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Cobalt(III)-catalyzed synthesis of isoquinolines from oximes and alkynes in deep eutectic solvents

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Contents

General Experimental

Unless otherwise noted, all chemicals were purchased from commercial suppliers (Aladdin) and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded at ambient temperature on a Bruker AVANCE Ⅲ 300 spectrometer. Chemical shifts are reported in δ units, parts per million (ppm), and were referenced to $CDCl_3$. The coupling constants *J* are given in Hz. Column chromatography was performed using EM Silica gel 60 (300-400 mesh). Chromatograph-Mass Spectrometer (LCMS) was performed on a Shimadzu LCMS-2020 instrument with an ESI source. Melting points (m.p.) are determined with an Optimelt MPA 100 apparatus and are not corrected.

Experimental procedures, spectral and analytical data

General procedure for the synthesis of **3a-h, 5a,b, 7a,b**

DES betaine/HFIP (1:2, mol/mol, HFIP is $(CF_3)_2CHOH$) was prepared by mixing the corresponding components and heating at 80 °C until a clear solution was formed. Then, oxime **1** or **4** (0.2 mmol), alkyne **2** or diyne **6** (0.24 mmol), [Cp*Co(CO)I_2] (10 mol%) and AcONa (20 mol%) were added to this system (1 ml). The mixture was stirred at 80 °C under magnetic stirring for 12 h. Once the reaction was finished, it was quenched with water (3.0 ml) and extracted with EtOAc (3 × 5 ml). The combined organic extracts were dried over $MgSO_4$. The organic phase was concentrated under reduced pressure to leave the crude product, which was purified by column chromatography using light petroleum/ethyl acetate (8:1, v/v) as the eluent to afford products **3a-h, 5a,b, 7a,b**.

Recovery procedure

Once the reaction was finished, the reaction mixture was cooled to room temperature, and EtOAc (3 × 5 ml) was added to the reaction vessel. The biphasic mixture was stirred for 10 min. The organic layer was separated by decantation. The betaine/HFIP DES was dried under vacuum. A new batch of fresh oxime, alkyne and NaOAc were then added in the recovered DES, without the addition of any more Co catalyst.

Characterization data

1-Methyl-3,4-diphenylisoquinoline (3a).[S1] Yellow solid (55 mg, 93%); m.p. 155-157 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.23 – 8.18 (m, 1H), 7.68 (dt, *J* = 6.9, 3.5 Hz, 1H), 7.62 – 7.56 (m, 2H), 7.40 (d, *J* = 7.4 Hz, 2H), 7.38 – 7.31 (m, 3H), 7.27 – 7.15 (m, 5H), 3.09 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.7, 149.4, 141.1,

137.6, 136.0, 131.4, 130.3, 129.9, 129.2, 128.2, 127.6, 127.1, 126.9, 126.5, 126.2, 126.1, 125.5, 22.8; MS (ESI) m/z 296.1 $[M + H]^+$.

1,6-Dimethyl-3,4-diphenylisoquinoline (3b).[S1] Yellow solid (56 mg, 91%); m.p. 164-167 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.12 – 8.05 (m, 1H), 7.44 – 7.39 (m, 2H), 7.38 – 7.28 (m, 5H), 7.24 – 7.13 (m, 5H), 3.04 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.4, 149.6, 141.2, 140.2, 137.8, 136.2, 131.5, 130.3, 128.8, 128.7, 128.2, 127.6, 127.0, 126.8, 125.5, 125.1, 124.6, 22.7, 22.2; MS (ESI) m/z 310.2 $[M + H]^+$.

6-Methoxy-1-methyl-3,4-diphenylisoquinoline (3c).[S1] Yellow solid (57 mg, 88%); m.p. 173-175 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 (d, *J* = 9.1 Hz, 1H), 7.41 – 7.27 (m, 5H), 7.25 – 7.19 (m, 3H), 7.19 – 7.12 (m, 3H), 6.91 (d, *J* = 2.5 Hz, 1H), 3.71 (s, 3H), 3.01 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.6, 157.0, 150.2, 141.2, 138.1, 137.9, 131.3, 130.3, 128.6, 128.3, 127.6, 127.5, 127.1, 126.9, 121.9, 118.7, 104.5, 55.2, 22.7; MS (ESI) m/z 326.3 $[M + H]^+$.

6-Chloro-1-methyl-3,4-diphenylisoquinoline (3d).[S1] Yellow solid (56 mg, 85%); m.p. 178-180 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.9 Hz, 1H), 7.54 (d, *J* = 1.9 Hz, 1H), 7.42 (dd, *J* = 8.9, 2.1 Hz, 1H), 7.30 – 7.22 (m, 5H), 7.14 – 7.07 (m, 5H), 2.96 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.7, 150.7, 140.7, 137.2, 136.9, 136.4, 131.3, 130.2, 128.5 (2C), 127.7 (2C), 127.5, 127.4, 127.2, 125.2, 124.4, 22.8; MS (ESI) m/z 330.8 $[M + H]^+$.

1-Methyl-6-nitro-3,4-diphenylisoquinoline (3e).[S2] Yellow solid (53 mg, 78%); m.p. 174-176 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.49 (d, *J* = 1.4 Hz, 1H), 8.29 – 8.18 (m, 2H), 7.37 – 7.23 (m, 5H), 7.19 – 7.06 (m, 5H), 3.03 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.1, 151.6, 148.3, 140.0, 136.0, 135.8, 131.2, 130.5, 130.2, 128.8, 128.1, 127.8, 127.7 (2C), 127.6, 122.7, 119.9, 23.0; MS (ESI) m/z 341.3 $[M + H]^+$.

1,8-Dimethyl-3,4-diphenylisoquinoline (3f).[S3] Yellow solid (53 mg, 86%); mp.121-122 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 (dd, *J* = 7.7, 2.1 Hz, 1H), 7.42 – 7.33 (m, 5H), 7.30 (dd, *J* = 5.3, 1.2 Hz, 2H), 7.22 – 7.14 (m, 5H), 3.24 (s, 3H), 2.99 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.7, 148.6, 140.8, 138.3, 138.1, 136.0, 131.5, 130.2, 130.1, 129.5, 129.2, 128.2, 127.6, 127.1, 126.9, 125.1, 30.0, 26.0; MS (ESI) m/z 310.2 $[M + H]^+$.

1-Ethyl-3,4-diphenylisoquinoline (3g).[S4] Yellow solid (54 mg, 87%); m.p. 111-113 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.27 – 8.16 (m, 1H), 7.69 – 7.61 (m, 1H), 7.59 – 7.50 (m, 2H), 7.39 (dd, *J* = 9.2, 2.3 Hz, 2H), 7.36 – 7.27 (m, 3H), 7.25 – 7.10 (m, 5H), 3.43 (q, *J* = 7.6 Hz, 2H), 1.53 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.3, 149.3, 141.2, 137.8, 136.4, 131.5, 130.4, 129.8, 129.0, 128.3, 127.6, 127.2, 127.0, 126.5, 126.4, 125.4, 125.2, 28.9, 14.0; MS (ESI) m/z 310.2 $[M + H]^+$.

1,3,4-Triphenylisoquinoline (3h).[S2] Yellow solid (64 mg, 89%); m.p. 172-174 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.08 – 8.02 (m, 1H), 7.73 – 7.66 (m, 2H), 7.59 (d, *J* = 8.1 Hz, 1H), 7.46 – 7.35 (m, 4H), 7.35 – 7.28 (m, 3H), 7.25 – 7.19 (m, 3H), 7.19 – 7.14 (m, 2H), 7.09 – 7.00 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.9, 149.7, 141.0, 139.9, 137.7, 137.1, 131.5, 130.6, 130.4, 130.1, 129.9, 128.7, 128.5, 128.4, 127.7, 127.6, 127.4, 127.1, 126.7, 126.1, 125.5; MS (ESI) m/z 358.2 $[M + H]^+$.

1-Methyl-3,4-diphenylbenzo[*h*]isoquinoline (5a).[S4] Yellow solid (58 mg, 84%); m.p. 146-148 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.87 (d, *J* = 8.4 Hz, 1H), 7.86 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.74 – 7.66 (m, 2H), 7.65 – 7.57 (m, 1H), 7.53 (d, *J* = 9.1 Hz, 1H), 7.46 – 7.39 (m, 2H), 7.37 – 7.29 (m, 3H), 7.24 – 7.16 (m, 5H), 3.41 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.5, 151.0, 140.7, 138.1, 137.3, 133.0, 131.8, 131.2, 130.3, 130.2, 129.7, 128.8, 128.4, 127.8, 127.4, 127.3, 127.2, 126.9, 126.7, 124.3, 124.0, 30.6; MS (ESI) m/z 346.2 $[M + H]^+$.

7-Methyl-4,5-diphenylthieno[2,3-*c*]pyridine (5b).[S3] Yellow solid (45 mg, 75%); m.p. 141-143 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59 (d, *J* = 5.5 Hz, 1H), 7.37 – 7.32 (m, 2H), 7.32 – 7.26 (m, 3H), 7.25 – 7.17 (m, 6H),

2.90 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.4, 151.0, 145.7, 140.5, 138.3, 134.3, 131.0, 130.6, 130.4, 128.3, 127.8, 127.2, 127.1, 124.3, 23.7; MS (ESI) m/z 302.1 $[M + H]^+$.

1-Methyl-4-phenyl-3-(phenylethynyl)isoquinoline (7a).[S5] Brown oil (43 mg, 68%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.43 (d, *J* = 8.0 Hz, 1H), 8.06 (ddd, *J* = 8.1, 4.8, 1.0 Hz, 3H), 7.72 (ddd, *J* = 8.3, 6.9, 1.2 Hz, 1H), 7.56 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H), 7.47 – 7.38 (m, 5H), 7.27 (dd, *J* = 5.0, 1.9 Hz, 3H), 2.96 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.1, 153.4, 140.3, 136.6, 131.4, 130.8, 130.0, 128.4 (2C), 127.9, 127.3, 126.3, 125.9, 125.6, 123.4, 111.0, 98.5, 86.2. 22.7; MS (ESI) m/z 320.1 $[M + H]^+$.

4-(4-Methoxyphenyl)-3-[(4-methoxyphenyl)ethynyl]-1-methylisoquinoline (7b).[S6] Brown oil (48 mg, 64%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.4 Hz, 1H), 8.19 – 8.08 (m, 3H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.65 – 7.57 (m, 1H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.04 (d, *J* = 8.7 Hz, 2H), 6.89 (d, *J* = 8.6 Hz, 2H), 3.89 (s, 3H), 3.83 (s, 3H), 3.02 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.8, 159.7, 157.5, 152.5, 136.7, 133.0, 132.8, 131.3, 130.6, 126.9, 126.3, 125.8, 125.4, 115.7, 114.1, 113.3, 110.5, 98.5, 85.1, 55.4, 55.3, 22.8; MS (ESI) m/z 380.2 $[M + H]^+$.

References

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S2. D. S. Deshmukh, P. A. Yadav and B. M. Bhanage, *Org. Biomol. Chem.*, 2019, **17**, 3489.
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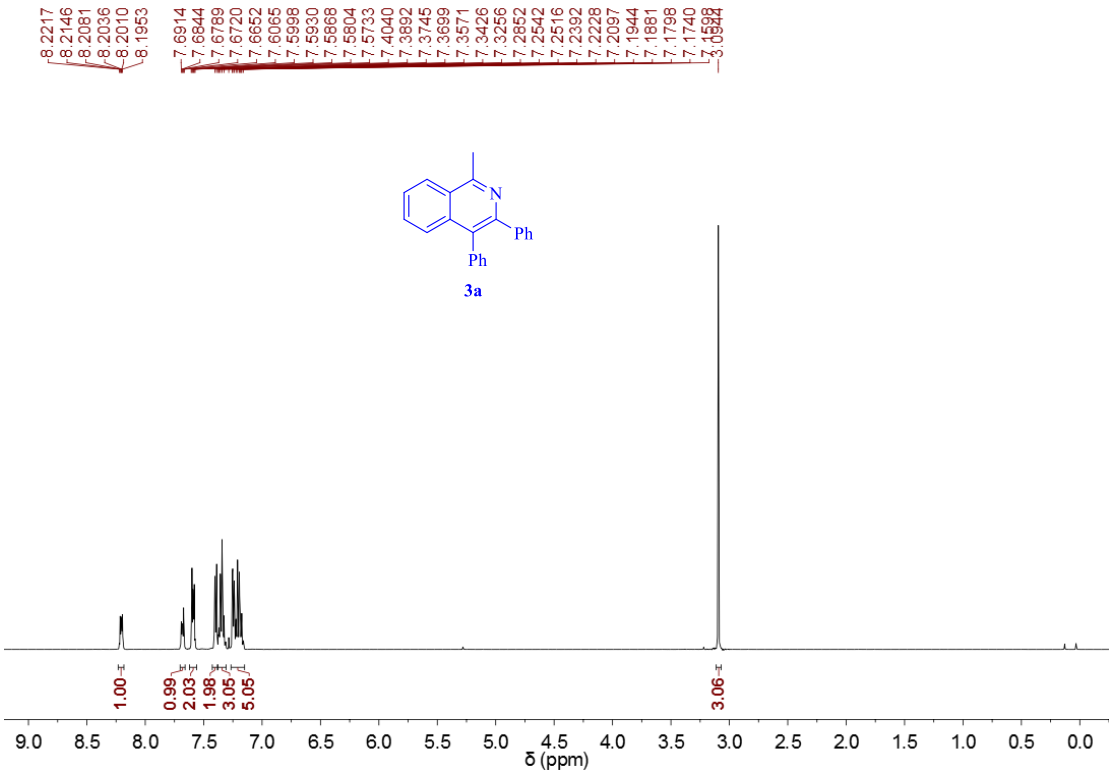
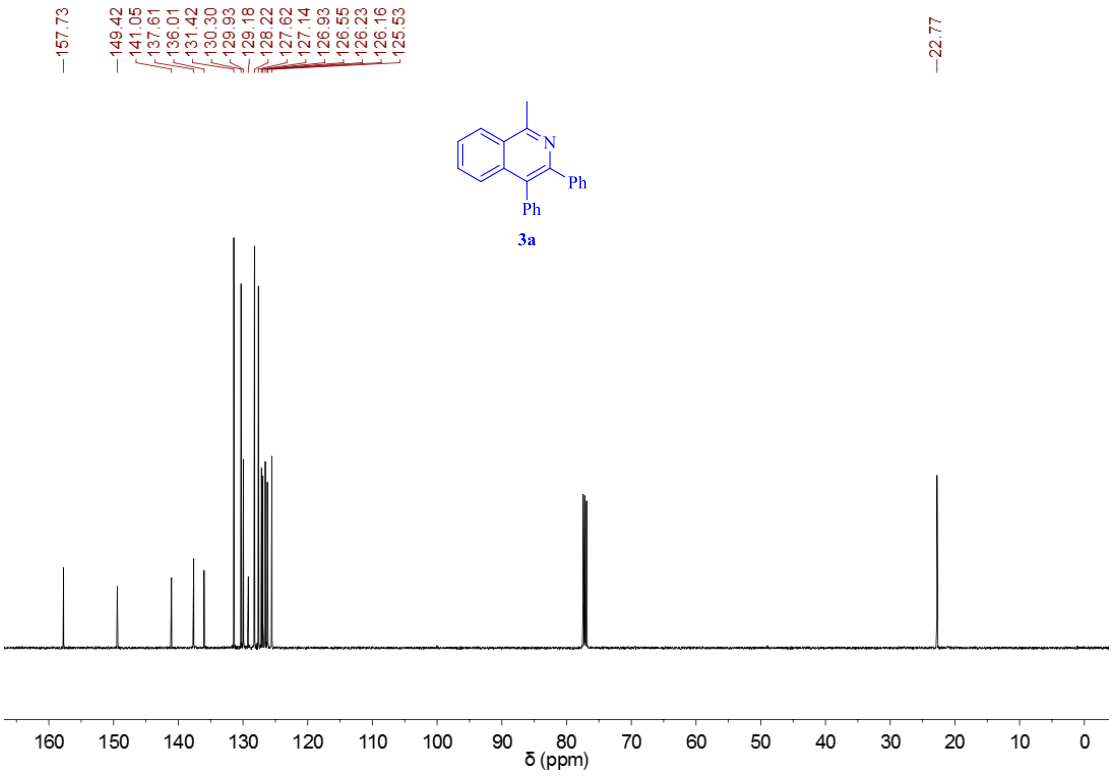
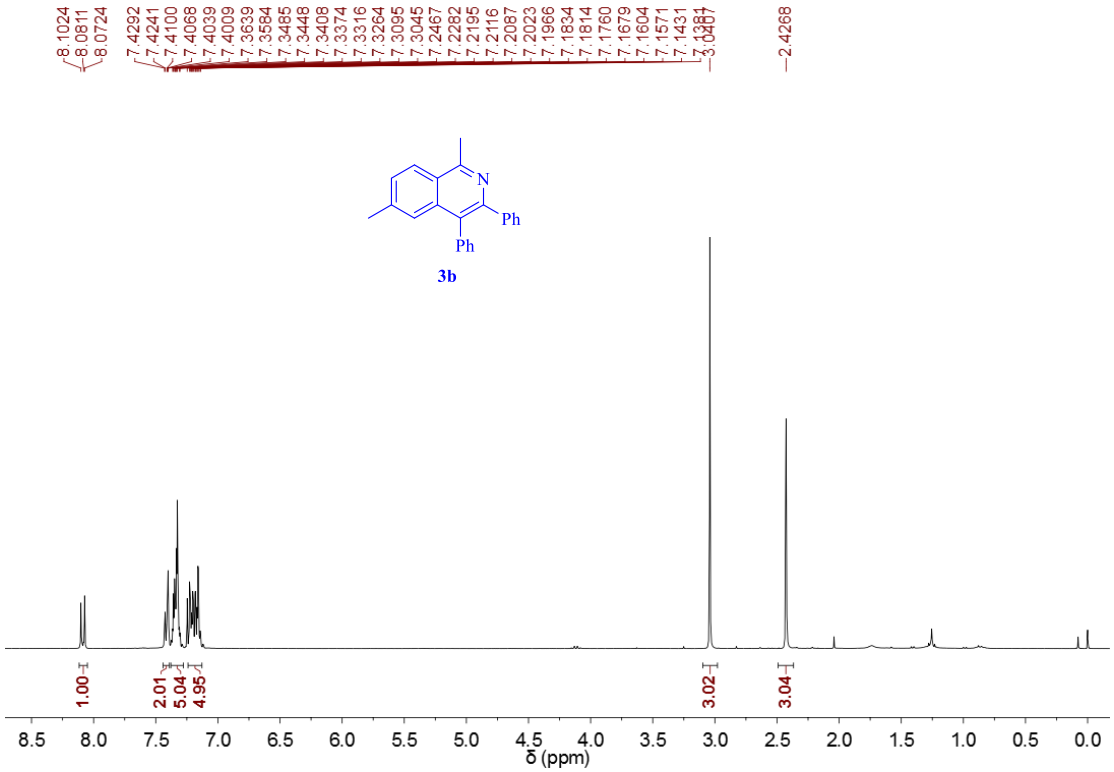
S5. S. Kumar, A. M. Nair and C. M. R. Volla, *Org. Lett.*, 2020, **22**, 2141.
S6. K. Jiang, L. Wang, Q. Chen, M. He, M. Shen and Z. Zhang, *Synth. Commun*. 2021, **51**, 94.

Copies of ^{1}H and ^{13}C NMR Spectra



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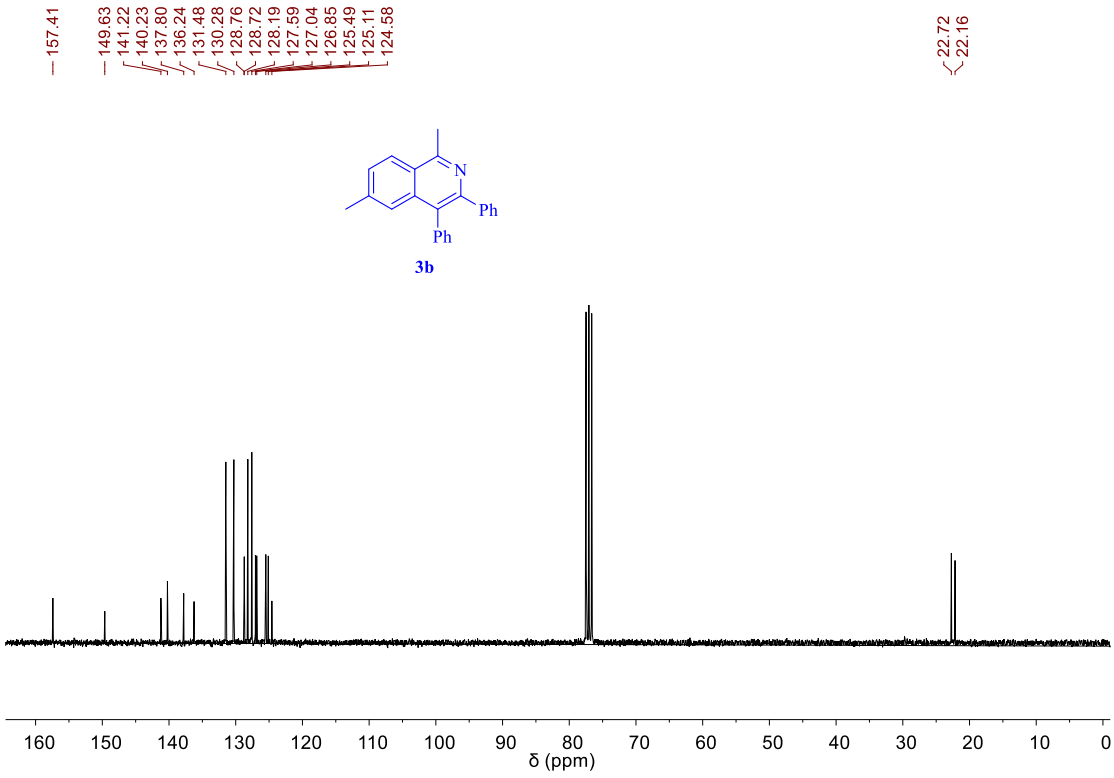
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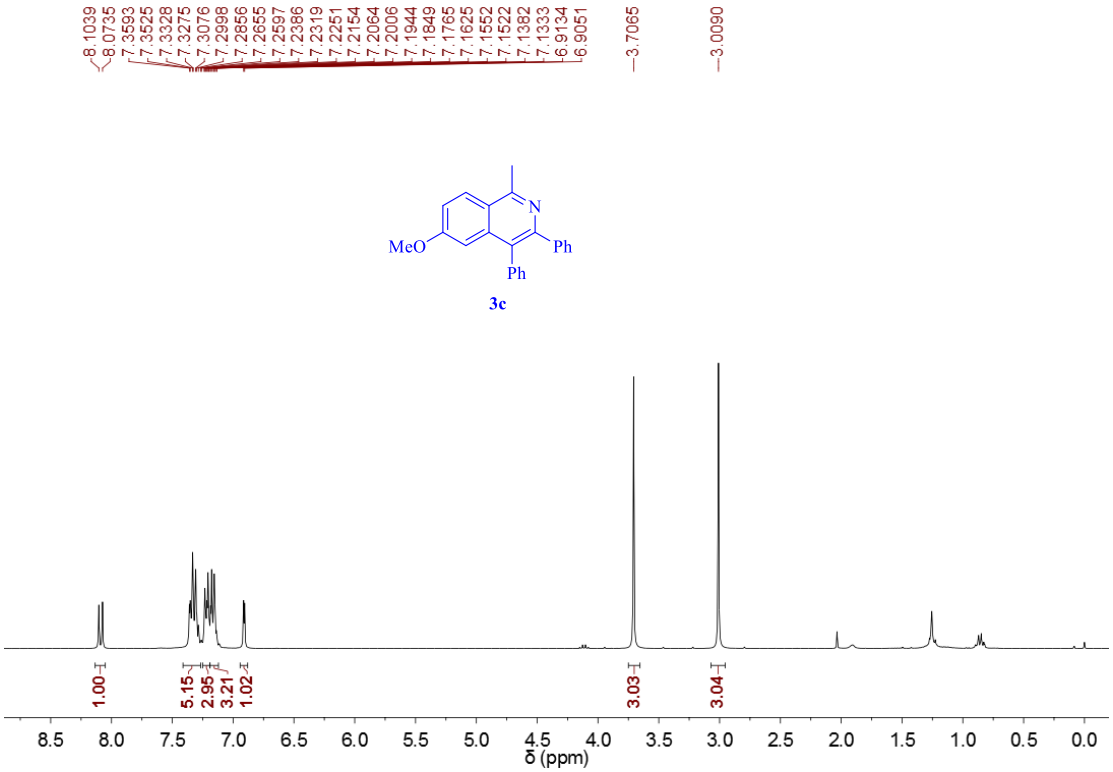
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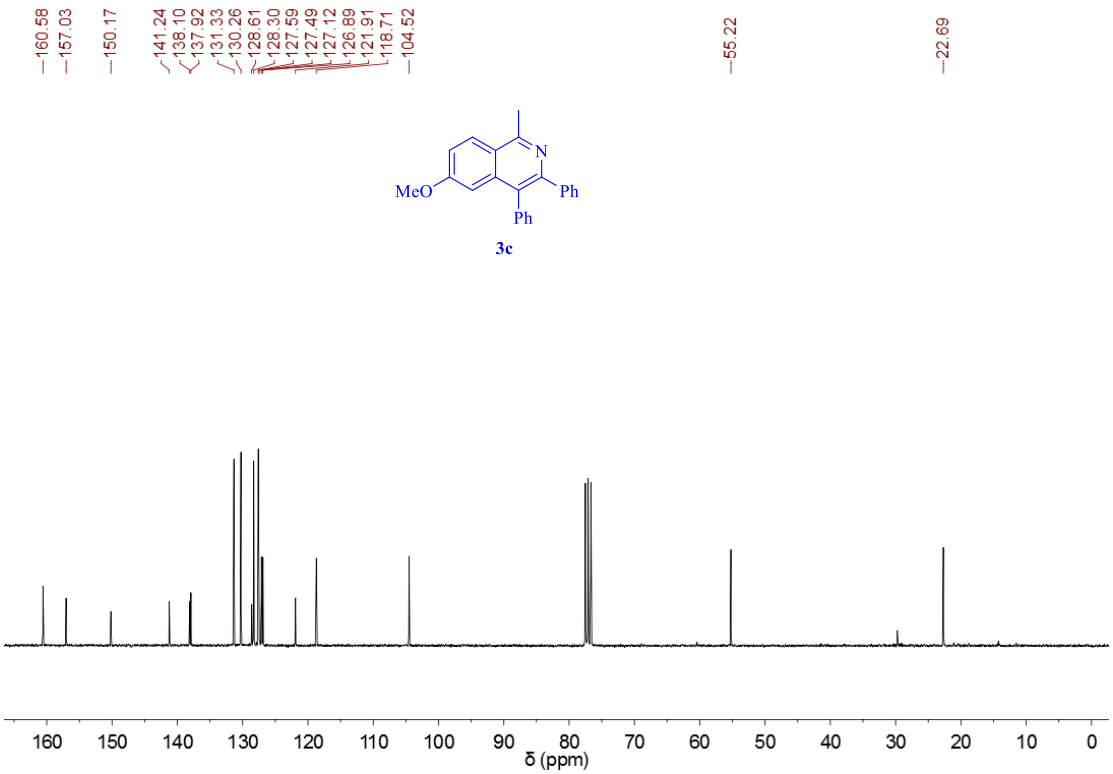
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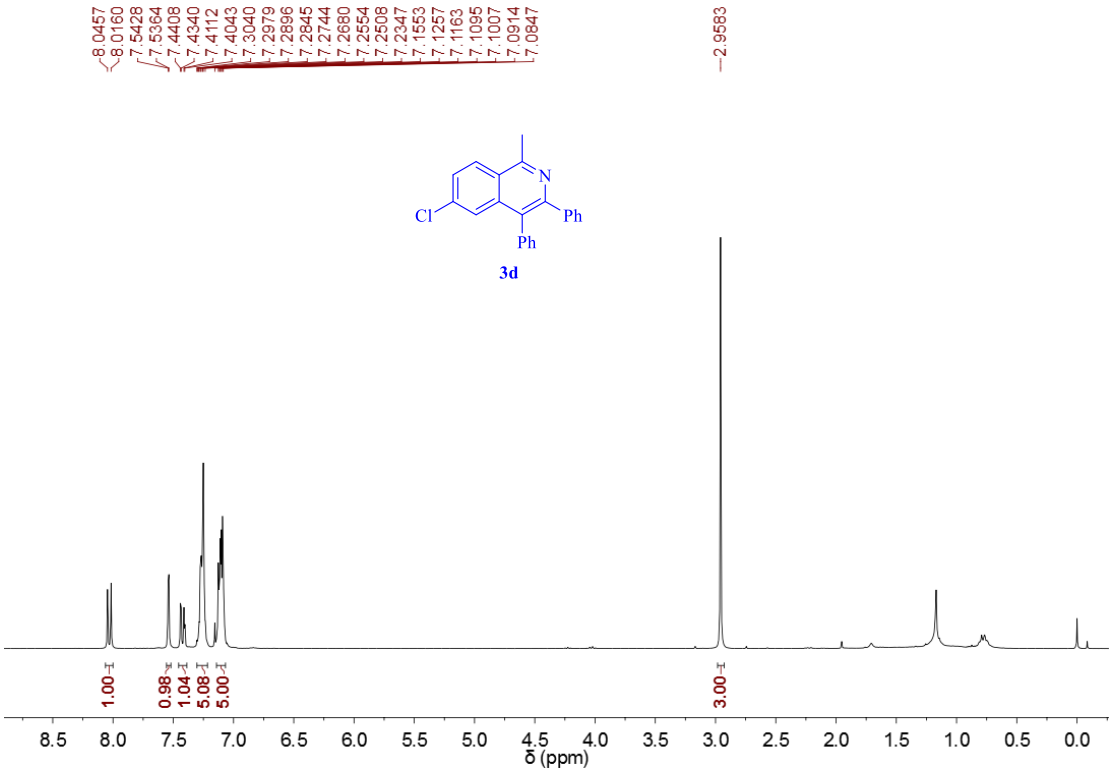
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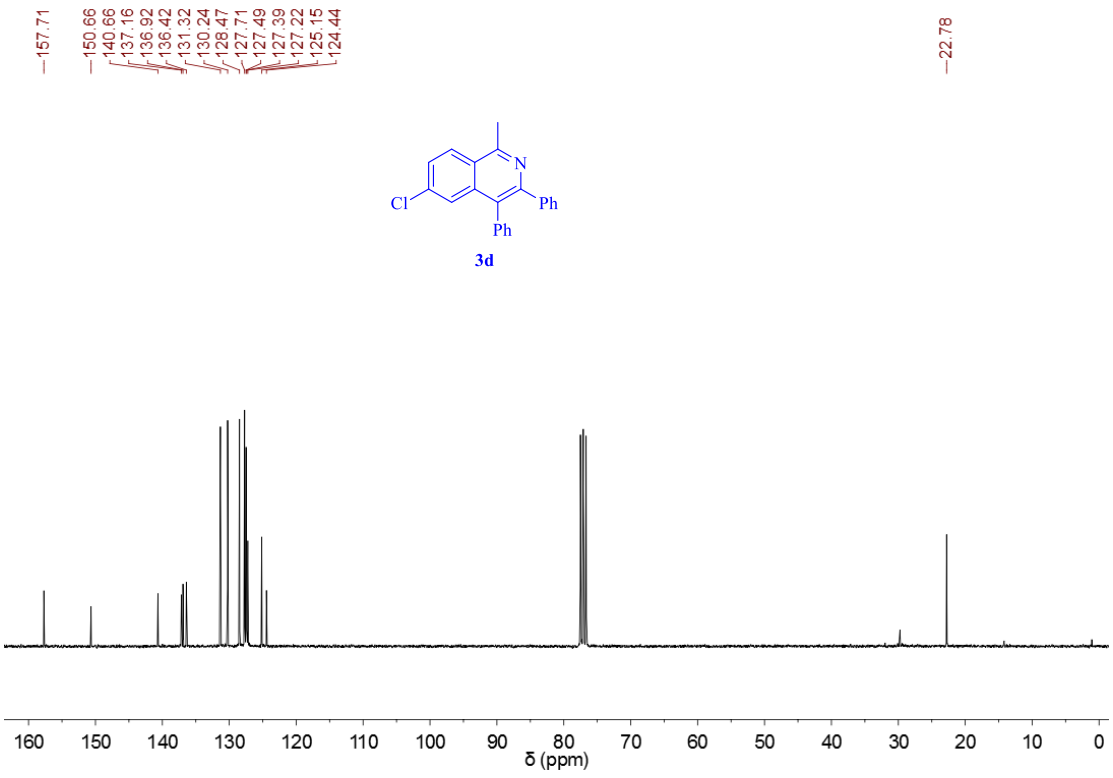
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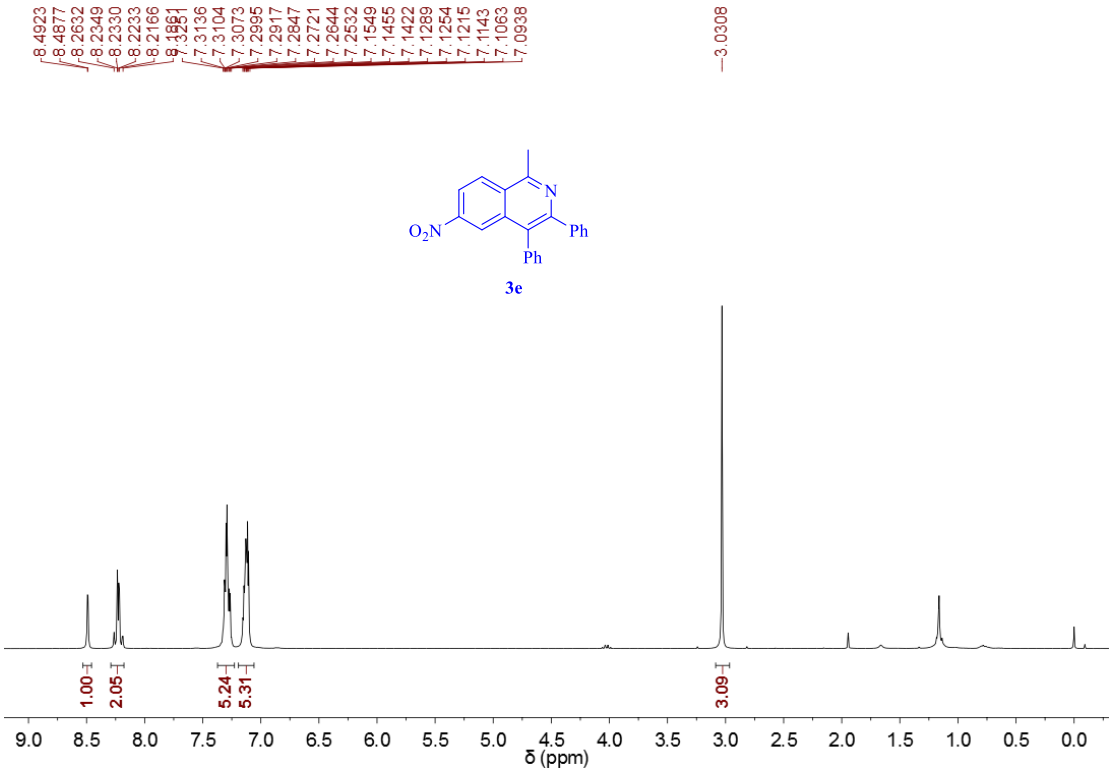
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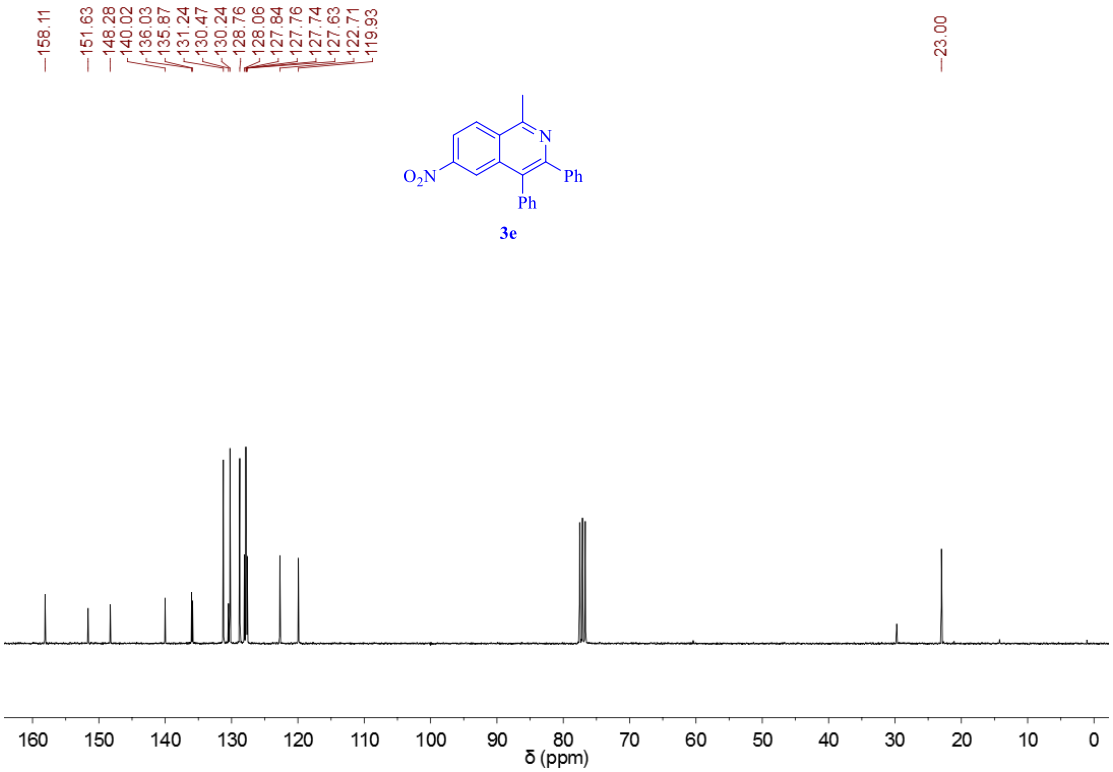
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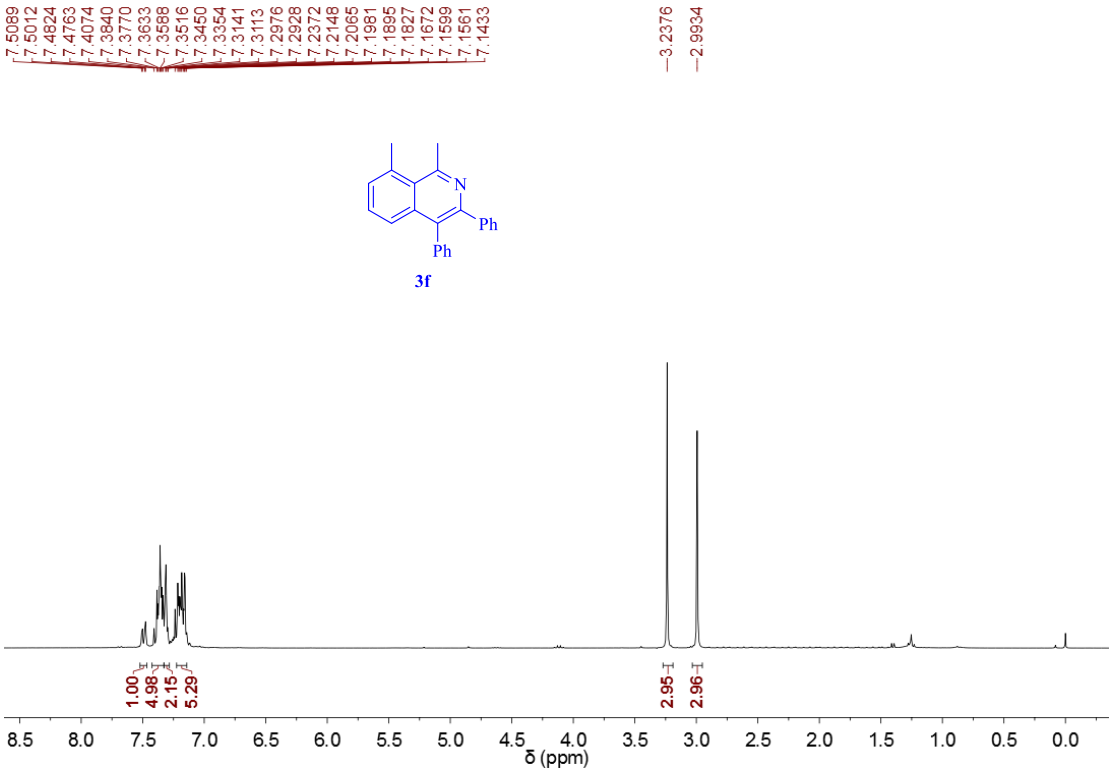
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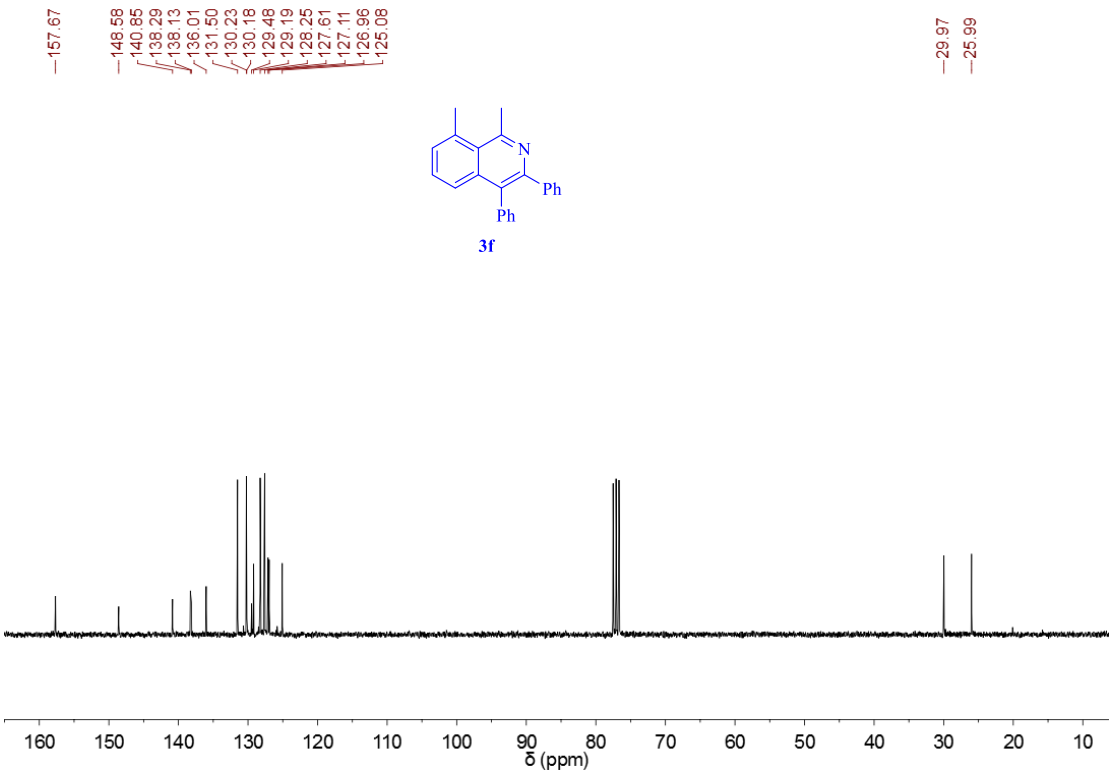
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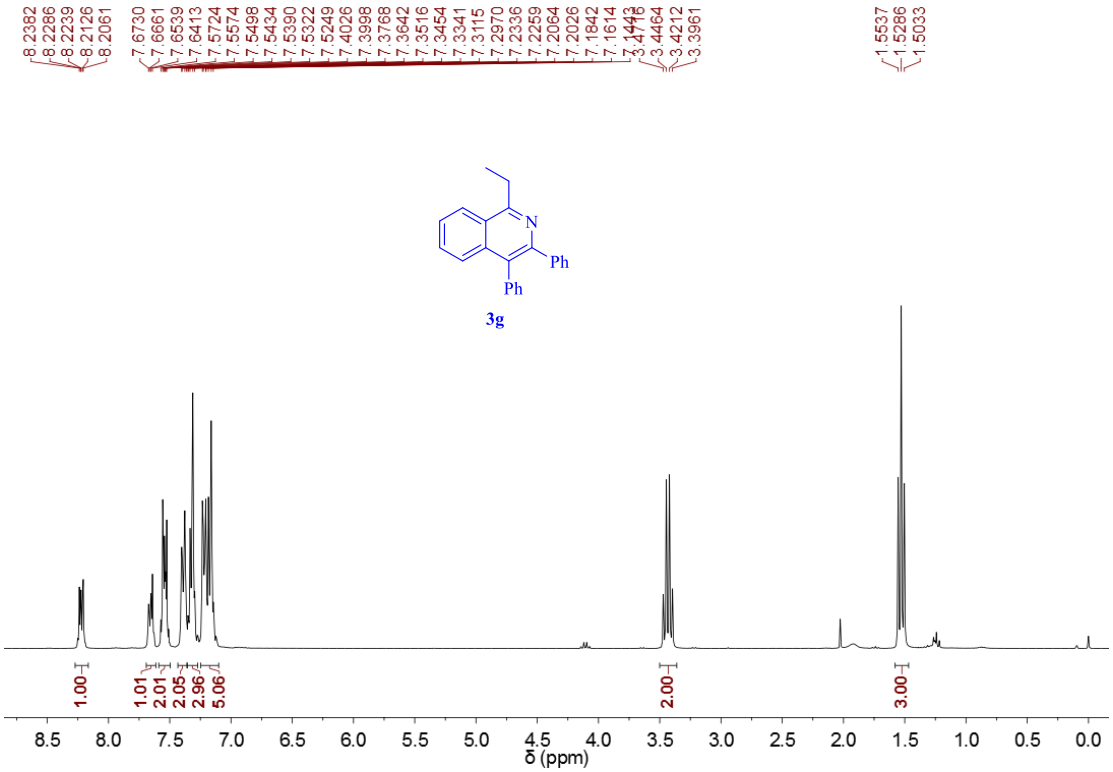
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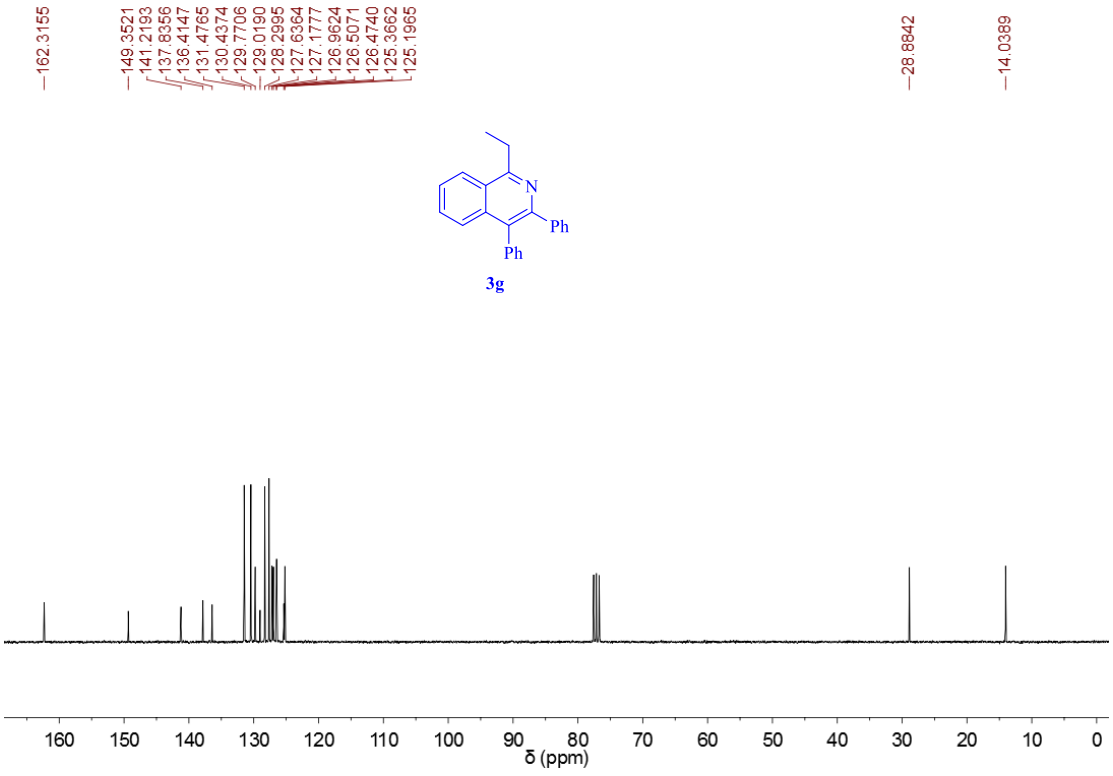
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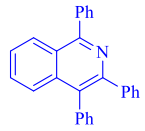
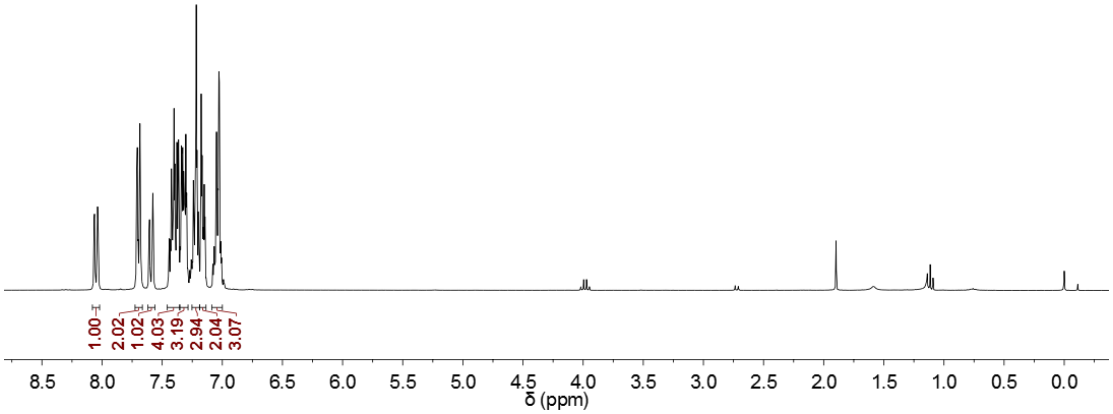
N
Ph
Ph
3g
δ (ppm)

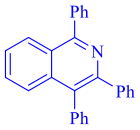

8.0630
8.0374
8.0347
7.7122
7.7067
7.7001
7.6899
7.6850
7.6806
7.6051
7.5781
7.4450
7.4405
7.4309
7.4229
7.4178
7.4119
7.4019
7.3949
7.3887
7.3819
7.3776
7.3641
7.3506
7.3397
7.3346
7.3294
7.3217
7.3165
7.3119
7.3030
7.2975
7.2584
7.2482
7.2406
7.2348
7.2165
7.2104
7.1992
7.1758
7.1680
7.1595
7.1559
7.1503
7.1443
7.0788
7.0666
7.0607
7.0484
7.0357
7.0287
7.0247
7.0122
7.0067


Ph
N
Ph
Ph

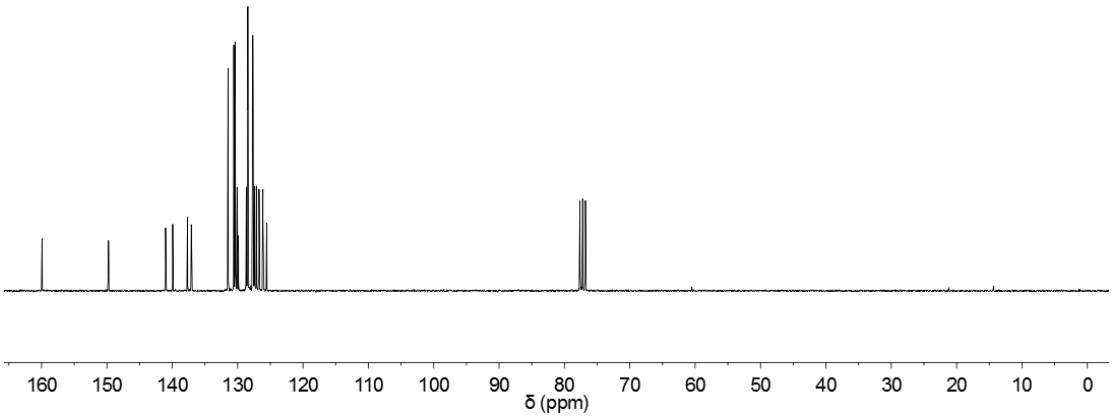
3h

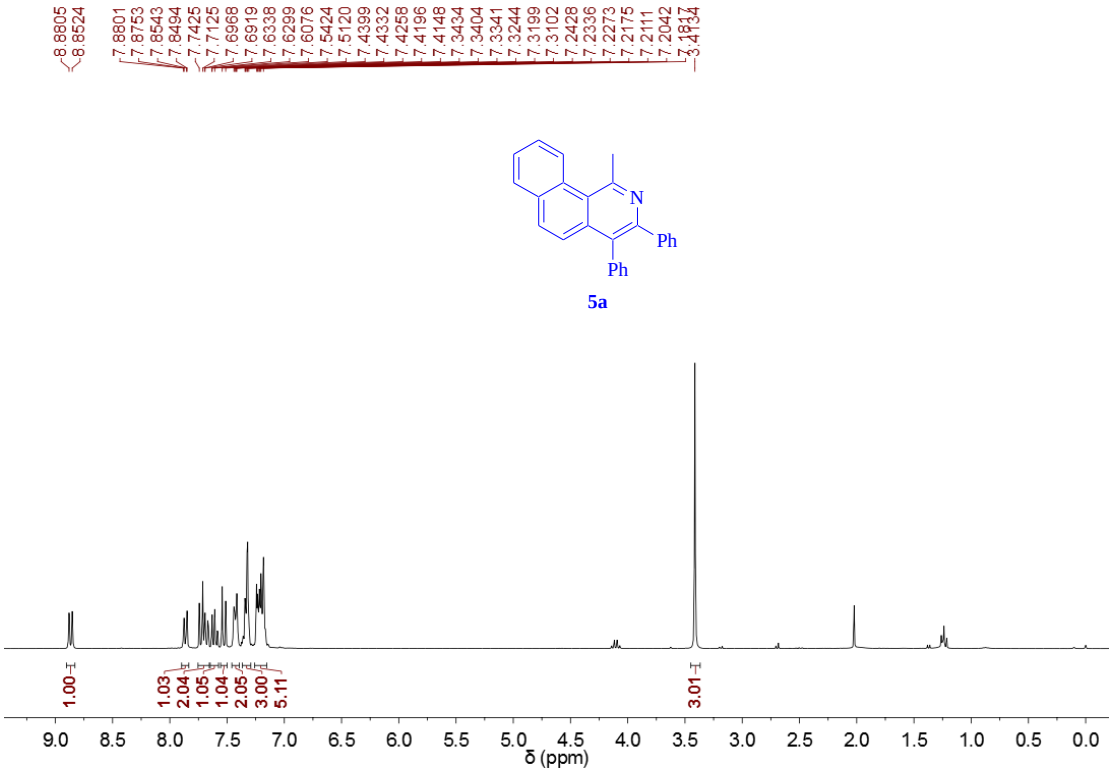

1.00
2.02
1.02
4.03
3.19
2.94
2.04
3.07
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)


159.92
149.76
141.02
139.93
137.67
137.09
131.47
130.58
130.36
130.07
129.88
128.66
128.46
128.44
127.68
127.60
127.42
127.12
126.72
126.14
125.54

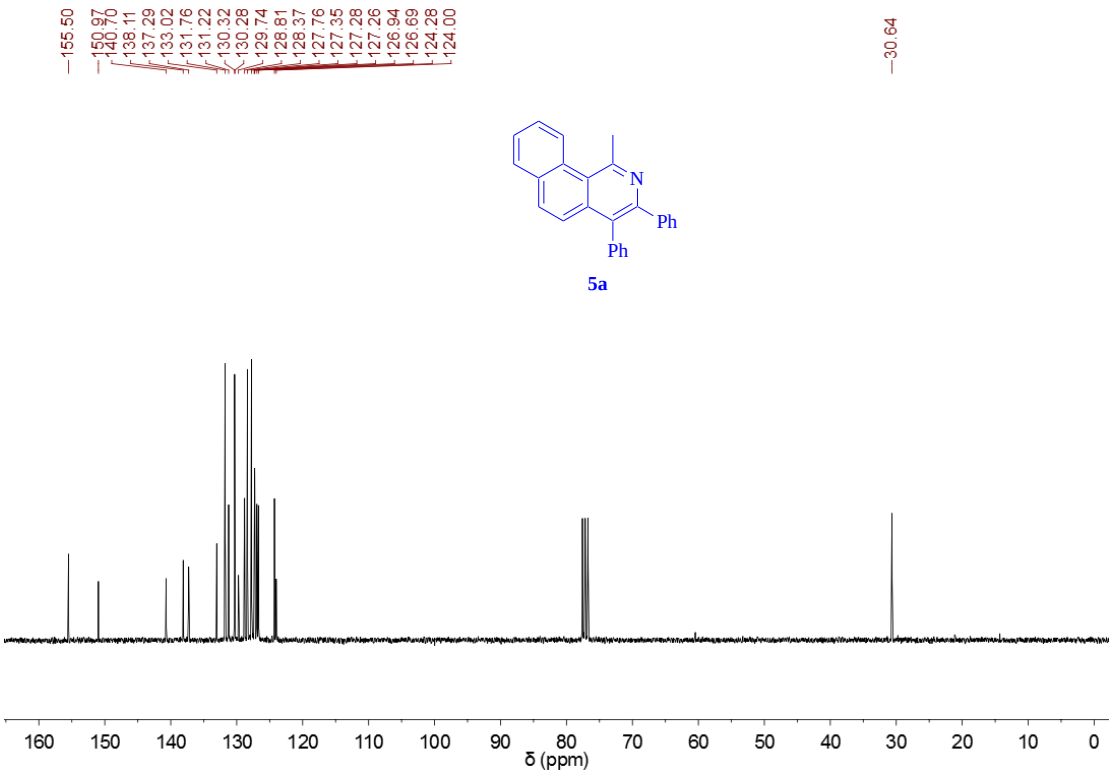

Ph
N
Ph
Ph

3h

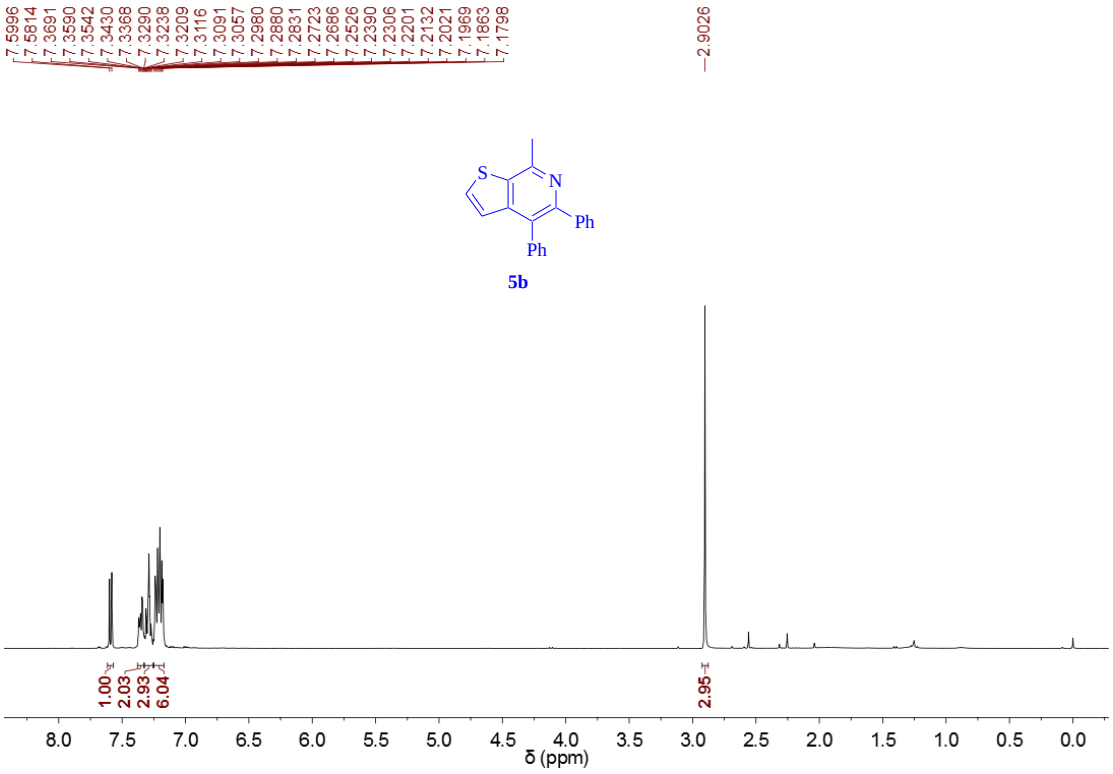

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ (ppm)


8.8805
8.8524
7.8801
7.8753
7.8543
7.8494
7.7425
7.7125
7.6968
7.6919
7.6338
7.6299
7.6076
7.5424
7.5120
7.4399
7.4332
7.4258
7.4196
7.4148
7.3434
7.3404
7.3341
7.3244
7.3199
7.3102
7.2428
7.2336
7.2273
7.2175
7.2111
7.2042
7.1817
3.4134
N
Ph
Ph
1.00
1.03
2.04
1.05
1.04
2.05
3.00
5.11
3.01
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
δ (ppm)

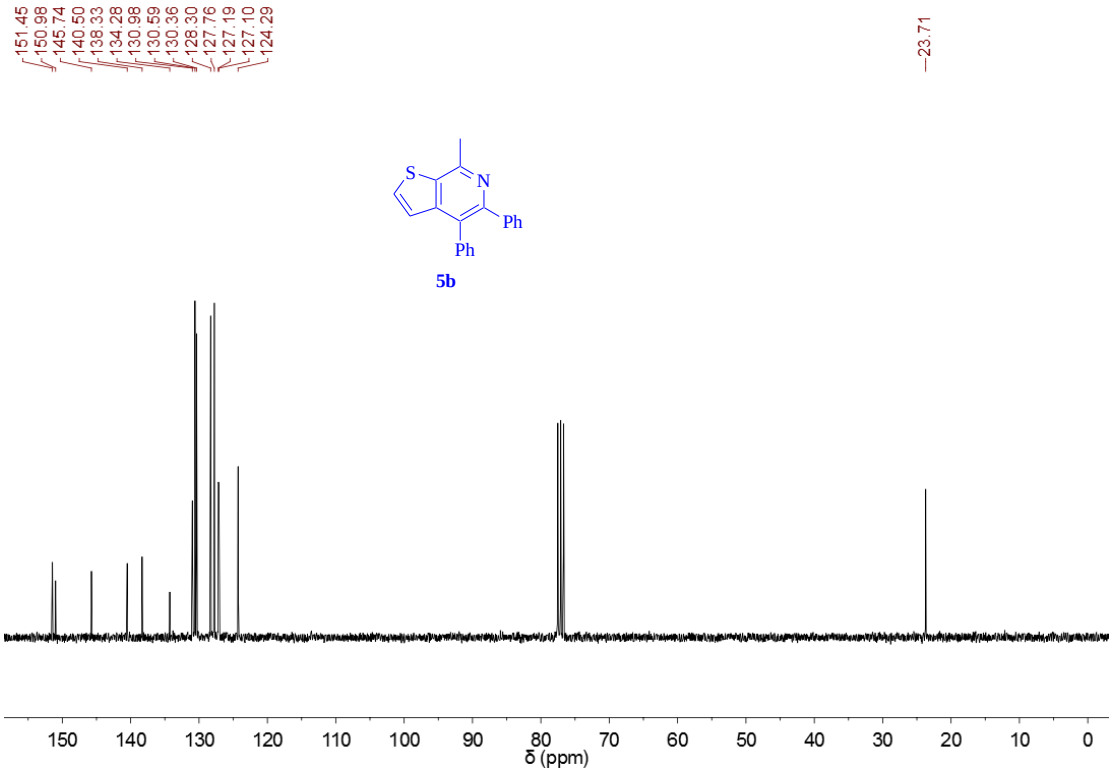
5a


155.50
150.97
140.70
138.11
137.29
133.02
131.76
131.22
130.32
130.28
129.74
128.81
128.37
127.76
127.35
127.28
127.26
126.94
126.69
124.28
124.00
30.64
N
Ph
Ph
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)

5a

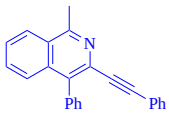

7.5996
7.5814
7.3691
7.3590
7.3542
7.3430
7.3368
7.3290
7.3238
7.3209
7.3116
7.3091
7.3057
7.2980
7.2880
7.2831
7.2723
7.2686
7.2526
7.2390
7.2306
7.2201
7.2132
7.2021
7.1969
7.1863
7.1798
2.9026
S
N
Ph
Ph
1.00
2.03
2.93
6.04
2.95
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)

5b

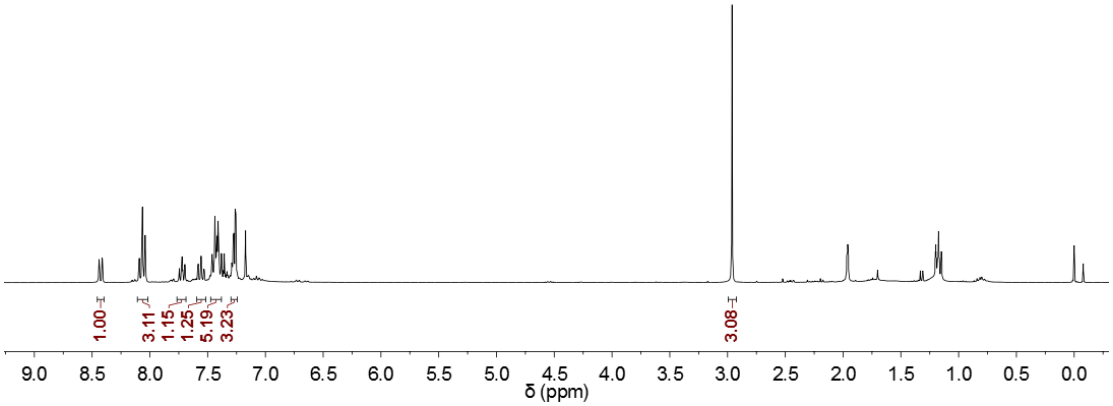

151.45
150.98
145.74
140.50
138.33
134.28
130.98
130.59
130.36
128.30
127.76
127.19
127.10
124.29
23.71
S
N
Ph
Ph
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ (ppm)

5b

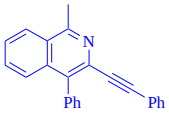

8.4394
8.4128
8.0917
8.0894
8.0688
8.0641
8.0575
8.0462
8.0411
8.0370
7.7253
7.7209
7.7163
7.6974
7.6933
7.5842
7.5801
7.5612
7.5567
7.5523
7.4658
7.4612
7.4559
7.4376
7.4346
7.4273
7.4231
7.4192
7.4128
7.4094
7.4021
7.3853
7.3804
7.3757
7.2782
7.2724
7.2621
7.2552
2.9611


N
Ph
Ph

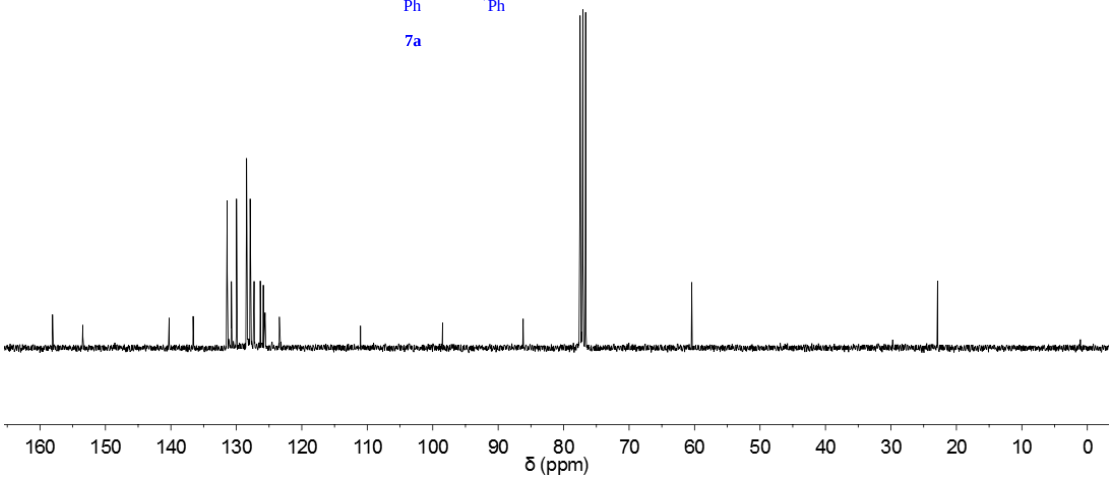
7a

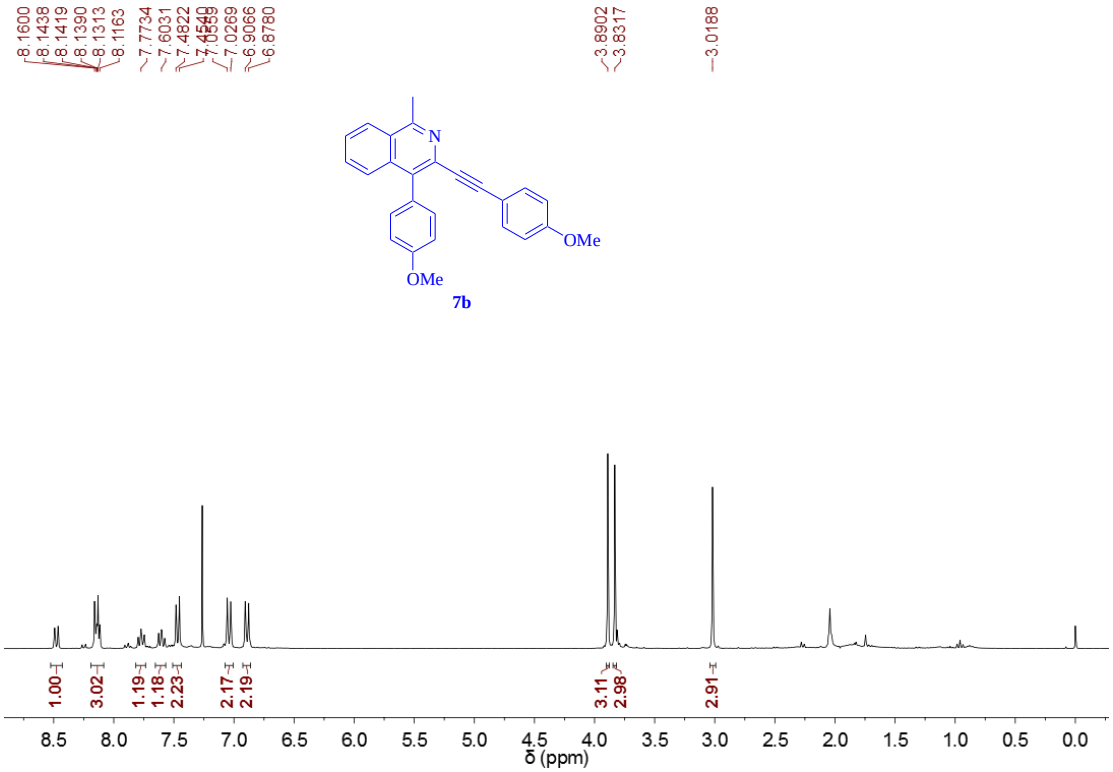

1.00
3.11
1.15
1.25
5.19
3.23
3.08
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)

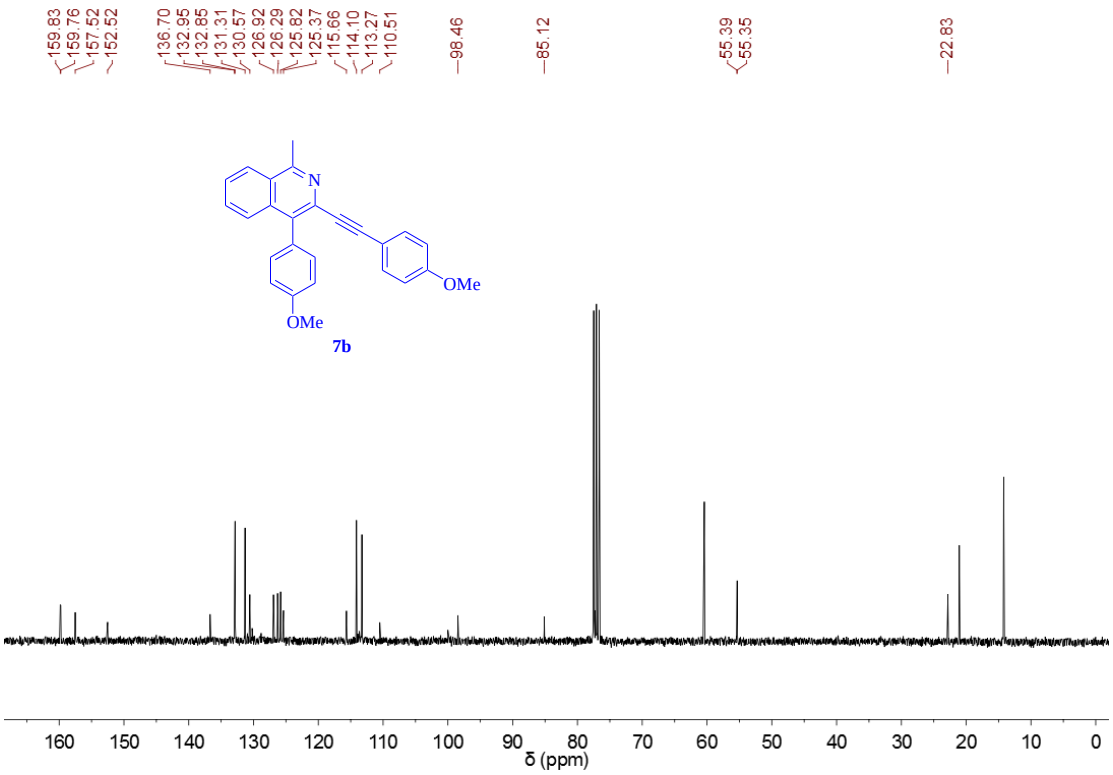

158.08
153.45
140.26
136.60
131.40
130.76
129.97
128.44
128.41
127.89
127.29
126.34
125.88
125.61
123.43
111.03
98.49
86.18
22.66


N
Ph
Ph

7a


160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)


8.1600
8.1438
8.1419
8.1390
8.1313
8.1163
7.7734
7.6031
7.4822
7.0269
6.9066
6.8780
3.8902
3.8317
3.0188
N
OMe
OMe
7b
1.00
3.02
1.19
1.18
2.23
2.17
2.19
3.11
2.98
2.91
δ (ppm)


159.83
159.76
157.52
152.52
136.70
132.95
132.85
131.31
130.57
126.92
126.29
125.82
125.37
115.66
114.10
113.27
110.51
98.46
85.12
55.39
55.35
22.83
N
OMe
OMe
7b
δ (ppm)