Supporting Information

Rapid Access to Benzimidazo[1,2-*a*]quinoline Fused Isoxazoles *via* Pd(II)-Catalyzed Intramolecular Cross Dehydrogenative Coupling: Synthetic Versatility and Photophysical Studies

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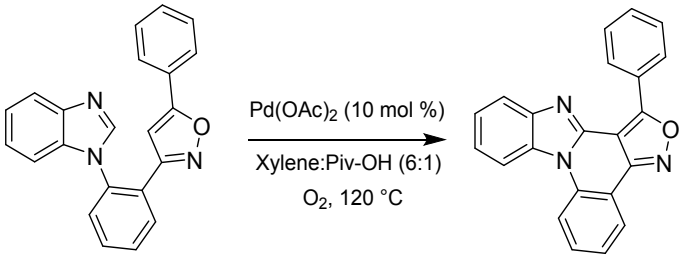
III) Mechanistic studies:

i) Determination of the kinetic isotope effect (k_H/k_D): (Parallel experiment)

As per the general procedure two parallel reactions were performed using **2a** or **2a-C_2D**. The reaction was carried out using **2a** or **2a-C_2D** (1 mmol), 10 mole % $Pd(OAc)_2$, xylene (1.2 ml) pivalic acid (0.2 ml) and allowed to rotate at 120 ˚C under oxygen atmosphere. Nitromethane (5 µl in 12 ml $CDCl_3$) was used as an internal standard in reaction mixture. Samples of 50 µL each were withdrawn from the reaction mixture after every 2 hour and analysed by ^{1}H-NMR.



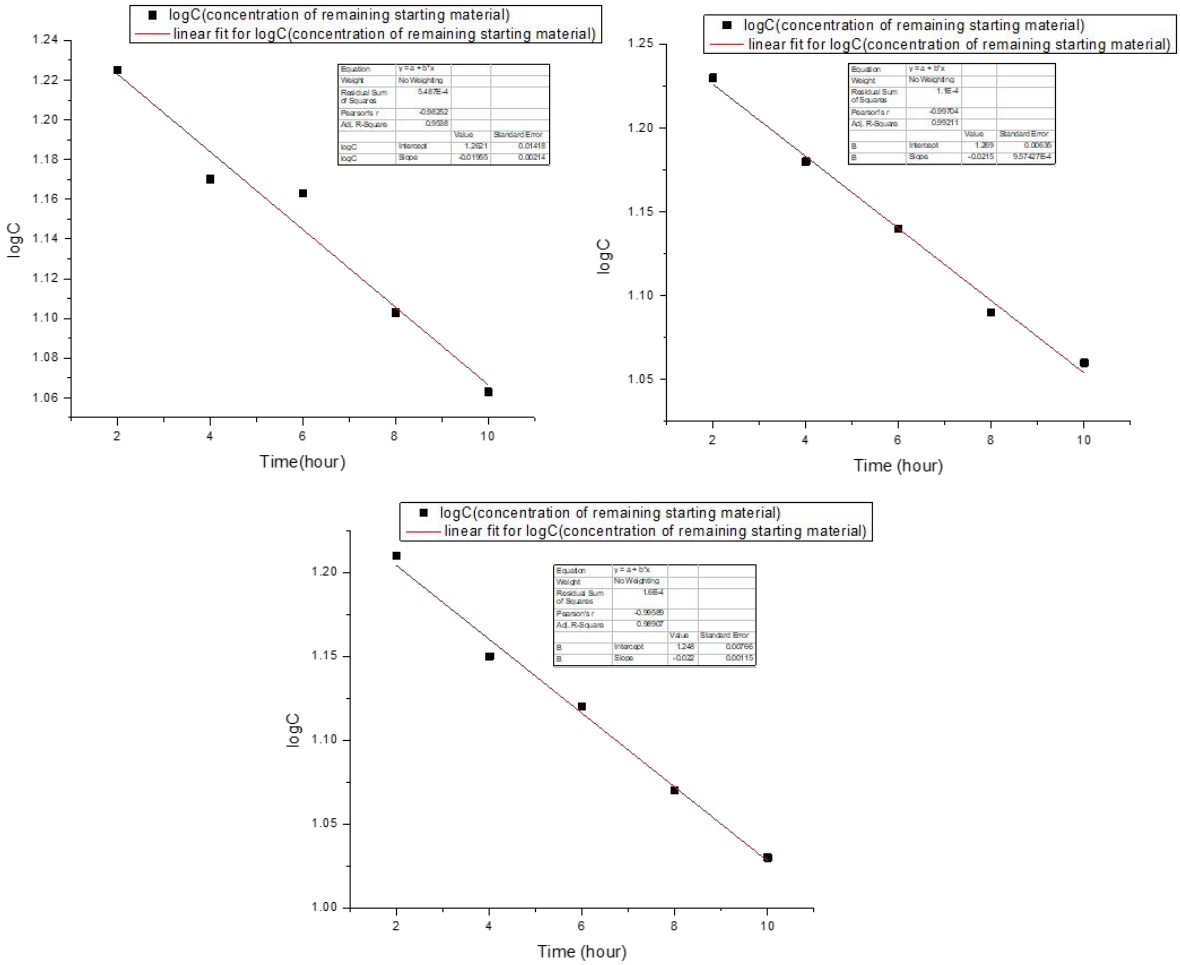
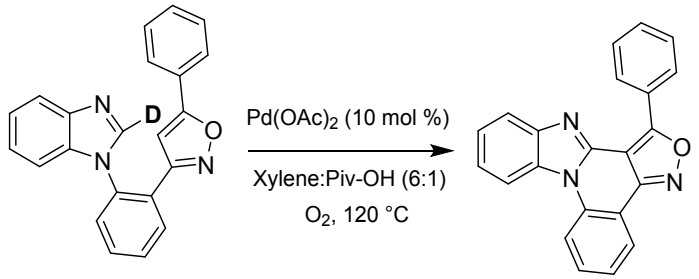


Figure S1 Initial rate measurement w.r.t C-H substrate for the determination of KIE



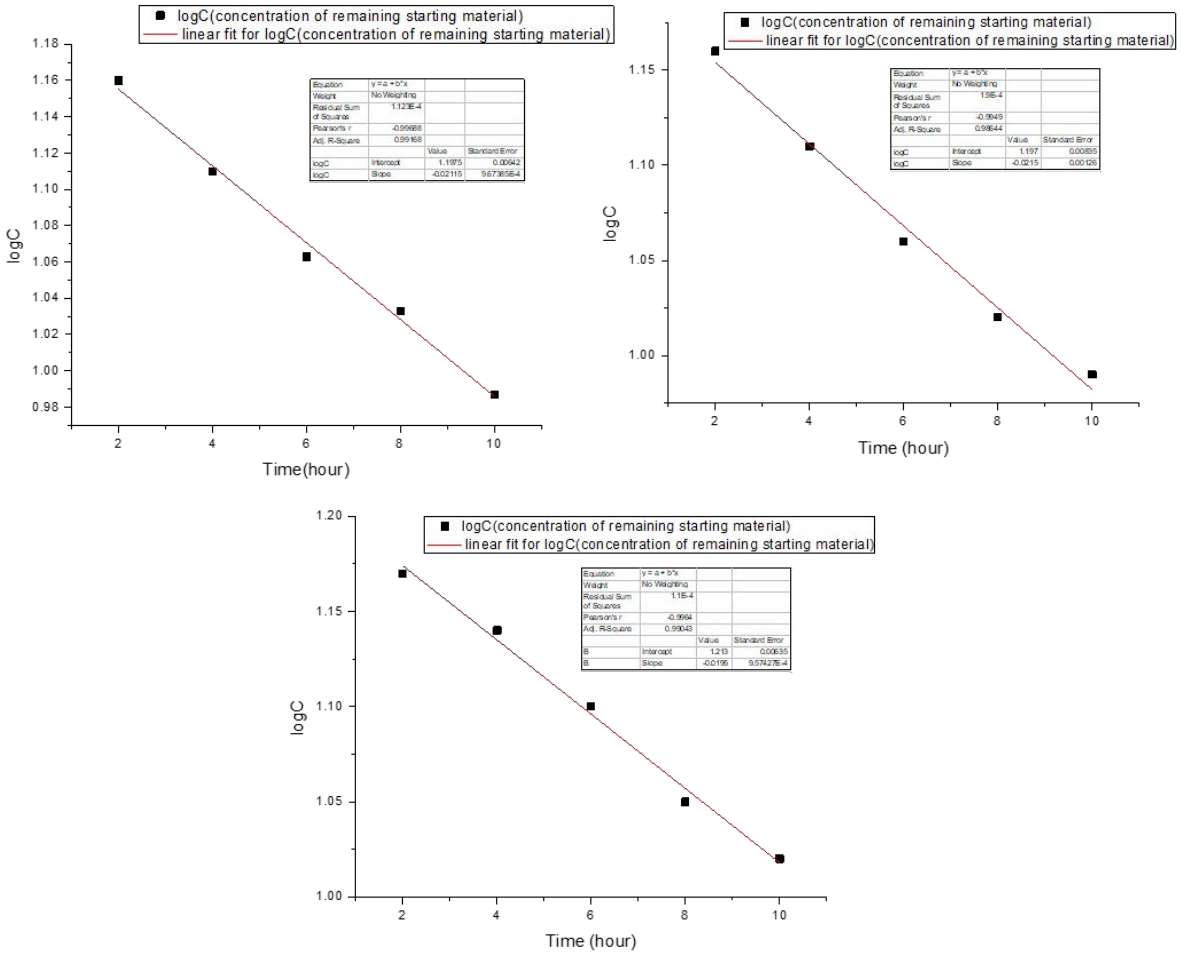
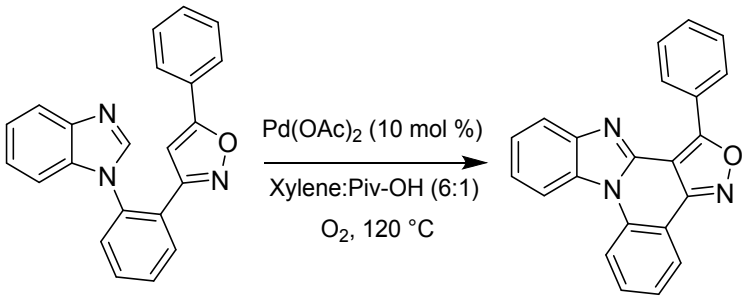


Figure S2 Initial rate measurement w.r.t C-D substrate for the determination of KIE

Kinetic isotope effect K_H/K_D = 1.01 (Average value of 3 experiment)

(ii) Determination of the kinetic isotope effect (k_H/k_D): (Parallel experiment)

As per the general procedure two parallel reactions were performed using **2a** or **2a-C_4D**. The reaction was carried out using **2a** or **2a-C_4D** (1 mmol), 10 mole % $Pd(OAc)_2$, xylene (1.2 ml) pivalic acid (0.2 ml) and allowed to rotate at 120 °C under oxygen atmosphere. Nitromethane (5 µl in 12 ml $CDCl_3$) was used as an internal standard in reaction mixture. Samples of 50 µL each were withdrawn from the reaction mixture after every 2 hour and analysed by ^{1}H-NMR.



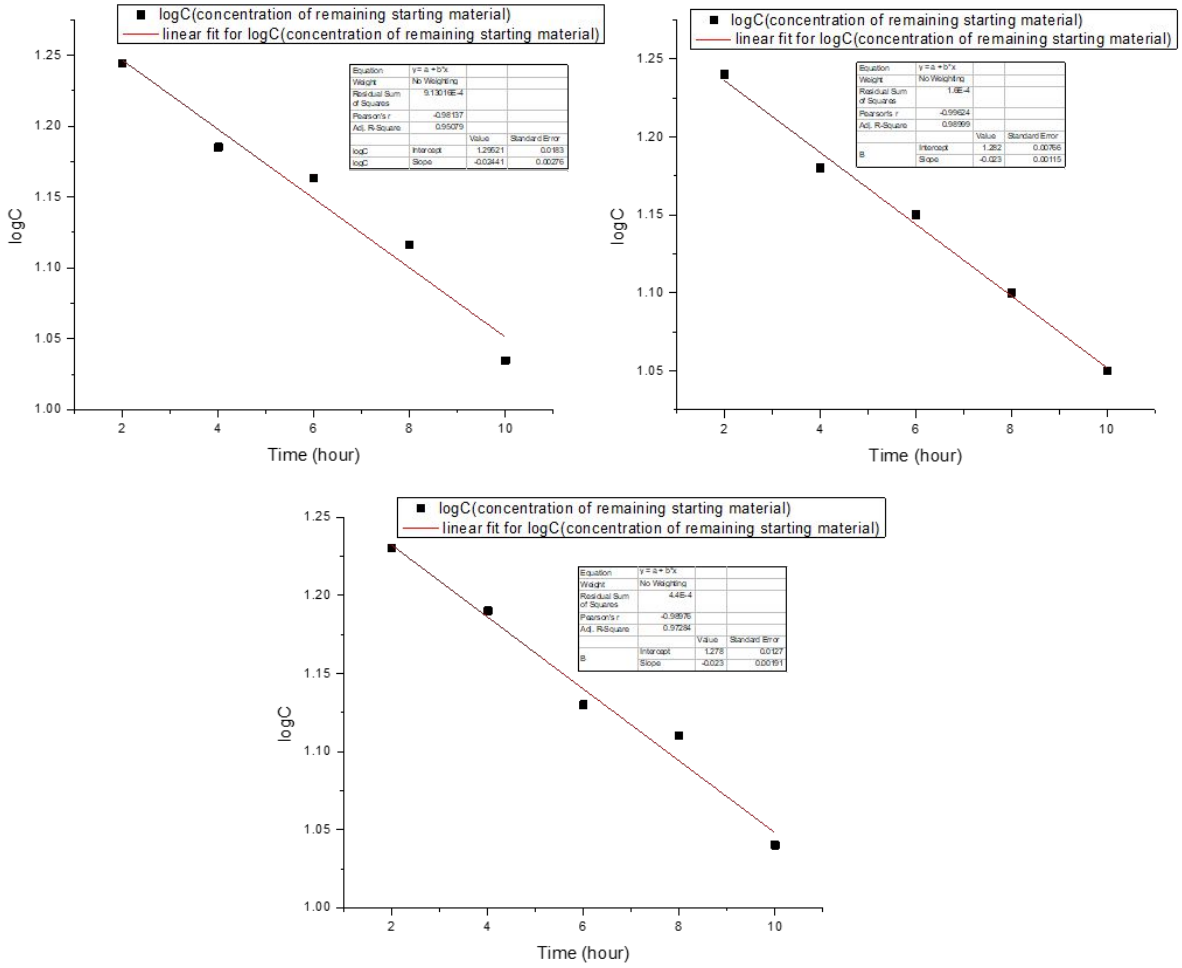
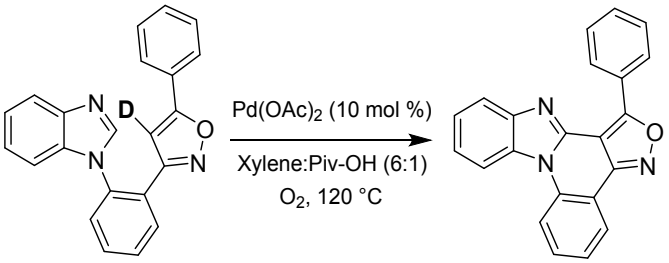


Figure S3 Initial rate measurement w.r.t C-H substrate for the determination of KIE



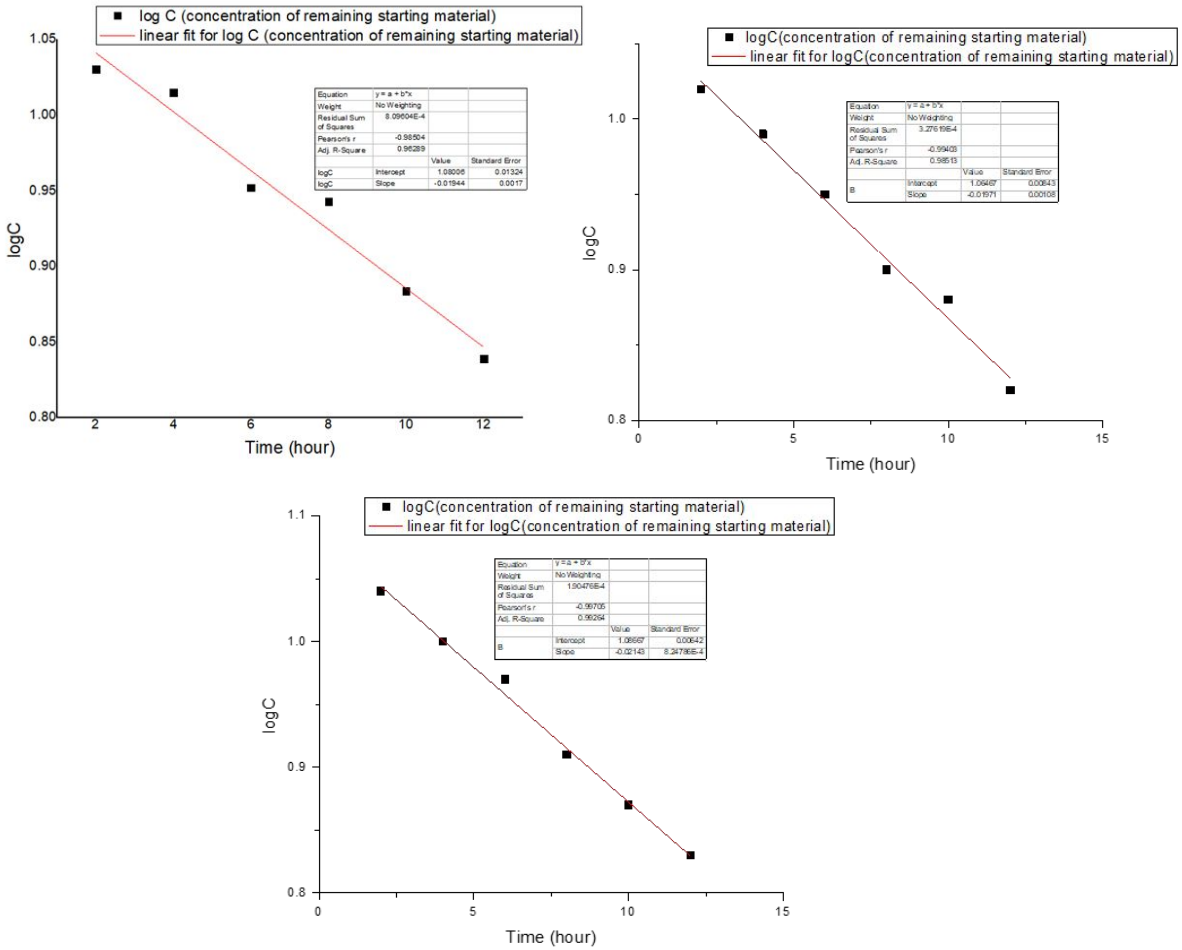
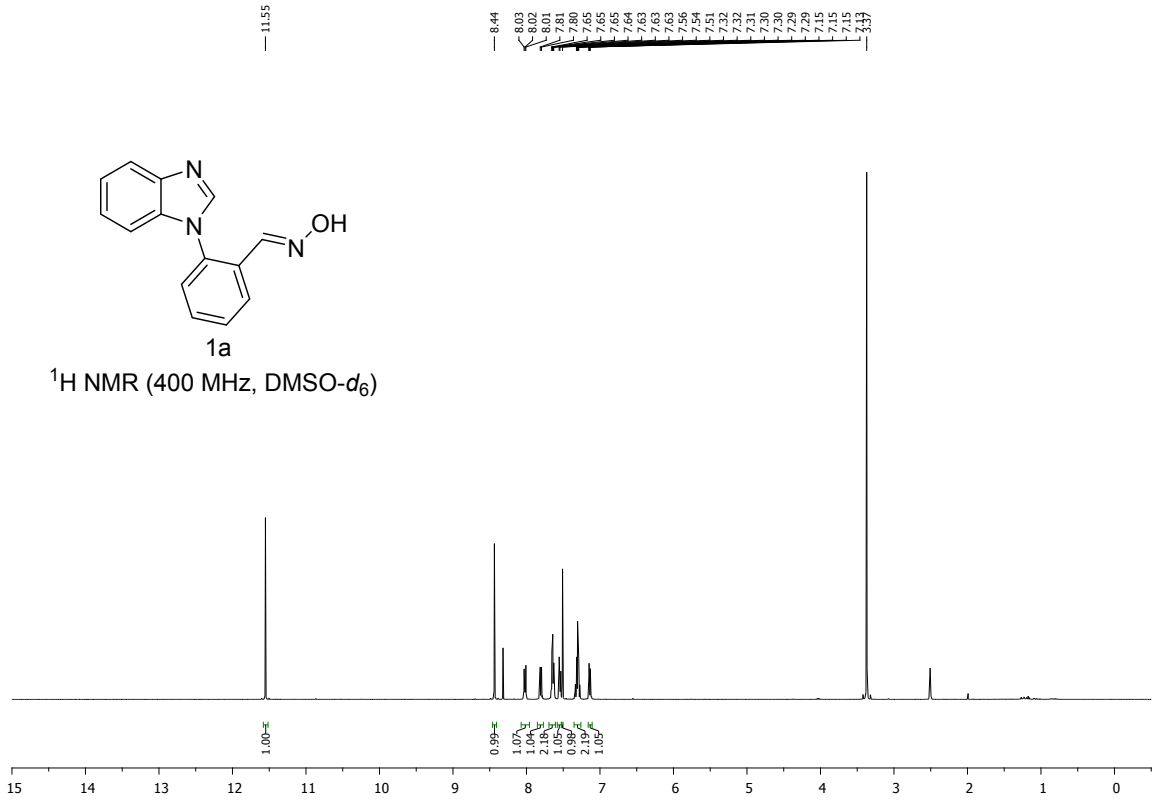


Figure S4 Initial rate measurement w.r.t C-D substrate for the determination of KIE

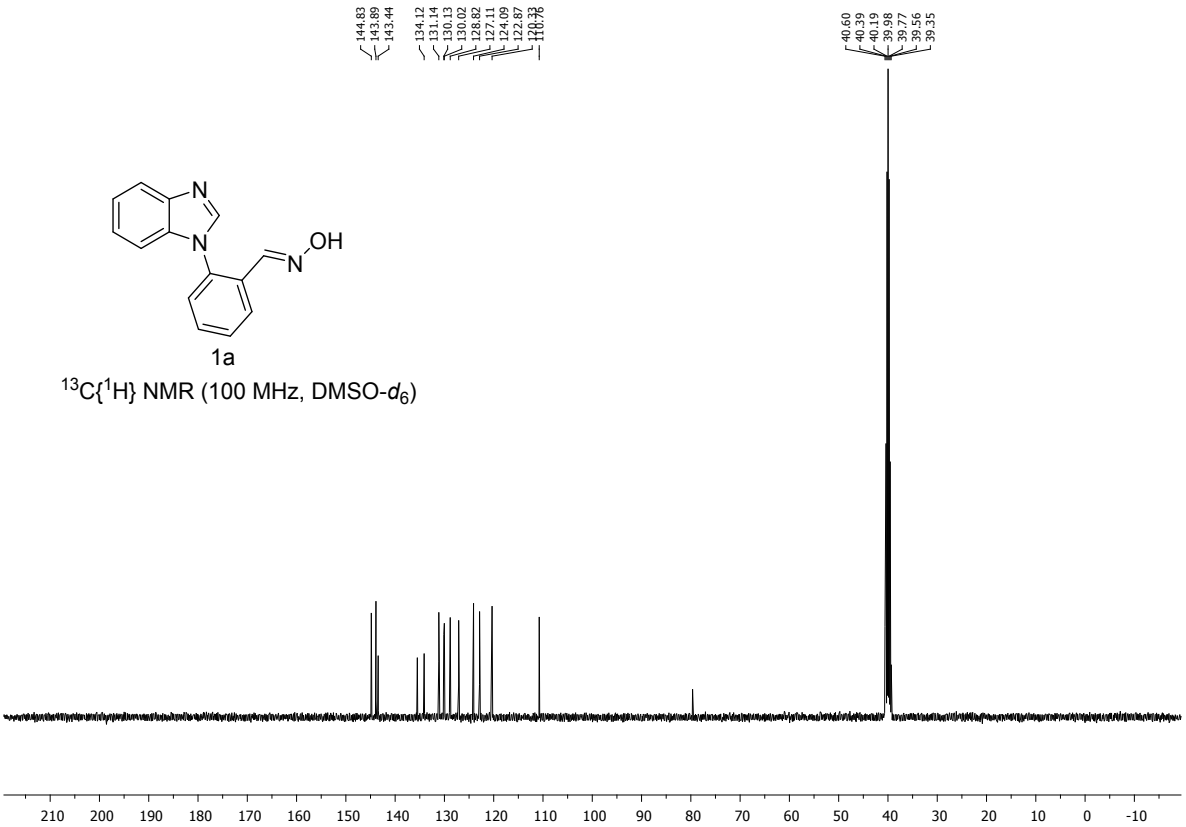
Kinetic isotope effect K_H/K_D = 1.17 (Average value of three experiment)

V) Copy of ^{1}H NMR and ^{13}C NMR Spectres



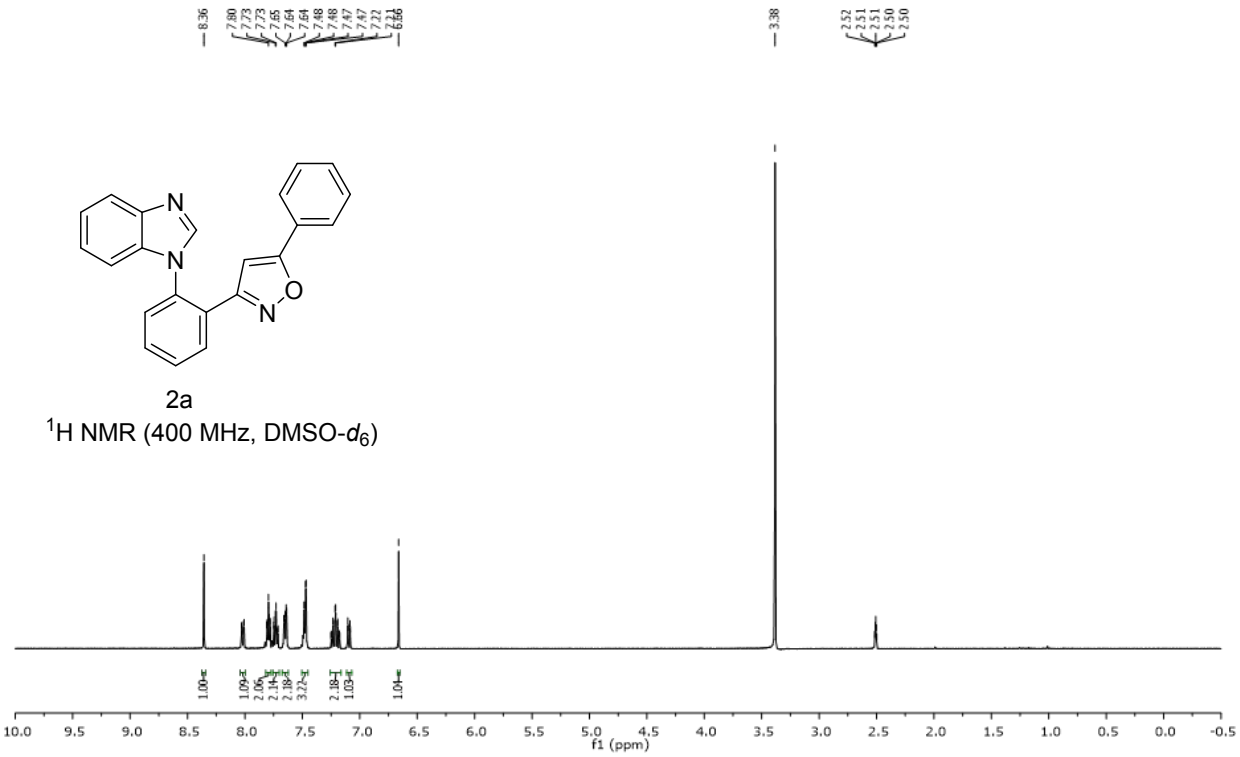
1a

^{1}H NMR (400 MHz, DMSO-d_6)



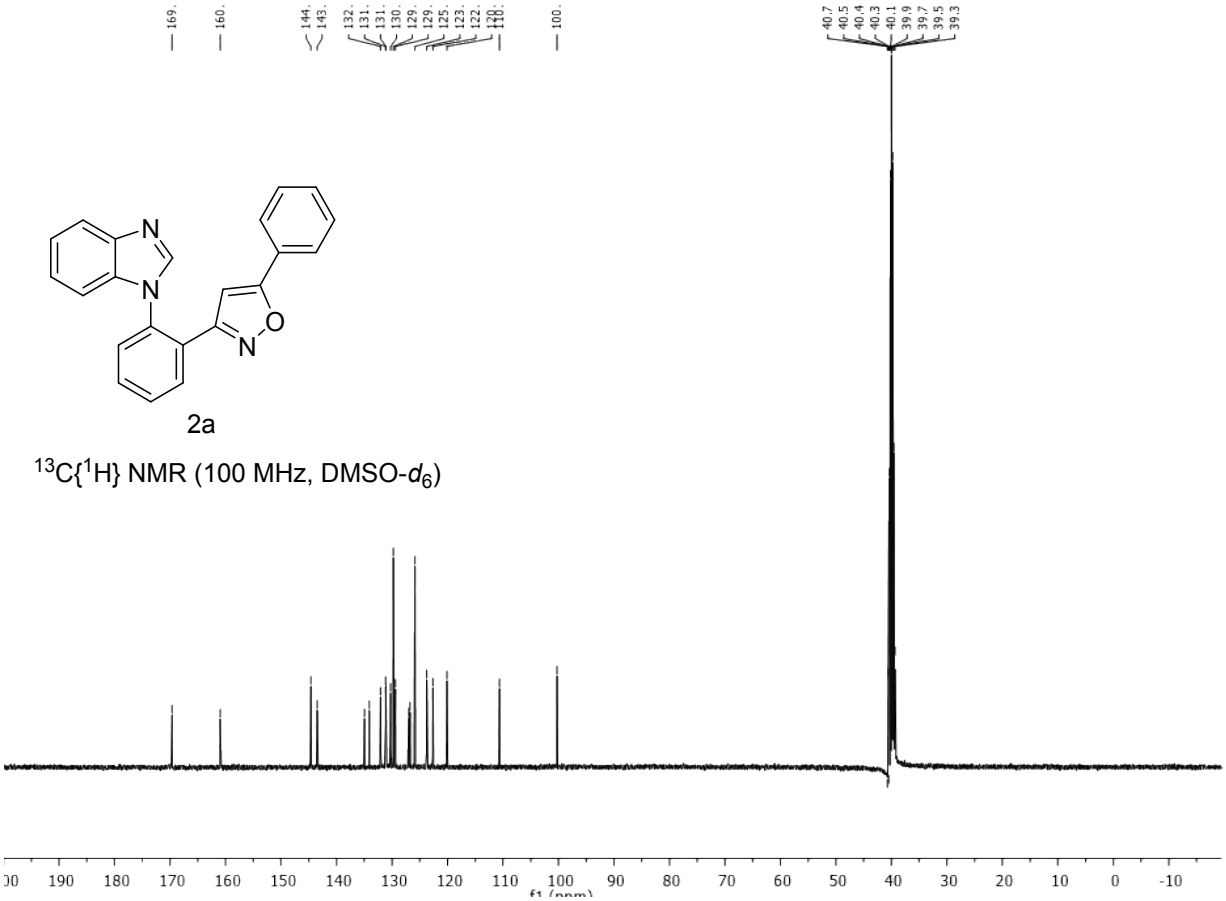
1a

^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6)



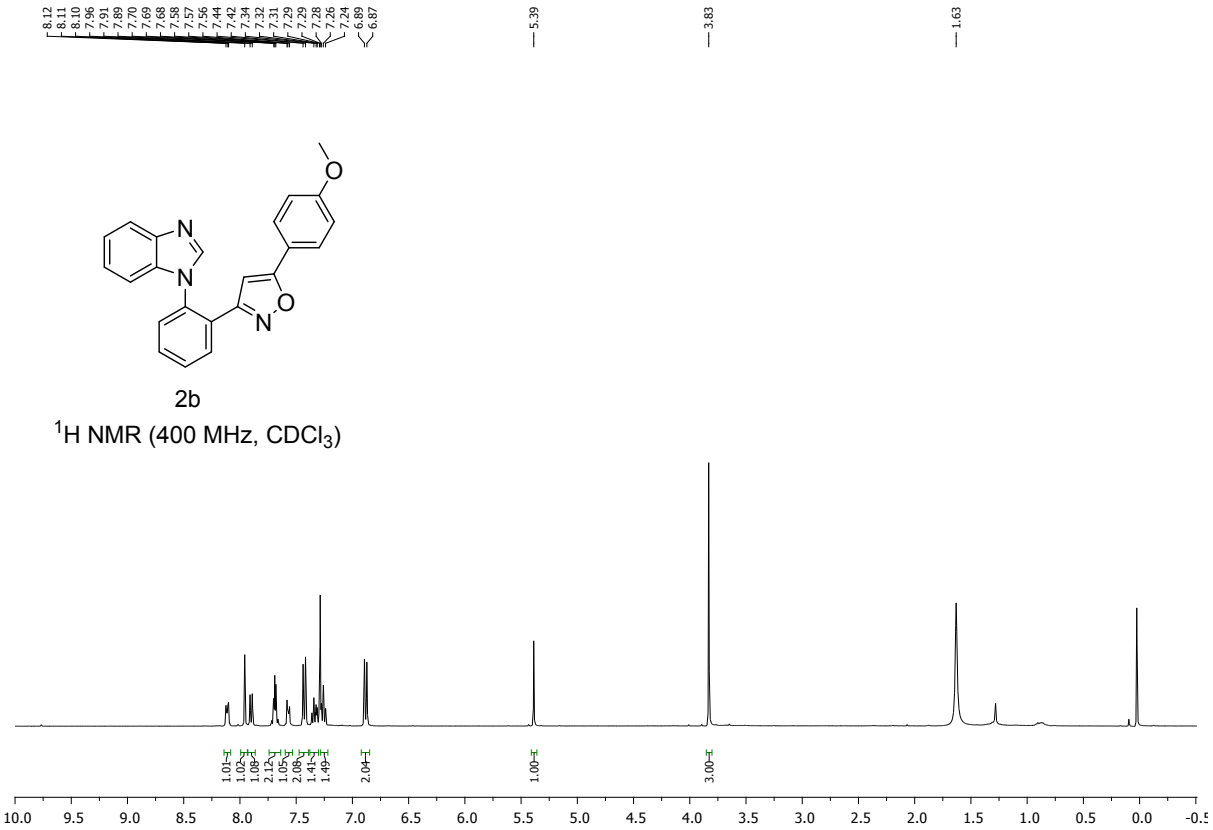
2a

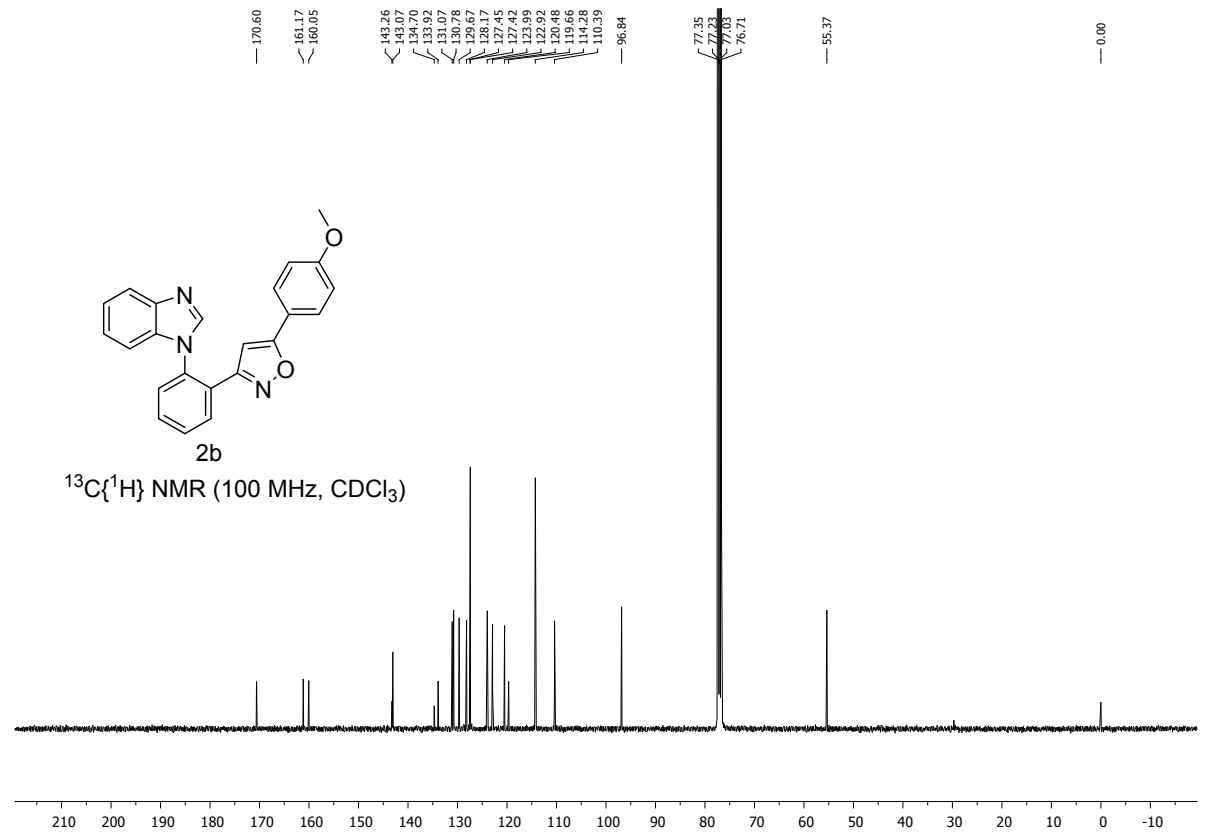
^{1}H NMR (400 MHz, DMSO-d_6)

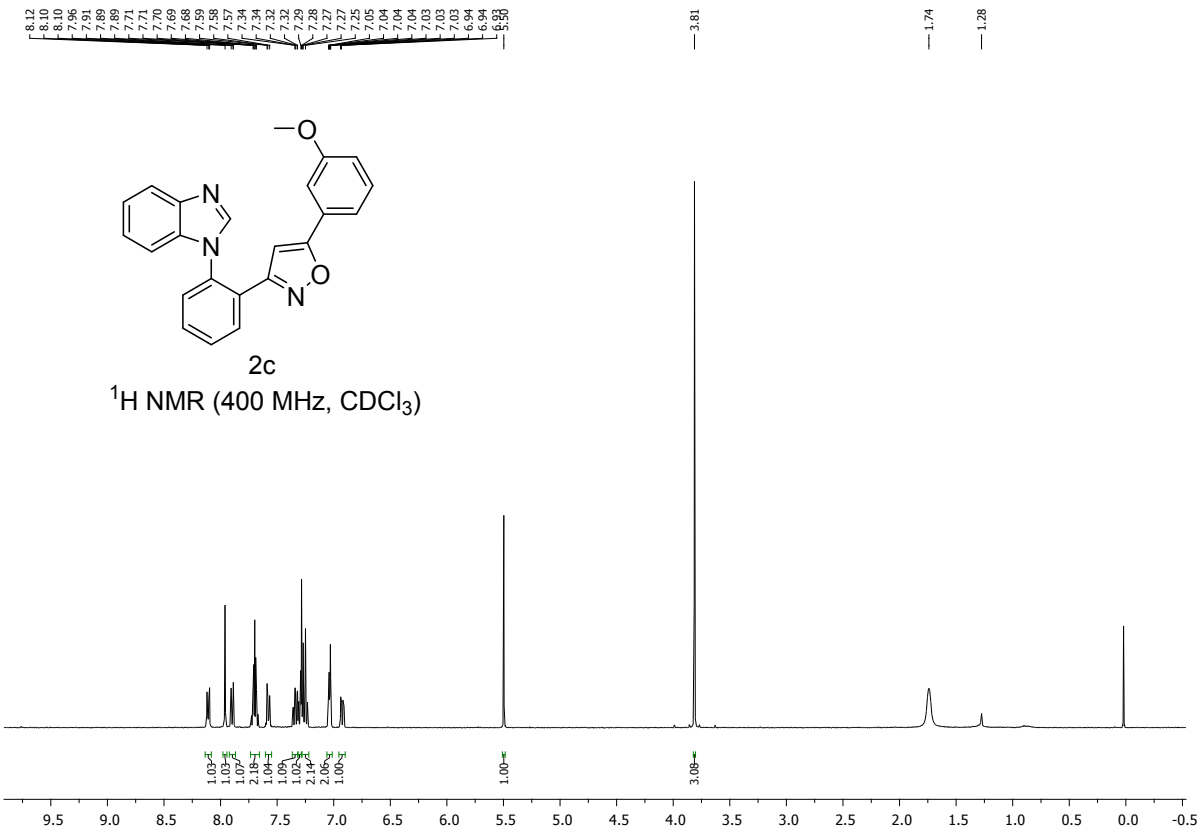


2a

^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6)

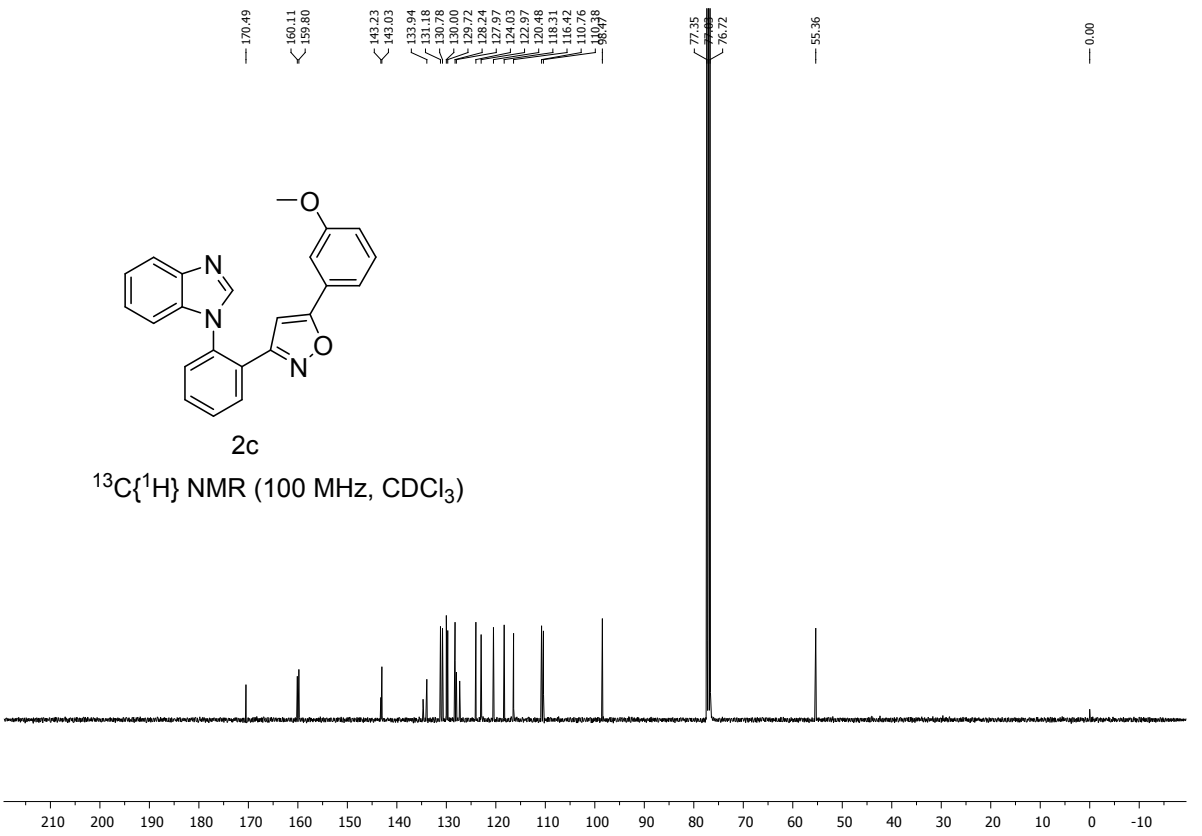

8.12
8.11
8.10
7.96
7.91
7.89
7.70
7.69
7.68
7.58
7.57
7.56
7.44
7.42
7.34
7.32
7.31
7.29
7.29
7.28
7.26
7.24
6.89
6.87
5.39
3.83
1.63
N
N
O
N
O
2b
^{1}H NMR (400 MHz, $CDCl_3$)
1.01
1.02
1.08
2.12
1.05
2.08
1.41
1.49
2.04
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


170.60
161.17
160.05
143.26
143.07
134.70
133.92
131.07
130.78
129.67
128.17
127.45
127.42
123.99
122.92
120.48
119.66
114.28
110.39
96.84
77.35
77.23
77.03
76.71
55.37
0.00
N
N
O
N
O
2b
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10



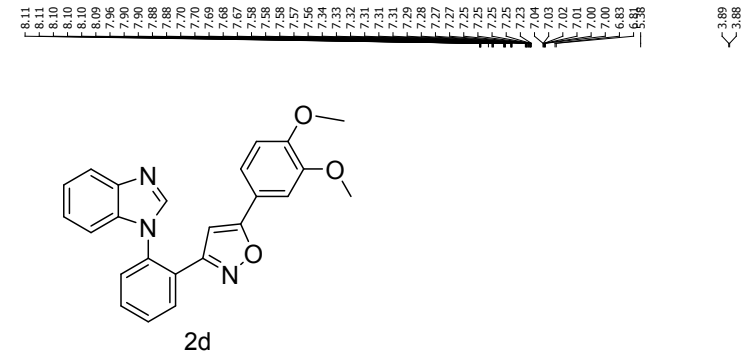
2c

^{1}H NMR (400 MHz, $CDCl_3$)



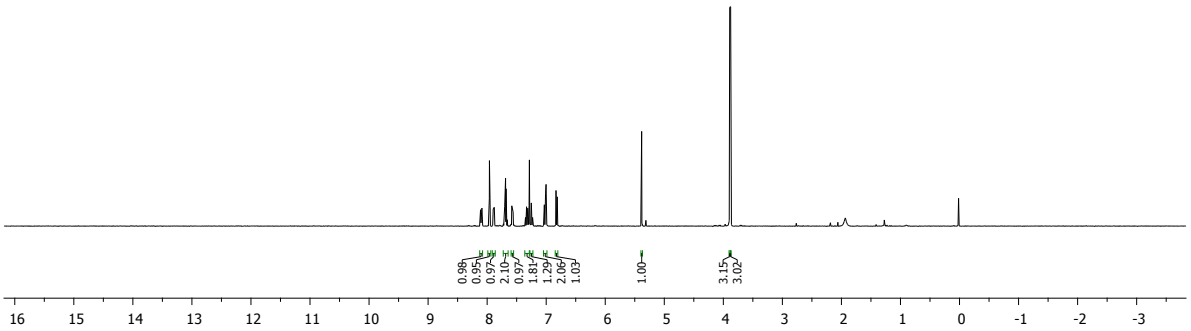
2c

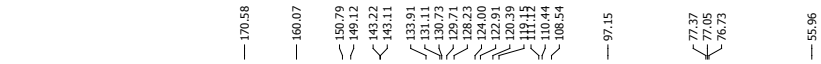
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



2d

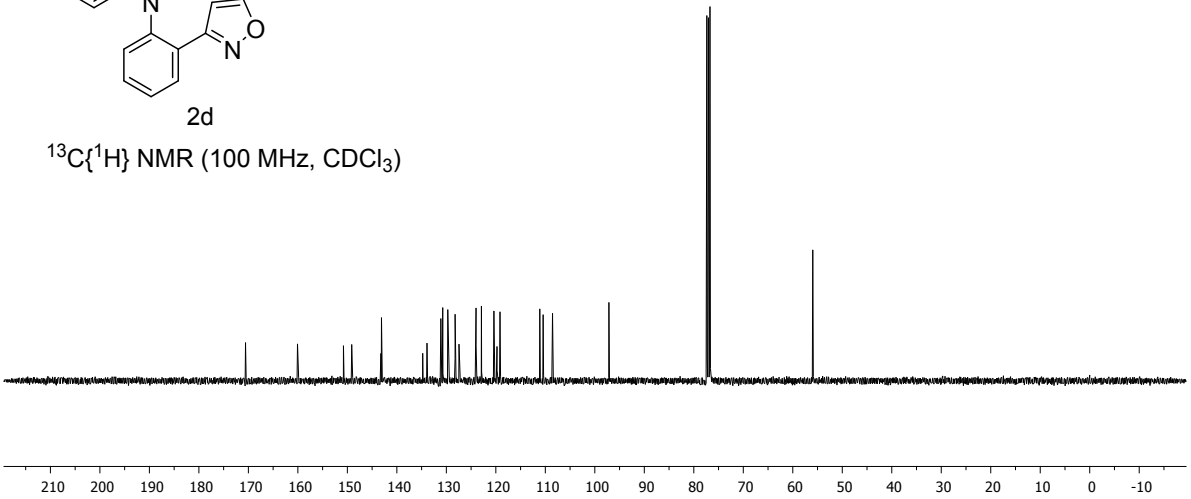
^{1}H NMR (400 MHz, $CDCl_3$)

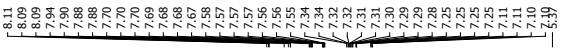


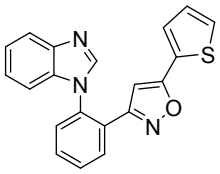


2d

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

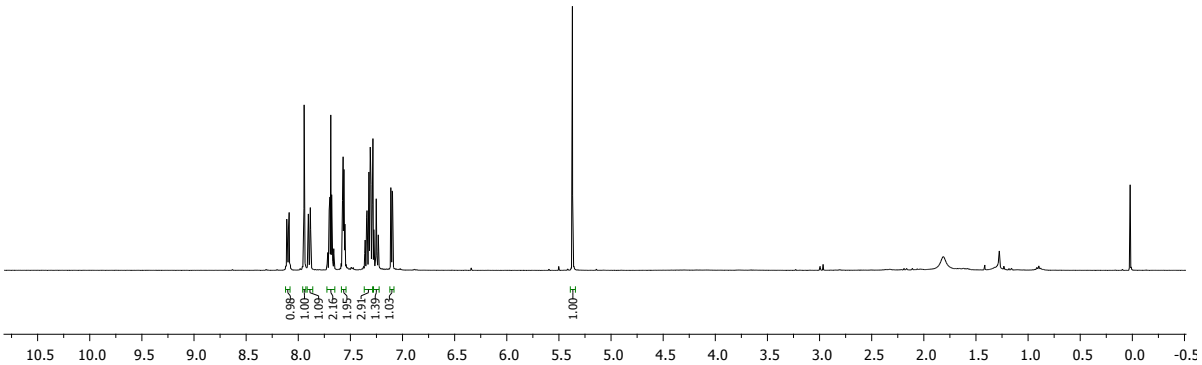


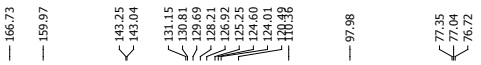


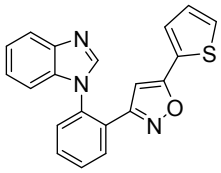


2e

^{1}H NMR (400 MHz, $CDCl_3$)

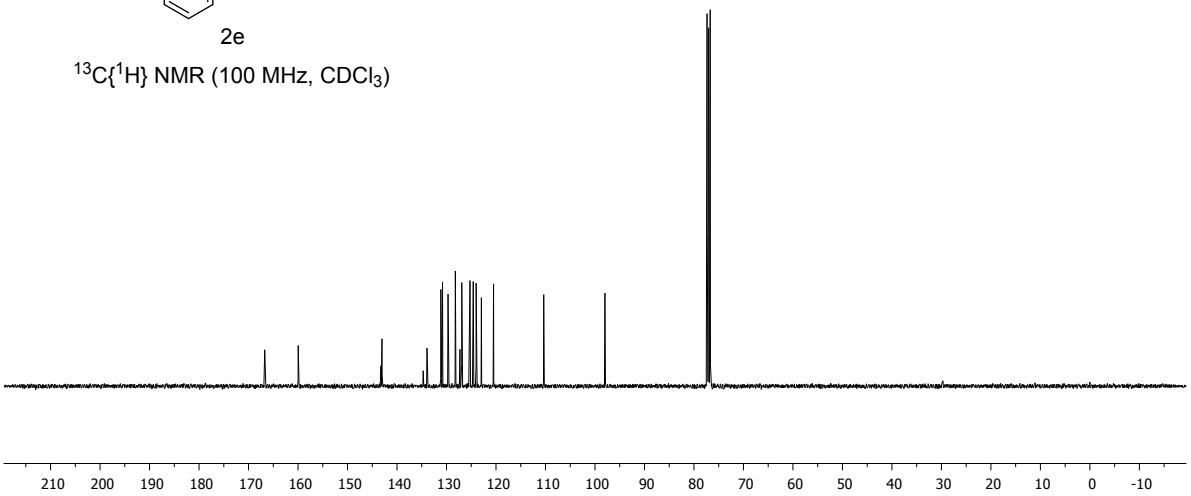


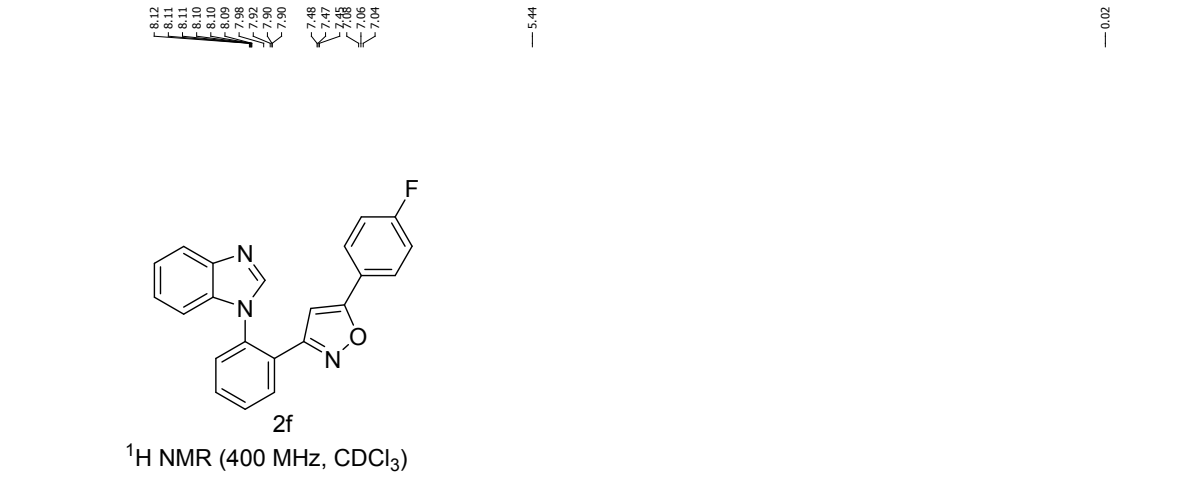




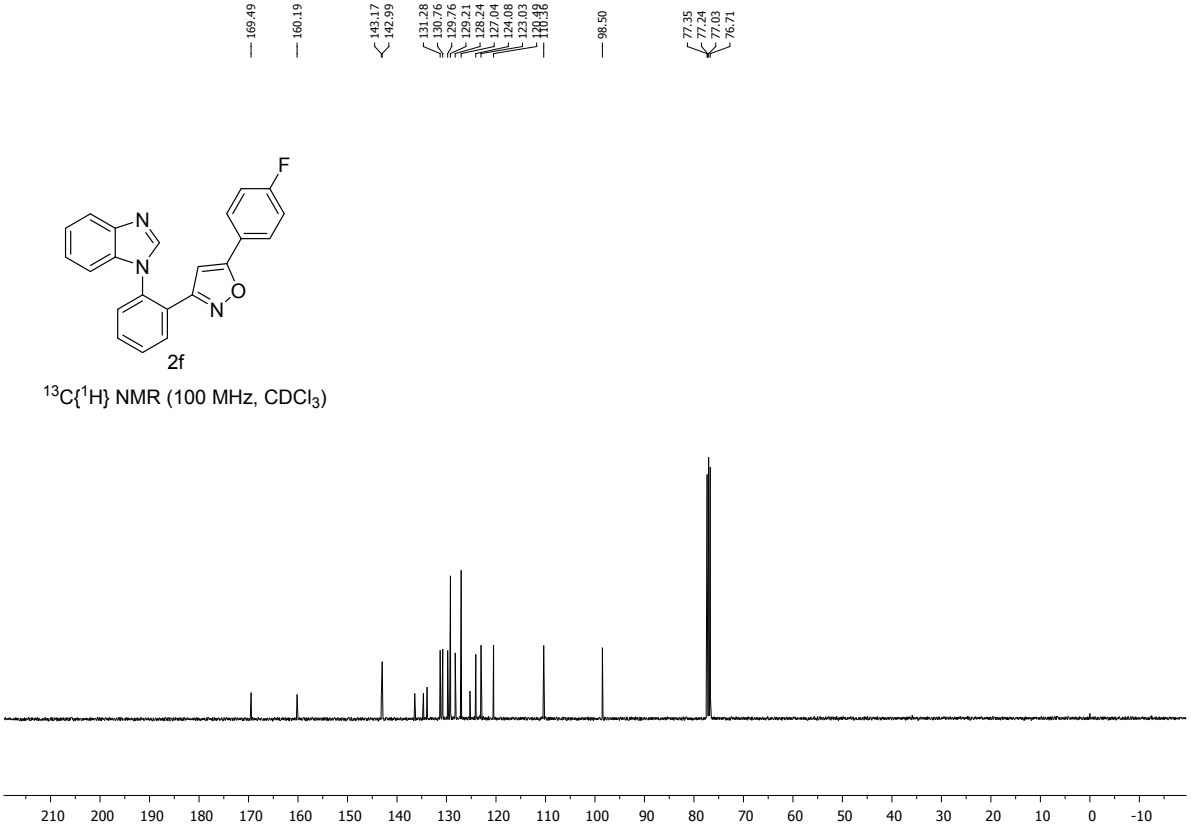
2e

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)





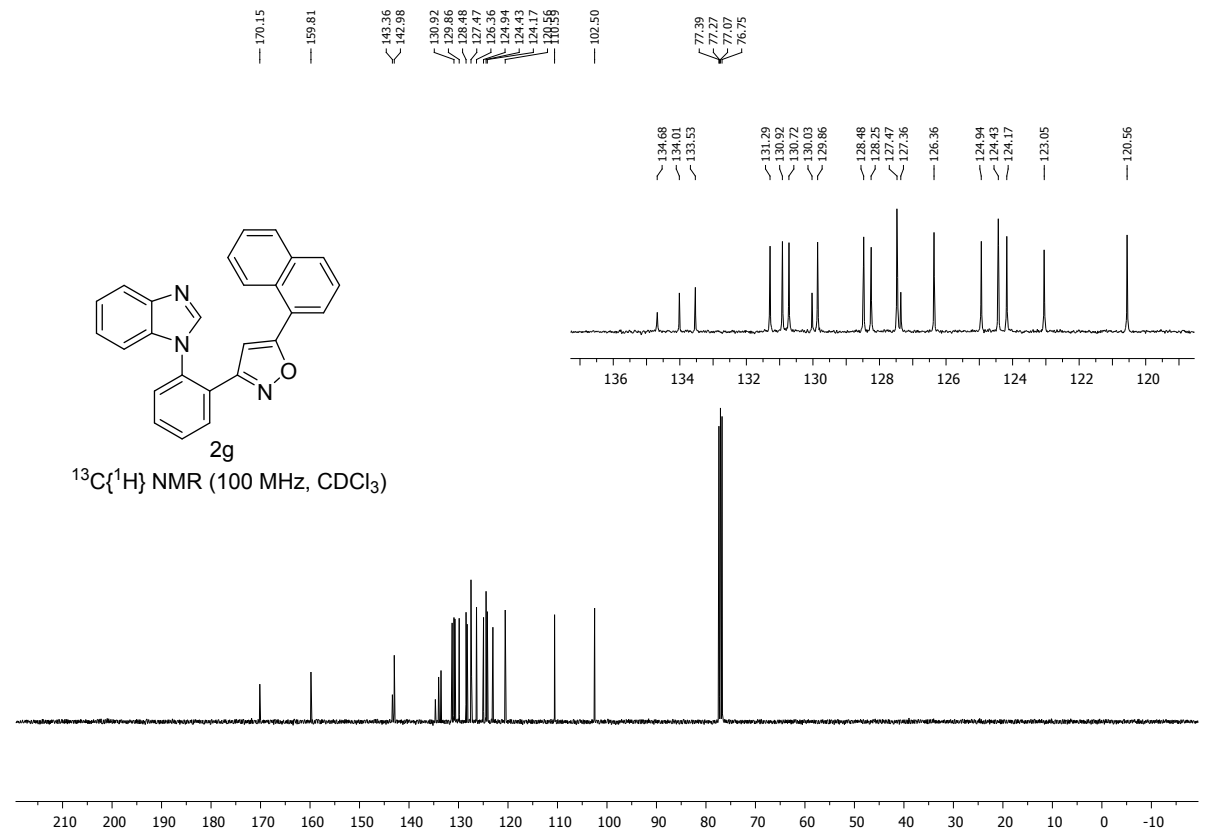
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

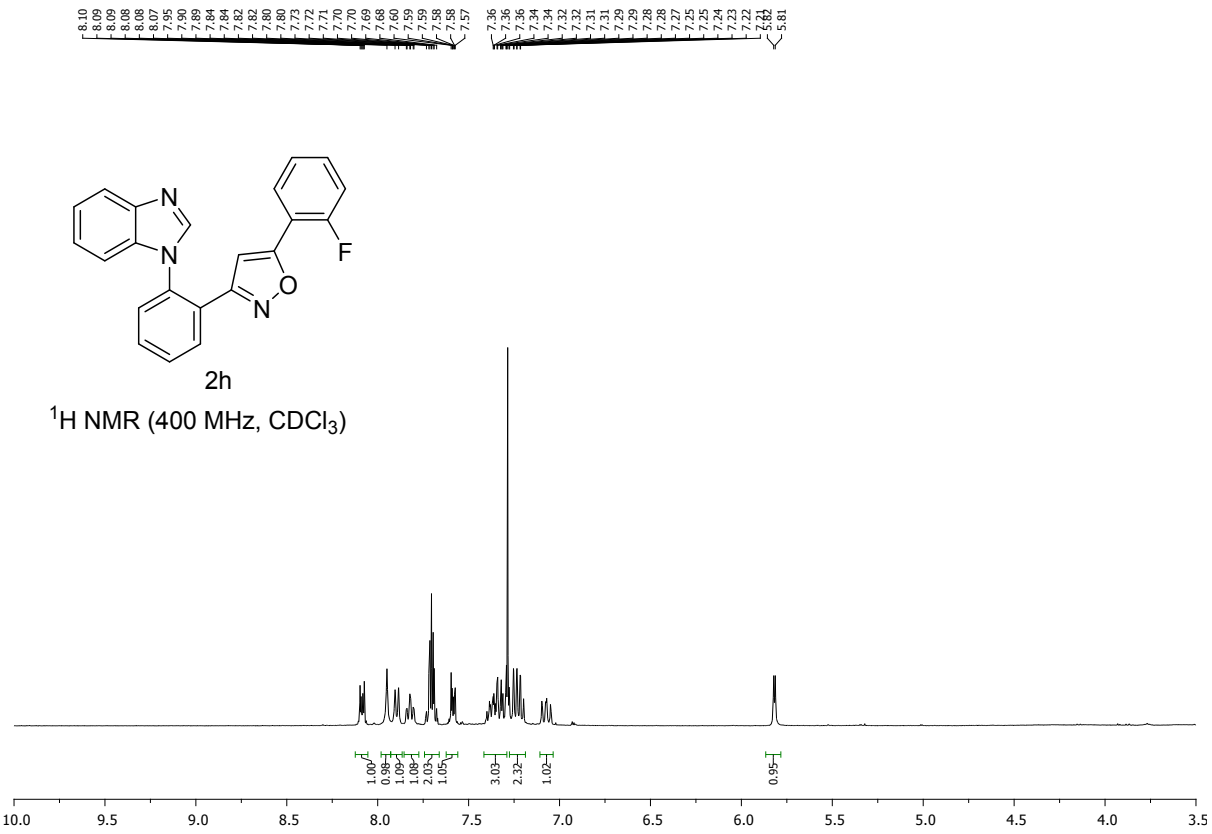
2g

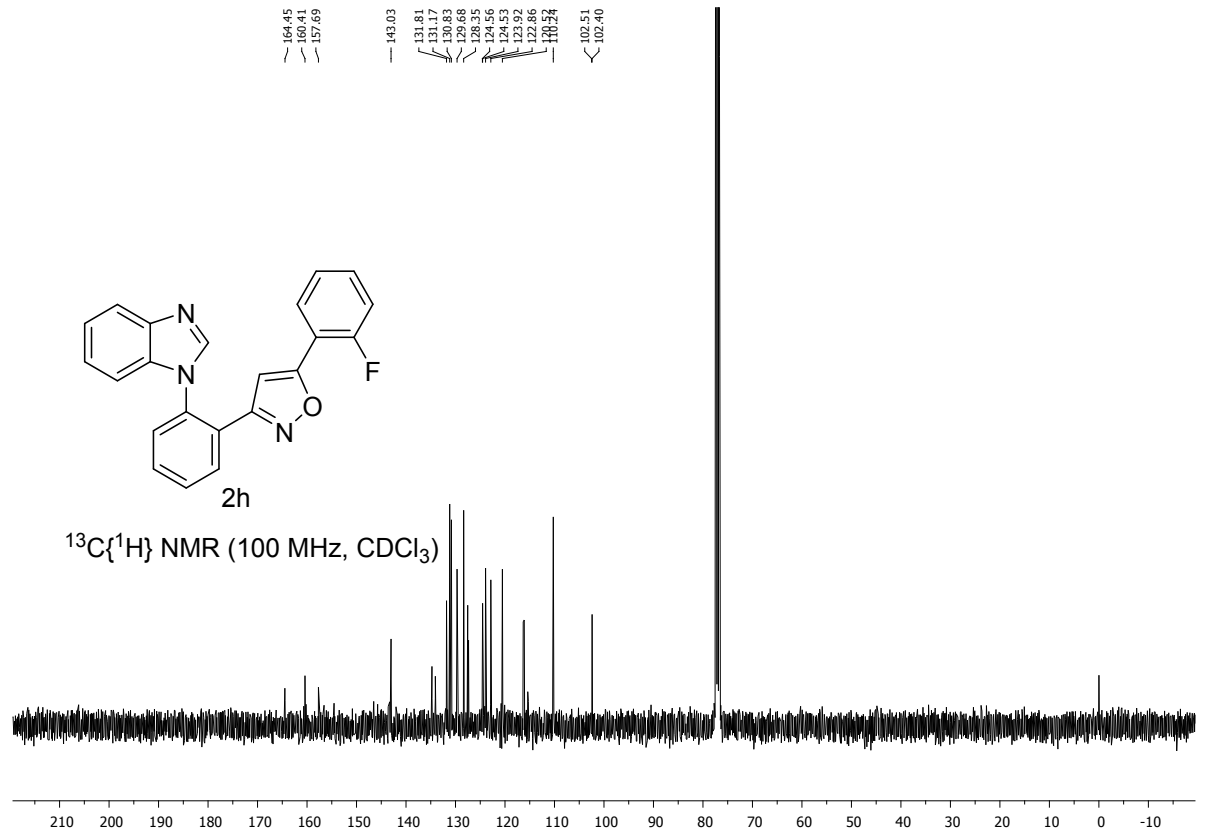
^{1}H NMR (400 MHz, $CDCl_3$)

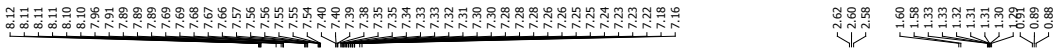


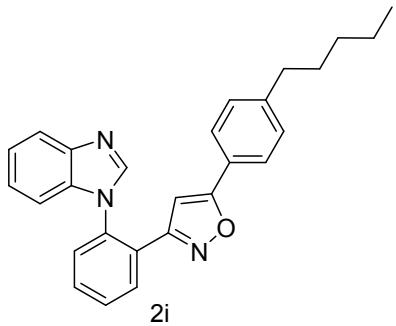
2g

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)


2h
^{1}H NMR (400 MHz, $CDCl_3$)

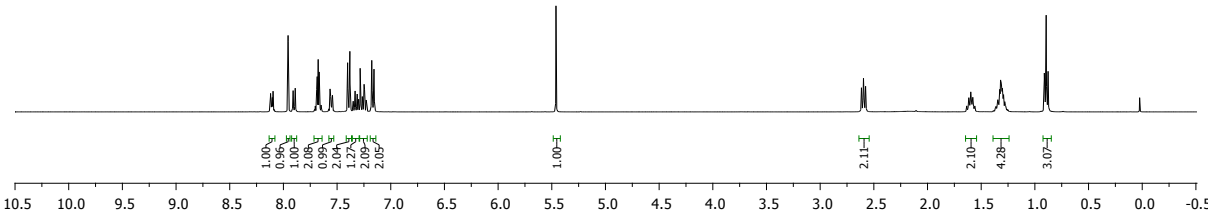

2h
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

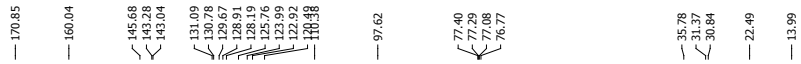


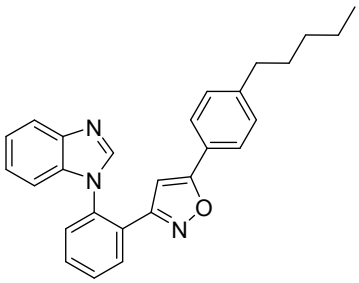


2i

^{1}H NMR (400 MHz, $CDCl_3$)

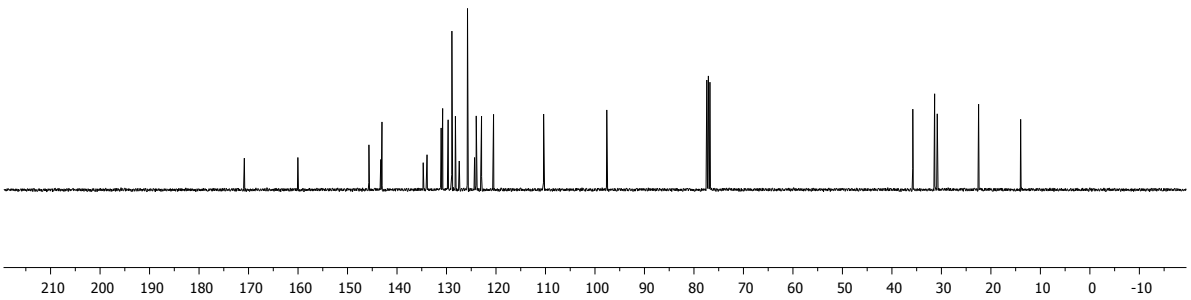


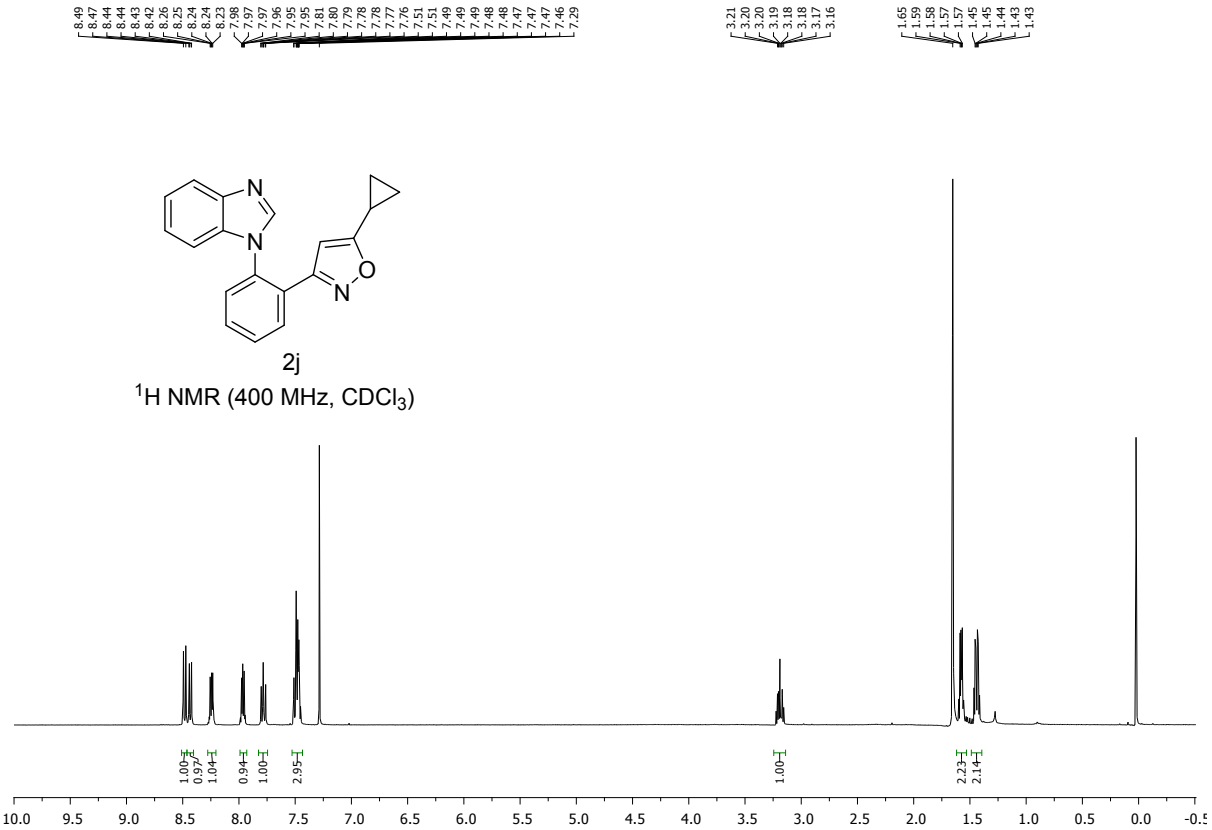




2i

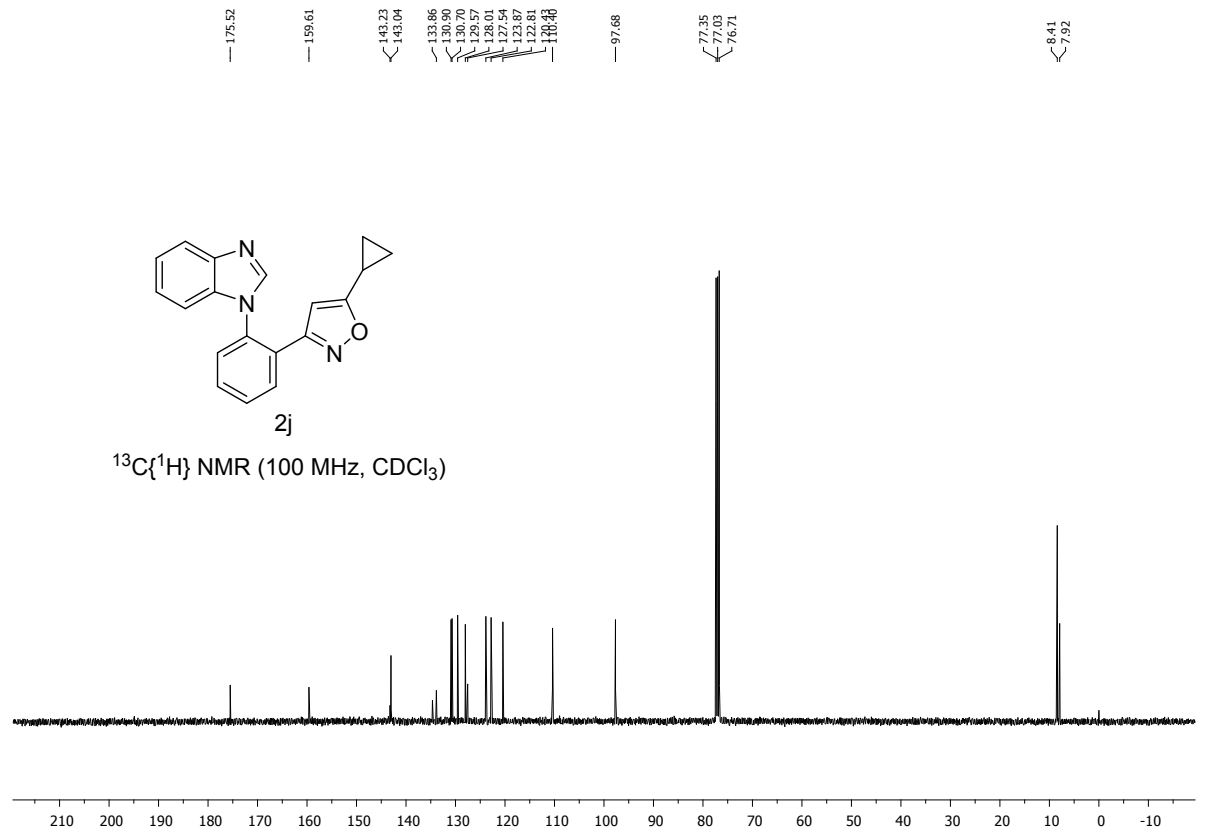
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)





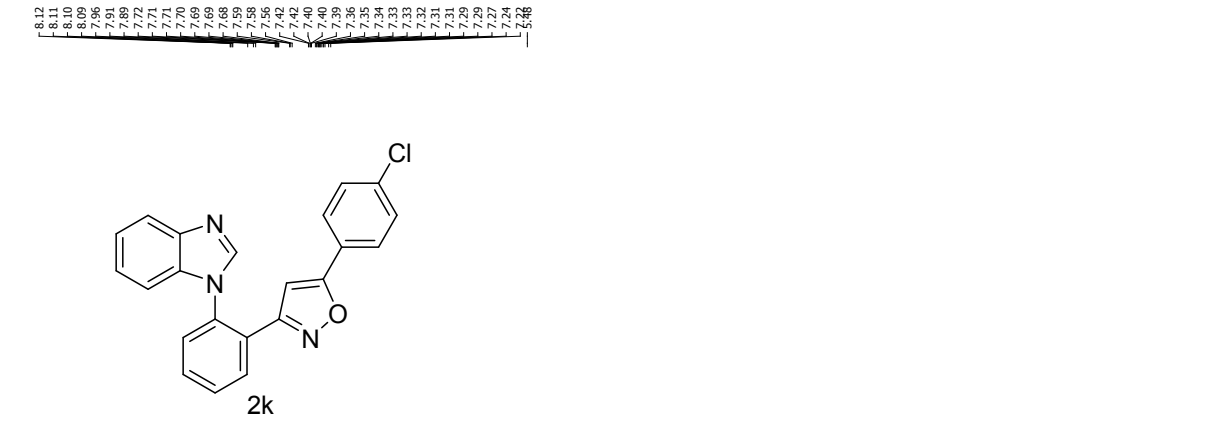
2j

^{1}H NMR (400 MHz, $CDCl_3$)

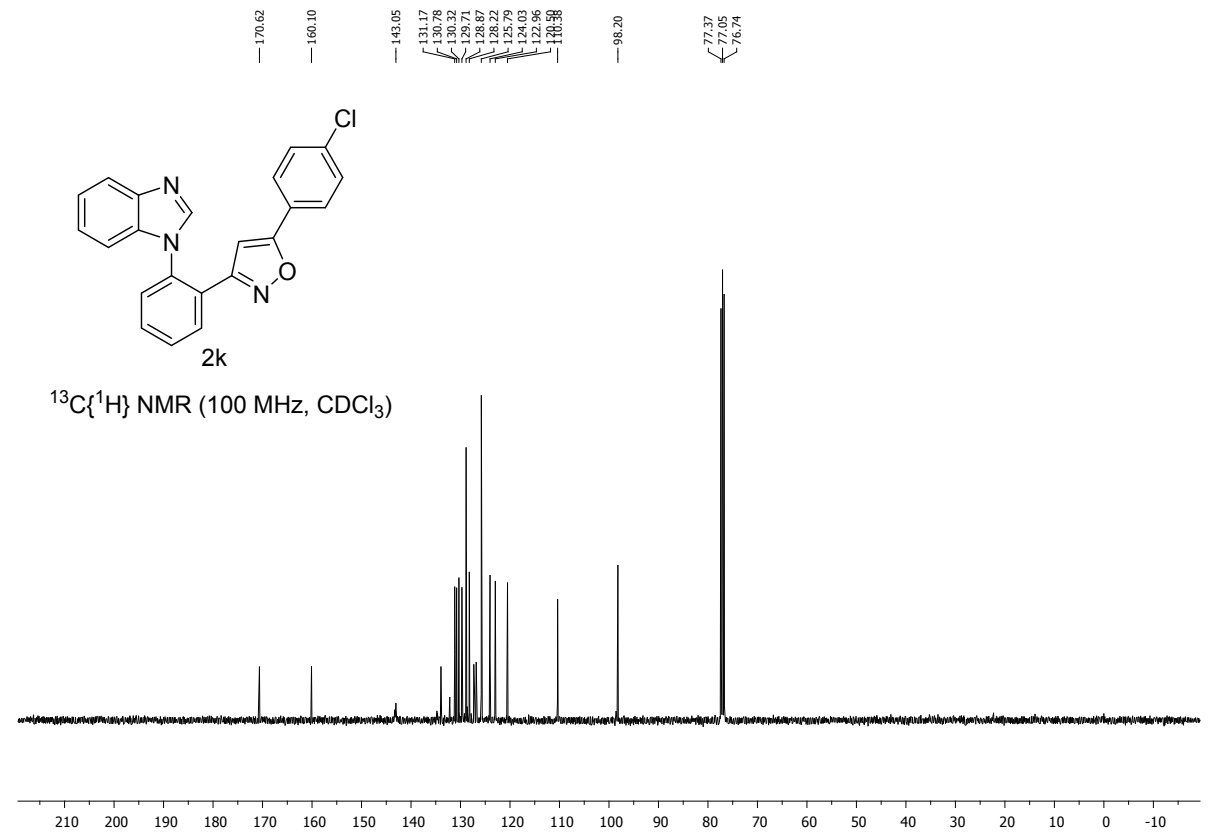


2j

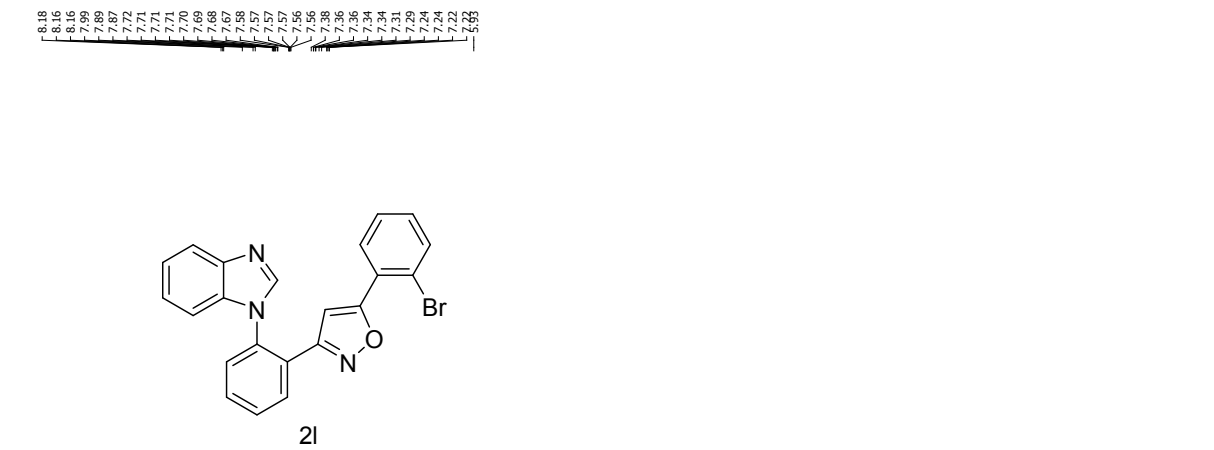
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



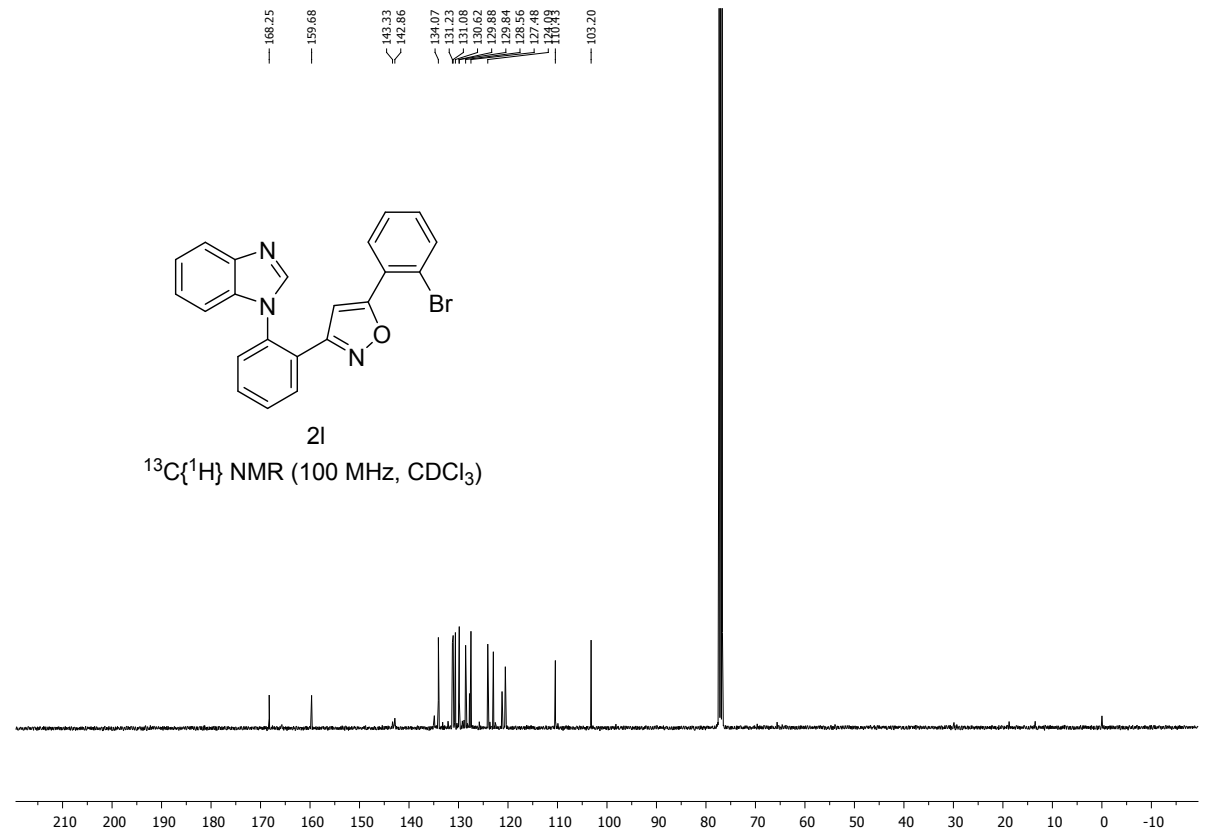
^{1}H NMR (400 MHz, $CDCl_3$)



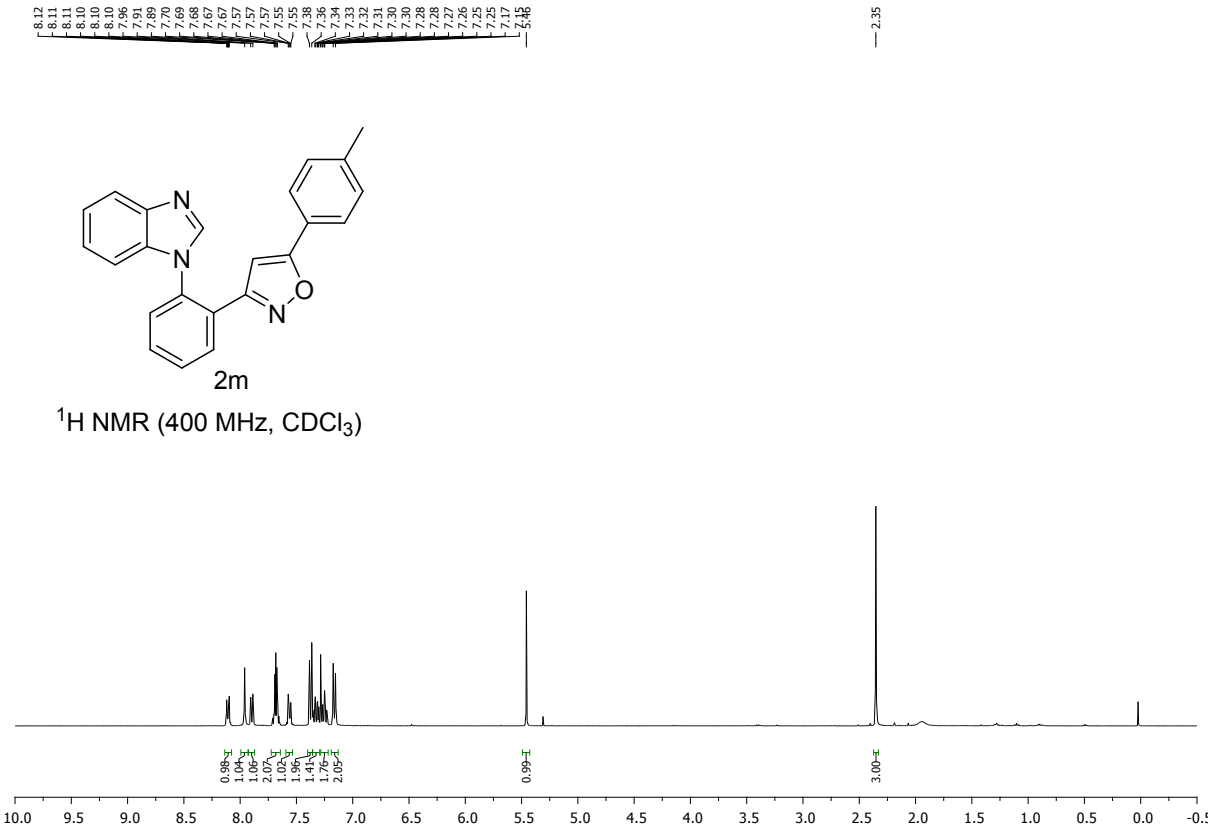
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



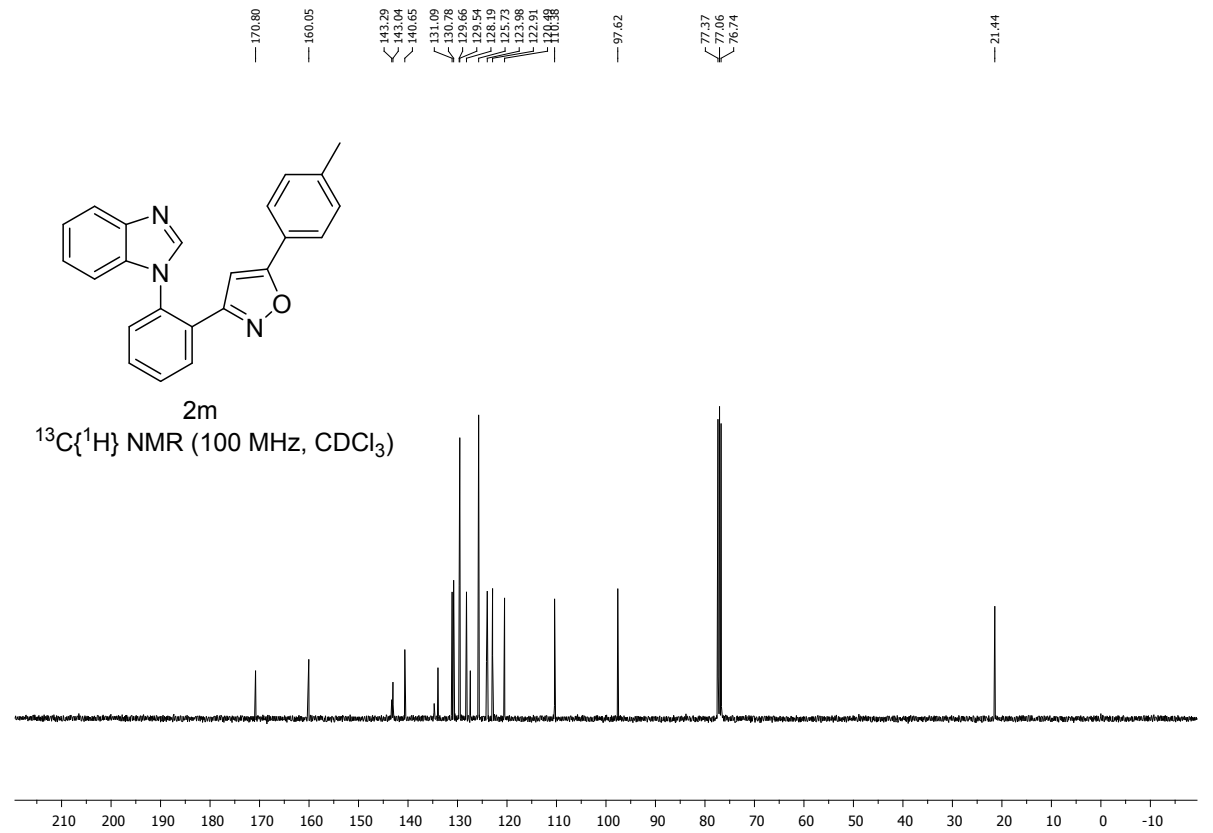
^{1}H NMR (400 MHz, $CDCl_3$)



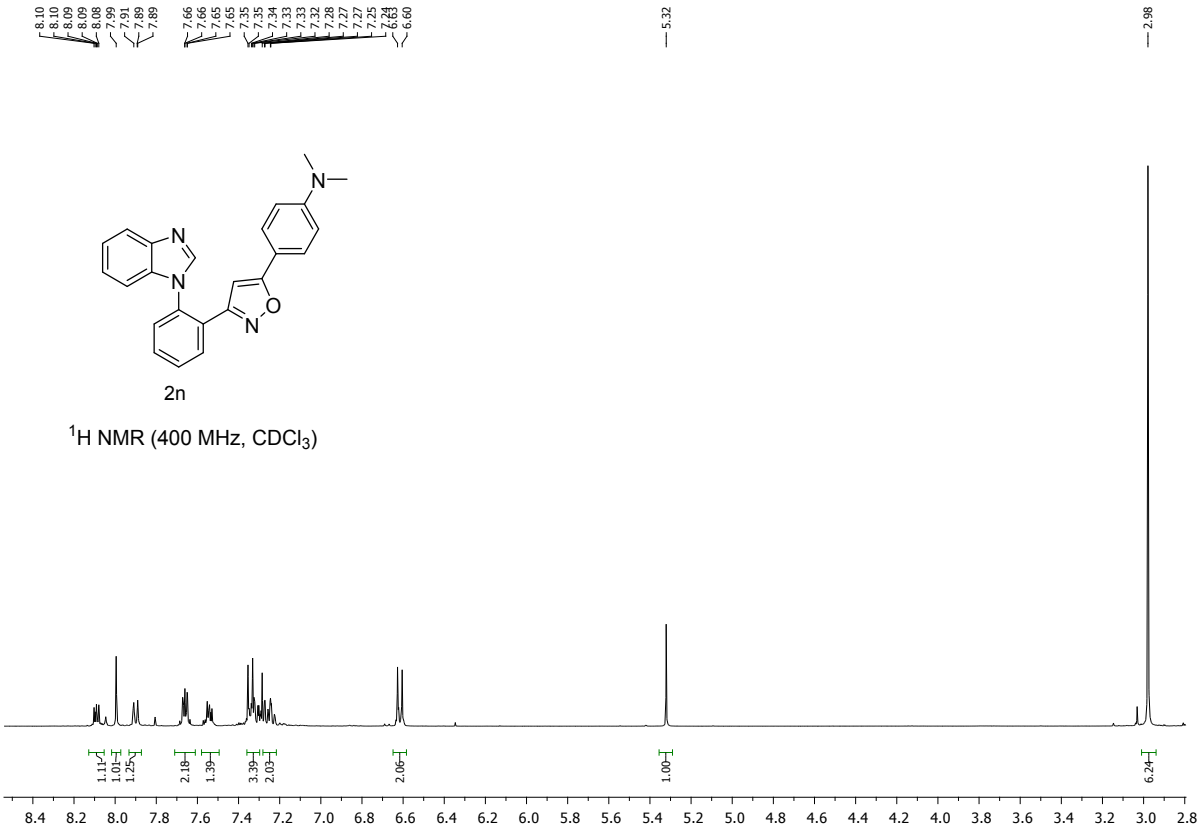
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)

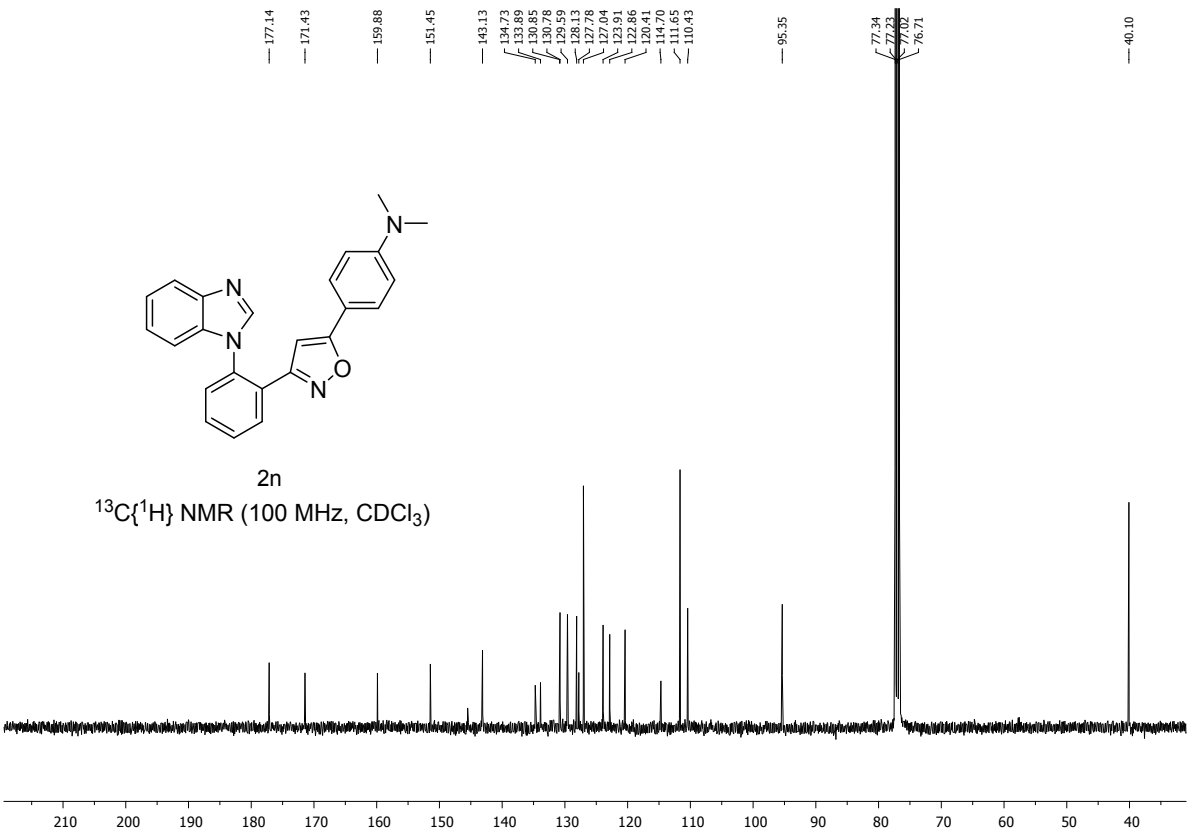


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



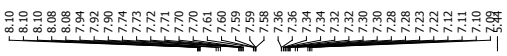
2n

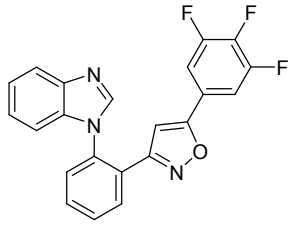
^{1}H NMR (400 MHz, $CDCl_3$)



2n

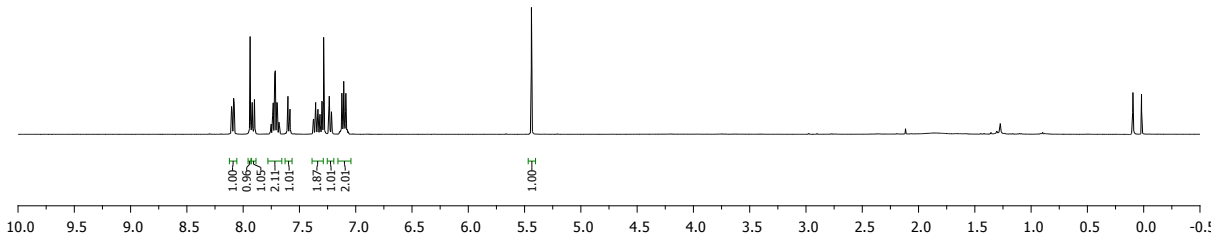
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)





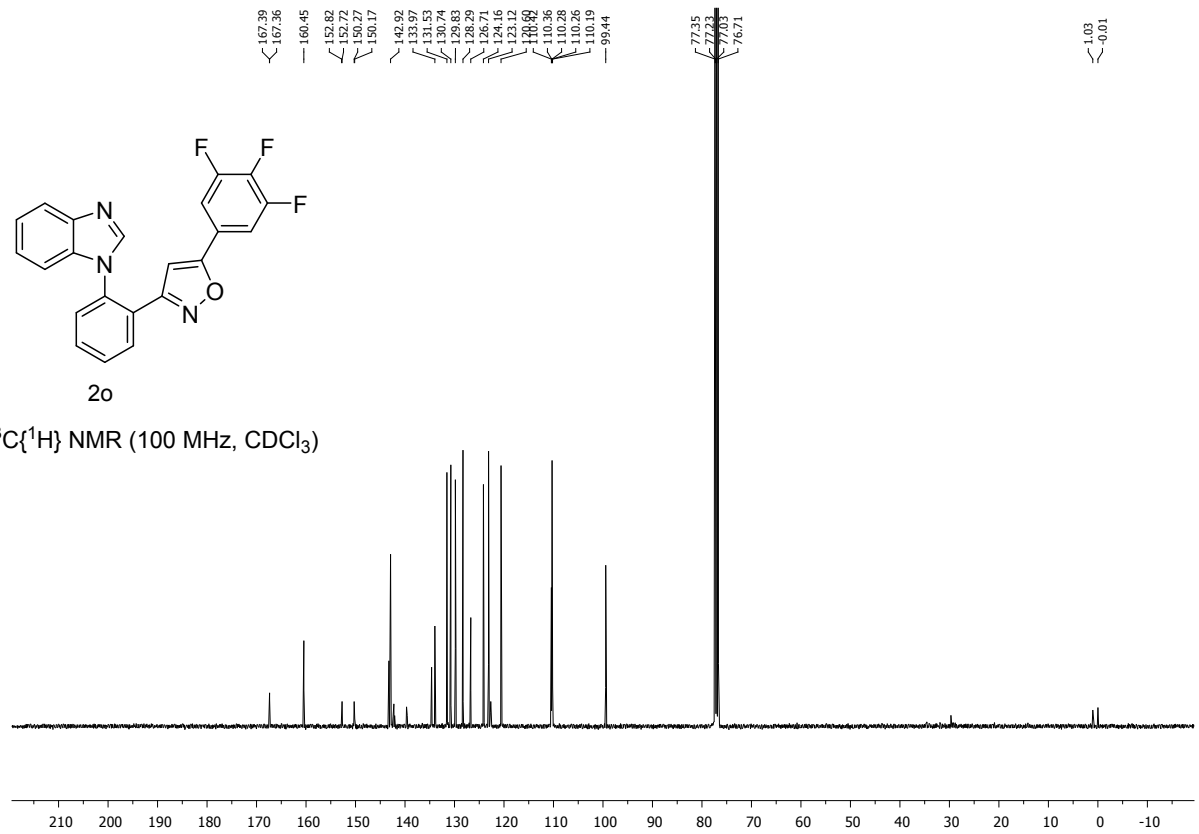
2o

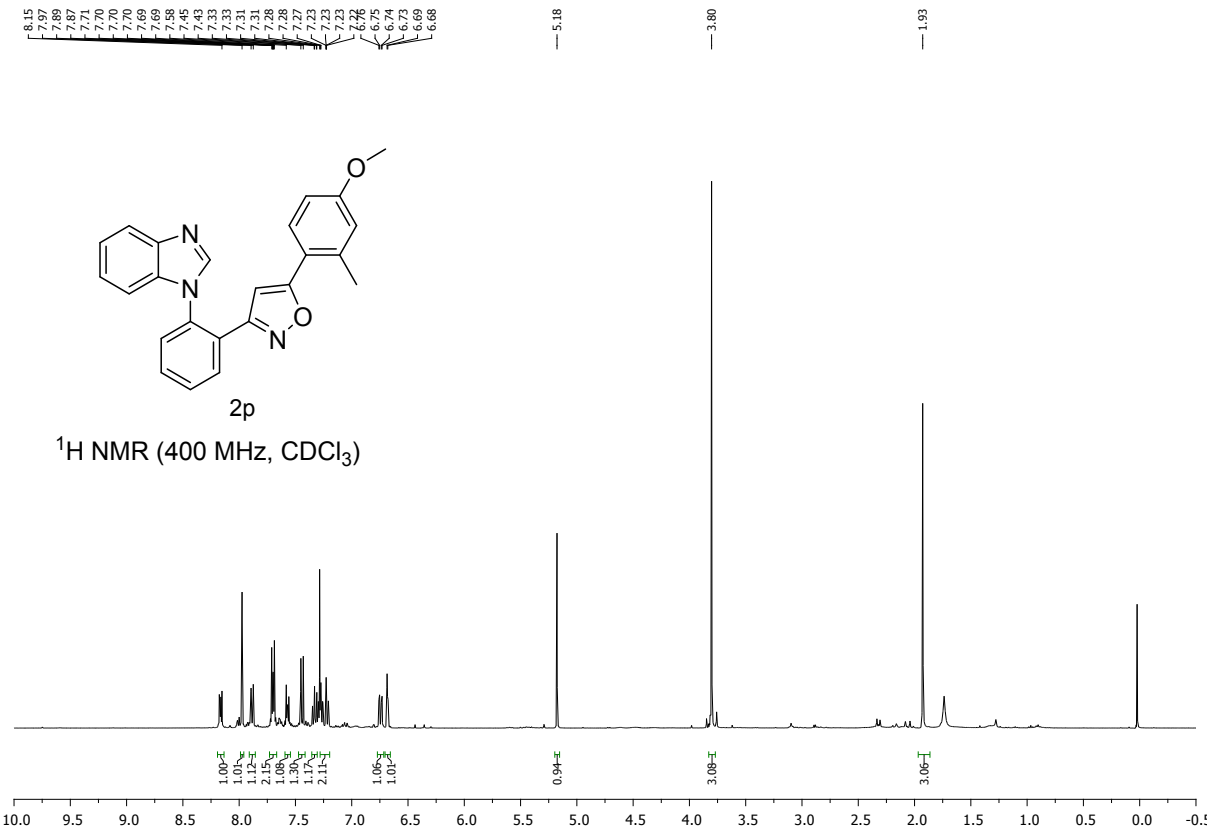
^{1}H NMR (400 MHz, $CDCl_3$)



2o

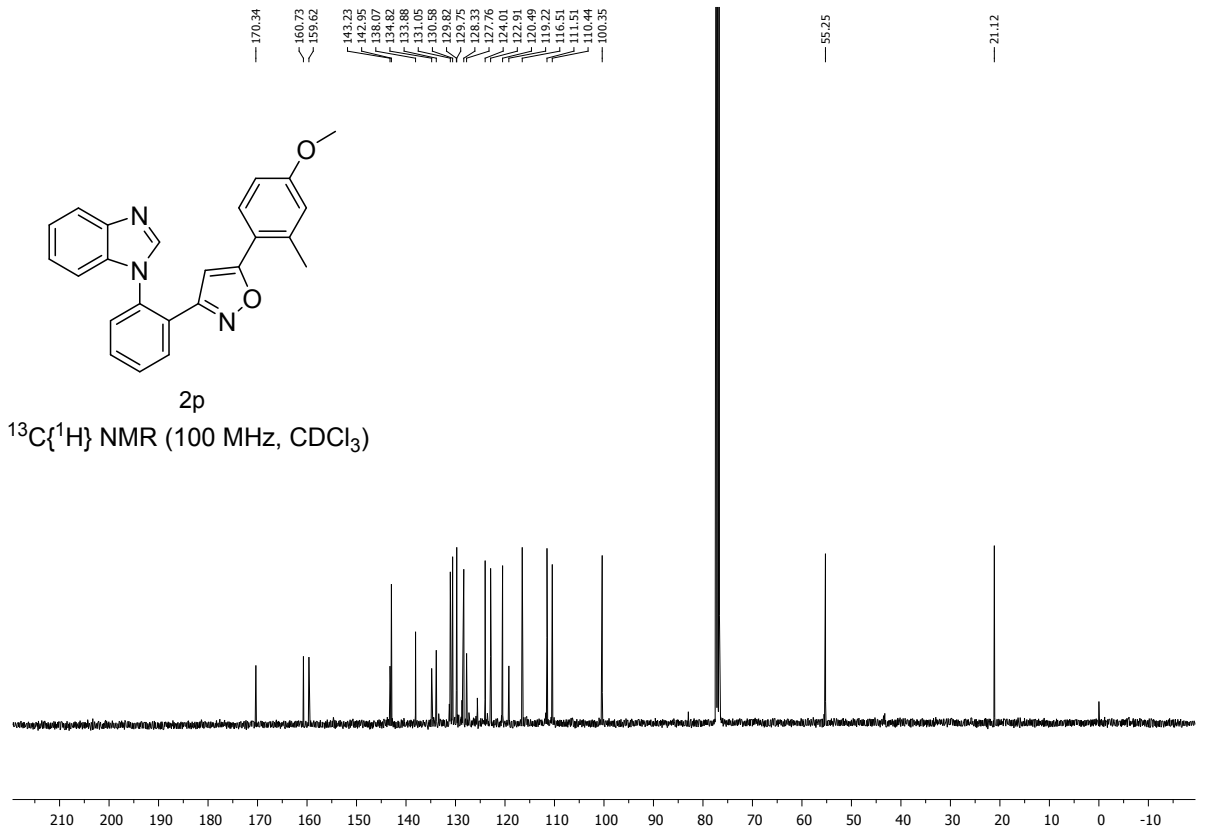
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)





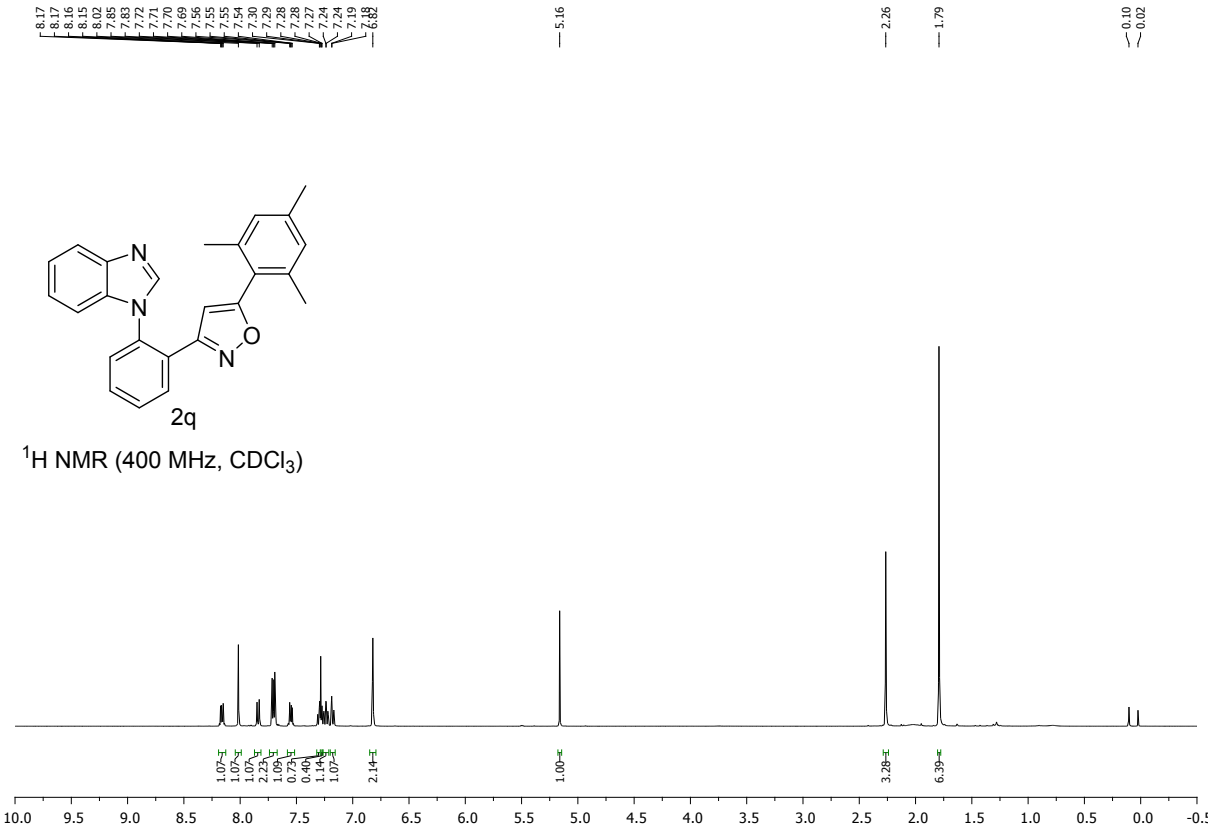
2p

^{1}H NMR (400 MHz, $CDCl_3$)

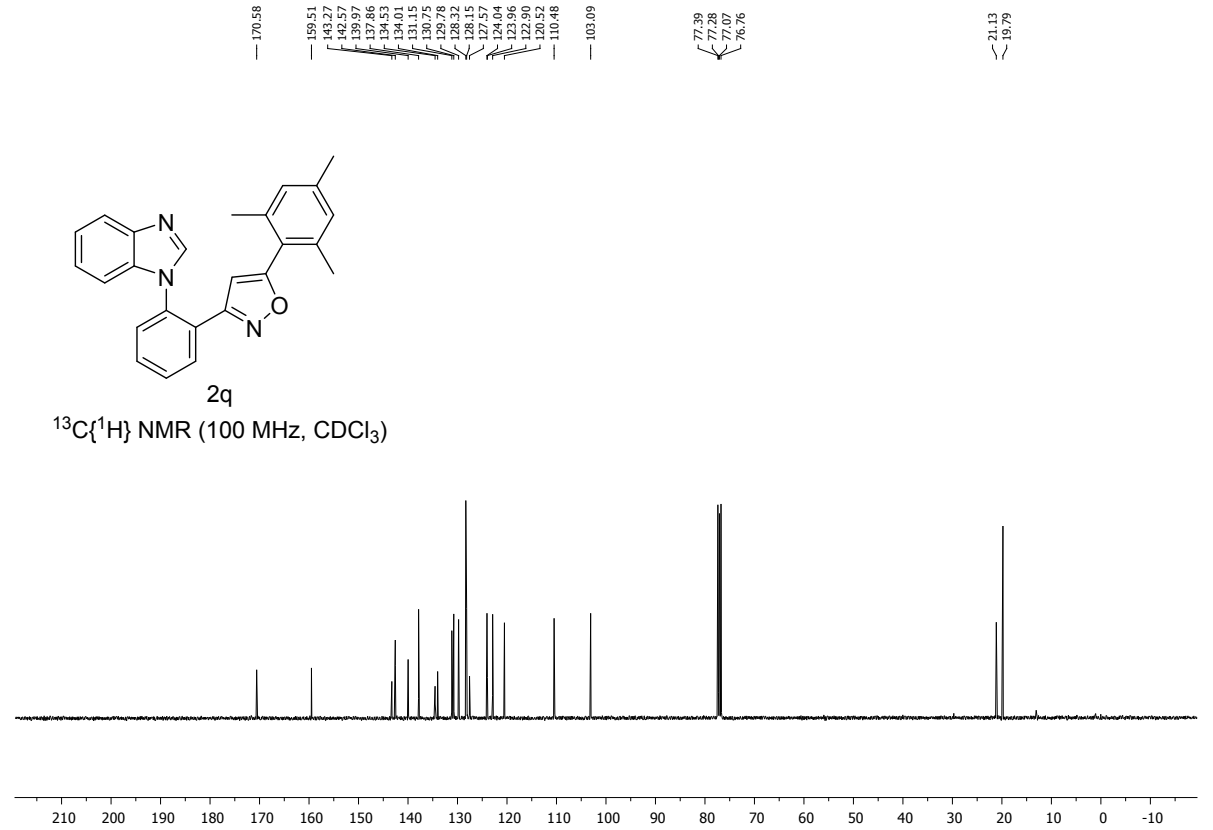


2p

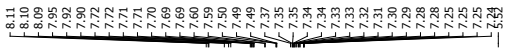
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

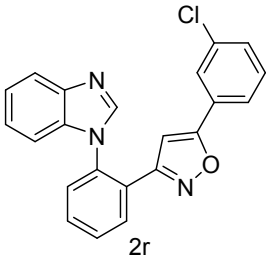


^{1}H NMR (400 MHz, $CDCl_3$)



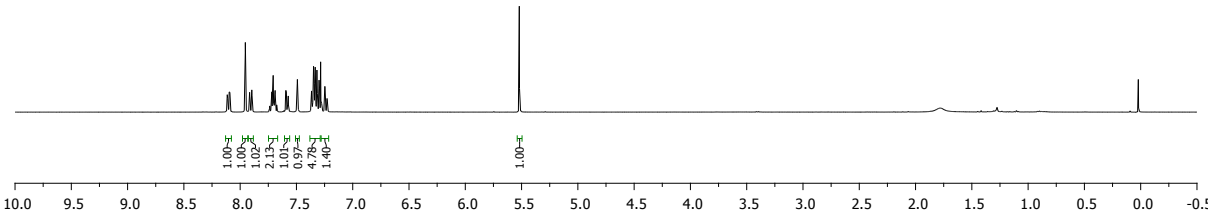
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

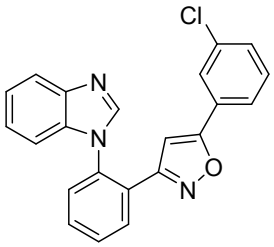




2r

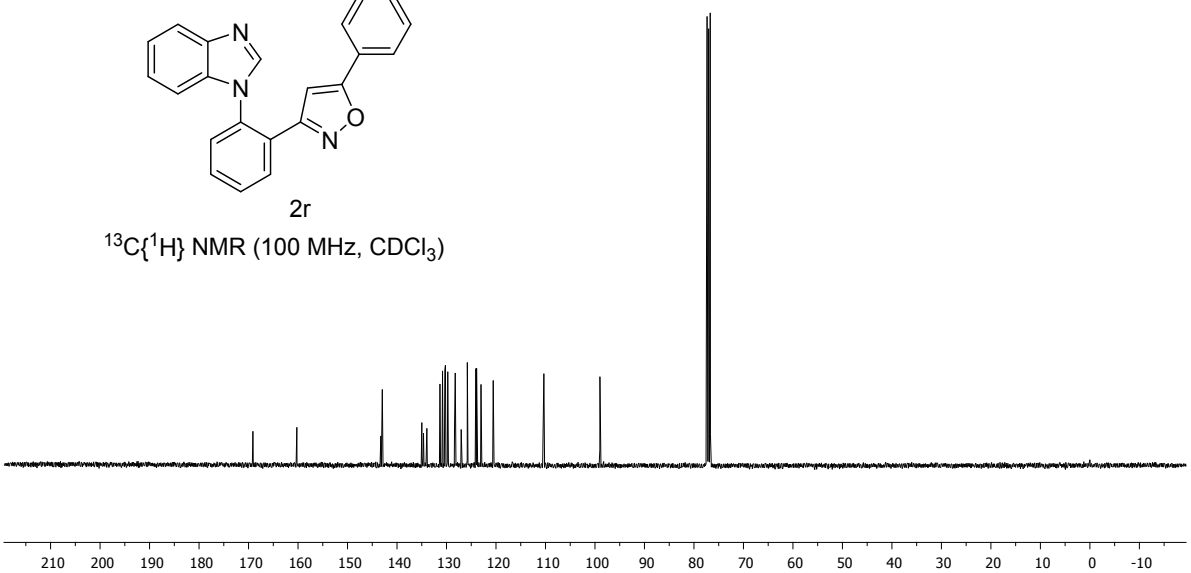
^{1}H NMR (400 MHz, $CDCl_3$)

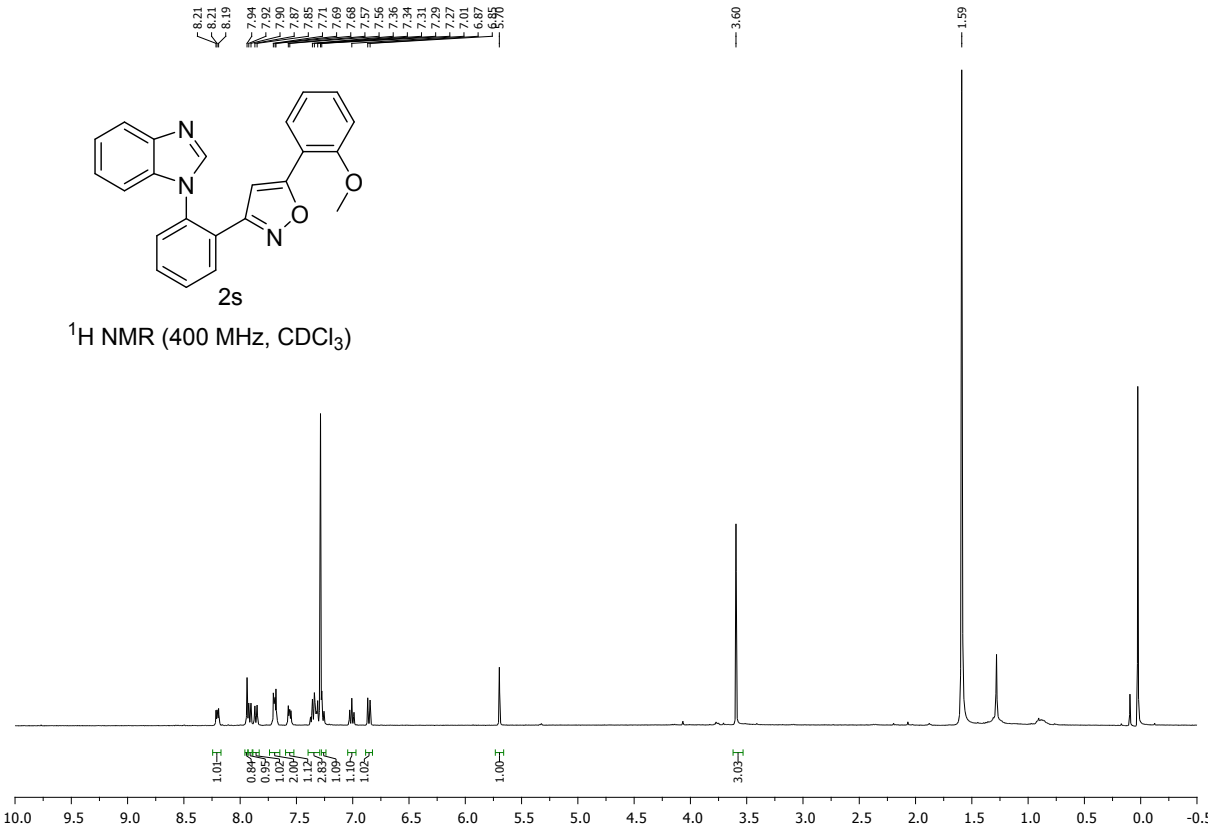




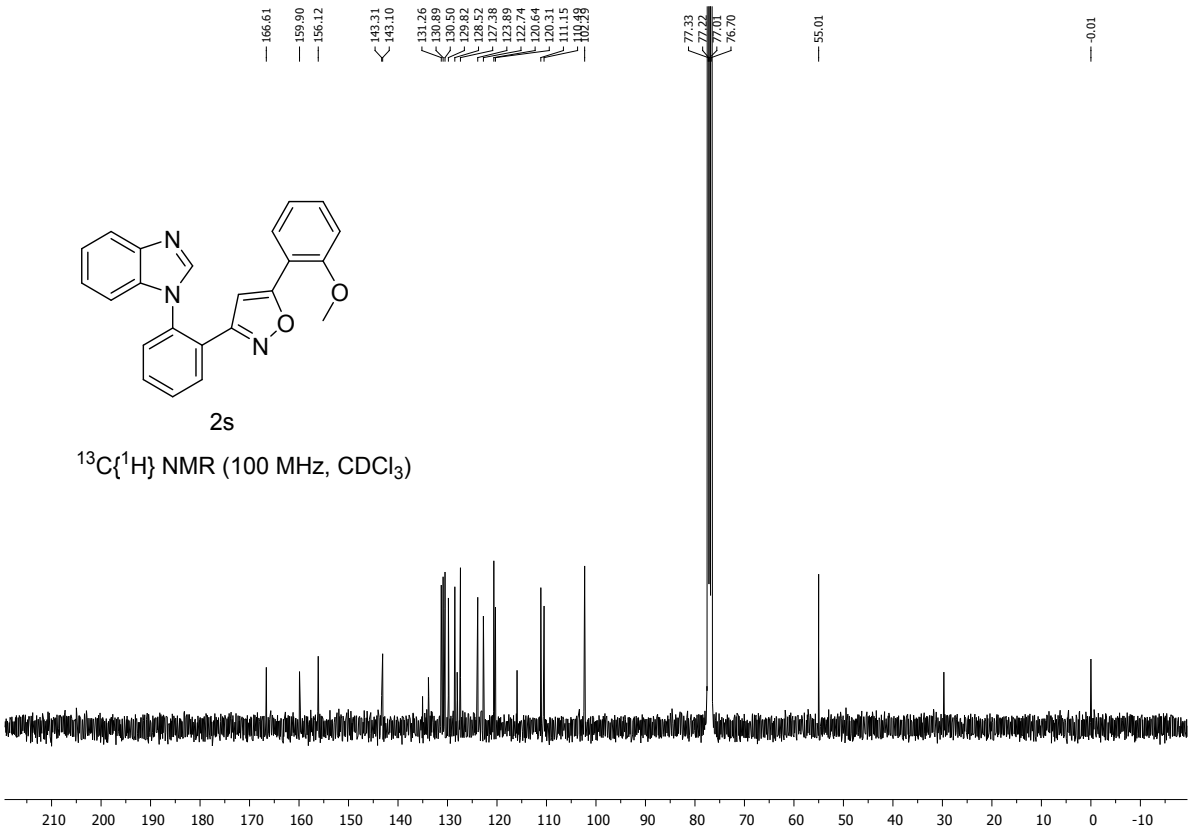
2r

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

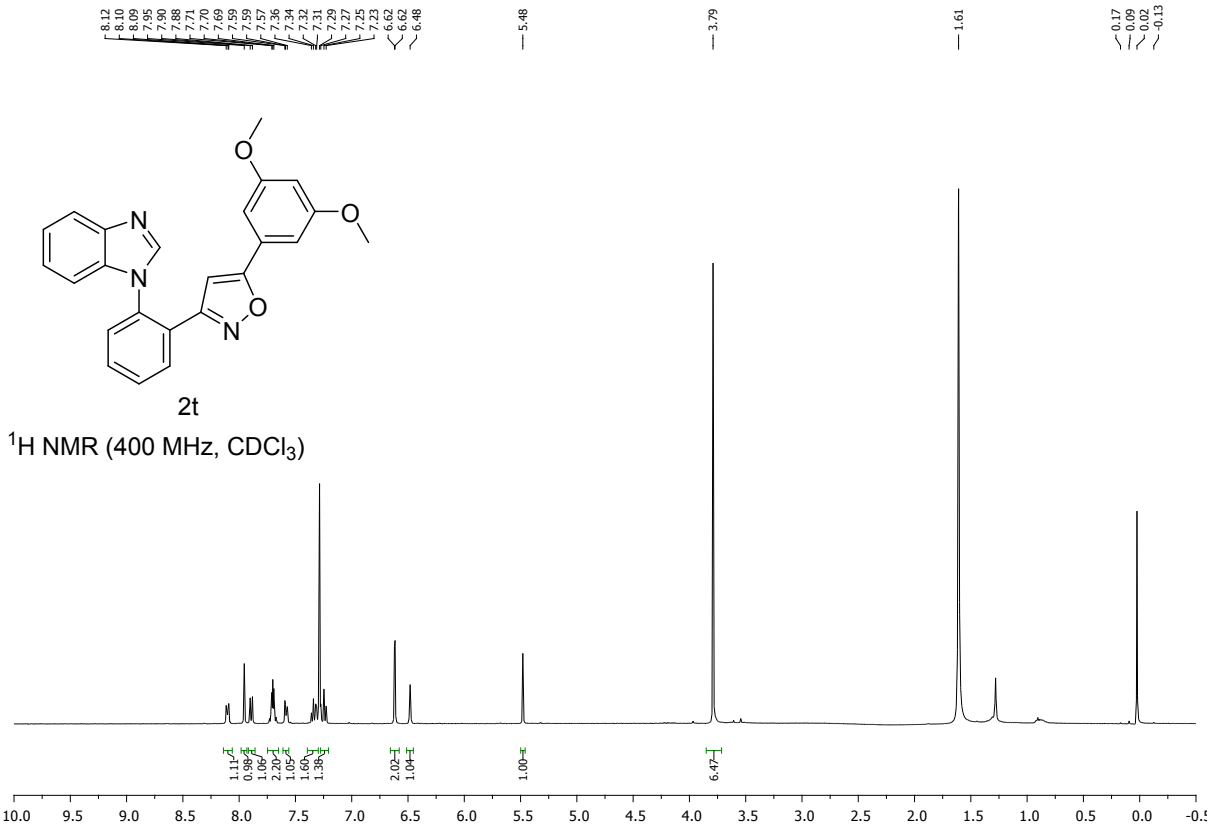




^{1}H NMR (400 MHz, $CDCl_3$)

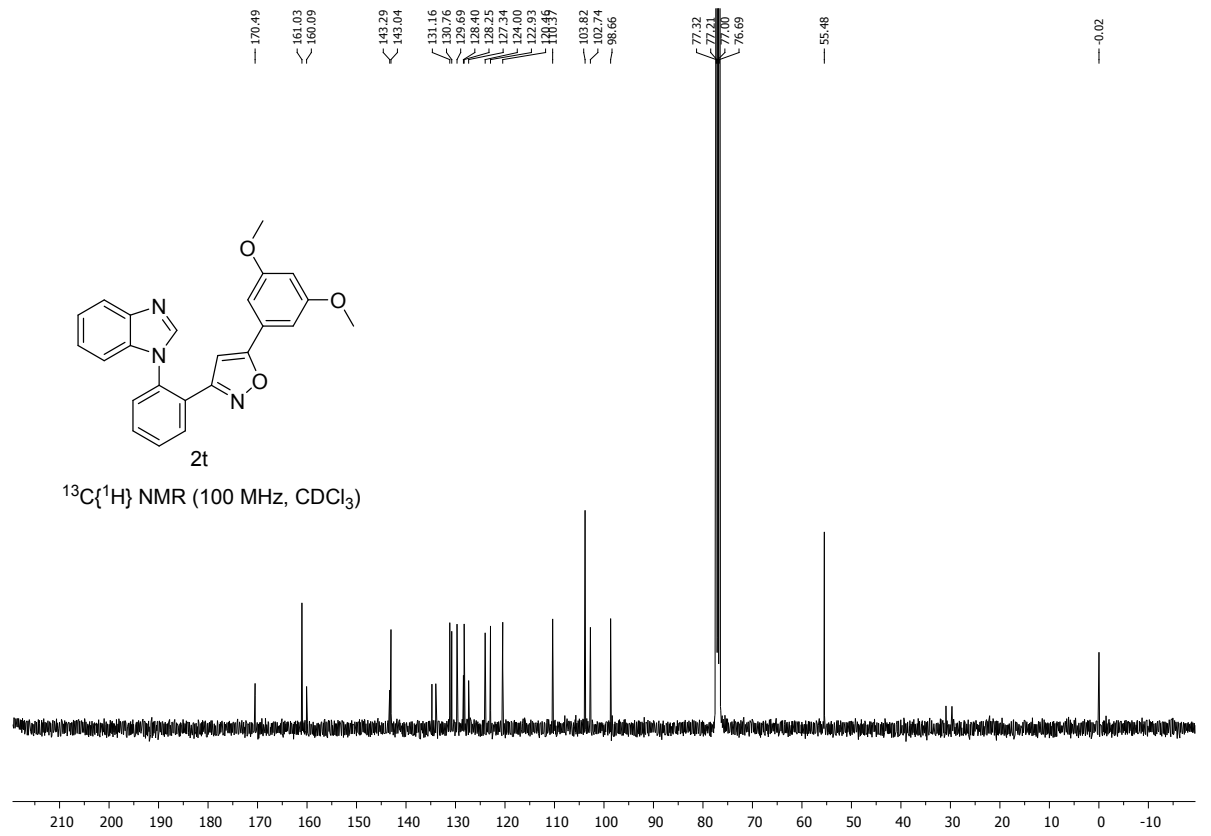


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



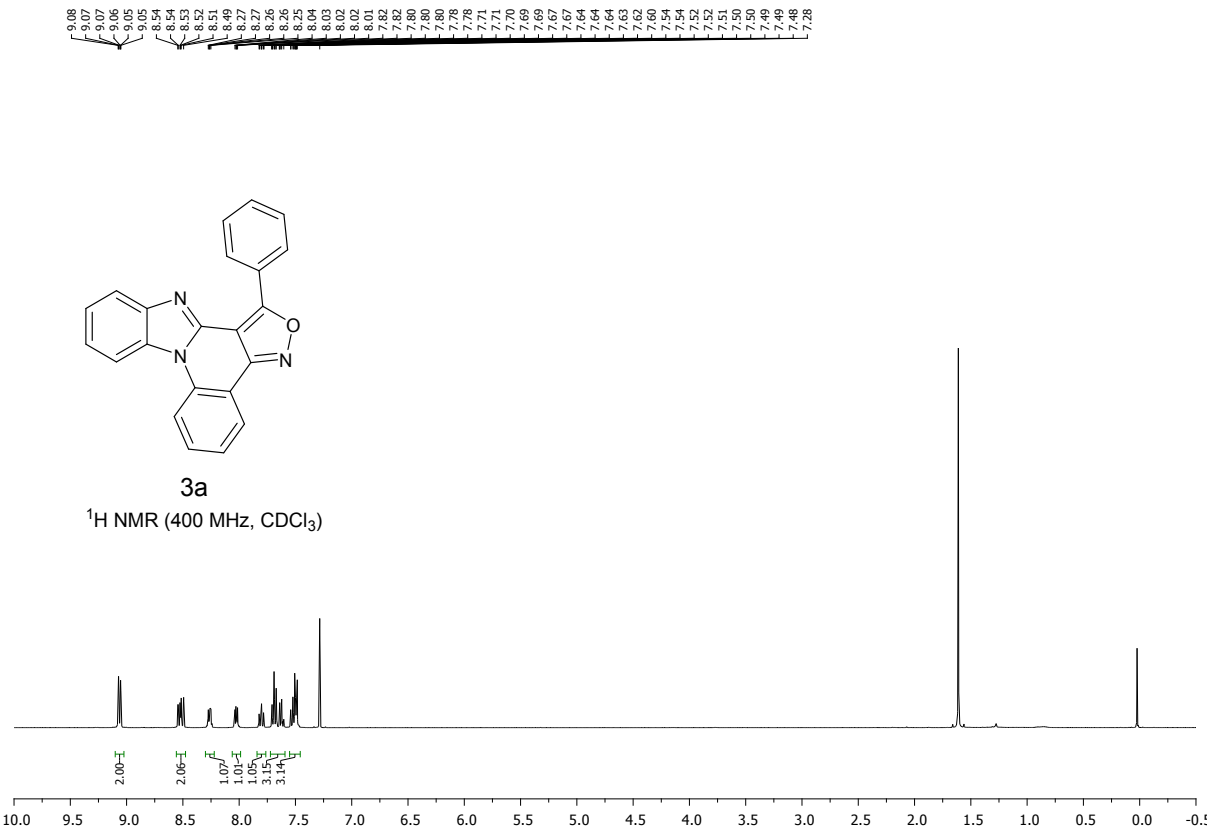
2t

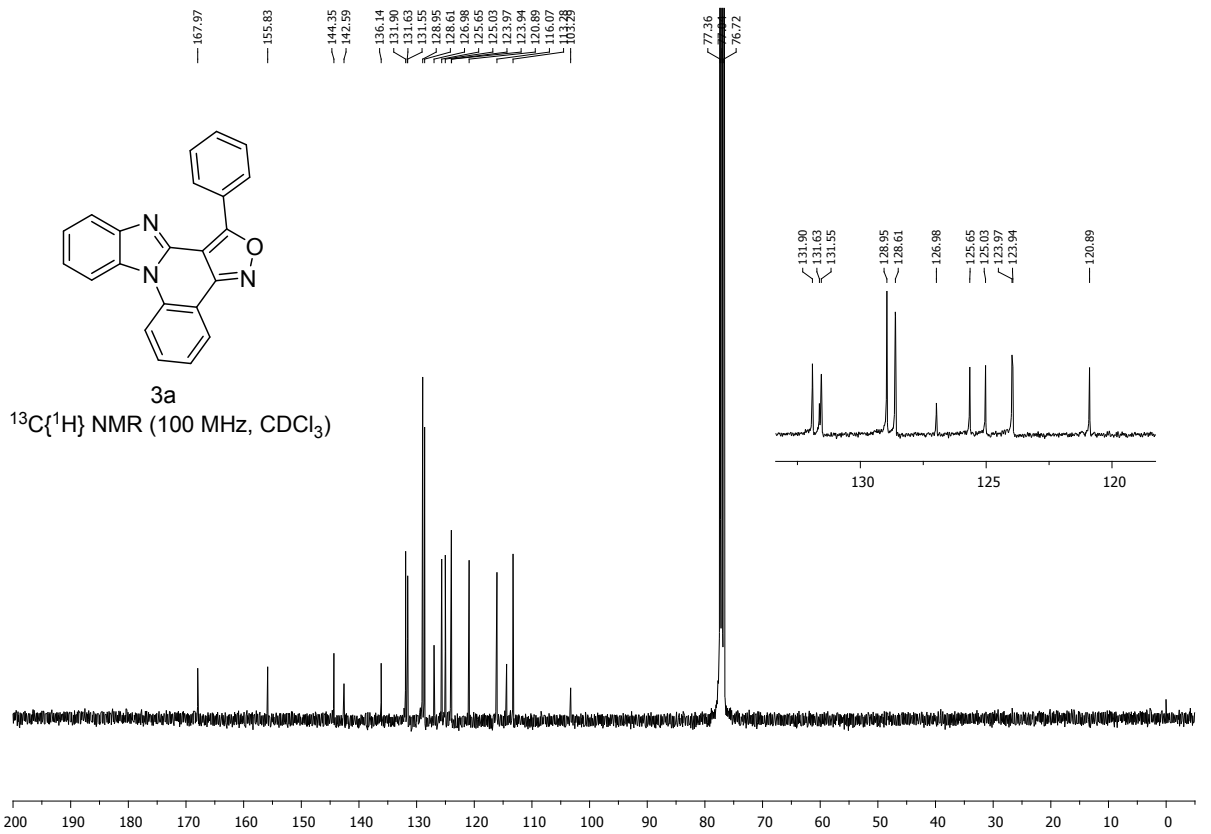
^{1}H NMR (400 MHz, $CDCl_3$)

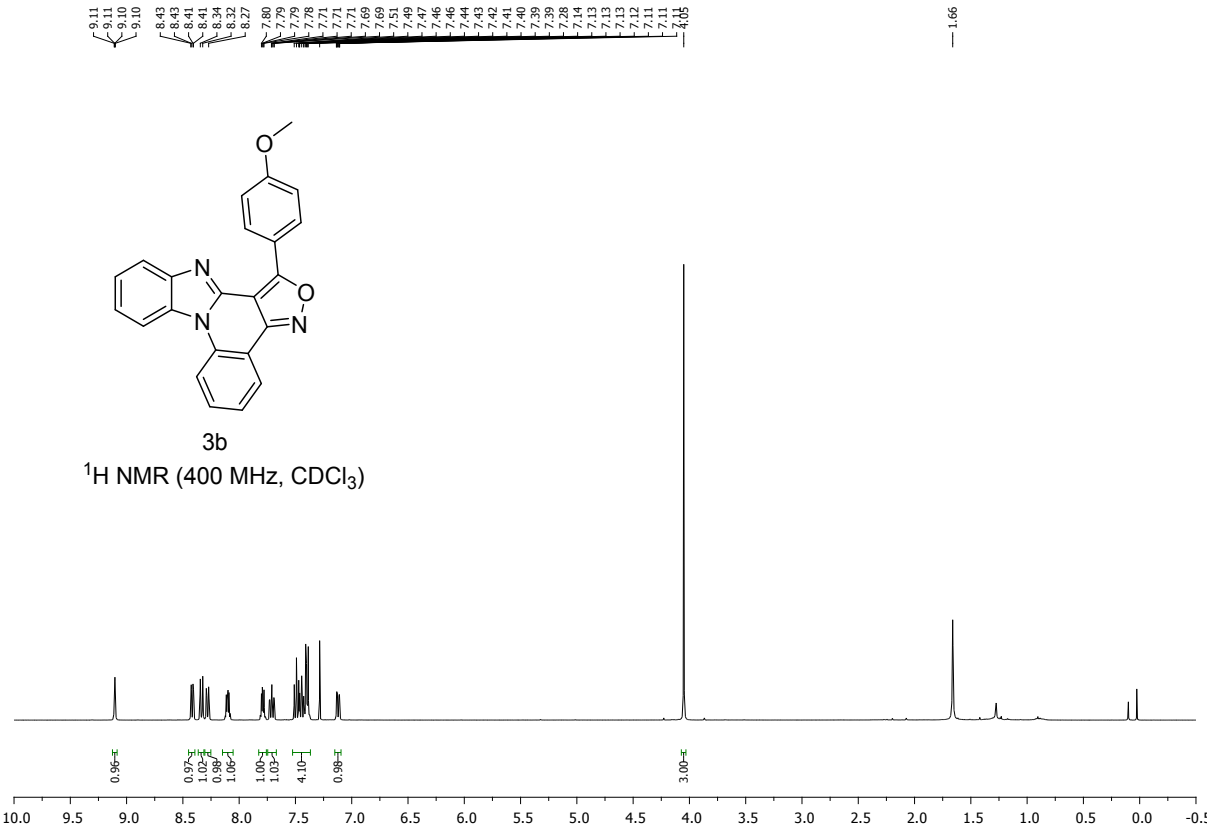


2t

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

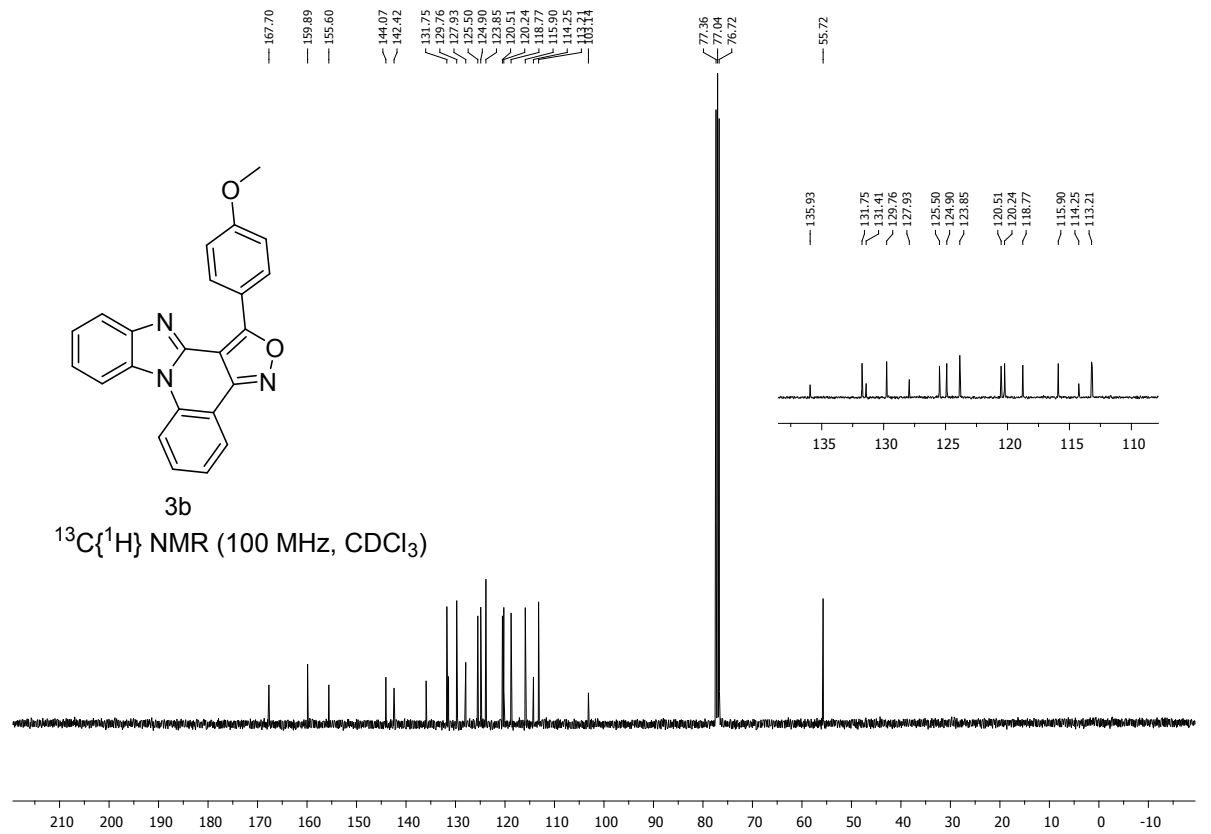

3a
^{1}H NMR (400 MHz, CDCl$_3$)


3a
^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$)



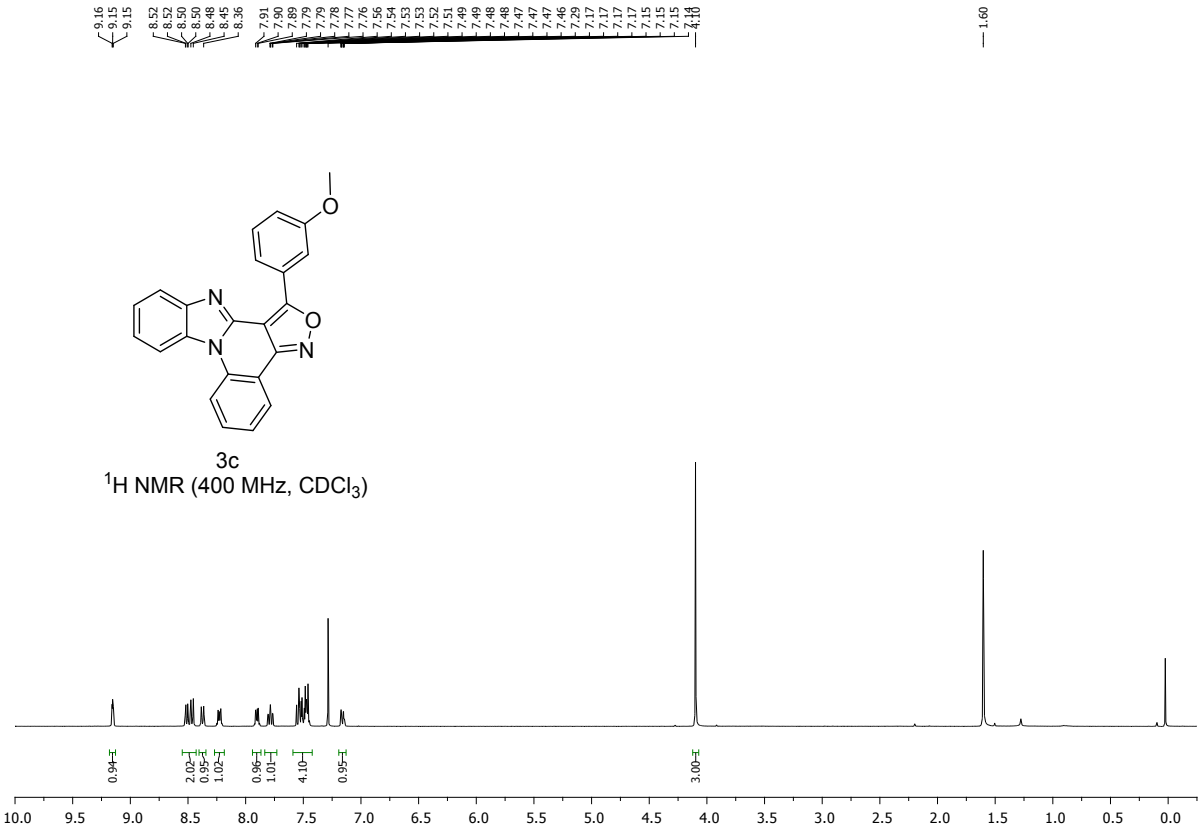
3b

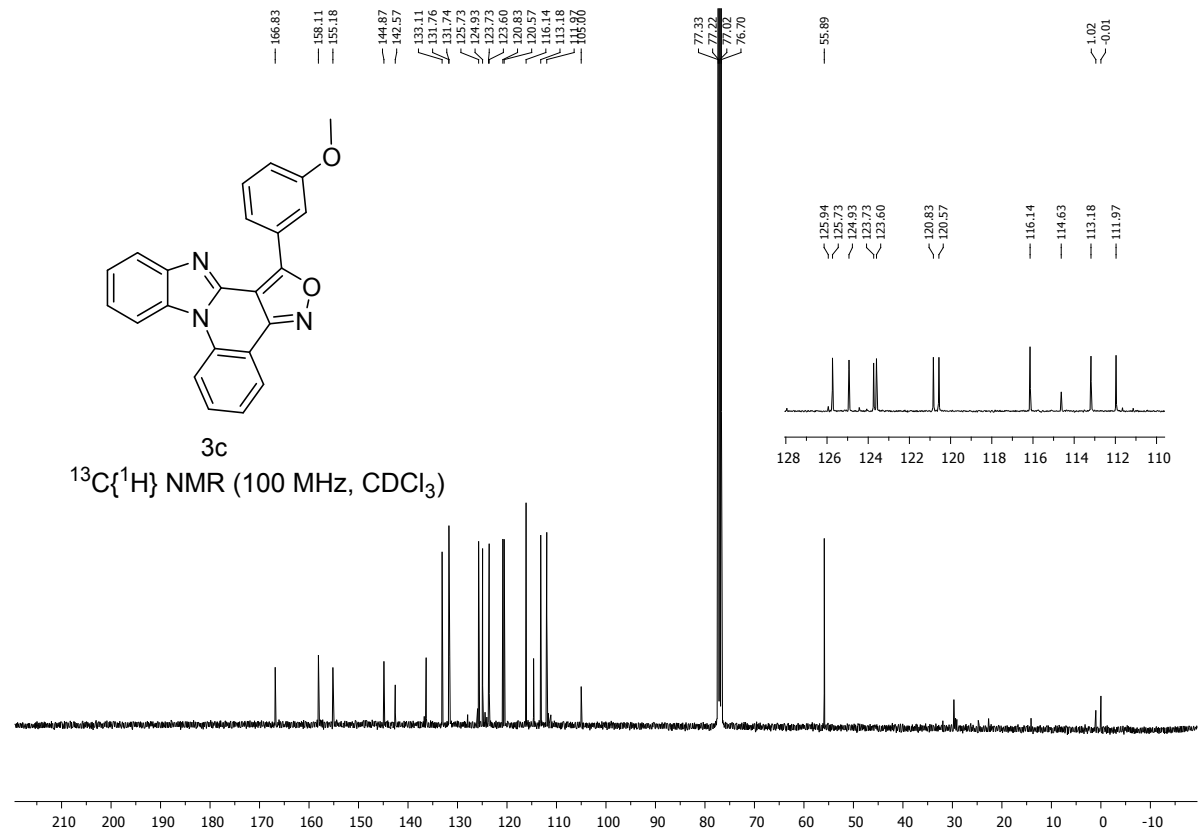
^{1}H NMR (400 MHz, $CDCl_3$)

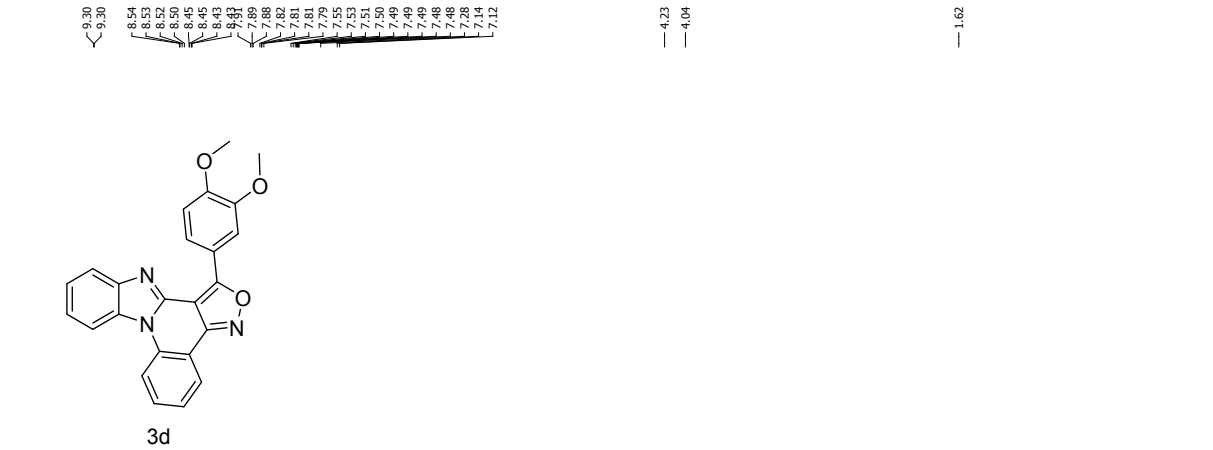


3b

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

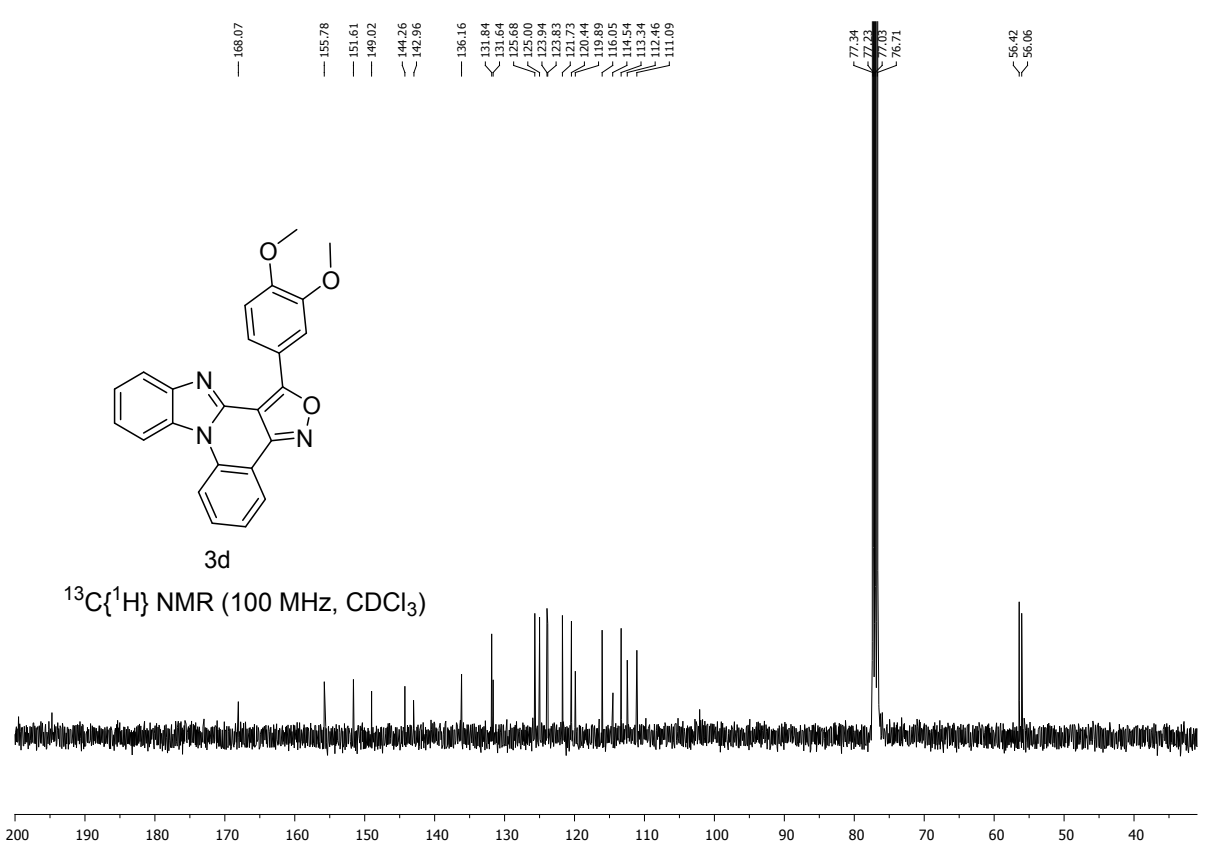

3c
^{1}H NMR (400 MHz, CDCl$_3$)


3c
^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$)



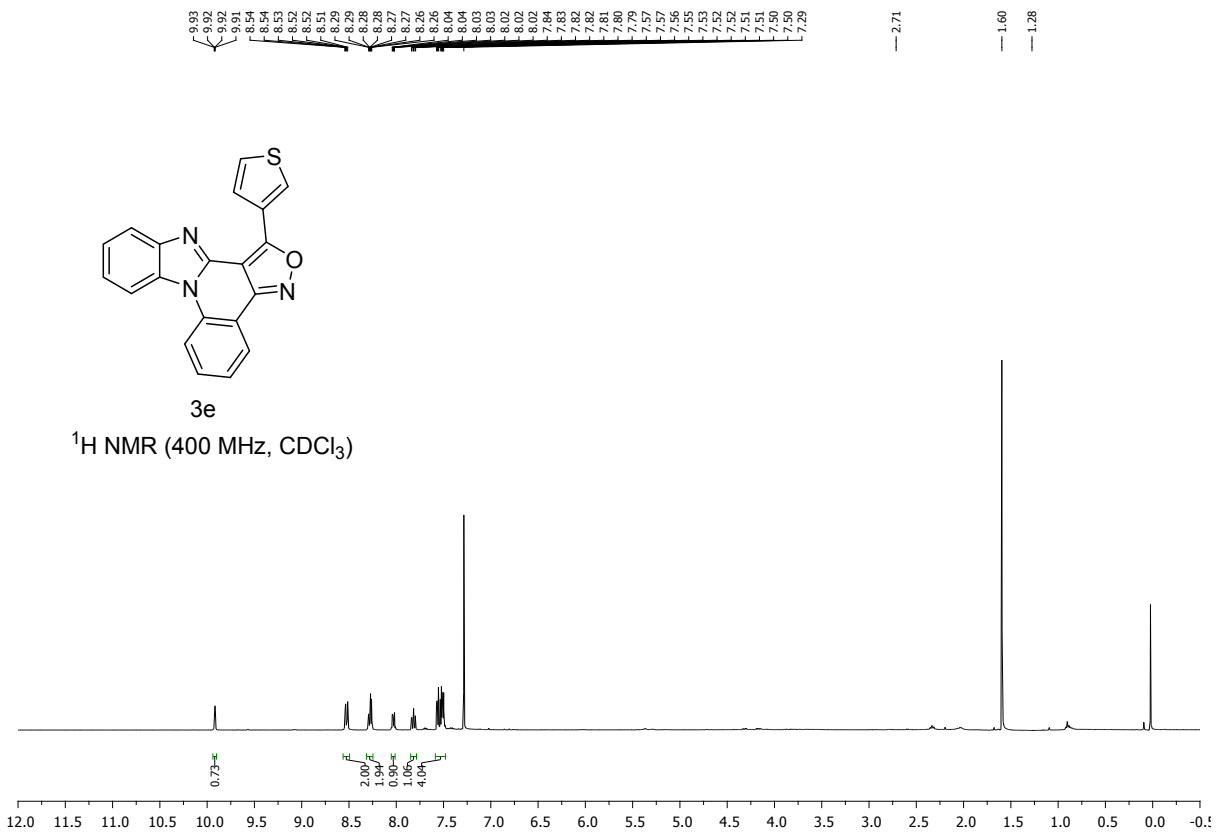
3d

^{1}H NMR (400 MHz, $CDCl_3$)



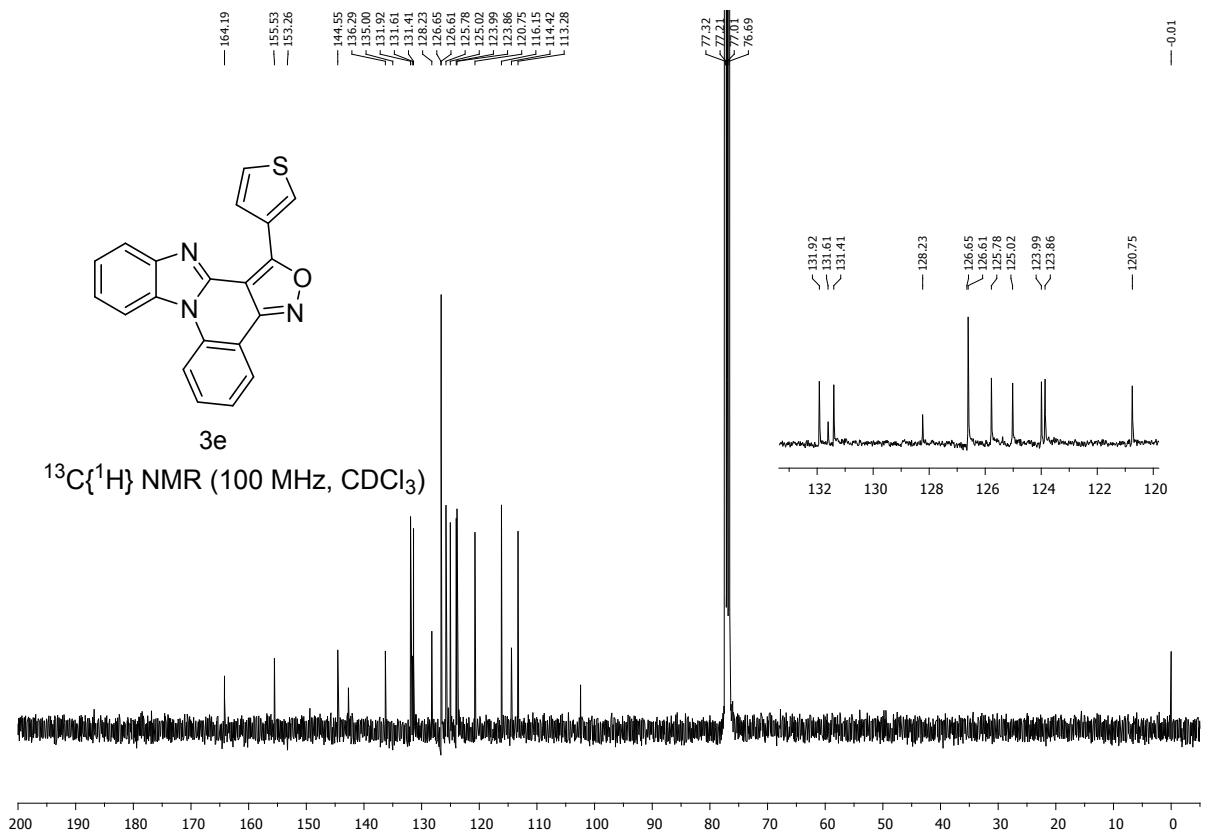
3d

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



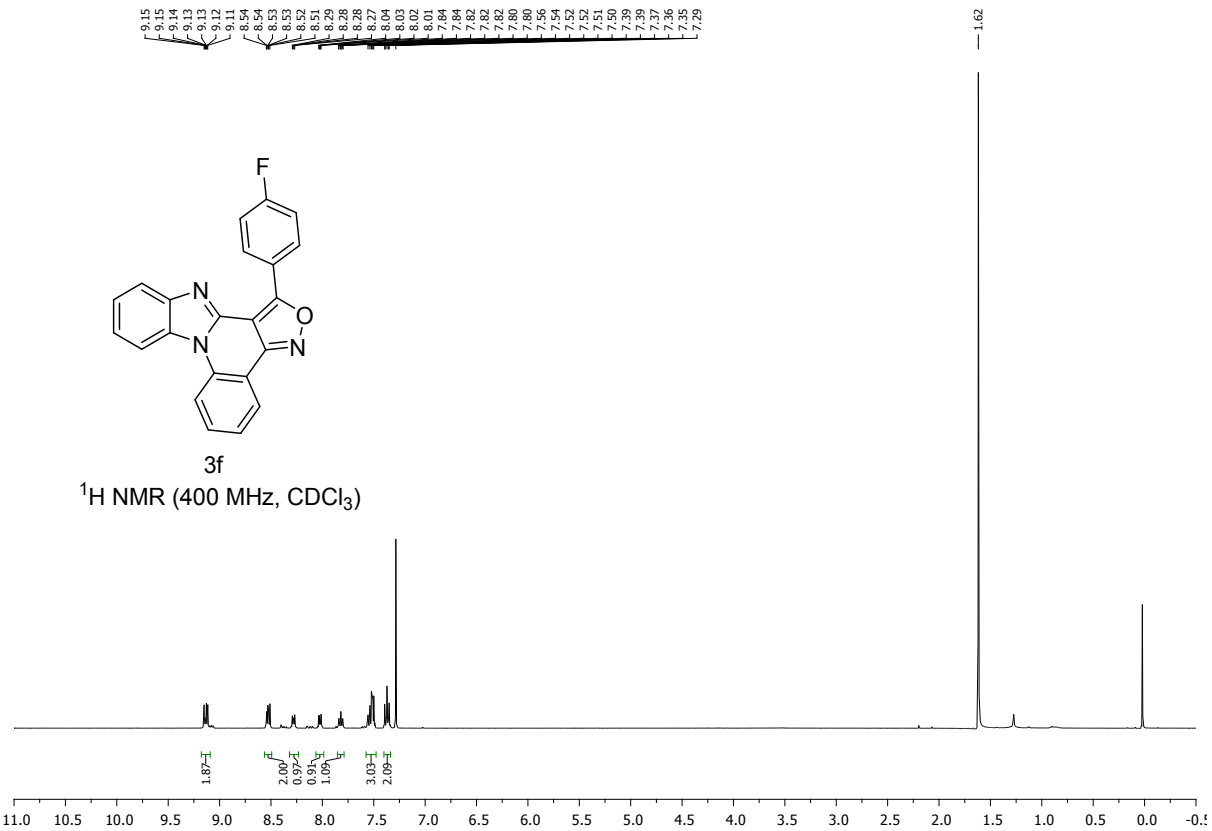
3e

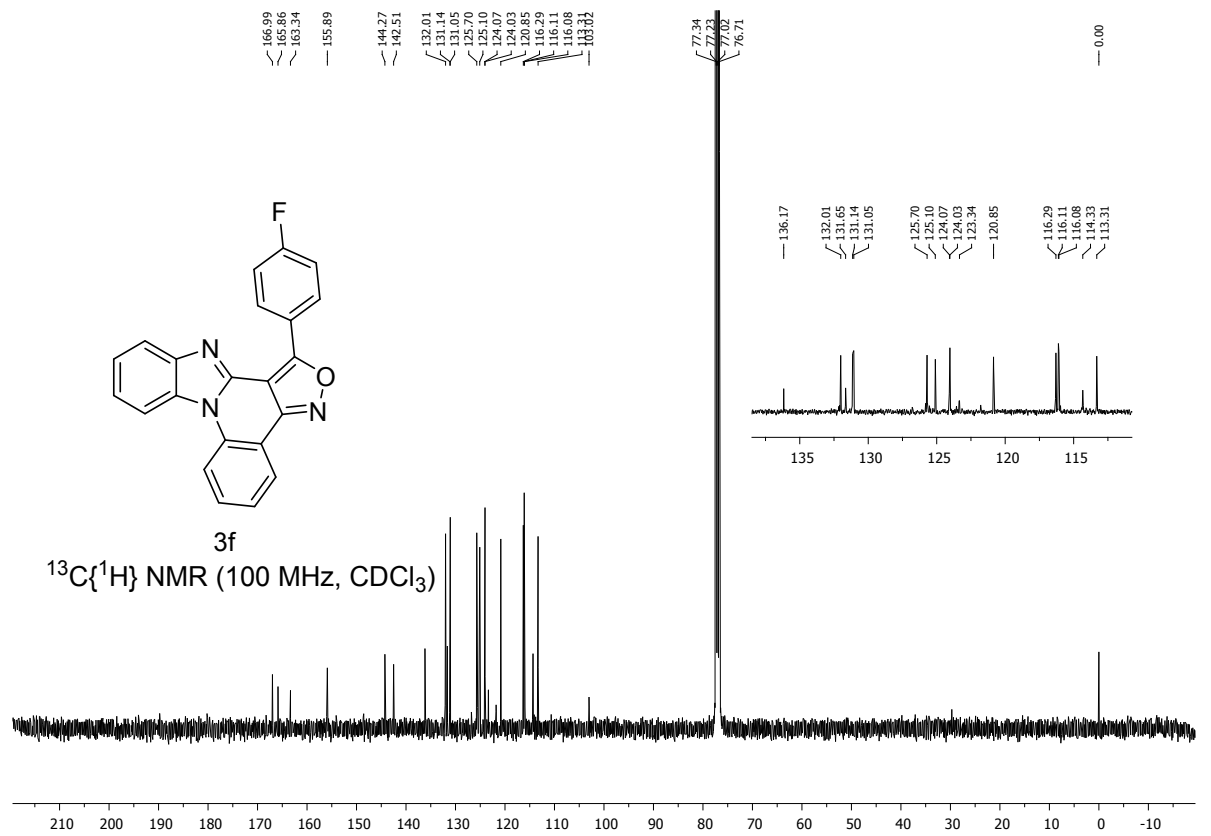
^{1}H NMR (400 MHz, $CDCl_3$)

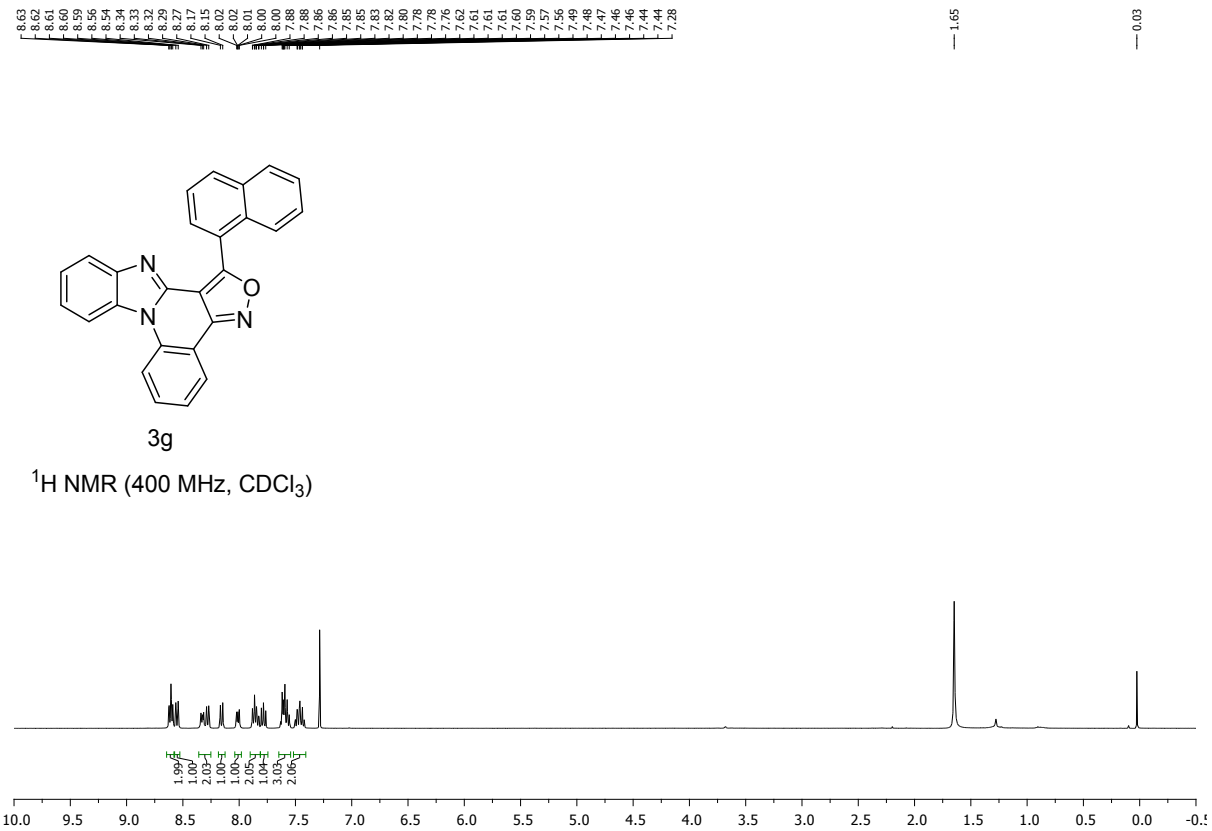


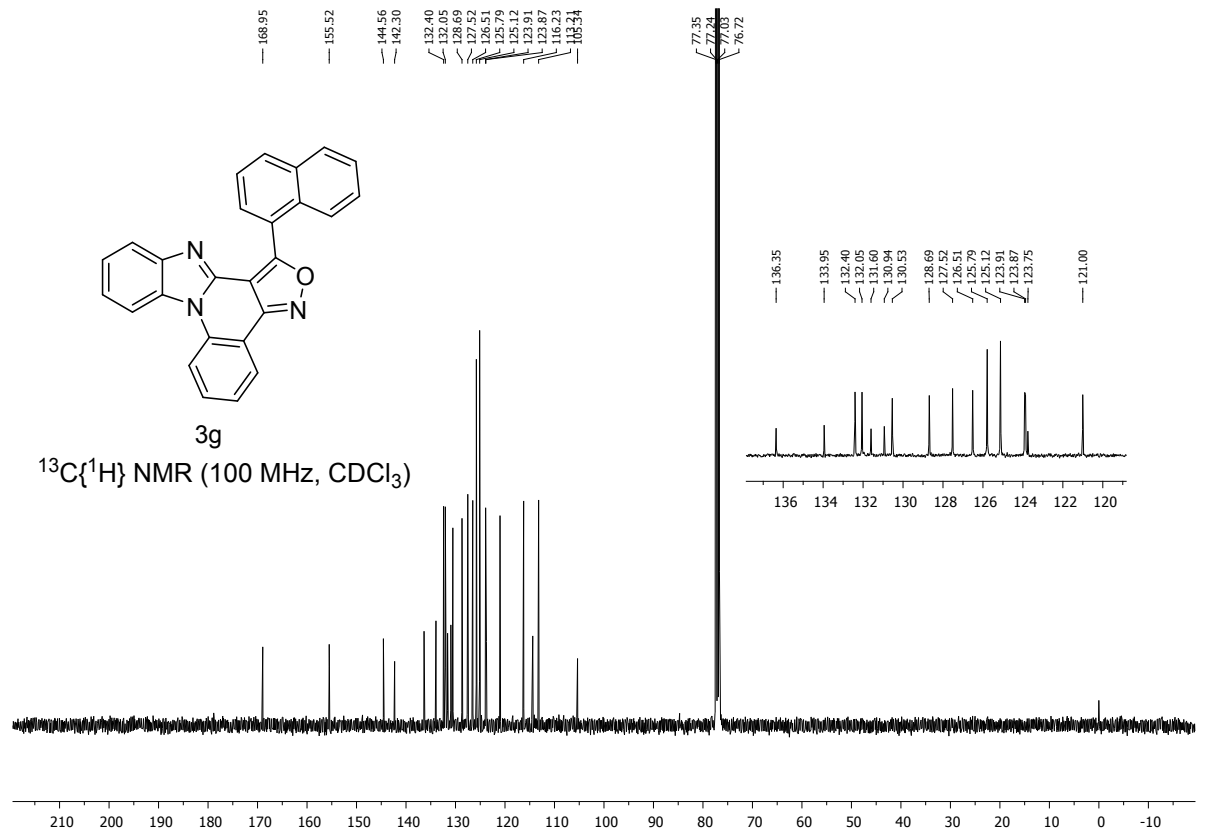
3e

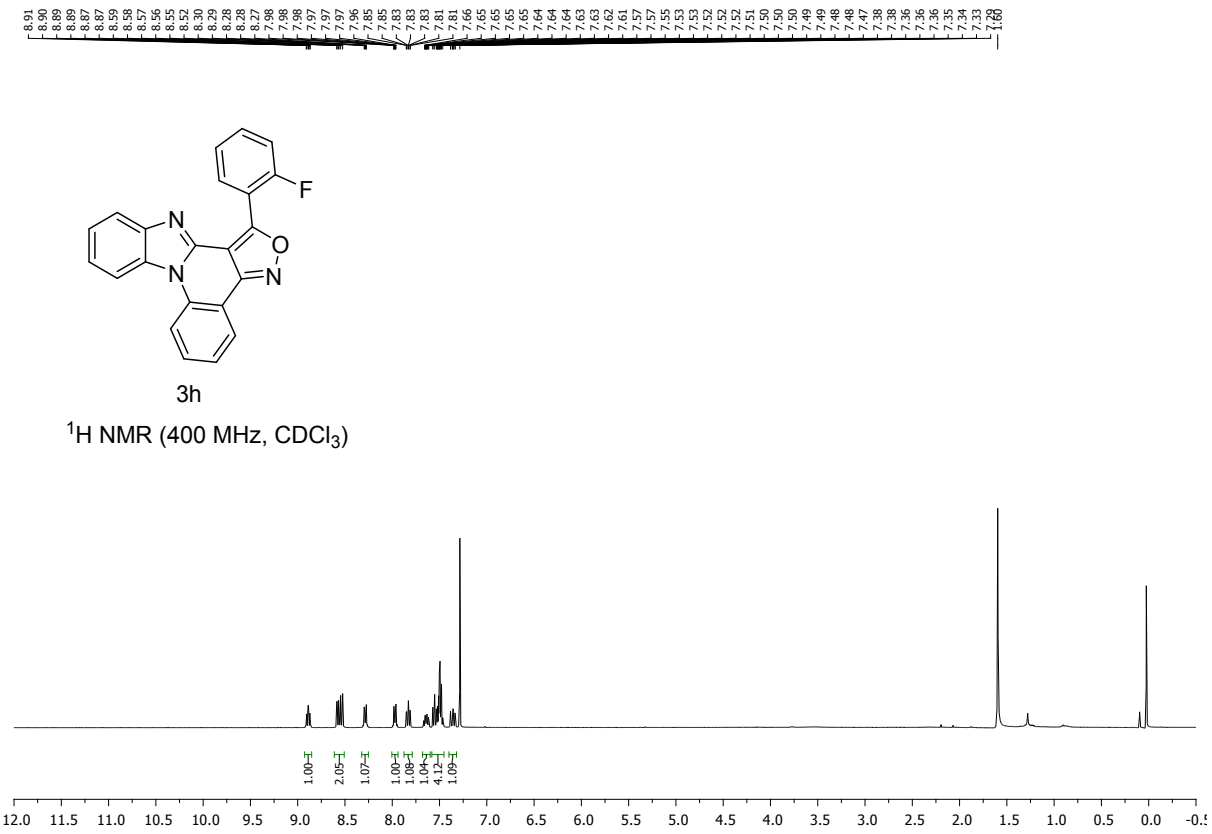
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

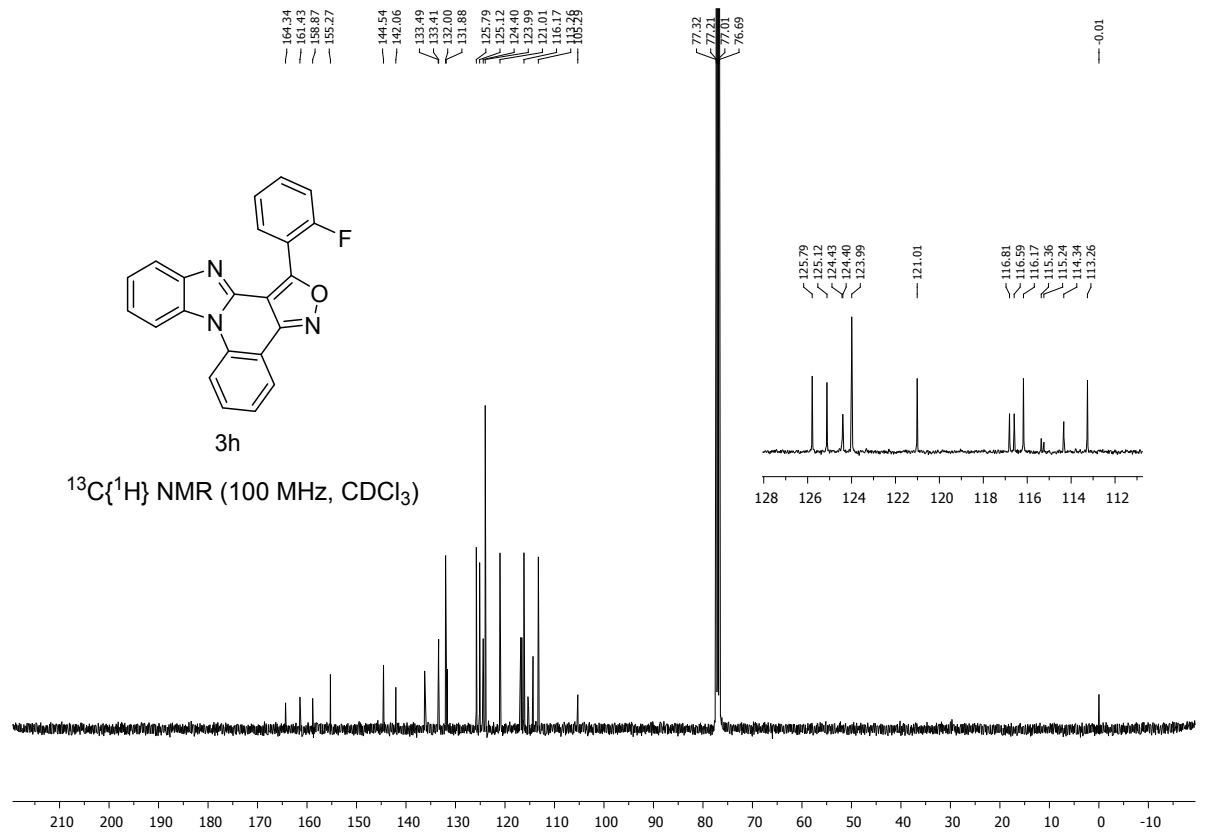

F
N
N
O
N
3f
1H NMR (400 MHz, CDCl3)

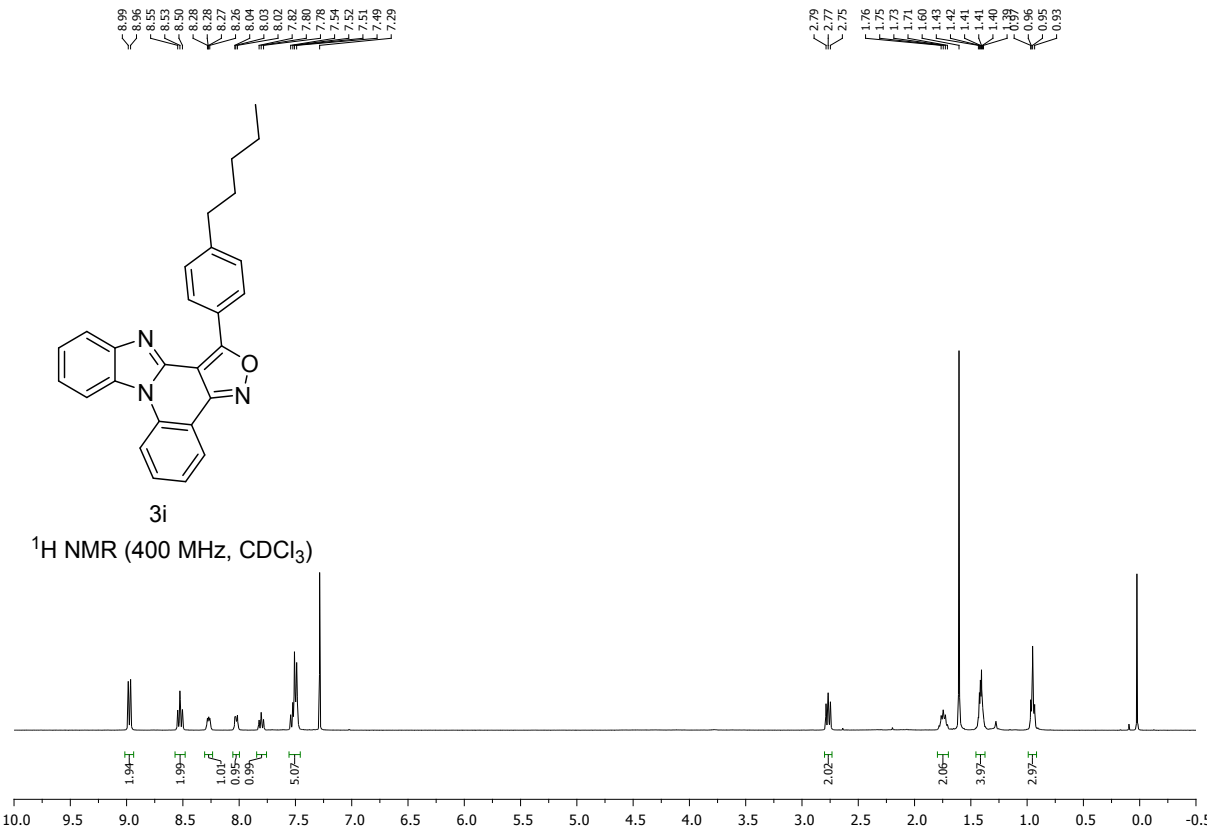

F
N
N
O
N
3f
13C{1H} NMR (100 MHz, CDCl3)

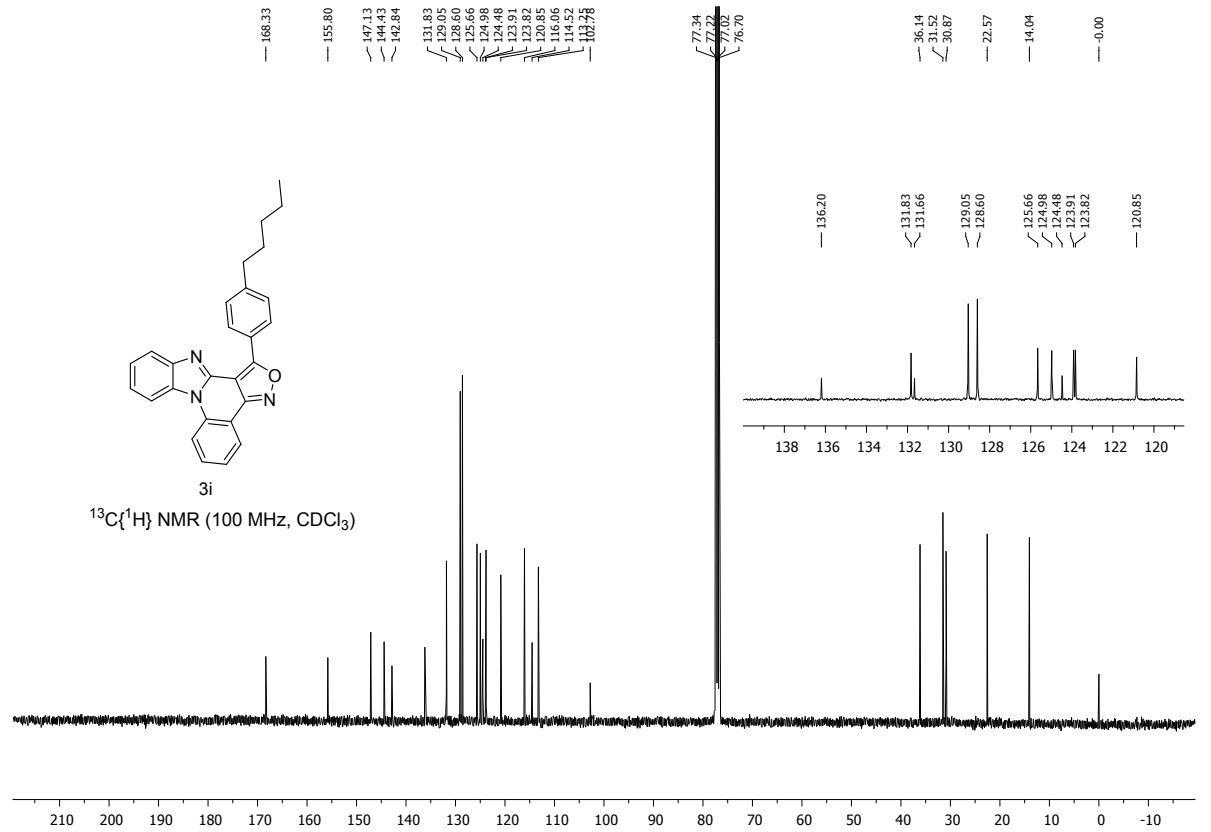

8.63 8.62 8.61 8.60 8.59 8.56 8.54 8.34 8.33 8.32 8.29 8.27 8.17 8.15 8.02 8.02 8.01 8.00 8.00 7.88 7.88 7.86 7.86 7.85 7.85 7.83 7.82 7.80 7.78 7.78 7.76 7.62 7.61 7.61 7.61 7.60 7.59 7.57 7.56 7.49 7.48 7.47 7.46 7.46 7.44 7.44 7.28
1.65
0.03
N
O
N
N
3g
^{1}H NMR (400 MHz, $CDCl_3$)
1.99 1.00 2.03 1.00 1.00 2.05 1.04 3.03 2.06
10.0 9.5 9.0 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

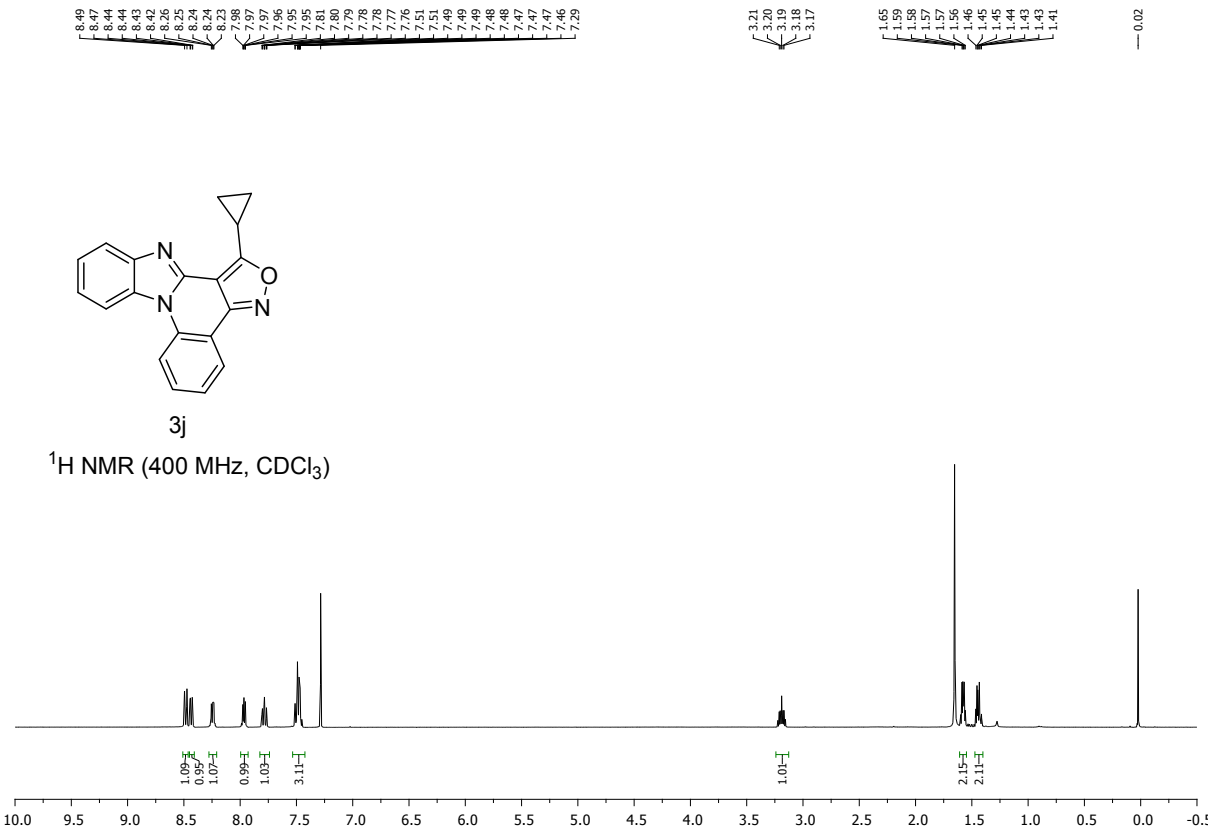

168.95
155.52
144.56
142.30
132.40
132.05
128.69
127.52
126.51
125.79
125.12
123.91
123.87
116.23
103.34
105.34
77.35
77.24
77.03
76.72
136.35
133.95
132.40
132.05
131.60
130.94
130.53
128.69
127.52
126.51
125.79
125.12
123.91
123.87
123.75
121.00
N
O
N
N
3g
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)
136 134 132 130 128 126 124 122 120
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

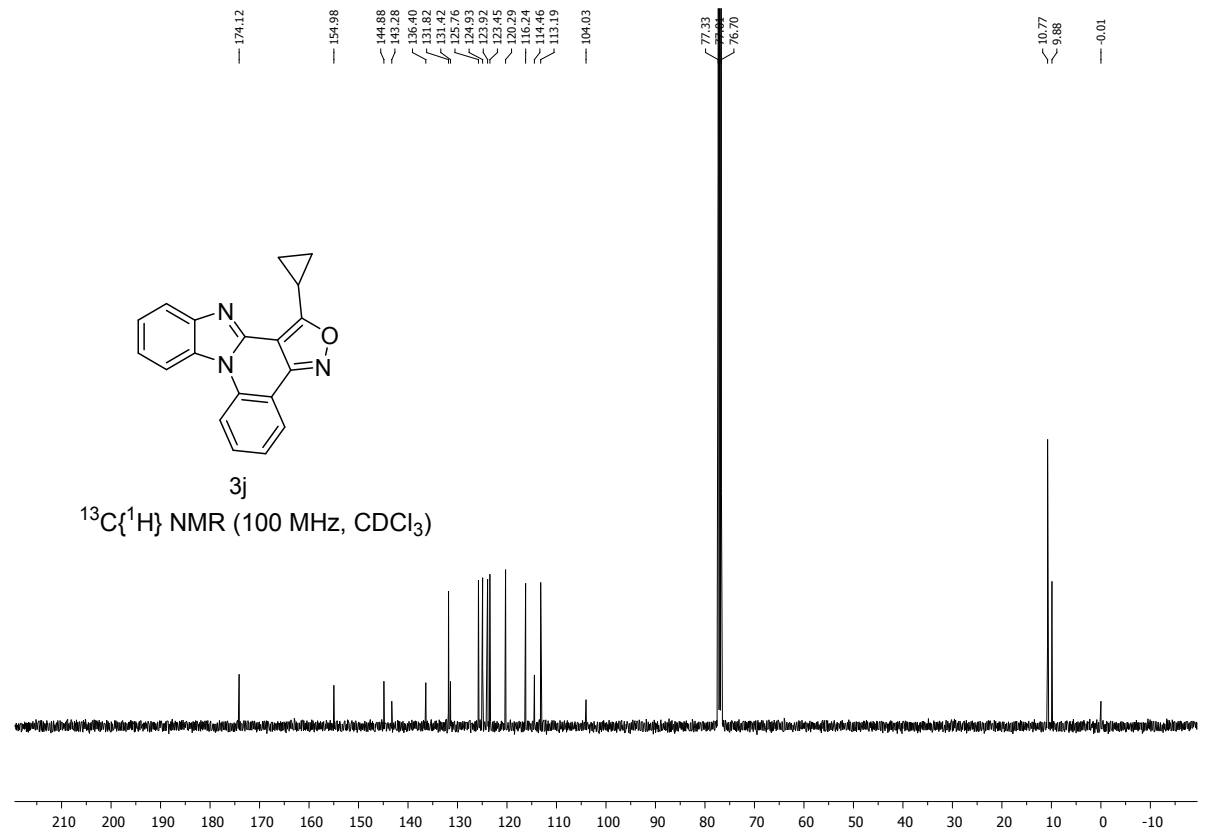

F
N
O
N
N
3h
^{1}H NMR (400 MHz, CDCl$_3$)

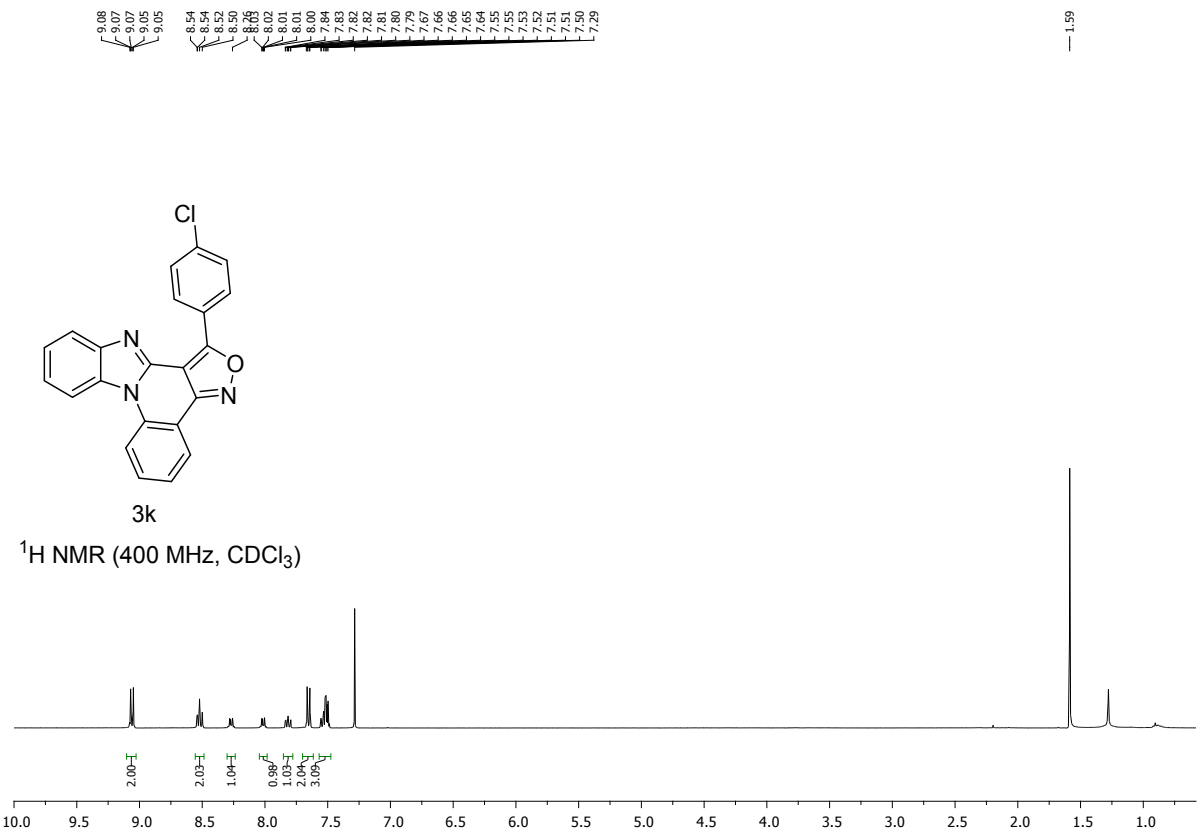

F
N
O
N
N
3h
^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$)

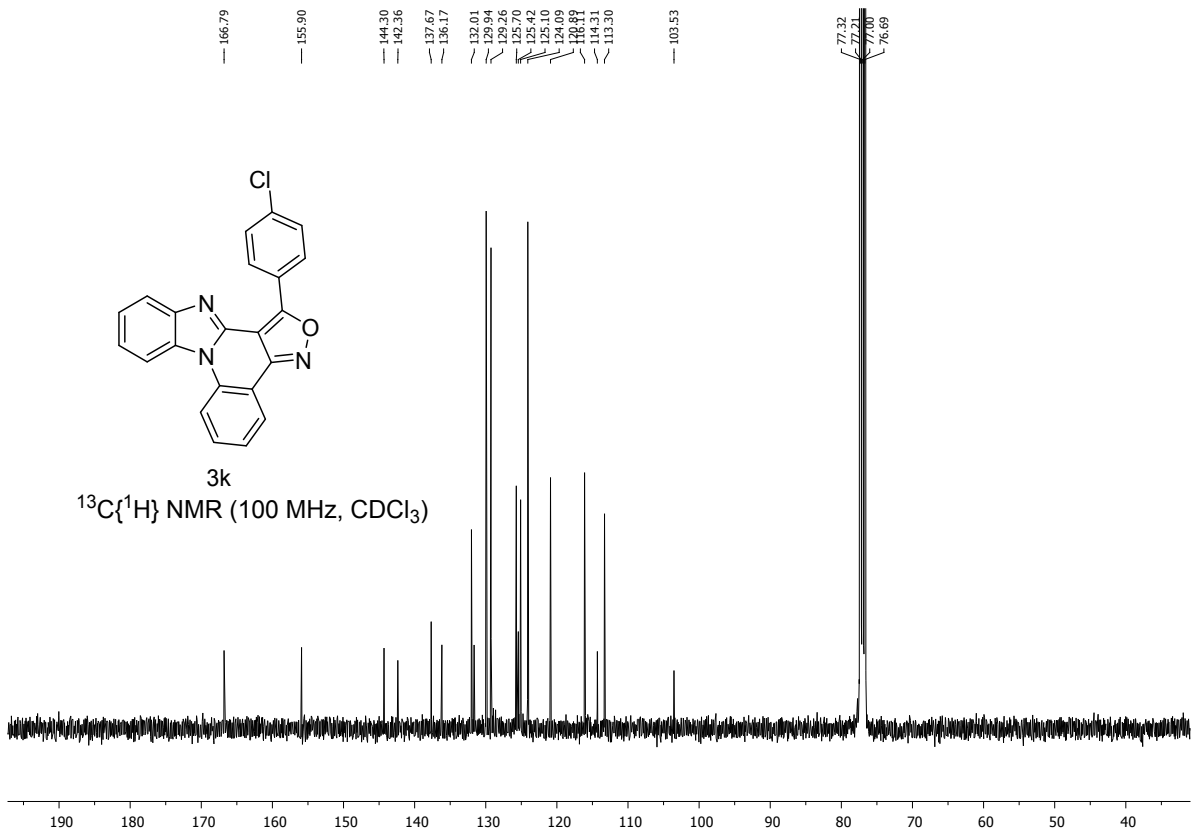

3i
^{1}H NMR (400 MHz, $CDCl_3$)

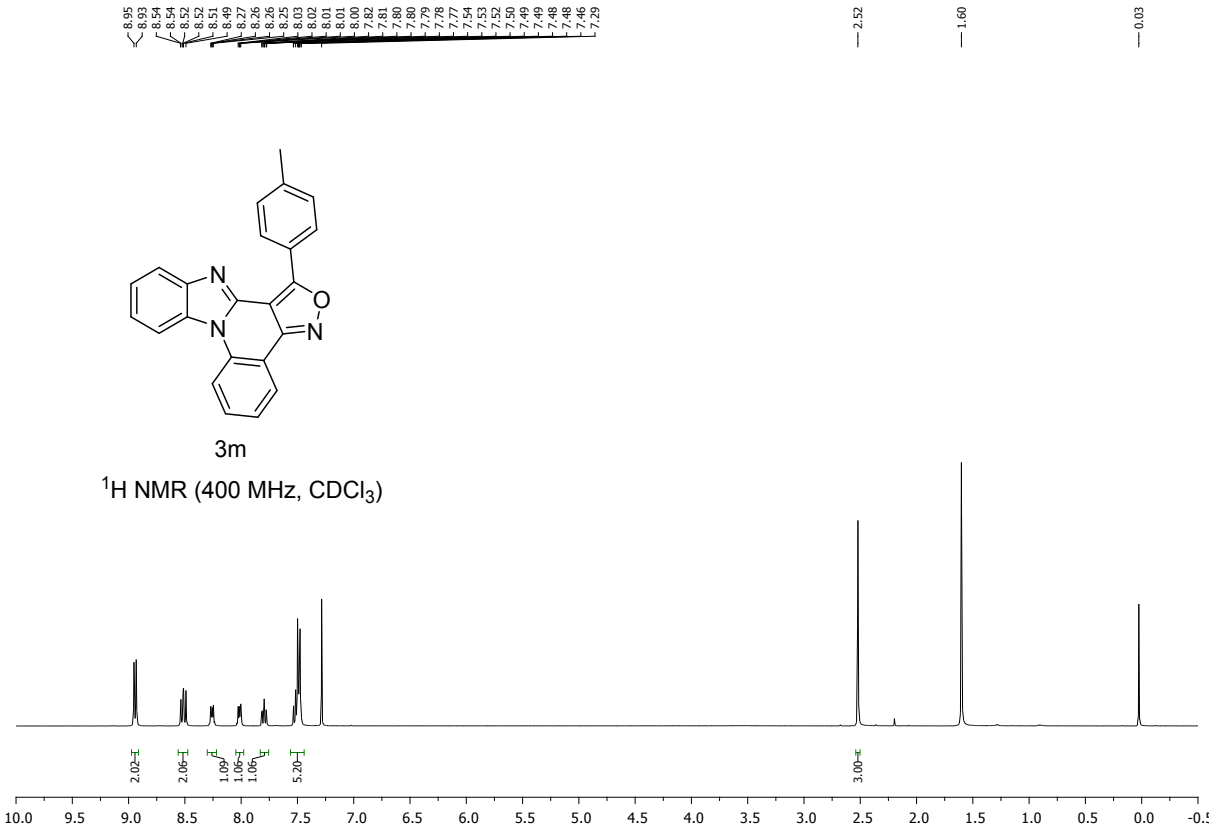

3i
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

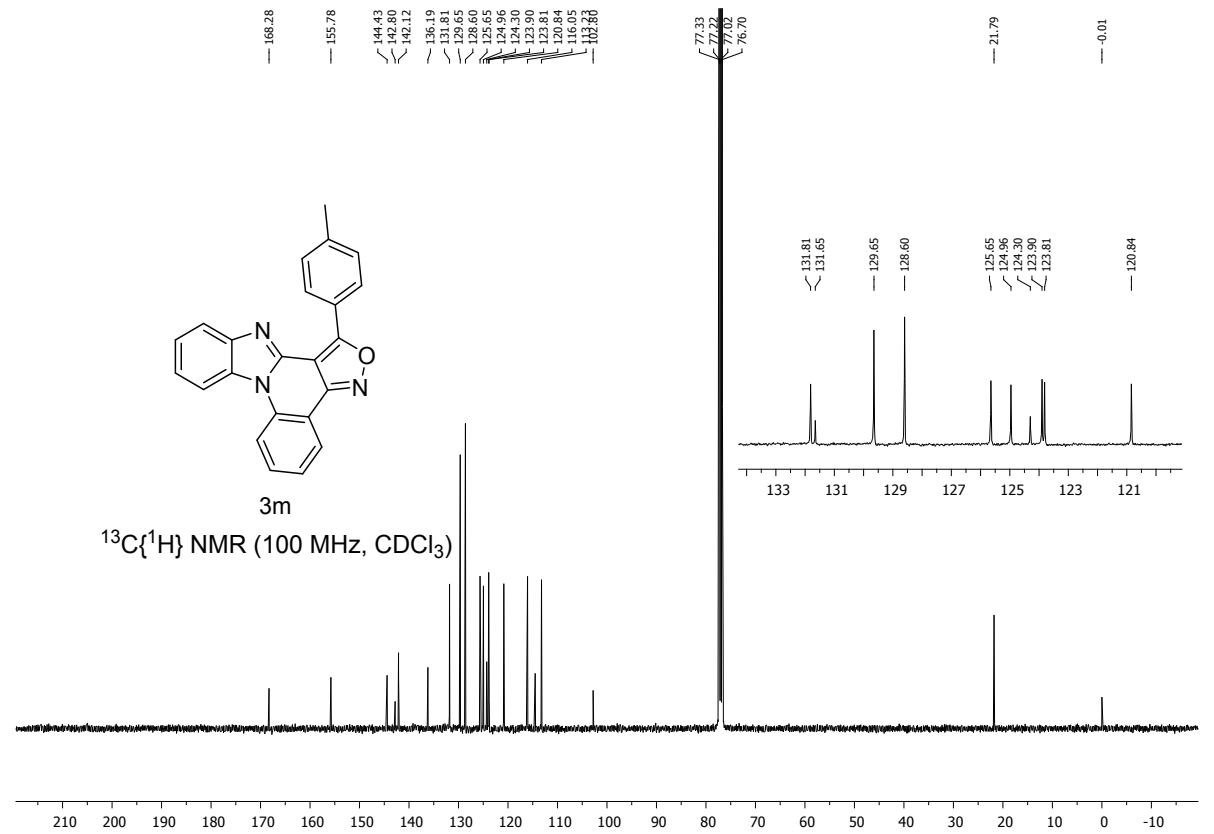

3j
^{1}H NMR (400 MHz, CDCl$_3$)

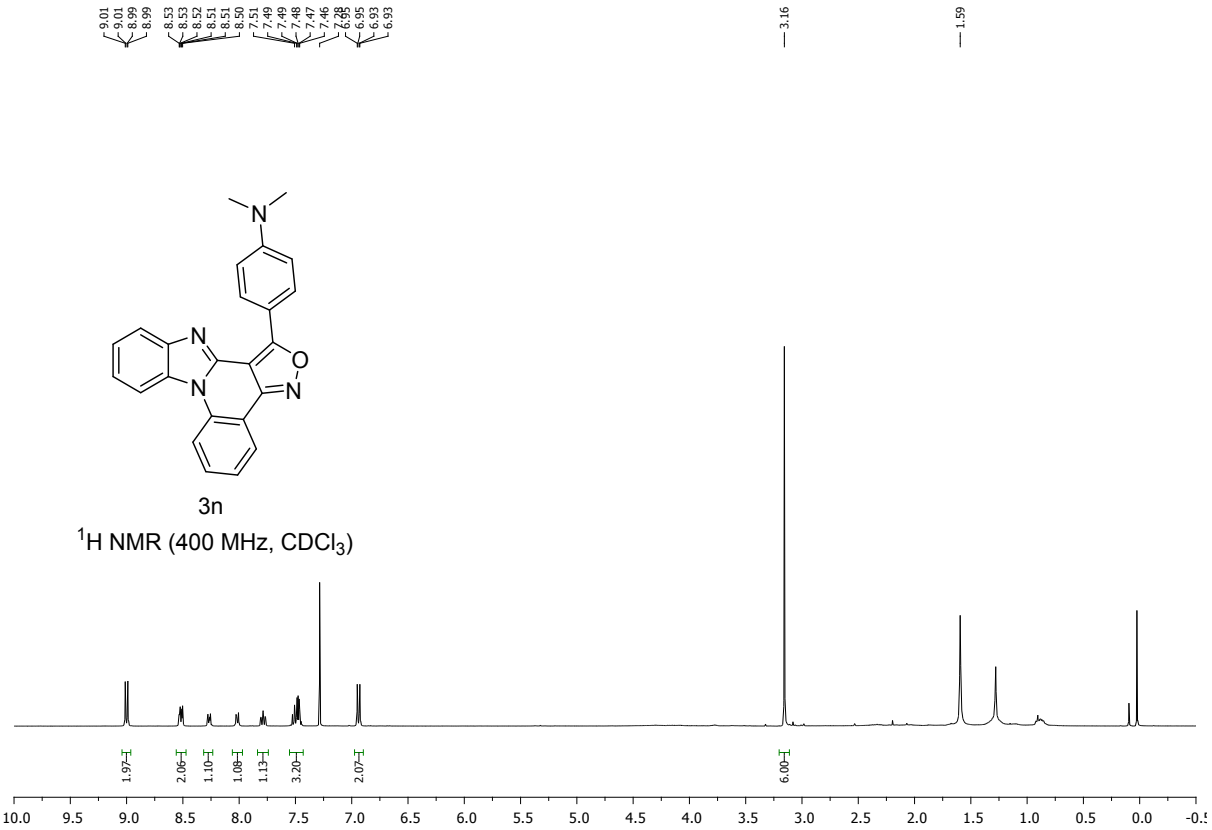

3j
^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$)

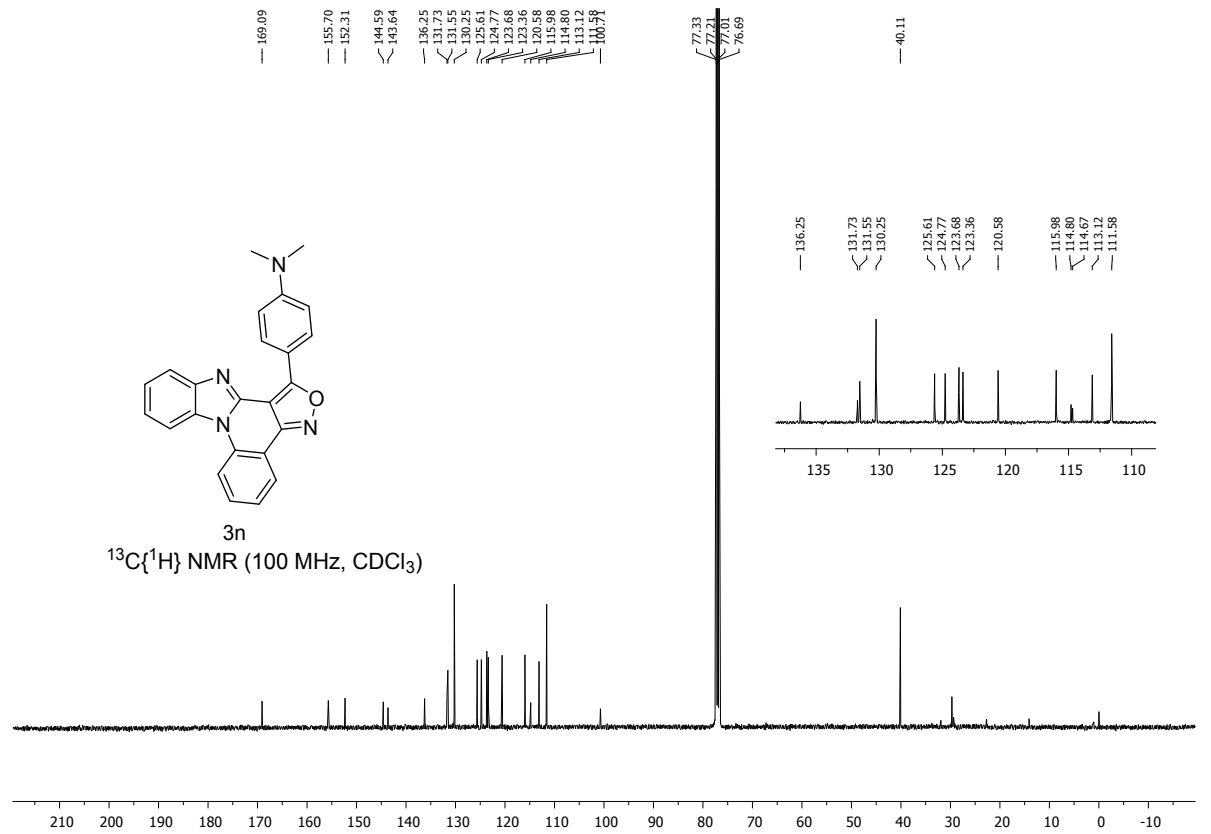

9.08
9.07
9.07
9.05
9.05
8.54
8.54
8.52
8.50
8.03
8.02
8.01
8.01
8.00
7.84
7.83
7.82
7.82
7.81
7.80
7.79
7.67
7.66
7.66
7.65
7.64
7.55
7.55
7.53
7.52
7.51
7.51
7.50
7.29
1.59
Cl
N
N
O
N
3k
^{1}H NMR (400 MHz, $CDCl_3$)
2.00
2.03
1.04
0.99
1.03
2.04
3.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0

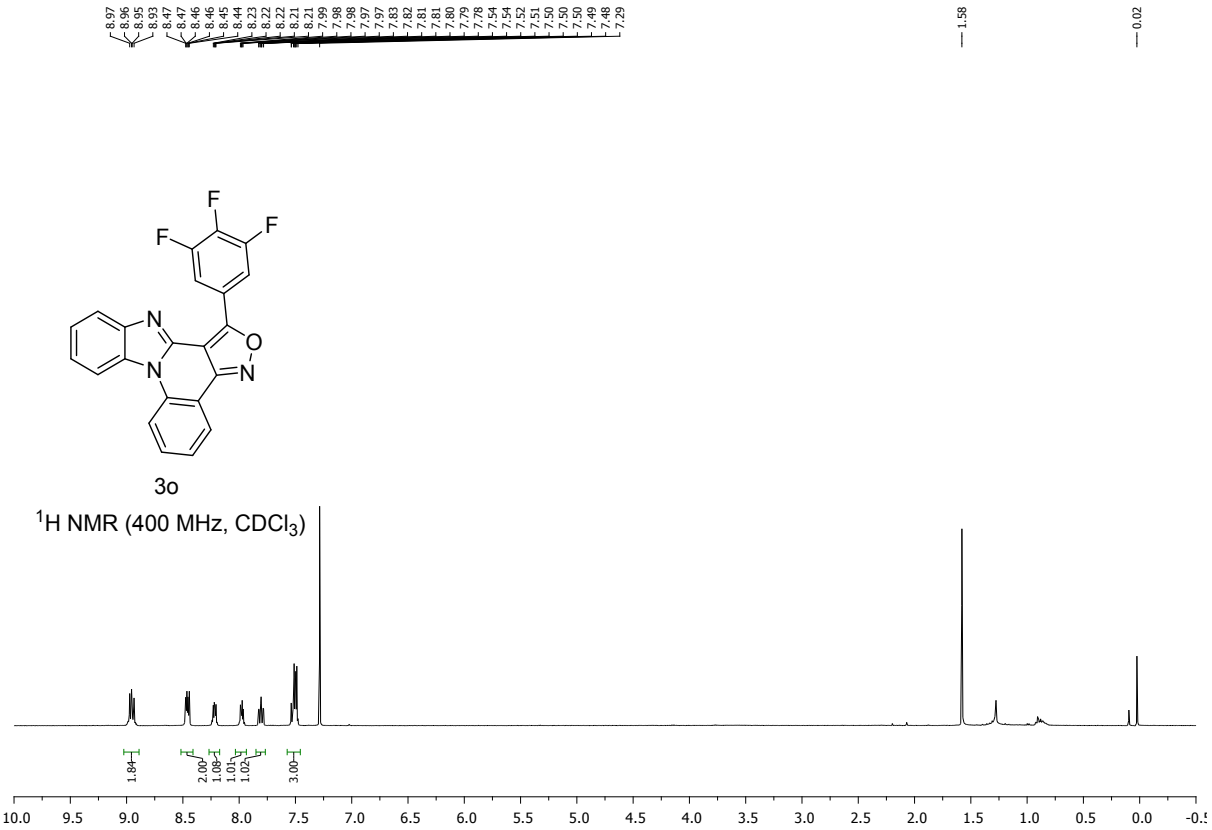

166.79
155.90
144.30
142.36
137.67
136.17
132.01
129.94
129.26
125.70
125.42
125.10
124.09
120.89
116.11
114.31
113.30
103.53
77.32
77.21
77.00
76.69
Cl
N
N
O
N
3k
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40

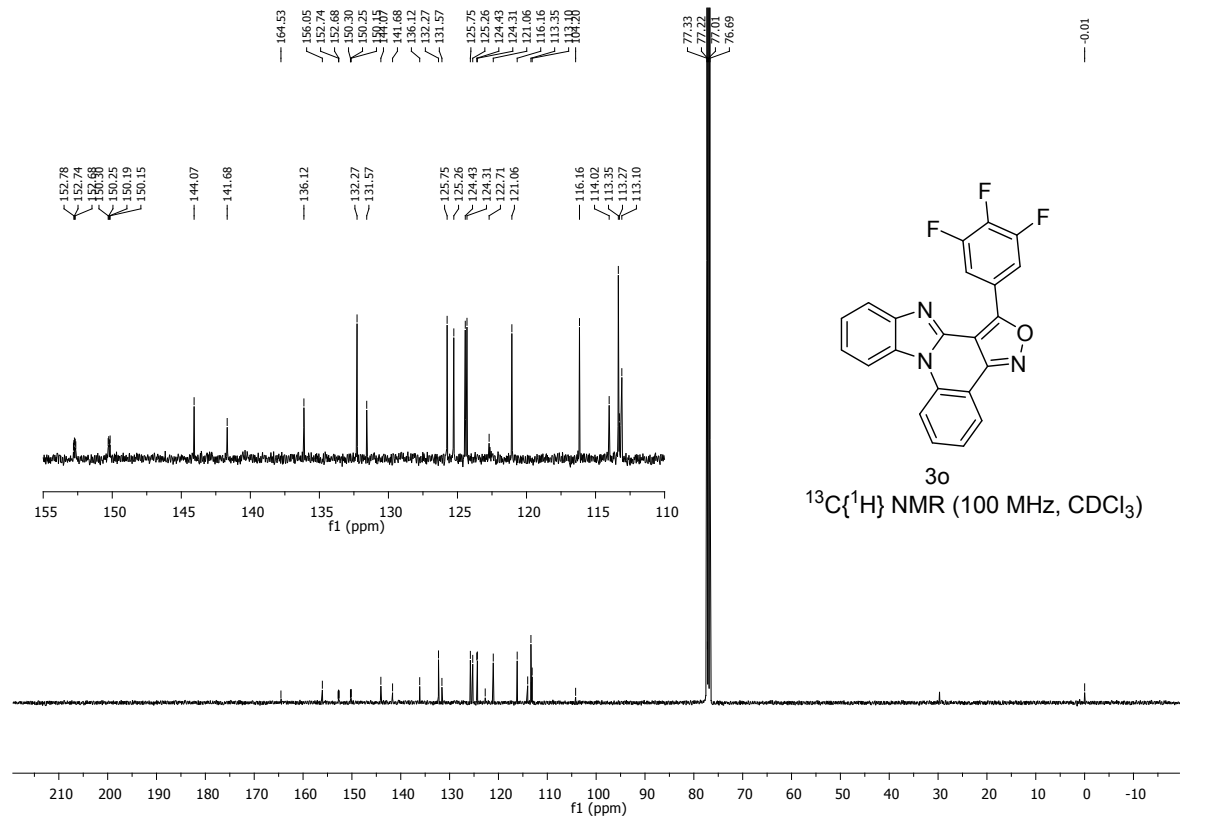

8.95
8.93
8.54
8.54
8.52
8.52
8.51
8.49
8.27
8.26
8.26
8.25
8.03
8.02
8.01
8.01
8.00
7.82
7.81
7.80
7.80
7.79
7.78
7.77
7.54
7.53
7.52
7.50
7.49
7.49
7.48
7.48
7.46
7.29
2.52
1.60
0.03
N
N
O
N
3m
^{1}H NMR (400 MHz, CDCl$_3$)
2.02
2.06
1.09
1.06
1.06
5.20
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

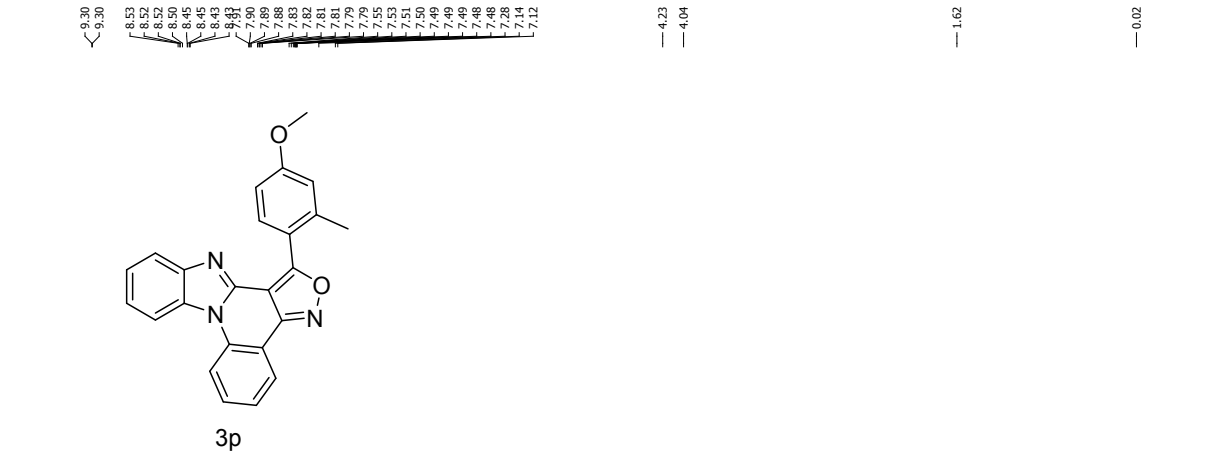

168.28
155.78
144.43
142.80
142.12
136.19
131.81
129.65
128.60
125.65
124.96
124.30
123.90
123.81
120.84
116.05
77.33
77.22
77.02
76.70
21.79
-0.01
131.81
131.65
129.65
128.60
125.65
124.96
124.30
123.90
123.81
120.84
133 131 129 127 125 123 121
N
N
O
N
3m
^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


3n
^{1}H NMR (400 MHz, $CDCl_3$)


3n
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

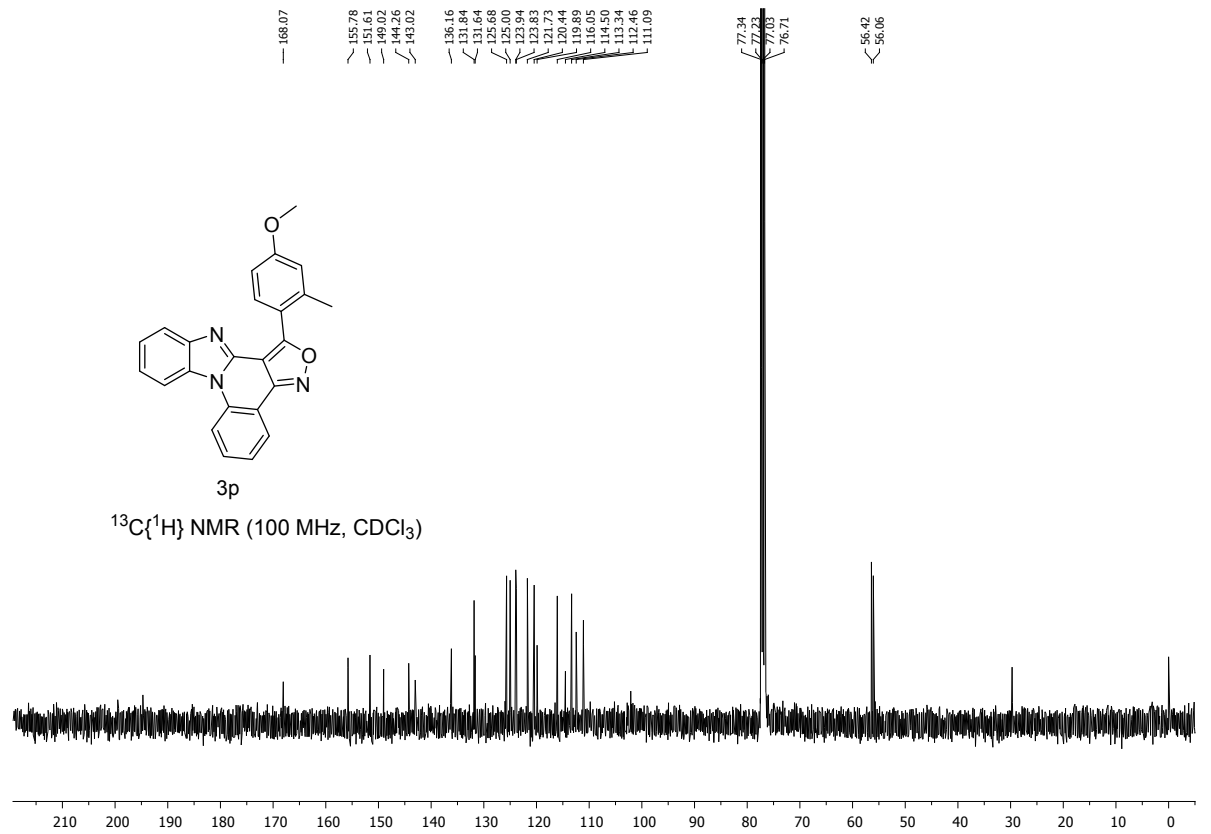

3o
^{1}H NMR (400 MHz, $CDCl_3$)


3o
$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$)
f1 (ppm)



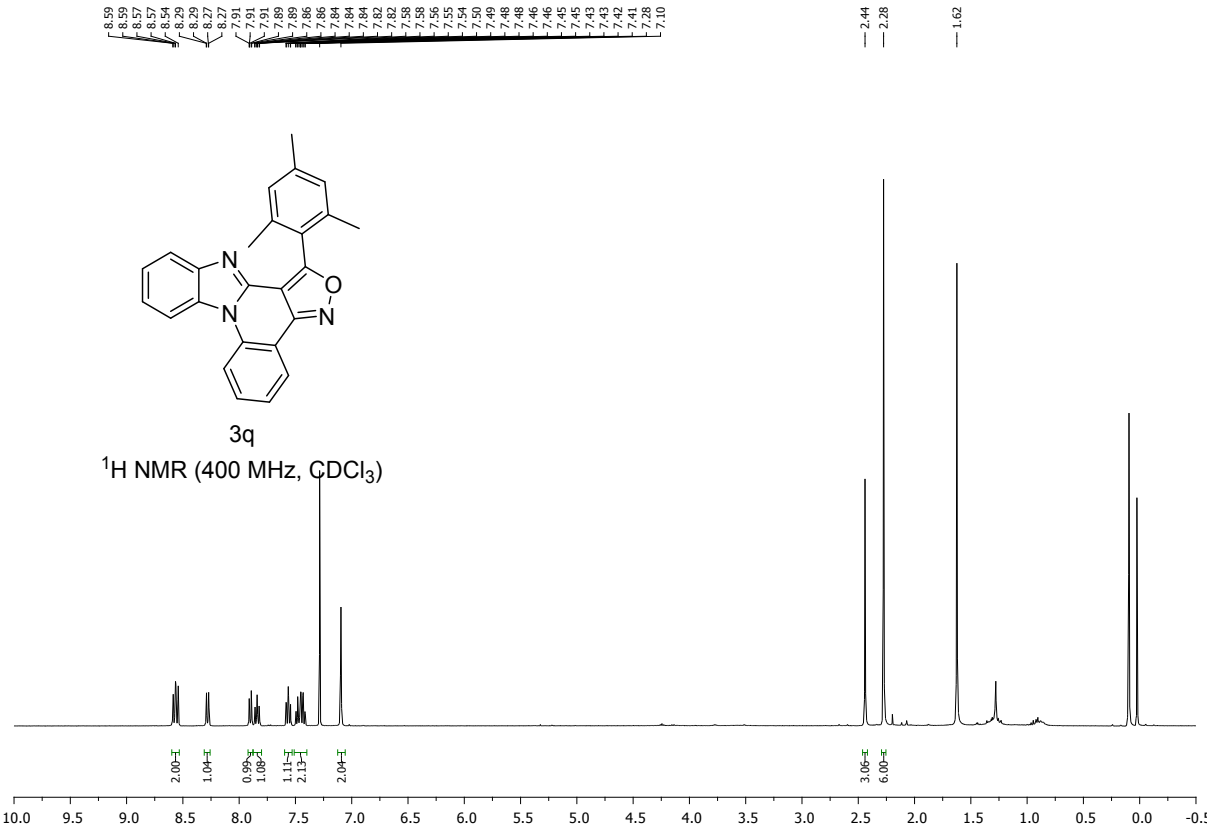
3p

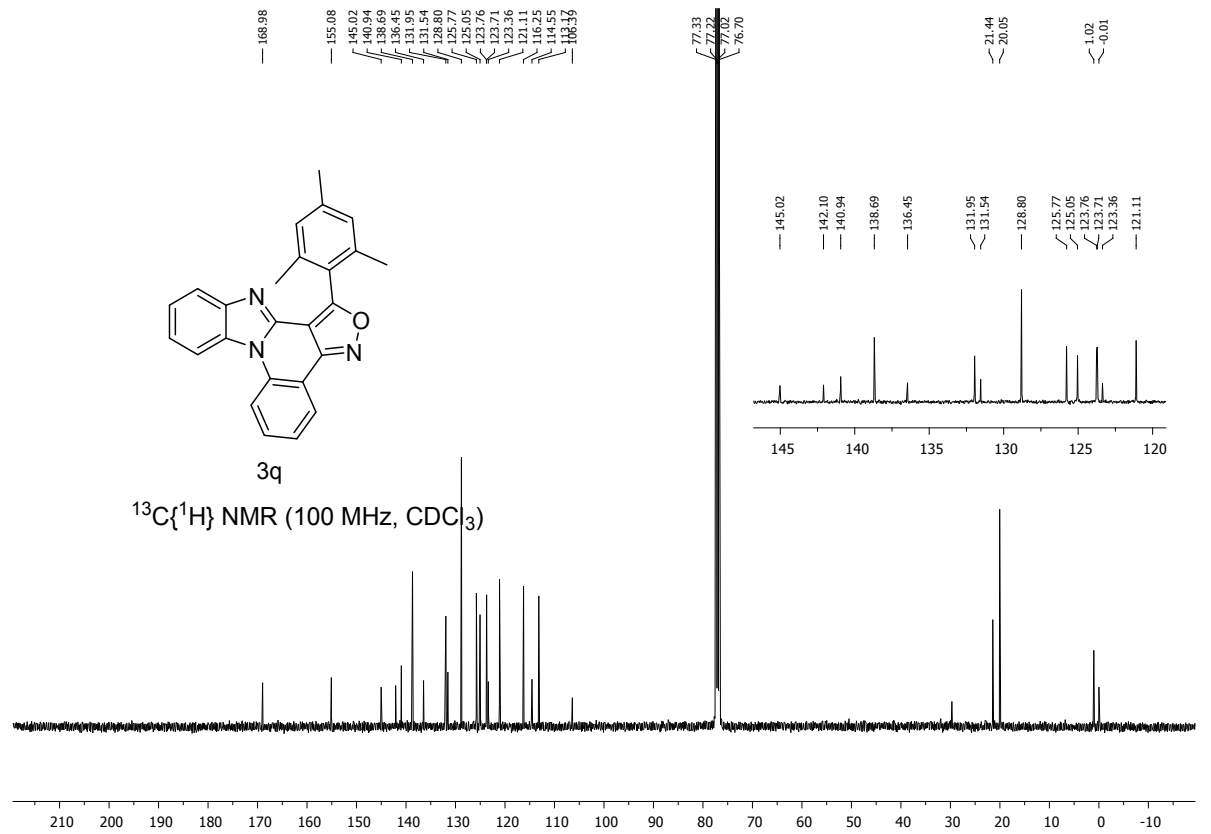
^{1}H NMR (400 MHz, $CDCl_3$)

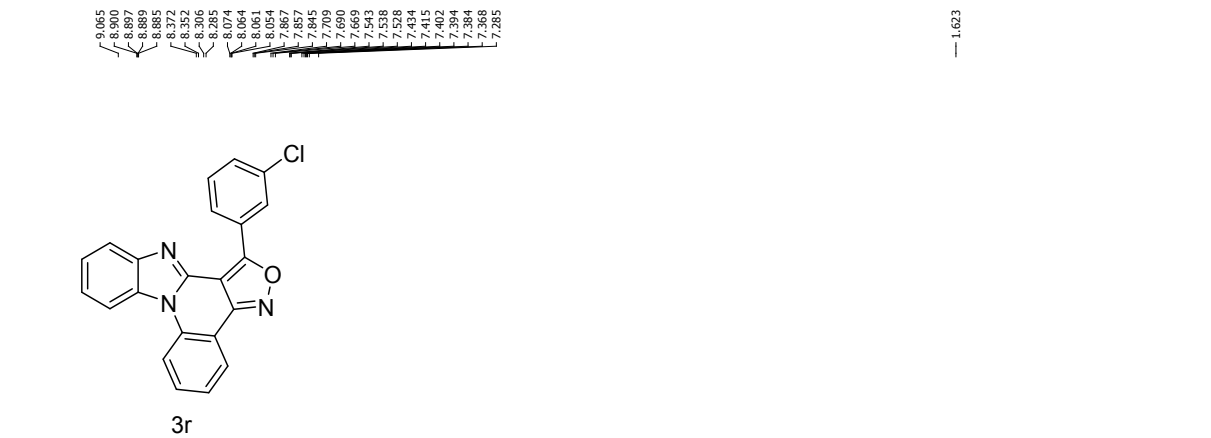


3p

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

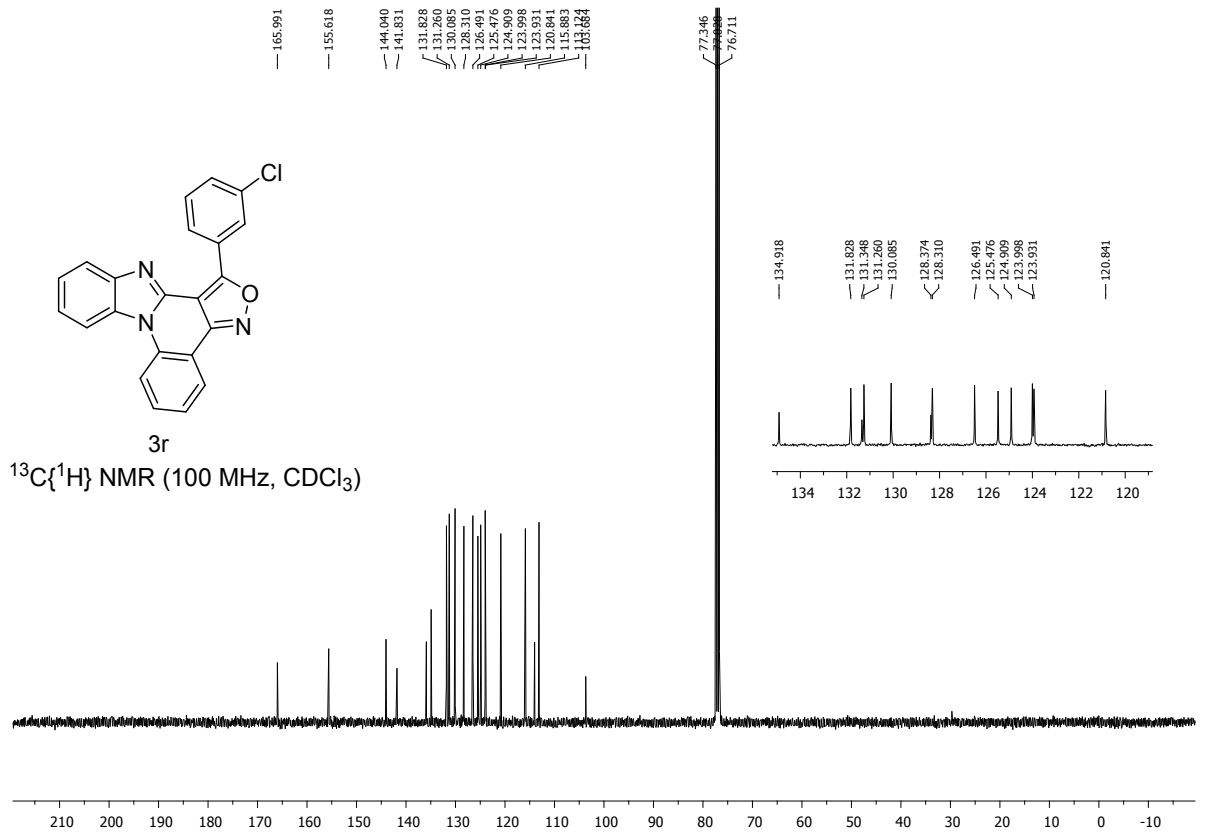

3q
^{1}H NMR (400 MHz, CDCl$_3$)


3q
^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$)



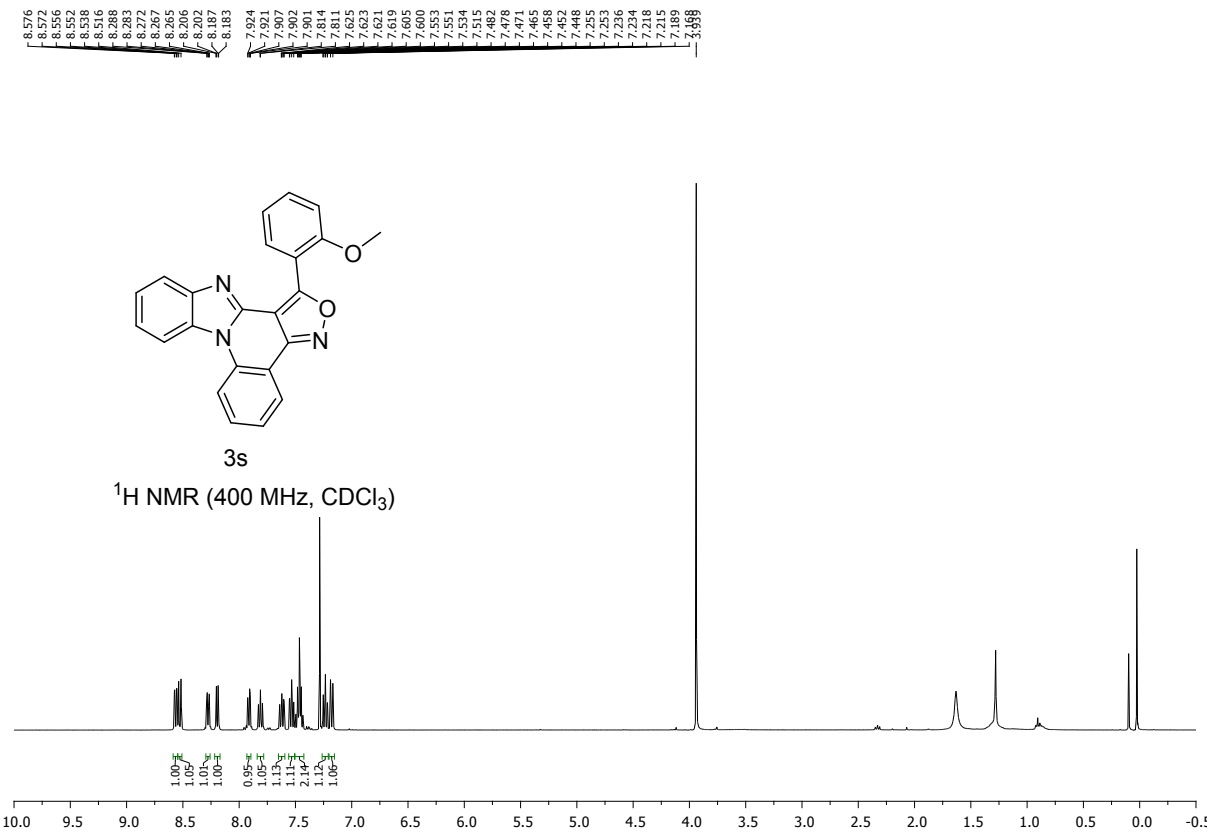
3r

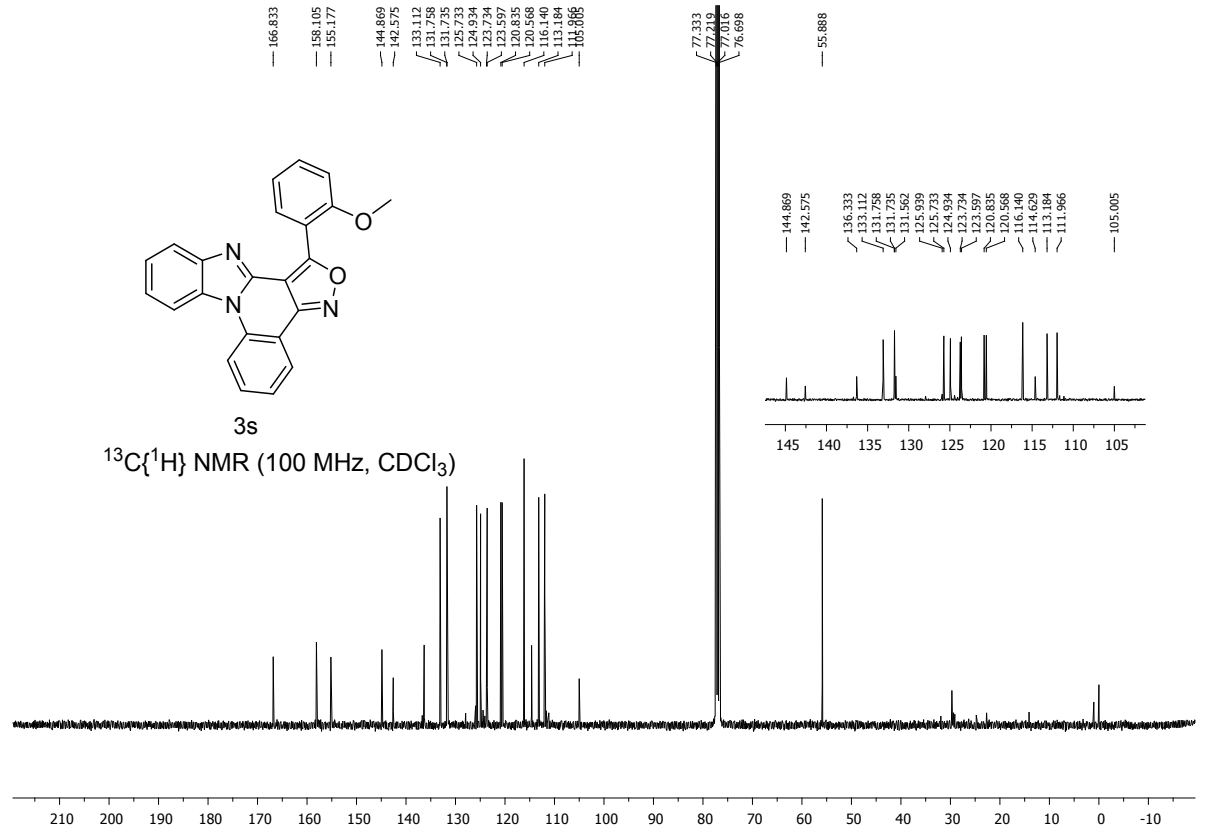
^{1}H NMR (400 MHz, $CDCl_3$)

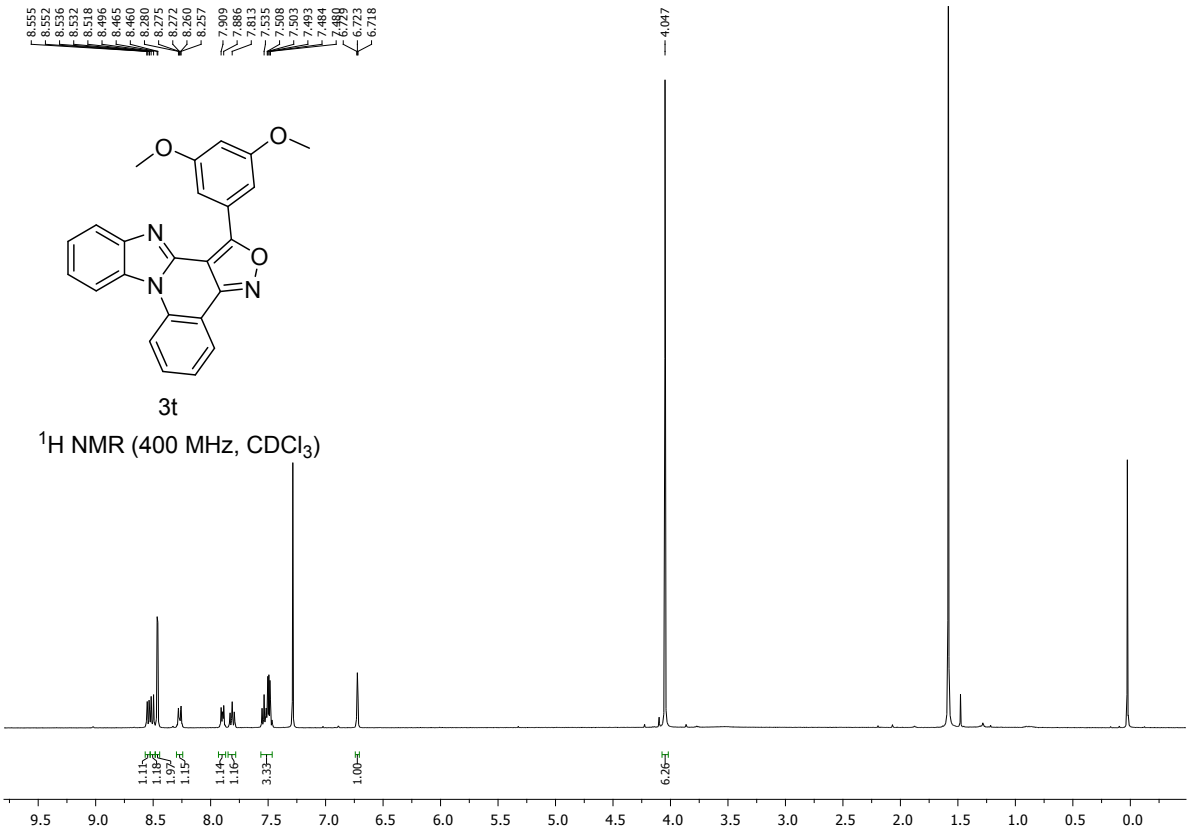


3r

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

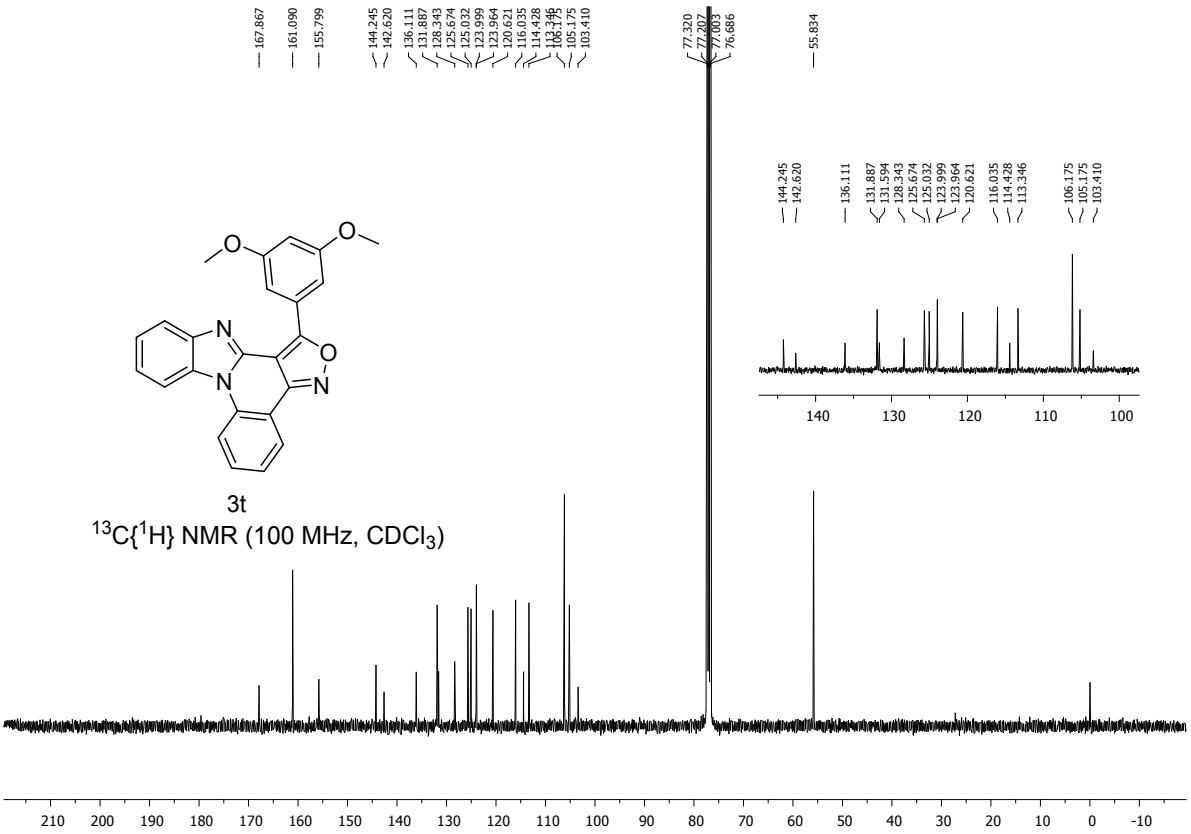

3s
^{1}H NMR (400 MHz, CDCl$_3$)


3s
^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$)



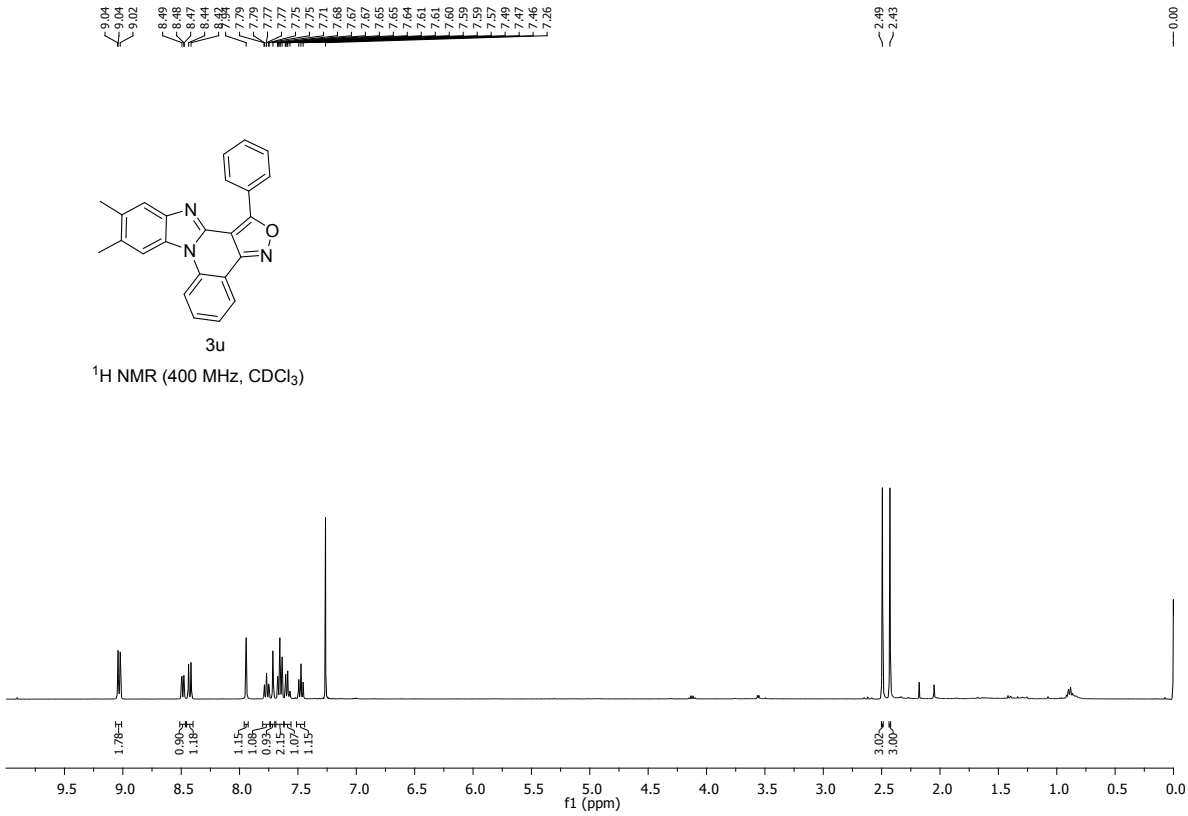
3t

^{1}H NMR (400 MHz, $CDCl_3$)



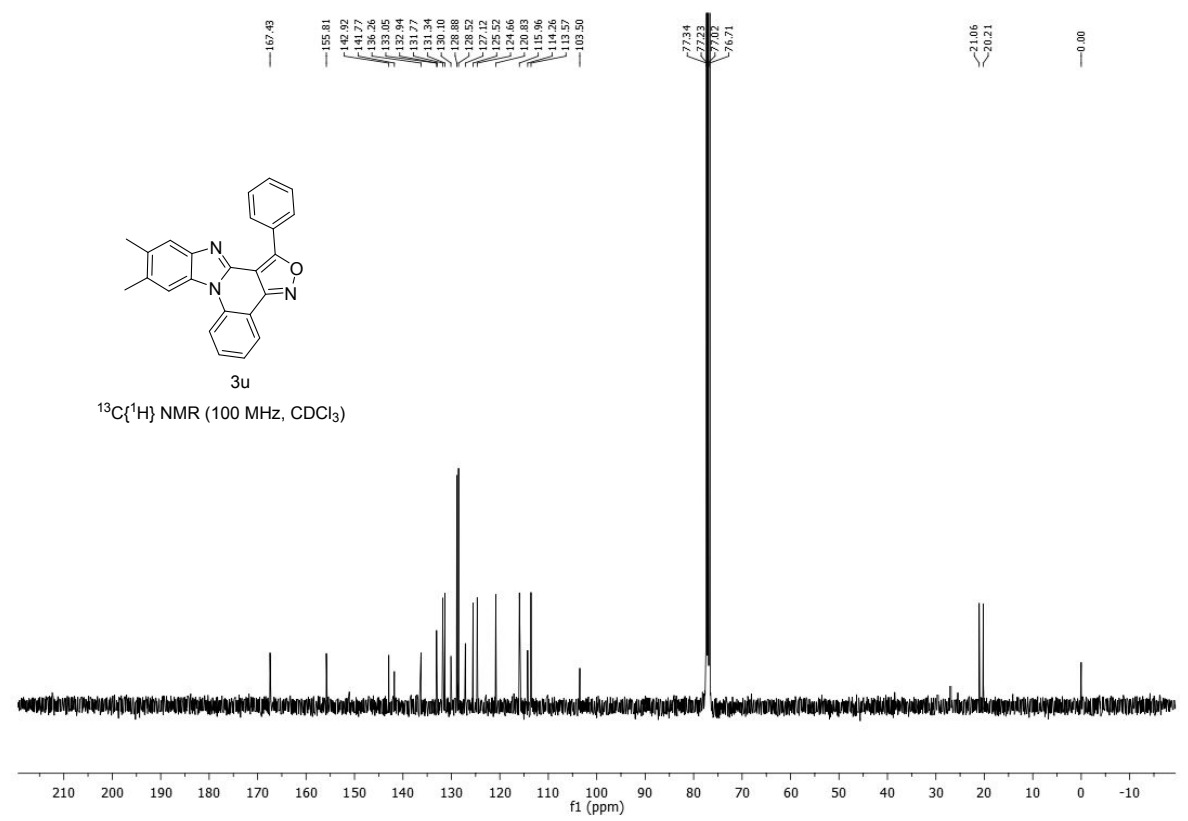
3t

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



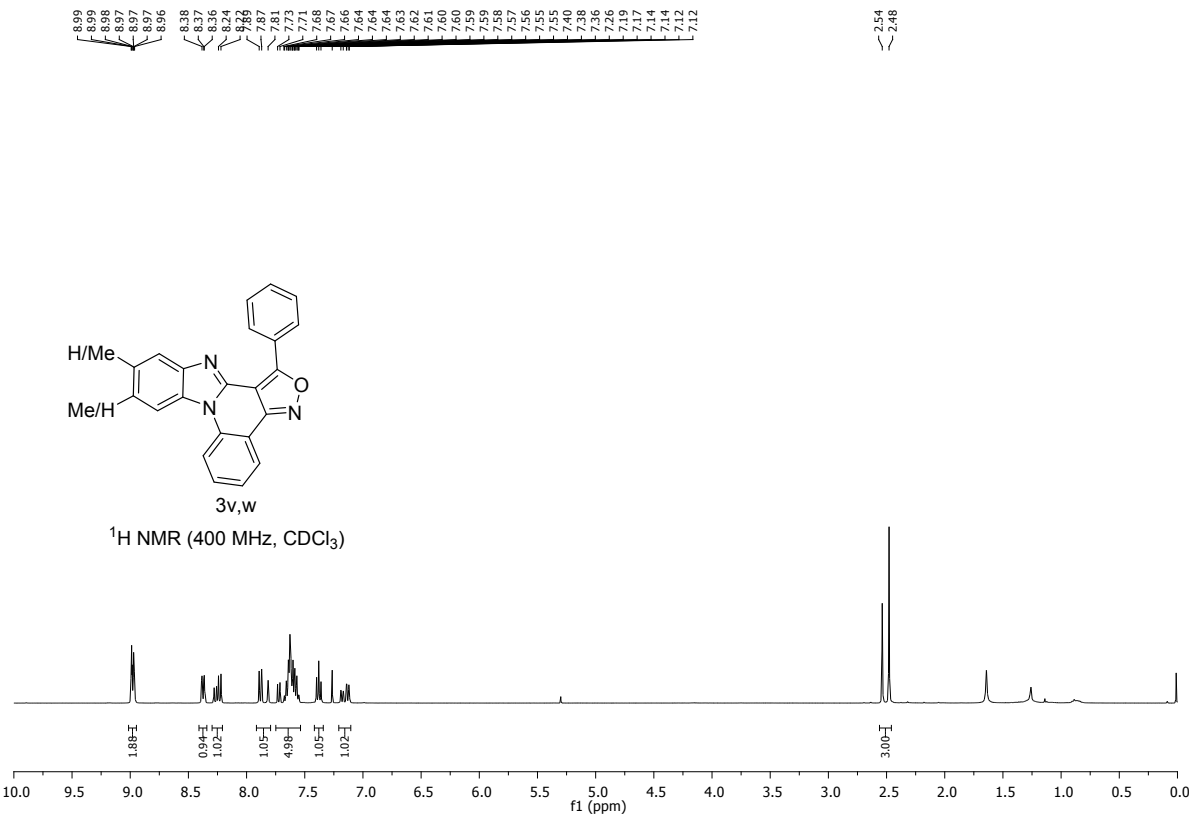
3u

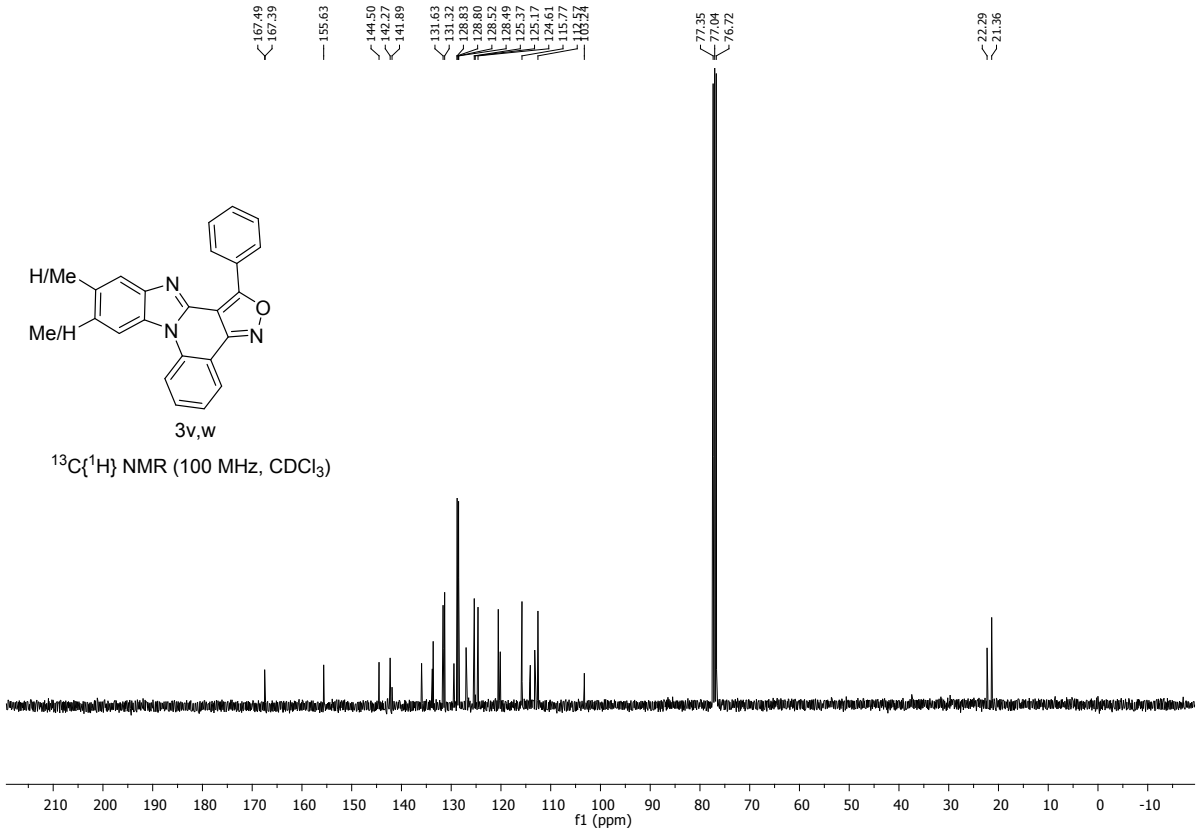
^{1}H NMR (400 MHz, $CDCl_3$)

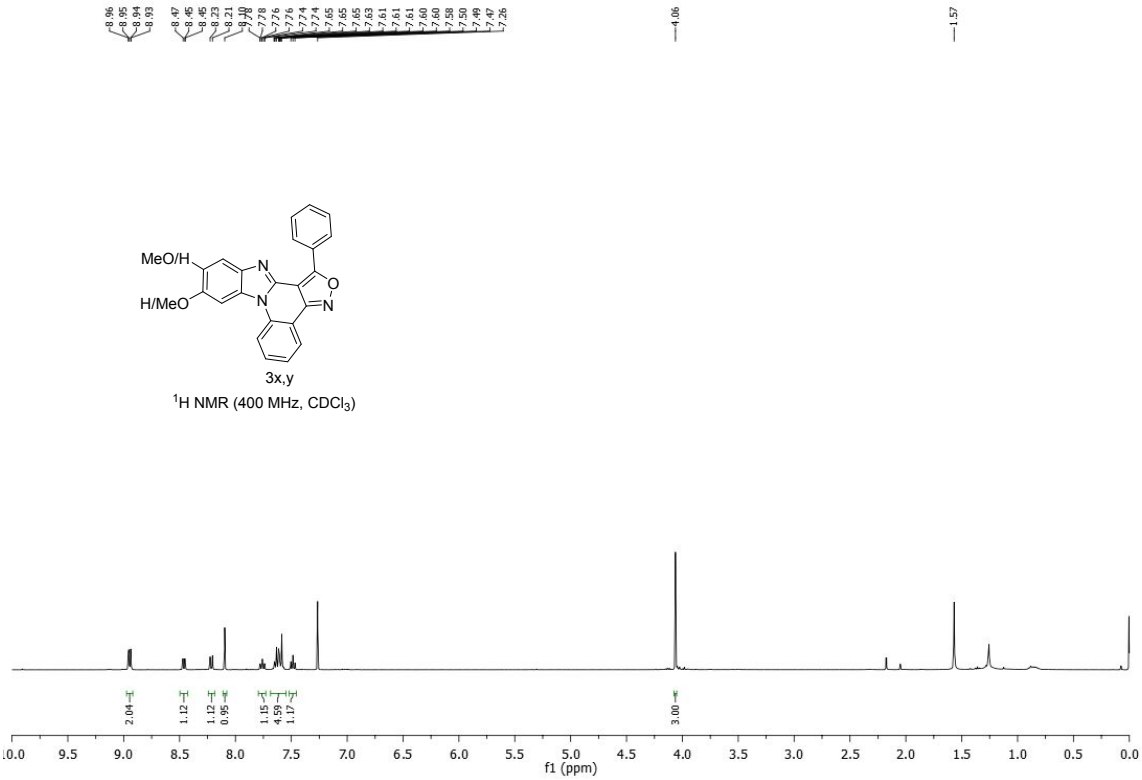


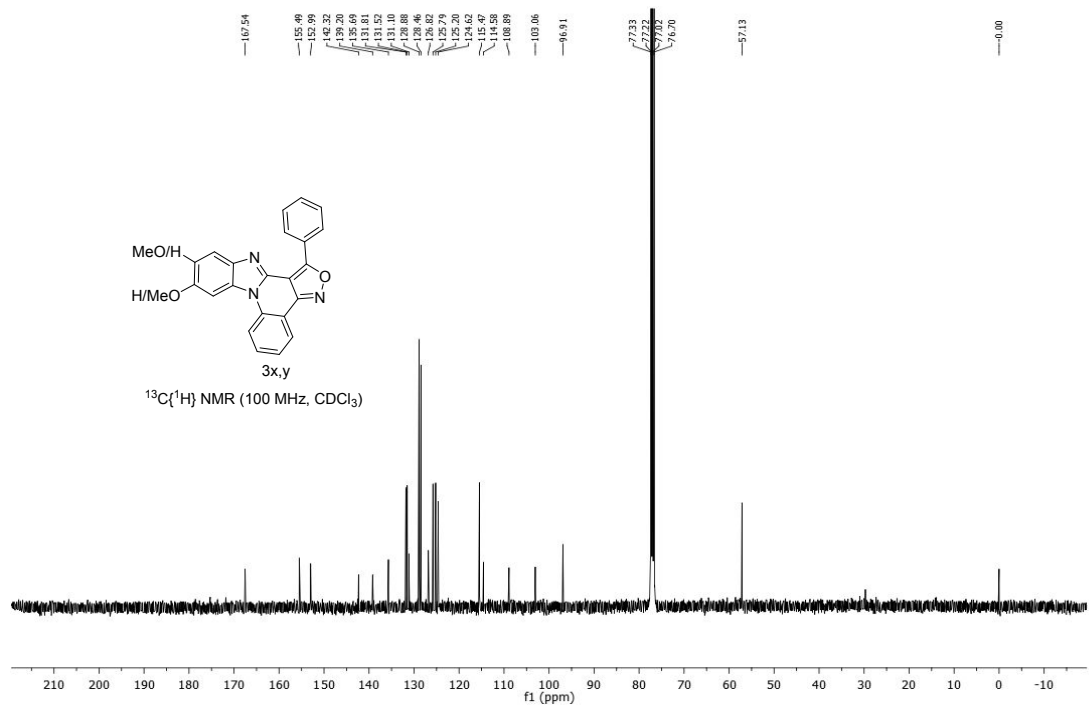
3u

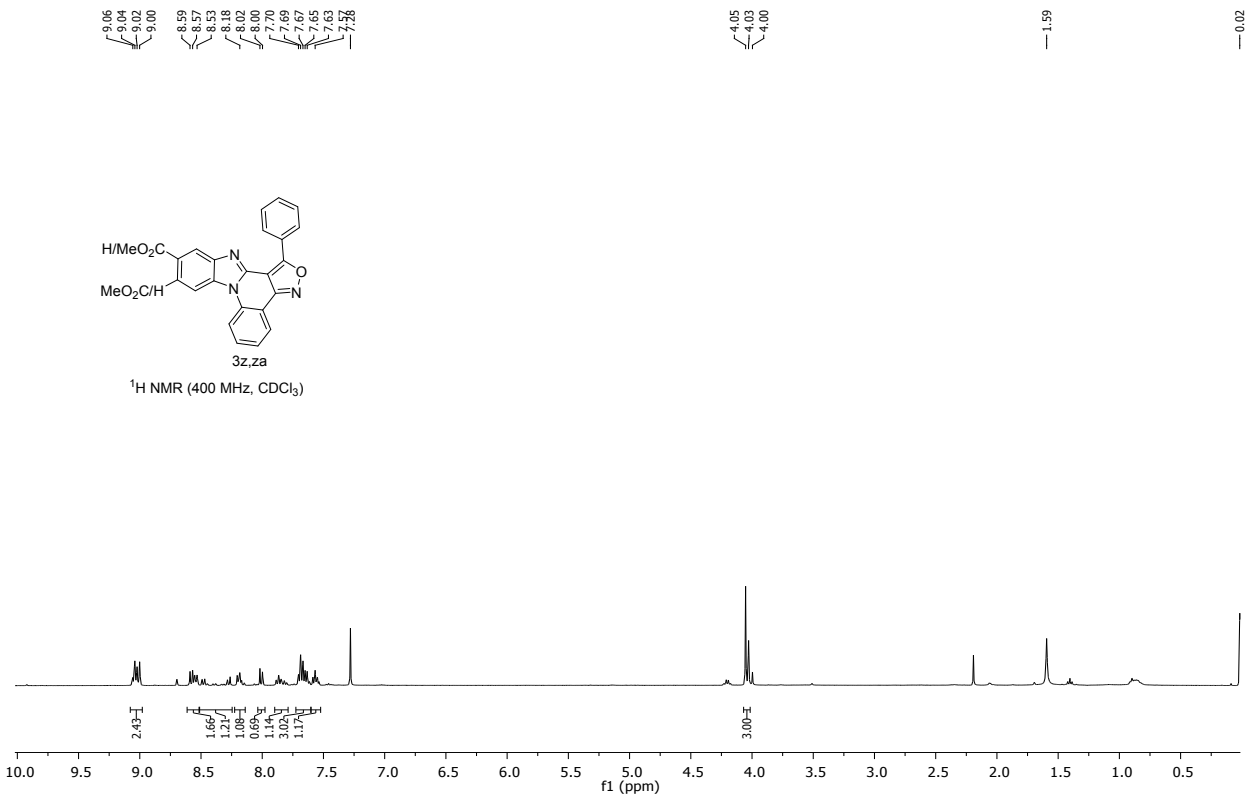
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

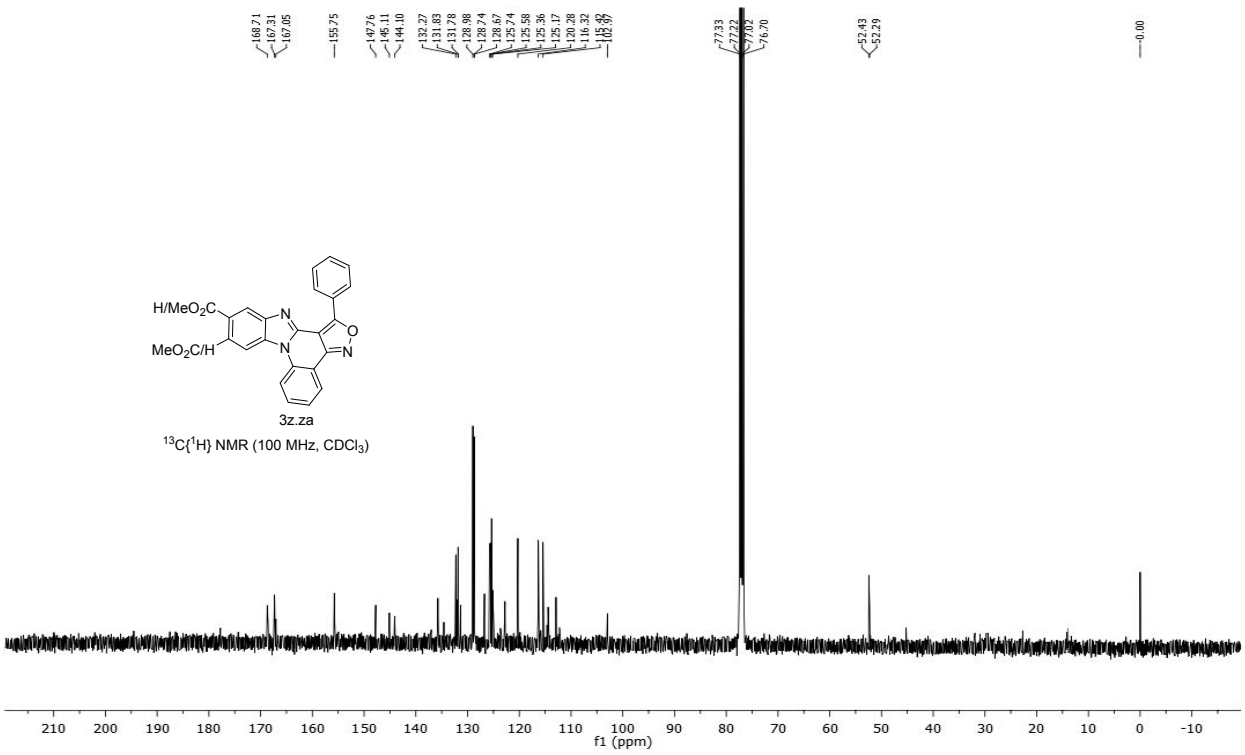

H/Me
Me/H
N
N
O
N
3v,w
^{1}H NMR (400 MHz, $CDCl_3$)
f1 (ppm)

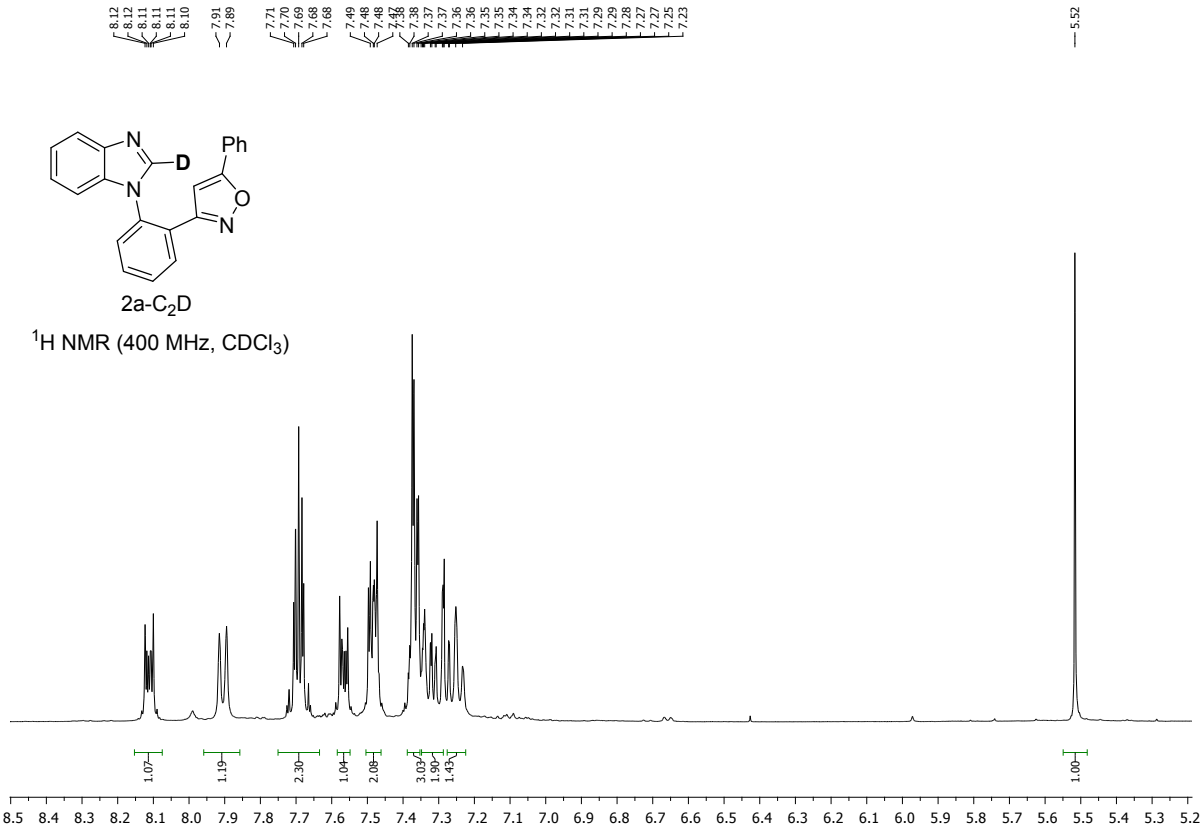

H/Me
Me/H
N
N
O
N
3v,w
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)
f1 (ppm)

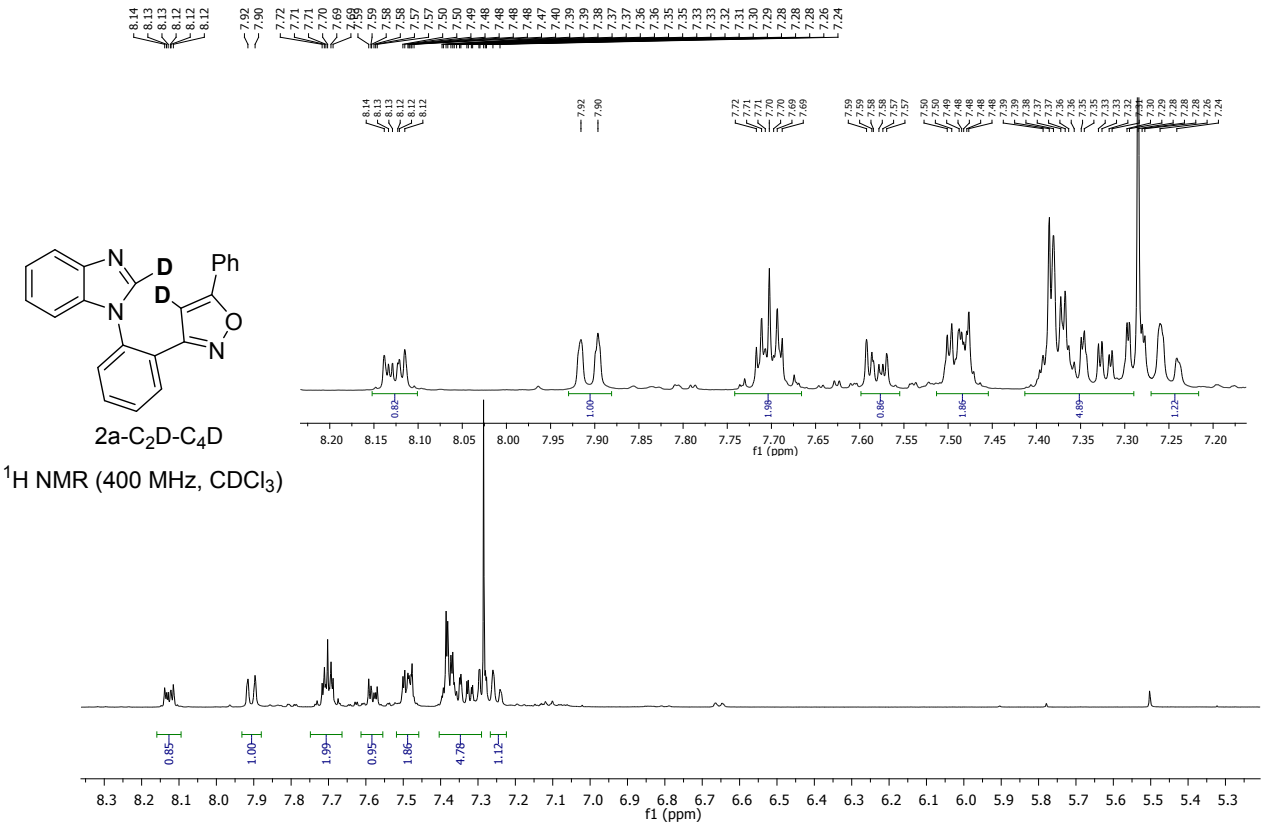

MeO/H
H/MeO
N
N
O
N
3x,y
^{1}H NMR (400 MHz, $CDCl_3$)
f1 (ppm)

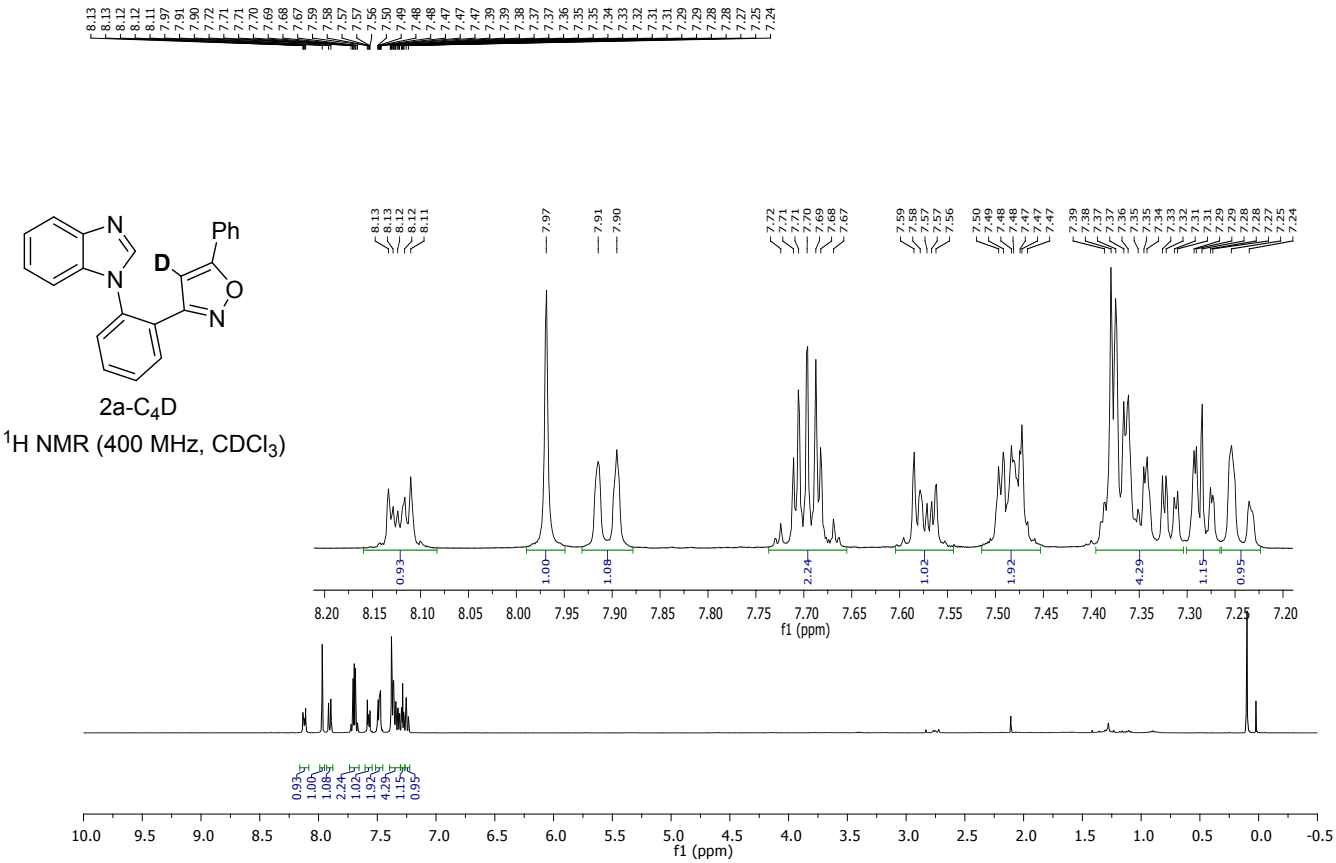

MeO/H
H/MeO
N
N
O
N
3x,y
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)
f1 (ppm)

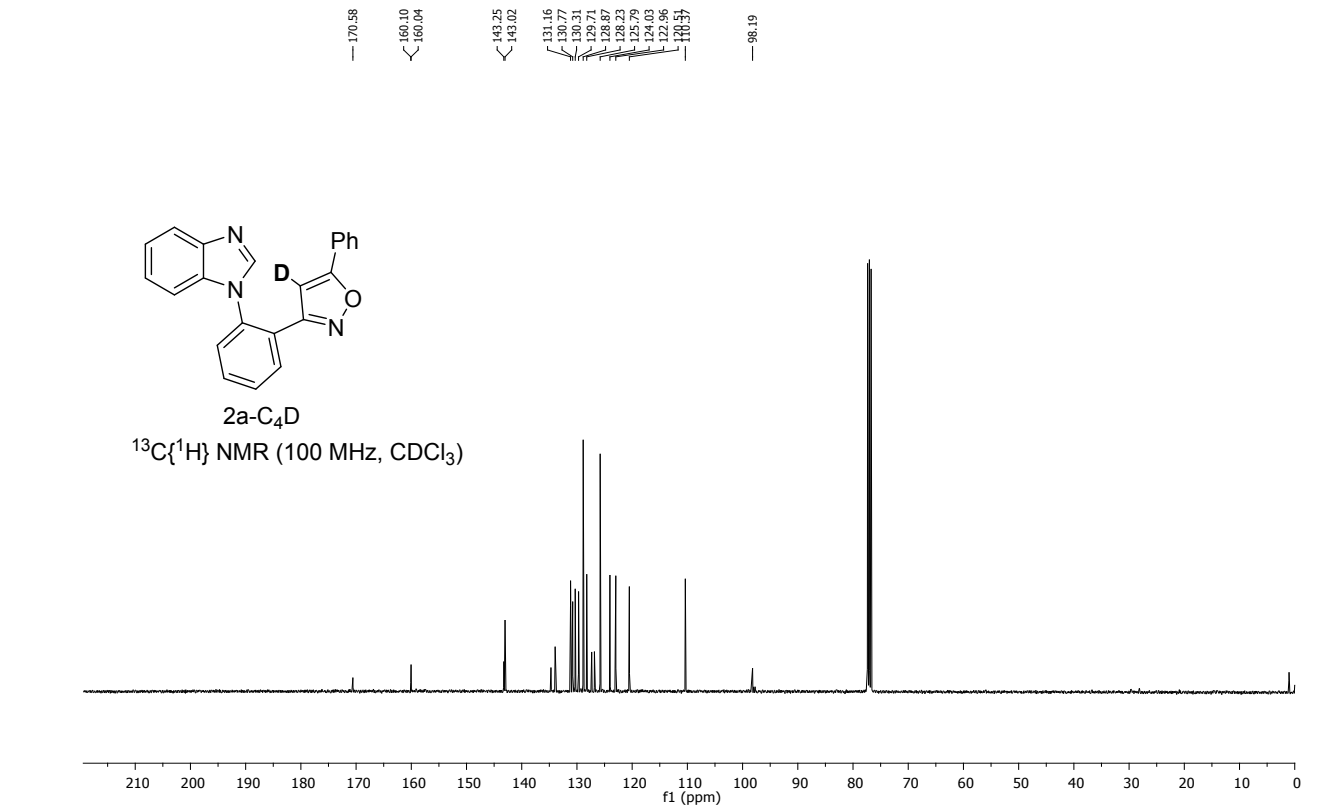

9.06
9.04
9.02
9.00
8.59
8.57
8.53
8.18
8.02
8.00
7.70
7.69
7.67
7.65
7.63
4.05
4.03
4.00
1.59
0.02
H/MeO2C
MeO2C/H
3z,za
1H NMR (400 MHz, CDCl3)
2.43
1.66
1.21
1.08
0.69
1.14
3.02
1.17
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

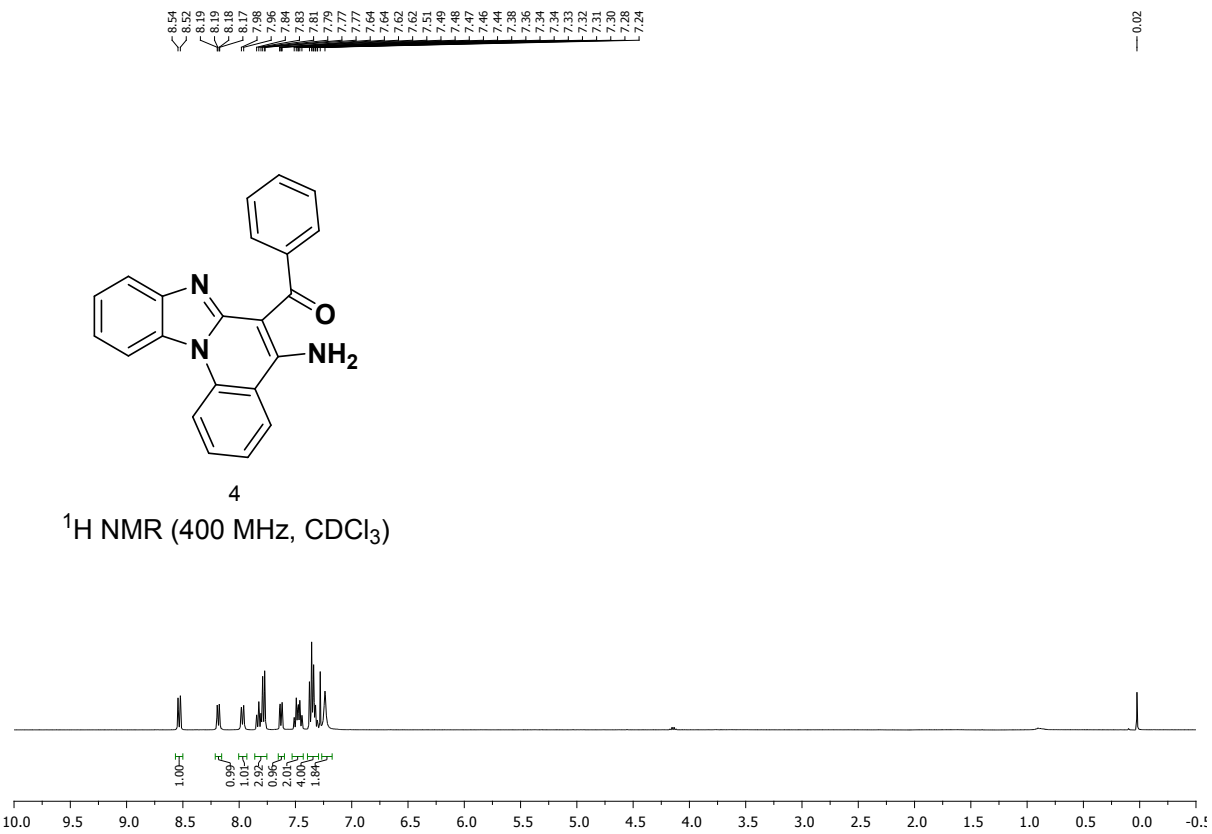

168.71
167.31
167.05
155.75
147.76
145.11
144.10
132.27
131.83
131.78
128.98
128.74
128.67
125.74
125.58
125.36
125.17
120.28
116.32
115.42
102.97
77.33
77.22
77.02
76.70
52.43
52.29
0.00
H/MeO2C
MeO2C/H
3z.za
13C{1H} NMR (100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


2a-C2D
1H NMR (400 MHz, CDCl3)


2a-C2D-C4D
1H NMR (400 MHz, CDCl3)
f1 (ppm)

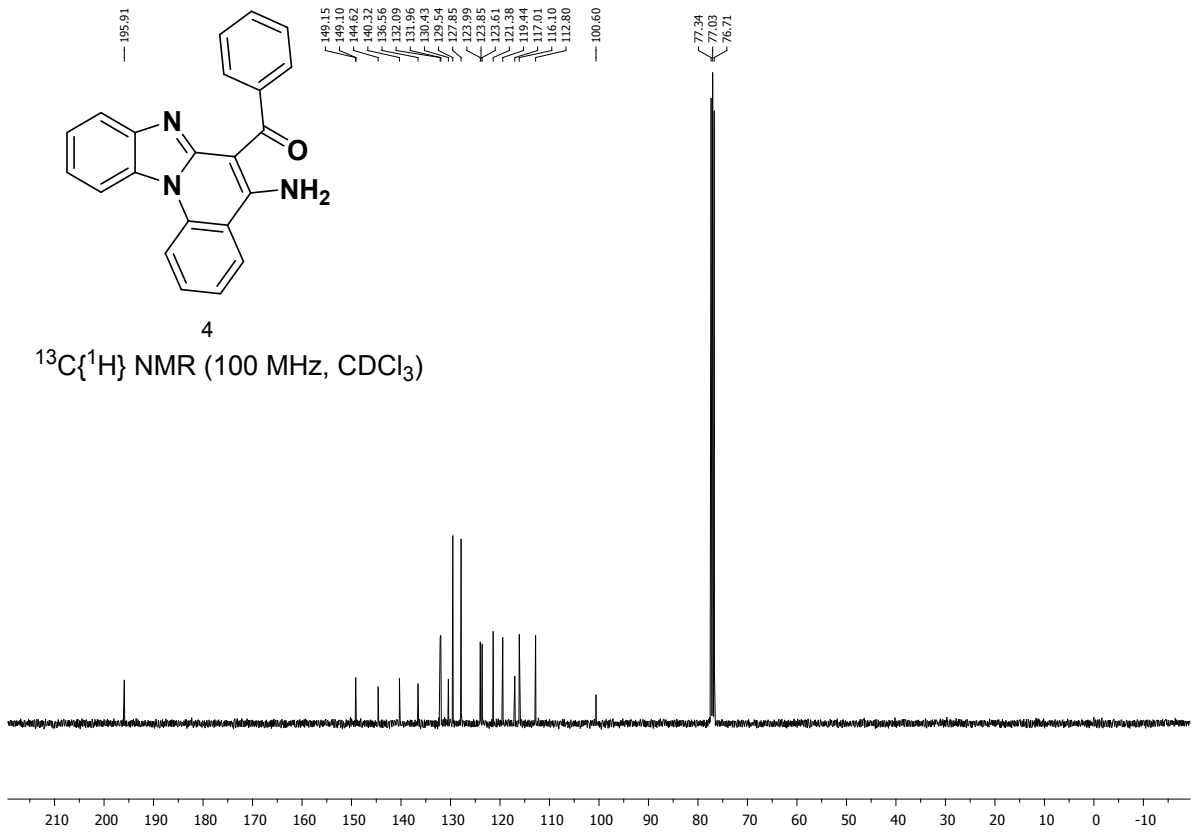

Ph
D
N
N
O
N
2a-C4D
1H NMR (400 MHz, CDCl3)
f1 (ppm)


Ph
D
N
N
O
N
2a-C4D
13C{1H} NMR (100 MHz, CDCl3)
f1 (ppm)



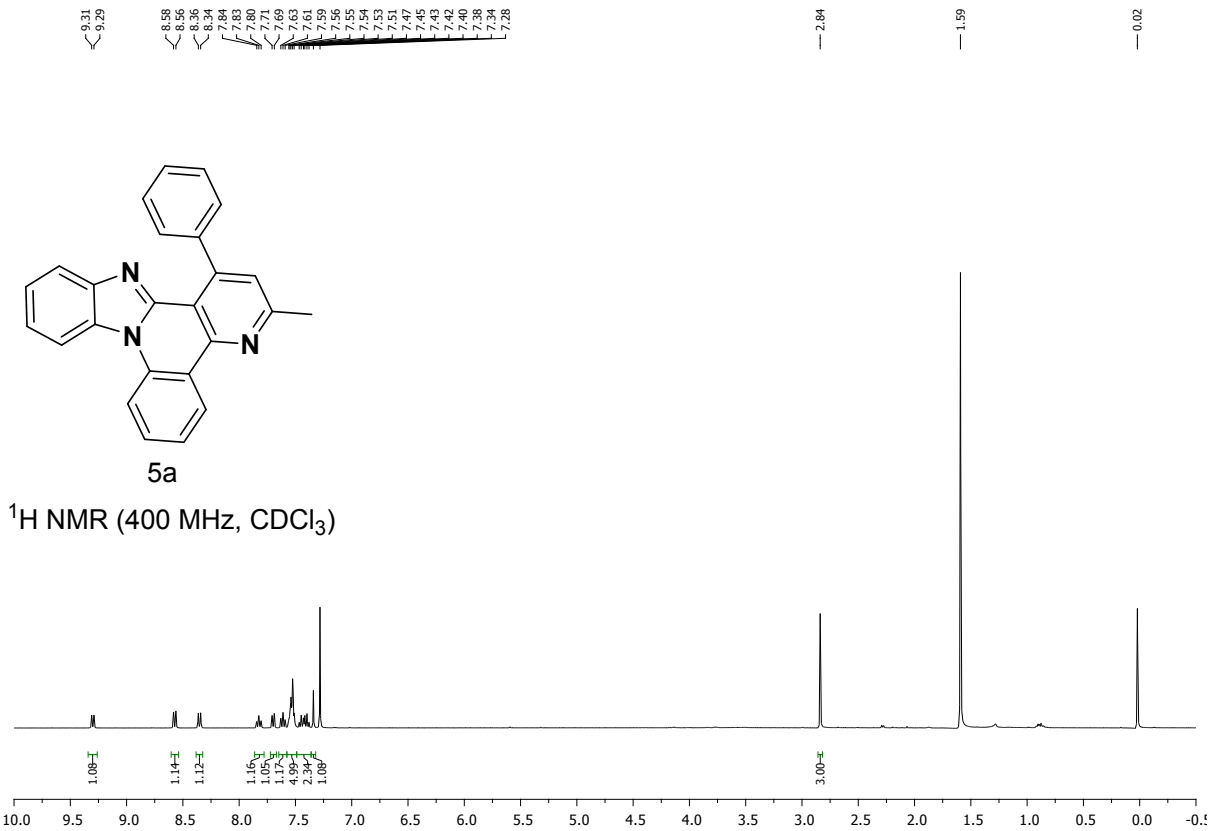
4

^{1}H NMR (400 MHz, $CDCl_3$)



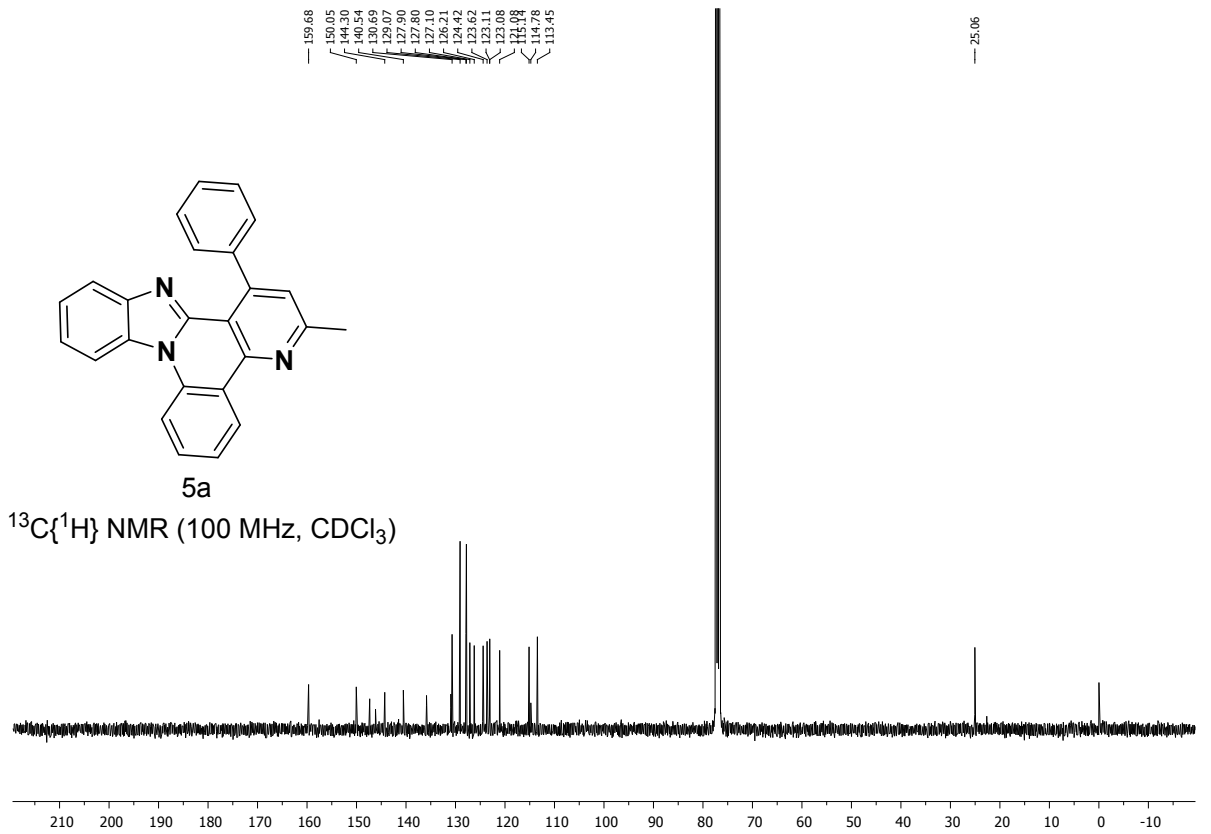
4

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



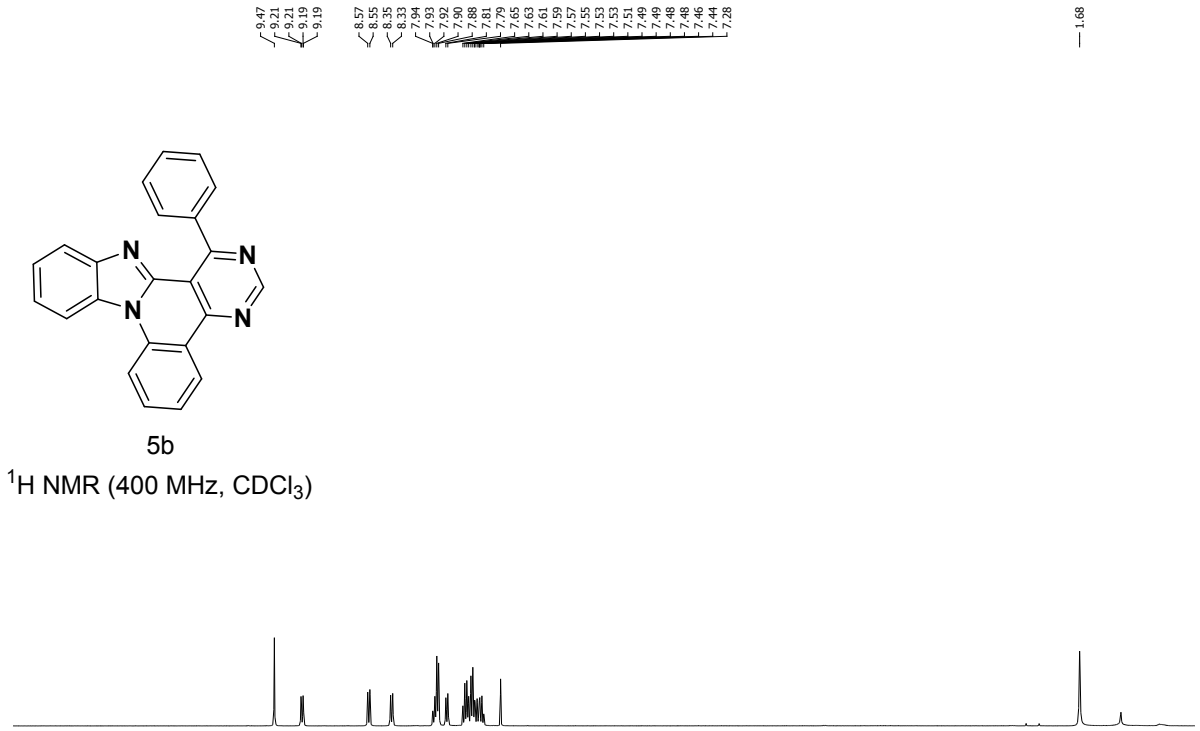
5a

^{1}H NMR (400 MHz, $CDCl_3$)



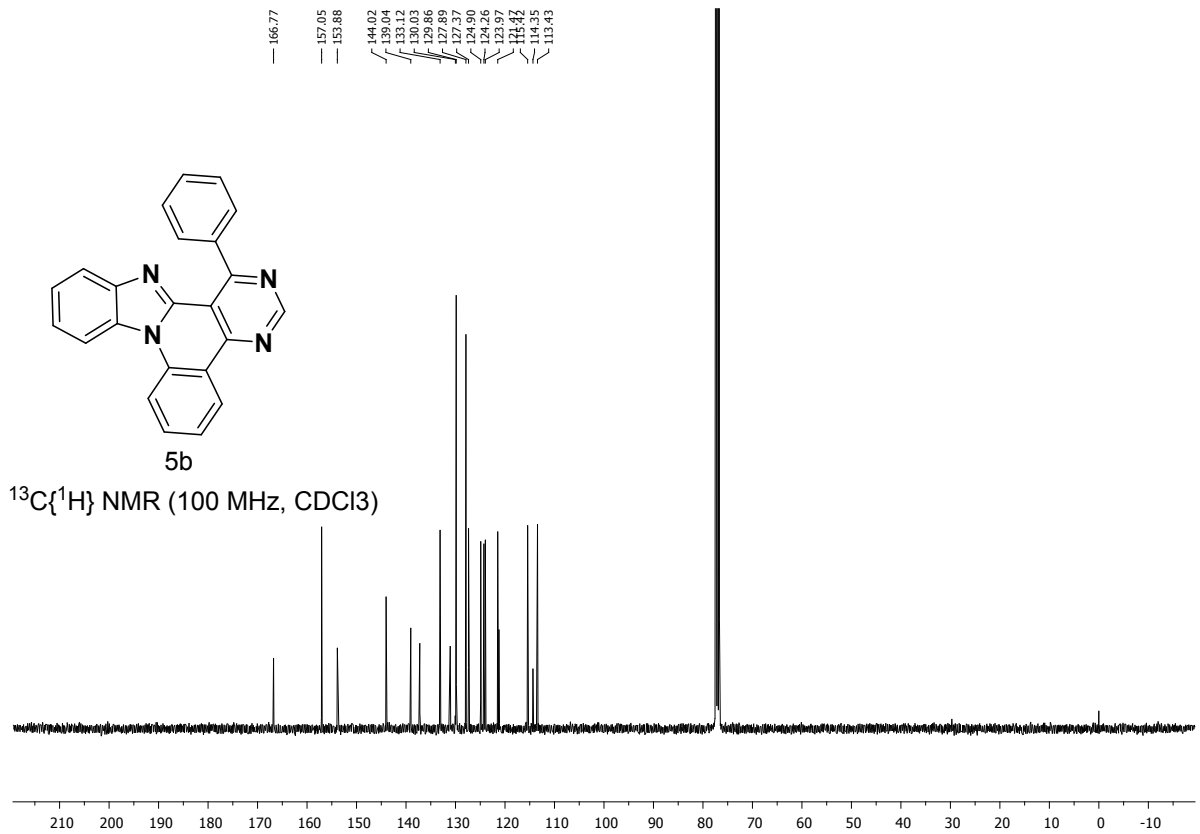
5a

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



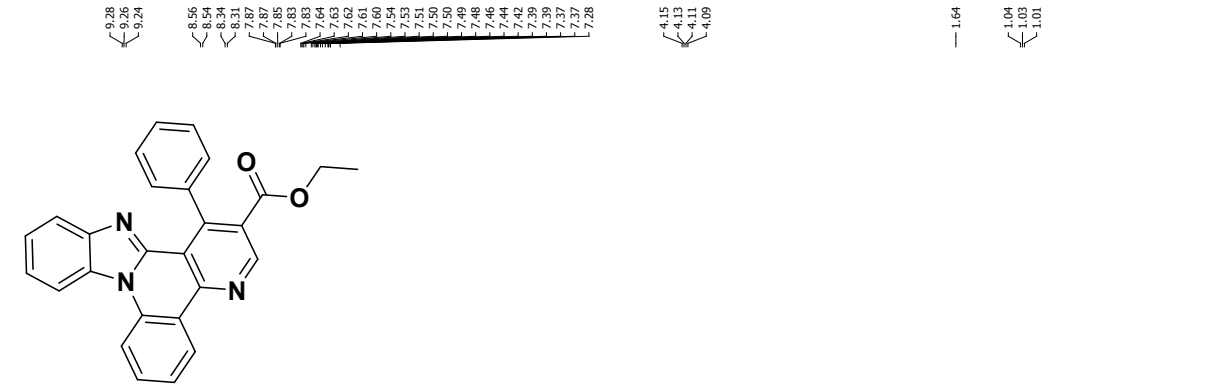
5b

^{1}H NMR (400 MHz, $CDCl_3$)



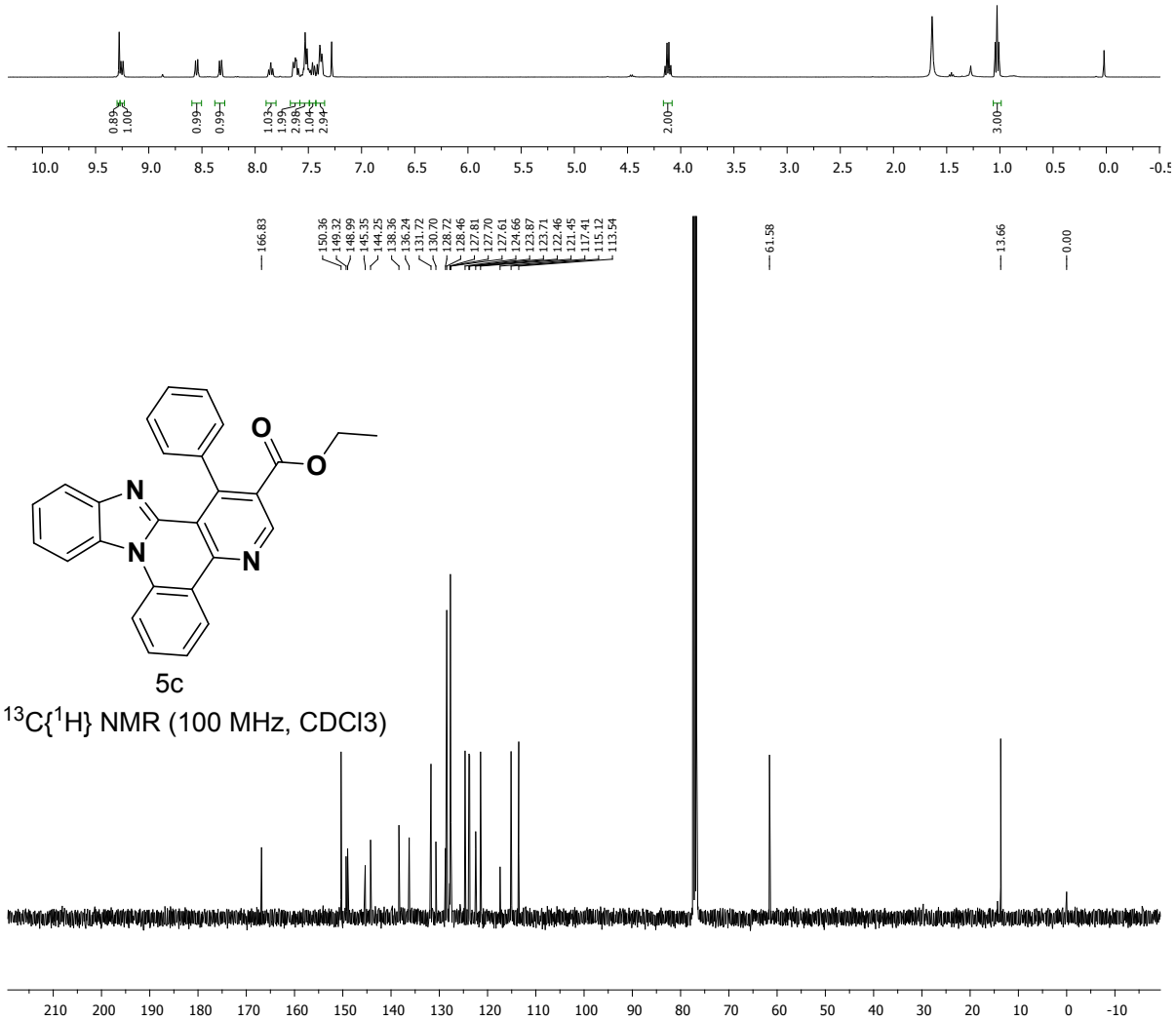
5b

^{13}C{^{1}H} NMR (100 MHz, CDCl3)



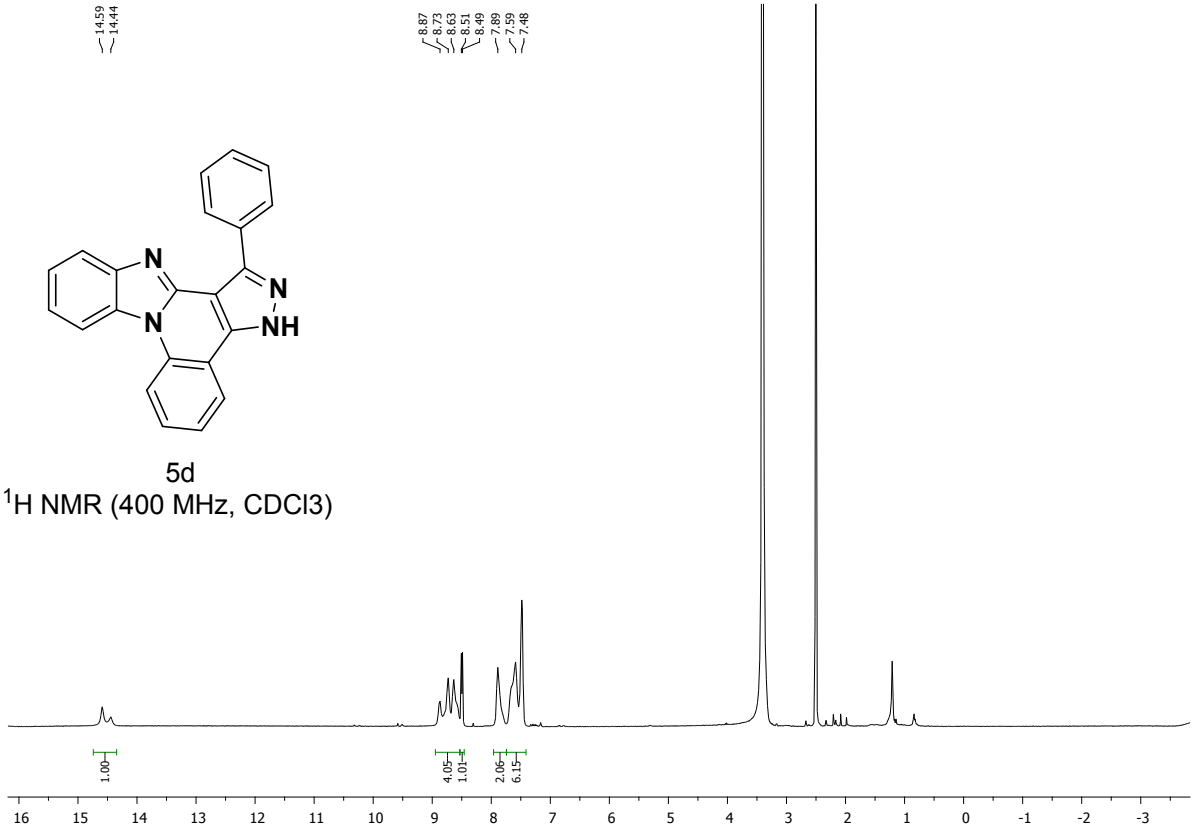
5c

^{1}H NMR (400 MHz, $CDCl_3$)



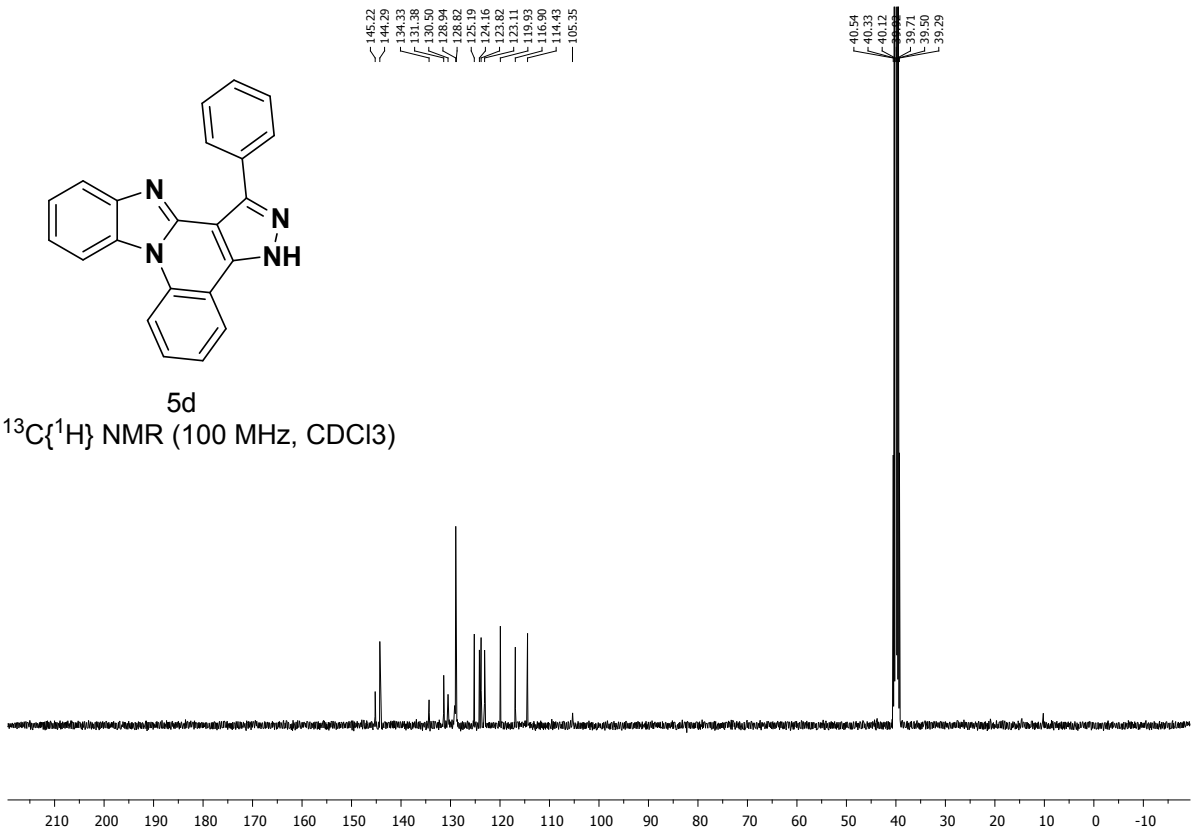
5c

^{13}C{^{1}H} NMR (100 MHz, CDCl3)



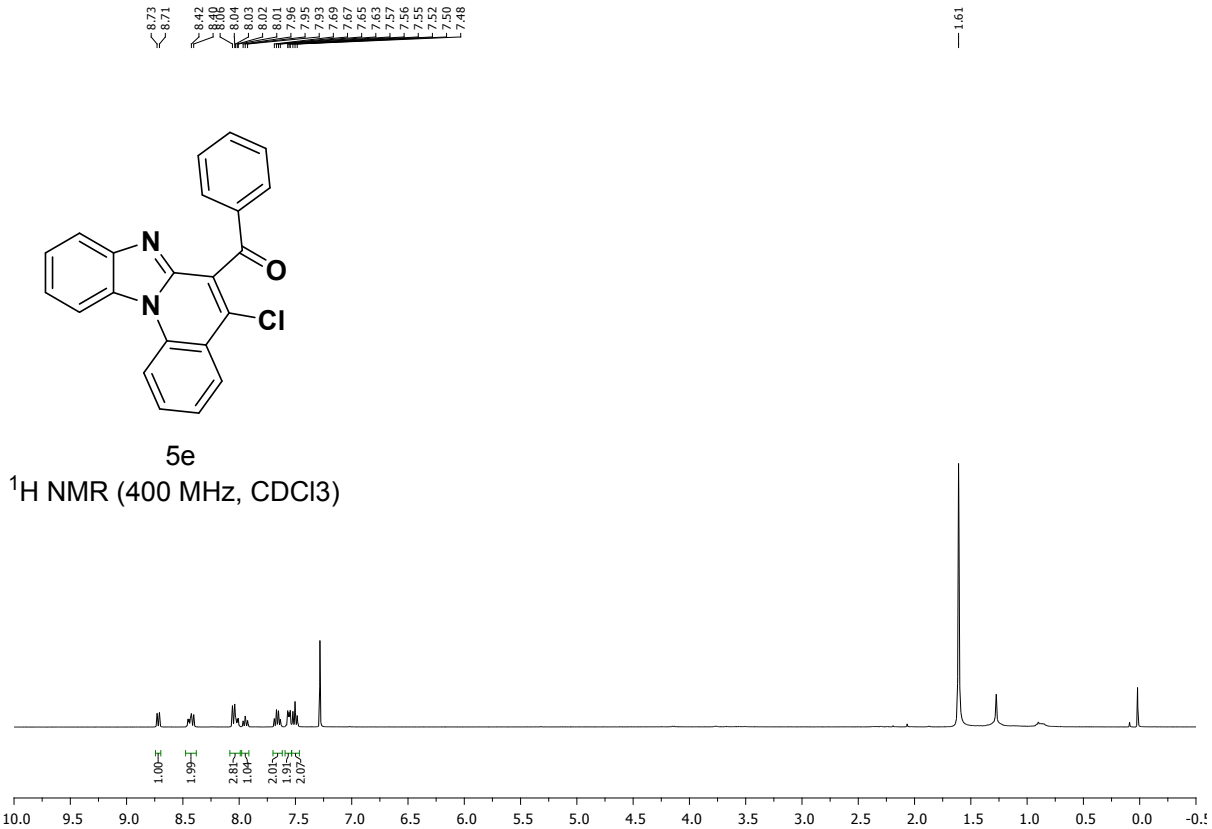
5d

^{1}H NMR (400 MHz, CDCl3)



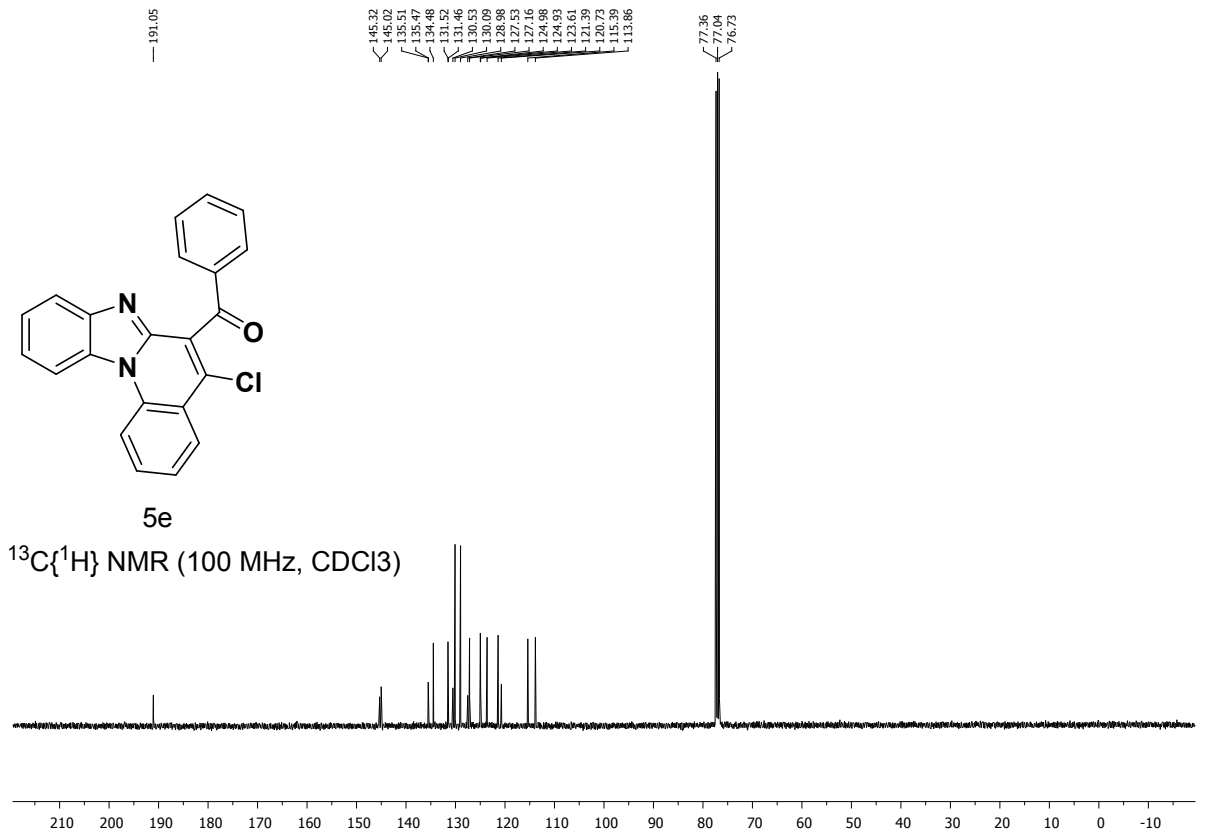
5d

^{13}C{^{1}H} NMR (100 MHz, CDCl3)



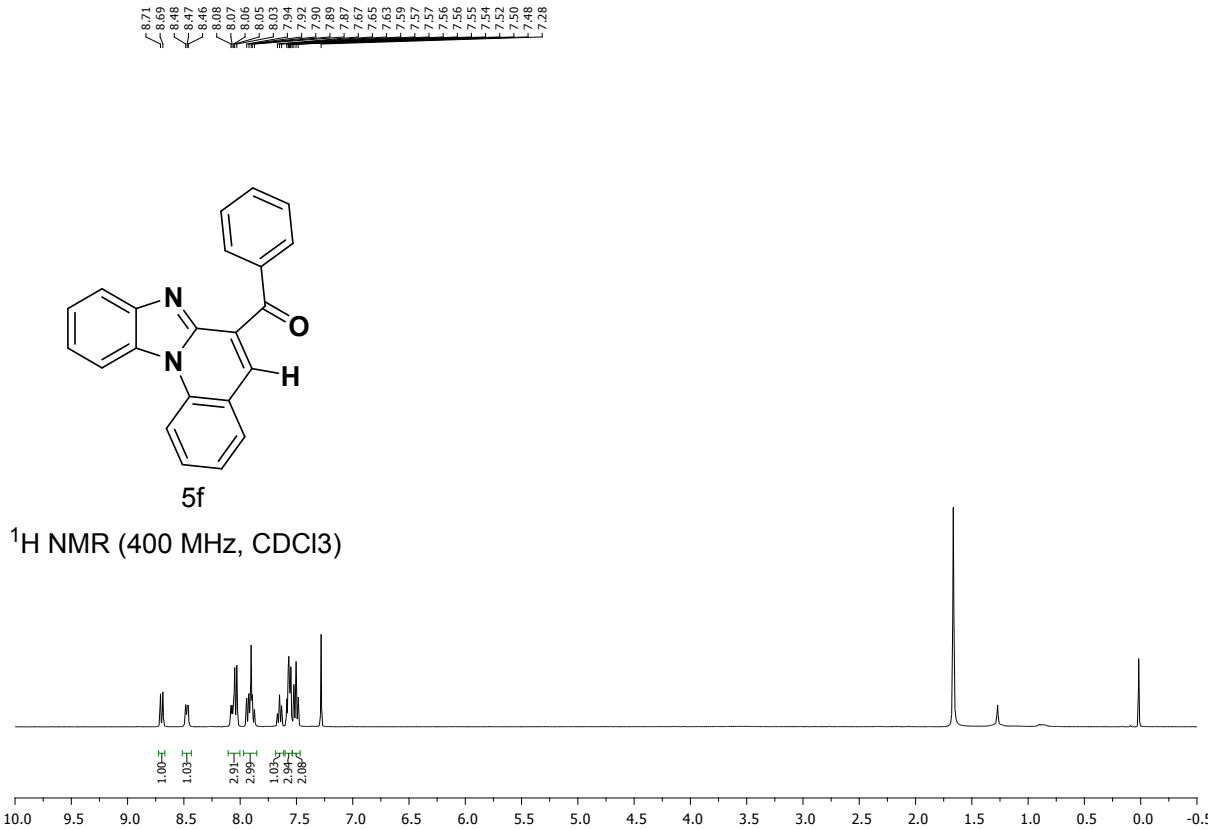
5e

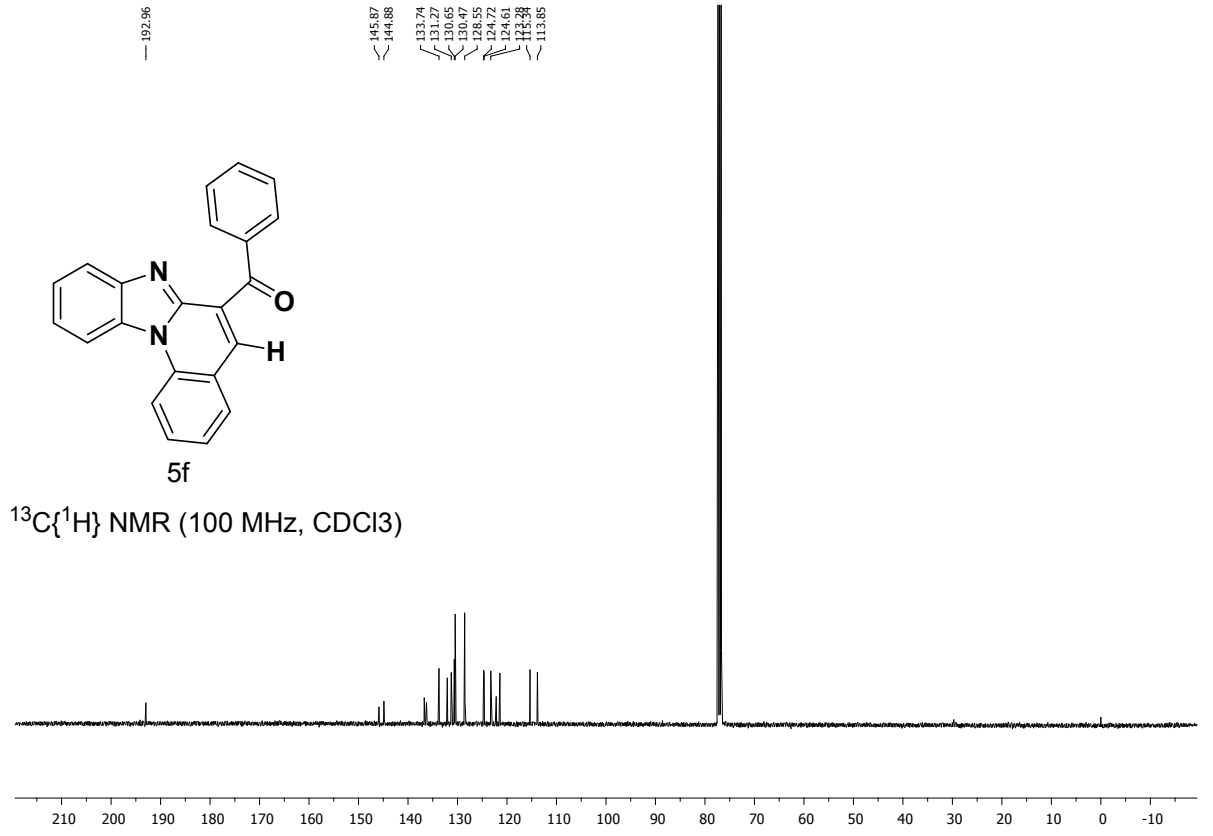
^{1}H NMR (400 MHz, CDCl3)

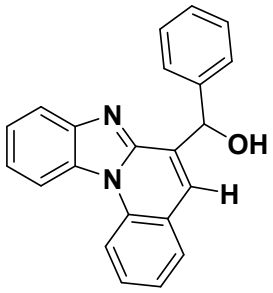


5e

^{13}C{^{1}H} NMR (100 MHz, CDCl3)

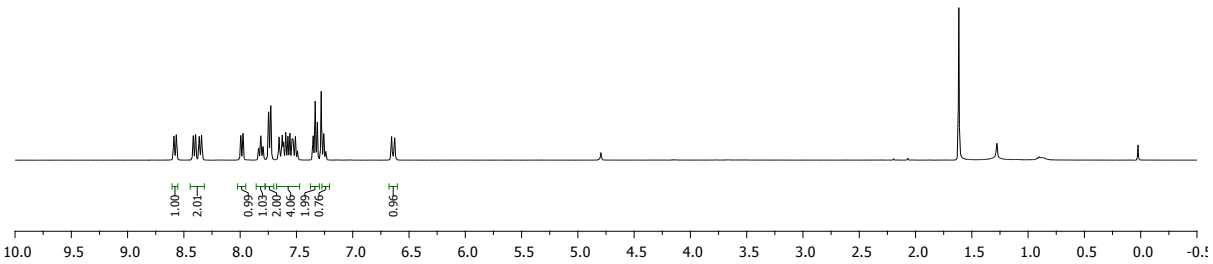

8.71
8.69
8.48
8.47
8.46
8.08
8.07
8.06
8.05
8.03
7.94
7.92
7.90
7.89
7.87
7.67
7.65
7.63
7.59
7.57
7.57
7.57
7.56
7.56
7.55
7.54
7.52
7.50
7.48
7.28
N
N
O
H
5f
^{1}H NMR (400 MHz, CDCl3)
1.00
1.03
2.91
2.99
1.03
2.94
2.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


192.96
145.87
144.88
133.74
131.27
130.65
130.47
128.55
124.72
124.61
113.85
N
N
O
H
5f
^{13}C{^{1}H} NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10



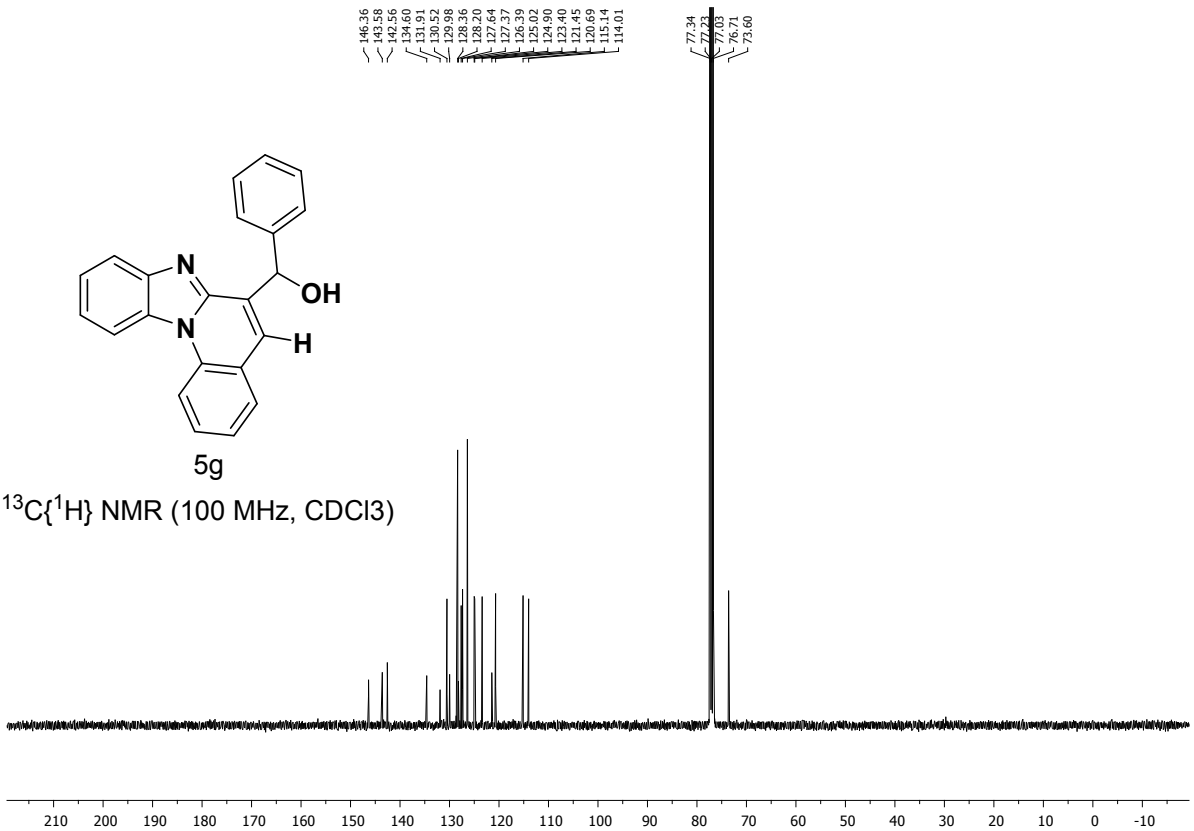
5g

^{1}H NMR (400 MHz, CDCl3)

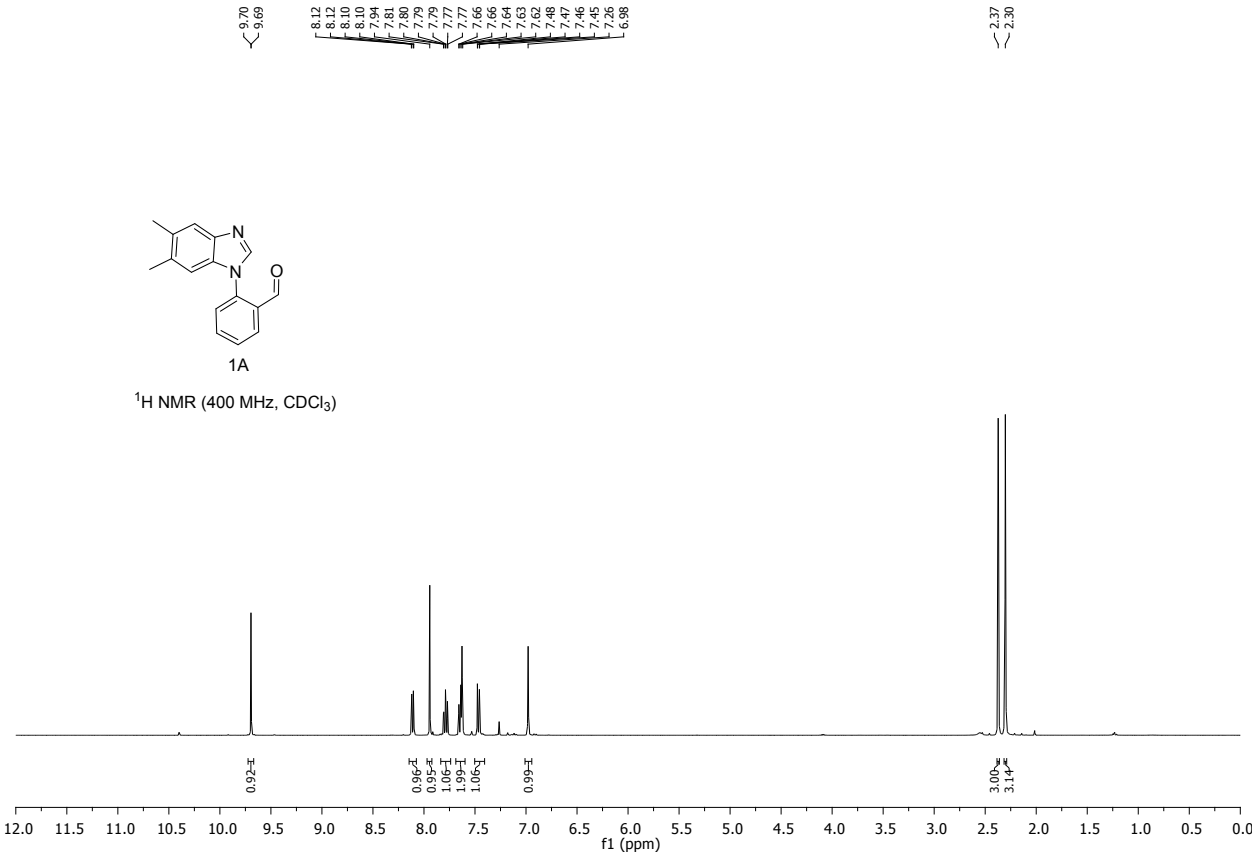


5g

^{13}C{^{1}H} NMR (100 MHz, CDCl3)

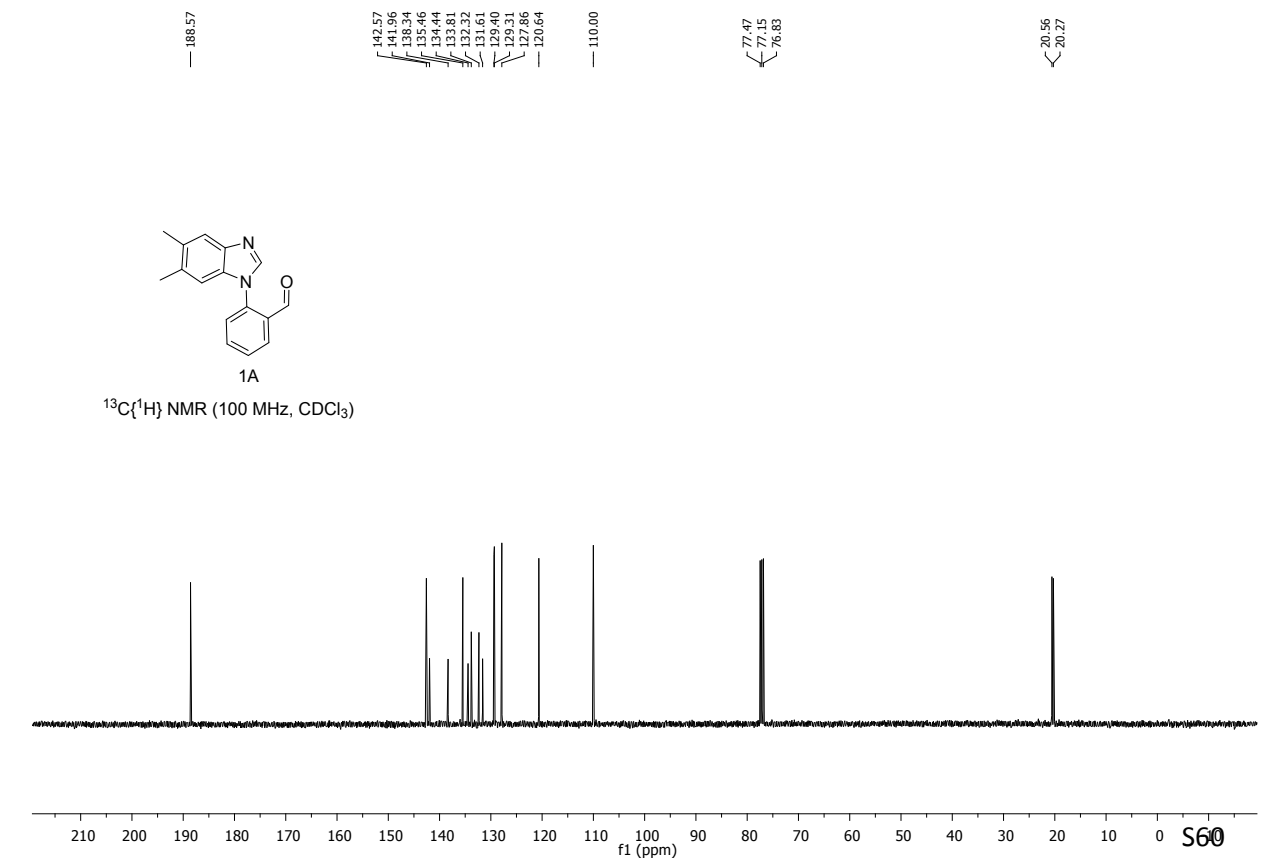


Spectra of compounds 1A-E, 1c-k, 2u-2zc:



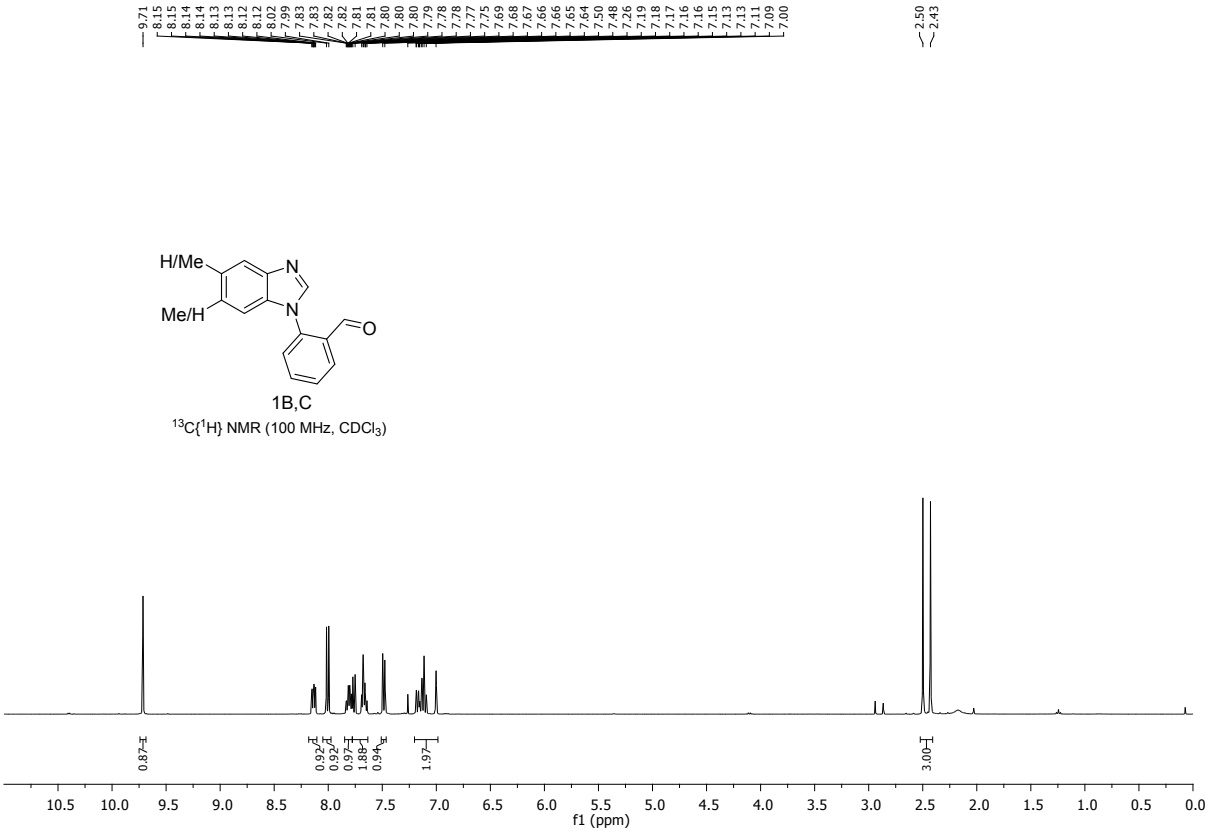
1A

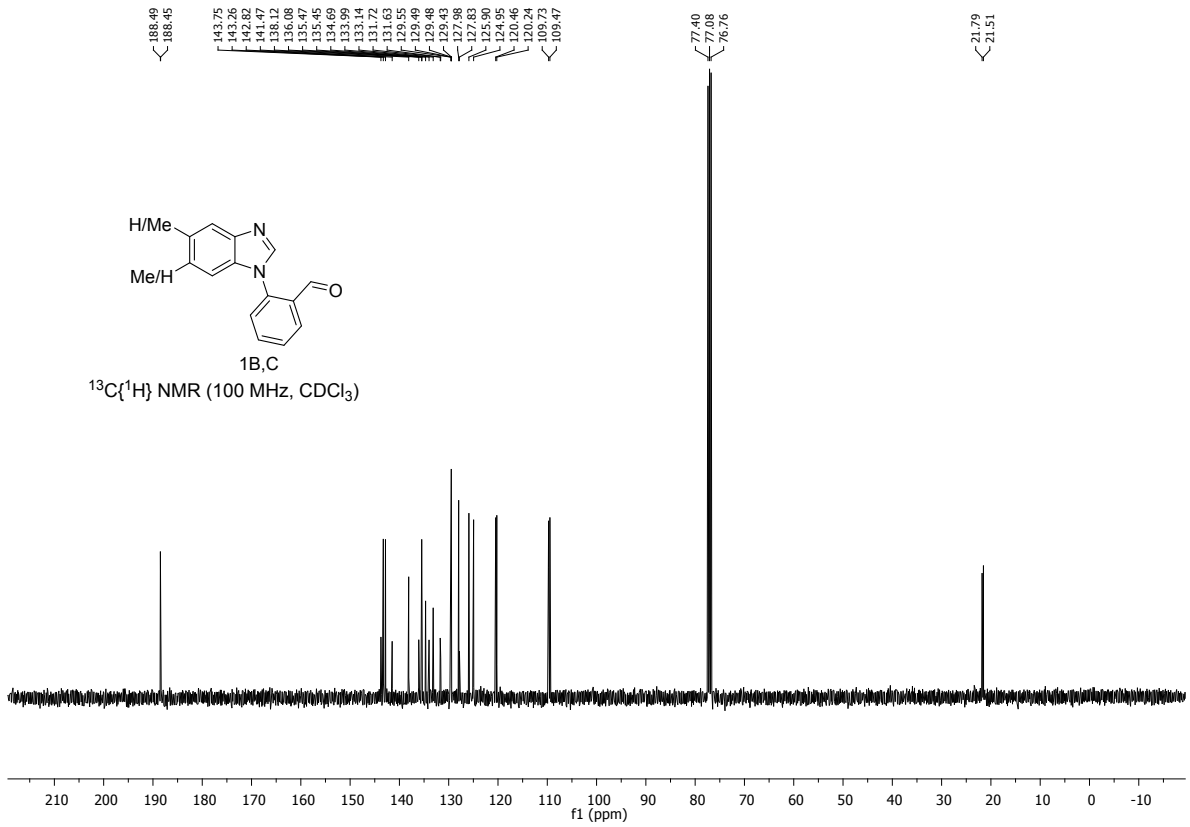
^{1}H NMR (400 MHz, $CDCl_3$)

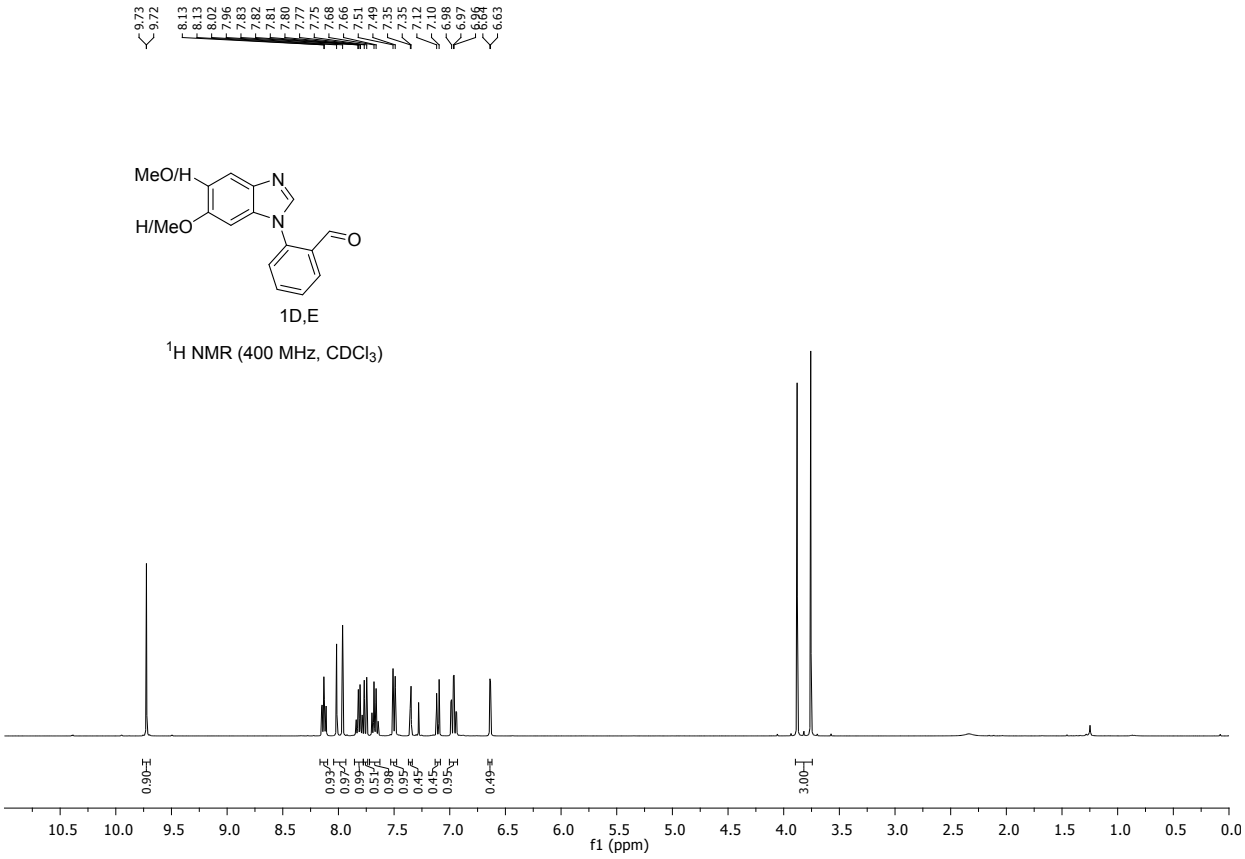


1A

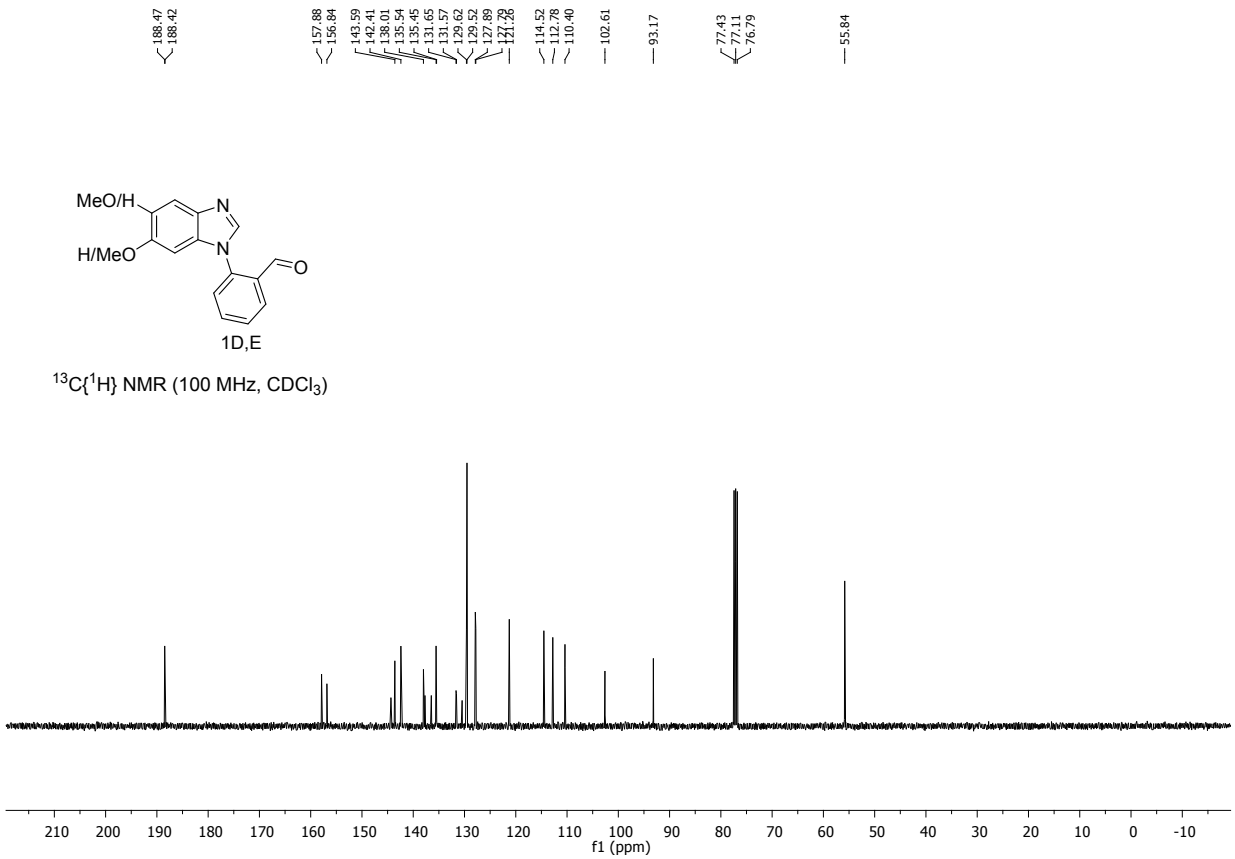
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)


H/Me
Me/H
N
N
O
1B,C
13C{1H} NMR (100 MHz, CDCl3)
f1 (ppm)

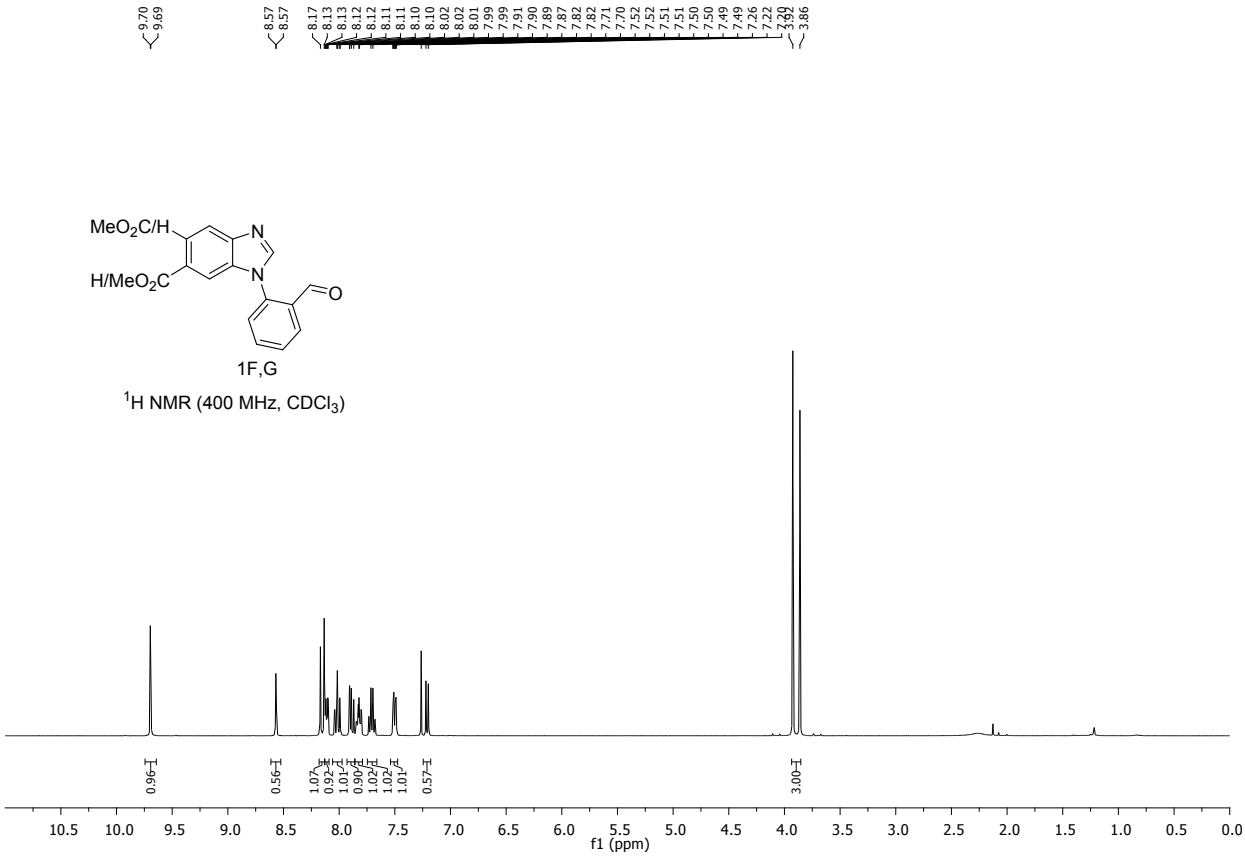

H/Me
Me/H
N
N
O
1B,C
13C{1H} NMR (100 MHz, CDCl3)
f1 (ppm)

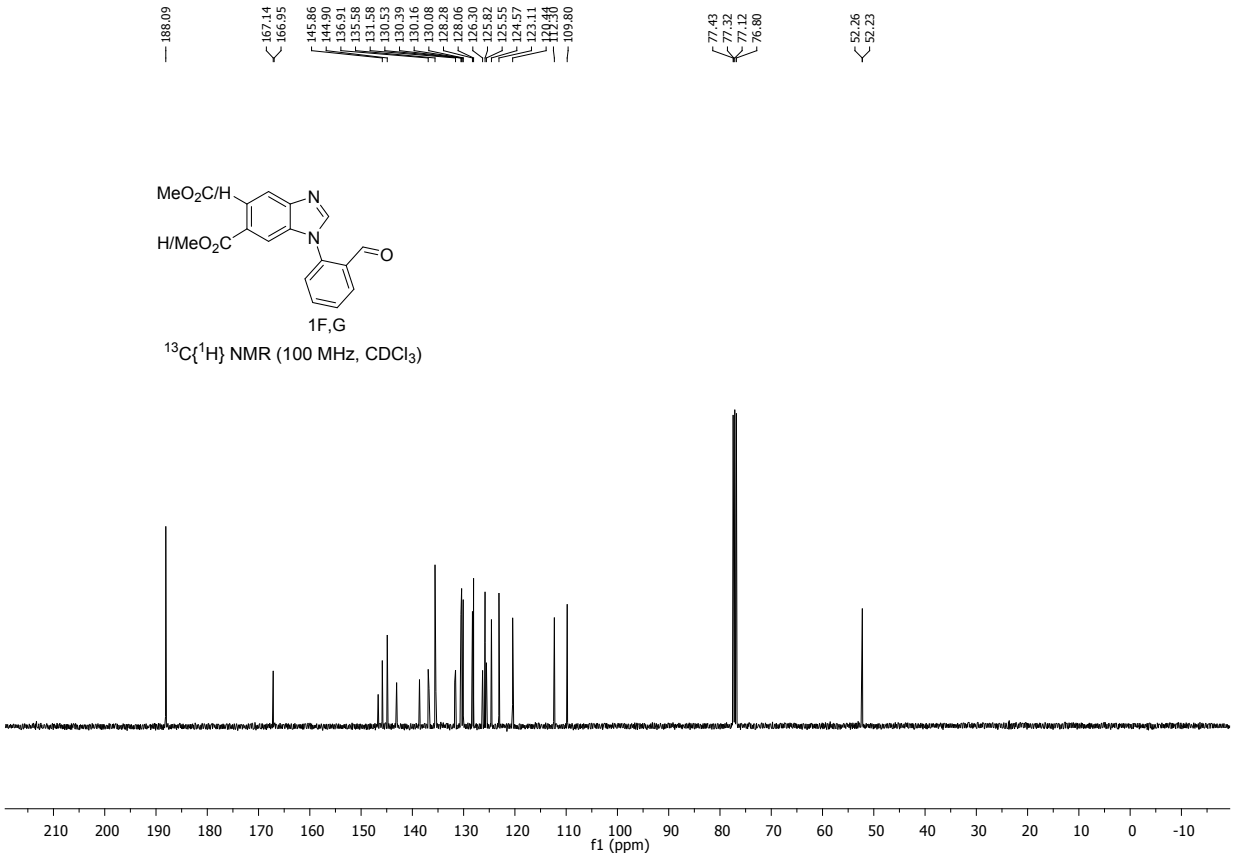


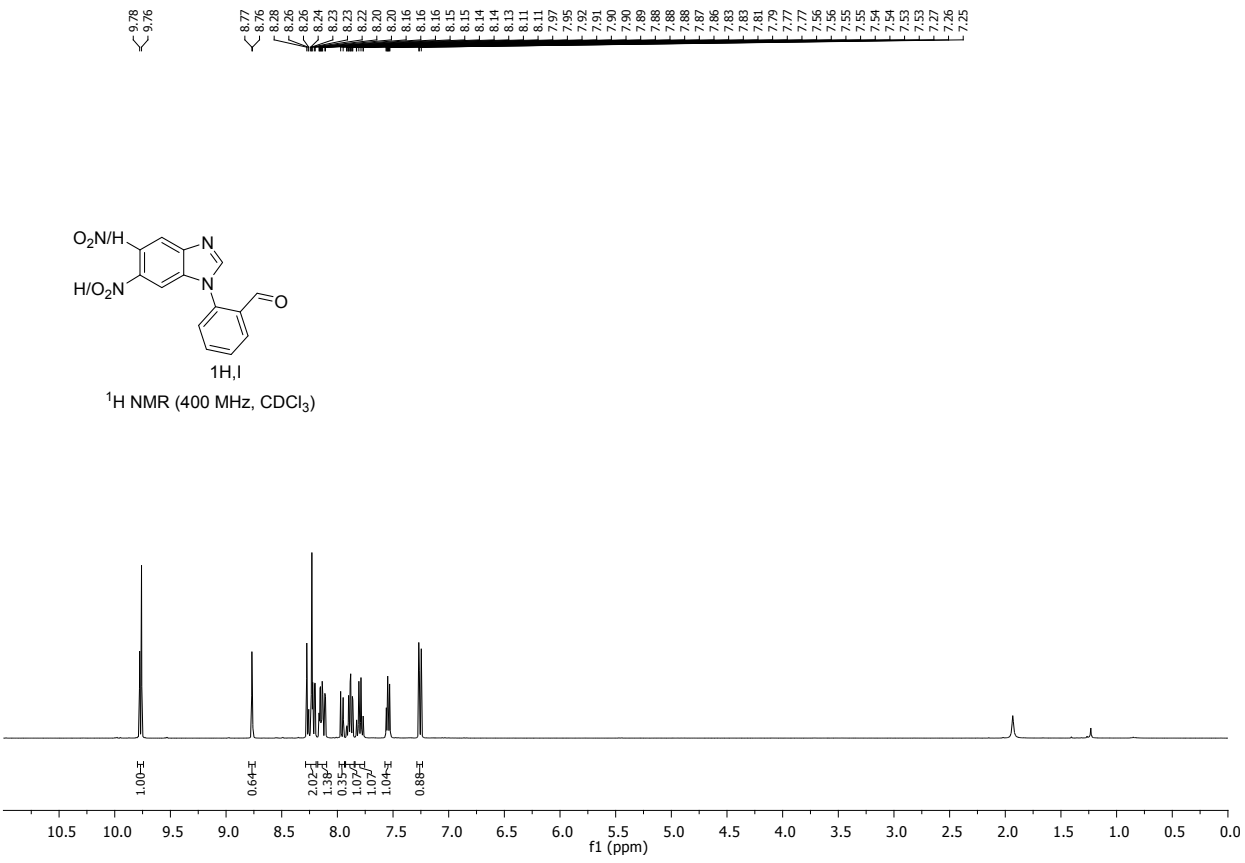
^{1}H NMR (400 MHz, $CDCl_3$)

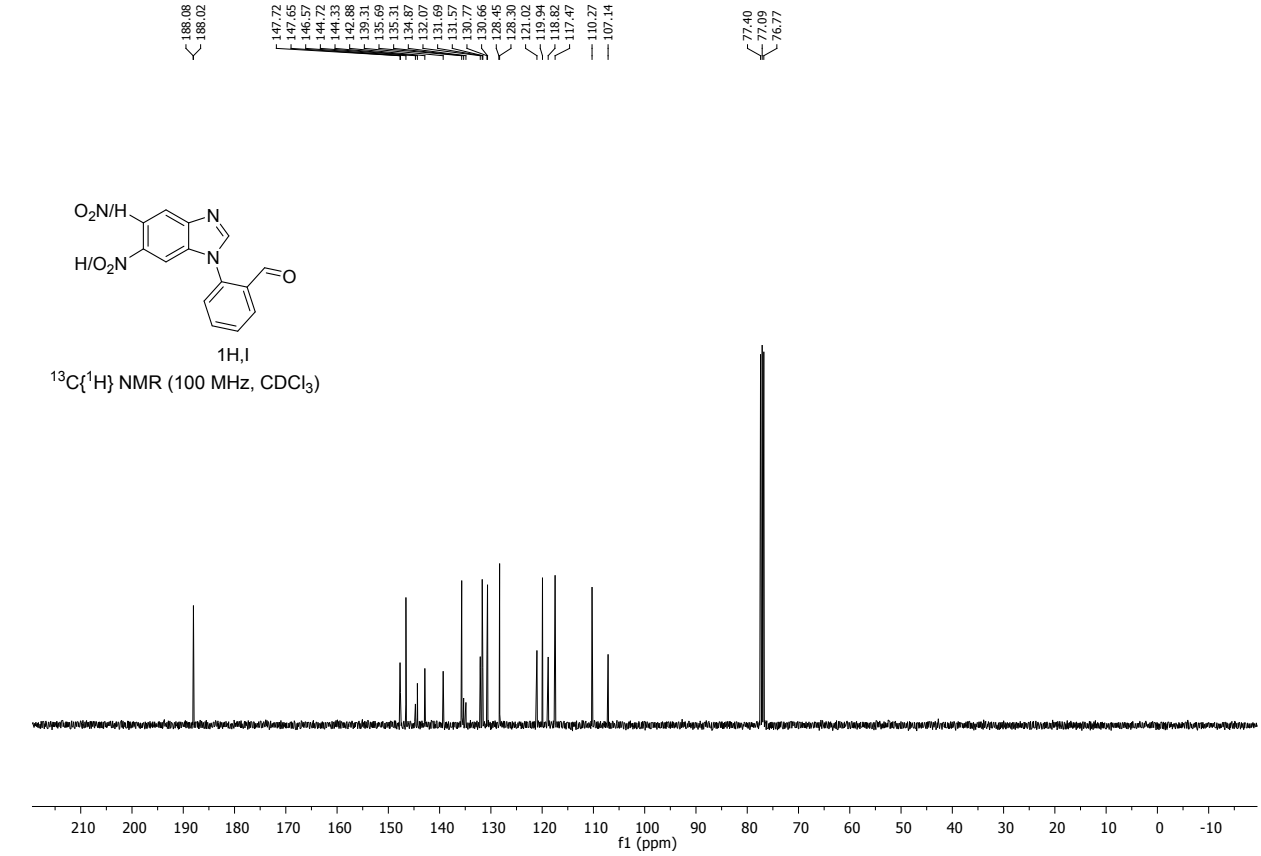


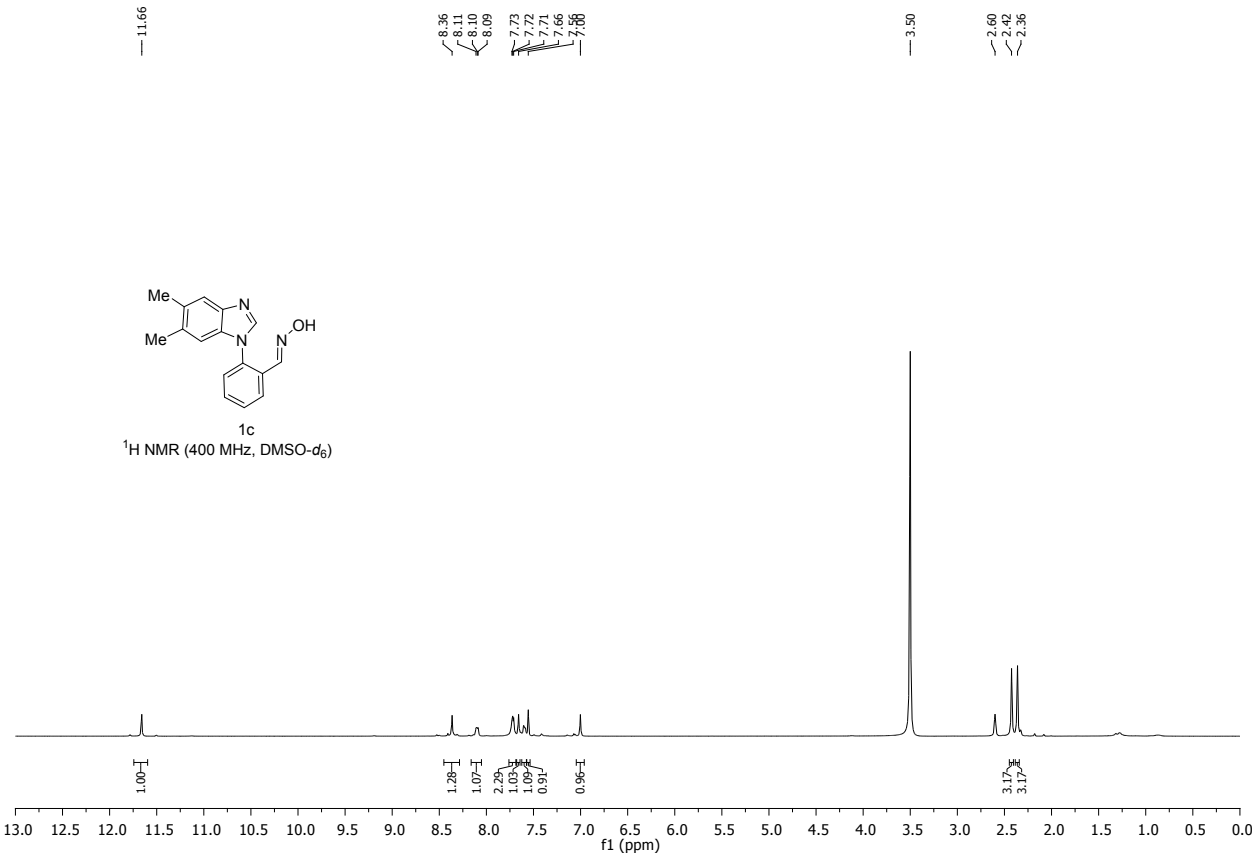
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)


9.70
9.69
8.57
8.57
8.17
8.13
8.13
8.12
8.12
8.11
8.11
8.10
8.10
8.02
8.02
8.01
7.99
7.99
7.91
7.90
7.89
7.87
7.82
7.82
7.71
7.70
7.52
7.52
7.51
7.51
7.50
7.50
7.49
7.49
7.26
7.22
3.92
3.86
MeO2C/H
H/MeO2C
N
N
O
1F,G
1H NMR (400 MHz, CDCl3)
0.96
0.56
1.07
0.92
1.01
0.90
1.02
1.02
1.01
0.57
3.00
10.5
10.0
9.5
9.0
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)

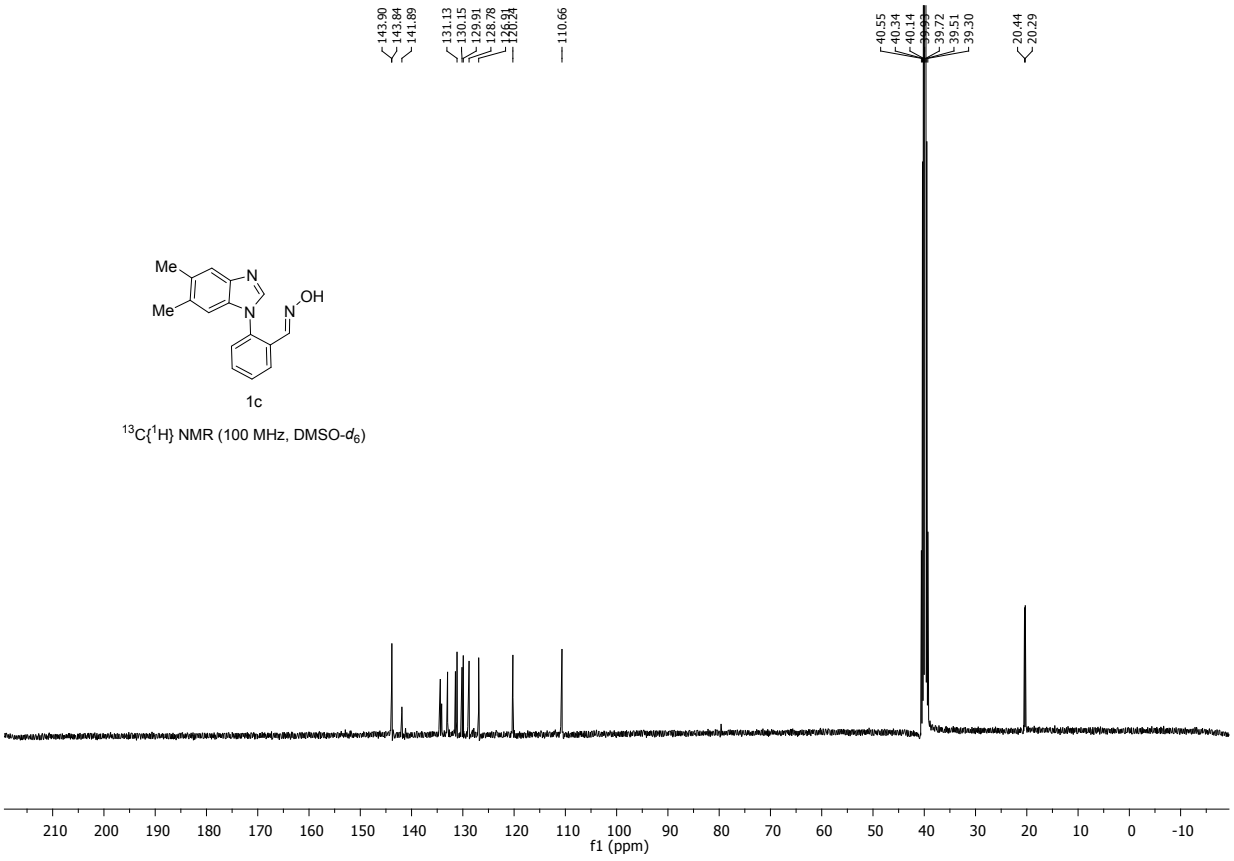

188.09
167.14
166.95
145.86
144.90
136.91
135.58
131.58
130.53
130.39
130.16
130.08
128.28
128.06
126.30
125.82
125.55
124.57
123.11
120.44
112.30
109.80
77.43
77.32
77.12
76.80
52.26
52.23
MeO2C/H
H/MeO2C
N
N
O
1F,G
13C{1H} NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


9.78
9.76
8.77
8.76
8.28
8.26
8.26
8.24
8.23
8.23
8.22
8.20
8.20
8.16
8.16
8.16
8.15
8.15
8.14
8.14
8.13
8.11
8.11
7.97
7.95
7.92
7.91
7.90
7.90
7.89
7.88
7.88
7.88
7.87
7.86
7.83
7.83
7.81
7.79
7.77
7.77
7.56
7.56
7.55
7.55
7.54
7.54
7.53
7.53
7.27
7.26
7.25
O2N/H
H/O2N
N
N
O
1H,I
1H NMR (400 MHz, CDCl3)
1.00
0.64
2.02
1.38
0.35
1.07
1.07
1.04
0.88
10.5
10.0
9.5
9.0
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)

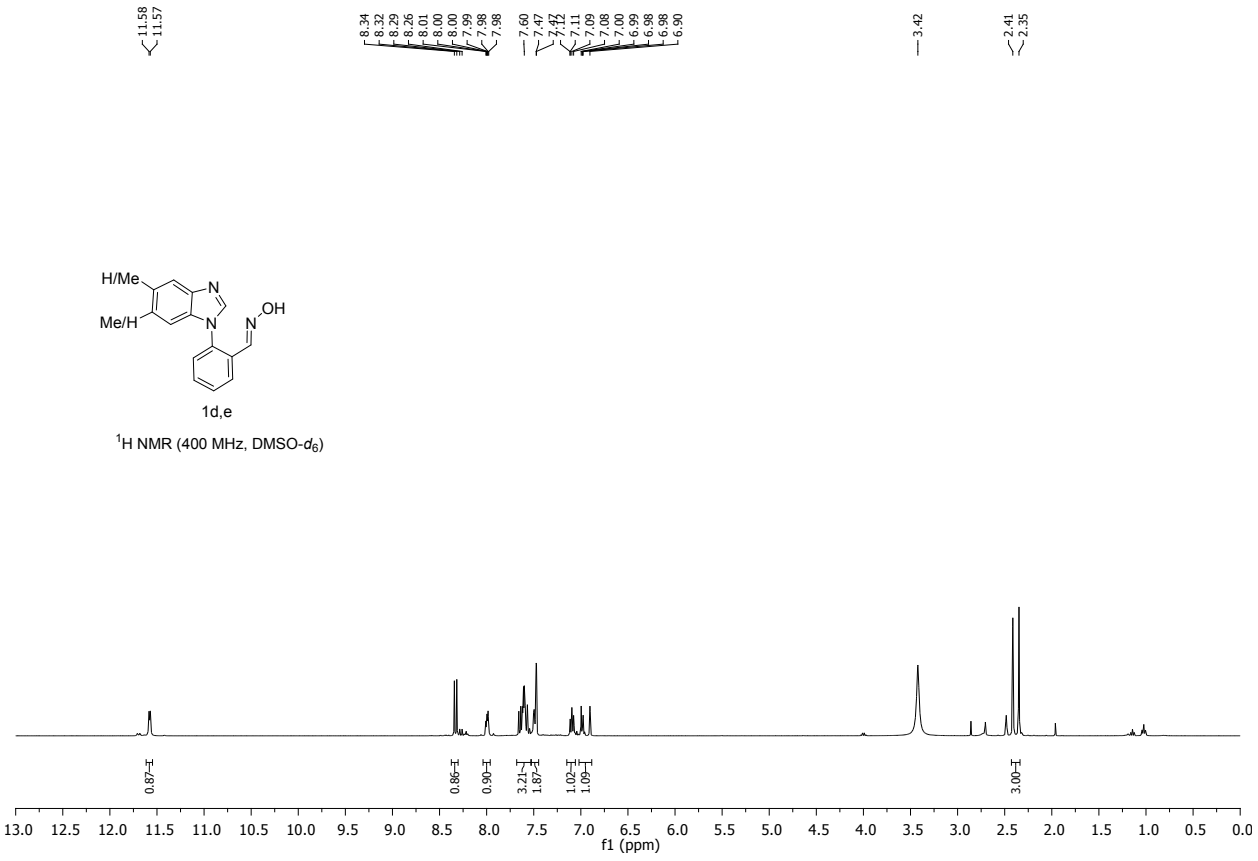

188.08
188.02
147.72
147.65
146.57
144.72
144.33
142.88
139.31
135.69
135.31
134.87
132.07
131.69
131.57
130.77
130.66
128.45
128.30
121.02
119.94
118.82
117.47
110.27
107.14
77.40
77.09
76.77
O2N/H
H/O2N
N
N
O
1H,I
13C{1H} NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



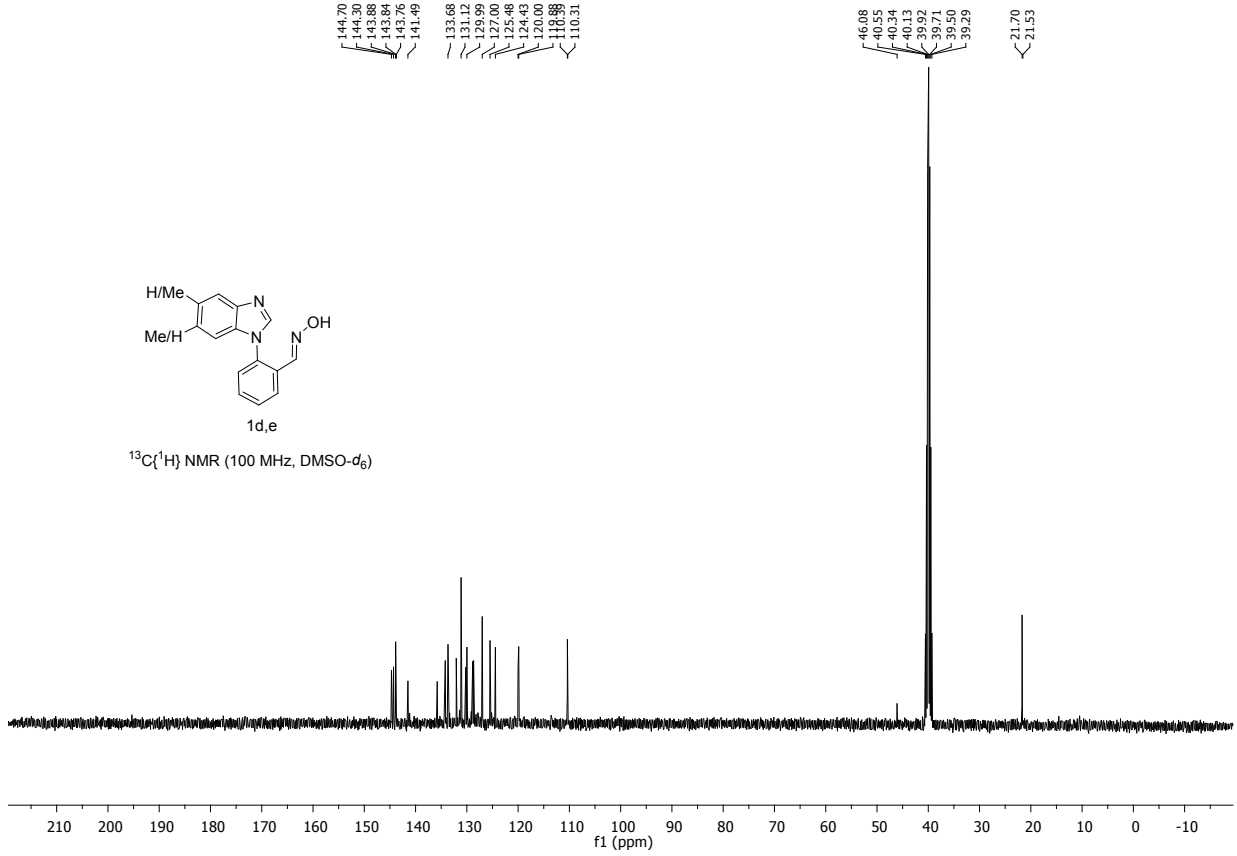
^{1}H NMR (400 MHz, DMSO-d_6)



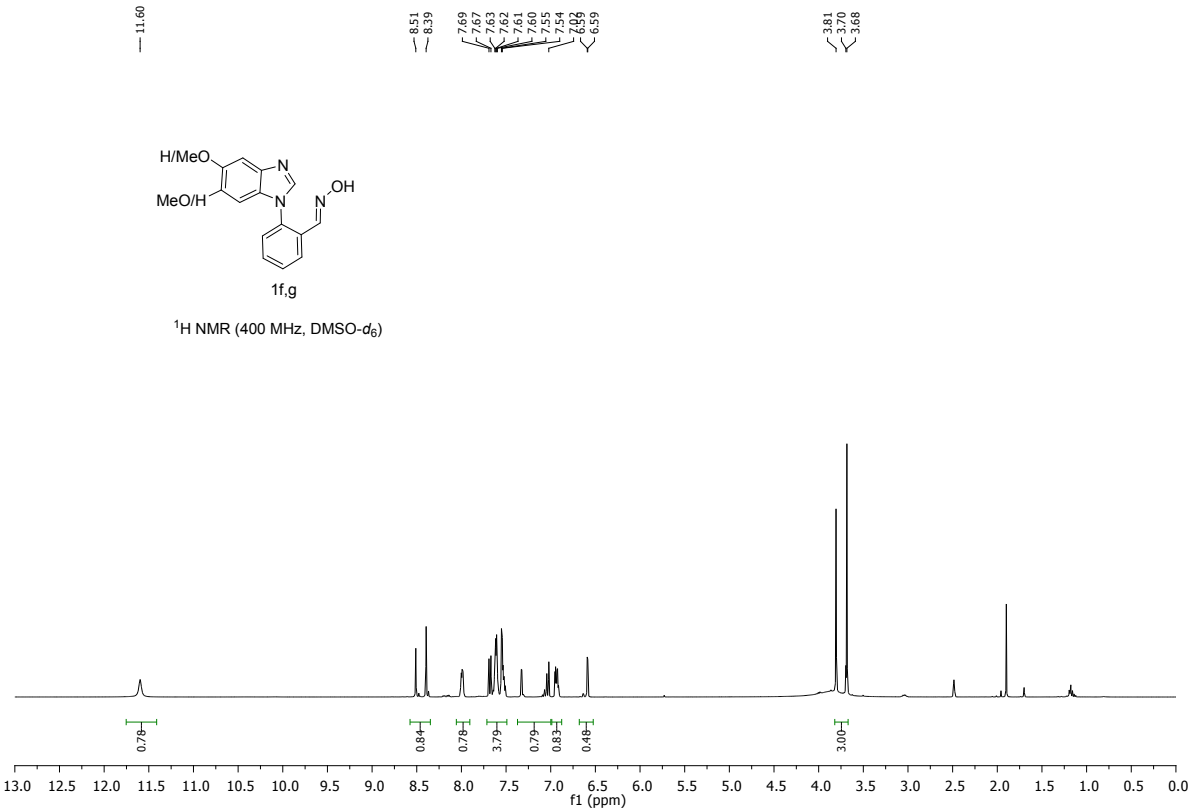
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6)

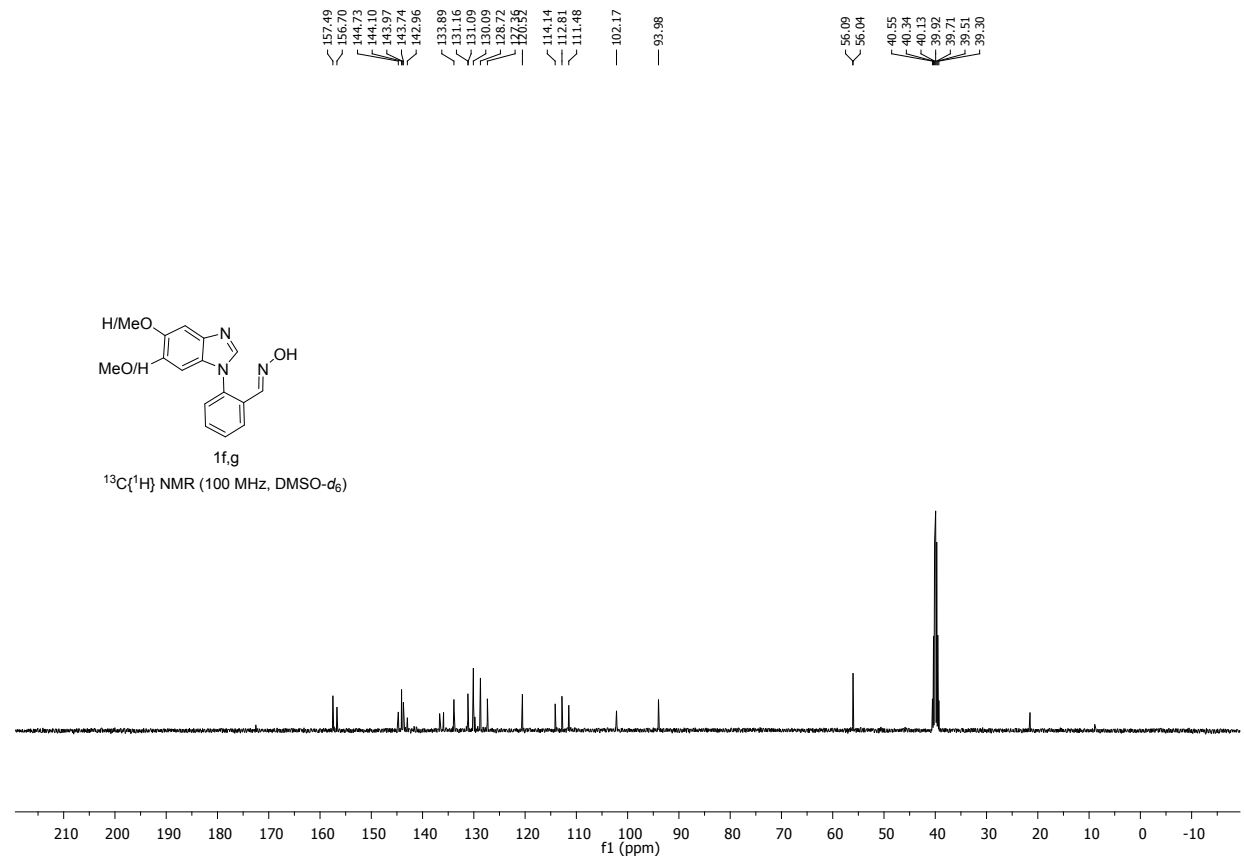


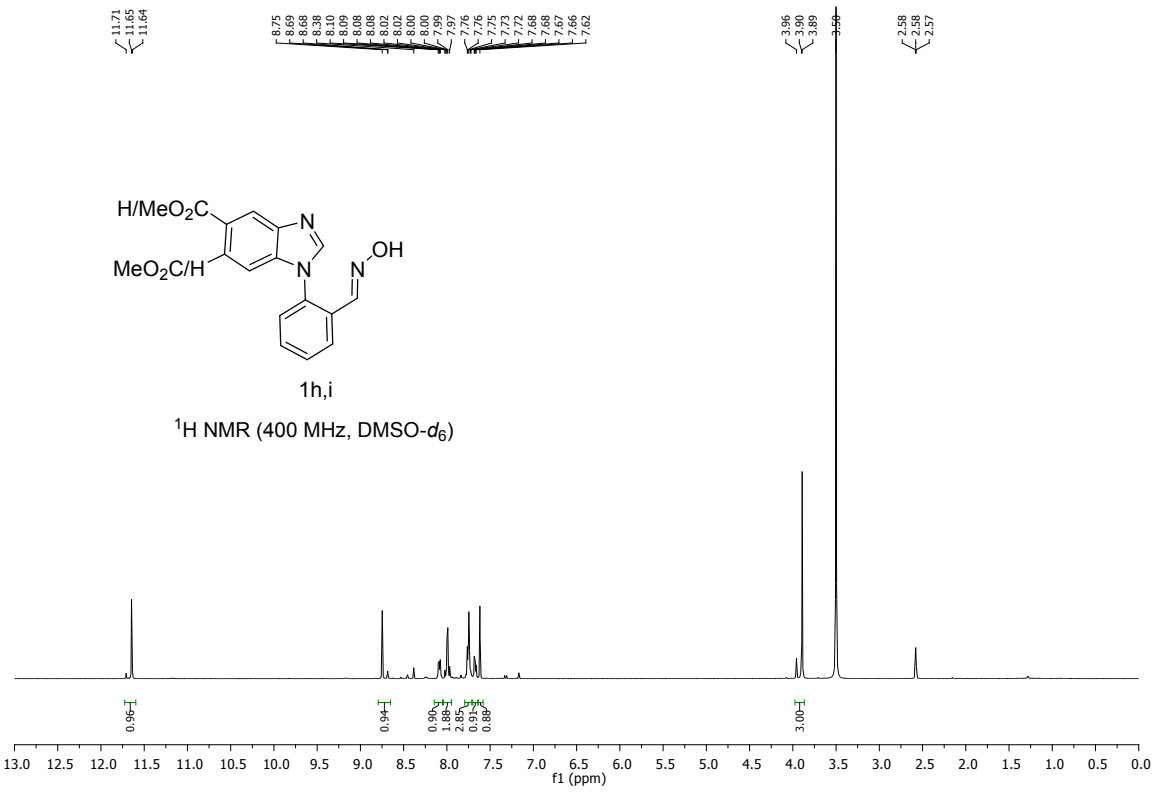
^{1}H NMR (400 MHz, DMSO-d_6)



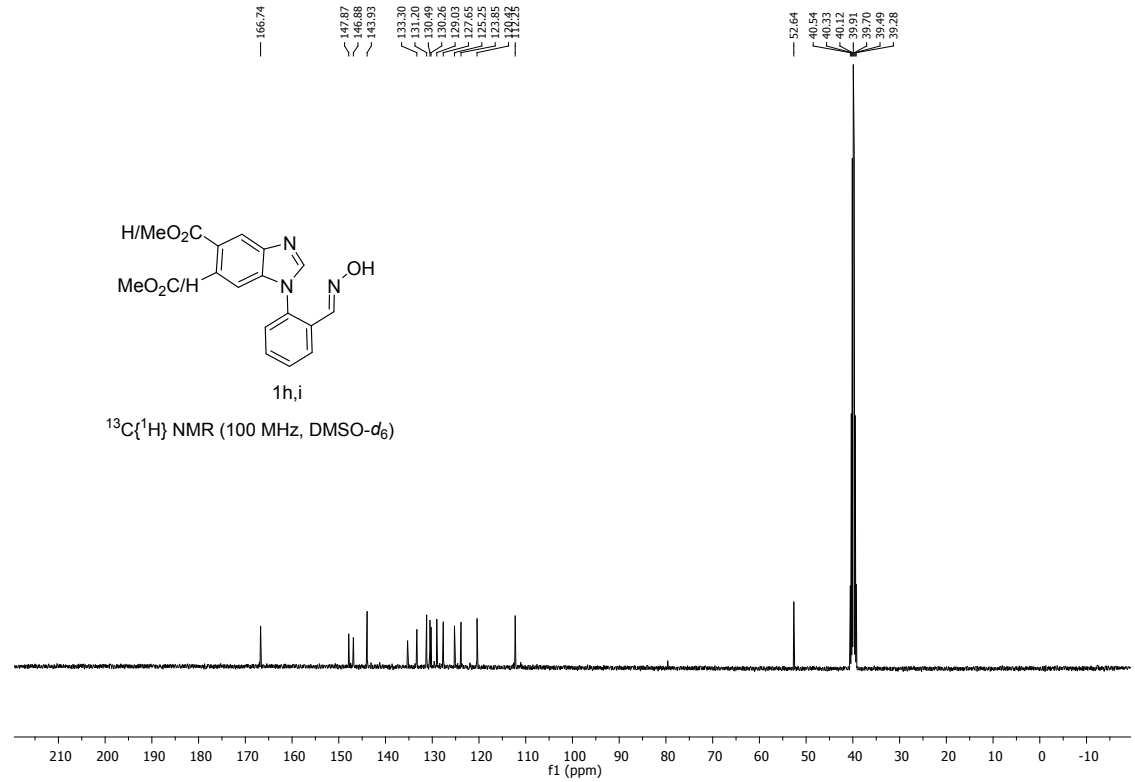
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6)


11.60
8.51
8.39
7.69
7.67
7.63
7.62
7.61
7.60
7.55
7.54
6.59
3.81
3.70
3.68
H/MeO
MeO/H
N
N
N
OH
1f,g
^{1}H NMR (400 MHz, DMSO-d_6)
0.78
0.84
0.78
3.79
0.79
0.83
0.48
3.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 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)

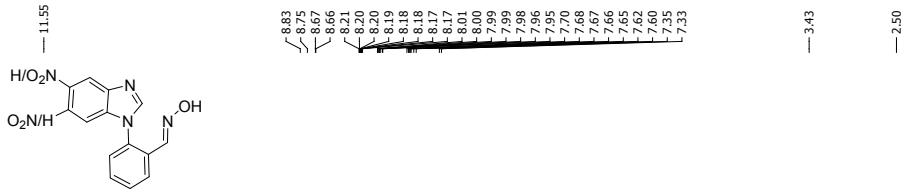

157.49
156.70
144.73
144.10
143.97
143.74
142.96
133.89
131.16
131.09
130.09
128.72
114.14
112.81
111.48
102.17
93.98
56.09
56.04
40.55
40.34
40.13
39.92
39.71
39.51
39.30
H/MeO
MeO/H
N
N
N
OH
1f,g
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



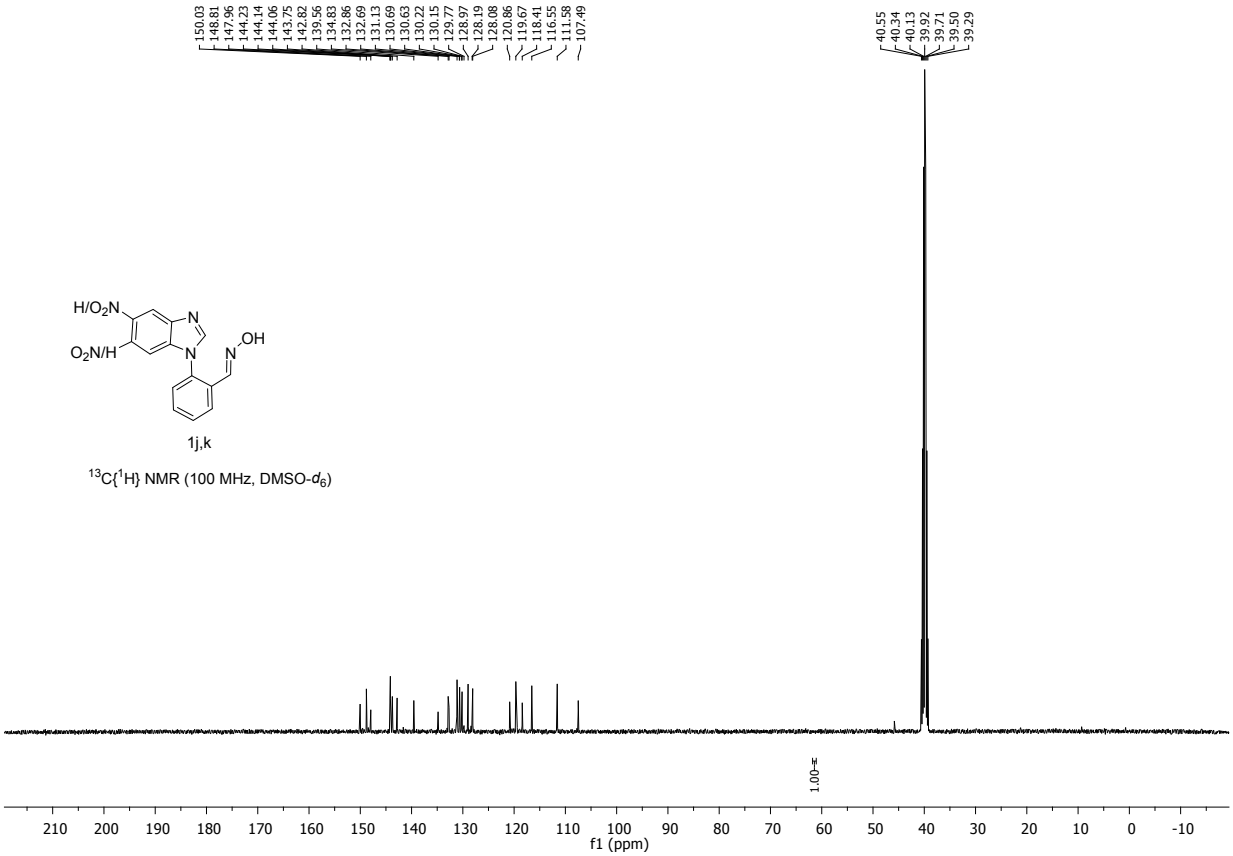
^{1}H NMR (400 MHz, DMSO-d_6)



^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6)

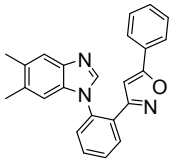


^{1}H NMR (400 MHz, DMSO-d_6)



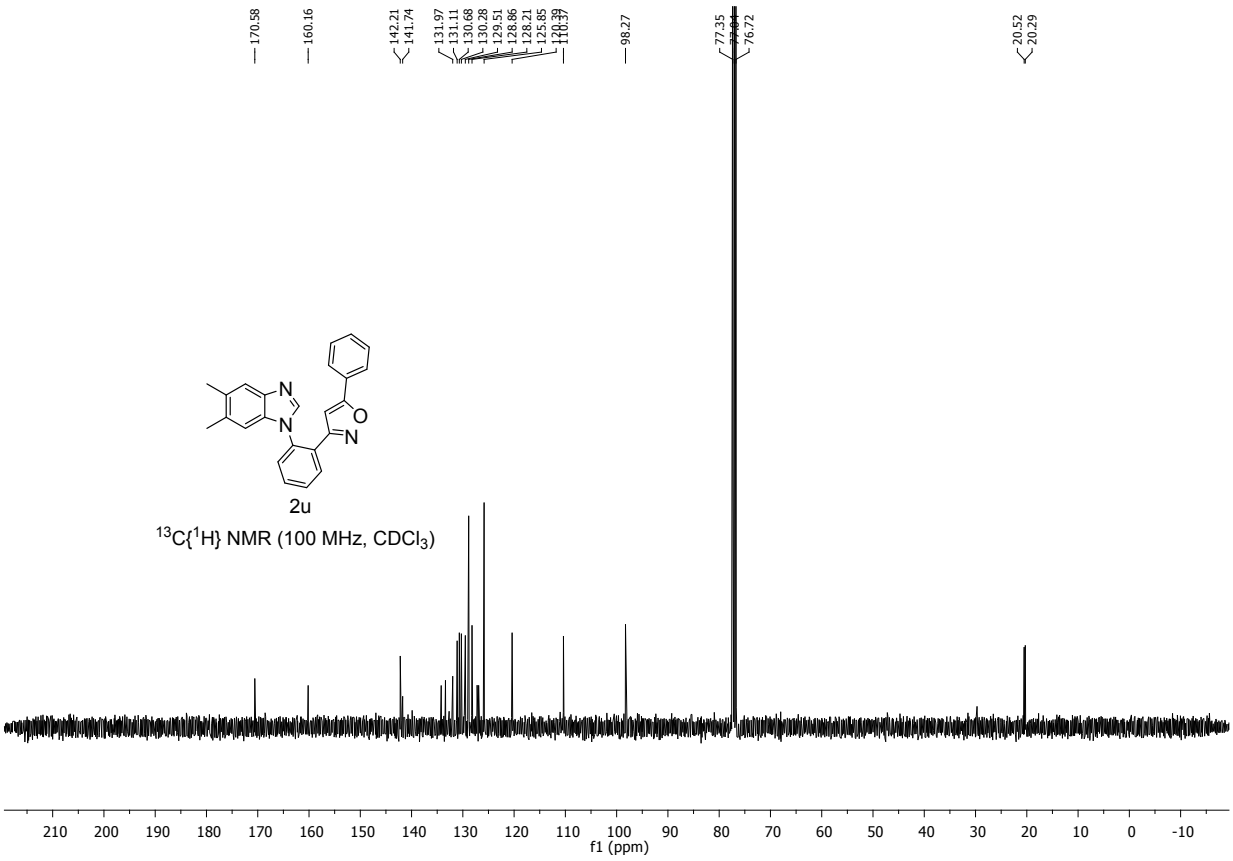
1j,k

$^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6)



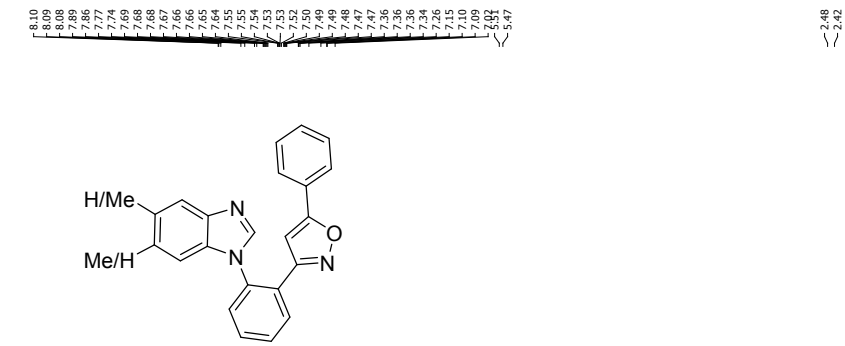
2u

^{1}H NMR (400 MHz, $CDCl_3$)



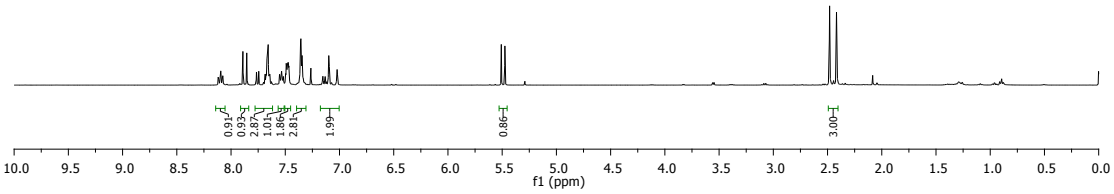
2u

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



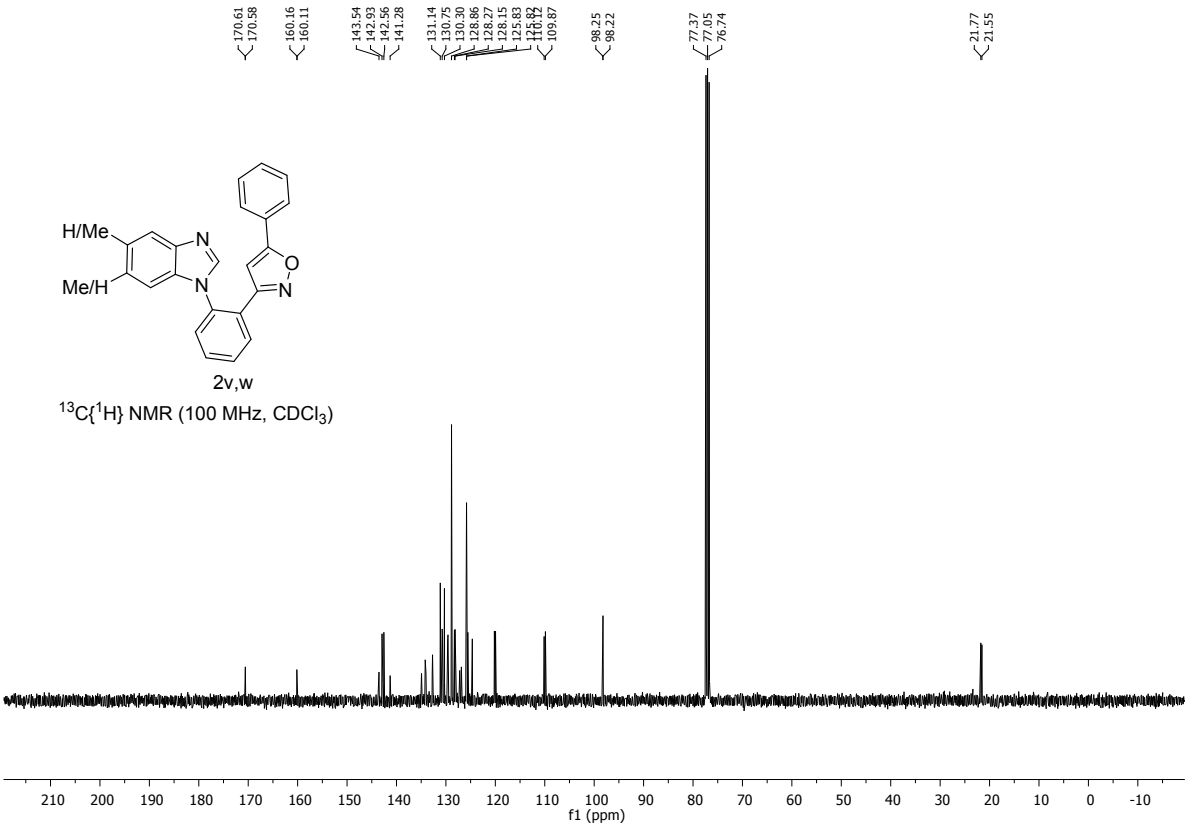
2v,w

^{1}H NMR (400 MHz, $CDCl_3$)

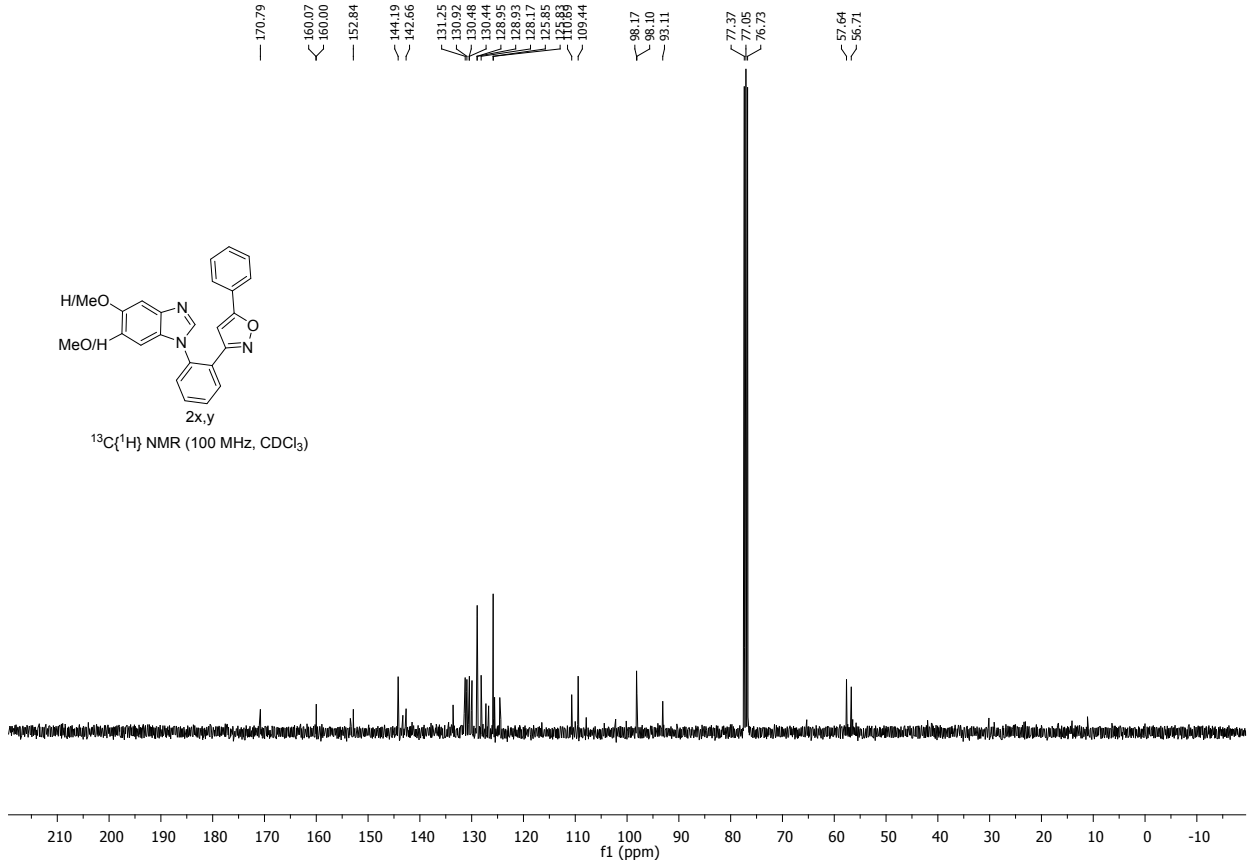


2v,w

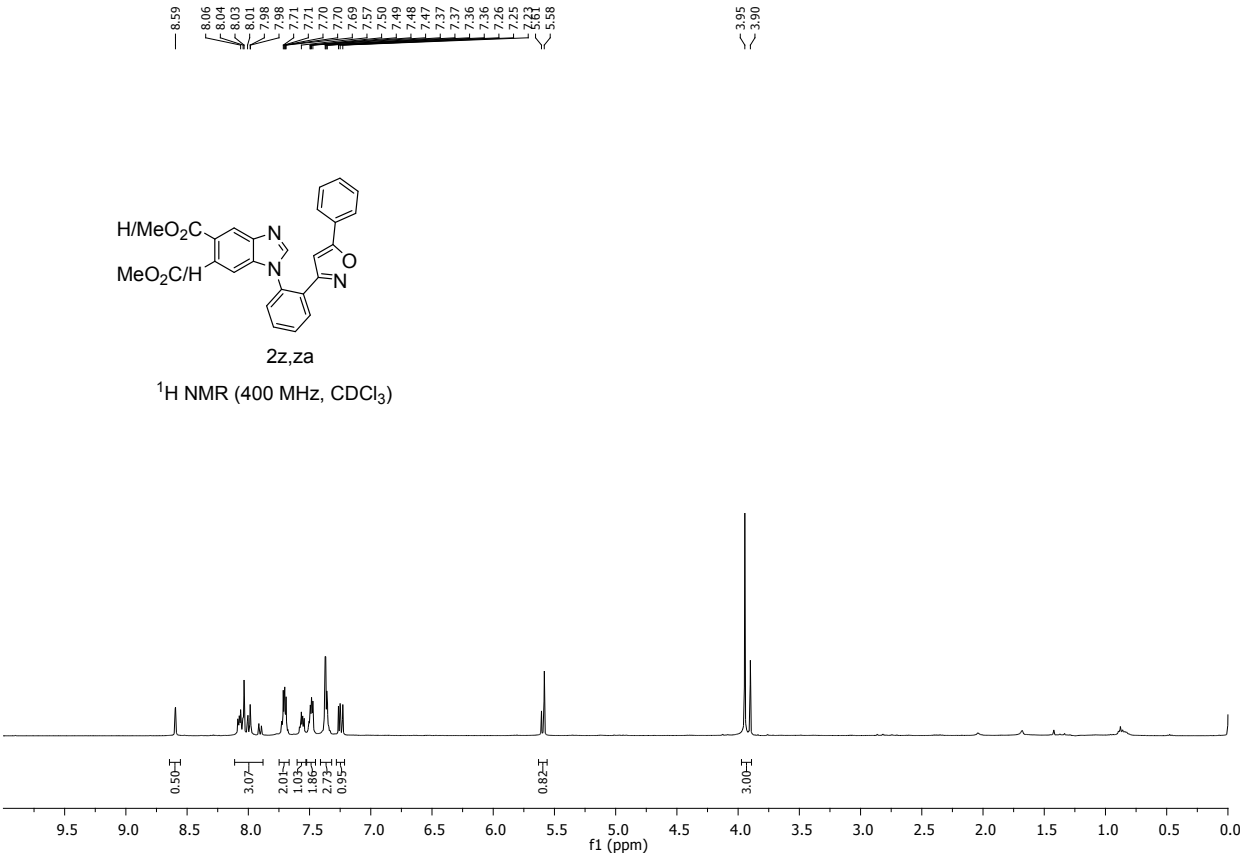
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

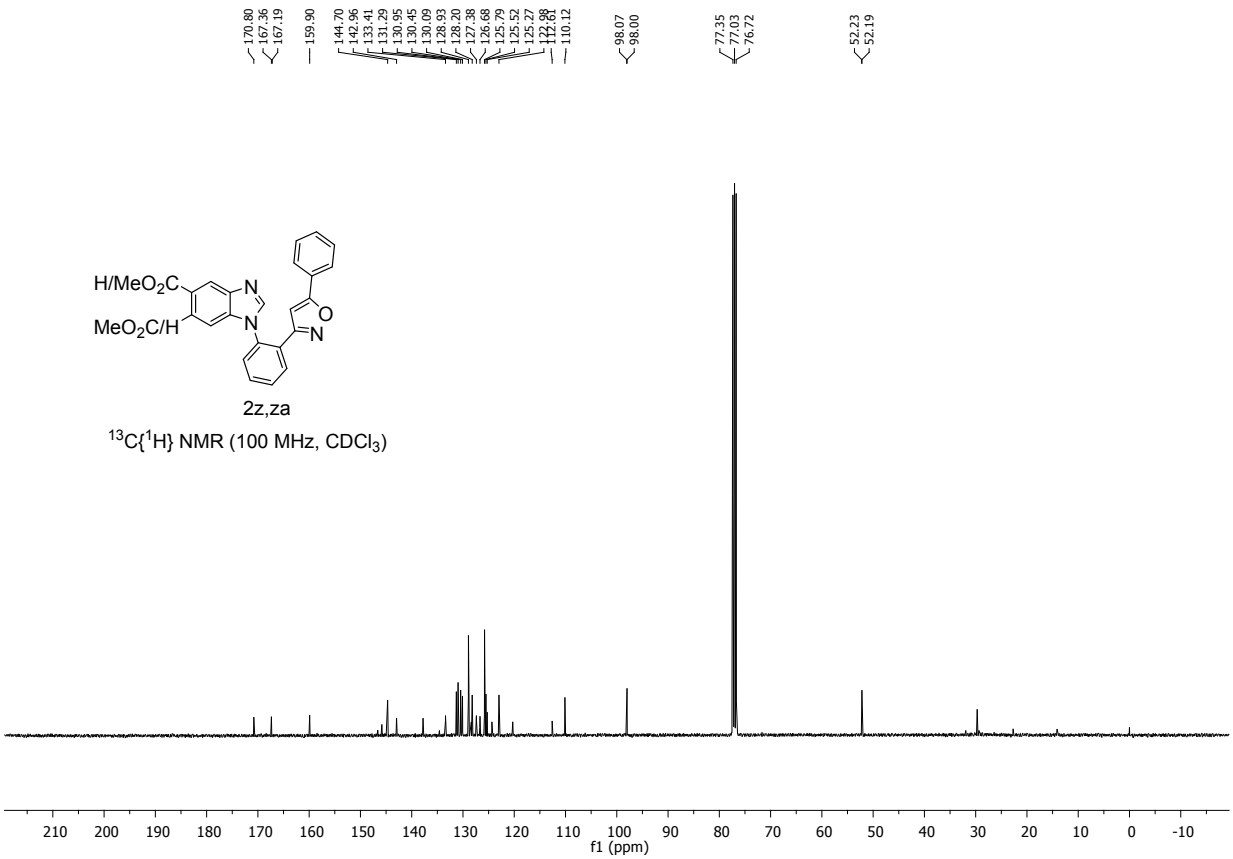


^{1}H NMR (400 MHz, $CDCl_3$)



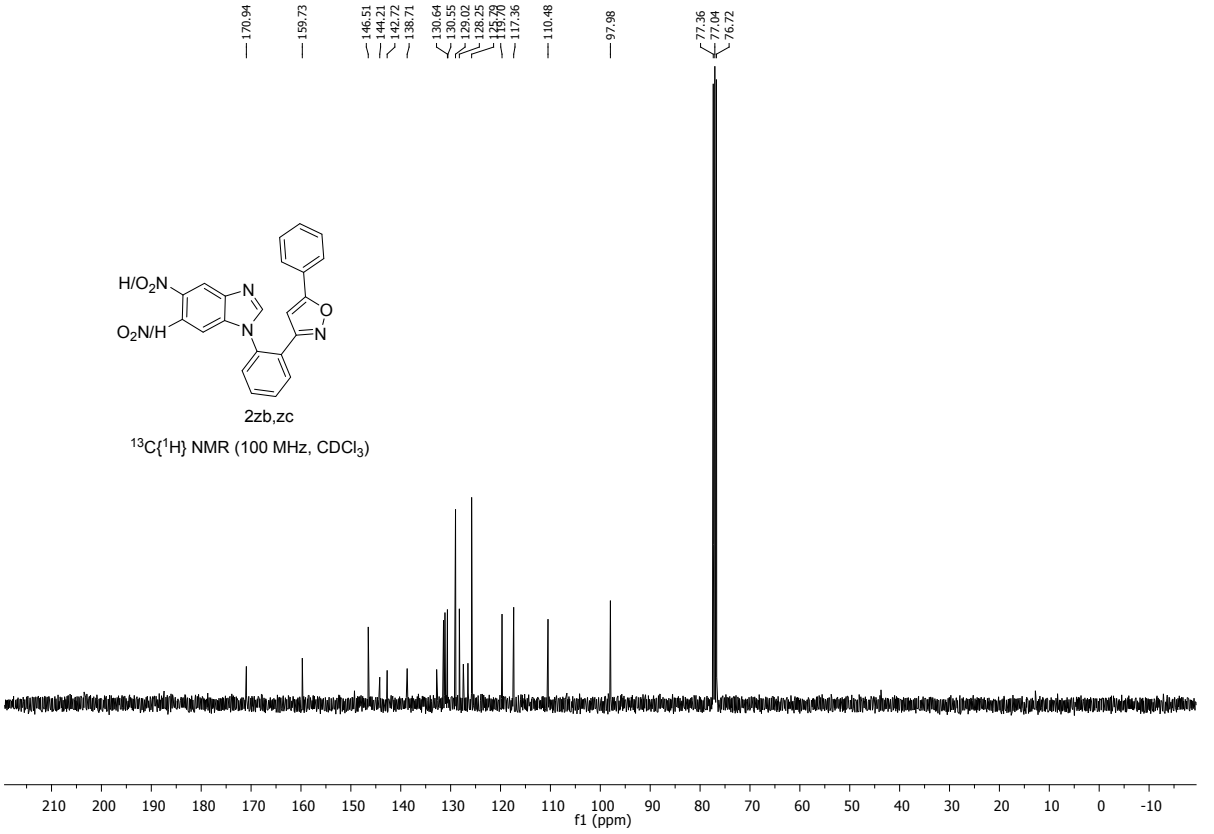
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)


8.59
8.06
8.04
8.03
8.01
7.98
7.98
7.71
7.71
7.70
7.70
7.69
7.57
7.50
7.49
7.48
7.47
7.37
7.37
7.36
7.36
7.26
7.25
5.61
5.58
3.95
3.90
H/MeO2C
MeO2C/H
N
N
O
N
2z,za
1H NMR (400 MHz, CDCl3)
0.50
3.07
2.01
1.03
1.86
2.73
0.95
0.82
3.00
9.5 9.0 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)


170.80
167.36
167.19
159.90
144.70
142.96
133.41
131.29
130.95
130.45
130.09
128.93
128.20
127.38
126.68
125.79
125.52
125.27
112.98
112.61
110.12
98.07
98.00
77.35
77.03
76.72
52.23
52.19
H/MeO2C
MeO2C/H
N
N
O
N
2z,za
13C{1H} NMR (100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2zb.zc

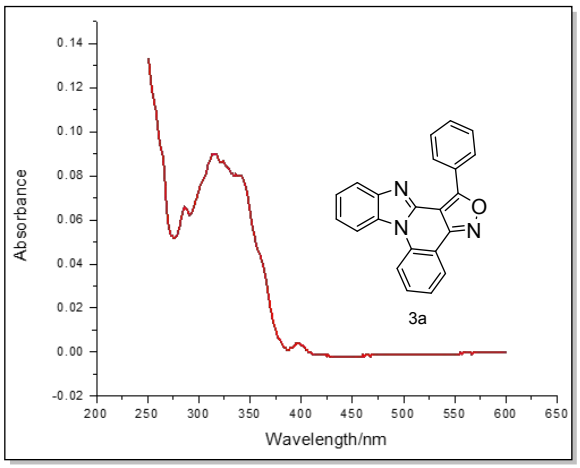
^{1}H NMR (400 MHz, $CDCl_3$)

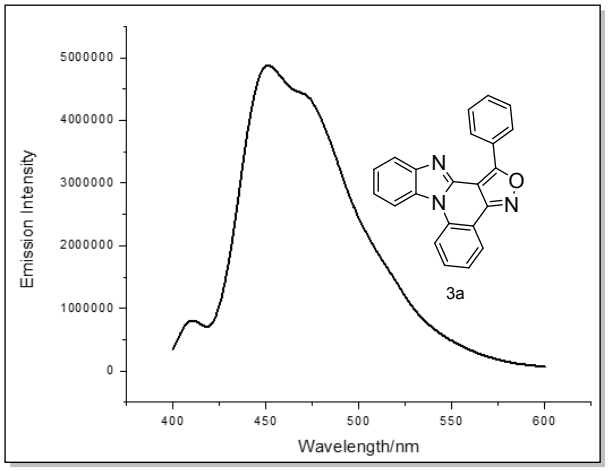


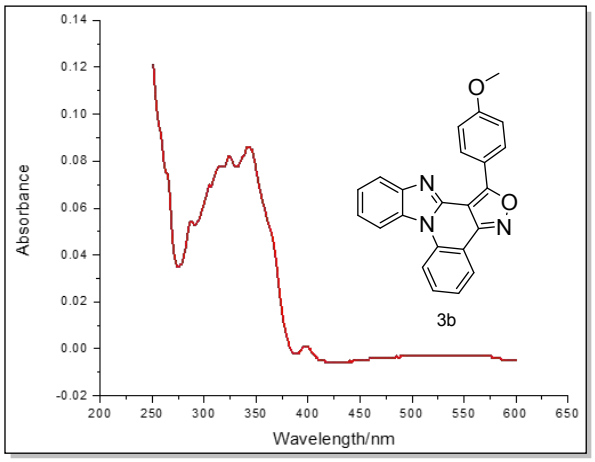
2zb,zc

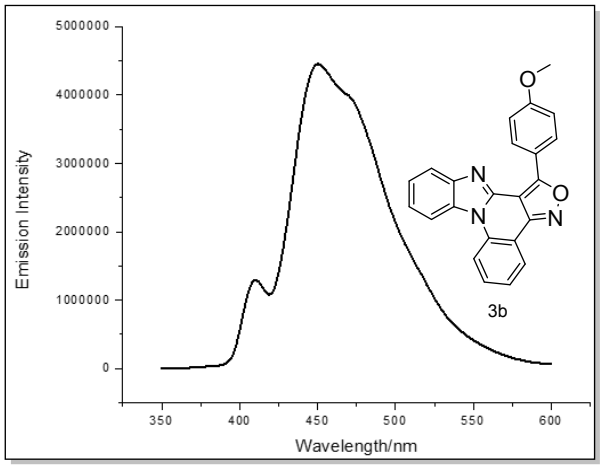
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

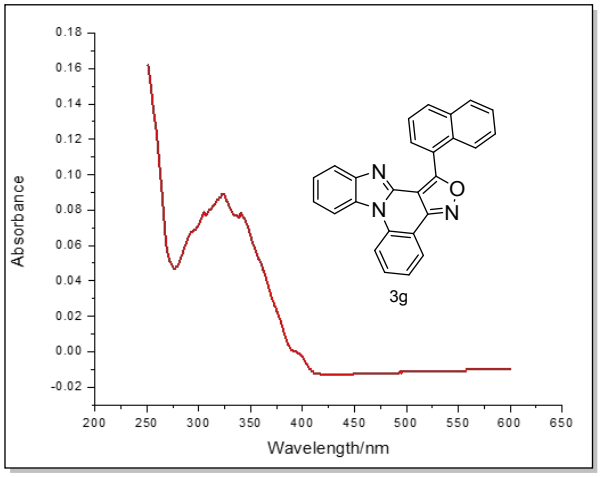
VII) UV-Vis and Emission spectres

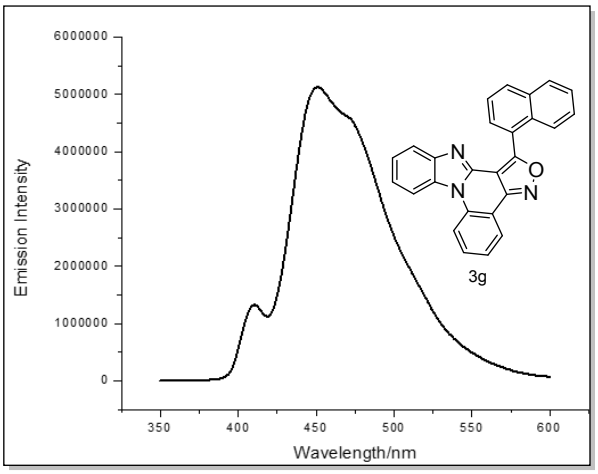


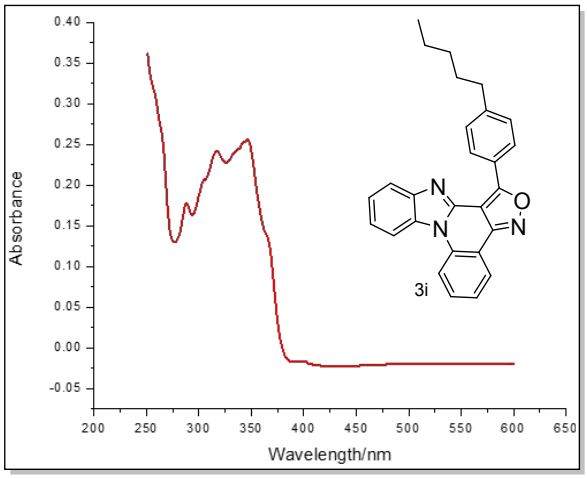


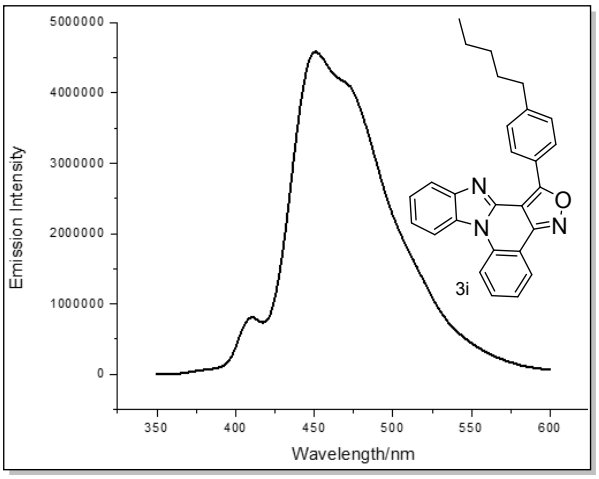


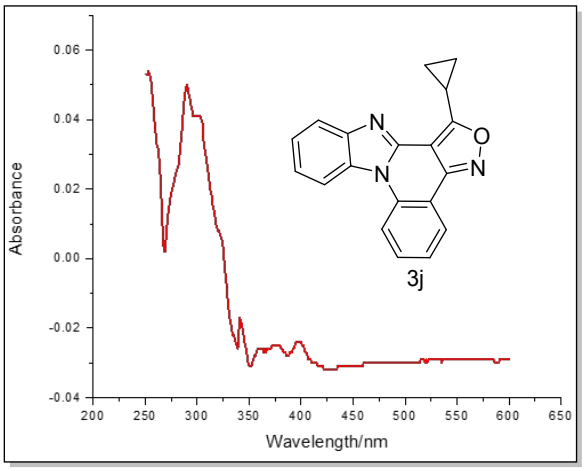







Absorbance
Wavelength/nm
3i


Emission Intensity
Wavelength/nm
3i


Absorbance
Wavelength/nm
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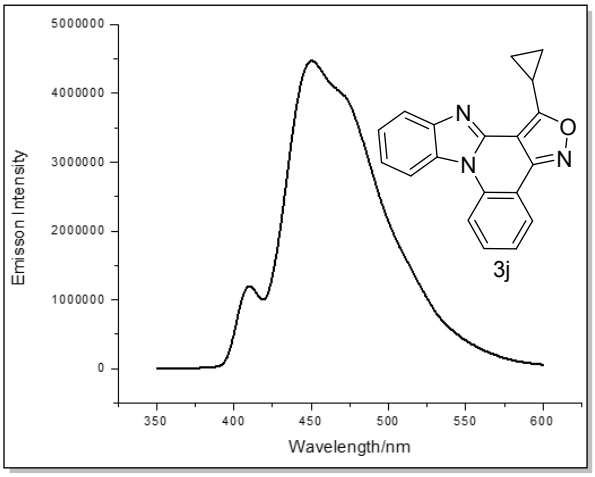
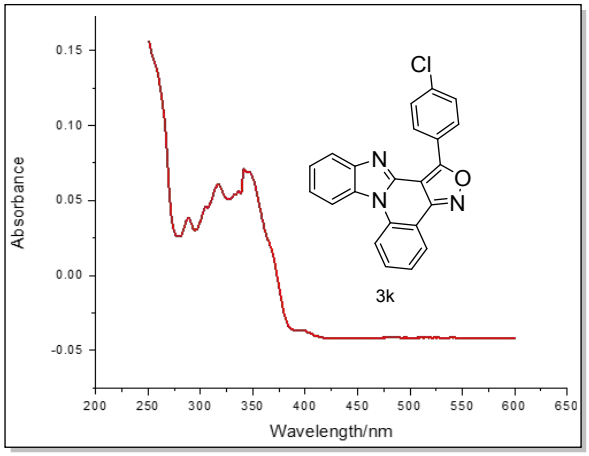
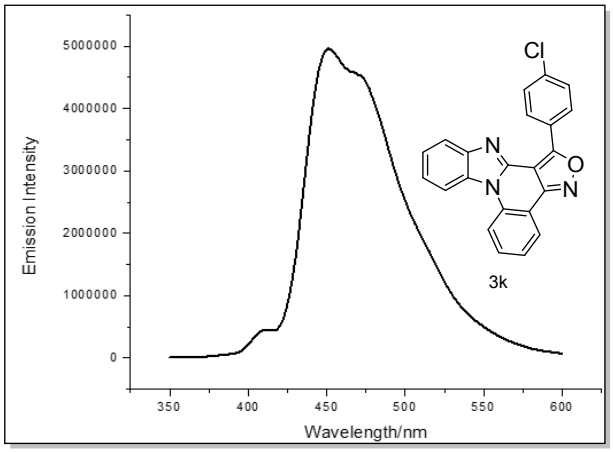
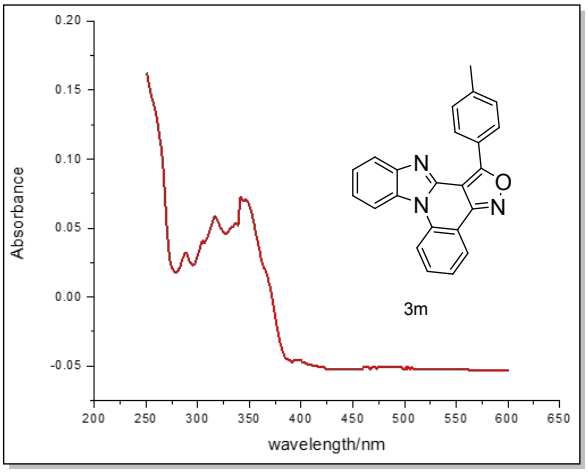
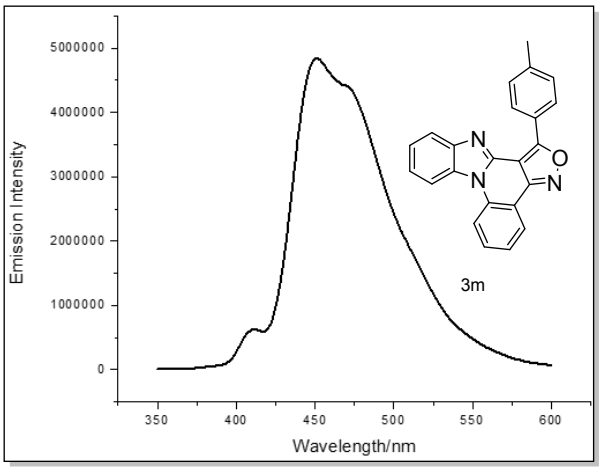
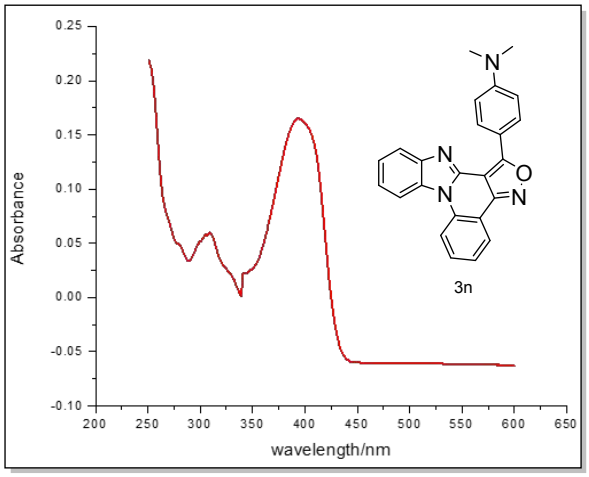

Emisson Intensity
Wavelength/nm
3j

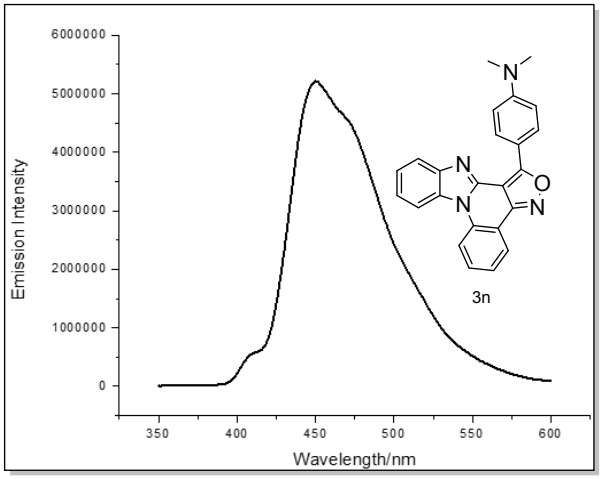

Absorbance
Wavelength/nm
Cl
3k

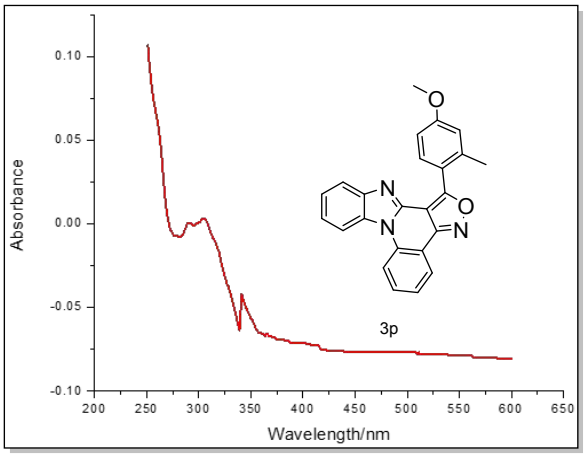

Emission Intensity
Wavelength/nm
Cl
3k

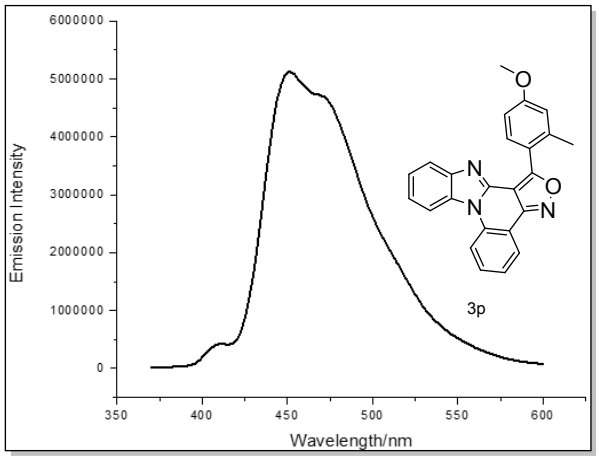

Absorbance
wavelength/nm
3m


Emission Intensity
Wavelength/nm
3m


Absorbance
wavelength/nm
3n


Emission Intensity
Wavelength/nm
3n


Absorbance
Wavelength/nm
3p


Emission Intensity
Wavelength/nm
3p

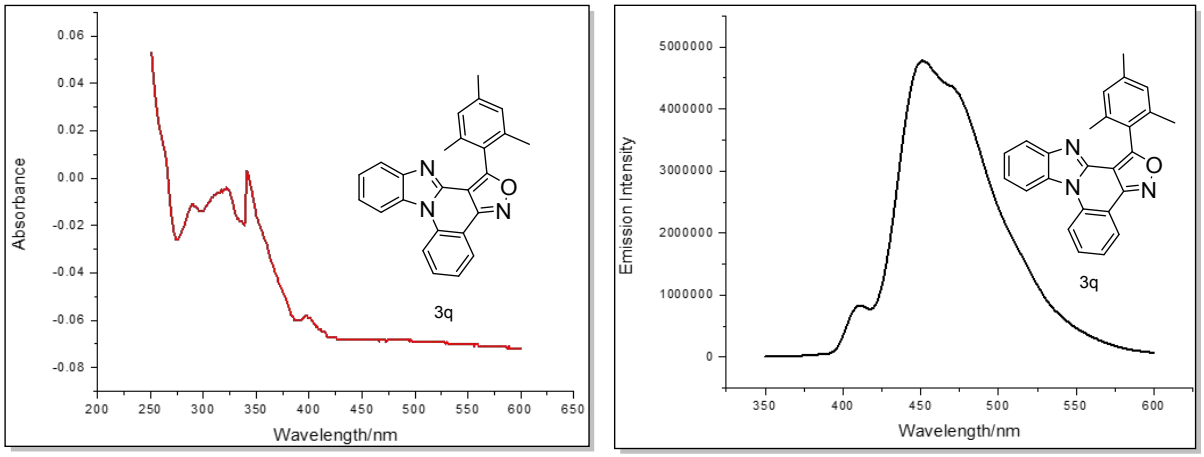


Figure S5 Absorption and fluorescence emission spectra in $CHCl_3$ at 1×10^{-6} mol/L.

V. X-ray diffraction data:

Sample preparation: 20 mg of **3q** (off white solid) was added to a 10 mL conical flask and dissolved in minimal amount of ethanol. Hexane (3 mL) was added to the conical along the wall. The conical was capped loosely and kept at room temperature for slow evaporation. After 7 days, single crystal (pale yellow colour) was obtained and then subjected to X-ray diffraction.

Single crystal X-ray diffraction data were collected on a Bruker APEXXII CCD diffractometer with graphite monochromated Mo-Kα radiation (0.71073 Å). The data collection was smooth without any complication and crystal was stable throughout the data collection period. The data sets were reduced in Bruker Apex2. Crystal structure were solved by direct methods and refined with full matrix least-squares based on F^2, both using SHELXL software package.

Table S1 Crystalographic data for compound 3q:

Compound	**3q**
CCDC	**2036437**
Empirical Formula	**$C_{25}H_{19}N_3O$**
Formula Weight	**377.43**
Temperature/K	**293 K**
Crystal System	**Triclinic**
Space Group	**P -1**
a/Å	**8.2690(15)**

b/Å	**9.1156(13)**
c/Å	**13.023(2)**
α/°	**79.560(5)**
β/°	**87.474(6)**
γ/°	**79.665(6)**
Volume/Å^3	**949.7(3)**
Z	**2**
ρ_{calc}g/cm^3	**1.320**
μ/mm^{-1}	**0.082**
F(000)	**396.0**
Radiation	**MoKα (λ = 0.71073)**
Diffractometer	**Bruker APEX-II CCD**
R(reflections)	**0.0584(1909)**
wR2(reflections)	**0.1654(4588)**

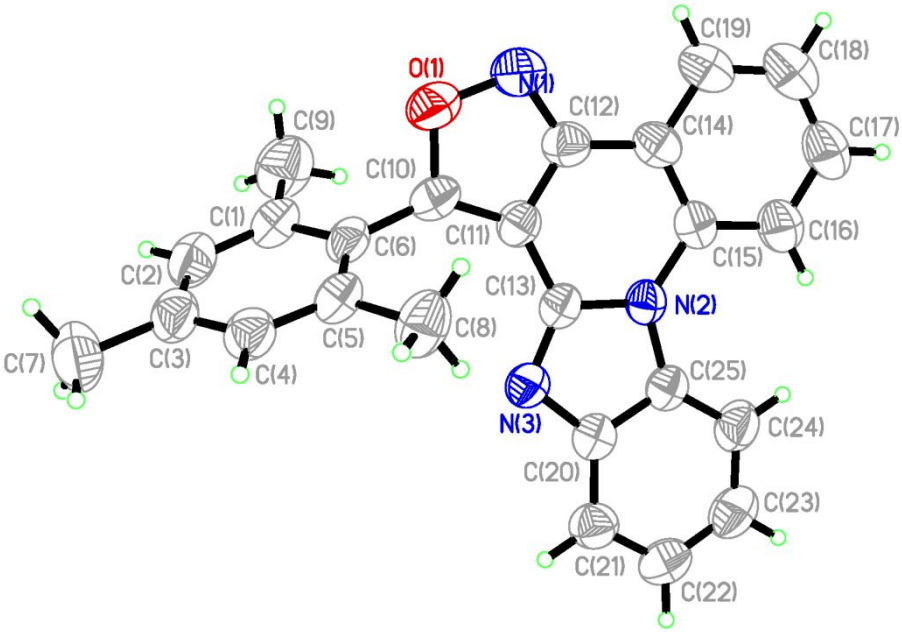


Figure S6 X-ray structure of **3q** (drawn at 50 % probality)