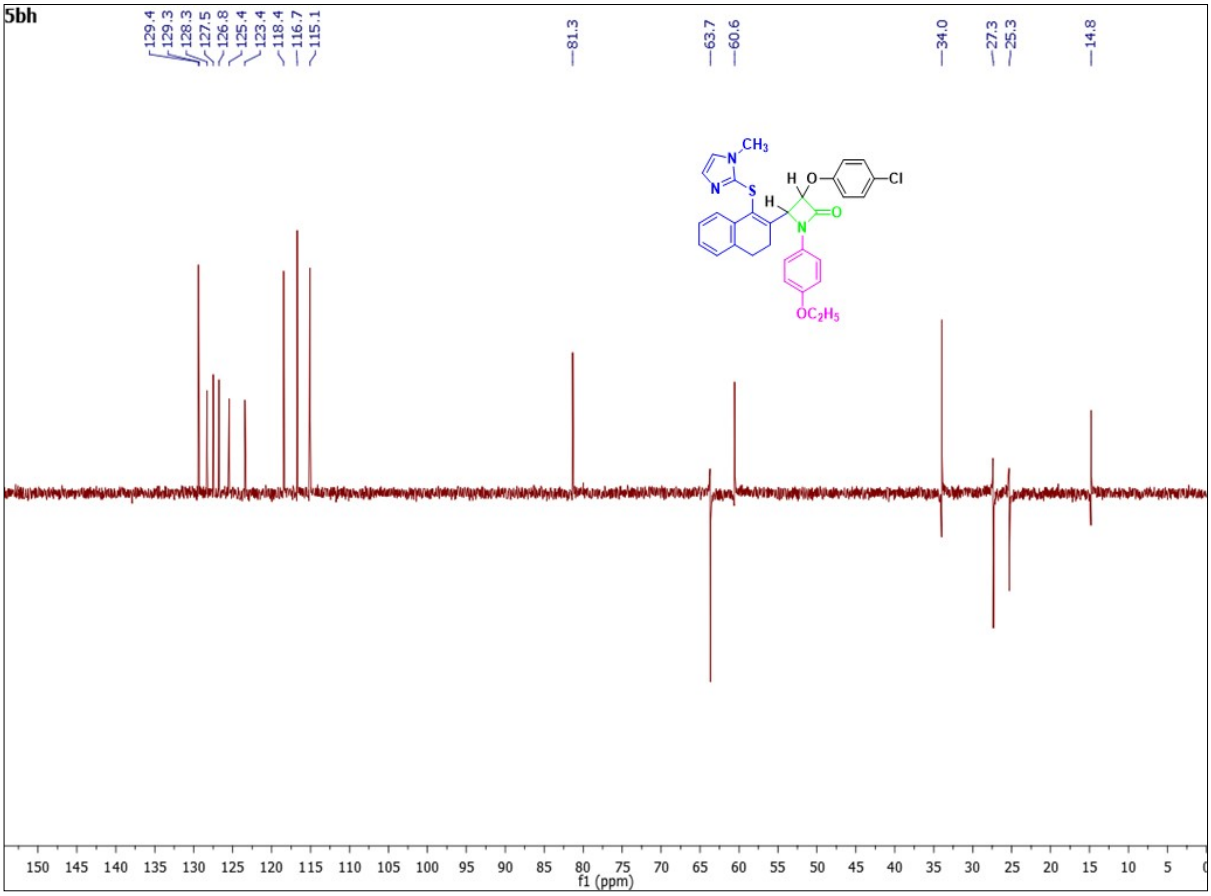


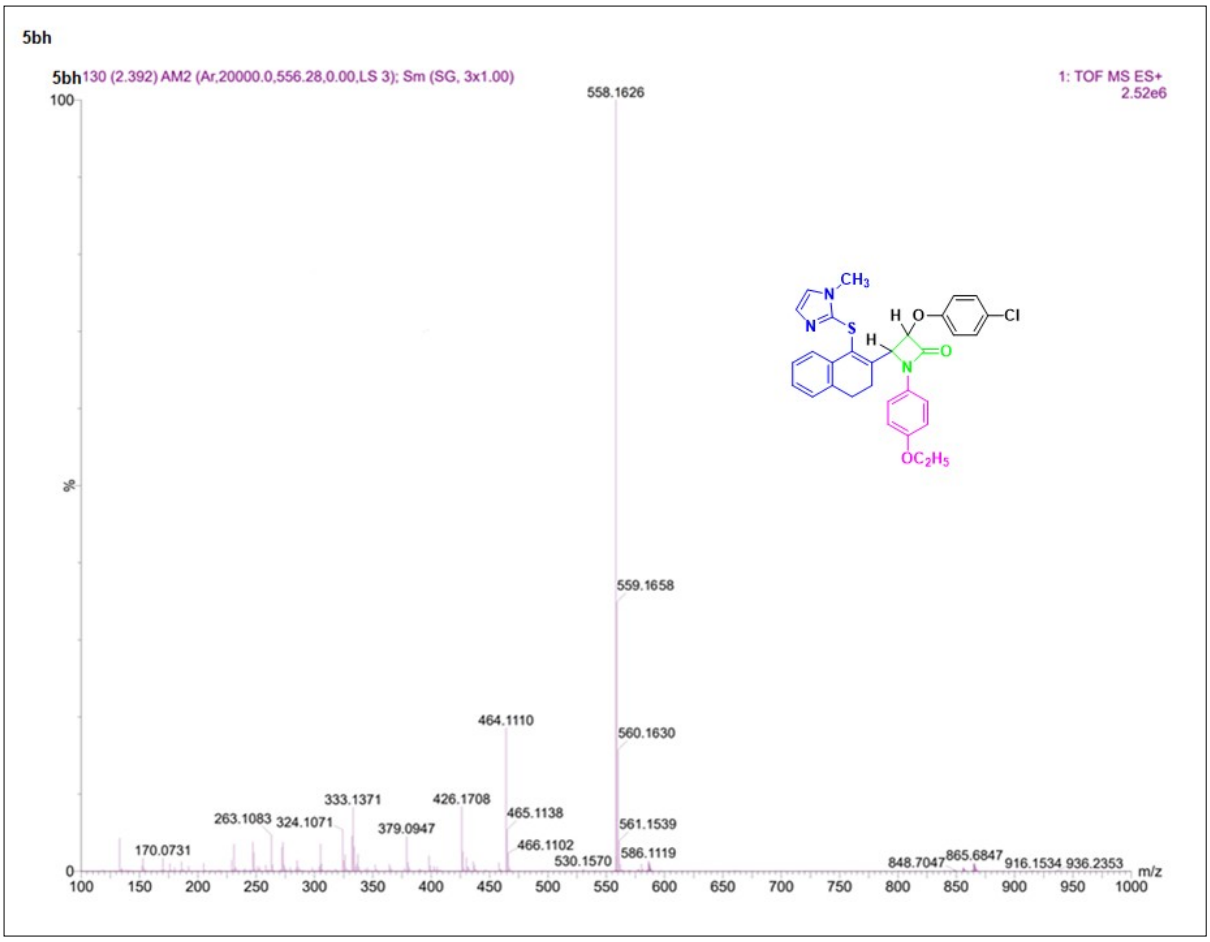


^{1}H NMR spectra, ^{13}C NMR spectra, DEPT-135 spectra, and HRMS data of compound (5bh)

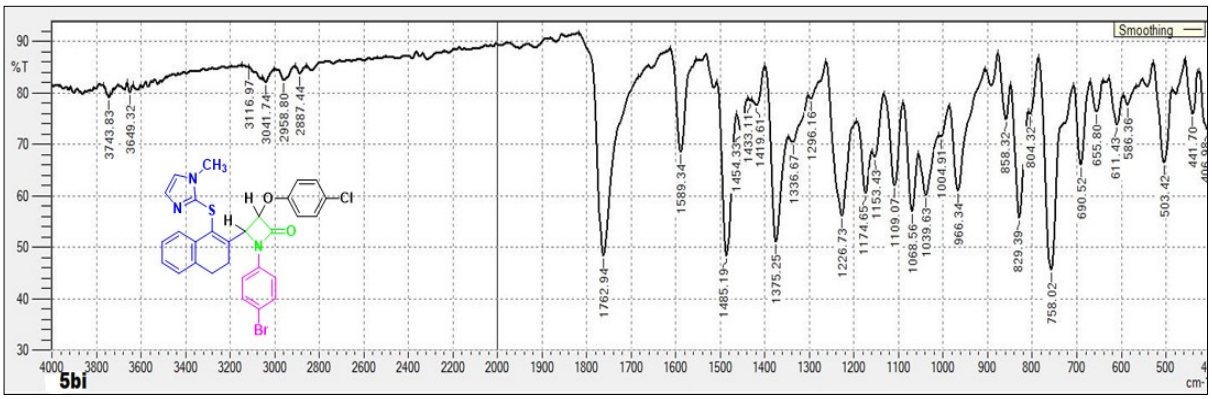


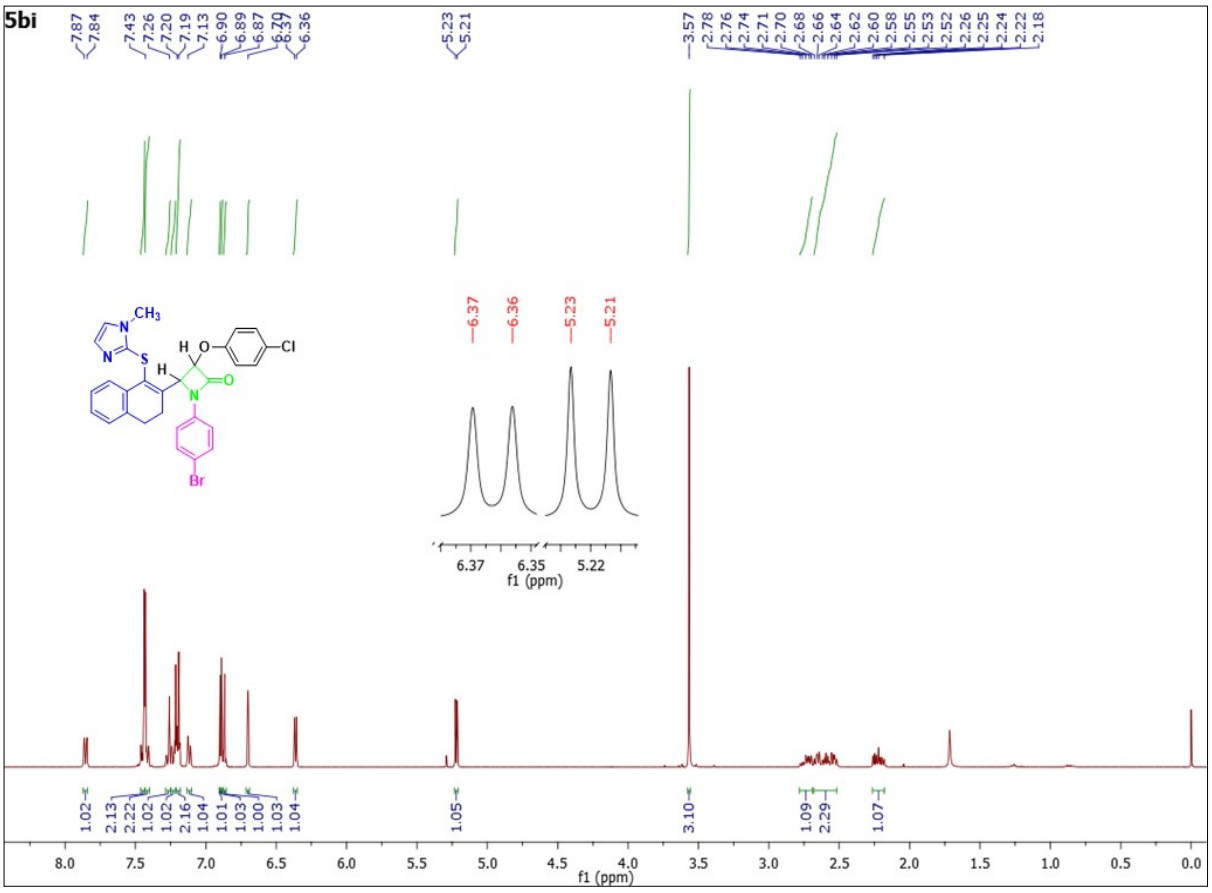

5bh
162.2
156.1
155.9
142.4
139.2
136.7
134.3
130.7
129.8
129.4
129.3
128.3
127.5
127.1
126.8
125.4
123.4
118.4
116.7
115.1
81.4
77.4
77.0
76.7
63.7
60.6
34.0
27.4
25.3
14.8
f1 (ppm)

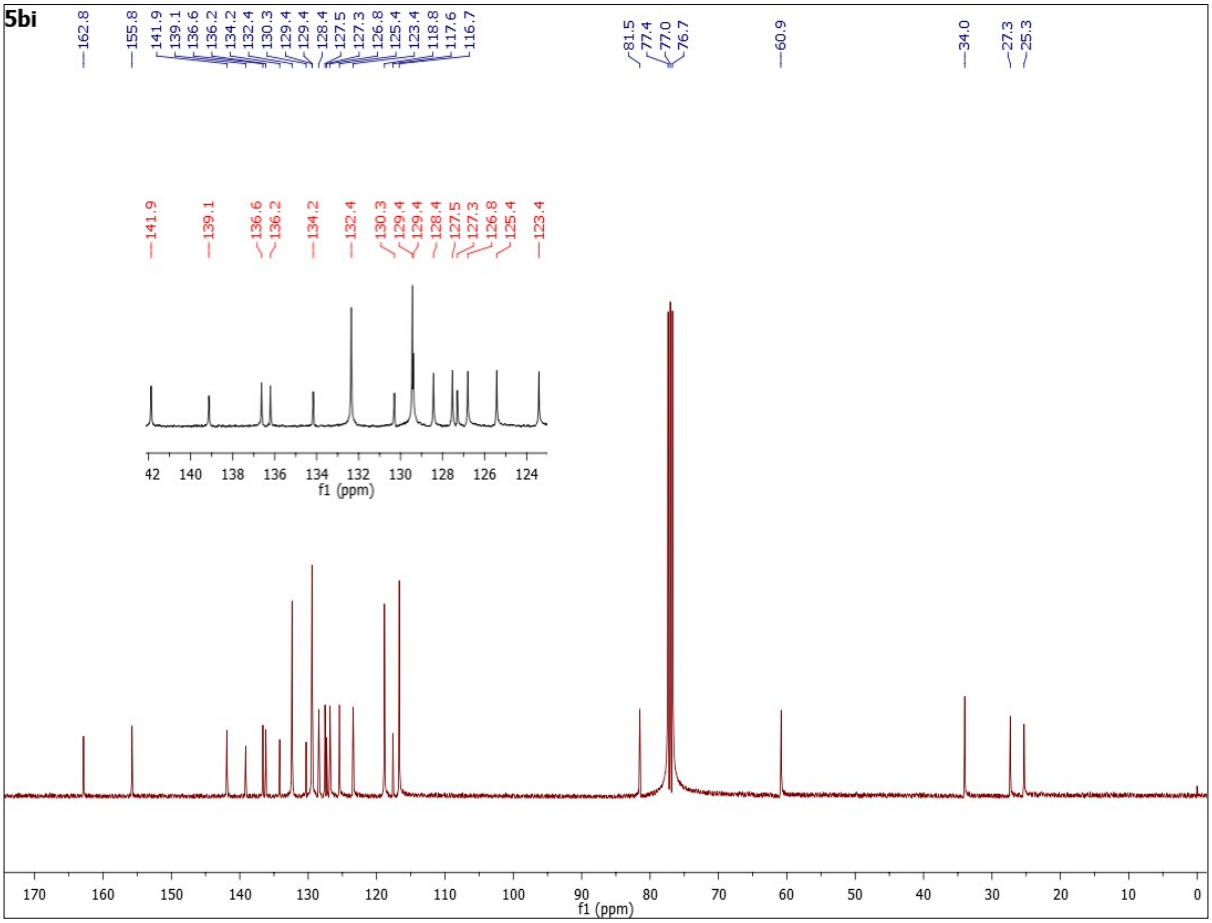

5bh
129.4
129.3
128.3
127.5
126.8
125.4
123.4
118.4
116.7
115.1
81.3
63.7
60.6
34.0
27.3
25.3
14.8
f1 (ppm)

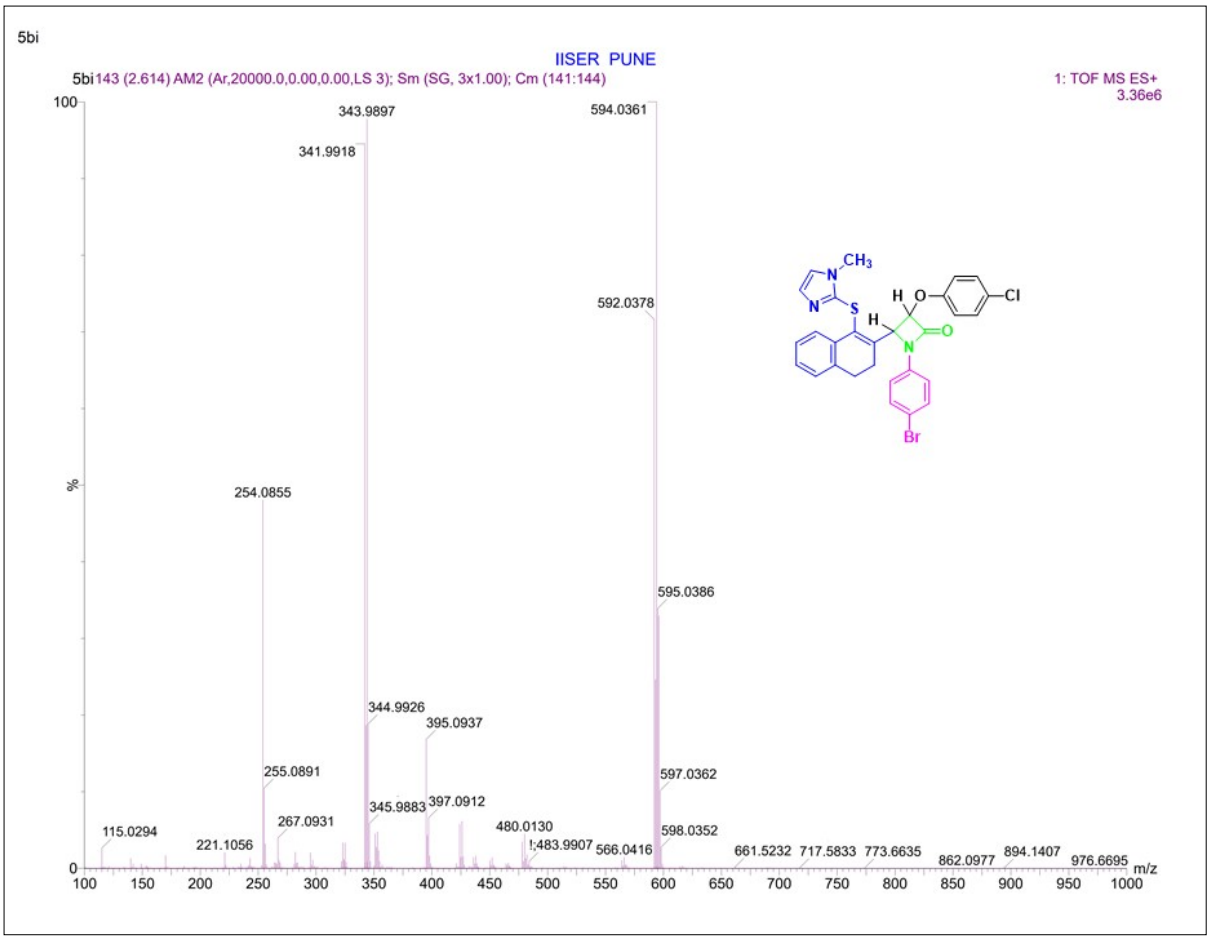


FT-IR, ^{1}H NMR spectra, ^{13}C NMR spectra, DEPT-135 spectra, and HRMS data of compound (5bi)




5bi
7.87
7.84
7.43
7.26
7.20
7.19
7.13
6.90
6.89
6.87
6.36
5.23
5.21
3.57
2.78
2.76
2.74
2.71
2.70
2.68
2.66
2.64
2.62
2.60
2.58
2.55
2.53
2.52
2.26
2.25
2.24
2.22
2.18
6.37
6.36
5.23
5.21
6.37
6.35
5.22
f1 (ppm)
1.02
2.13
2.22
1.02
1.02
2.16
1.04
1.01
1.03
1.00
1.03
1.04
1.05
3.10
1.09
2.29
1.07
f1 (ppm)


5bi
162.8
155.8
141.9
139.1
136.6
136.2
134.2
132.4
130.3
129.4
129.4
128.4
127.5
127.3
126.8
125.4
123.4
118.8
117.6
116.7
81.5
77.4
77.0
76.7
60.9
34.0
27.3
25.3
141.9
139.1
136.6
136.2
134.2
132.4
130.3
129.4
129.4
128.4
127.5
127.3
126.8
125.4
123.4
f1 (ppm)
f1 (ppm)


5bi
IISER PUNE
5bi143 (2.614) AM2 (Ar,20000.0,0.00,0.00,LS 3); Sm (SG, 3x1.00); Cm (141:144)
1: TOF MS ES+
3.36e6
100
%
0
343.9897
341.9918
594.0361
592.0378
254.0855
595.0386
344.9926
395.0937
255.0891
597.0362
345.9883
397.0912
267.0931
480.0130
598.0352
115.0294
221.1056
483.9907
566.0416
661.5232
717.5833
773.6635
862.0977
894.1407
976.6695
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
CH3
N
N
S
H
O
H
O
Cl
N
Br

4. Report for a single crystal XRD of compound (5ad) and (5ae)

The name, crystal data of compounds (5ad) and (5ae)

4-(1-((1-methyl-1*H*-imidazol-2-yl)thio)-3,4-dihydronaphthalen-2-yl)-3-phenoxy-1-(p-tolyl)azetidin-2-one (**5ad**)

1-(4-chlorophenyl)-4-(1-((1-methyl-1*H*-imidazol-2-yl)thio)-3,4-dihydronaphthalen-2-yl)-3-phenoxyazetidin-2-one (**5ae**)

Table 1: The crystal data and structure refinement of the compounds (**5ad**) and (**5ae**)

Compound	**5ad**	**5ae**
Empirical formula	$C_{30}H_{27}N_3O_2S$	$C_{29}H_{24}ClN_3O_2S$
Formula weight	493.6250	514.0400
Temperature (K)	135	232
Wave length (Å)	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic
Space group	P -1	P -1
Unit cell dimensions		
a (Å)	10.3342 (16) Å	10.440 (3) Å
b (Å)	11.9217 (19) Å	11.519 (3) Å
c (Å)	12.4260 (16) Å	12.207 (3) Å
α (°)	115.186 (4)	112.745 (10)
β (°)	111.605 (4)	91.875 (10)
γ (°)	92.280 (6)	106.279 (9)
Volume ($Å^3$)	1252.4 (3)	1282.9 (6)
D calc. (g/cm^{-3})	1.593	1.717
Z	16	12
Absorption coefficient (mm^{-1})	0.762	1.192
F (000)	608.0	660.0
Crystal size (mm)	0.23×0.39×0.73	0.48×0.37×0.82
υ Range for data collection (°)	2.335-24.998	2.335-24.997
Limiting index	h = -12 → 12	h = -12 → 12
	k = -14 → 14	k = -13 → 13
	l = -14 → 14	l = -14 → 14
Reflections collected/ unique [R_{int}]	4333/3881 [0.0772]	4483/3681[0.0741]
Completeness to θ	24.998-98.1%	24.997-98.9%
Absorption correction	Multi-scan	Multi-scan
Max. and min. transmission	0.690 and 0.595	0.645 and 0.595
Refinement method	Full-matrix	Full-matrix
	Least-squares	Least-squares
Data/restraints/parameters	4333/0/327	4483/0/326
Goodness-to-fit on F^2	1.018	1.332
Final R index [1>2 σ(I)]	R_1 = 0.0772,	R_1 = 0.0741,
	${}_wR_2$ = 0.2199	${}_wR_2$ = 0.2147
R index (all data)	R_1 = 0.0772,	R_1 = 0.0741,
	${}_wR_2$ = 0.2199	${}_wR_2$ = 0.2147
Largest diff. peak and hole ($e.Å^{-3}$)	0.680 and -0.450	0.630 and -0.455

5. Structure of the compound (5ad)

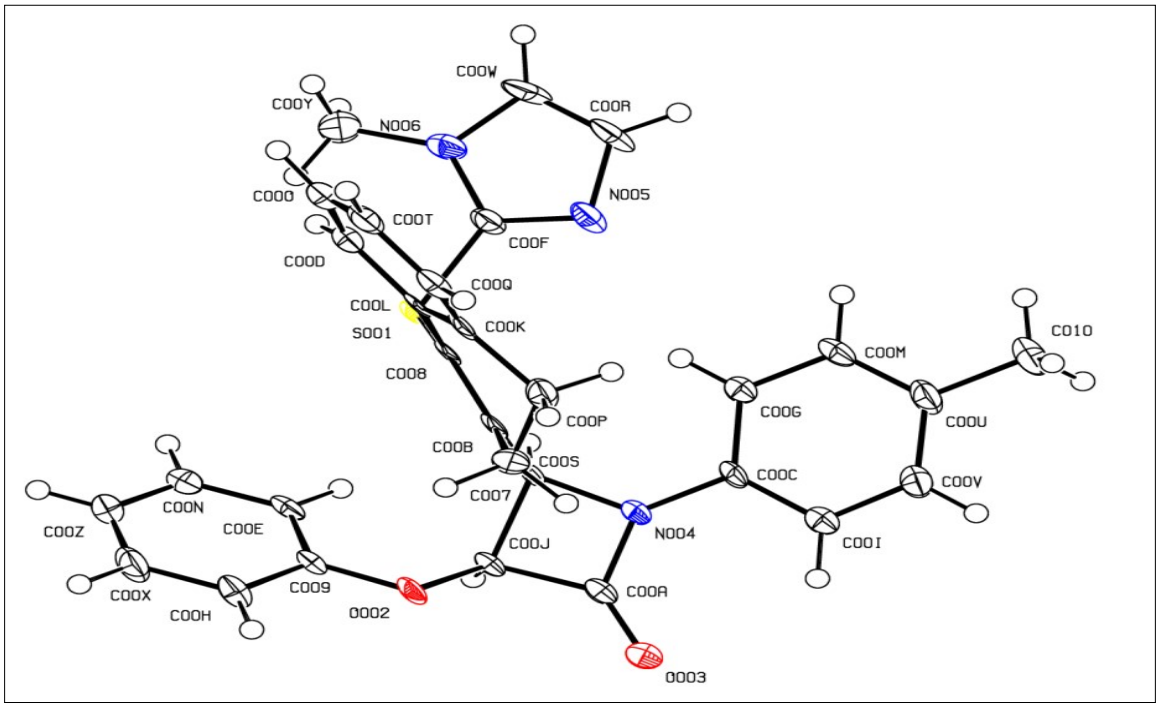


Figure 1: ORTEP diagram of compound **5ad** (**2065586**).

6. Structure of the compound (5ae)

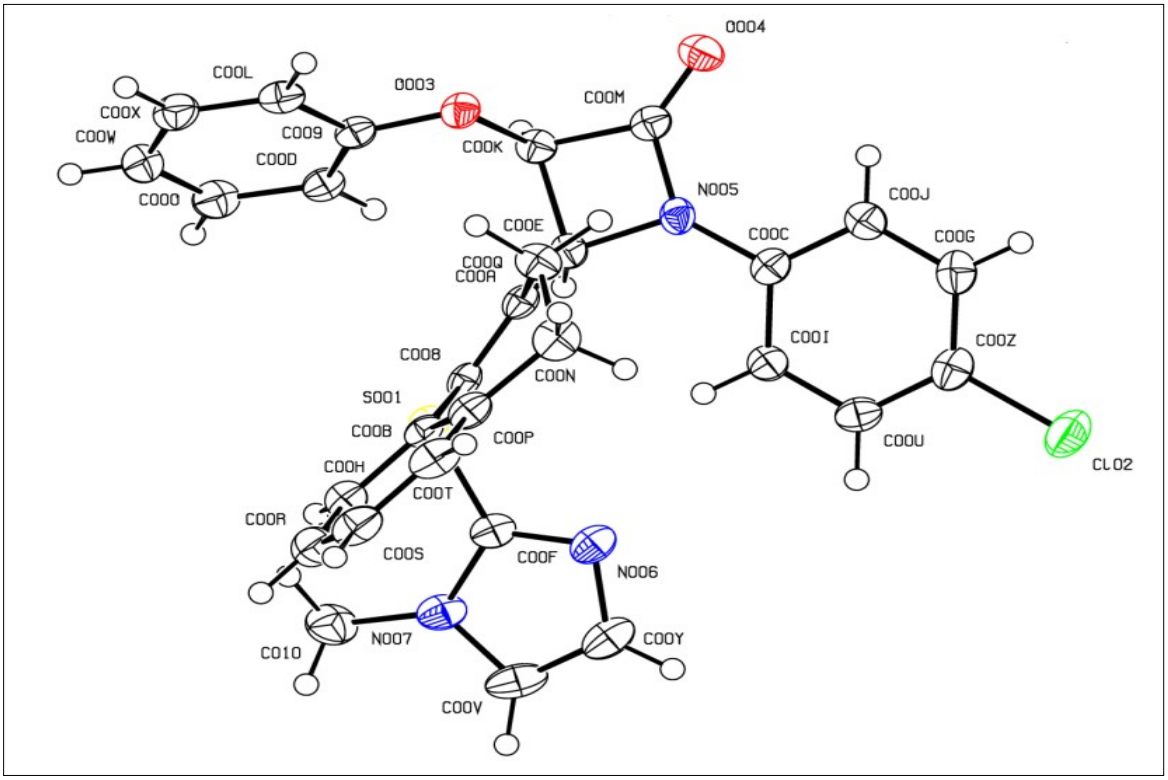


Figure 2: OETEP diagram of compound **5ae** (**2065587**).