

# Supporting Information

## Efficient Approach To Construct Unsymmetrical Biaryls through Oxidative Coupling Reactions of Aromatic Primary Alcohols and Arylboronic Acids with a Rhodium Catalyst

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### Table of Contents

General Information	S4
IR spectra for the reaction mixture	S5
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of Materials	S6-S15
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>1aa</b>	S6
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>1ba</b>	S7
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>1bb</b>	S8
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>1bc</b>	S9
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>1bd</b>	S10
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>1be</b>	S11
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>1bf</b>	S12
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>1c</b>	S13
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>1d</b>	S14
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>1aa'</b>	S15

Experimental Procedure for Products	S16
<sup>1</sup> H NMR, <sup>13</sup> C NMR and <sup>19</sup> F NMR Spectra of Product	S17-S48
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3aa</b>	S17
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3ab</b>	S18
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3ac</b>	S19
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3ad</b>	S20
<sup>19</sup> F NMR Spectra of <b>3ad</b>	S21
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3ae</b>	S22
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3af</b>	S23
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3ag</b>	S24
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3ah</b>	S25
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3ai</b>	S26
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3aj</b>	S27
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3ak</b>	S28
<sup>19</sup> F NMR Spectra of <b>3ak</b>	S29
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3al</b>	S30
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3am</b>	S31
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3an</b>	S32
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3ao</b>	S33
<sup>19</sup> F NMR Spectra of <b>3ao</b>	S34
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3ap</b>	S35
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3aq</b>	S36
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3ar</b>	S37
<sup>19</sup> F NMR Spectra of <b>3ar</b>	S38
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3as</b>	S39
<sup>19</sup> F NMR Spectra of <b>3as</b>	S40
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3at</b>	S41
<sup>19</sup> F NMR Spectra of <b>3at</b>	S42
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3ba</b>	S43
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra of <b>3bb</b>	S44

$^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of <b>3bc</b>	S45
$^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of <b>3bd</b>	S46
$^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of <b>3be</b>	S47
$^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of <b>3bf</b>	S48

**General Information.** The starting materials were synthesized and purified according to the literature procedures.<sup>1-4</sup> Other chemicals and reagents were obtained from commercial sources. All reactions were monitored by analytical thin layer chromatography on 0.20 mm Yantai Huagong silica gel plates and spots were detected by UV-absorption. Silica gel (200-300 mesh) (from Yantai Huagong Chem. Company, Ltd.) was used for flash chromatography.

NMR spectra were obtained on 400 MHz spectrometer with CDCl<sub>3</sub> as solvent. The chemical shifts are reported in ppm relative to CDCl<sub>3</sub> ( $\delta$  = 7.26) for <sup>1</sup>H NMR and relative to the central CDCl<sub>3</sub> resonance ( $\delta$  = 77.0) for <sup>13</sup>C NMR. For <sup>19</sup>F NMR, the (trifluoromethyl)benzene was used as an external standard. Coupling constants (J) are quoted in Hz for <sup>1</sup>H. Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), quartet (q), and multiplet (m). Conversions were obtained by <sup>1</sup>H NMR analysis of the sample. NMR data of known compounds is in agreement with literature values. Infrared spectra were recorded on FT-IR spectrophotometer. Elemental analyses were performed by the Elemental Analysis Section of Tianjin University.

## IR spectra for the reaction mixture

To an oven-dried screwed vial were added benzo[h]quinoline-10-ylmethanol (0.3 mmol), Rh(PPh<sub>3</sub>)<sub>3</sub>Cl (19.5 mg) and xylene 3 mL under air atmosphere. The mixture was vigorously stirred at 130 °C for 5 h. Organic solvents were removed in vacuo, and then the residue was detected by IR (Figure S1) and an absorption peak of Rh-CO was found at 1976 cm<sup>-1</sup>.<sup>5</sup>

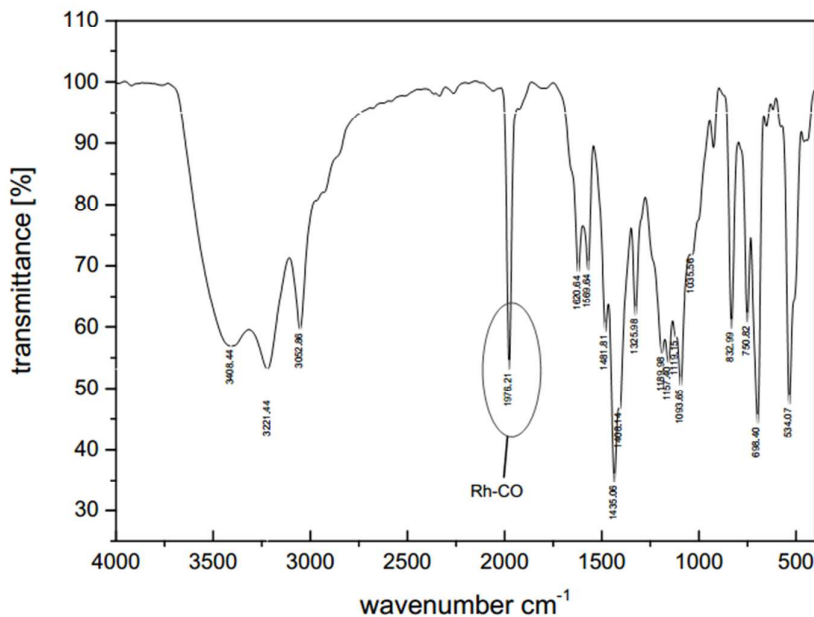


Figure S1. IR for the reaction mixture

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- [2] Kochi, T.; Urano, S.; Seki, H.; Mizushima, E.; Sato, M.; Kakiuchi, F. *J. Am. Chem. Soc.* **2009**, 131, 2792–2793.
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- [5] Ginsberg, A. P.; Edward Lindsell, W.; McCullough, K. J.; Sprinkle, C. R.; Welch, A. J. *J. Am. Chem. Soc.* **1986**, 108, 403–416.

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 1aa

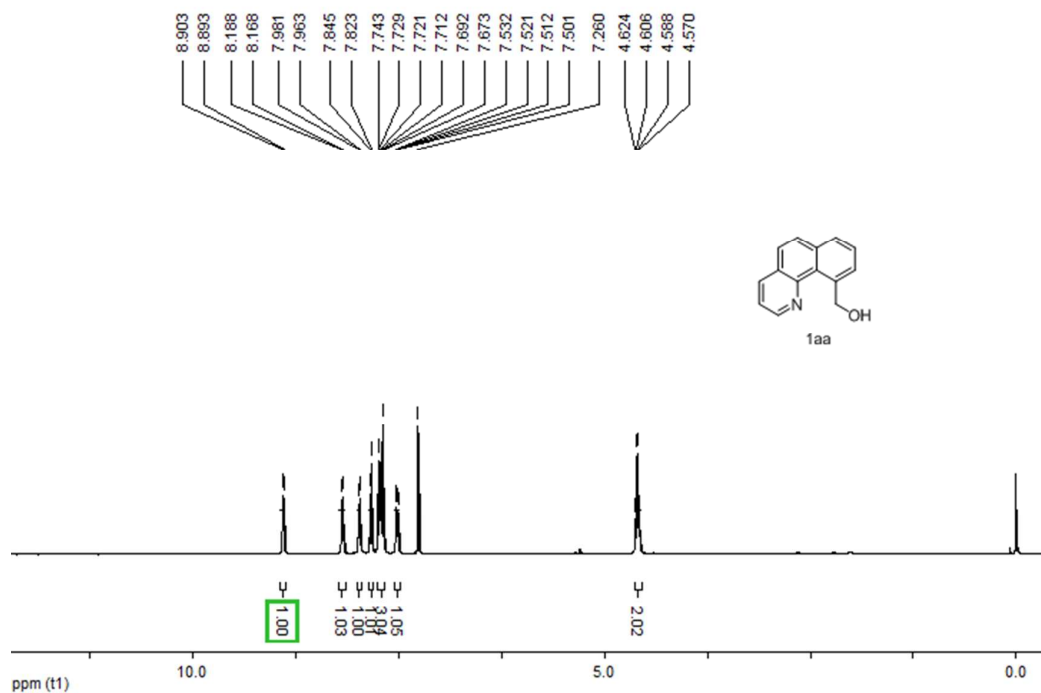


Figure S2. <sup>1</sup>H NMR for compound 1aa

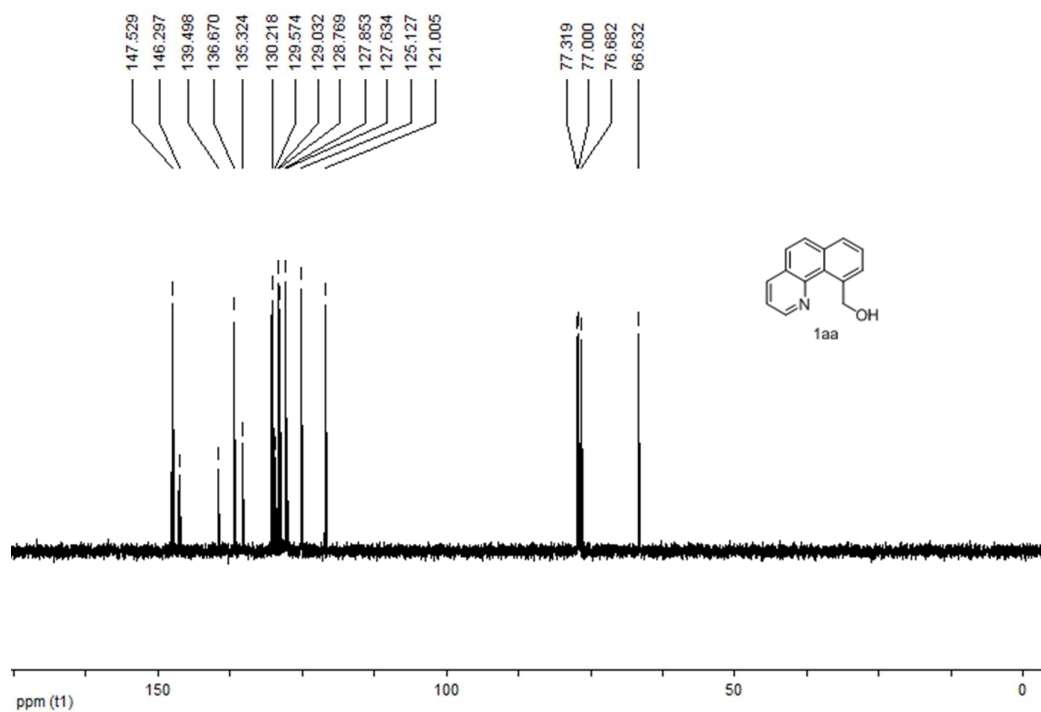
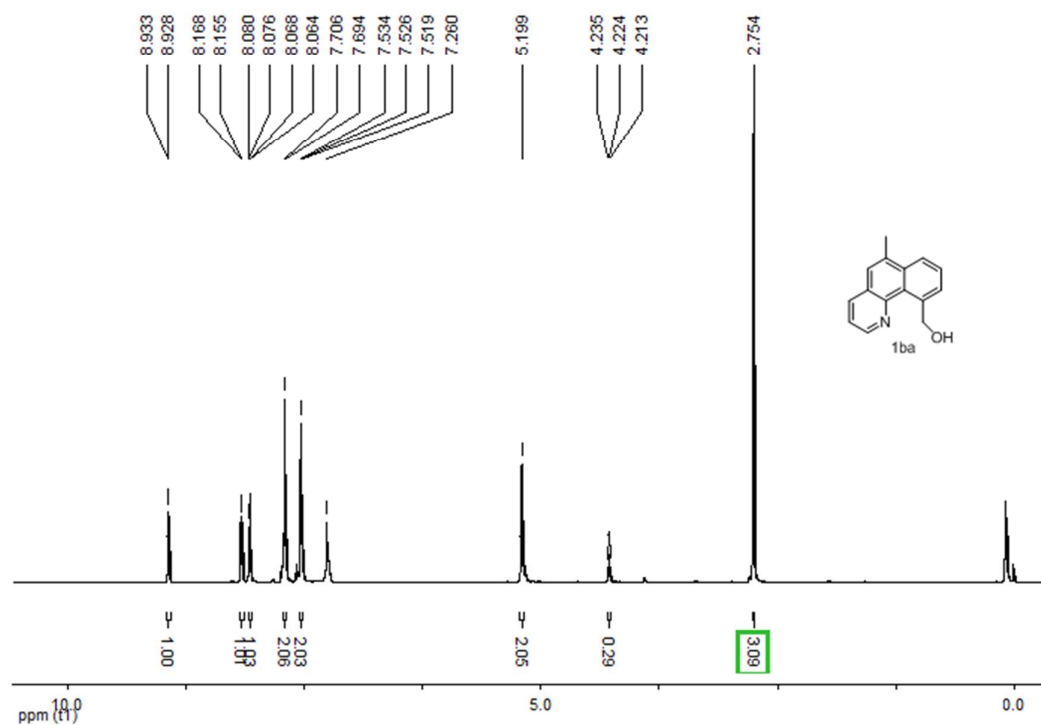
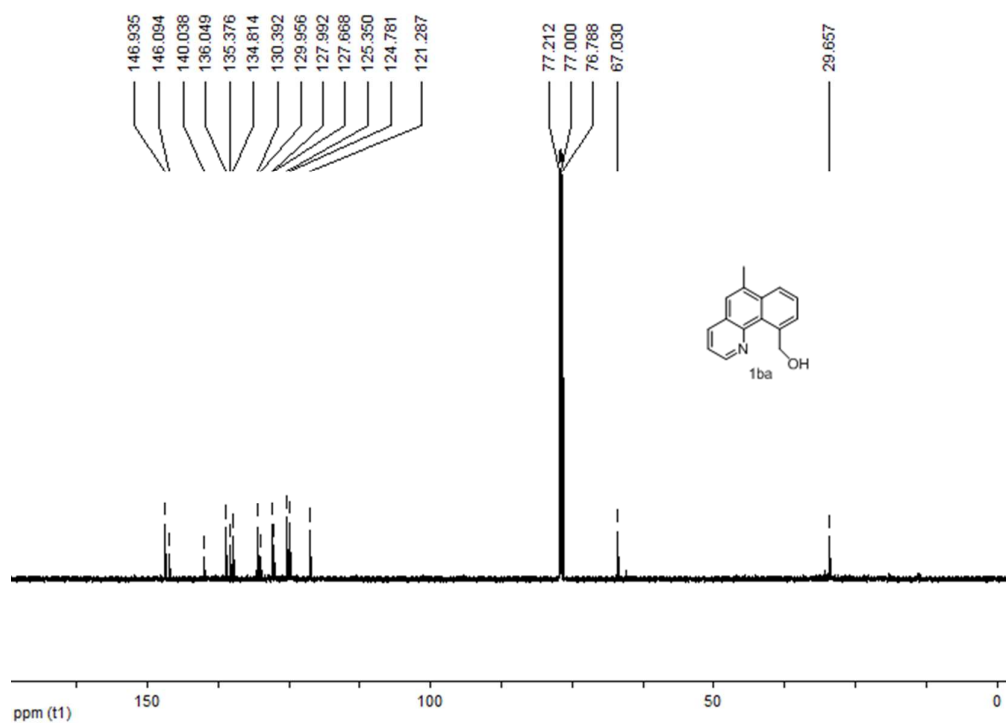


Figure S3. <sup>13</sup>C NMR for compound 1aa

# **$^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of 1ba**



**Figure S4.  $^1\text{H}$  NMR for compound 1ba**



**Figure S5.  $^{13}\text{C}$  NMR for compound 1ba**

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 1bb

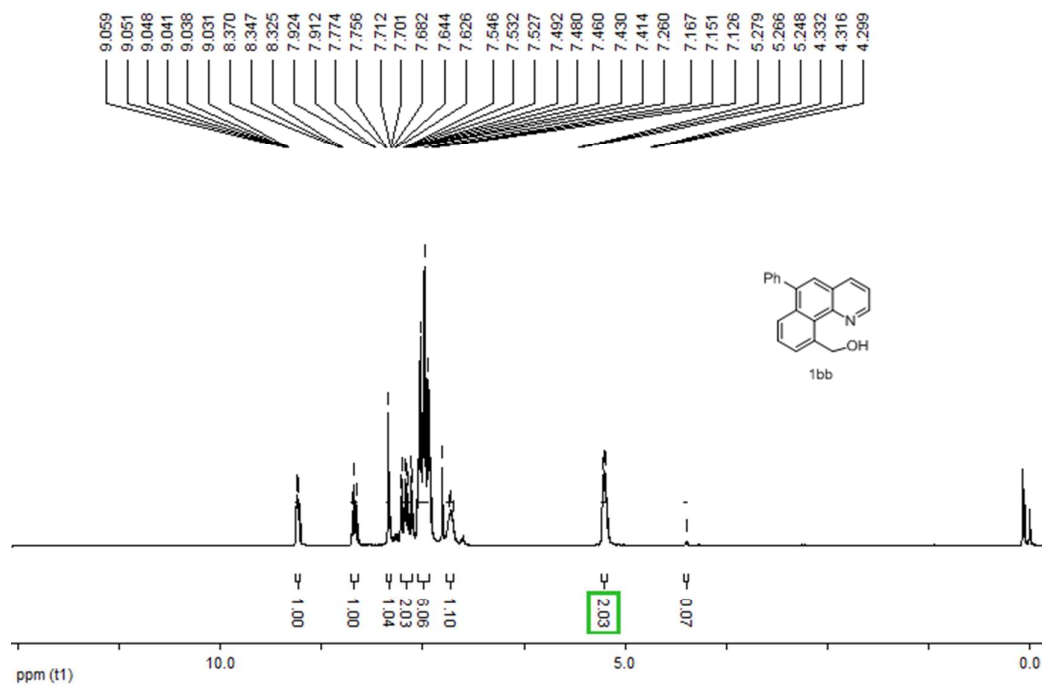


Figure S6. <sup>1</sup>H NMR for compound 1bb

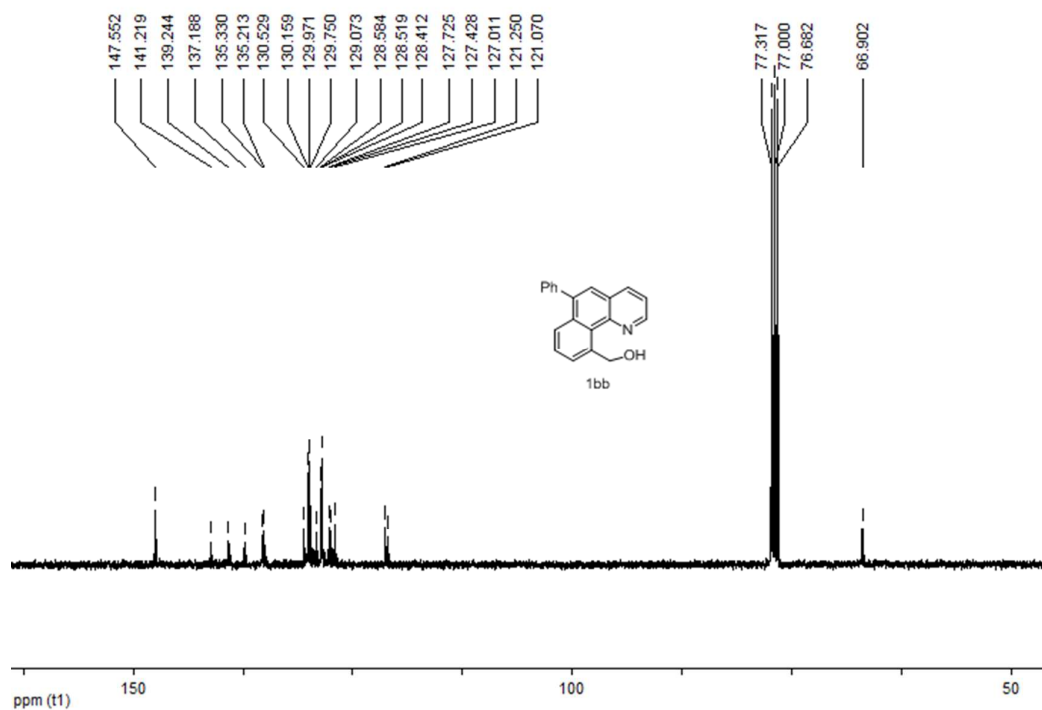


Figure S7. <sup>13</sup>C NMR for compound 1bb



## $^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of 1bc

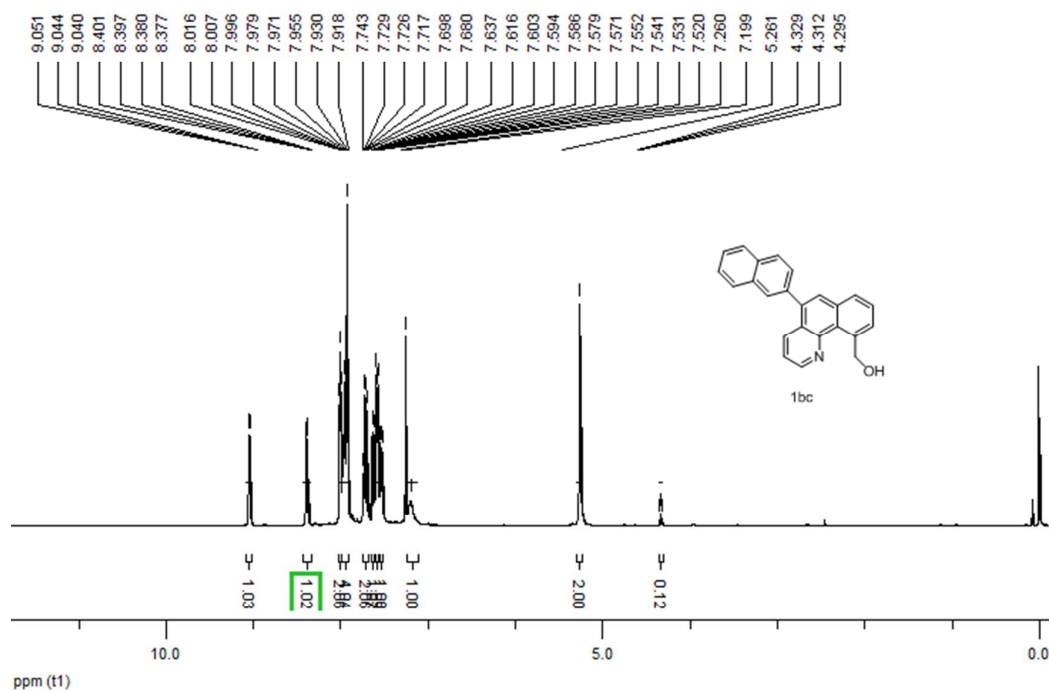


Figure S8.  $^1\text{H}$  NMR for compound 1bc

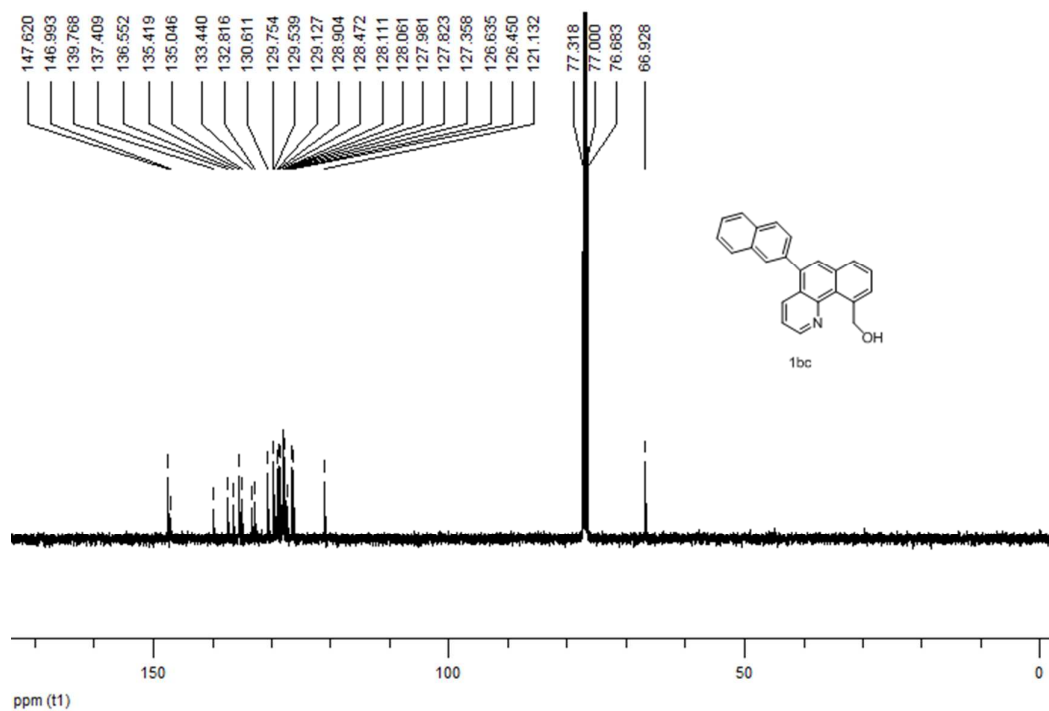


Figure S9.  $^{13}\text{C}$  NMR for compound 1bc

Chemical structure of 1bd: COc1ccc2c(c1)cnc3ccccc23

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) of compound 1bd. The x-axis represents chemical shift in ppm (t1), ranging from 0.0 to 10.0. The spectrum shows several peaks, with integration values indicated below the baseline. A peak at approximately 4.3 ppm is highlighted with a green box, showing an integration of 1.00.

Chemical Shift (ppm)	Integration
~8.9	1.00
~8.3	1.00
~7.7	1.00
~7.6	1.07
~5.0	1.99
~4.3 (highlighted)	1.00
~4.0	0.03
~3.9	3.05

Chemical structure of **1bd** (2-(hydroxymethyl)-6-methoxy-1,2,3,4-tetrahydroquinoline) is shown as an inset.

<sup>13</sup>C NMR spectrum (CDCl<sub>3</sub>) peaks (ppm):

Peak (ppm)
155.335
147.695
146.436
136.804
131.774
130.807
130.686
128.020
126.517
124.491
122.464
121.317
106.968
77.318
77.000
76.683
66.608
55.793

S10

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 1be

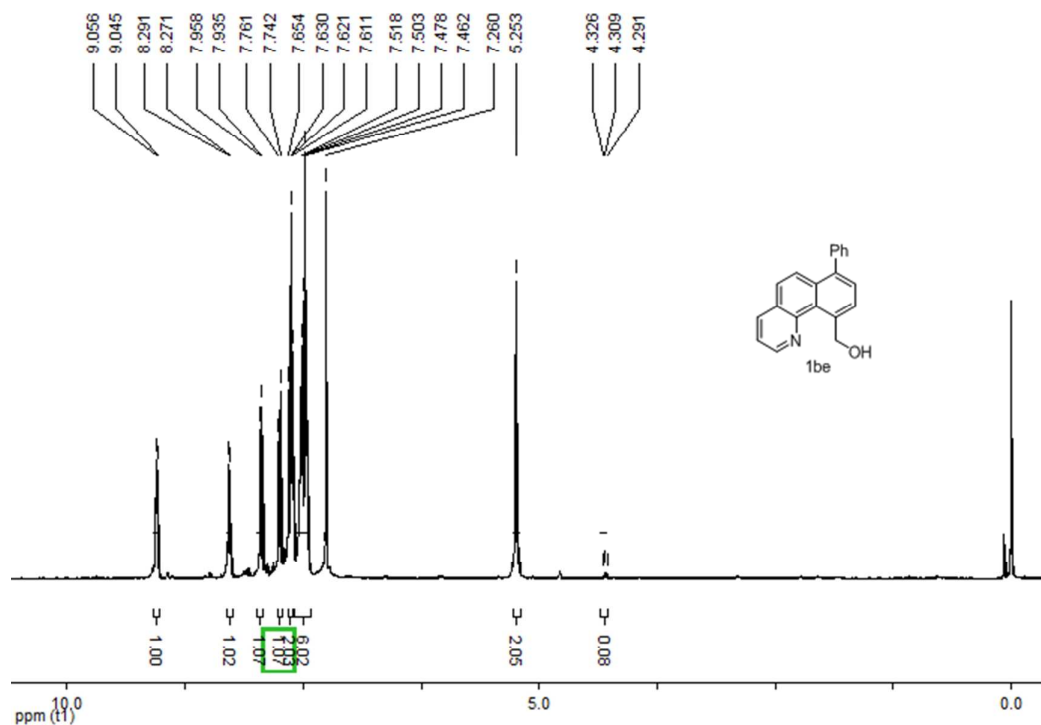


Figure S12. <sup>1</sup>H NMR for compound 1be

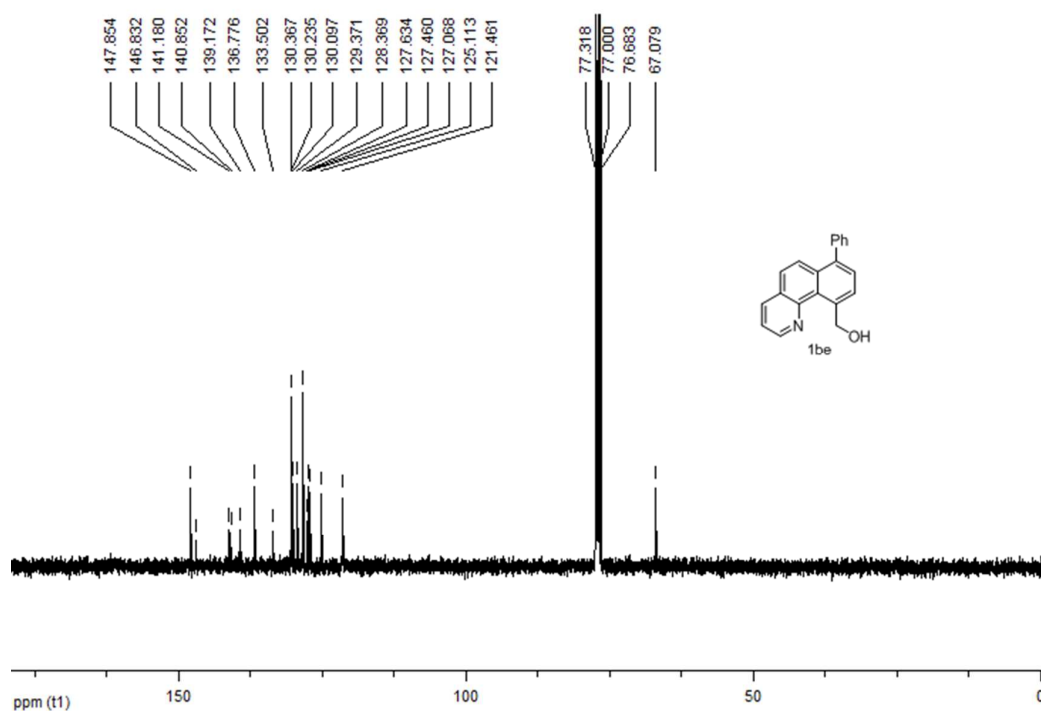


Figure S13. <sup>13</sup>C NMR for compound 1be

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 1bf

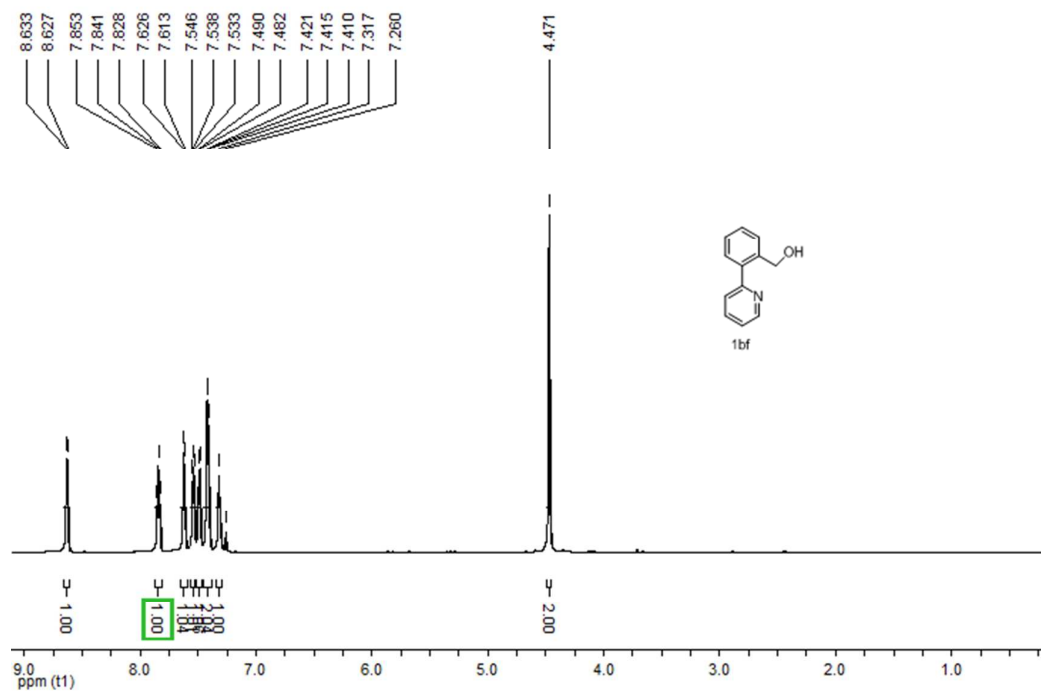


Figure S14. <sup>1</sup>H NMR for compound 1bf

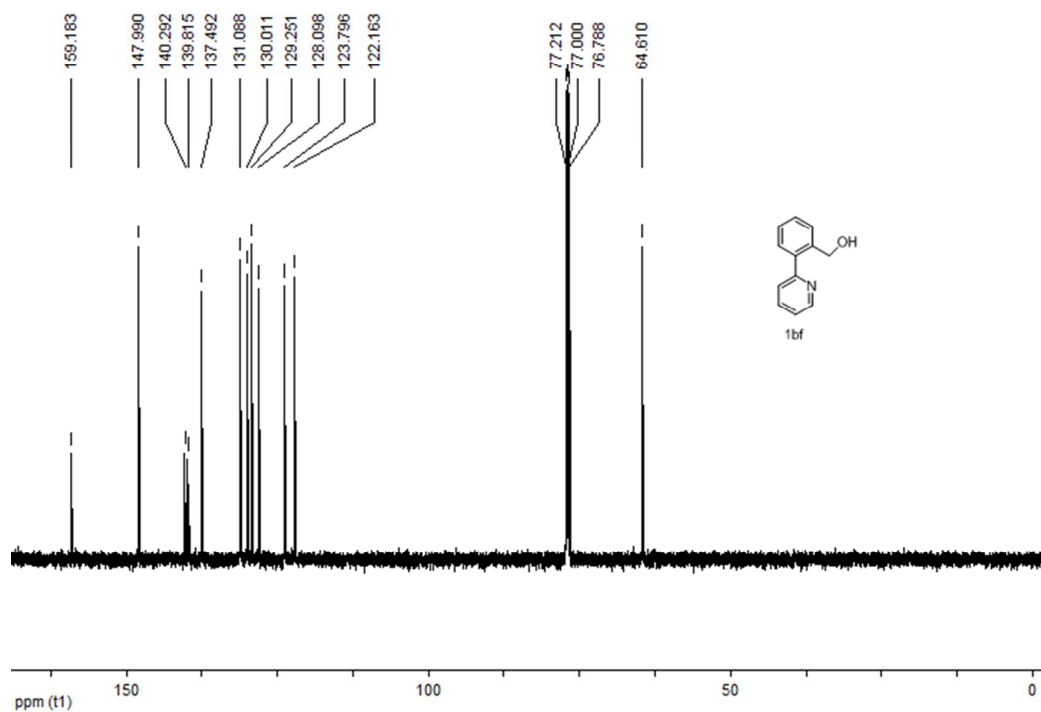


Figure S15. <sup>13</sup>C NMR for compound 1bf

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 1c

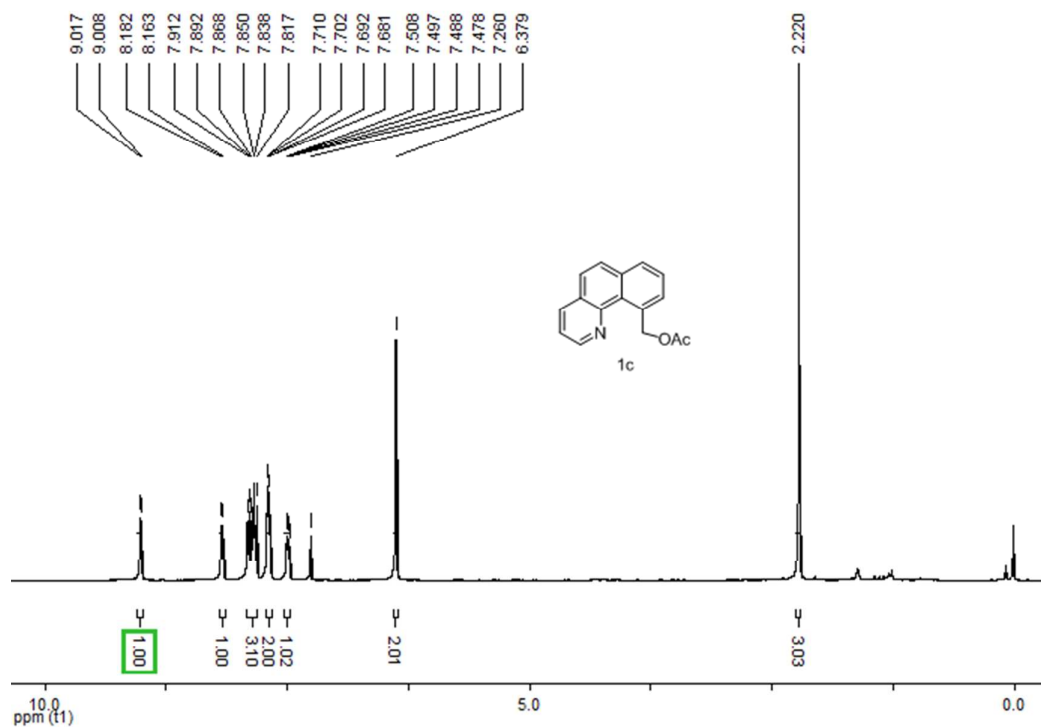


Figure S16. <sup>1</sup>H NMR for compound 1c

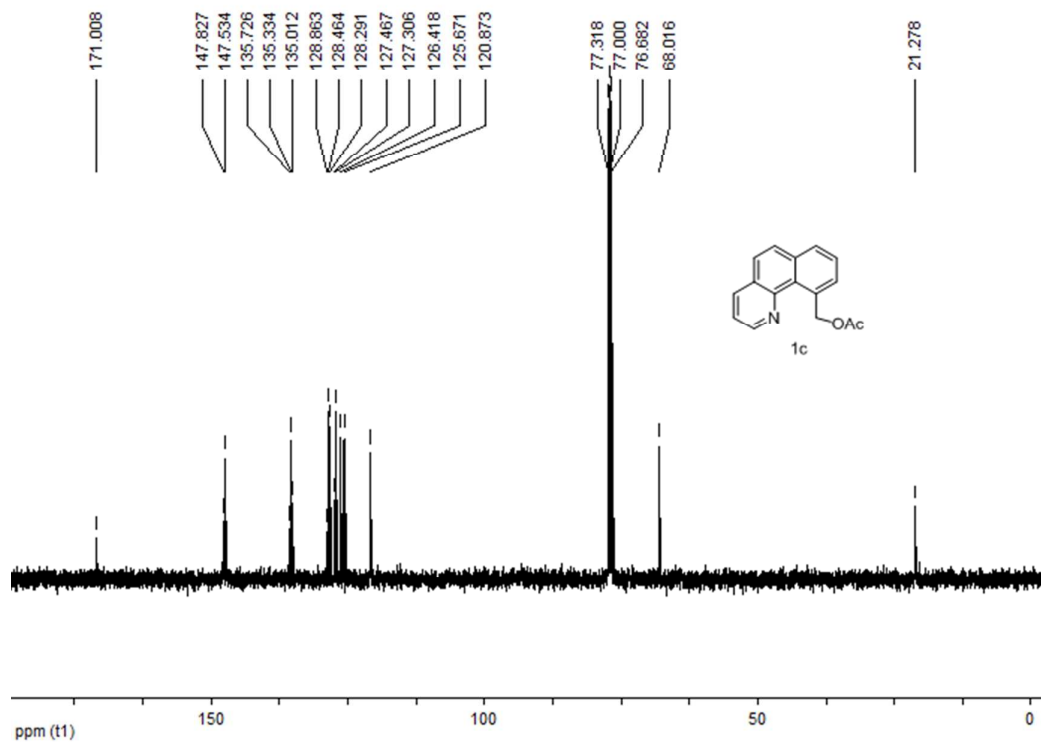


Figure S17. <sup>13</sup>C NMR for compound 1c

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 1d

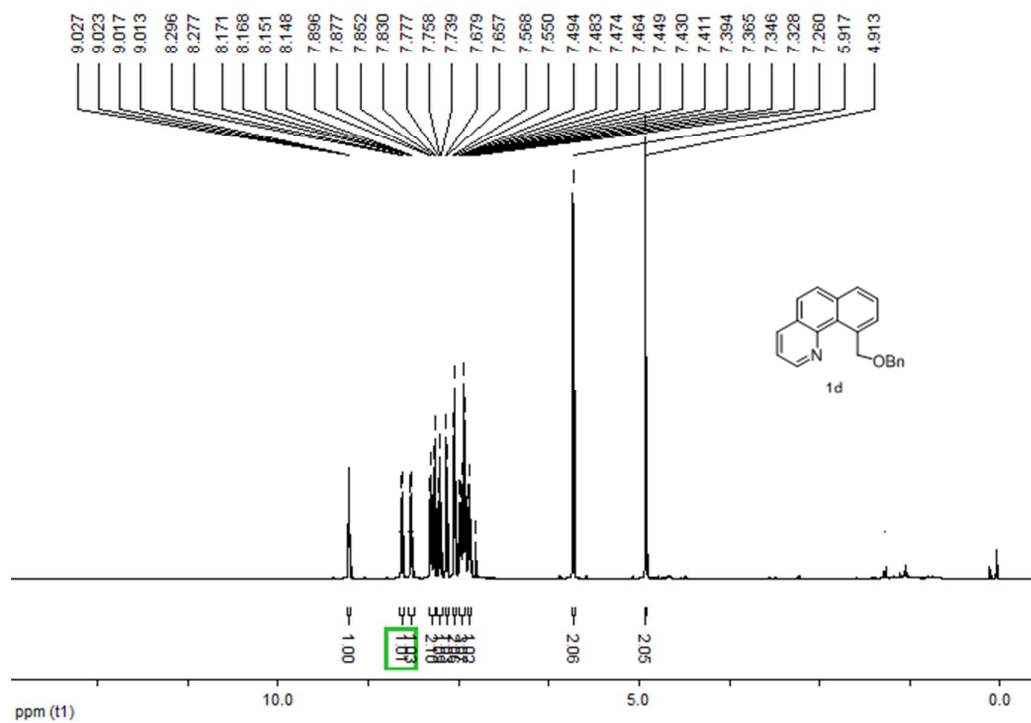


Figure S18. <sup>1</sup>H NMR for compound 1d

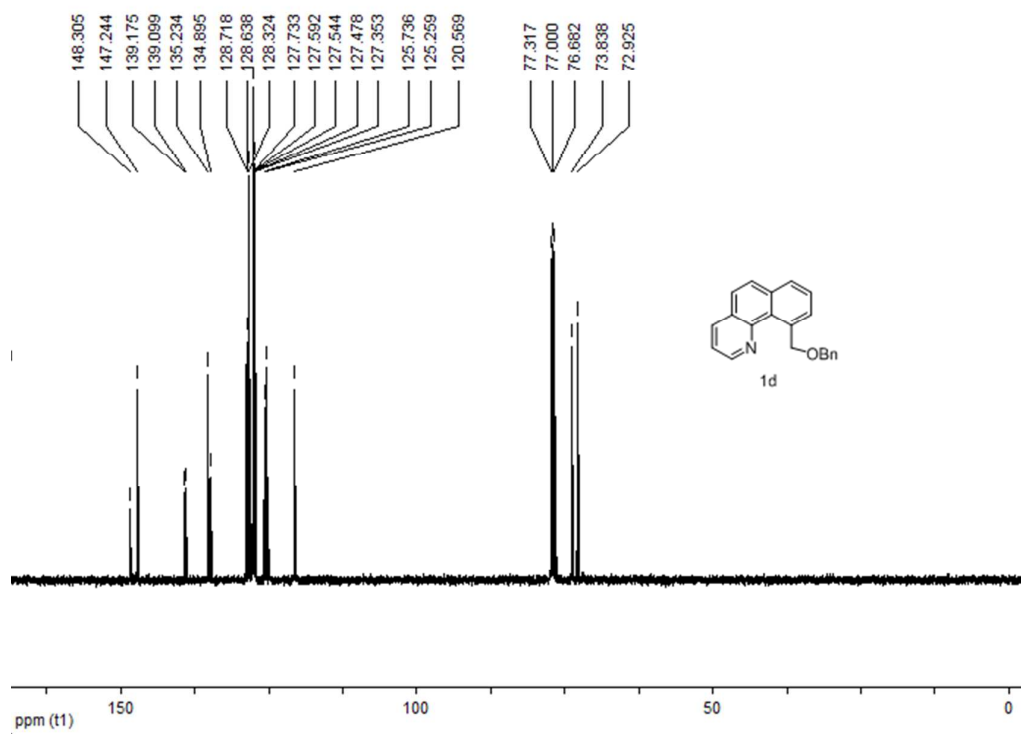


Figure S19. <sup>13</sup>C NMR for compound 1d

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 1aa'

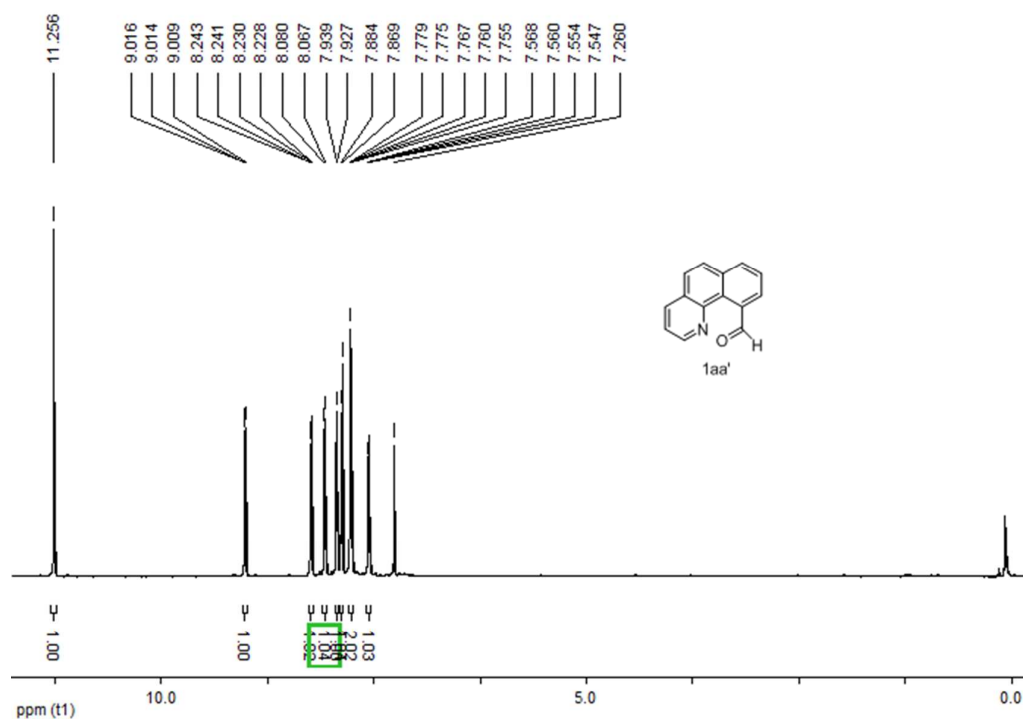


Figure S20. <sup>1</sup>H NMR for compound 1aa'

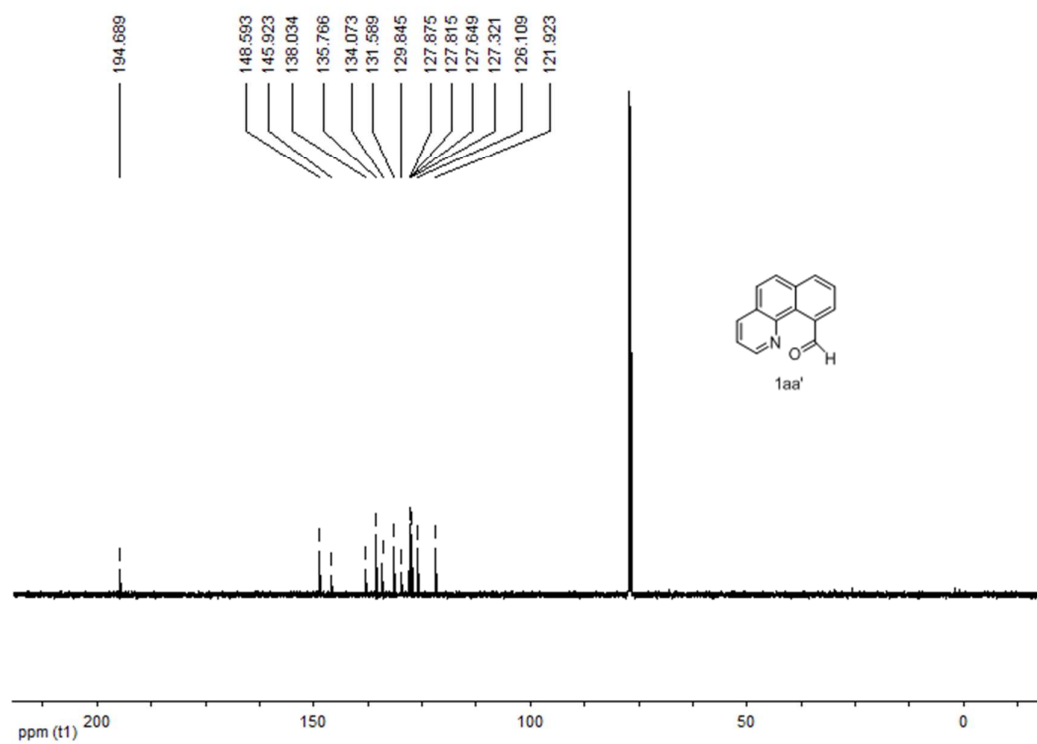


Figure S21. <sup>13</sup>C NMR for compound 1aa'

**Experimental Procedure for Rhodium-catalyzed Direct Arylation with Organoboron Compounds via Primary alcohols**

To an oven-dried screwed vial were added primary alcohol (0.1 mmol), substituted phenylboronic acid (0.2 mmol), copper (I) chloride (9.9 mg, 0.1 mmol),  $\text{Rh}(\text{PPh}_3)_3\text{Cl}$  (6.5 mg, 0.007 mmol) and xylene 1 mL under air atmosphere. The mixture was vigorously stirred at 130 °C to the end of the reaction. Organic solvents were removed in vacuo, and then the residue was purified by a silica gel column chromatography to give the desired product.



# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 3aa

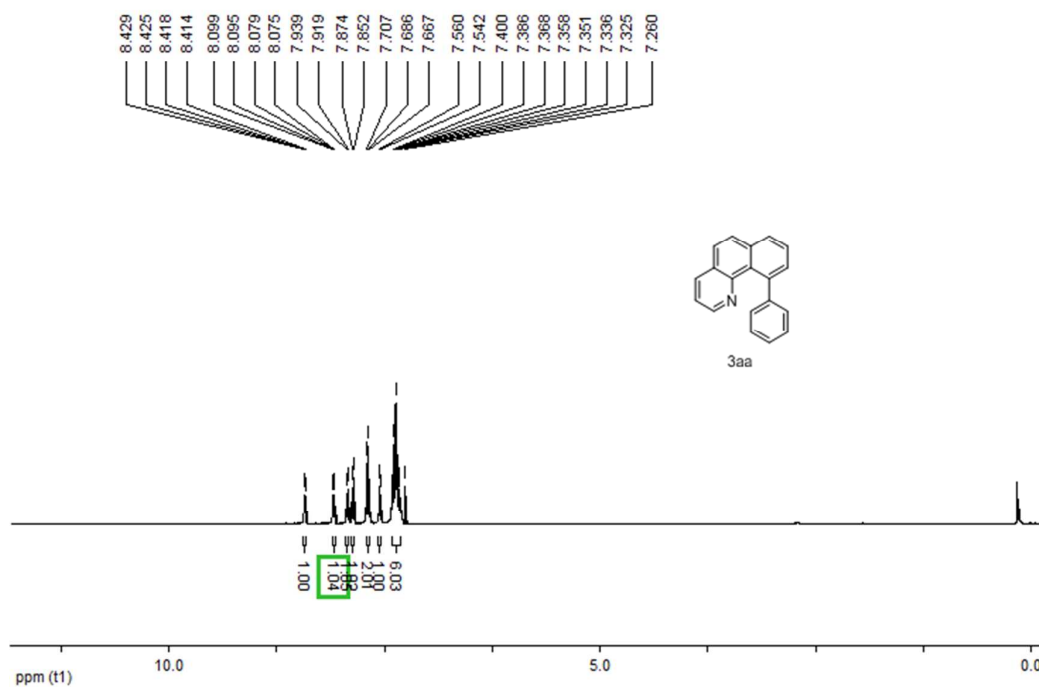


Figure S22. <sup>1</sup>H NMR for compound 3aa

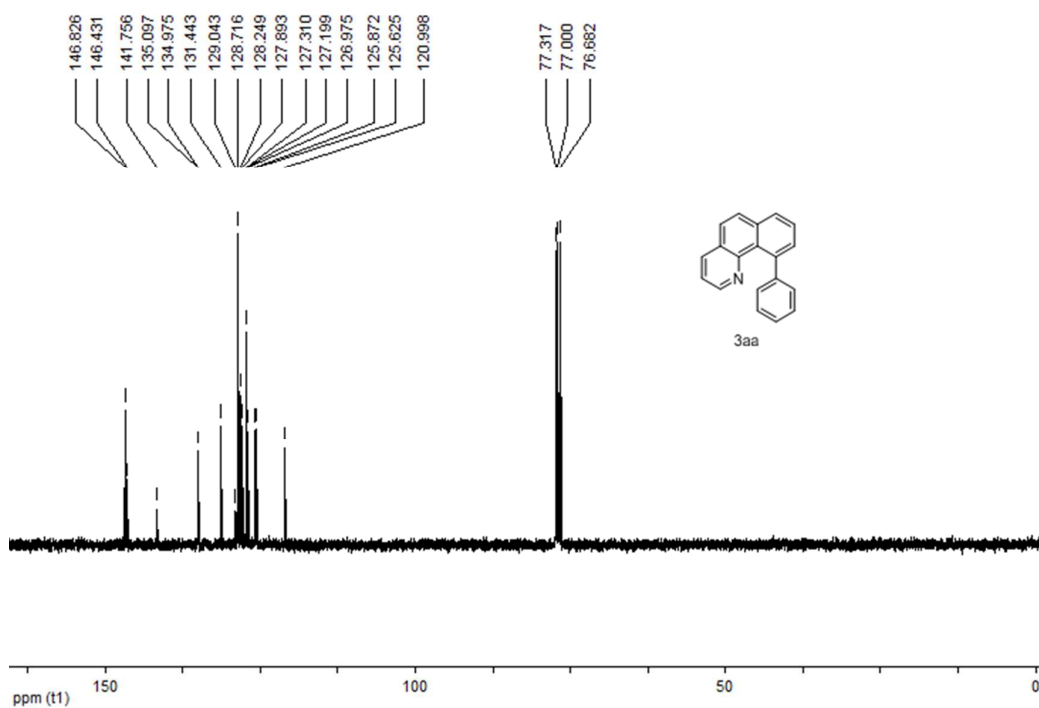


Figure S23. <sup>13</sup>C NMR for compound 3aa

**<sup>1</sup>H NMR spectrum of compound 3ab in CDCl<sub>3</sub>.**

**Chemical structure of 3ab:** Cc1ccc(cc1)-c2ccc3c(c2)nc4ccccc34

**Peak list (ppm):** 8.449, 8.442, 8.439, 8.439, 8.095, 8.075, 7.923, 7.903, 7.867, 7.845, 7.702, 7.695, 7.677, 7.657, 7.559, 7.541, 7.354, 7.321, 7.310, 7.292, 7.281, 7.260, 7.209, 7.179, 7.159, 7.140, 2.404.

**Integration values:** 1.00, 2.06, 2.09, 2.08, 3.06, 3.06, 3.00.

Chemical structure of **3ab**: Cc1ccc(cc1)-c2ccc3c(c2)cc[nH]3

<sup>13</sup>C NMR peaks (ppm): 146.853, 146.277, 141.888, 139.493, 135.115, 131.505, 129.342, 128.807, 128.298, 128.235, 127.819, 127.145, 126.996, 126.384, 125.995, 125.853, 121.019, 77.318, 77.000, 76.683, 21.566.

S18

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 3ac

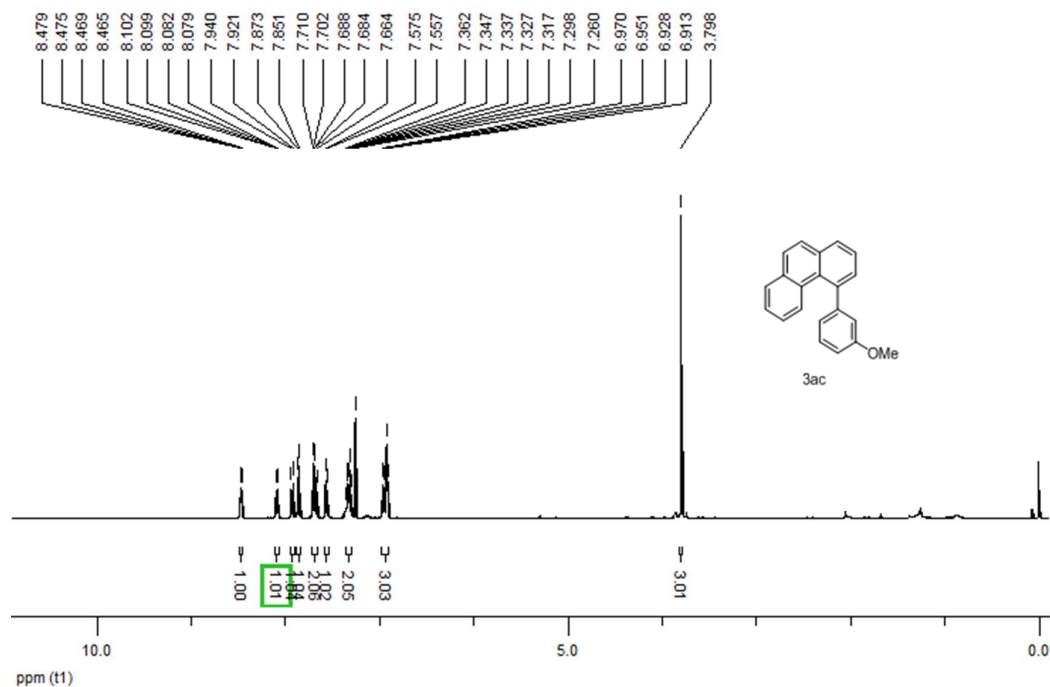


Figure S26. <sup>1</sup>H NMR for compound 3ac

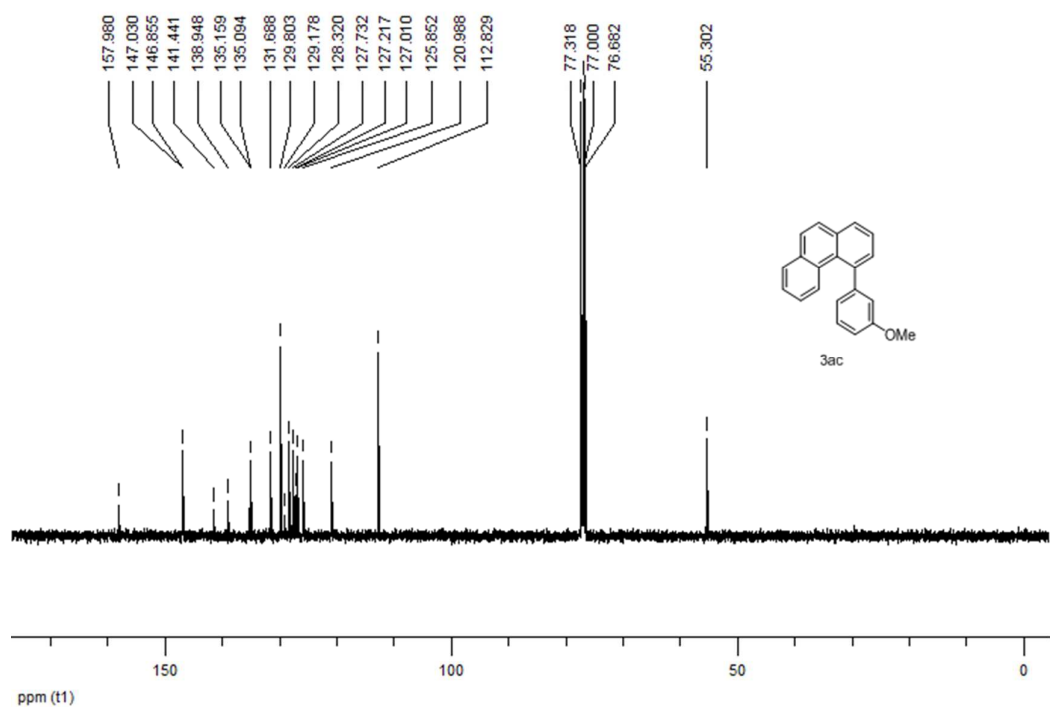


Figure S27. <sup>13</sup>C NMR for compound 3ac

Chemical structure of **3ad** is shown: 2-(4-(trifluoromethoxy)phenyl)quinoline.

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) of **3ad** is displayed, showing aromatic signals between 7.2 and 8.5 ppm. The integration values are provided below the peaks, with 1.03 highlighted in a green box.

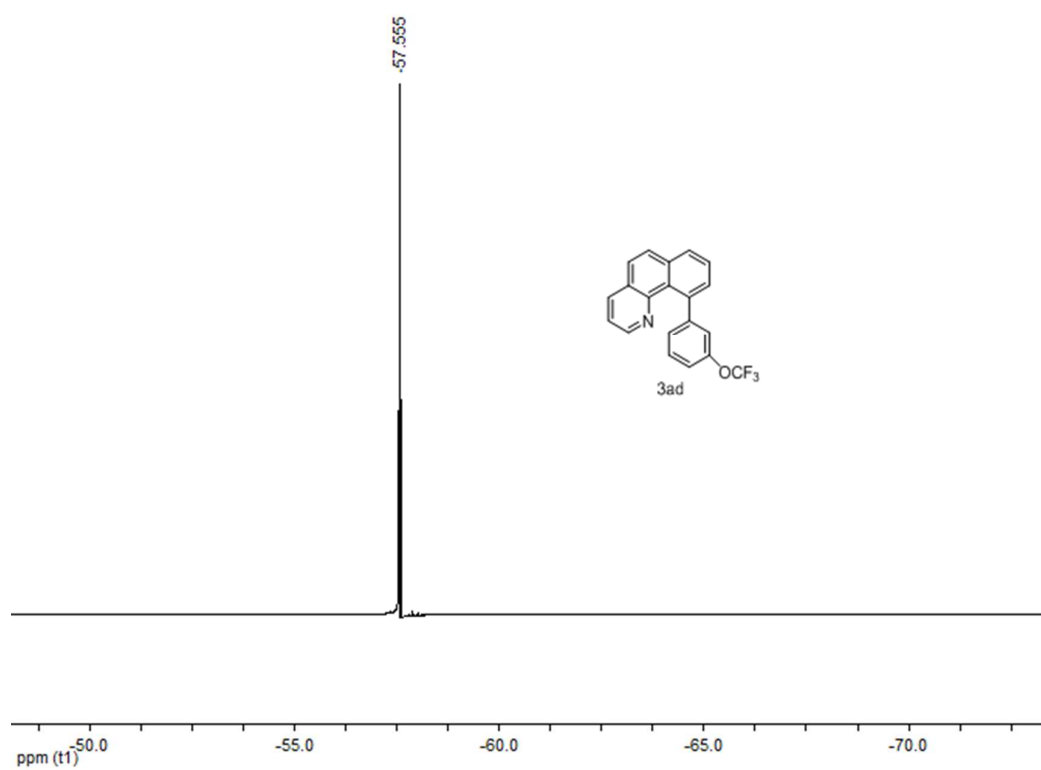
148.577  
148.327  
146.959  
146.470  
140.008  
135.234  
134.980  
131.155  
128.892  
128.663  
128.488  
128.178  
127.279  
127.014  
126.855  
126.114  
122.127  
121.973  
121.221  
119.425  
118.264  
77.318  
77.000  
76.683

3ad

COc1ccc(cc1C2=CNc3ccccc23)OC(F)(F)F

S20

**$^{19}\text{F}$  NMR for compound 3ad**



**Figure S30.  $^{19}\text{F}$  NMR for compound 3ad**

Chemical structure of **3ae** is shown as an inset: c1ccc(cc1-c2ccc3ccccc3n2)-c4ccc(cc4)[N+](=O)[O-].

The <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) displays the following chemical shifts (ppm) and integration values:

Chemical Shift (ppm)	Integration
8.365	1.00
8.359	1.00
8.356	1.00
8.241	1.00
8.125	1.00
8.105	1.00
8.010	1.00
7.990	1.00
7.902	1.00
7.880	1.00
7.748	1.00
7.723	1.00
7.696	1.00
7.676	1.00
7.562	1.00
7.541	1.00
7.529	1.00
7.511	1.00
7.359	1.00
7.348	1.00
7.340	1.00
7.329	1.00
7.260	1.00

Chemical structure of **3ae** (2-(4-nitrophenyl)quinoline) is shown in the top right corner.

The <sup>13</sup>C NMR spectrum (CDCl<sub>3</sub>) displays the following chemical shifts (ppm):

Chemical Shift (ppm)
147.952
147.760
146.890
146.224
138.971
135.446
135.041
134.995
131.144
128.951
128.725
128.202
127.924
127.352
127.098
126.262
123.946
121.373
120.756
77.317
77.000
76.682

S22

[illegible]

Chemical structure of **3af** is shown as an inset: Cc1ccc(cc1)-c2ccc3c(c2)c4ccccc4n3.

13C NMR spectrum (ppm (t1)) showing peaks at the following chemical shifts (ppm):

- 147.424
- 147.058
- 146.427
- 141.079
- 135.848
- 135.014
- 134.664
- 130.714
- 128.709
- 128.411
- 127.922
- 127.849
- 127.207
- 126.953
- 125.882
- 125.795
- 125.408
- 125.064
- 120.922
- 77.317
- 77.000
- 76.682
- 20.147

S23

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 3ag

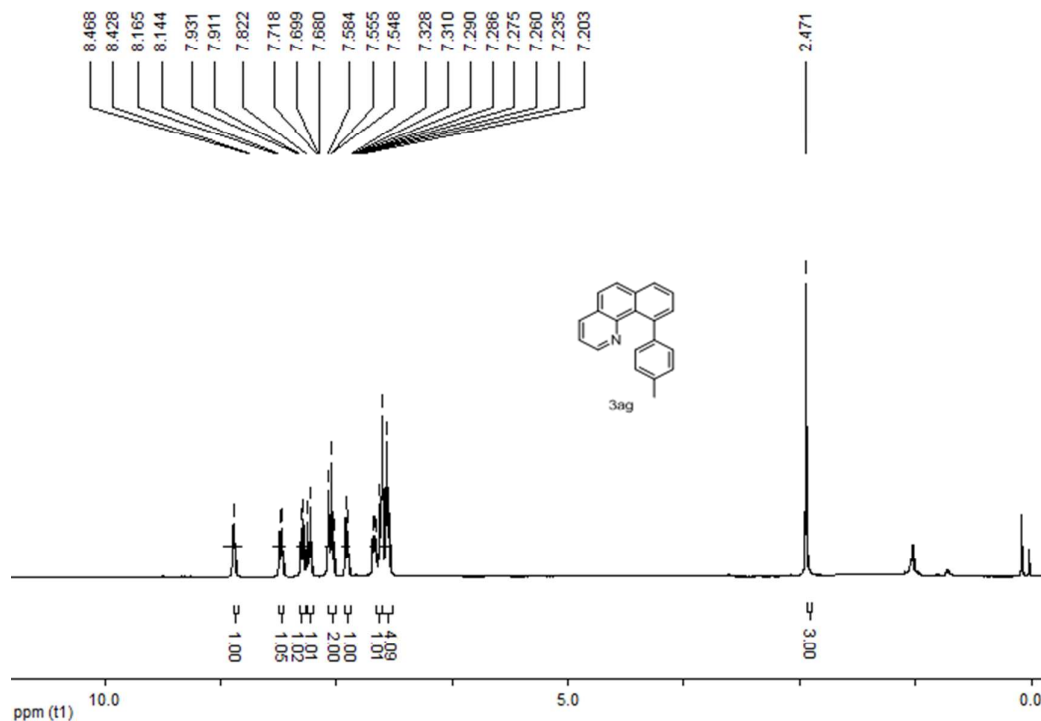


Figure S35. <sup>1</sup>H NMR for compound 3ag

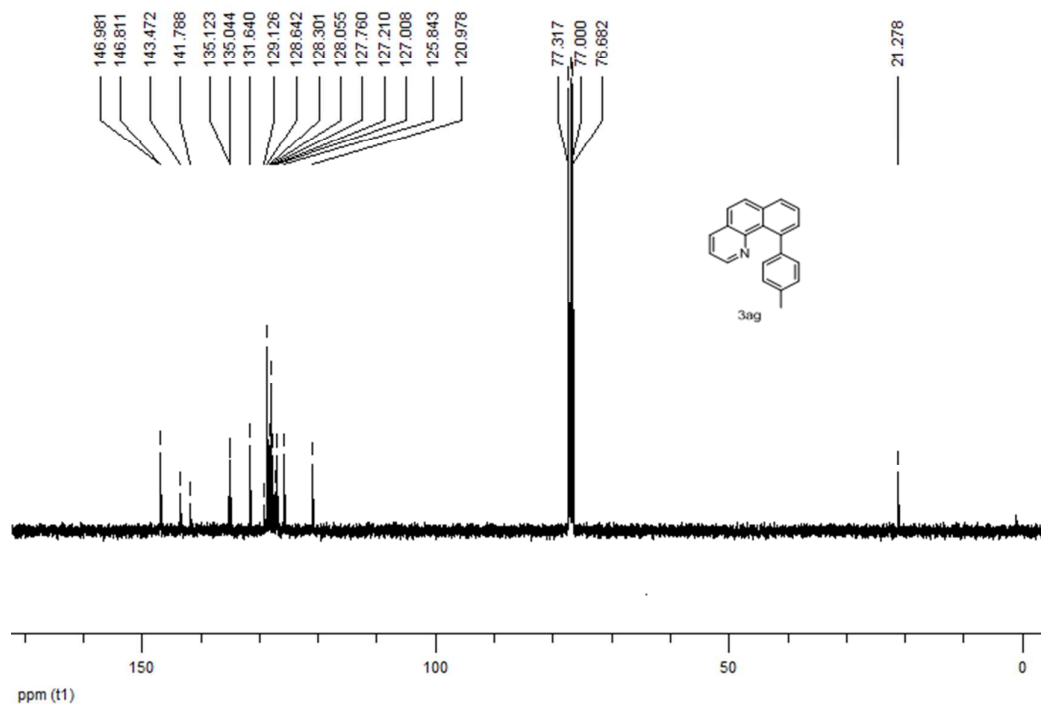


Figure S36. <sup>13</sup>C NMR for compound 3ag



[illegible]

148.426  
146.956  
146.805  
143.301  
141.787  
135.107  
135.030  
131.538  
129.180  
128.343  
128.300  
127.727  
127.163  
127.004  
125.828  
124.189  
120.961

77.317  
77.000  
76.882

34.511  
31.551

3ah

ppm (t1)

S25

[illegible]

Chemical structure of 3ai is shown in the top right corner. The structure is a tricyclic system consisting of a benzene ring fused to a pyridine ring, which is further fused to another benzene ring. A methoxy group (OMe) is attached to the benzene ring at the 3-position.

The <sup>13</sup>C NMR spectrum (ppm (t1)) shows the following peaks (ppm):

- 157.990
- 147.039
- 146.864
- 138.957
- 135.168
- 135.104
- 131.694
- 129.810
- 129.192
- 128.329
- 127.736
- 127.228
- 127.018
- 125.859
- 120.994
- 112.837
- 77.318
- 77.000
- 76.683
- 55.313

S26

[illegible]

Chemical structure of **3aj** is shown in the upper right. The structure is a benzimidazole derivative with an ethyl ester group (COOEt) attached to the benzene ring.

The <sup>13</sup>C NMR spectrum (ppm (t1)) shows the following peaks (ppm):

- 166.266
- 151.477
- 146.853
- 144.270
- 135.180
- 134.893
- 130.949
- 130.122
- 130.047
- 128.688
- 128.359
- 128.150
- 127.223
- 127.151
- 126.984
- 126.040
- 121.170
- 77.318
- 77.000
- 76.682
- 61.035
- 14.309

S27

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 3ak

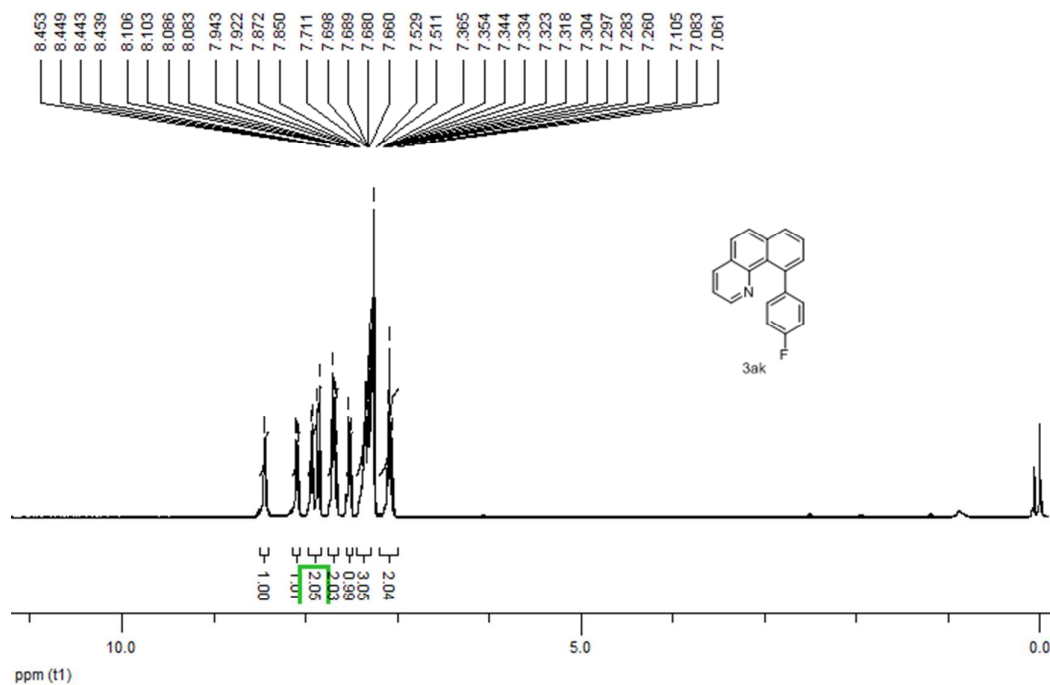


Figure S43. <sup>1</sup>H NMR for compound 3ak

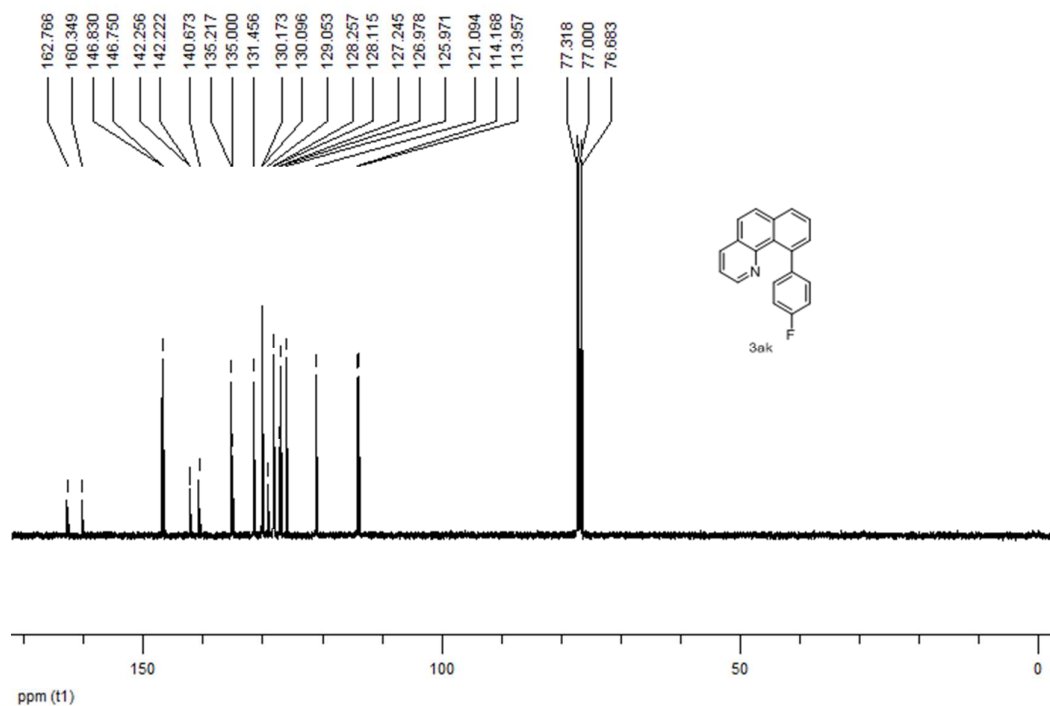
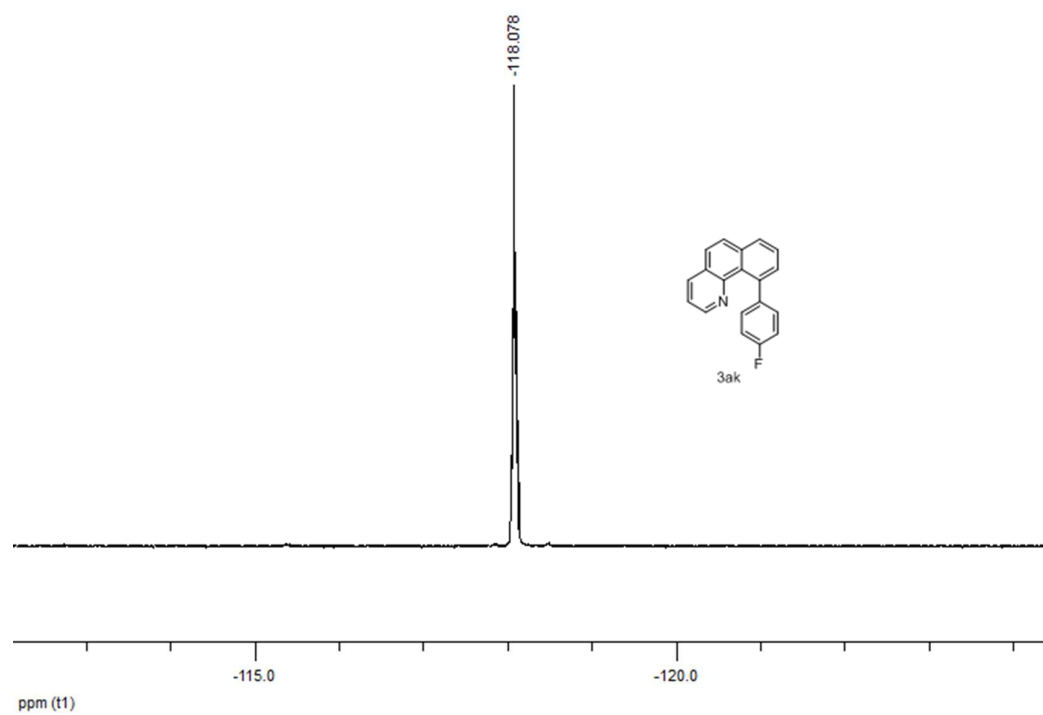


Figure S44. <sup>13</sup>C NMR for compound 3ak

**$^{19}\text{F}$  NMR for compound 3ak**



**Figure S45.  $^{19}\text{F}$  NMR for compound 3ak**

Chemical structure of **3al** (2-(4-chlorophenyl)quinoline) is shown. The <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) displays aromatic signals in the range of 7.2–8.5 ppm. The integration values for the peaks are 1.00, 1.06, 1.04, 1.01, and 1.05. The chemical shifts (ppm) for the peaks are listed at the top: 8.490, 8.483, 8.108, 8.088, 7.960, 7.941, 7.881, 7.859, 7.719, 7.695, 7.675, 7.530, 7.512, 7.408, 7.388, 7.333, 7.321, 7.300, and 7.260.

Chemical structure of 3al: c1ccc(cc1)-c2nc3ccccc3n2

<sup>13</sup>C NMR peaks (ppm):

Peak Label	Chemical Shift (ppm)
146.838	146.838
146.810	146.810
146.593	146.593
146.561	146.561
144.861	144.861
140.336	140.336
135.213	135.213
134.953	134.953
131.471	131.471
131.284	131.284
130.090	130.090
130.058	130.058
128.852	128.852
128.205	128.205
127.414	127.414
127.215	127.215
127.182	127.182
126.989	126.989
125.992	125.992
121.130	121.130
77.319	77.319
77.000	77.000
76.883	76.883

S30

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 3am

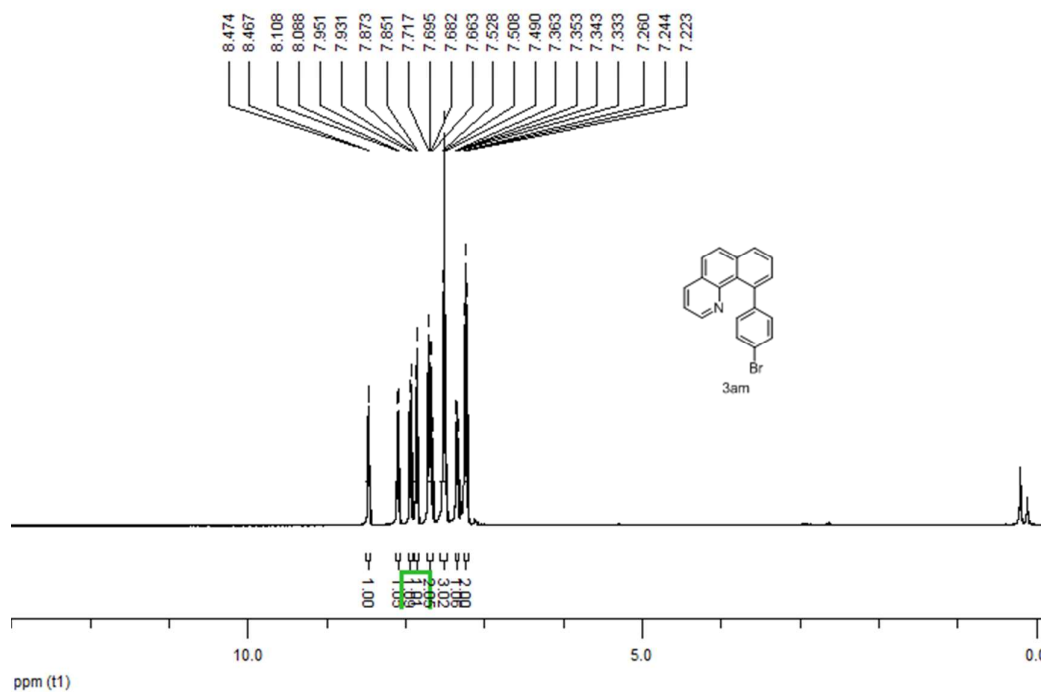


Figure S48. <sup>1</sup>H NMR for compound 3am

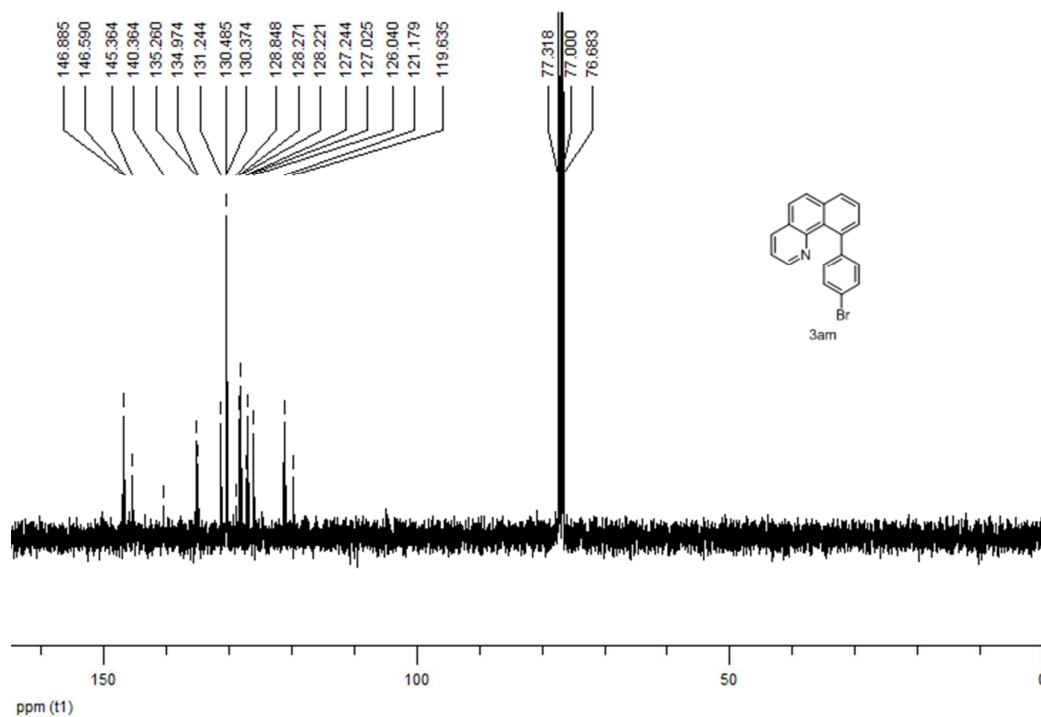


Figure S49. <sup>13</sup>C NMR for compound 3am

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 3an

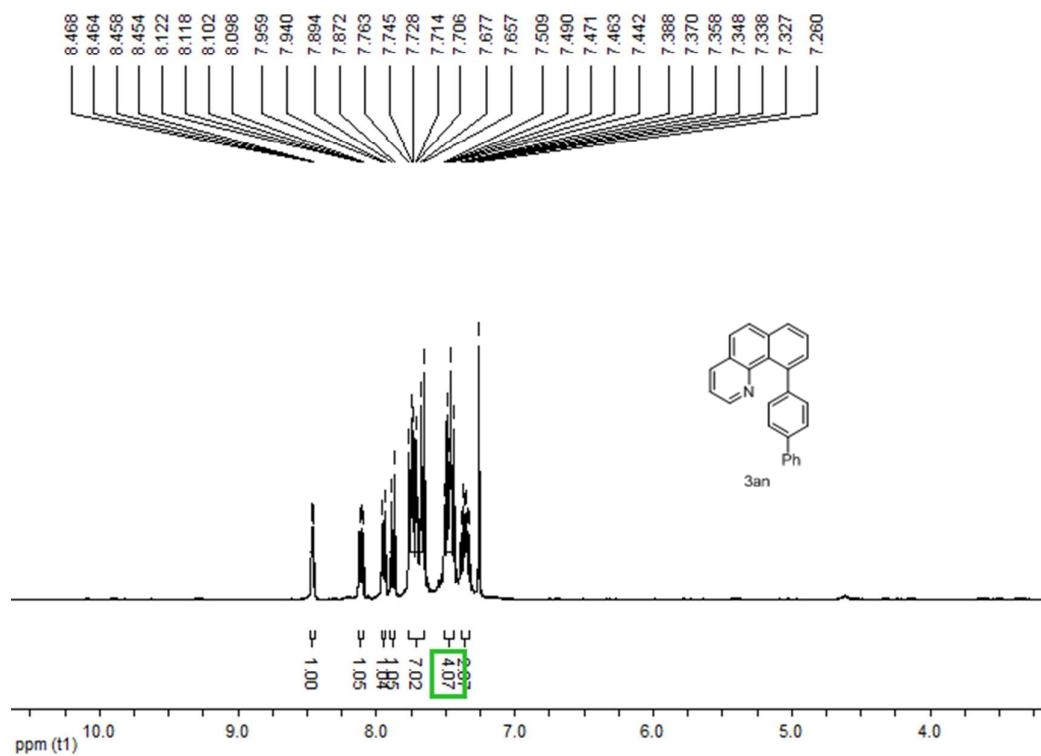


Figure S50. <sup>1</sup>H NMR for compound 3an

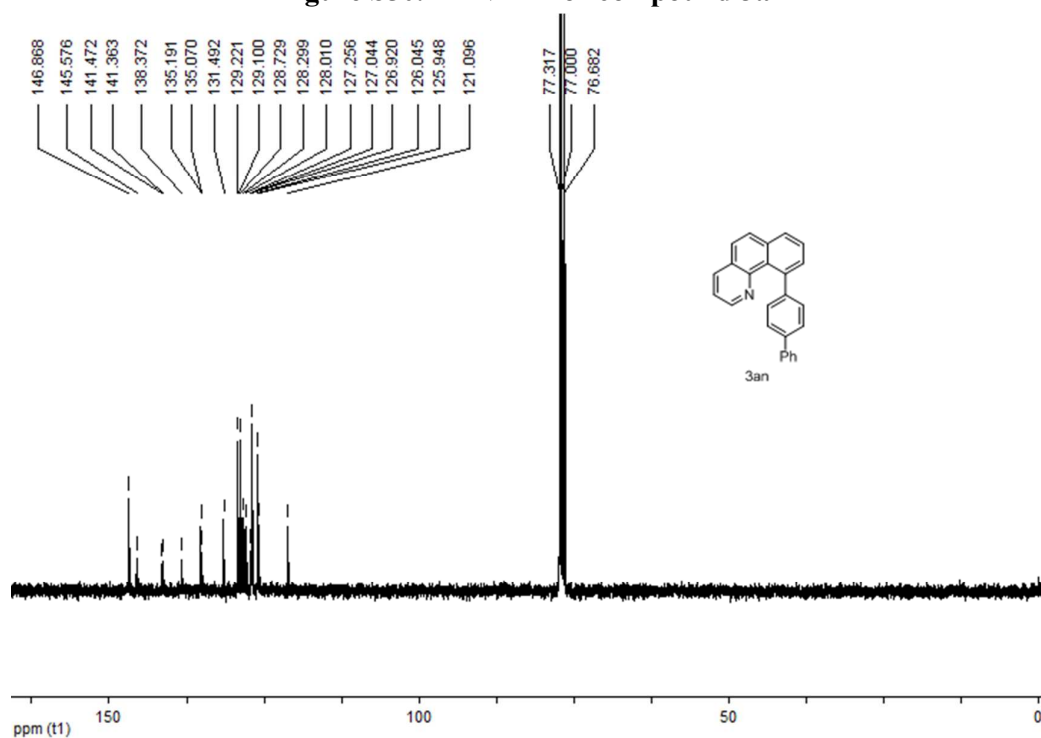


Figure S51. <sup>13</sup>C NMR for compound 3an



Chemical structure of **3ao** (2-(4-(trifluoromethyl)phenyl)quinoline) is shown in the top right. The <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) displays aromatic signals between 7.2 and 8.4 ppm. A green box highlights the peaks at 7.260, 7.331, 7.341, 7.350, 7.448, 7.468, 7.516, 7.564, 7.589, 7.644, 7.684, 7.710, 7.717, 7.729, 7.739, 7.874, 7.896, 7.967, 7.987, 8.102, 8.122, 8.401, and 8.408 ppm. The chemical shift values (ppm) are listed above the peaks, and the integration values are shown below the peaks.

Chemical Shift (ppm)	Integration
7.260	1.00
7.331	1.00
7.341	1.00
7.350	1.00
7.448	1.00
7.468	1.00
7.516	1.00
7.564	1.00
7.589	1.00
7.644	1.00
7.684	1.00
7.710	1.00
7.717	1.00
7.729	1.00
7.739	1.00
7.874	1.00
7.896	1.00
7.967	1.00
7.987	1.00
8.102	1.00
8.122	1.00
8.401	1.00
8.408	1.00

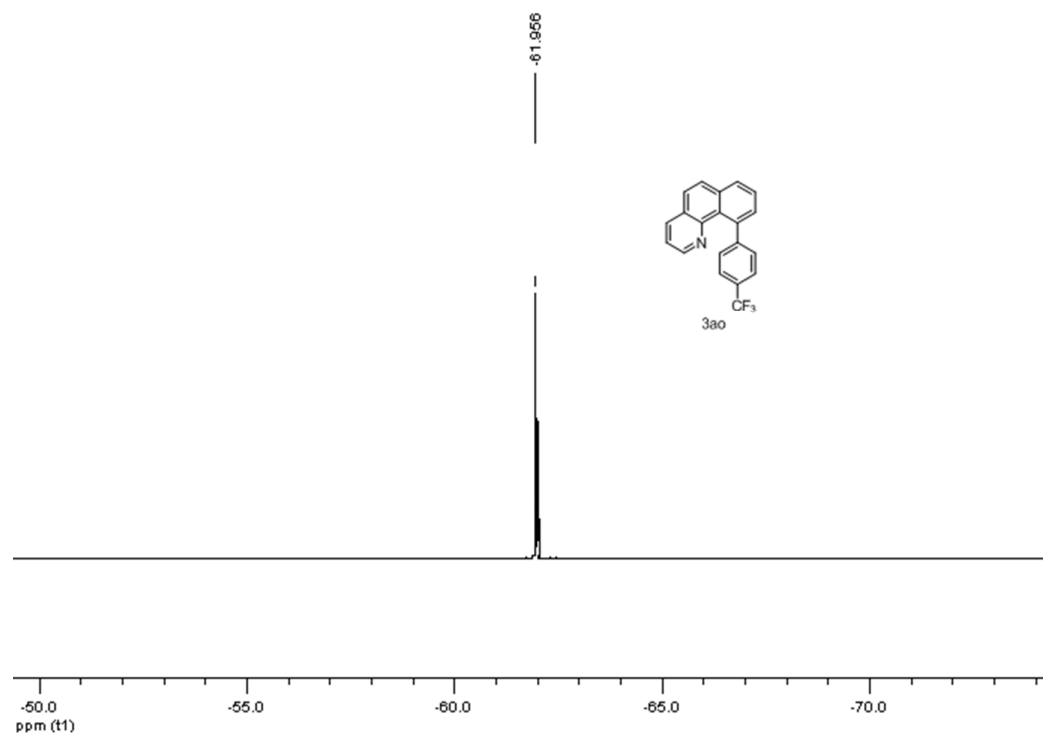
Chemical structure of 3ao: FC(F)(F)c1ccc(cc1)-c2ccc3c(c2)cccnc3

<sup>13</sup>C NMR spectrum (CDCl<sub>3</sub>) of compound 3ao. The spectrum shows a cluster of peaks between 120 and 150 ppm and a triplet for the CDCl<sub>3</sub> solvent at 77.000 ppm.

Chemical Shift (ppm)
150.236
146.915
146.442
140.251
135.286
134.963
131.082
128.990
128.874
128.526
128.207
127.981
127.863
127.293
127.053
126.135
124.776
124.239
124.202
124.152
121.251
77.317
77.000
76.682

S33

**$^{19}\text{F}$  NMR for compound 3ao**



**Figure S54.  $^{19}\text{F}$  NMR for compound 3ao**

[illegible]

Chemical structure of 3ap is shown as an inset. The structure is a tricyclic compound consisting of a pyridine ring fused to a benzene ring, which is further fused to another benzene ring. The label "3ap" is placed below the structure.

13C NMR spectrum (ppm (t1)) of compound 3ap. The spectrum shows a cluster of peaks between 120 and 150 ppm and a triplet of peaks around 77 ppm. The chemical structure of 3ap is shown as an inset.

Peak (ppm)
146.917
146.714
144.486
141.526
135.142
135.046
133.786
132.174
131.909
129.417
129.093
128.313
128.122
128.064
127.583
127.234
127.171
125.945
125.653
125.495
125.419
125.121
121.076
77.318
77.000
76.683

S35

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 3aq

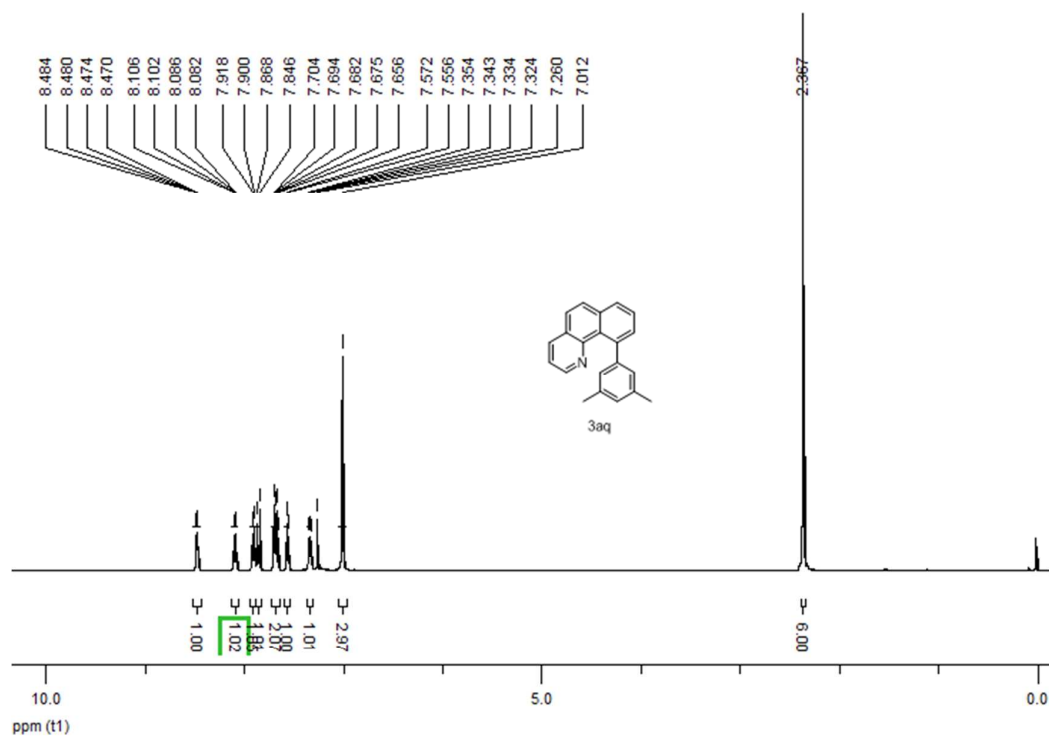


Figure S57. <sup>1</sup>H NMR for compound 3aq

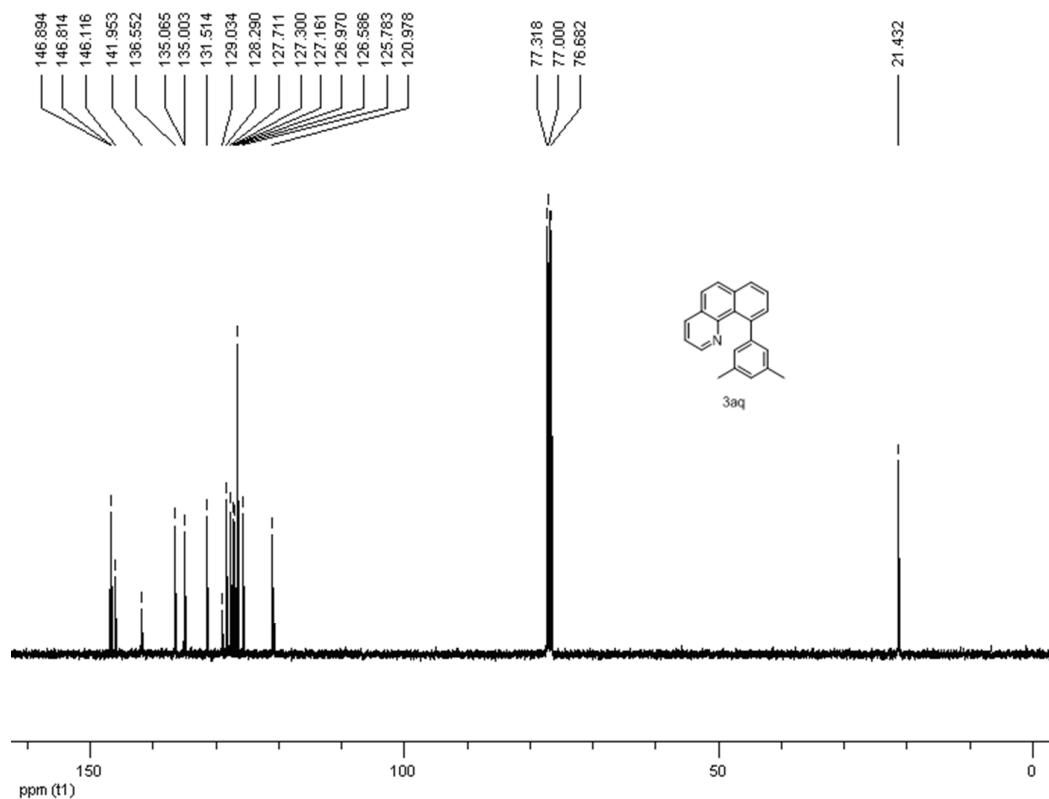


Figure S58. <sup>13</sup>C NMR for compound 3aq

Chemical structure of **3ar** is shown: 2-(4,4-difluorophenyl)quinoline.

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) of **3ar** is displayed, showing aromatic signals between 7.2 and 8.4 ppm. Integration values are provided below the peaks: 1.00, 1.00, 1.00, 2.03, 1.04, 1.00, 1.00.

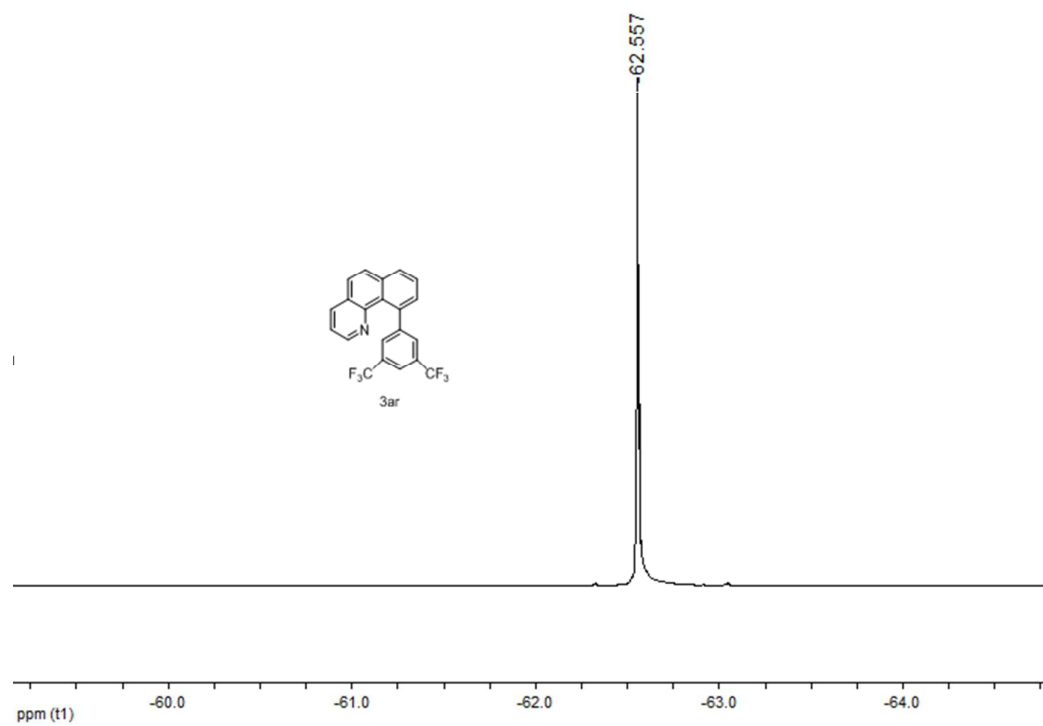
Chemical structure of **3ar** is shown in the top right corner. The structure is a tricyclic system consisting of a quinoline ring fused to a benzene ring, which is further substituted with a 4-(trifluoromethyl)phenyl group. The trifluoromethyl group is represented as  $\text{F}_3\text{C}$ .

The  $^{13}\text{C}$  NMR spectrum displays the following chemical shifts (ppm) for the peaks:

- 148.083
- 146.868
- 146.046
- 138.419
- 135.483
- 135.033
- 131.195
- 130.732
- 130.407
- 130.080
- 129.756
- 129.256
- 128.643
- 128.203
- 127.345
- 127.155
- 126.359
- 125.211
- 122.503
- 121.559
- 119.532
- 119.493
- 119.456
- 119.419
- 77.319
- 77.000
- 76.683

S37

**$^{19}\text{F}$  NMR for compound 3ar**



**Figure S61.  $^{19}\text{F}$  NMR for compound 3ar**

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 3as

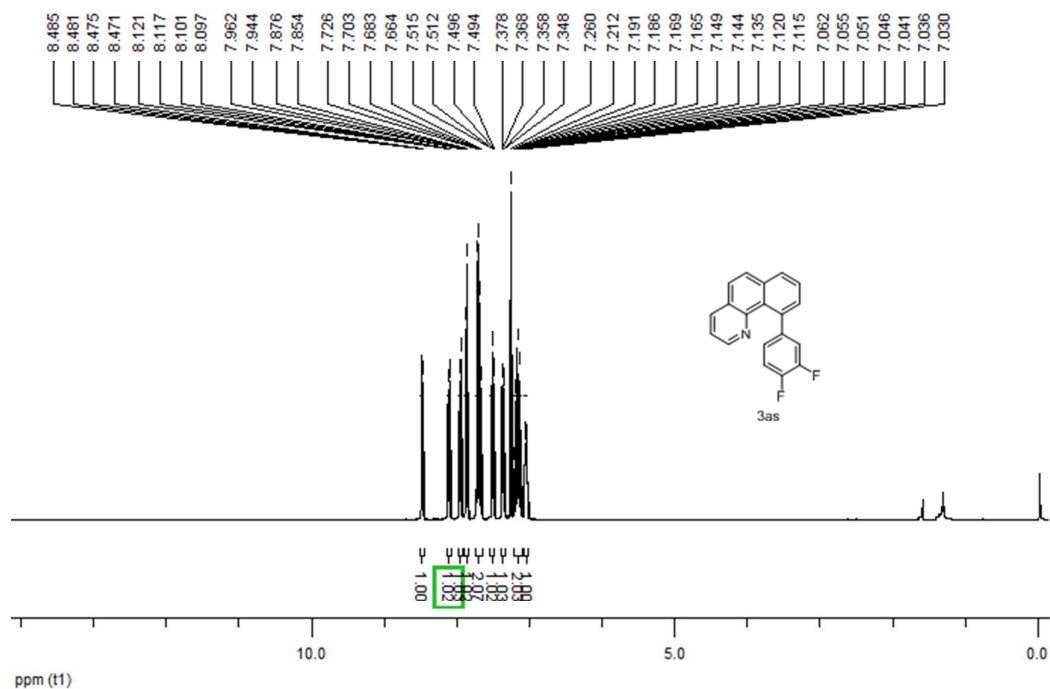


Figure S62. <sup>1</sup>H NMR for compound 3as

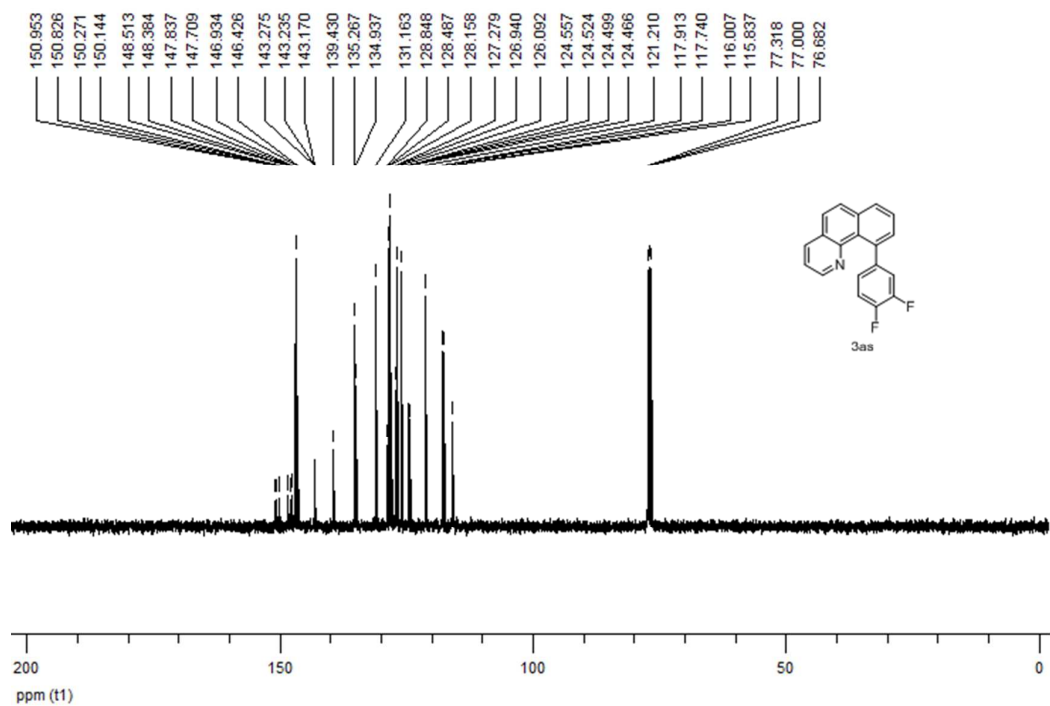
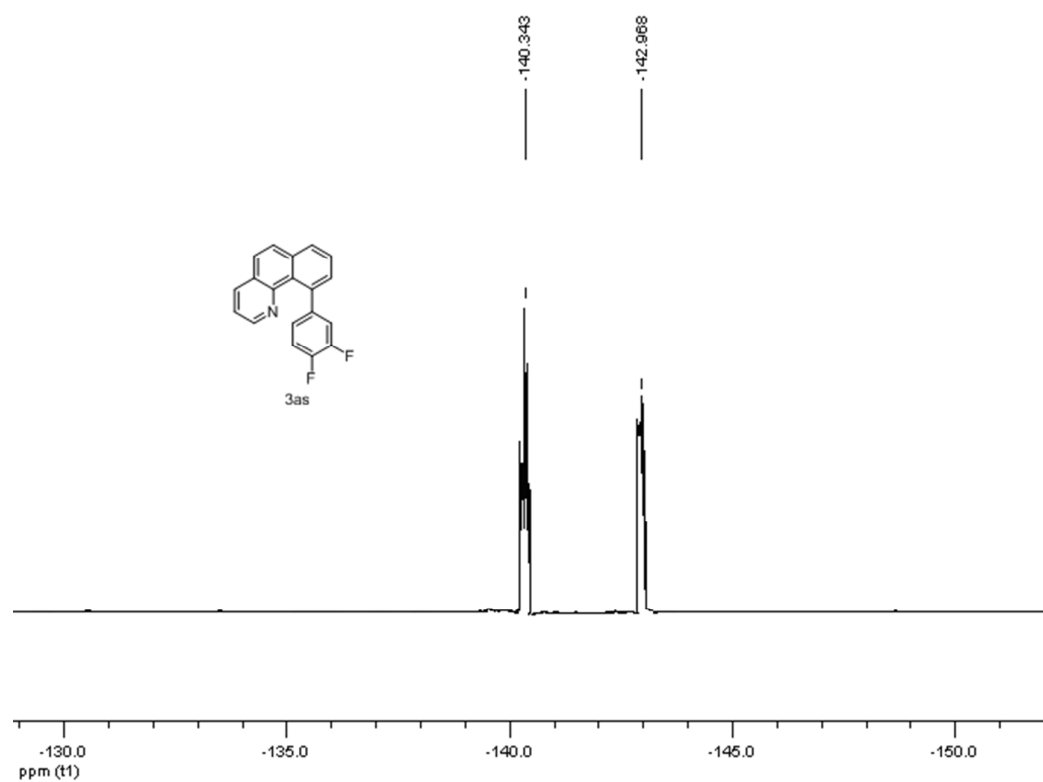


Figure S63. <sup>13</sup>C NMR for compound 3as

**$^{19}\text{F}$  NMR for compound 3as**



**Figure S64.  $^{19}\text{F}$  NMR for compound 3as**



Chemical structure of **3at** is shown in the top right corner of the spectrum.

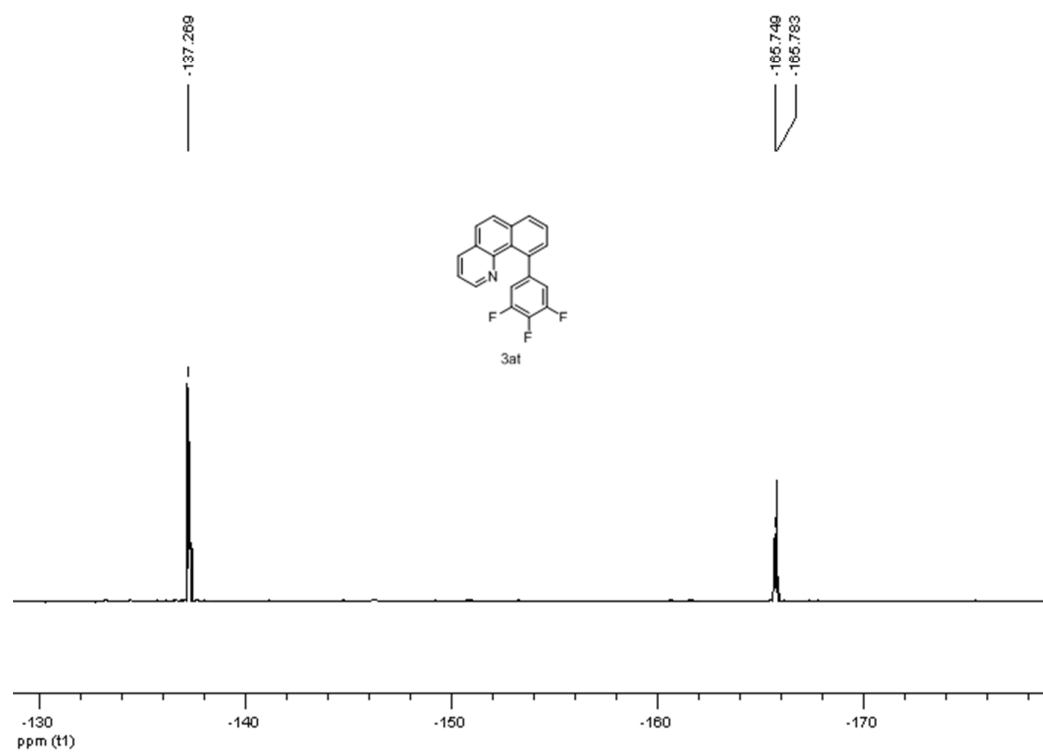
Chemical structure of **3at** is shown in the top right corner. The structure is a fluorene derivative with a 2,4,6-trifluorophenyl group attached to the 9-position.

The <sup>13</sup>C NMR spectrum (t1) shows the following chemical shifts (ppm) for the peaks:

- 151.898
- 151.855
- 151.798
- 151.757
- 149.440
- 149.398
- 149.340
- 149.298
- 147.125
- 146.192
- 142.451
- 142.398
- 142.364
- 142.313
- 142.281
- 142.228
- 139.751
- 139.597
- 139.441
- 138.538
- 135.368
- 134.945
- 130.838
- 128.871
- 128.735
- 128.136
- 127.374
- 126.978
- 126.280
- 121.390
- 112.961
- 112.908
- 112.804
- 112.751
- 77.318
- 77.000
- 76.683

S41

**$^{19}\text{F}$  NMR for compound 3at**



**Figure S67.  $^{19}\text{F}$  NMR for compound 3at**

Chemical structure of **3ba** is shown: Cc1ccc2c(c1)c3ccccc3n2.

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) of **3ba** is displayed, showing peaks in the aromatic region (7.2–8.4 ppm) and a singlet at 3.07 ppm. Integration values are provided below the peaks.

Chemical Shift (ppm)	Integration
8.371	1.00
8.364	1.00
8.360	1.00
8.121	1.00
8.100	1.00
8.009	1.00
8.006	1.00
7.989	1.00
7.966	1.00
7.766	1.00
7.747	1.00
7.728	1.00
7.601	1.00
7.583	1.00
7.554	1.00
7.439	1.00
7.419	1.00
7.403	1.00
7.382	1.00
7.372	1.00
7.355	1.00
7.298	1.00
7.288	1.00
7.278	1.00
7.268	1.00
7.260	1.00
3.07	3.07

Chemical structure of **3ba** is shown as an inset: Cc1ccc2c(c1)c3ccccc3n2.

<sup>13</sup>C NMR spectrum (CDCl<sub>3</sub>) of **3ba**. The x-axis represents the chemical shift in ppm (t1), ranging from 0 to 200. The spectrum displays several peaks corresponding to the aromatic and heterocyclic carbons of the molecule, with the following chemical shifts (ppm) labeled above the peaks:

- 146.898
- 146.307
- 146.008
- 142.096
- 134.832
- 134.274
- 133.624
- 131.168
- 128.613
- 127.355
- 127.055
- 126.895
- 125.836
- 125.478
- 123.776
- 121.077

The solvent peak (CDCl<sub>3</sub>) is visible as a triplet at 77.000 ppm. Other labeled peaks include 77.319, 76.884, and 20.519 ppm.

S43

Chemical structure of **3bb** (1-(2-phenyl-1H-indol-3-yl)benzene) is shown. The <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) displays aromatic signals. The chemical shift (ppm) and integration values are listed below the spectrum. A green box highlights the integration value for the peak at 7.583 ppm.

Chemical Shift (ppm)	Integration
8.433	1.00
8.430	1.00
8.423	1.00
8.162	1.00
8.159	1.00
8.141	1.00
8.138	1.00
7.944	1.00
7.923	1.00
7.827	1.00
7.728	1.00
7.709	1.00
7.690	1.00
7.583	1.00
7.554	1.00
7.546	1.00
7.463	1.00
7.431	1.00
7.414	1.00
7.394	1.00
7.374	1.00
7.278	1.00
7.268	1.00
7.260	1.00
7.247	1.00

146.526  
141.710  
139.502  
137.952  
134.397  
133.511  
131.435  
130.269  
129.976  
128.676  
128.569  
128.491  
128.333  
127.977  
127.869  
127.352  
127.302  
126.390  
125.910  
125.598  
120.814

77.318  
77.000  
76.683

Ph

3bb

ppm (t1)

S44

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 3bc

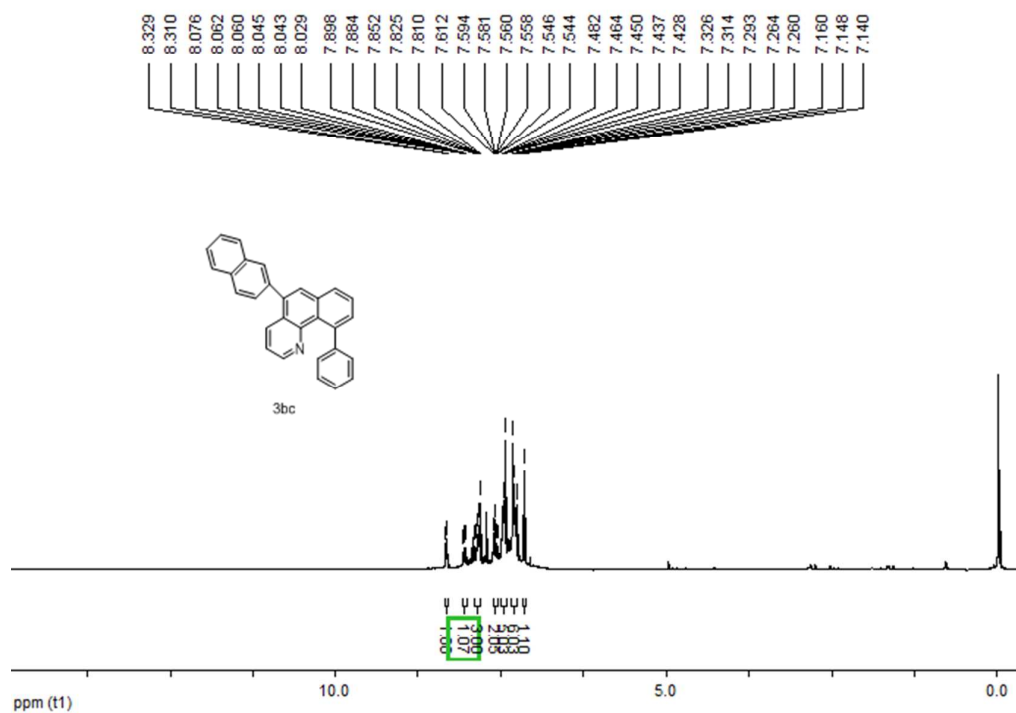


Figure S72. <sup>1</sup>H NMR for compound 3bc

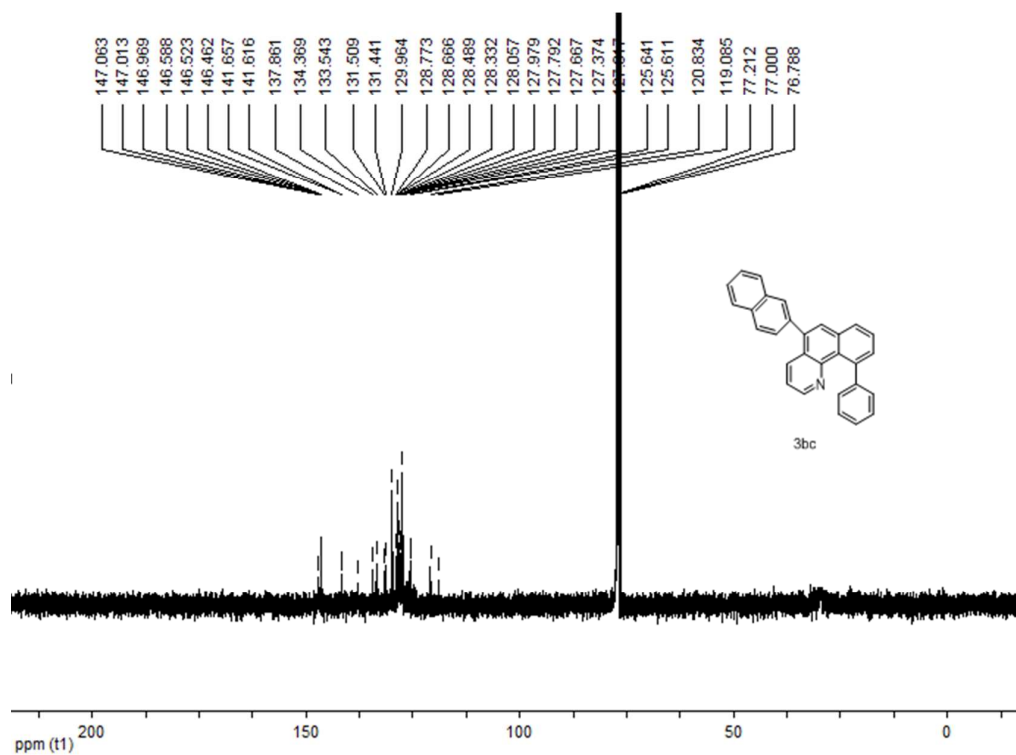


Figure S73. <sup>13</sup>C NMR for compound 3bc

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 3bd

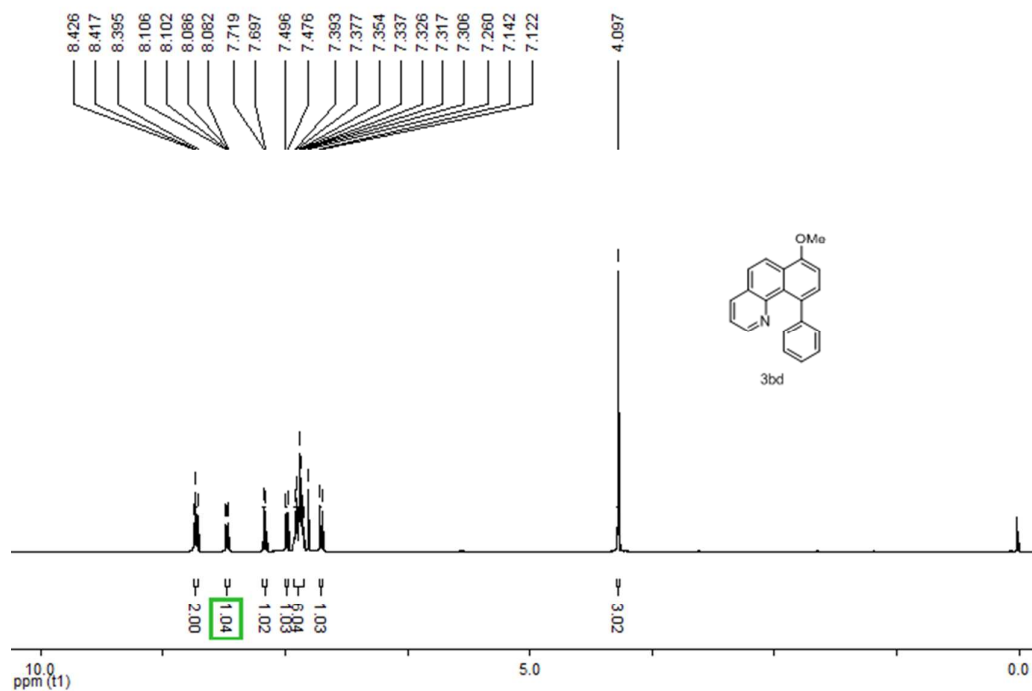


Figure S74. <sup>1</sup>H NMR for compound 3bd

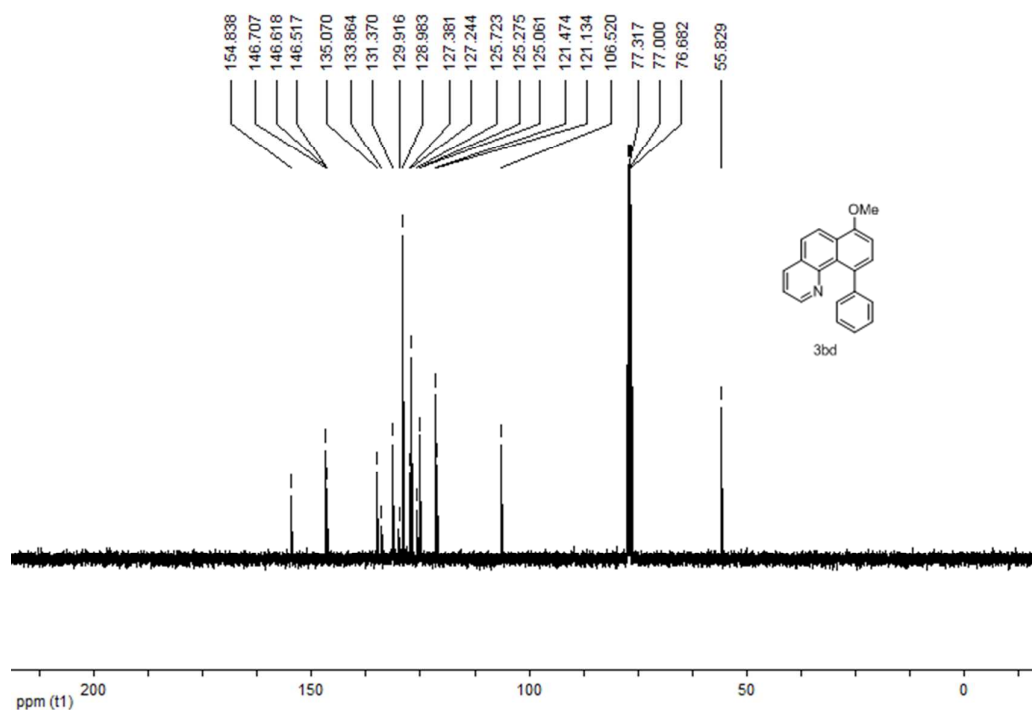


Figure S75. <sup>13</sup>C NMR for compound 3bd

[illegible]

148.881  
146.789  
146.757  
141.175  
141.004  
140.055  
134.922  
132.750  
130.801  
130.326  
129.467  
128.730  
128.639  
128.352  
127.414  
127.355  
126.872  
125.929  
125.681  
125.558  
121.205

77.318  
77.000  
76.683

3be

c1ccc(cc1)-c2ccc3c(c2)ccn3

S47

# <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 3bf

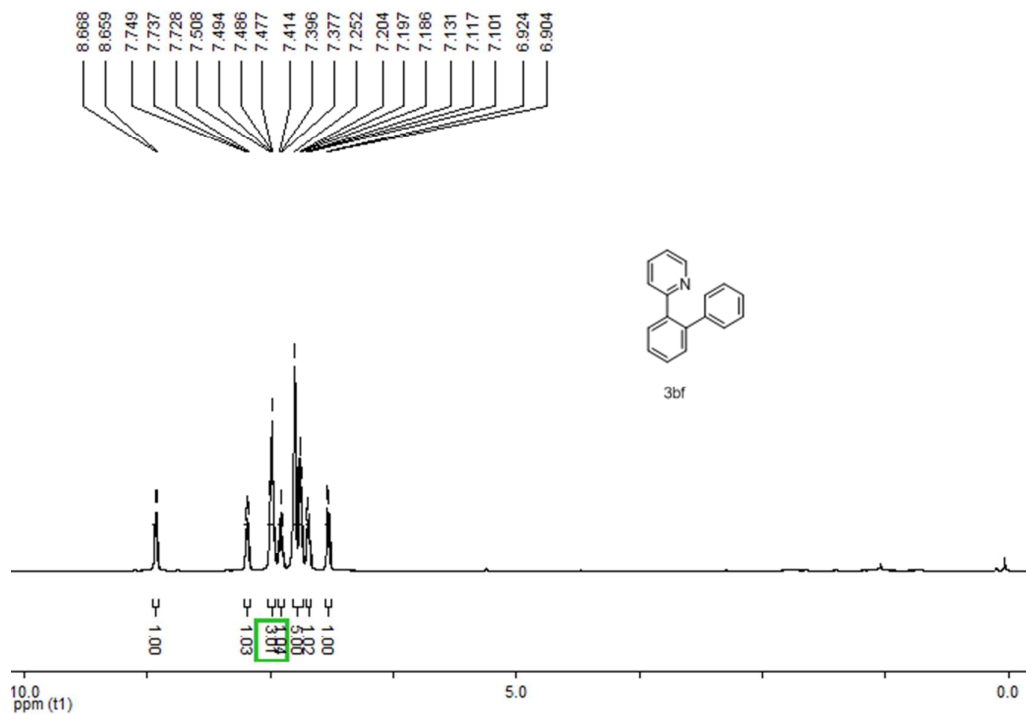


Figure S78. <sup>1</sup>H NMR for compound 3bf

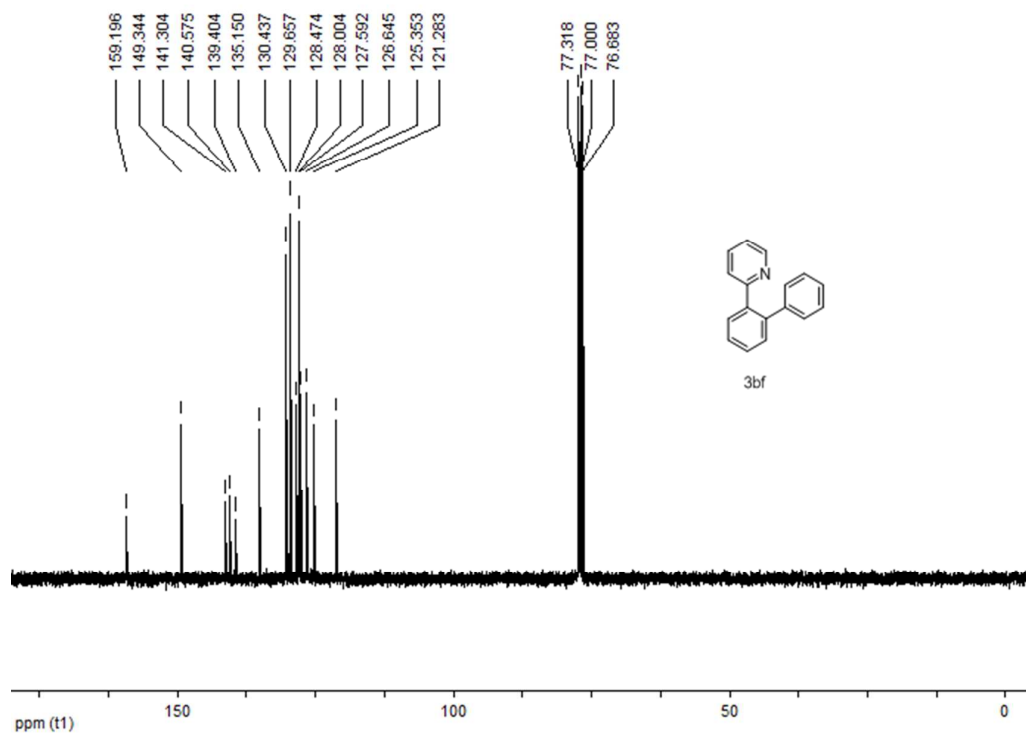


Figure S79. <sup>13</sup>C NMR for compound 3bf