Electronic Supplementary Information

Naphthol Synthesis: Annulation of Nitrones with Alkynes via Rhodium(III) Catalyzed C-H Activation

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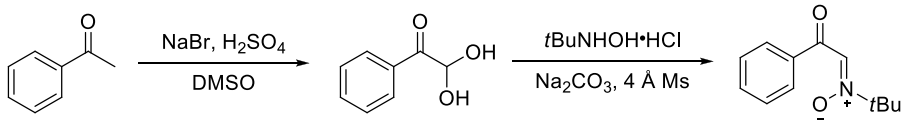
1. General Considerations

Unless otherwise stated, all reagents and solvents were used as received from commercial sources. All reactions were performed in flame-dried glassware using sealed tube or Schlenk tube. ^{1}H NMR spectra were recorded on Bruker AV 400 (400 MHz). Chemical shifts were reported in parts per million (ppm) referenced to the appropriate solvent peak. The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = double of doublet, dt = double of triplet, td = triple of doublet. Coupling constants, *J*, were reported in hertz unit (Hz). ^{13}C NMR spectra were recorded on Bruker AV 400 (100 MHz). Chemical shifts were reported in ppm referenced to the center line of a triplet at 77.0 ppm of chloroform-*d*, 29.9, 206.7 of acetone-d_6.

2. Synthesis of Substrates

2.1 Synthesis of Nitrones



According to reported literatures,[1,2] we described a modified method here. Ketone (20 mmol) and sodium bromide (0.5 g) were dissolved in DMSO (10 mL) in a 100 mL round bottom flask equipped a reflux condensor. The mixture was heated to 85 ℃ with stirring and then ~0.5 mL of concentrated sulfuric acid was quickly added to the reaction. The reaction mass foamed due to dimethyl sulfide gas formation and the reaction temperature began to rise. The mixture was stirred at 115 ℃ for 30 min. After cooling, 50 mL of ice cold water was added, and the mixture was extracted by EtOAc three times. The organic layer was washed with water and brine then dried by anhydrous Na_2SO_4. The solvent was removed under reduced pressure to afford crude product glyoxal, which will be used directly to the next step. To a stirred solution of a glyoxal in dichloromethane (20 mL) was added 4 Å MS (5 g) under N_2 atmosphere. The reaction mixture was stirred at room temperature for 2 h, then *t*BuNHOH·HCl (2.5 g, 20 mmol) and Na_2CO_3 (2.2 g, 20 mmol) was added. After stirring at 35 °C for 6 h, 50 mL water was added. Then the organic layer was separated and the aqueous layer was extracted by EtOAc three times. The combined organic layers were washed with water and brine then dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure to get the crude product, further purification by recrystallization afforded the final product almost in quantitative yield.

2.2 Representative Procedure for the Rh-Catalyzed Cyclization between Nitrones and Alkynes

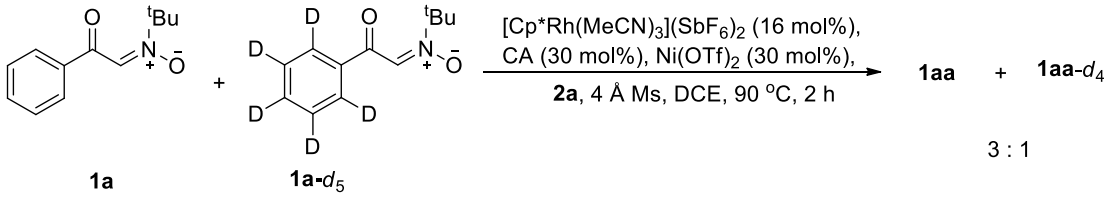
A pressure tube was charged with $[Cp^*Rh(MeCN)_3](SbF_6)_2$ (0.0138 g, 0.016 mmol), $Ni(OTf)_2$ (0.0215 g, 0.06 mmol), nitrone (**1**, 0.2 mmol), alkyne (**2**, 0.21 mmol), citric acid (0.0116 g, 0.060

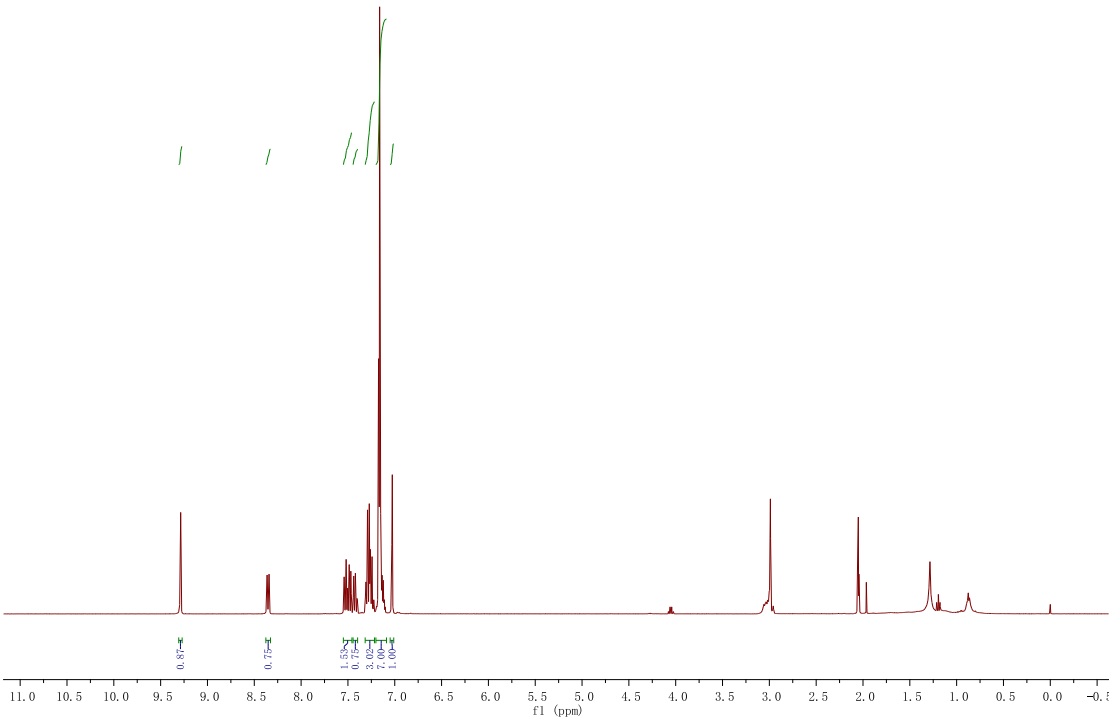
mmol), HOPiv (0.0245 g, 0.24 mmol) and 4 Å MS (100 mg). DCE (5 mL) was then added and the mixture was stirred at 90 °C for 12 h. Then the solvent was evaporated and the crude residue was purified through column chromatography on silica gel to afford the desired product **3**.

3. Mechanistic Studies

3.1.1 Intermolecular competition

An equimolar mixture of 2-methyl-*N*-(2-oxo-2-phenylethylidene)propan-2-amine oxide **1a** (0.1 mmol) and **1a**-d_5 (0.1 mmol), $[Cp^*Rh(MeCN)_3](SbF_6)_2$ (0.0138 g, 0.016 mmol), $Ni(OTf)_2$ (0.0215 g, 0.06 mmol), alkyne **2a** (0.0373 g, 0.21 mmol), citric acid (0.0116 g, 0.060 mmol), HOPiv (0.0245 g, 0.24 mmol) and 4 Å MS (100 mg). DCE (5 mL) were charged into a pressure tube. The reaction mixture was stirred under nitrogen at 90 °C for 1 h. The solvent was rapidly removed under reduced pressure and the residue was purified by silica gel chromatography to afford the mixed product. The KIE value (k_H/k_D = 3.0) was determined by ^{1}H NMR spectroscopic on the basis of the analysis of the product mixture.

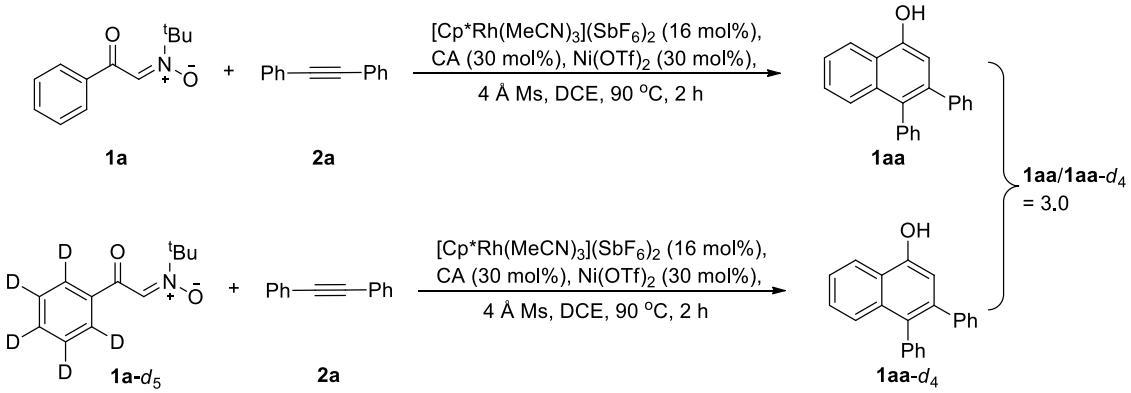


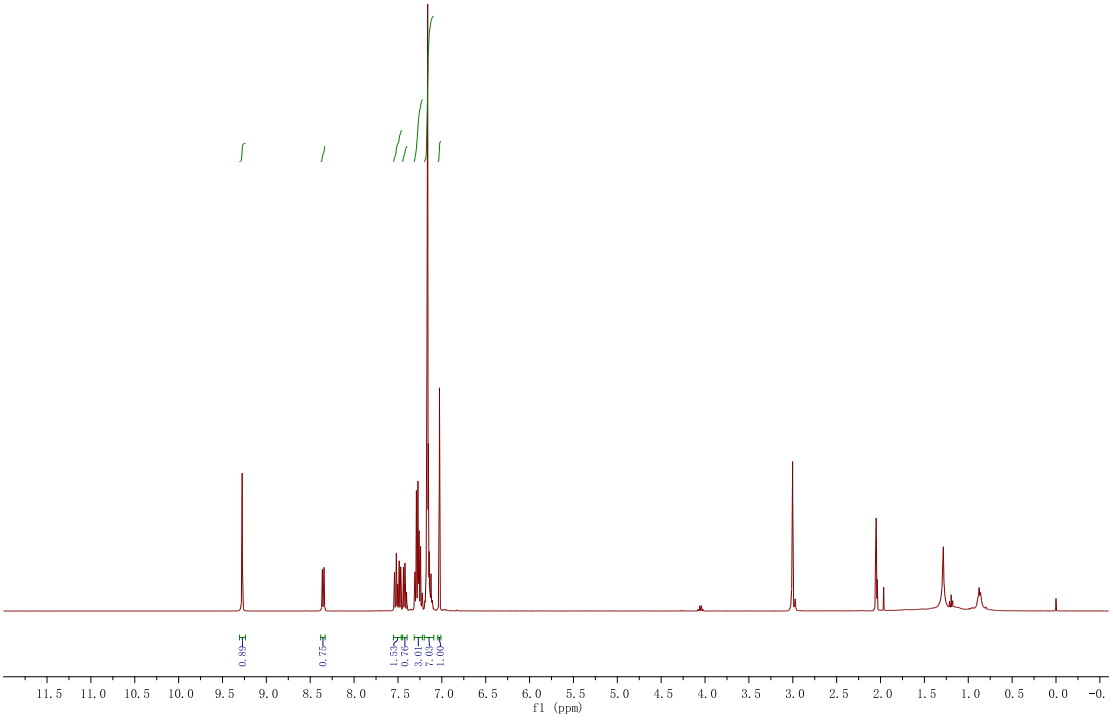


3.1.2 Parallel Experiment

Two independent reactions with **1a** or deuterated substrate **1a**-d_5 under the standard conditions were performed. Suspensions of 2-methyl-*N*-(2-oxo-2-phenylethylidene)propan-2-amine oxide **1a**

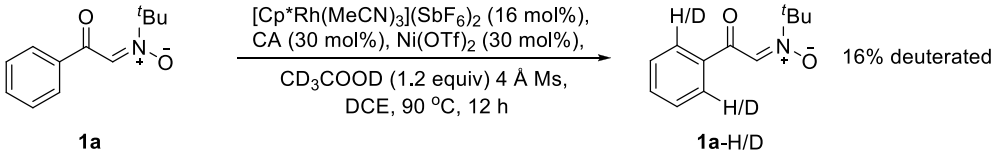
(0.0205 g, 0.1 mmol) or **1a**-d_5 (0.0210, 0.1 mmol), [Cp*Rh(MeCN)$_3$](SbF$_6$)$_2$ (0.0069 g, 0.008 mmol), Ni(OTf)$_2$ (0.0108 g, 0.030 mmol), alkyne **2a** (0.0187 g, 0.105 mmol), citric acid (0.0058 g, 0.030 mmol), HOPiv (0.0122 g, 0.12 mmol) and 4 Å MS (100 mg) and DCE (5 mL) were stirred at 90 °C for 1 h under nitrogen. Both reactions were quenched at the same time and these two mixtures were rapidly combined and the volatiles were removed under reduced pressure and the residue was purified by silica gel chromatography. KIE value (k_H/k_D = 3.0) was determined on the basis of ^{1}H NMR analysis.



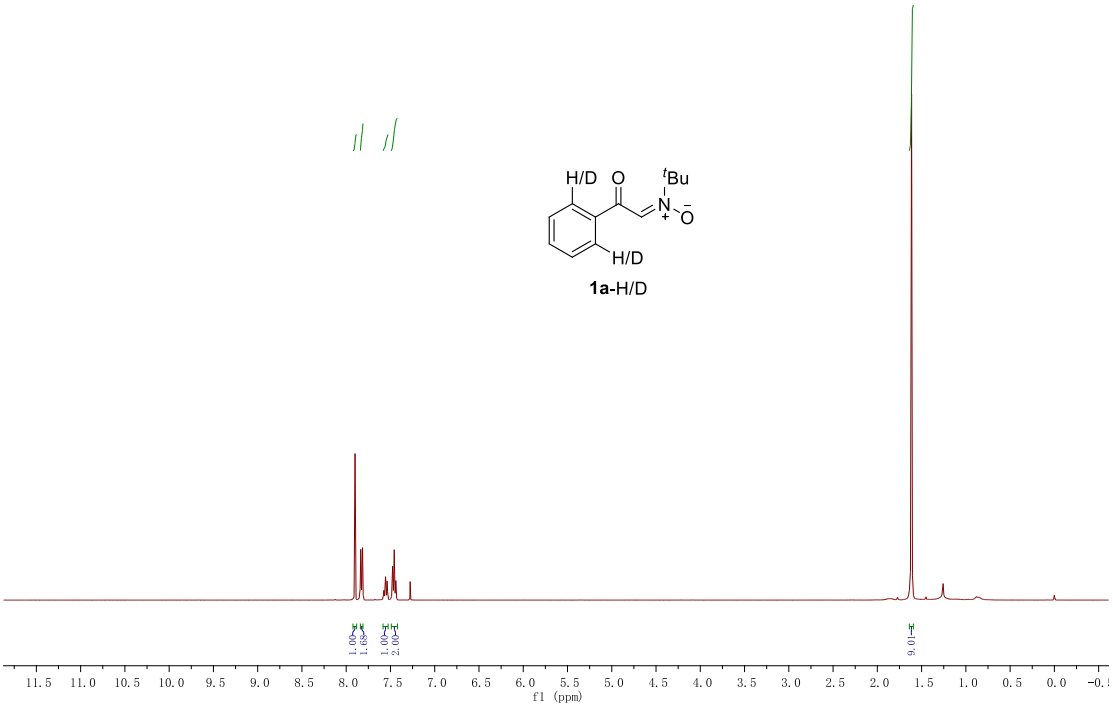


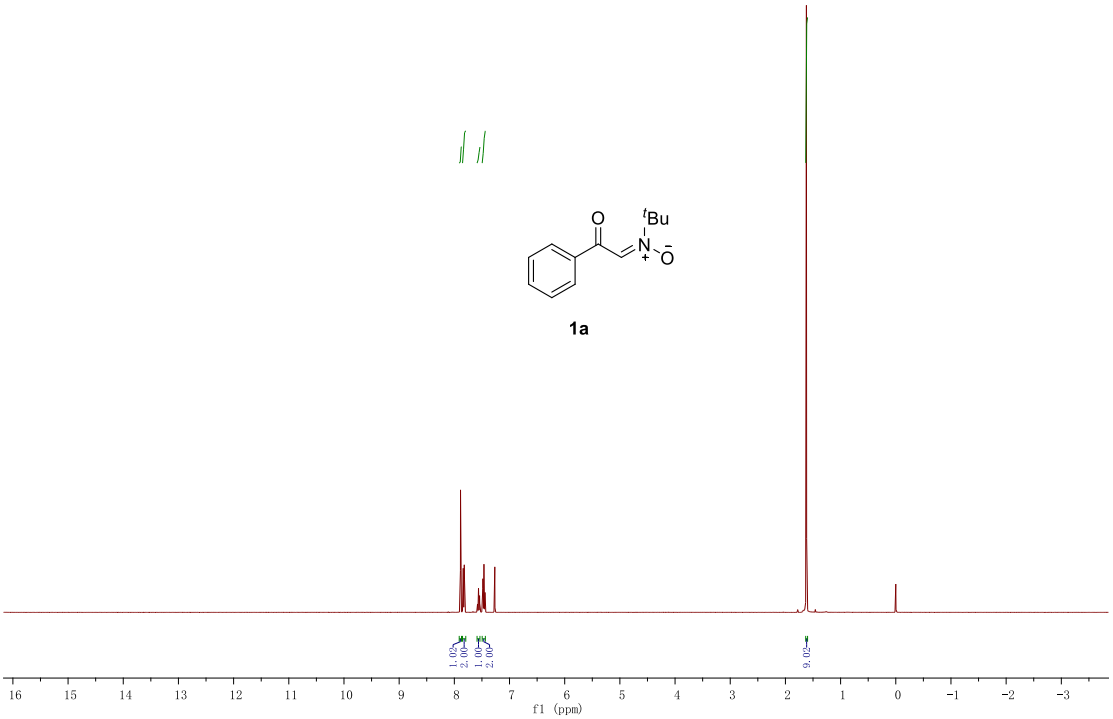
3.1.2 H/D Exchange Experiment

The reaction was run using CD_3COOD as acid additive following the standard procedure for cyclization reaction. The analysis of ^{1}H NMR indicating 16% of deuterium at ortho positions.

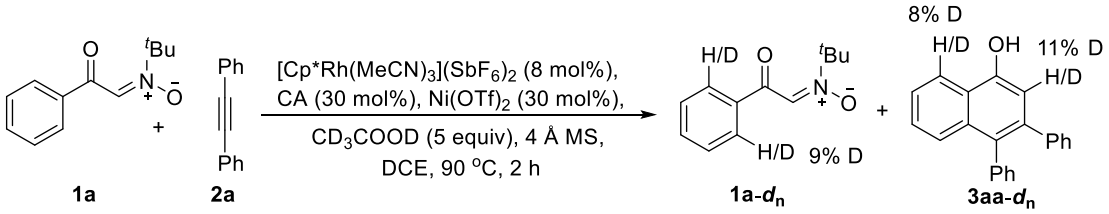

[Cp*Rh(MeCN)3](SbF6)2 (16 mol%),
CA (30 mol%), Ni(OTf)2 (30 mol%),
CD3COOD (1.2 equiv) 4 Å Ms,
DCE, 90 °C, 12 h
16% deuterated

1a **1a**-H/D

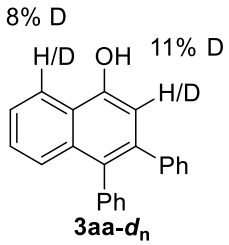

H/D
H/D
1a-H/D
f1 (ppm)

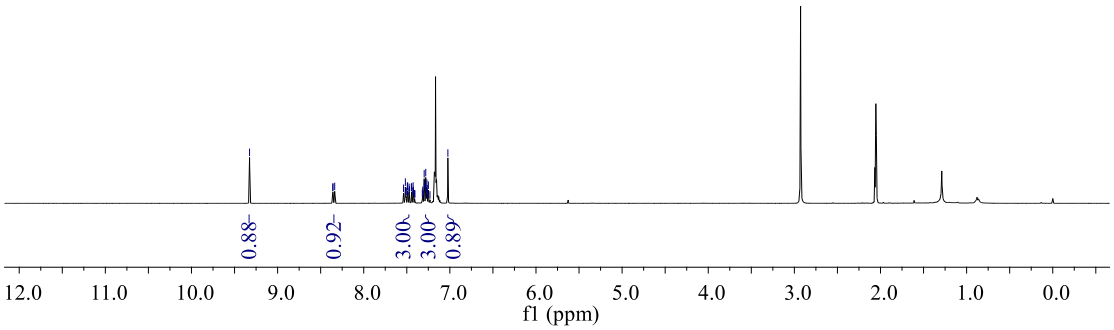

1a
f1 (ppm)

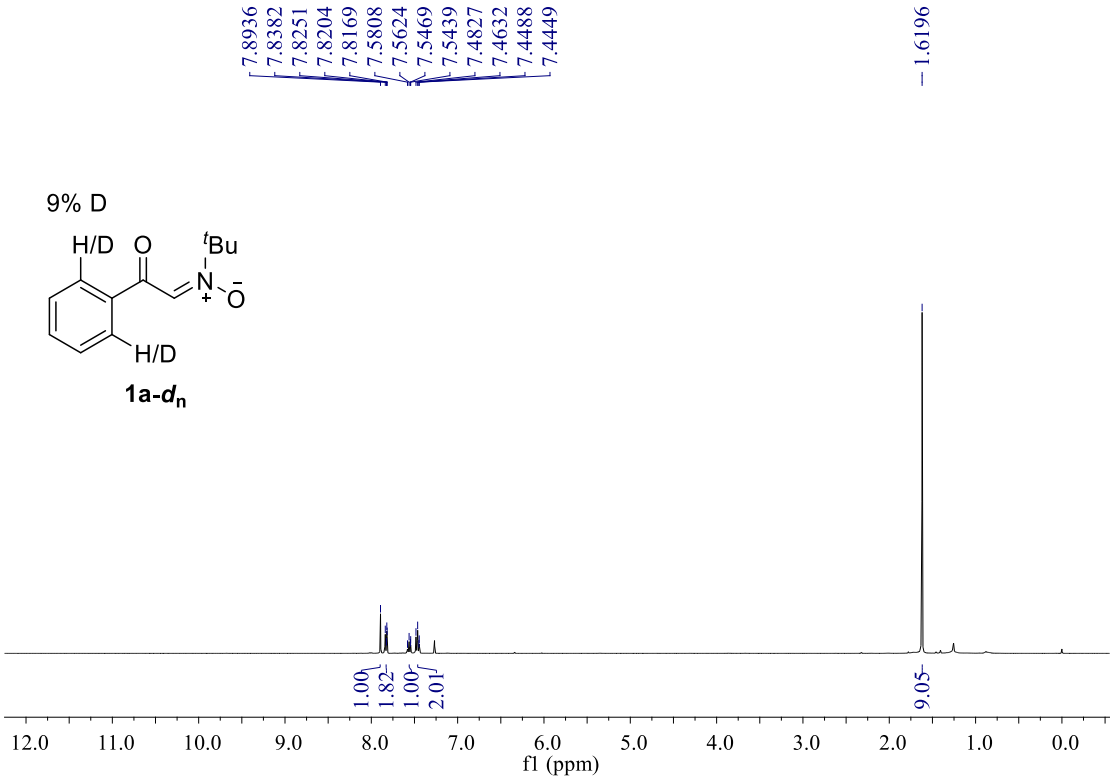
H/D Exchange Experiment in the Presence of an Alkyne



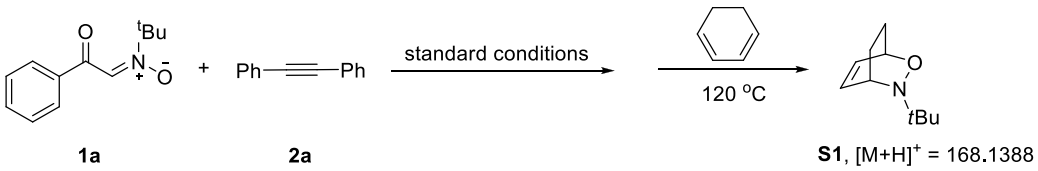
A pressure tube was charged with $[Cp^*Rh(MeCN)_3](SbF_6)_2$ (0.0138 g, 0.016 mmol), $Ni(OTf)_2$ (0.0215 g, 0.06 mmol), nitrone (**1a**, 0.2 mmol), alkyne (**2a**, 0.21 mmol), citric acid (0.0116 g, 0.060 mmol), CD_3COOD (0.0640 g, 1.0 mmol) and 4 Å MS (100 mg). DCE (5 mL) was then added and the mixture was stirred at 90 °C for 2 h. The solvent was rapidly removed under reduced pressure and the residue was purified by silica gel chromatography to afford **3aa-*d*$_n$** and the recovered **1a-*d***.



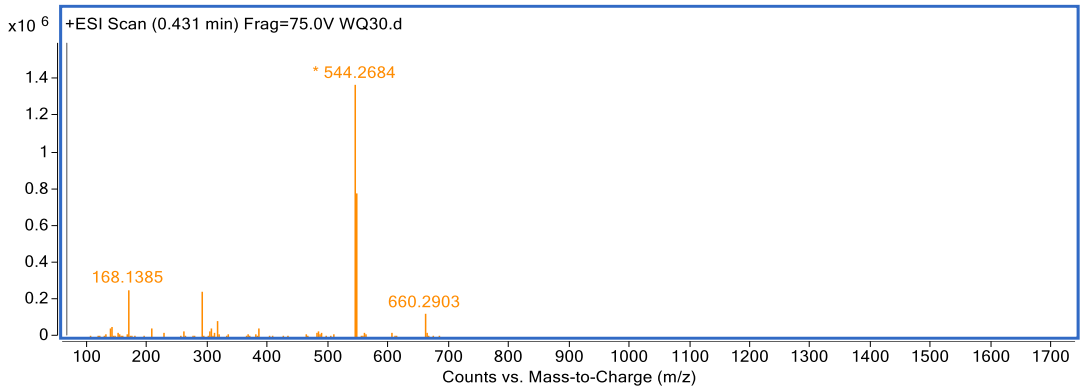




5. Trapping Experiment

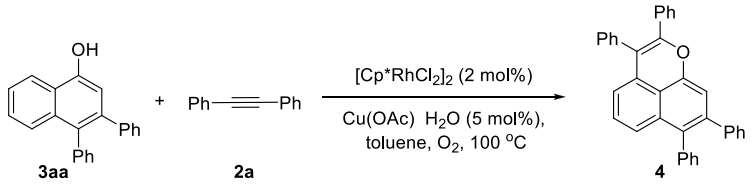


nitrone **1a** (0.0410g, 0.2 mmol), alkyne **2a** (0.0373g, 0.21 mmol) reacted in standard conditions for 12 h. After the reaction was cooled to 0 °C, to the mixture was added cyclohexa-1,3-diene (0.0400g, 0.5 mmol) under nitrogen. Then the reaction mixture was further stirred at 120°C for 4 h. The HRMS spectrum was recorded after the mixture was cooled to room temperature. HRMS (ESI) calculated for $C_{10}H_{18}NO$ $[M + H]^+$: 168.1388, found:168.1385.

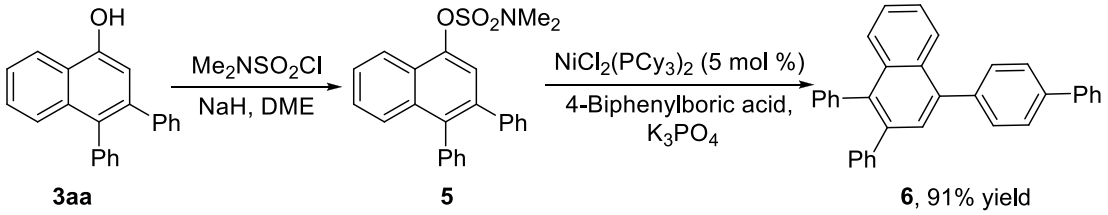


4. The Oxidative Annulation of 3aa with Alkyne

A dried schlenk tube equipped with a stir bar was loaded with naphthol **3aa** (0.0592 g, 0.2 mmol), 1,2-diphenylethyne (0.0178 g, 0.1 mmol), $[Cp^*RhCl_2]_2$ (0.0025 g, 0.004 mmol) $Cu(OAc)_2$ (0.002 g, 0.01 mmol) and toluene (3 mL) under the atmosphere of O_2 (1 atm). The tube was then stirred at 100 °C for 12 h. After cooling down to room temperature, the solvent was evaporated in vacuum, the residue was purified through flash column chromatography on silica gel to afford the pure product **4**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.39 (m, 2H), 7.38 – 7.34 (m, 3H), 7.31 (m, 4H), 7.28 – 7.25 (m, 1H), 7.24 – 7.15 (m, 11H), 7.11 (dd, *J* = 8.6, 7.2 Hz, 1H), 7.06 (s, 1H), 6.52 (dd, *J* = 7.2, 0.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 149.3, 141.7, 140.2, 138.9, 135.6, 134.1, 133.9, 131.8, 131.5, 131.0, 130.0, 129.7, 129.1, 128.9, 128.5, 128.1, 128.0, 127.7, 127.63, 127.61, 126.6, 126.3, 122.9, 122.0, 117.5, 115.9, 109.3. HRMS (ESI)**:** calcd for $C_{36}H_{25}O$ ($[M+H]^+$) 473.1905, found 473.1906.

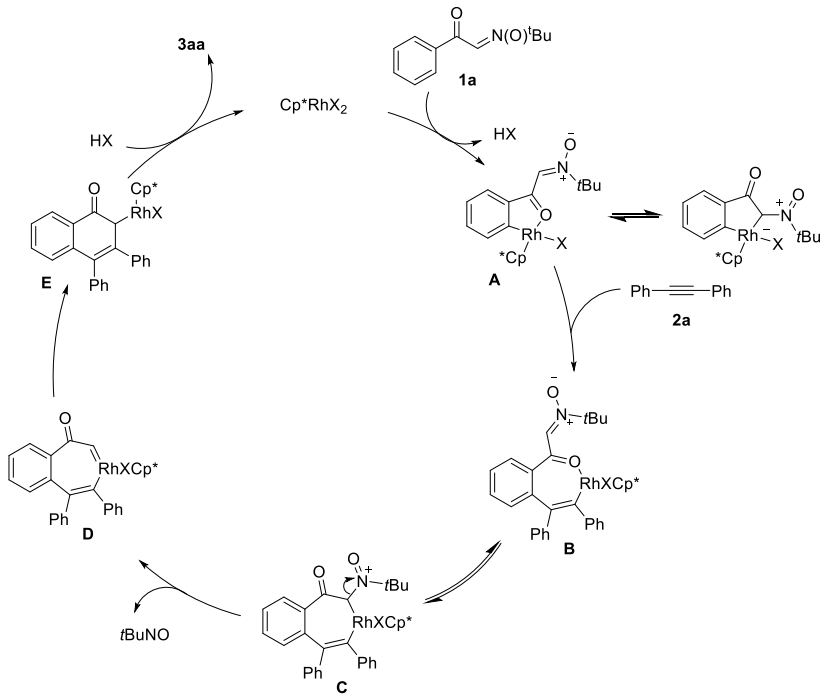


5. The Nickel-Catalyzed Cross-Coulpling



Sulfamate **5** was prepared according to the report literature[3] as a white solid. A sealed tube with a magnetic stir bar was charged with sulfamate **5** (0.0806 g, 0.2 mmol), 4-biphenylboric acid (0.0990 g, 2.5 mmol), $NiCl_2(PCy_3)_2$ (0.0069 g, 0.001 mmol), anhydrous powdered K_3PO_4 (0.1910 g, 0.9 mmol) and 5 mL CH_3CN. The mixture was allowed to stir rapidly at 23 °C for 1 h, and then heated to 100 °C for 12 h. After cooling down to room temperature, the solvent was was evaporated in vacuum, the residue was purified through flash column chromatography on silica gel to afford the pure product **6**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.1 Hz, 1H), 7.78 – 7.69 (m, 3H), 7.66 (m, 4H), 7.59 (d, *J* = 4.7 Hz, 1H), 7.50 – 7.34 (m, 5H), 7.33 – 7.21 (m, 5H), 7.21 – 7.06 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.9, 140.9, 140.3, 139.7, 139.5, 139.1, 138.0, 137.3, 133.2, 131.6, 131.0, 130.7, 130.2, 129.5, 128.9, 127.9, 127.7, 127.5, 127.3, 127.2, 127.1, 126.9, 126.3, 126.2, 126.1, 125.9.

6. Alternative Proposed Mechanism Involving α-oxo Carbene Species



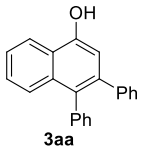
7. References

(1) S. V. Karpov, A. A. Grigor'ev, Y. S. Kayukov, I. V. Karpova, O. E. Nasakin and V. A. Tafeenko, *J. Org. Chem.*, **2016**, *81*, 6402.

(2) P. Wang, W. -J. Tao, X. -L. Sun, S. Liao and Y. Tang, *J. Am. Chem. Soc*., **2013**, *135*, 16849.

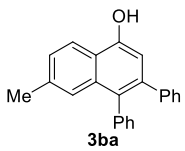
(3) S. D. Ramgren, L. Hie, Y. Ye and N. K. Garg. *Org. Lett.*, **2013**, *15*, 3950.

8. Spectroscopic Data



3aa

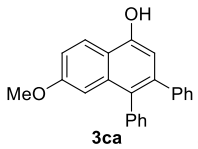
3,4-diphenylnaphthalen-1-ol **3aa** was purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 81% yield (47.6 mg, 0.16 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.23 (brs, 1H), 8.35 (d, *J* = 8.2 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.51 – 7.46 (m, 1H), 7.45 – 7.39 (m, 1H), 7.27 (m, 3H), 7.16 (m, 7H), 7.03 (s, 1H). ^{13}C NMR (100 MHz, Acetone) δ 152.3, 142.3, 139.4, 138.8, 134.0, 131.8, 129.8, 129.2, 127.7, 127.5, 126.5, 126.4, 126.2, 126.1, 124.5, 124.2, 122.0, 110.2. HRMS (ESI)**:** calcd for $C_{22}H_{15}O$ ([M-H]$^-$) 295.1123, found 295.1126.



3ba

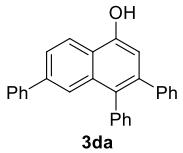
6-methyl-3,4-diphenylnaphthalen-1-ol **3ba** was purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 82% yield (50.9 mg, 0.16

mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.16 (brs, 1H), 8.25 (d, *J* = 8.9 Hz, 1H), 7.33 (dd, *J* = 3.9, 3.2 Hz, 2H), 7.30 – 7.21 (m, 3H), 7.19 – 7.08 (m, 7H), 6.95 (s, 1H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, Acetone) δ 152.4, 142.5, 139.5, 139.0, 135.9, 134.2, 131.9, 129.8, 128.6, 127.7, 127.5, 126.6, 126.3, 126.0, 125.2, 122.5, 122.0, 109.5, 21.1. HRMS (ESI)**:** calcd for $C_{23}H_{17}O$ ([M-H]$^-$) 309.1279, found 309.1282.



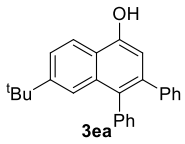
3ca

6-methoxy-3,4-diphenylnaphthalen-1-ol **3ca** was purified via silica gel column chromatography (hexane/ethyl acetate = 10/1, v/v) as a yellow solid in 73% yield (47.6 mg, 0.15 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.12 (brs, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.40 (t, *J* = 8.0 Hz, 1H), 7.14 – 6.99 (m, 10H), 6.94 (s, 1H), 6.88 (d, *J* = 7.6 Hz, 1H), 3.33 (s, 3H). ^{13}C NMR (100 MHz, Acetone) δ 157.1, 151.8, 143.5, 142.9, 139.8, 130.6, 129.9, 127.7, 127.1, 126.1, 125.8, 125.7, 125.3, 125.0, 124.6, 114.6, 110.8, 107.4, 54.7. HRMS (ESI)**:** calcd for $C_{23}H_{17}O_2$ ([M-H]$^-$) 325.1229, found 325.1233.



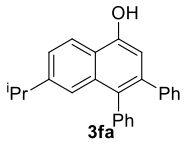
3da

3,4,6-triphenylnaphthalen-1-ol **3da** was purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 73% yield (54.3 mg, 0.15 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.35 (brs, 1H), 8.45 (d, *J* = 9.2 Hz, 1H), 7.84 – 7.73 (m, 2H), 7.56 (d, *J* = 7.4 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.30 (m, 3H), 7.27 – 7.20 (m, 3H), 7.19 – 7.10 (m, 5H), 7.06 (s, 1H). ^{13}C NMR (100 MHz, Acetone) δ 152.4, 142.3, 141.1, 139.5, 139.3, 139.0, 134.3, 131.9, 129.8, 129.5, 128.8, 127.8, 127.5, 127.3, 127.0, 126.5, 126.2, 124.1, 123.9, 123.4, 122.9, 110.5. HRMS (ESI)**:** calcd for $C_{28}H_{19}O$ ([M-H]$^-$) 371.1436, found 371.1439.



3ea

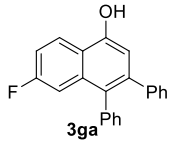
6-tert-butyl-3,4-diphenylnaphthalen-1-ol **3ea** was purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 82% yield (57.8 mg, 0.16 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.28 – 8.95 (br, 1H), 8.29 (dd, *J* = 8.8, 3.2 Hz, 1H), 7.62 (dd, *J* = 8.8, 1.9 Hz, 1H), 7.57 (d, *J* = 1.9 Hz, 1H), 7.35 – 7.21 (m, 3H), 7.20 – 7.06 (m, 7H), 7.00 – 6.89 (m, 1H), 1.26 (s, 9H). ^{13}C NMR (100 MHz, Acetone) δ 152.2, 148.8, 142.6, 139.6, 138.8, 133.9, 131.9, 129.9, 129.2, 127.6, 127.5, 126.3, 126.0, 123.2, 122.4, 121.8, 121.4, 109.7, 34.6, 30.5. HRMS (ESI)**:** calcd for $C_{26}H_{23}O$ ([M-H]$^-$) 351.1749, found 351.1749.



3fa

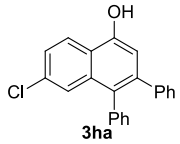
6-isopropyl-3,4-diphenylnaphthalen-1-ol **3fa** was purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 73% yield (49.5

mg, 0.15 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.18 (brs, 1H), 8.29 (d, *J* = 8.6 Hz, 1H), 7.47 – 7.37 (m, 2H), 7.29 (dt, *J* = 6.8, 1.7 Hz, 1H), 7.25 – 7.20 (m, 1H), 7.19 – 7.08 (m, 7H), 6.97 (s, 1H), 2.90 (m, 1H), 1.19 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (100 MHz, Acetone) δ 152.3, 146.8, 142.5, 139.5, 138.9, 134.2, 131.9, 129.8, 128.9, 127.6, 127.5, 126.3, 126.0, 123.8, 122.9, 122.7, 122.2, 109.6, 34.3, 23.3. HRMS (ESI)**:** calcd for $C_{25}H_{21}O$ ([M-H]$^-$) 337.1592, found 337.1595.



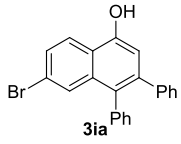
3ga

6-fluoro-3,4-diphenylnaphthalen-1-ol **3ga** was purified via silica gel column chromatography (hexane/ethyl acetate = 60/1, v/v) as a yellow solid in 66% yield (41.5 mg, 0.13 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.44 (brs, 1H), 8.56 – 8.28 (m, 1H), 7.38 – 7.23 (m, 4H), 7.23 – 7.08 (m, 8H), 7.05 – 6.99 (m, 1H). ^{13}C NMR (100 MHz, Acetone) δ 161.4 (d, *J* = 242 Hz), 152.61, 142.0, 140.5, 138.9, 135.3 (d, *J* = 9 Hz), 131.7, 129.7, 128.7 (d, *J* = 5 Hz), 127.9, 127.6, 126.6, 126.3, 125.2 (d, *J* = 10 Hz), 121.3, 114.3 (d, *J* = 25 Hz), 109.7, 109.3 (d, *J* = 22 Hz). ^{19}F NMR (376 MHz, Acetone) δ -114.92. HRMS (ESI)**:** calcd for $C_{22}H_{14}FO$ ([M-H]$^-$) 313.1029, found 313.1033.



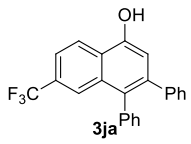
3ha

6-chloro-3,4-diphenylnaphthalen-1-ol **3ha** was purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 72% yield (47.5 mg, 0.14 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.49 (brs, 1H), 8.35 (d, *J* = 8.9 Hz, 1H), 7.56 – 7.43 (m, 2H), 7.37 – 7.25 (m, 3H), 7.25 – 7.12 (m, 7H), 7.05 (s, 1H). ^{13}C NMR (100 MHz, Acetone) δ 152.5, 141.9, 140.5, 138.6, 134.8, 132.2, 131.7, 129.7, 128.5, 127.9, 127.6, 126.7, 126.4, 125.0, 124.8, 124.4, 122.5, 110.7. HRMS (ESI)**:** calcd for $C_{22}H_{14}ClO$ ([M-H]$^-$) 329.0733, found 329.0733.



3ia

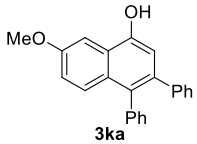
6-bromo-3,4-diphenylnaphthalen-1-ol **3ia** was purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 77% yield (57.7 mg, 0.15 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.50 (brs, 1H), 8.28 (d, *J* = 8.9 Hz, 1H), 7.68 (d, *J* = 1.8 Hz, 1H), 7.59 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.30 (m, 3H), 7.24 – 7.11 (m, 7H), 7.07 (s, 1H). ^{13}C NMR (100 MHz, Acetone) δ 152.5, 141.8, 140.5, 138.6, 135.2, 131.7, 129.7, 128.5, 128.1, 127.9, 127.6, 127.6, 126.8, 126.4, 124.5, 122.7, 120.7, 110.9. HRMS (ESI)**:** calcd for $C_{22}H_{14}BrO$ ([M-H]$^-$) 373.0228, found 373.0228, 375.0212.



3ja

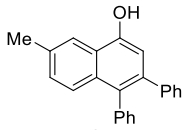
3,4-diphenyl-6-(trifluoromethyl)naphthalen-1-ol **3ja** was purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 71% yield (51.7 mg, 0.14 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.65 (brs, 1H), 8.55 (d, *J* = 8.8 Hz, 1H), 7.90

(s, 1H), 7.73 (dd, *J* = 8.8, 1.5 Hz, 1H), 7.47 – 7.27 (m, 3H), 7.24 – 7.12 (m, 8H). ^{13}C NMR (100 MHz, Acetone) δ 152.4, 141.6, 140.7, 138.3, 131.7, 131.5 (q, *J* = 278 Hz), 129.7, 128.0, 127.7 (q, *J* =32 Hz), 127.6, 126.9, 126.5, 126.0, 125.5, 123.9, 123.7 (q, *J* = 5 Hz), 123.3, 119.7 (q, *J* = 3 Hz), 112.5. ^{19}F NMR (376 MHz, Acetone) δ -62.90. HRMS (ESI)**:** calcd for $C_{23}H_{14}F_3O$ ([M-H]$^-$) 363.0997, found 363.0999.



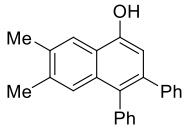
3ka

7-methoxy-3,4-diphenylnaphthalen-1-ol **3ka** was purified via silica gel column chromatography (hexane/ethyl acetate = 20/1, v/v) as a yellow solid in 71% yield (46.3 mg, 0.14 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.19 (brs, 1H), 7.96 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.44 – 7.35 (m, 1H), 7.15 – 6.97 (m, 10H), 6.94 (s, 1H), 6.88 (d, *J* = 7.1 Hz, 1H), 3.33 (s, 3H). ^{13}C NMR (100 MHz, Acetone) δ 157.1, 151.9, 143.4, 142.9, 139.8, 130.6, 129.9, 127.7, 127.1, 126.1, 125.8, 125.6, 125.3, 125.0, 124.6, 114.6, 110.8, 107.3, 54.7. HRMS (ESI)**:** calcd for $C_{23}H_{17}O_2$ ([M-H]$^-$) 325.1229, found 325.1229.



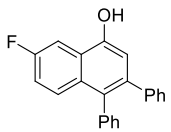
3la

7-methyl-3,4-diphenylnaphthalen-1-ol **3la** was purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 76% yield (47.1 mg, 0.15 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.18 (brs, 1H), 8.13 (s, 1H), 7.43 (d, *J* = 8.7 Hz, 1H), 7.30 – 7.21 (m, 4H), 7.18 – 7.10 (m, 7H), 6.99 (s, 1H), 2.51 (s, 3H). ^{13}C NMR (100 MHz, Acetone) δ 151.9, 142.5, 139.5, 137.8, 134.0, 132.2, 131.8, 129.9, 129.1, 128.5, 127.7, 127.5, 126.3, 126.2, 126.0, 124.4, 121.0, 110.2, 20.8. HRMS (ESI)**:** calcd for $C_{23}H_{17}O$ ([M-H]$^-$) 309.1279, found 309.1282.



3ma

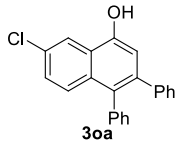
6,7-dimethyl-3,4-diphenylnaphthalen-1-ol **3ma** was purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 72% yield (46.9 mg, 0.14 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.09 (brs, 1H), 8.09 (s, 1H), 7.38 – 7.18 (m, 4H), 7.19 – 7.05 (m, 7H), 6.92 (s, 1H), 2.44 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, Acetone) δ 151.9, 142.6, 139.7, 137.9, 135.9, 134.0, 132.9, 131.8, 129.9, 128.4, 127.6, 127.5, 126.2, 125.94, 125.90, 123.1, 121.6, 109.5, 19.6, 19.3. HRMS (ESI)**:** calcd for $C_{24}H_{19}O$ ([M-H]$^-$) 323.1436, found 323.1440.



3na

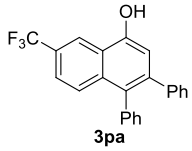
7-fluoro-3,4-diphenylnaphthalen-1-ol **3na** was purified via silica gel column chromatography (hexane/ethyl acetate = 50/1, v/v) as a yellow solid in 82% yield (51.5 mg, 0.16 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.49 (brs, 1H), 8.20 (dd, *J* = 8.4, 0.7 Hz, 1H), 7.46 (ddd, *J* =

8.4, 7.7, 4.6 Hz, 1H), 7.23 – 7.06 (m, 11H), 7.03 (s, 1H). ^{13}C NMR (100 MHz, Acetone) δ 159.5 (d, *J* = 253 Hz), 152.1 (d, *J* = 4 Hz), 142.1, 141.3 (d, *J* = 4 Hz), 140.9, 130.7 (d, *J* = 4 Hz), 129.8, 127.3, 126.7, 126.5 (d, *J* = 4 Hz), 126.1, 125.8, 125.7 (d, *J* = 2 Hz), 124.7 (d, *J* = 9 Hz), 123.5 (d, *J* = 9 Hz), 118.4 (d, *J* = 4 Hz), 112.2 (d, *J* = 23 Hz), 111.2 (d, *J* = 1 Hz). ^{19}F NMR (376 MHz, Acetone) δ -106.57. HRMS (ESI)**:** calcd for $C_{22}H_{14}FO$ ([M-H]$^-$) 313.1029, found 313.1028.



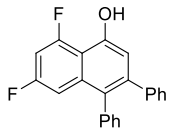
3oa

7-chloro-3,4-diphenylnaphthalen-1-ol **3oa** as purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 53% yield (35.1 mg, 0.11 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.48 (brs, 1H), 8.30 (d, *J* = 2.3 Hz, 1H), 7.53 (d, *J* = 9.1 Hz, 1H), 7.42 (dd, *J* = 9.1, 2.3 Hz, 1H), 7.33 – 7.23 (m, 3H), 7.20 – 7.12 (m, 7H), 7.08 (s, 1H). ^{13}C NMR (100 MHz, Acetone) δ 151.6, 141.9, 139.5, 138.8, 132.3, 131.7, 130.1, 129.8, 129.3, 128.5, 127.8, 127.6, 127.0, 126.6, 126.3, 124.9, 120.9, 111.4. HRMS (ESI)**:** calcd for $C_{22}H_{14}ClO$ ([M-H]$^-$) 329.0733, found 329.0735.



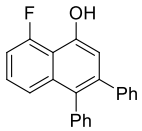
3pa

3,4-diphenyl-7-(trifluoromethyl)naphthalen-1-ol **3pa** as purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 61% yield (37.9 mg, 0.12 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.79 (brs, 1H), 8.69 (d, *J* = 0.8 Hz, 1H), 7.72 (d, *J* = 9.0 Hz, 1H), 7.67 (dd, *J* = 9.0, 1.9 Hz, 1H), 7.37 – 7.26 (m, 3H), 7.25 – 7.12 (m, 8H). ^{13}C NMR (100 MHz, Acetone) δ 153.0, 141.73, 141.71, 138.5, 135.2, 131.7, 129.7, 129.3, 127.9, 127.7, 127.6, 126.8, 126.5, 125.7 (q, *J* = 32 Hz), 124.9 (q, *J* = 305 Hz), 123.0, 121.8 (q, *J* = 3 Hz), 120.0 (q, *J* = 5 Hz), 111.6. ^{19}F NMR (376 MHz, Acetone) δ -62.60. HRMS (ESI)**:** calcd for $C_{23}H_{14}F_3O$ ([M-H]$^-$) 363.0997, found 363.0998.



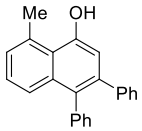
3qa

6,8-difluoro-3,4-diphenylnaphthalen-1-ol **3qa a**s purified via silica gel column chromatography (hexane/ethyl acetate = 50/1, v/v) as a yellow solid in 62% yield (41.2 mg, 0.12 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.30 (brs, 1H), 7.35 – 7.25 (m, 3H), 7.22 – 7.06 (m, 8H), 7.02 (s, 1H), 6.94 (ddd, *J* = 11.4, 2.5, 1.3 Hz, 1H). ^{13}C NMR (100 MHz, Acetone) δ 160.2 (dd, *J* =258 Hz, 243 Hz), 160.1 (dd, *J* = 258 Hz, 243 Hz), 152.5, 141.6, 141.4, 138.7, 136.7 (dd, *J* = 100 Hz, 6Hz), 131.6, 129.6, 128.6, 128.0, 127.6, 126.9, 126.6, 112.0, 111.5 (d, *J* = 10 Hz), 105.8 (dd, *J* = 23 Hz, 18 Hz), 101.0 (dd, *J* = 29 Hz, 3 Hz). ^{19}F NMR (376 MHz, Acetone) δ -108.27 (d, *J* = 2 Hz),-112.85 (d, *J* = 5 Hz). HRMS (ESI)**:** calcd for $C_{22}H_{13}F_2O$ ([M-H]$^-$) 331.0934, found 331.0936.



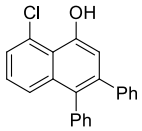
3ra

8-fluoro-3,4-diphenylnaphthalen-1-ol **3ra a**s purified via silica gel column chromatography (hexane/ethyl acetate = 60/1, v/v) as a yellow solid in 87% yield (54.6 mg, 0.17 mmol). ^{1}H NMR (400 MHz, Acetone) δ 8.95 (d, *J* = 1.4 Hz, 1H), 7.43 – 7.21 (m, 5H), 7.19 – 7.10 (m, 8H), 7.06 (s, 1H). ^{13}C NMR (100 MHz, Acetone) δ 159.4 (d, *J* = 252 Hz) , 152.0 (d, *J* = 3 Hz), 141.6, 140.3, 139.2, 136.7 (d, *J* = 4 Hz), 131.7, 129.7, 129.1, 127.8, 127.6, 126.6, 126.4, 126.3 (d, *J* = 9 Hz), 122.6 (d, *J* = 4 Hz), 114.1 (d, *J* = 10 Hz), 112.6, 109.8 (d, *J* = 22 Hz). ^{19}F NMR (376 MHz, Acetone) δ -114.62. HRMS (ESI)**:** calcd for $C_{22}H_{14}FO$ ([M-H]$^-$) 313.1029, found 313.1029.



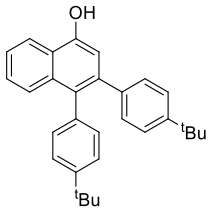
3sa

8-methyl-3,4-diphenylnaphthalen-1-ol **3sa** as purified via silica gel column chromatography (hexane/ethyl acetate = 50/1, v/v) as a yellow solid in 63% yield (39.1 mg, 0.13 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.08 (brs, 1H), 7.36 – 7.31 (m, 1H), 7.28 (m, 2H), 7.24 (dd, *J* = 5.1, 3.6 Hz, 1H), 7.22 – 7.17 (m, 2H), 7.14 (m, 7H), 6.99 (s, 1H), 3.01 (s, 3H). ^{13}C NMR (100 MHz, Acetone) δ 154.8, 142.1, 140.1, 138.6, 135.7, 135.2, 131.8, 129.7, 129.6, 127.7, 127.5, 127.4, 126.3, 126.1, 125.8, 124.8, 123.5, 111.6, 24.5. HRMS (ESI)**:** calcd for $C_{23}H_{17}O$ ([M-H]$^-$) 309.1279, found 309.1278.



3ta

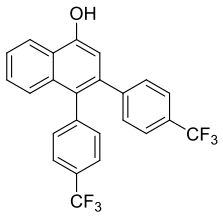
8-chloro-3,4-diphenylnaphthalen-1-ol **3ta** as purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 56% yield (37.0 mg, 0.11 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.18 (brs, 1H), 7.52 (dd, *J* = 7.4, 1.1 Hz, 1H), 7.46 (dd, *J* = 8.6, 1.1 Hz, 1H), 7.34 – 7.23 (m, 4H), 7.20 – 7.13 (m, 7H), 7.10 (s, 1H). ^{13}C NMR (100 MHz, Acetone) δ 152.9, 141.5, 140.0, 139.3, 136.7, 131.7, 129.9, 129.6, 129.5, 127.92, 127.90, 127.6, 126.7, 126.5, 126.1, 126.0, 120.8, 113.5. HRMS (ESI)**:** calcd for $C_{22}H_{14}ClO$ ([M-H]$^-$) 329.0733, found 329.0736.



3ab

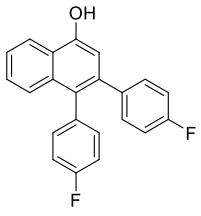
3,4-bis(4-*tert*-butylphenyl)naphthalen-1-ol **3ab** as purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 62% yield (50.1 mg, 0.12 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.18 (brs, 1H), 8.34 (dd, *J* = 8.2, 0.8 Hz, 1H), 7.60 – 7.54 (m, 1H), 7.46 (ddd, *J* = 8.2, 6.8, 1.3 Hz, 1H), 7.40 (ddd, *J* = 8.2, 6.8, 1.4 Hz, 1H), 7.34 – 7.27 (m, 2H), 7.18 (d, *J* = 8.4 Hz, 2H), 7.10 – 7.03 (m, 5H), 1.31 (s, 9H), 1.24 (s, 9H). ^{13}C NMR (100 MHz, Acetone) δ 152.2, 148.9, 148.6, 139.4, 138.8, 136.5, 134.1, 131.5, 129.6, 129.2, 126.36, 126.31, 124.4, 124.3, 124.2, 122.0, 110.2, 34.1, 33.9, 30.8, 30.7. HRMS (ESI)**:** calcd for $C_{30}H_{31}O$ ([M-H]$^-$)

407.2375, found 407.2378.



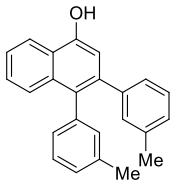
3ac

3,4-bis(4-(trifluoromethyl)phenyl)naphthalen-1-ol **3ac** as purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 69% yield (60.1 mg, 0.12 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.62 (brs, 1H), 8.41 (d, *J* = 8.3 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.58 – 7.50 (m, 3H), 7.49 – 7.44 (m, 2H), 7.37 (m, 4H), 7.06 (s, 1H). ^{13}C NMR (100 MHz, Acetone) δ 153.2, 146.05, 146.03, 143.3, 143.3, 137.7, 133.5, 132.5, 130.5, 128.3 (q, *J* = 32 Hz), 128.0 (q, *J* = 32 Hz), 127.8, 127.2, 124.7 (q, *J* = 4 Hz), 124.57 (q, *J* = 4 Hz), 124.5 (q, *J* = 270 Hz), 125.8, 125.8, 125.1, 124.4 (q, *J* = 269 Hz), 122.3, 109.6. ^{19}F NMR (376 MHz, Acetone) δ -62.80, -62.86. HRMS (ESI)**:** calcd for $C_{24}H_{13}F_6O$ ([M-H]$^-$) 431.0871, found 431.0872.



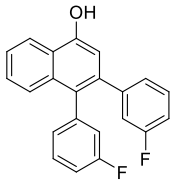
3ad

3,4-bis(4-fluorophenyl)naphthalen-1-ol **3ad** as purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 61% yield (40.6 mg, 0.12 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.32 (brs, 1H), 8.36 (dd, *J* = 8.6, 1.1 Hz, 1H), 7.57 – 7.48 (m, 2H), 7.48 – 7.41 (m, 1H), 7.21 – 7.13 (m, 4H), 7.07 (ddd, *J* = 8.8, 5.8, 2.4 Hz, 2H), 7.00 (s, 1H), 6.96 (ddd, *J* = 8.9, 5.9, 2.5 Hz, 2H). ^{13}C NMR (100 MHz, Acetone) δ 161.6 (d, *J* = 243 Hz), 161.2 (d, *J* = 243 Hz), 152.6, 138.4 (d, *J* = 3 Hz), 138.1, 135.3 (d, *J* = 3 Hz), 133.9, 133.5 (d, *J* = 8 Hz), 131.6 (d, *J* = 8 Hz), 128.2, 126.8, 125.9, 124.7, 124.3, 122.1, 114.6 (d, *J* = 21Hz), 114.3 (d, *J* = 21 Hz), 110.0. ^{19}F NMR (376 MHz, Acetone) δ -117.40, -117.82. HRMS (ESI)**:** calcd for $C_{22}H_{13}F_2O$ ([M-H]$^-$) 331.0934, found 331.0933.



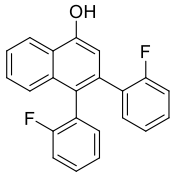
3ae

3,4-dim-tolylnaphthalen-1-ol **3ae** as purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 63% yield (39.5 mg, 0.12 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.19 (brs, 1H), 8.34 (dd, *J* = 8.3, 0.7 Hz, 1H), 7.56 – 7.51 (m, 1H), 7.47 (ddd, *J* = 8.2, 6.8, 1.3 Hz, 1H), 7.40 (ddd, *J* = 8.2, 6.8, 1.4 Hz, 1H), 7.17 (t, *J* = 7.5 Hz, 1H), 7.09 – 7.00 (m, 5H), 6.99 – 6.90 (m, 3H), 2.26 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (100 MHz, Acetone) δ 152.2, 142.3, 139.4, 138.8, 136.9, 136.7, 134.0, 132.5, 130.6, 129.3, 128.9, 127.5, 127.3, 127.03, 127.00, 126.7, 126.39, 126.35, 124.4, 124.2, 121.9, 110.2, 20.55, 20.50. HRMS (ESI)**:** calcd for $C_{24}H_{19}O$ ([M-H]$^-$) 323.1436, found 323.1435.



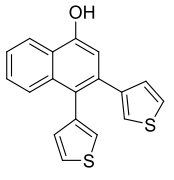
3af

3,4-bis(3-fluorophenyl)naphthalen-1-ol **3af** as purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 62% yield (41.1 mg, 0.12 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.44 (d, *J* = 2.5 Hz, 1H), 8.52 – 8.28 (m, 1H), 7.53 (ddd, *J* = 8.3, 6.4, 1.6 Hz, 1H), 7.50 – 7.41 (m, 2H), 7.36 – 7.27 (m, 1H), 7.21 (m, 3H), 7.12 – 7.05 (m, 2H), 7.00 (m, 3H). ^{13}C NMR (100 MHz, Acetone) δ 160.6 (d, *J* = 243 Hz), 159.5 (d, *J* = 243 Hz), 152.9, 134.1, 133.6, 133.3 (d, *J* = 3 Hz), 131.7 (d, *J* = 3 Hz), 129.4 (d, *J* = 8 Hz), 129.3 (d, *J* = 16 Hz), 129.1 (d, *J* =8 Hz), 126.9, 126.4 (d, *J* = 17 Hz), 125.6, 125.0, 124.5, 124.0, 123.7 (d, *J* = 3 Hz), 123.6 (d, *J* = 4 Hz), 122.2, 115.1 (d, *J* = 4 Hz), 114.9 (d, *J* = 3 Hz), 110.07. ^{19}F NMR (376 MHz, Acetone) δ -113.98, -115.65. HRMS (ESI)**:** calcd for $C_{22}H_{13}F_2O$ ([M-H]$^-$) 331.0934, found 331.0937.



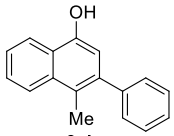
3ag

3,4-bis(2-fluorophenyl)naphthalen-1-ol **3ag** as purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 70% yield (46.5 mg, 0.14 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.44 (d, *J* = 2.5 Hz, 1H), 8.52 – 8.28 (m, 1H), 7.53 (ddd, *J* = 8.3, 6.4, 1.6 Hz, 1H), 7.50 – 7.41 (m, 2H), 7.36 – 7.27 (m, 1H), 7.21 (m, 3H), 7.12 – 7.05 (m, 2H), 7.00 (m, 3H). ^{13}C NMR (100 MHz, Acetone) δ 160.6 (d, *J* = 243 Hz), 159.5 (d, *J* = 243 Hz), 152.9, 134.1, 133.6, 133.3 (d, *J* = 3 Hz), 131.7 (d, *J* = 3 Hz), 129.4 (d, *J* = 8 Hz), 129.3 (d, *J* = 16 Hz), 129.1 (d, *J* =8 Hz), 126.9, 126.4 (d, *J* = 17 Hz), 125.6, 125.0, 124.5, 124.0, 123.7 (d, *J* = 3 Hz), 123.6 (d, *J* = 4 Hz), 122.2, 115.1 (d, *J* = 4 Hz), 114.9 (d, *J* = 3 Hz), 110.0. HRMS (ESI)**:** calcd for $C_{22}H_{13}F_2O$ ([M-H]$^-$) 331.0934, found 331.0935.



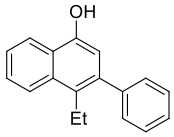
3ah

3,4-di(thiophen-3-yl)naphthalen-1-ol **3ah** as purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 37% yield (22.8 mg, 0.07 mmol). ^{1}H NMR (400 MHz, Acetone) δ 9.47 (brs, 1H), 8.52 – 8.00 (m, 1H), 7.66 – 7.57 (m, 2H), 7.53 – 7.43 (m, 2H), 7.40 – 7.33 (m, 1H), 7.28 (d, *J* = 3.0 Hz, 1H), 7.23 – 7.15 (m, 1H), 7.04 (dd, *J* = 3.4, 1.1 Hz, 1H), 6.99 (dd, *J* = 3.6, 0.7 Hz, 1H), 6.96 – 6.91 (m, 1H). ^{13}C NMR (100 MHz, Acetone) δ 153.6, 143.1, 139.7, 135.5, 133.4, 130.0, 127.2, 127.1, 127.0, 126.9, 126.7, 126.5, 126.2, 125.0, 124.3, 121.9, 120.3, 109.3. HRMS (ESI)**:** calcd for $C_{18}H_{11}OS_2$ ([M-H]$^-$) 307.0251, found 307.0252.



3ai

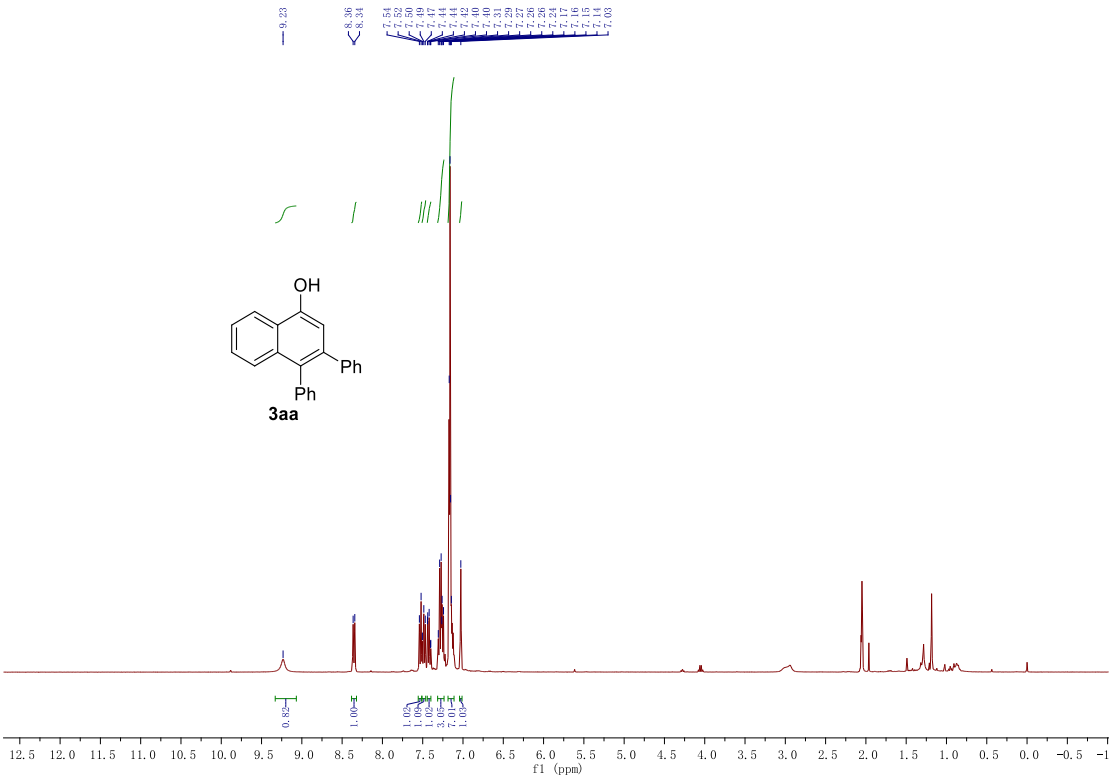
4-methyl-3-phenylnaphthalen-1-ol **3ai** as purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 85% yield (39.7 mg, 0.17 mmol). ^{1}H NMR (400 MHz, Acetone) δ 8.95 (brs, 1H), 8.32 (d, *J* = 8.3 Hz, 1H), 8.05 (d, *J* = 8.5 Hz, 1H), 7.58 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.53 – 7.44 (m, 3H), 7.42 – 7.34 (m, 3H), 6.85 (d, *J* = 1.7 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, Acetone) δ 150.9, 142.9, 139.1, 134.1, 129.5, 128.0, 126.7, 126.5, 124.5, 124.3, 124.2, 122.4, 121.2, 110.1, 14.9. HRMS (ESI)**:** calcd for $C_{17}H_{13}O$ ([M-H]$^-$) 233.0966, found 233.0969.

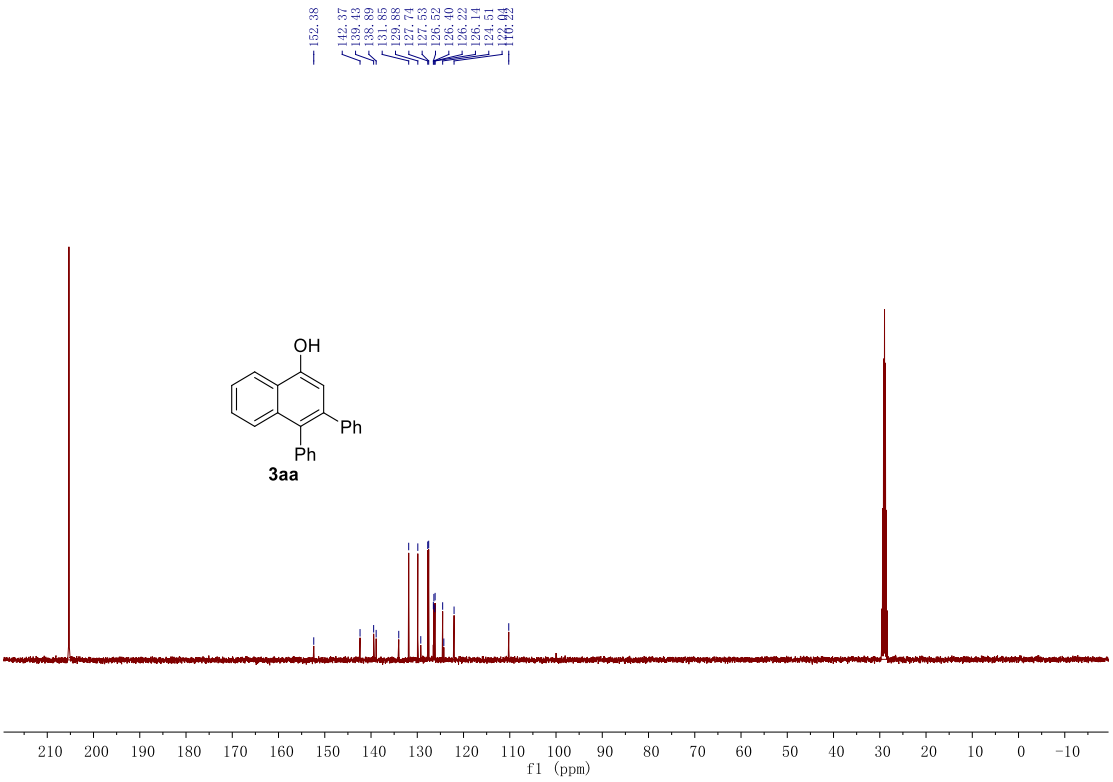


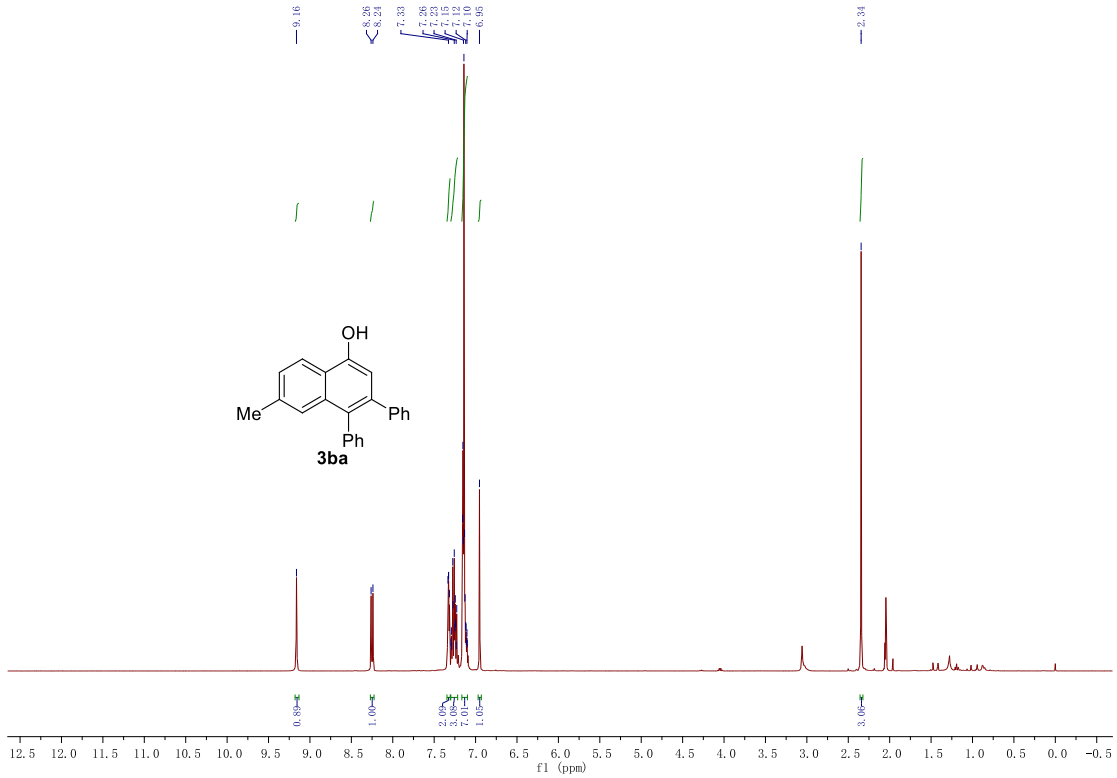
3aj

4-ethyl-3-phenylnaphthalen-1-ol **3aj** as purified via silica gel column chromatography (hexane/ethyl acetate = 30/1, v/v) as a yellow solid in 81% yield (40.1 mg, 0.16 mmol). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (dd, *J* = 8.3, 0.9 Hz, 1H), 8.07 (d, *J* = 8.5 Hz, 1H), 7.57 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.50 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H), 7.45 – 7.38 (m, 3H), 7.38 – 7.31 (m, 2H), 6.69 (s, 1H), 5.25 (s, 1H), 2.92 (q, *J* = 7.5 Hz, 2H), 1.20 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 142.6, 138.7, 132.9, 130.0, 129.2, 128.0, 126.8, 126.7, 124.7, 124.6, 124.2, 122.2, 111.1, 22.0, 16.1. HRMS (ESI)**:** calcd for $C_{18}H_{15}O$ ([M-H]$^-$) 247.1123, found 247.1128.

9. NMR Spectra of Products



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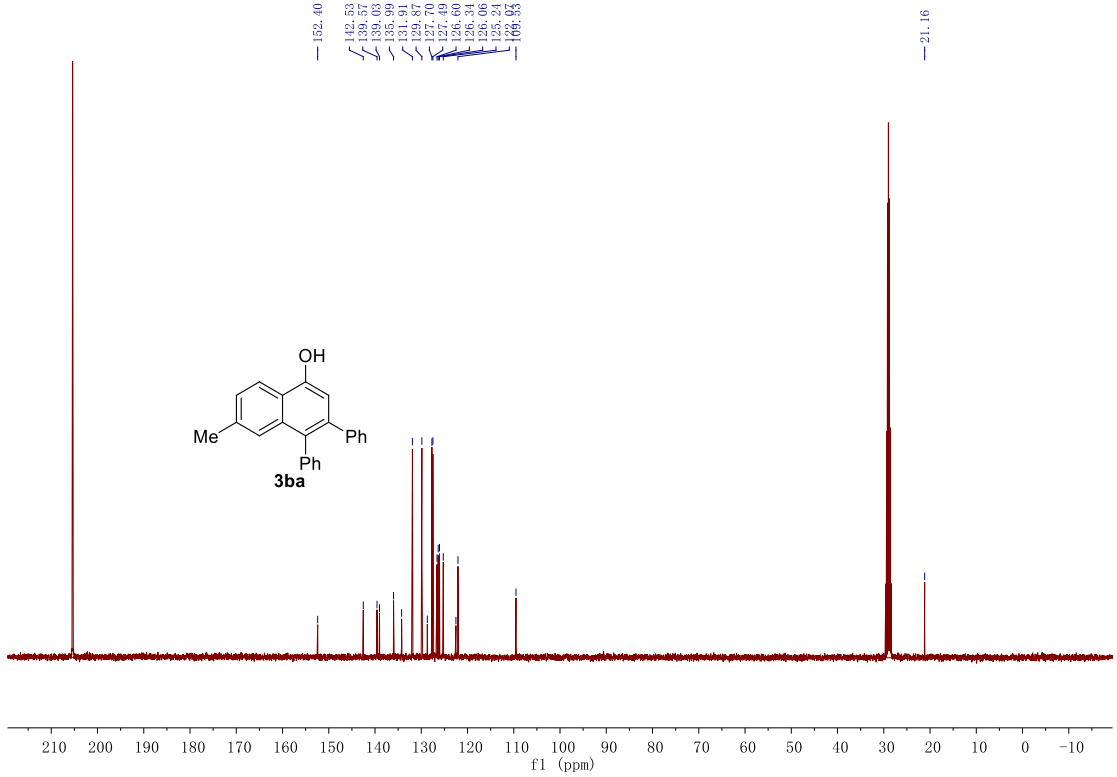
7.33
7.26
7.23
7.15
7.12
7.10
6.95
2.34
OH
Me
Ph
Ph
3ba
0.89
1.00
2.06
2.03
2.01
1.05
3.06
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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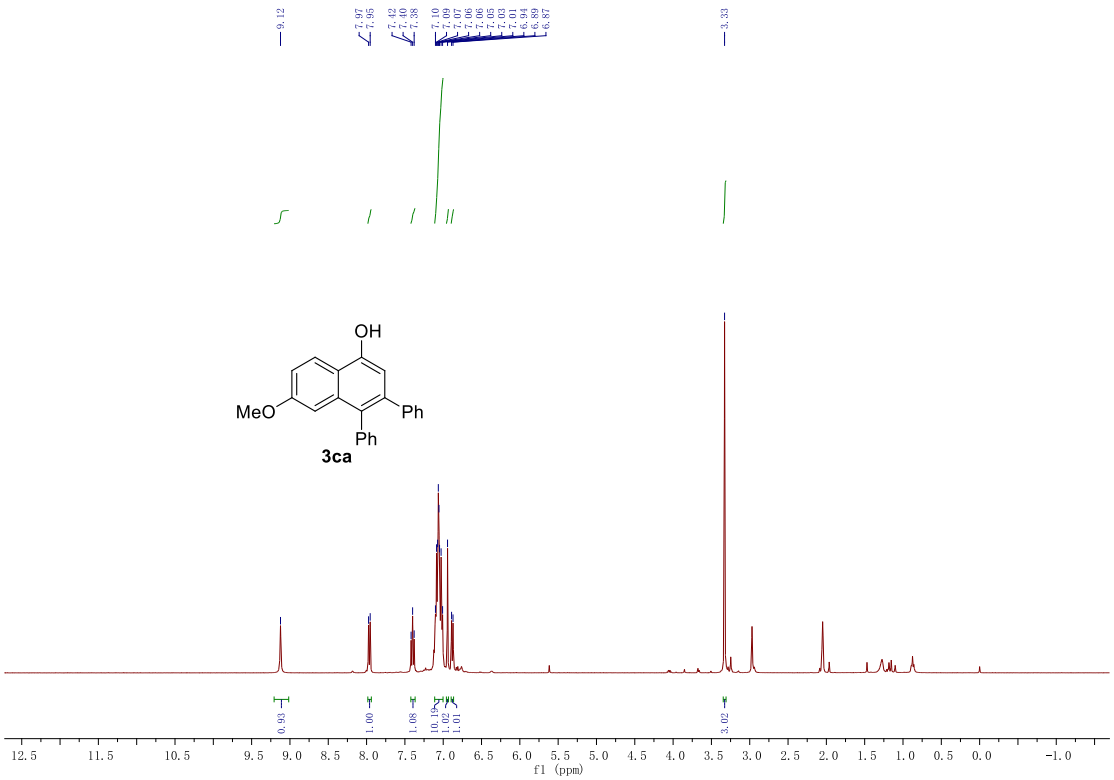
142.53
139.57
139.03
135.99
131.91
129.87
127.70
127.49
126.60
126.34
126.06
125.24
21.16
OH
Me
Ph
Ph
3ba
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.97
7.95
7.42
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7.38
7.10
7.09
7.07
7.06
7.06
7.05
7.03
7.01
6.94
6.89
6.87
3.33
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MeO
Ph
Ph
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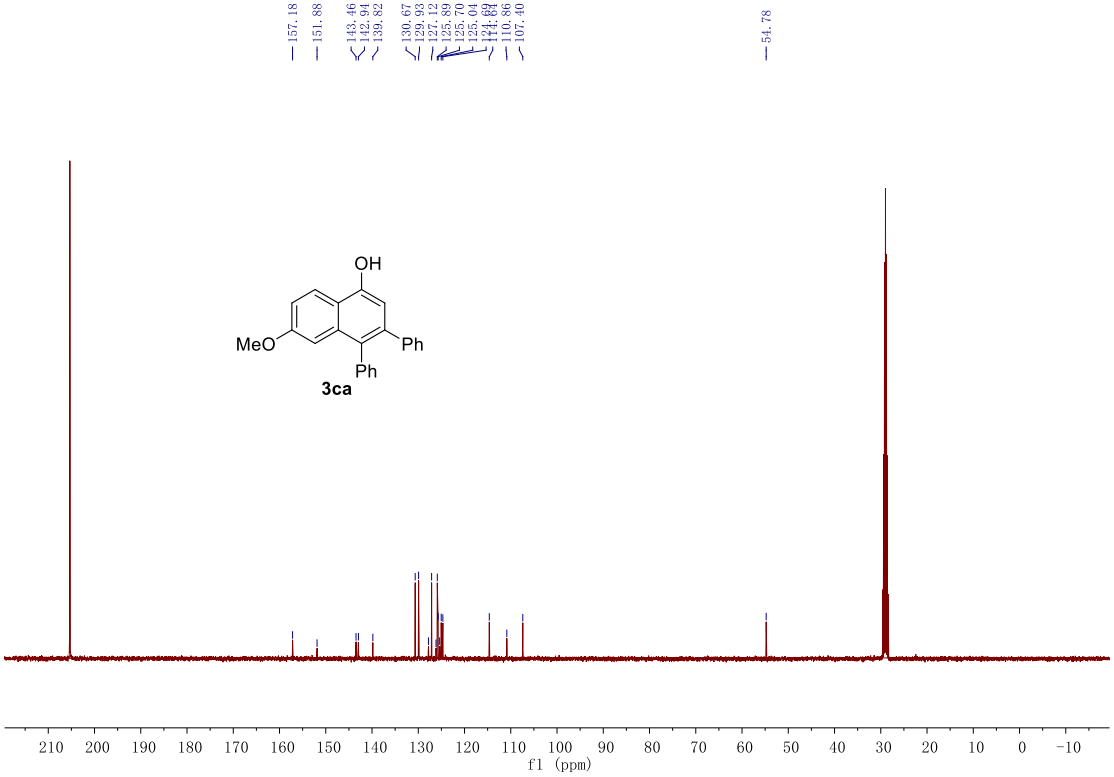
1.00
1.08
10.19
1.02
1.01
3.02
f1 (ppm)


157.18
151.88
143.46
142.94
139.82
130.67
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127.12
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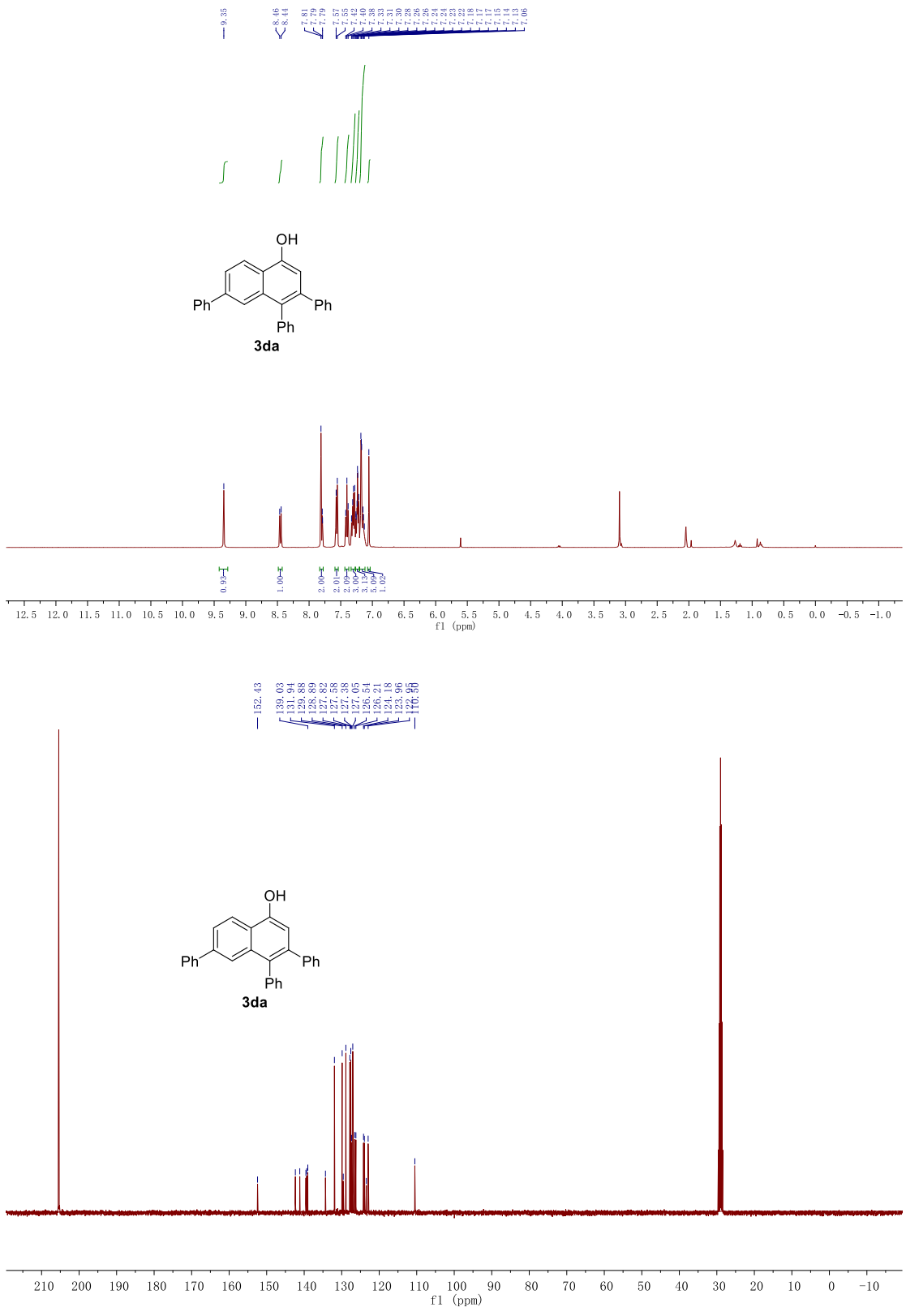
125.70
125.04
54.78
OH
MeO
Ph
Ph
3ca
f1 (ppm)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7.38
7.33
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7.26
7.26
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7.24
7.23
7.22
7.18
7.17
7.17
7.15
7.14
7.13
7.06
OH
Ph
Ph
Ph
3da
0.93
1.00
2.00
2.01
2.09
3.15
5.09
1.02
f1 (ppm)
152.43
139.03
131.94
129.88
128.89
127.82
127.58
127.38
127.15
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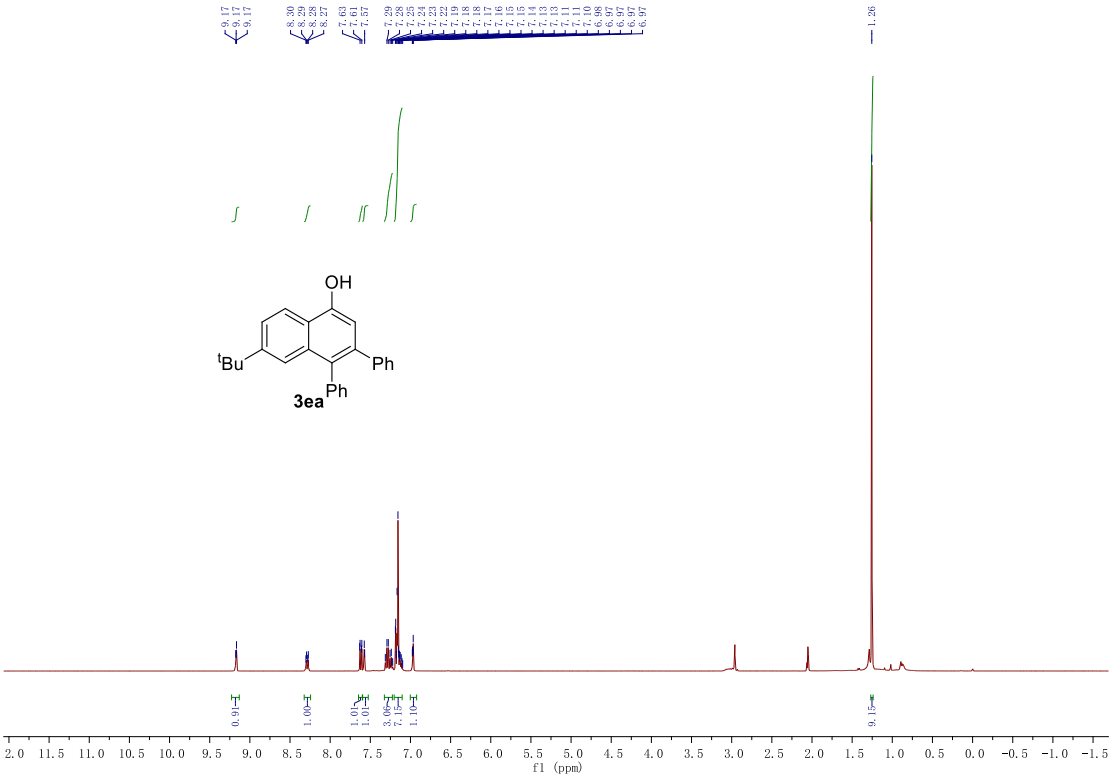
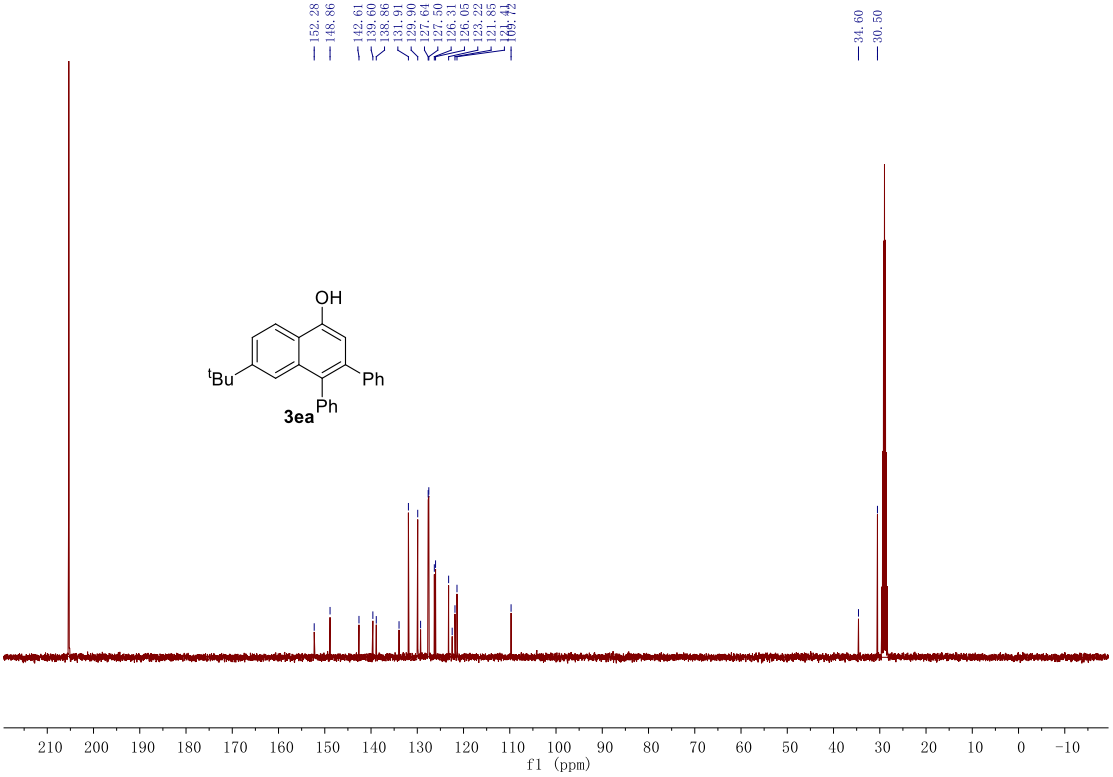
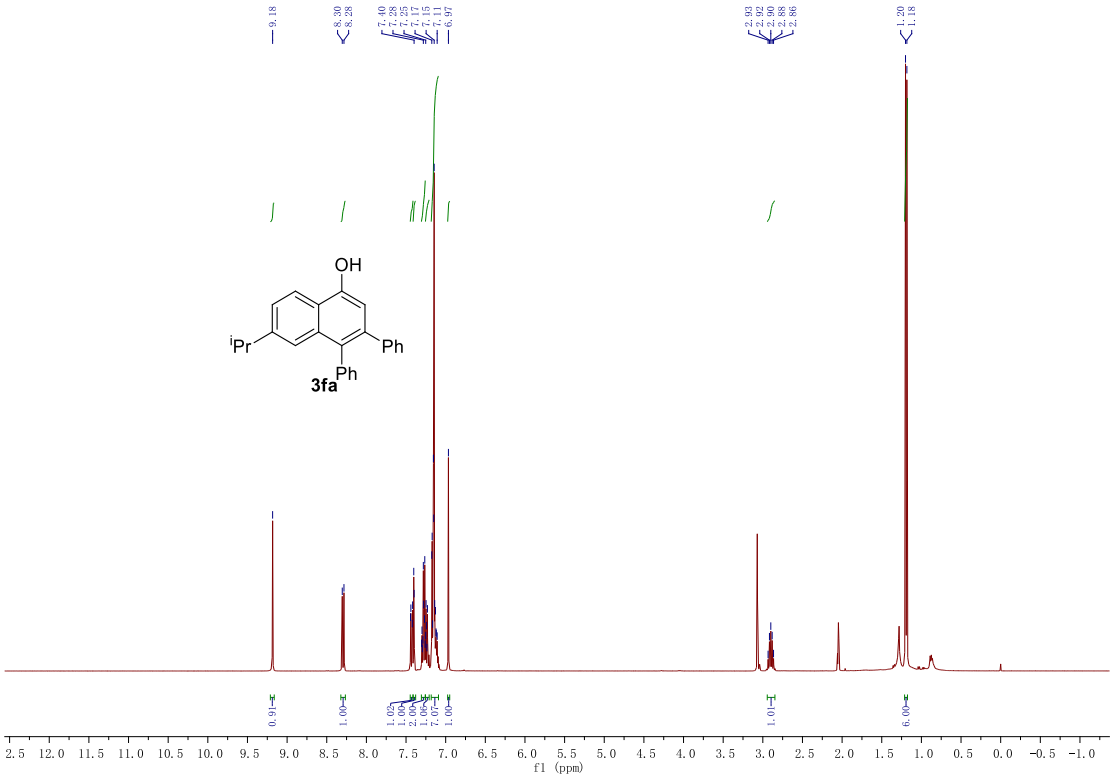
126.21
124.18
123.96
122.95
110.50
OH
Ph
Ph
Ph
3da
f1 (ppm)


OH
tBu
Ph
Ph
3ea
f1 (ppm)


OH
tBu
Ph
Ph
3ea
f1 (ppm)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8.28
7.40
7.38
7.25
7.17
7.15
7.11
6.97
2.93
2.92
2.90
2.88
2.86
1.20
1.18
OH
iPr
Ph
Ph
3fa
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1.00
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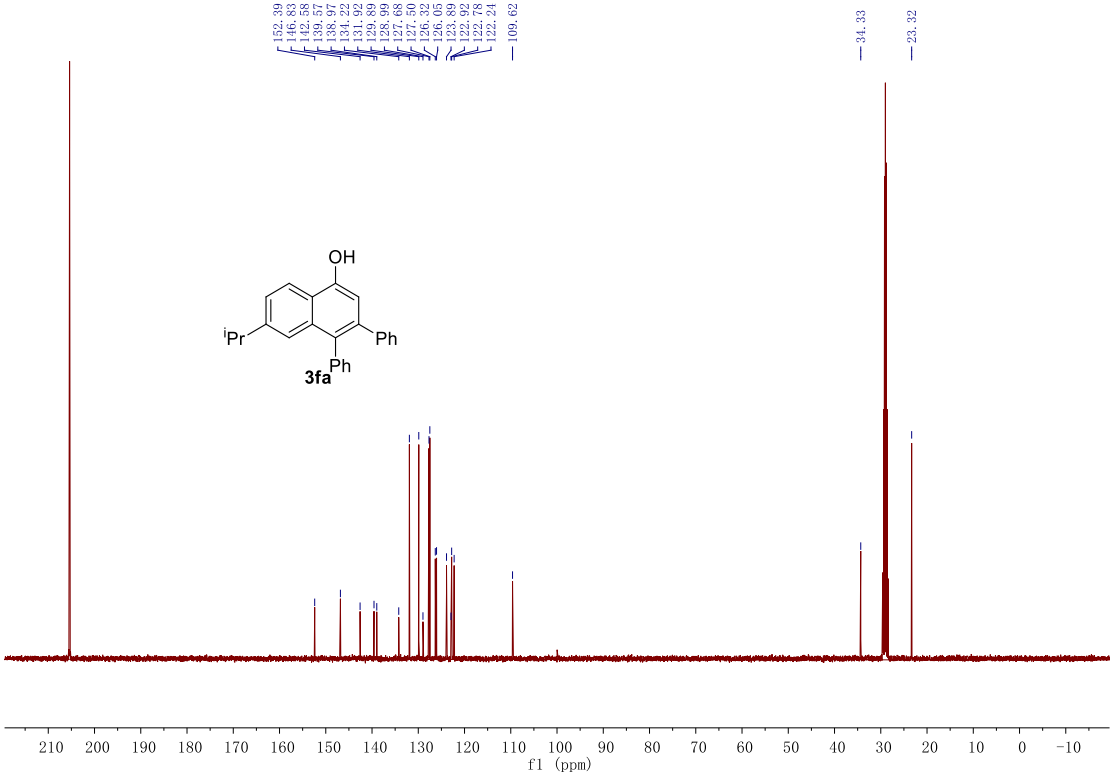
1.06
2.06
1.07
1.00
1.01
6.00
f1 (ppm)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129.89
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127.50
126.32
126.05
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122.78
122.24
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34.33
23.32
OH
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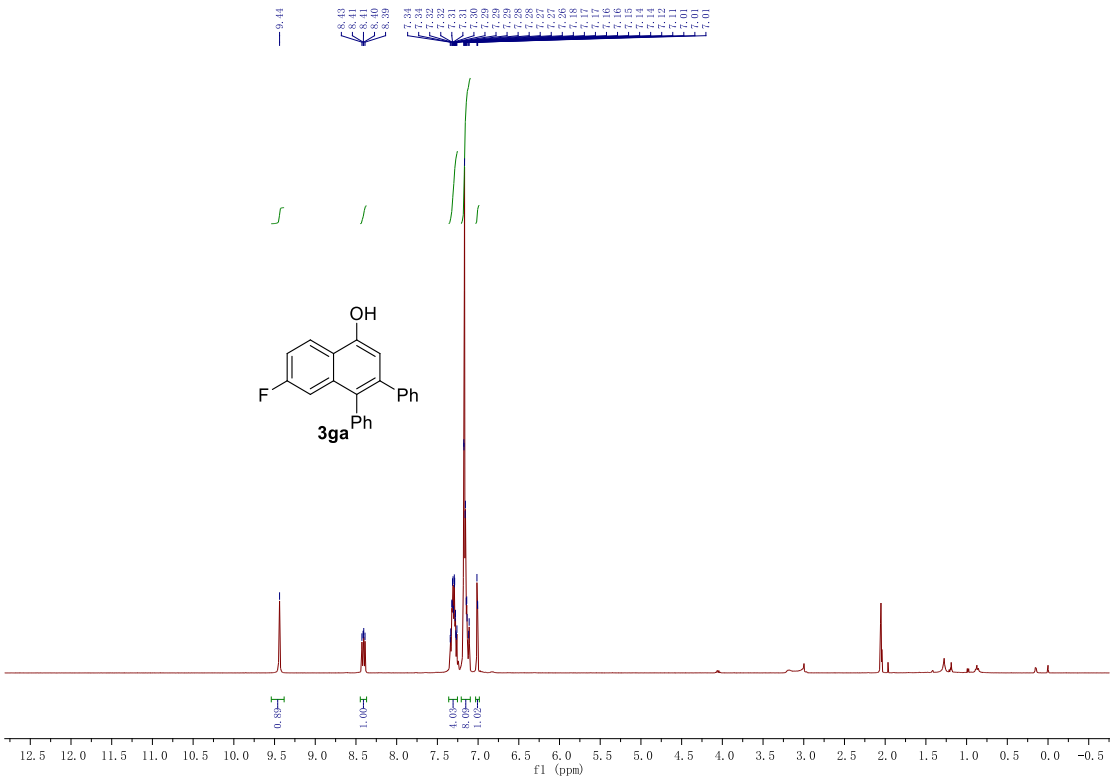
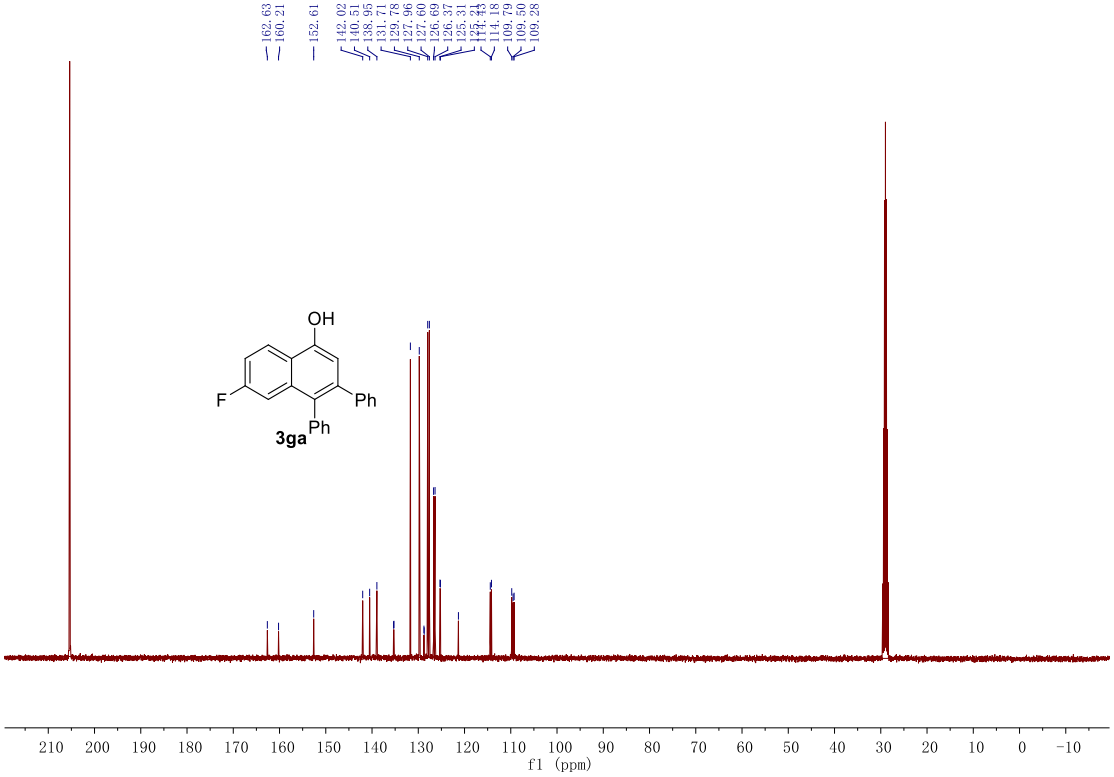
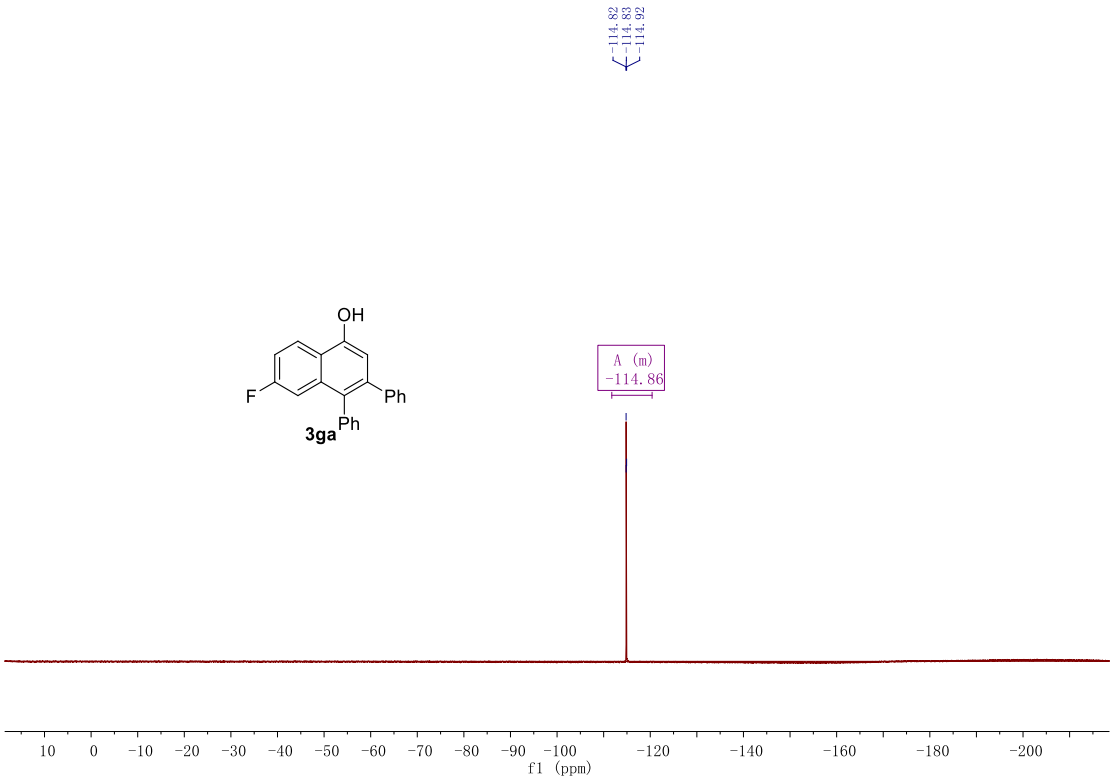
Ph
Ph
3fa
f1 (ppm)


OH
F
Ph
Ph
3ga
f1 (ppm)


OH
F
Ph
Ph
3ga
f1 (ppm)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-114.92
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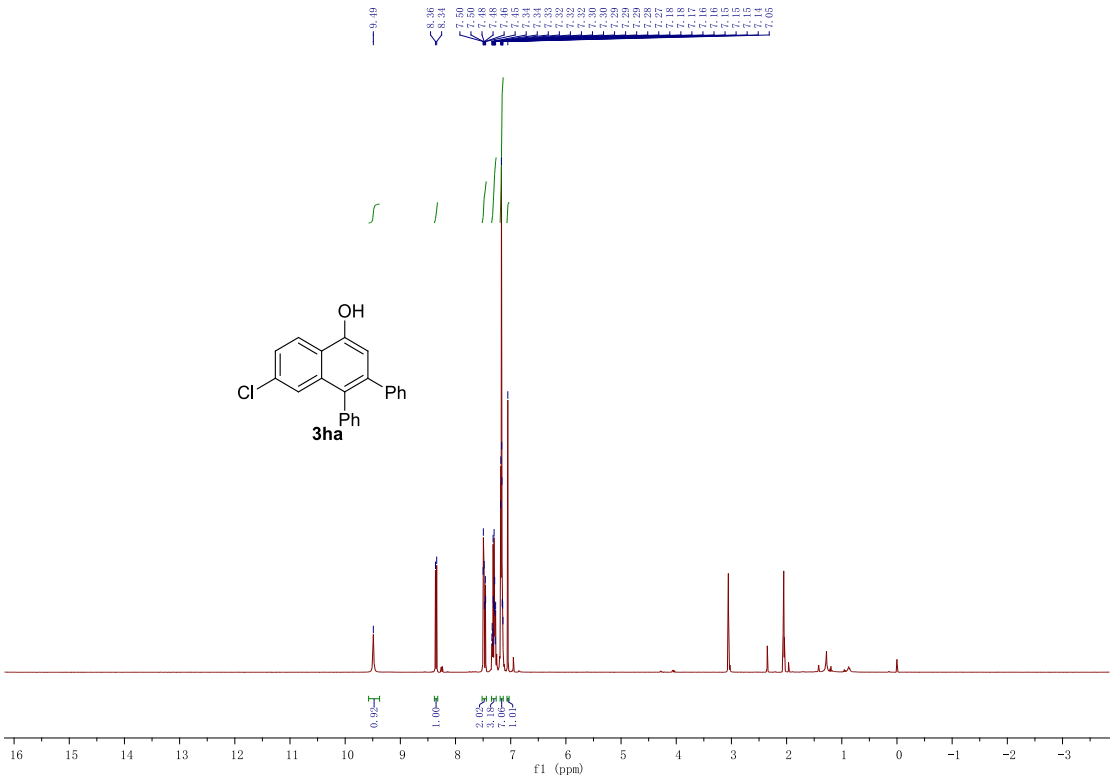
F
Ph
Ph
3ga
A (m)
-114.86
f1 (ppm)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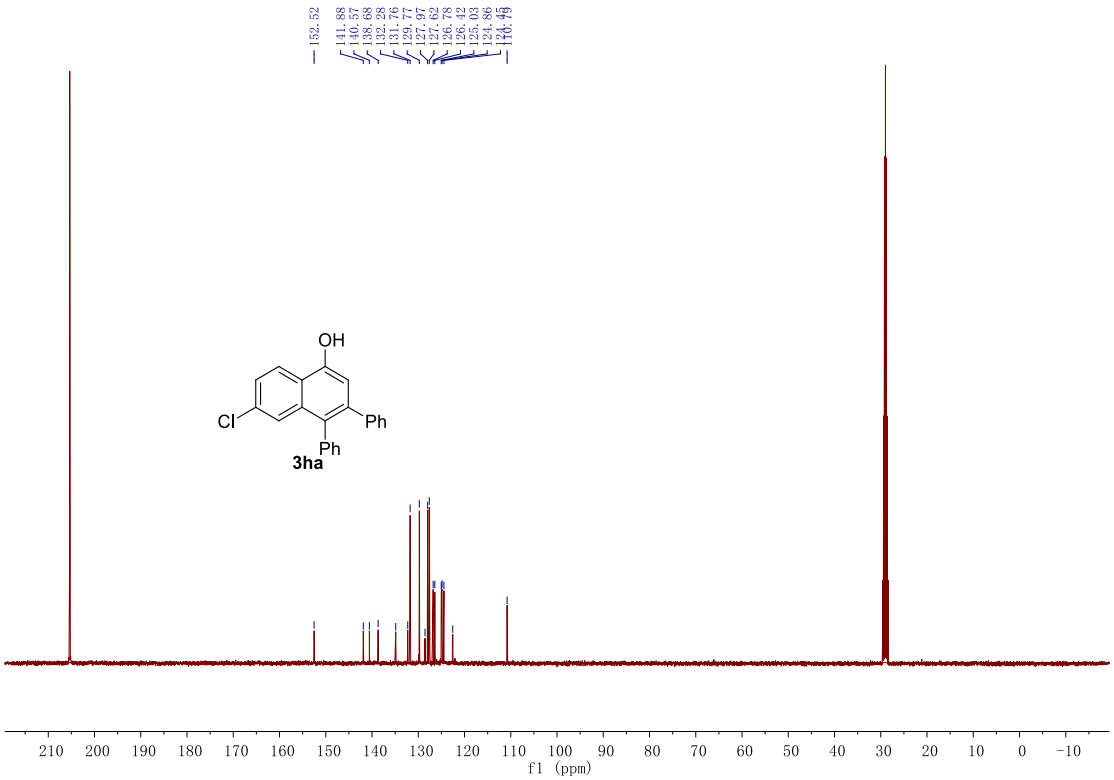
Cl
Ph
Ph
3ha
f1 (ppm)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138.68
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126.42
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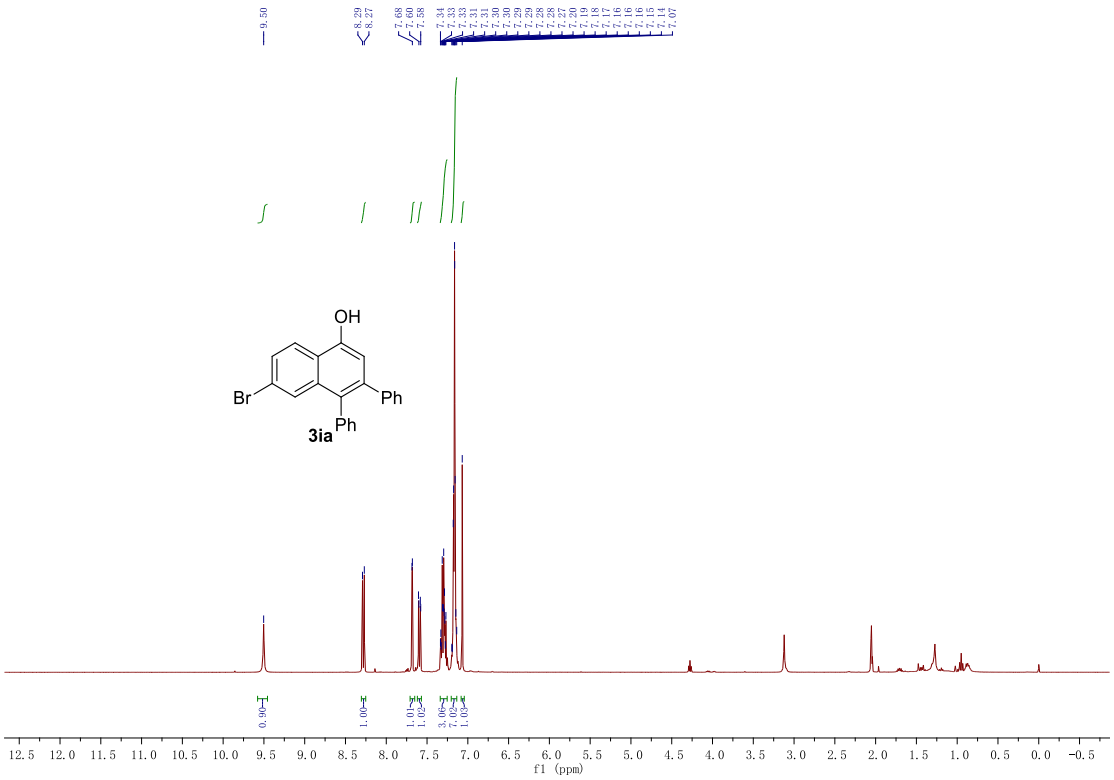
124.86
OH
Cl
Ph
Ph
3ha
f1 (ppm)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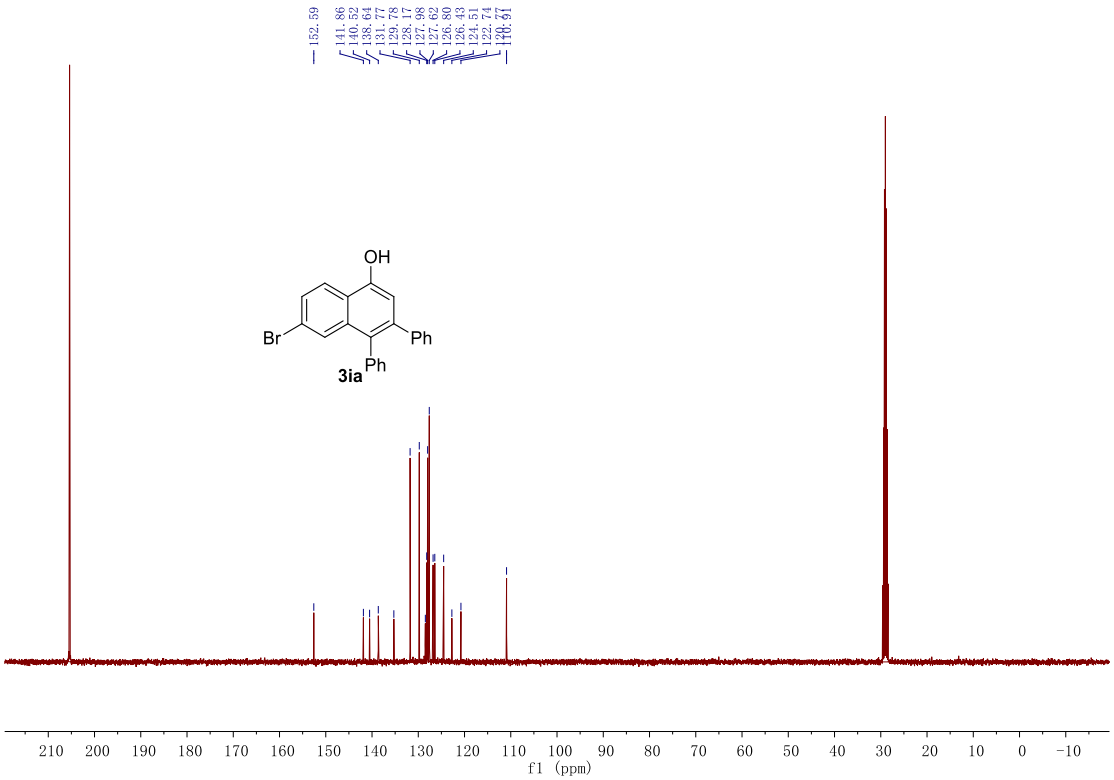
Br
Ph
Ph
3ia
f1 (ppm)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120.77
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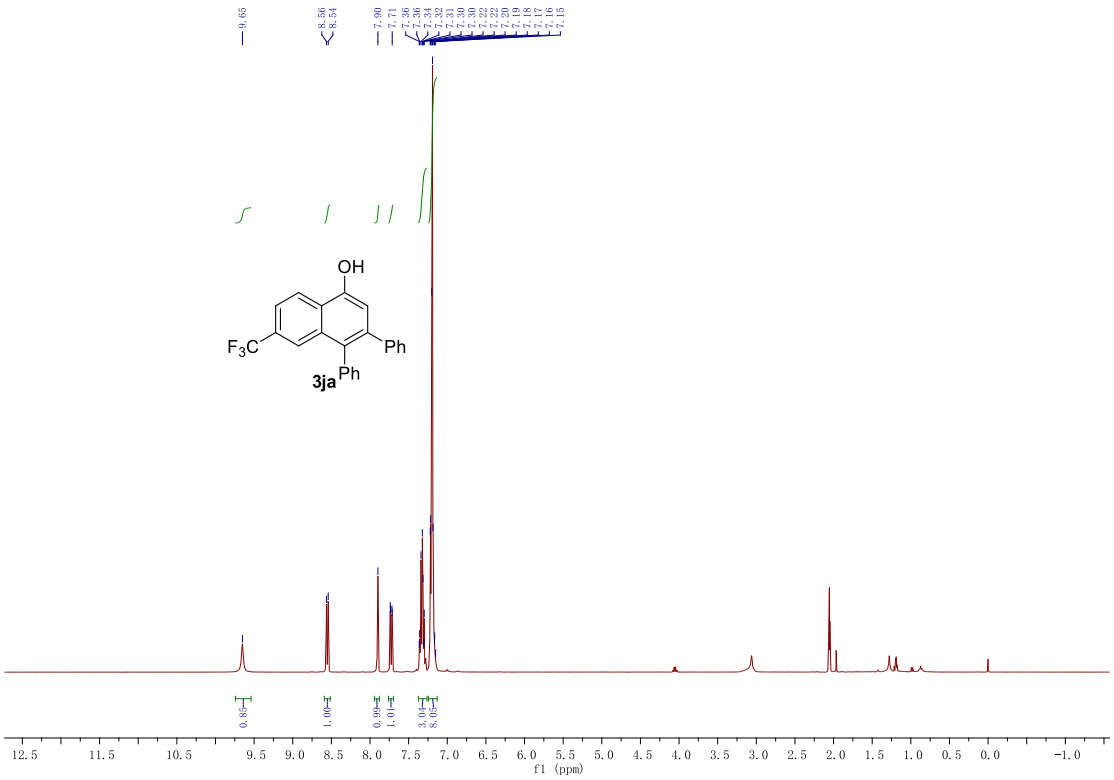
OH
Br
Ph
Ph
3ia
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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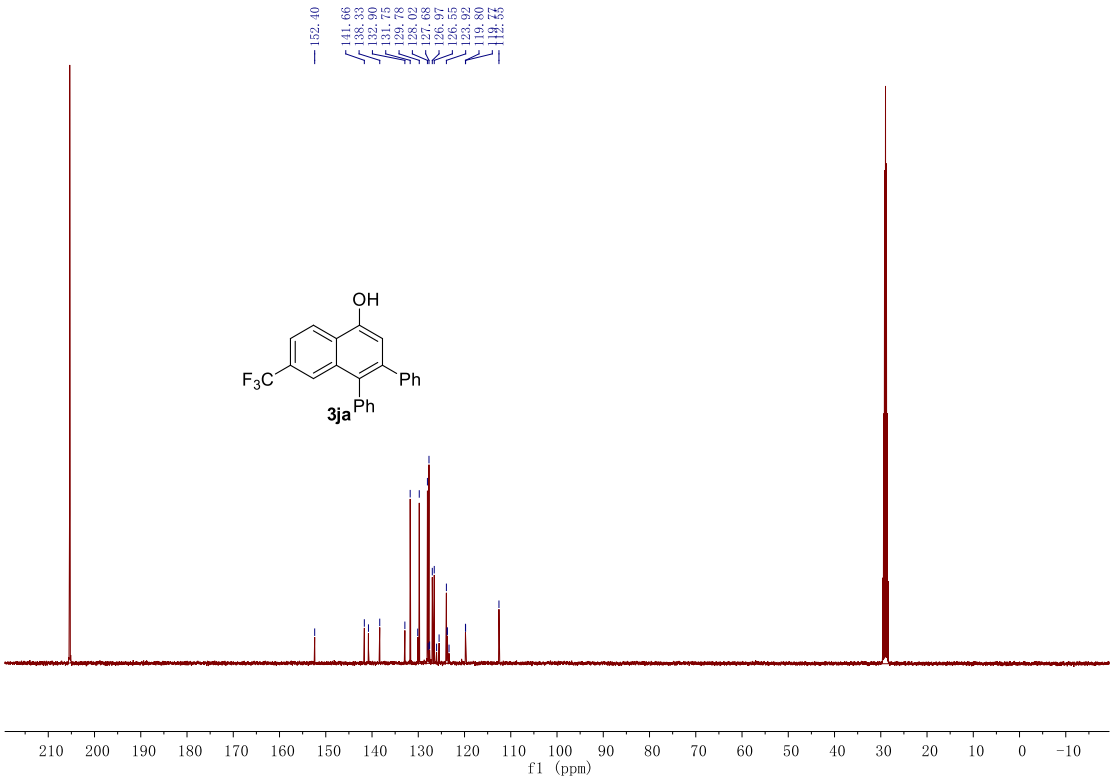
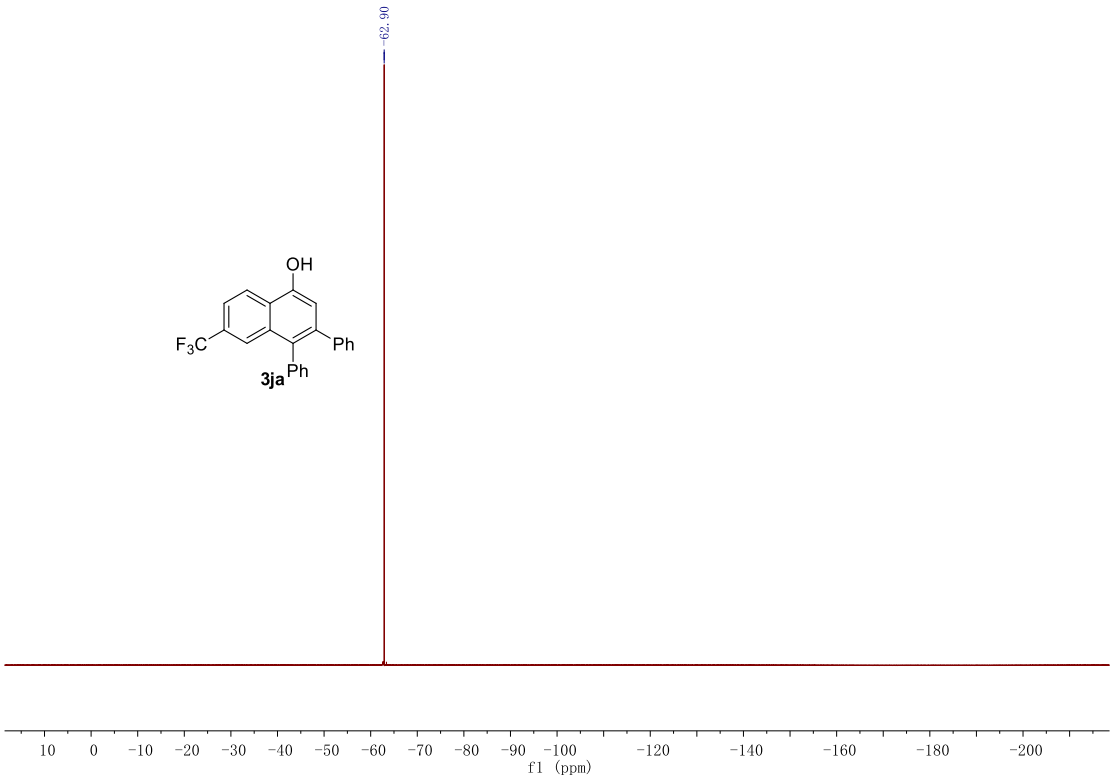
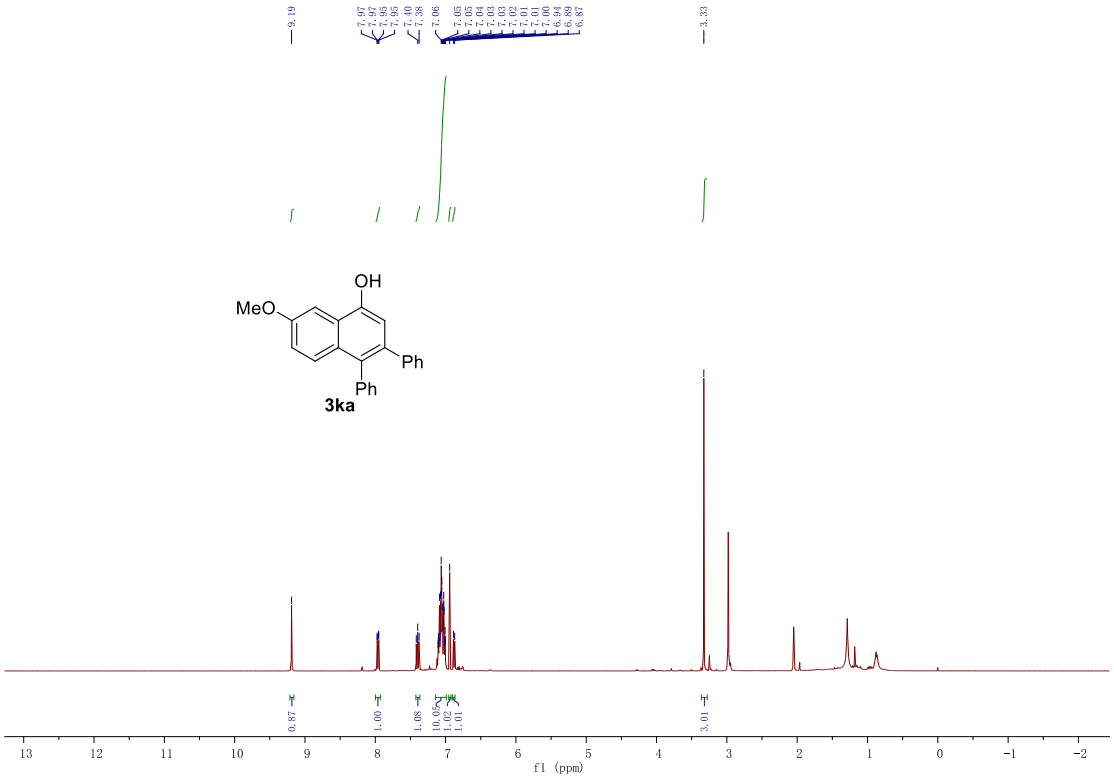
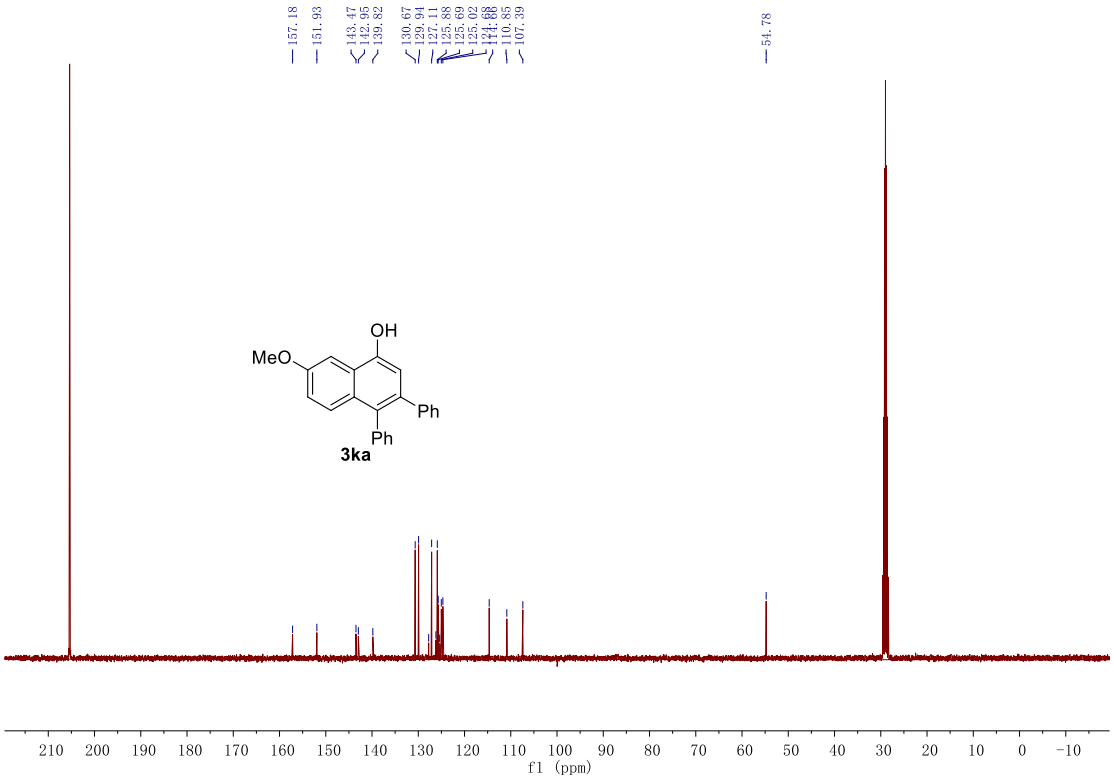
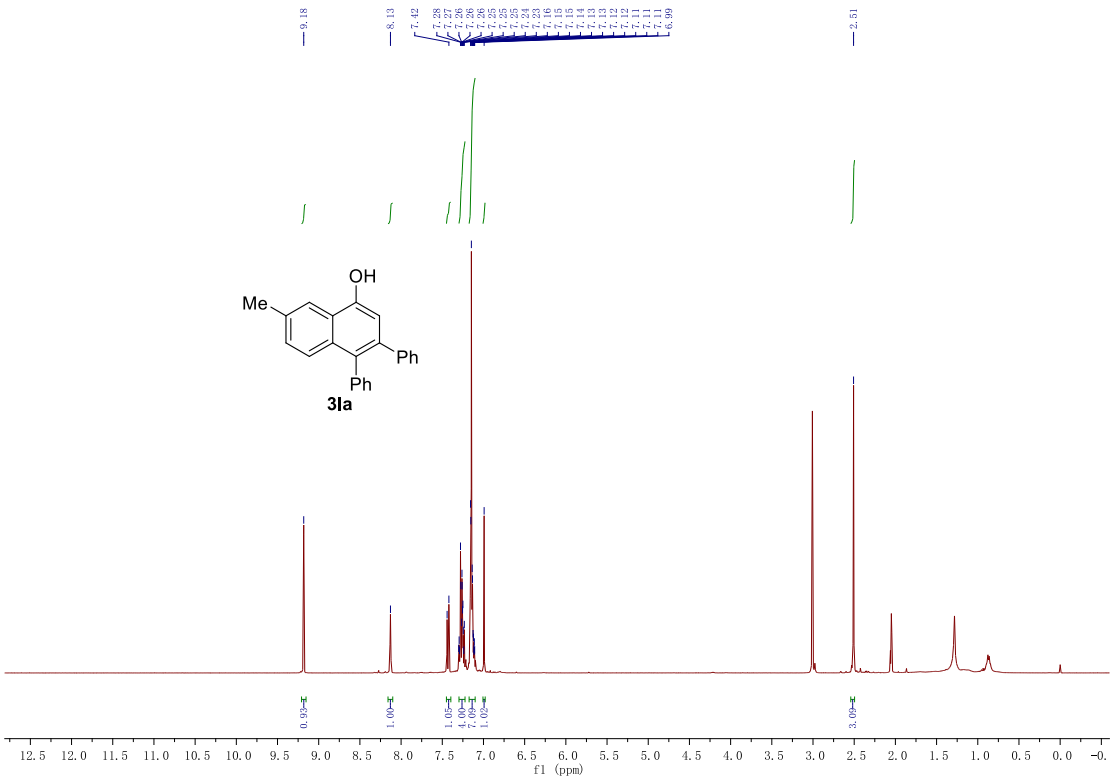
7.20
7.19
7.18
7.17
7.16
7.15
OH
F3C
Ph
Ph
3ja
0.85
1.00
0.99
1.01
3.04
8.05
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)

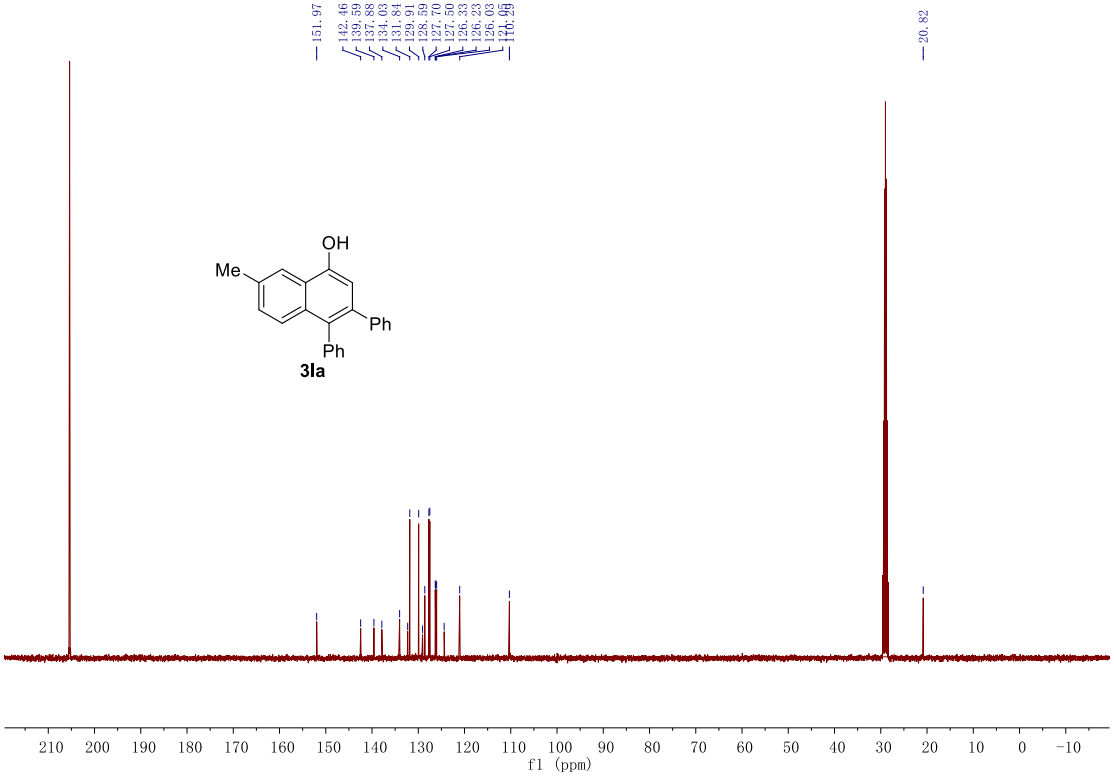

152.40
141.66
138.33
132.90
131.75
129.78
128.02
127.68
126.97
126.55
123.92
119.80
OH
F3C
Ph
Ph
3ja
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-62.90
OH
F3C
Ph
Ph
3ja
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)


9.19
7.97
7.97
7.95
7.95
7.40
7.38
7.06
7.05
7.05
7.04
7.04
7.03
7.03
7.02
7.02
7.01
7.01
7.00
7.00
6.94
6.89
6.87
3.33
OH
MeO
Ph
Ph
3ka
0.87
1.00
1.08
10.05
1.02
1.01
3.01
f1 (ppm)


157.18
151.93
143.47
142.95
139.82
130.67
129.94
127.11
125.88
125.69
125.02
114.68
114.66
110.85
107.39
54.78
OH
MeO
Ph
Ph
3ka
f1 (ppm)


9.18
8.13
7.42
2.51
OH
Me
Ph
Ph
3la
f1 (ppm)


151.97
142.46
139.59
137.88
134.03
131.84
129.91
128.59
127.70
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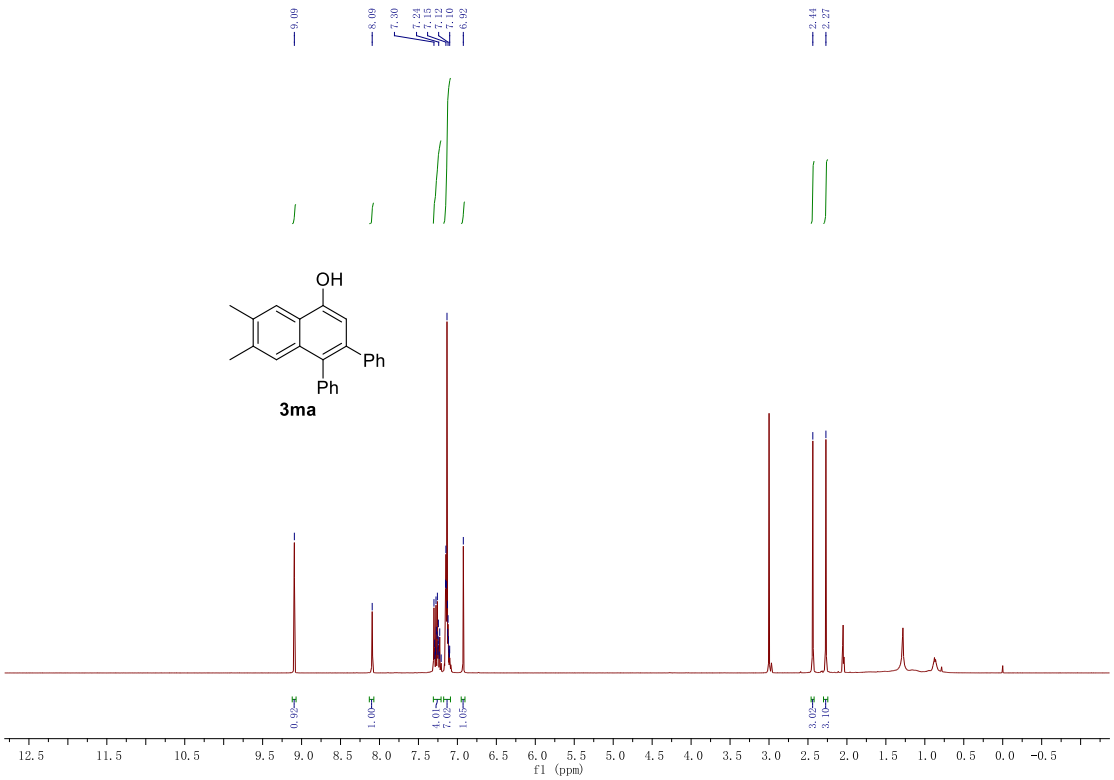
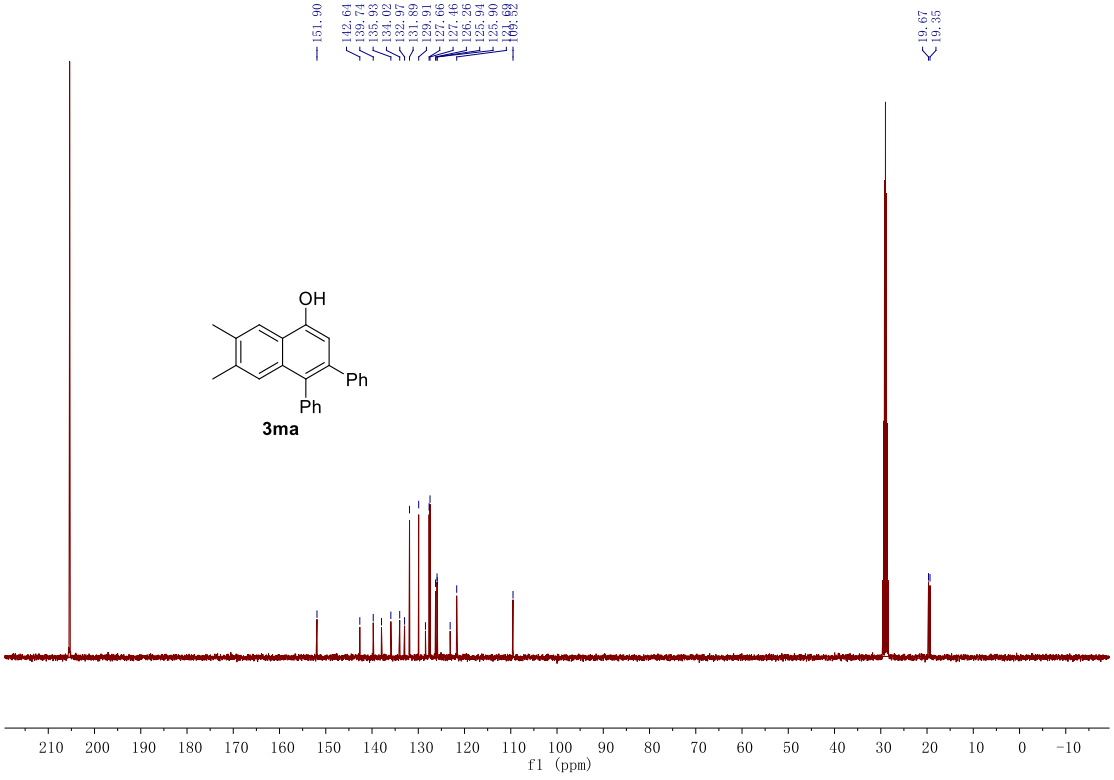
126.33
126.23
126.03
121.06
116.29
20.82
OH
Me
Ph
Ph
3la
f1 (ppm)


8.09
8.09
7.30
7.24
7.15
7.12
7.10
6.92
2.44
2.27
OH
Ph
Ph
3ma
0.98
1.00
4.01
2.00
1.05
3.02
3.10
12.5
11.5
10.5
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
f1 (ppm)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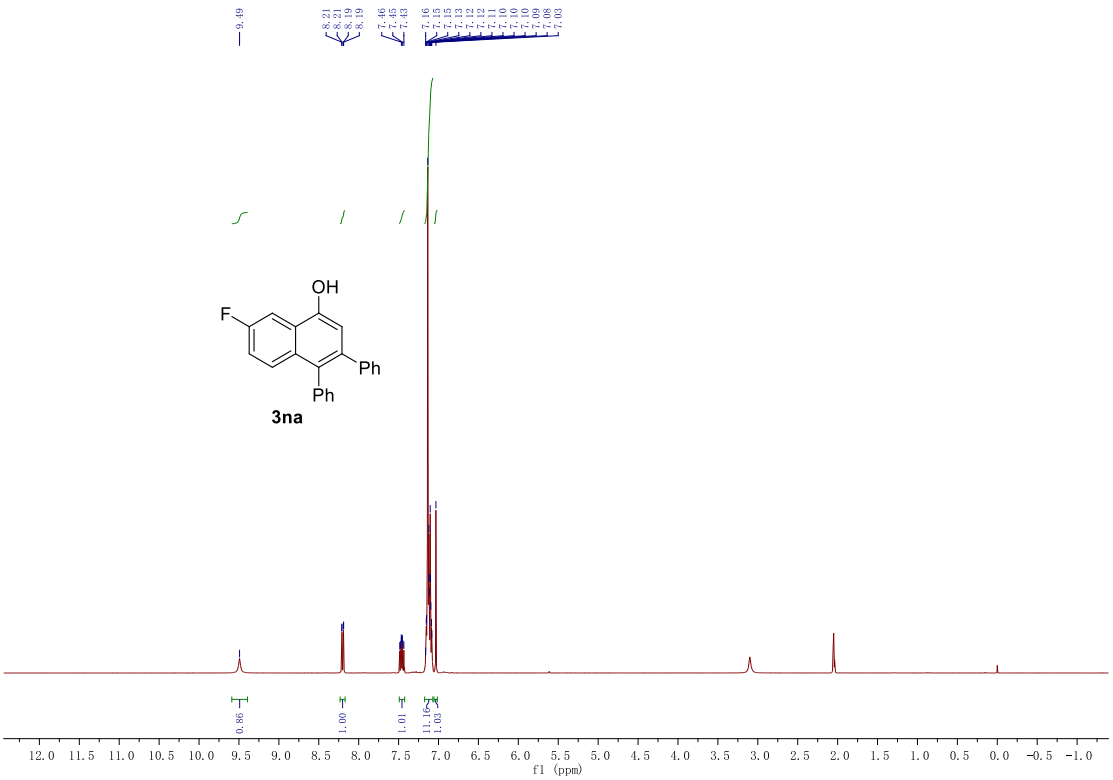
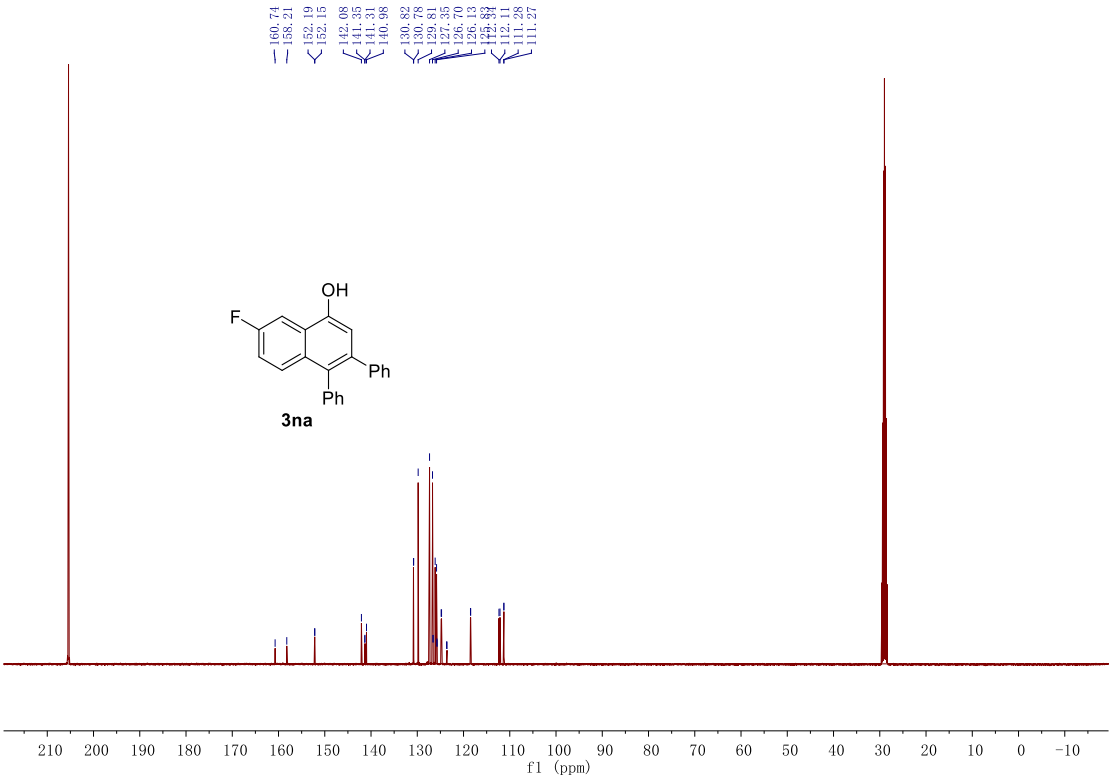
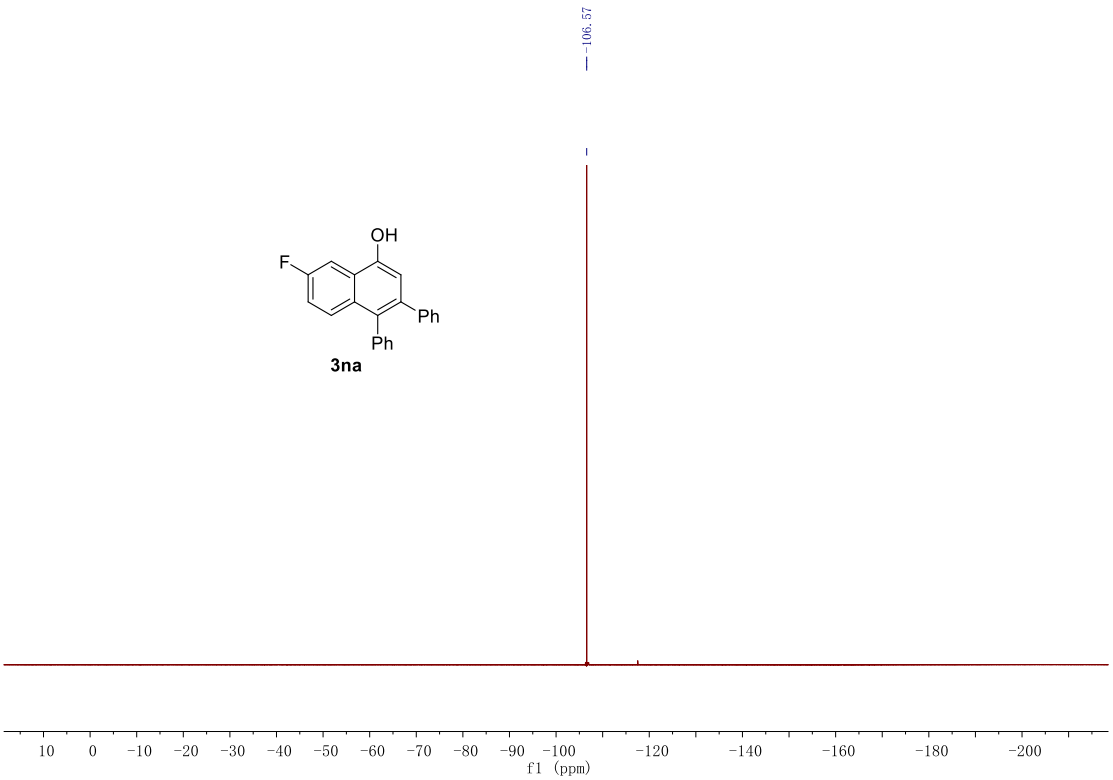
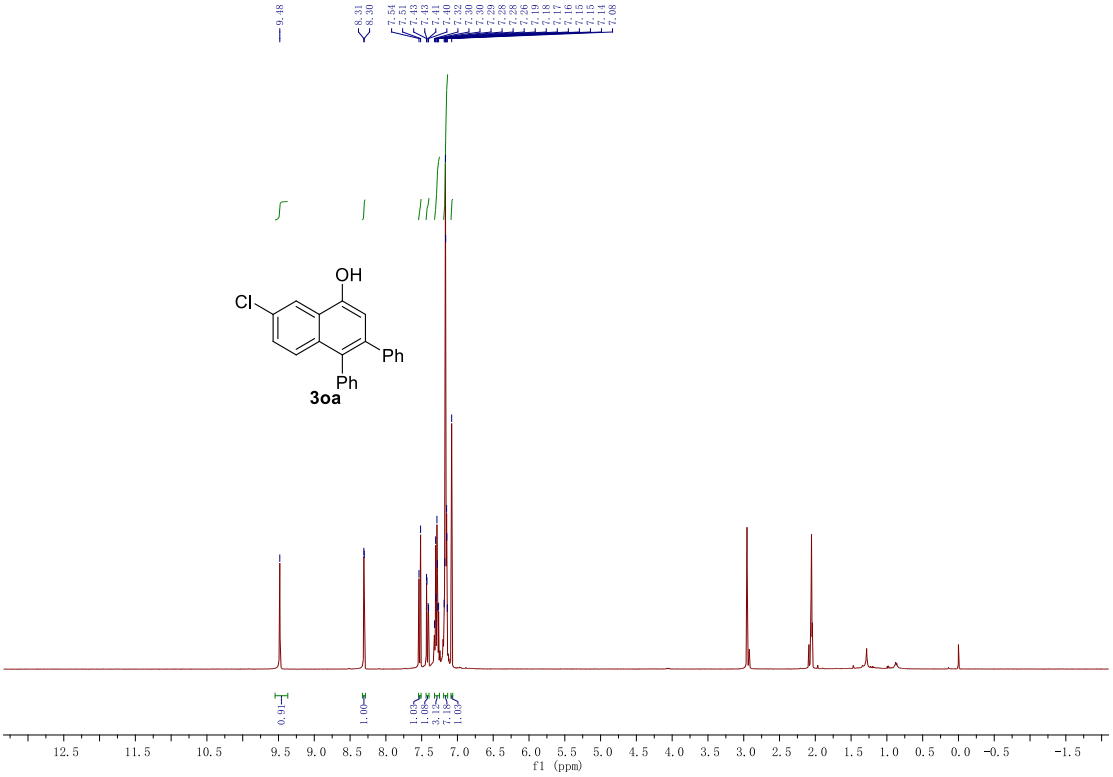
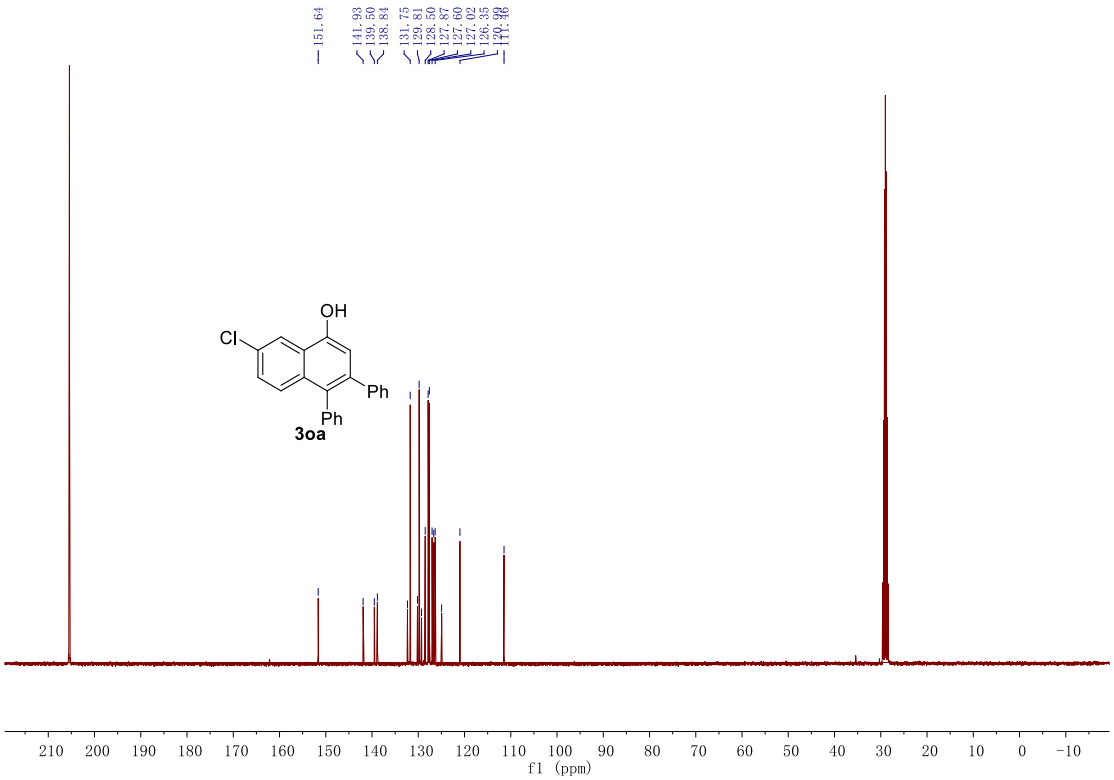
142.64
139.74
135.93
134.02
132.97
131.89
129.91
127.66
127.46
126.26
125.94
125.90
19.67
19.35
OH
Ph
Ph
3ma
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

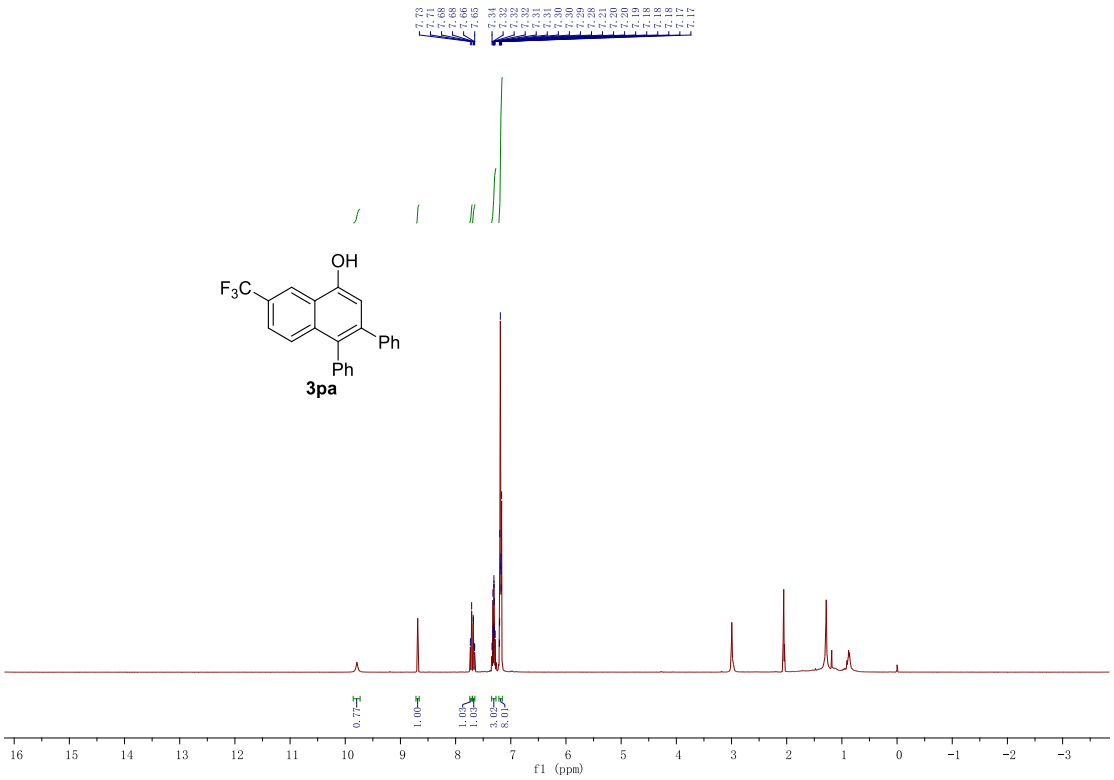

9.49
8.21
8.21
8.19
8.19
7.46
7.45
7.43
7.16
7.15
7.15
7.13
7.13
7.12
7.12
7.11
7.11
7.10
7.10
7.09
7.08
7.08
7.05
OH
F
Ph
Ph
3na
0.86
1.00
1.01
11.18
1.03
f1 (ppm)

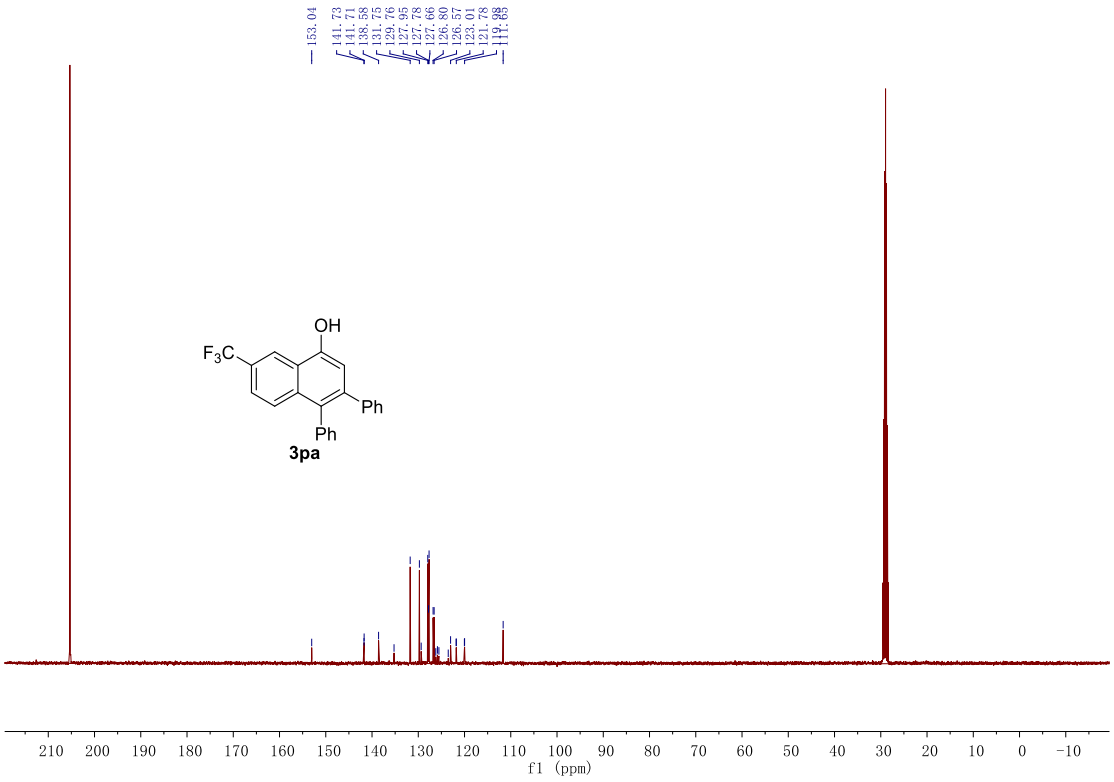

160.74
158.21
152.19
152.15
142.08
141.35
141.31
140.98
130.82
130.78
129.81
127.35
126.70
126.13
112.11
111.98
111.27
OH
F
Ph
Ph
3na
f1 (ppm)

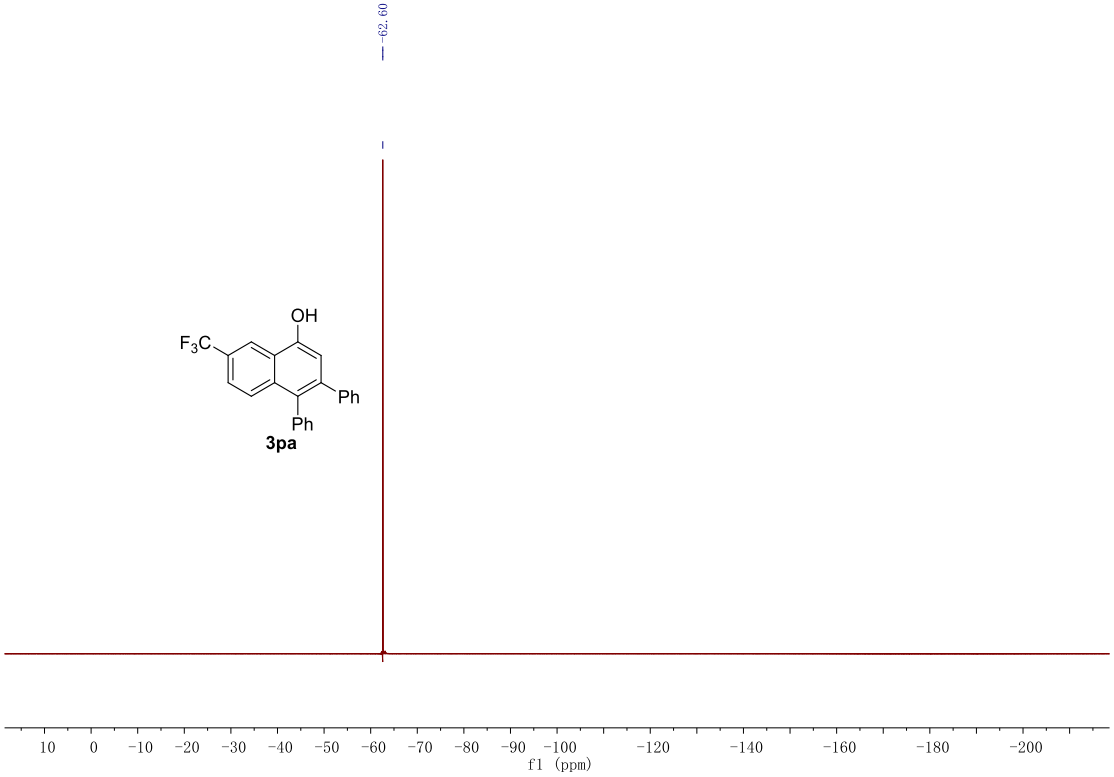

-106.57
OH
F
Ph
Ph
3na
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

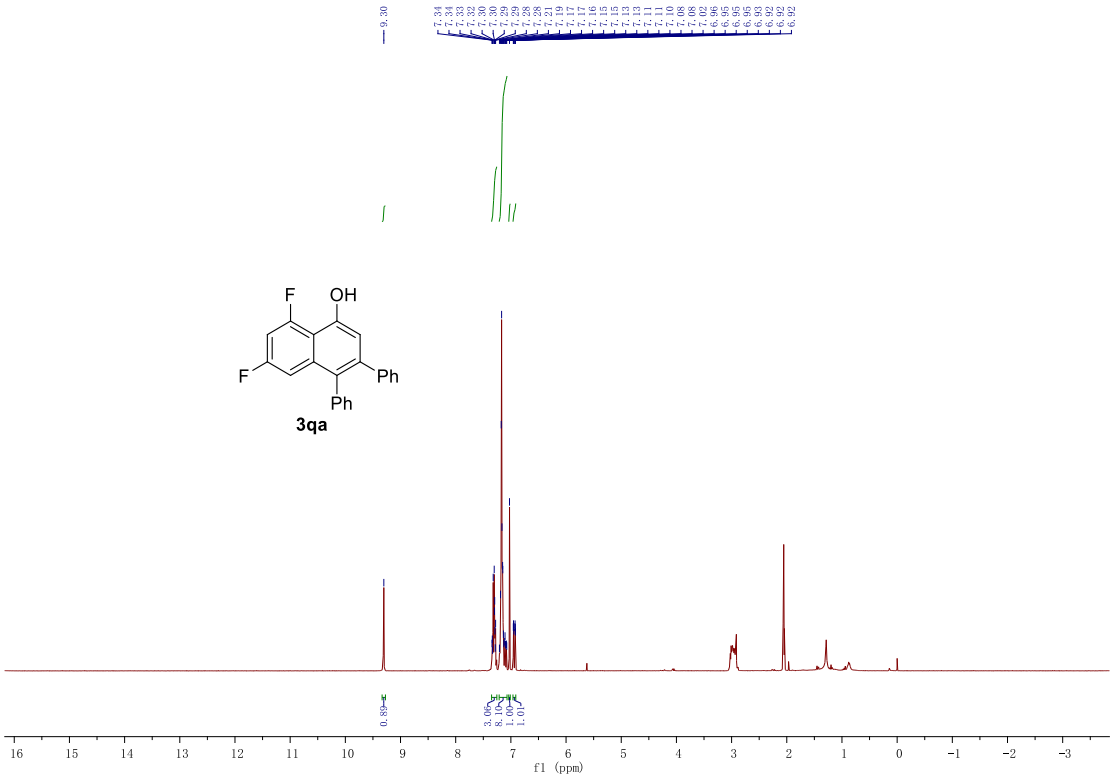

9.48
8.31
8.30
7.54
7.51
7.43
7.43
7.41
7.40
7.32
7.30
7.30
7.29
7.28
7.26
7.19
7.18
7.17
7.16
7.15
7.15
7.14
7.08
OH
Cl
Ph
Ph
3oa
0.91
1.00
1.03
1.08
2.12
2.14
1.02
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.5
f1 (ppm)

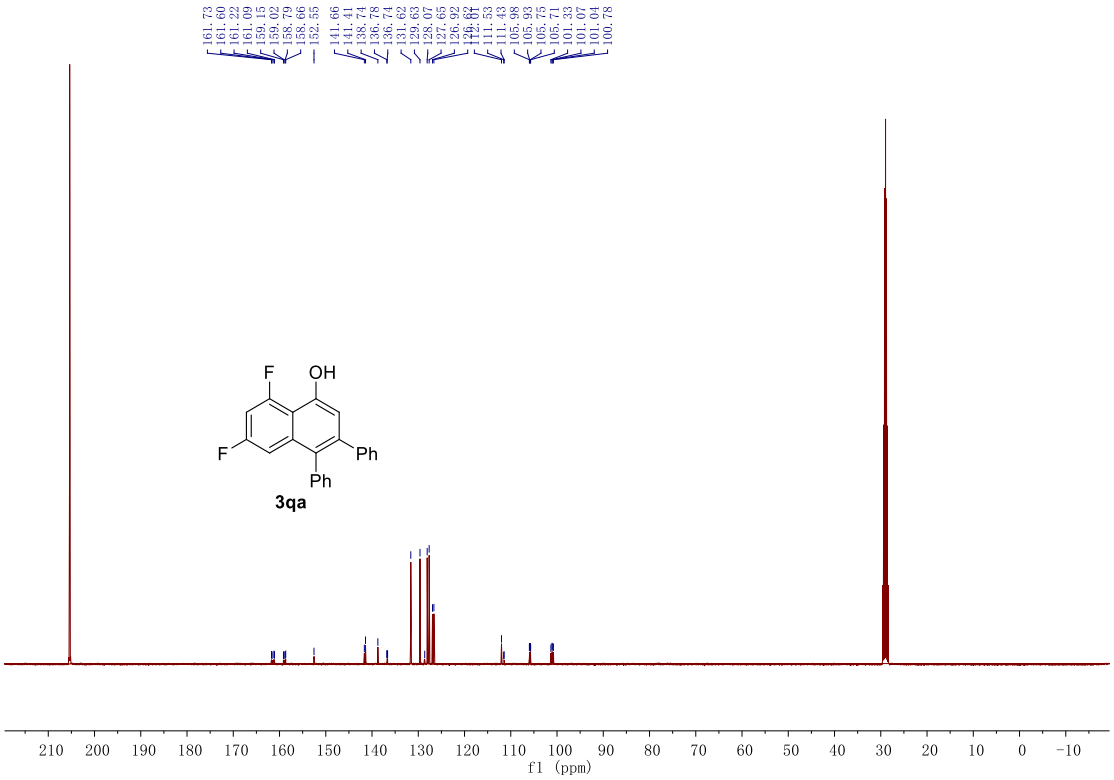

151.64
141.93
139.50
138.84
131.75
129.81
128.50
127.87
127.60
127.02
126.35
120.99
111.46
OH
Cl
Ph
Ph
3oa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

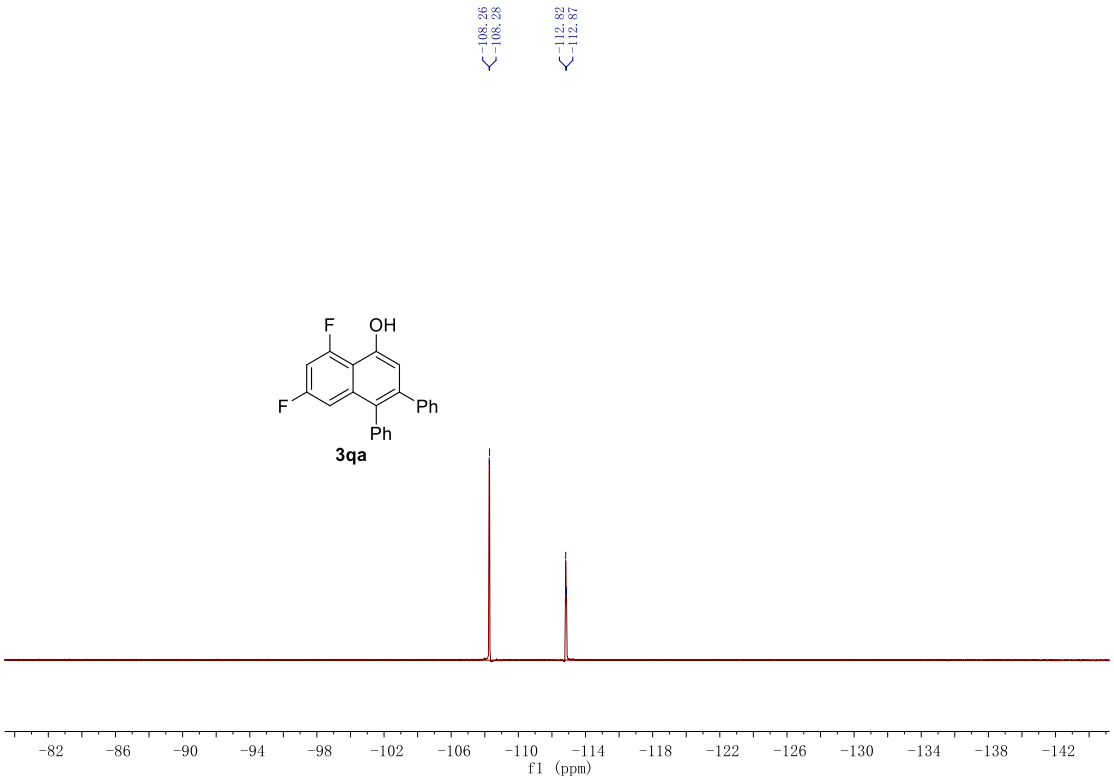

7.73
7.71
7.68
7.68
7.66
7.65
7.34
7.32
7.32
7.32
7.31
7.31
7.30
7.30
7.29
7.28
7.21
7.20
7.19
7.18
7.18
7.18
7.17
7.17
OH
F3C
Ph
Ph
3pa
0.77
1.00
1.03
1.03
3.02
8.01
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

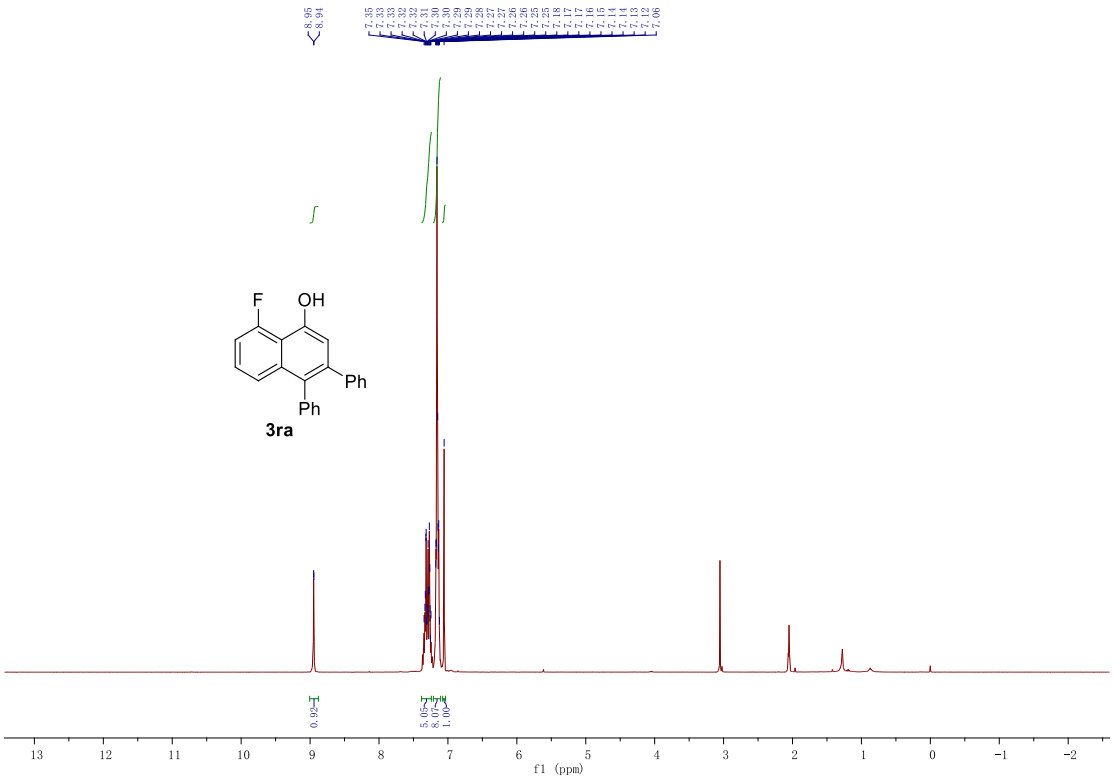

153.04
141.73
141.71
138.58
131.75
129.76
127.95
127.78
127.66
126.80
126.57
123.01
121.78
OH
F3C
Ph
Ph
3pa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

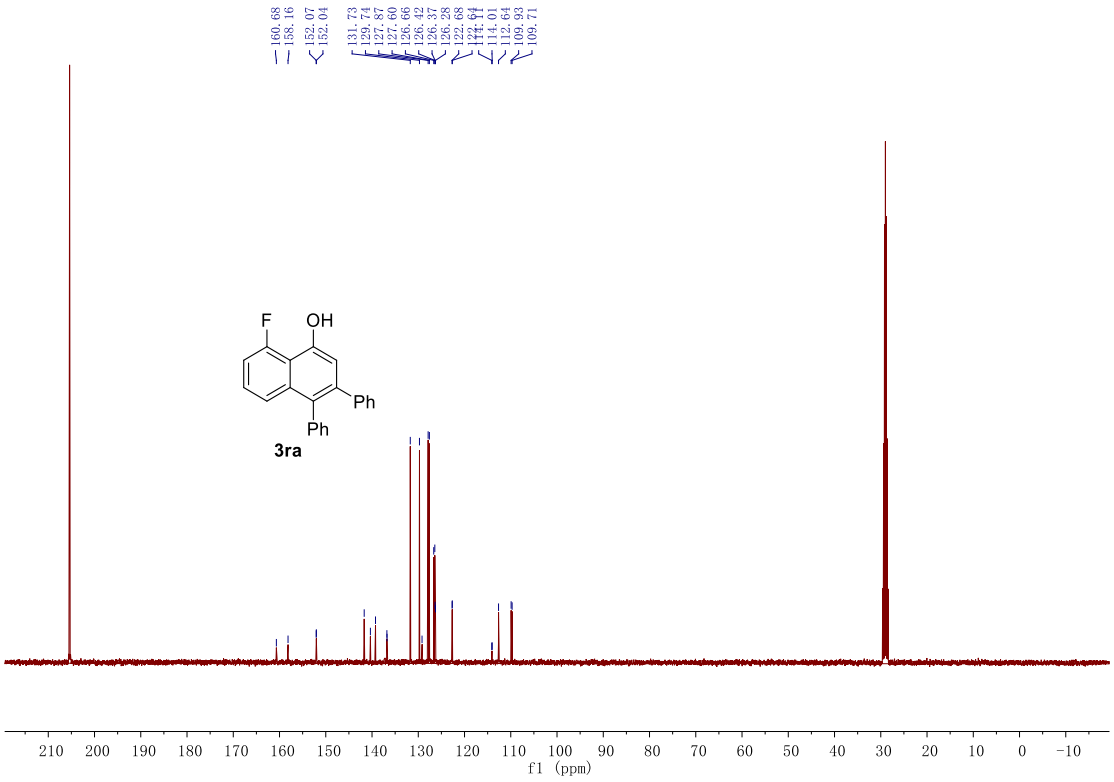

-62.60
OH
F3C
Ph
Ph
3pa
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

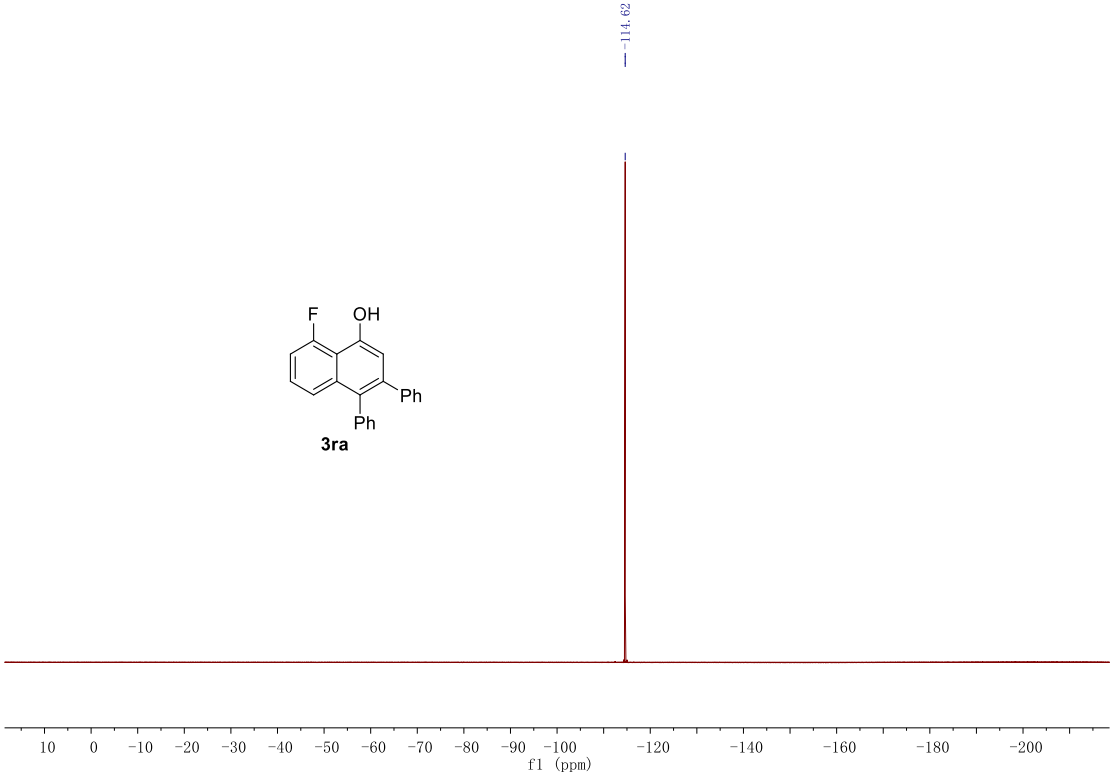

F
OH
F
Ph
Ph
3qa
f1 (ppm)

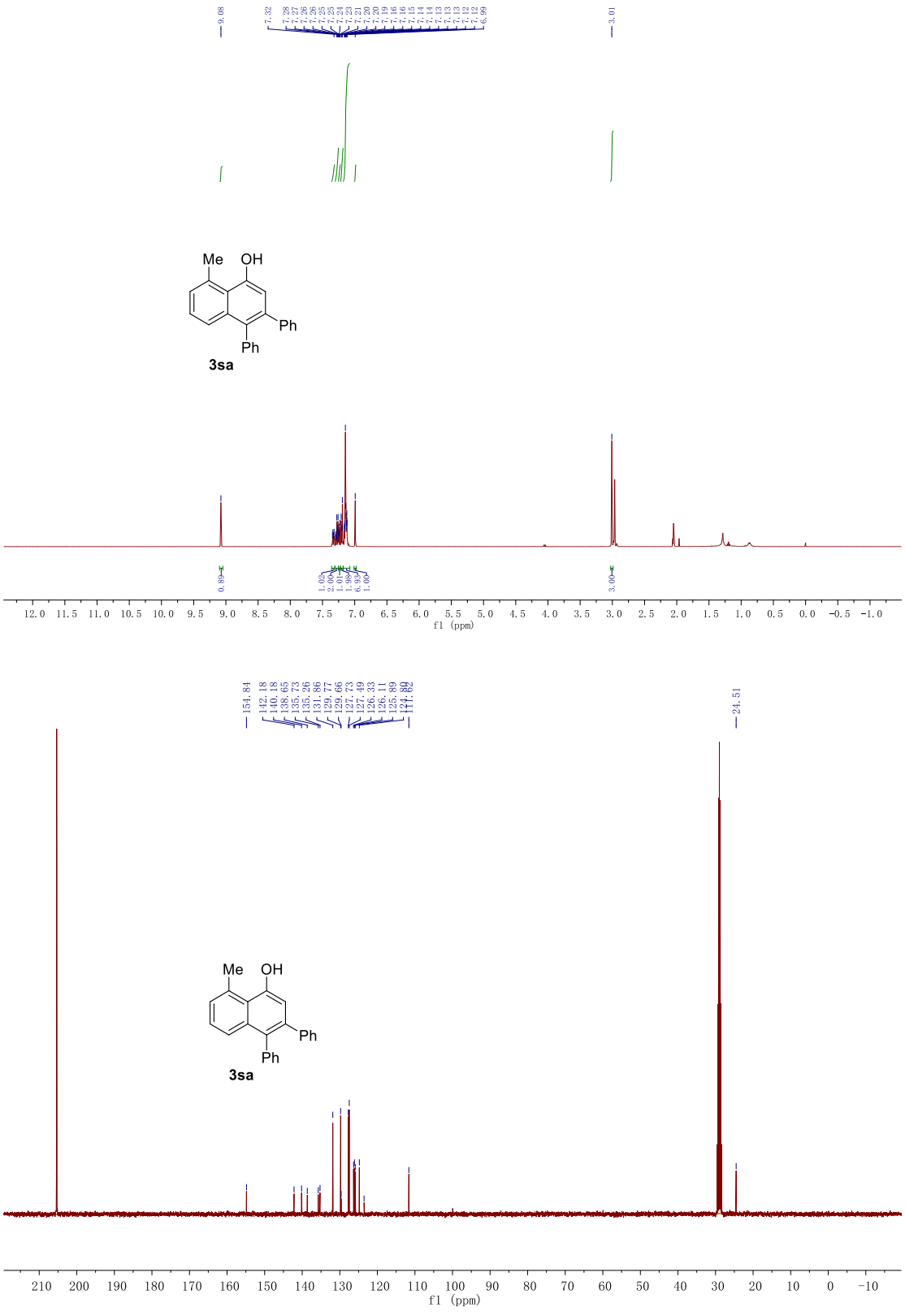

F
OH
F
Ph
Ph
3qa
f1 (ppm)

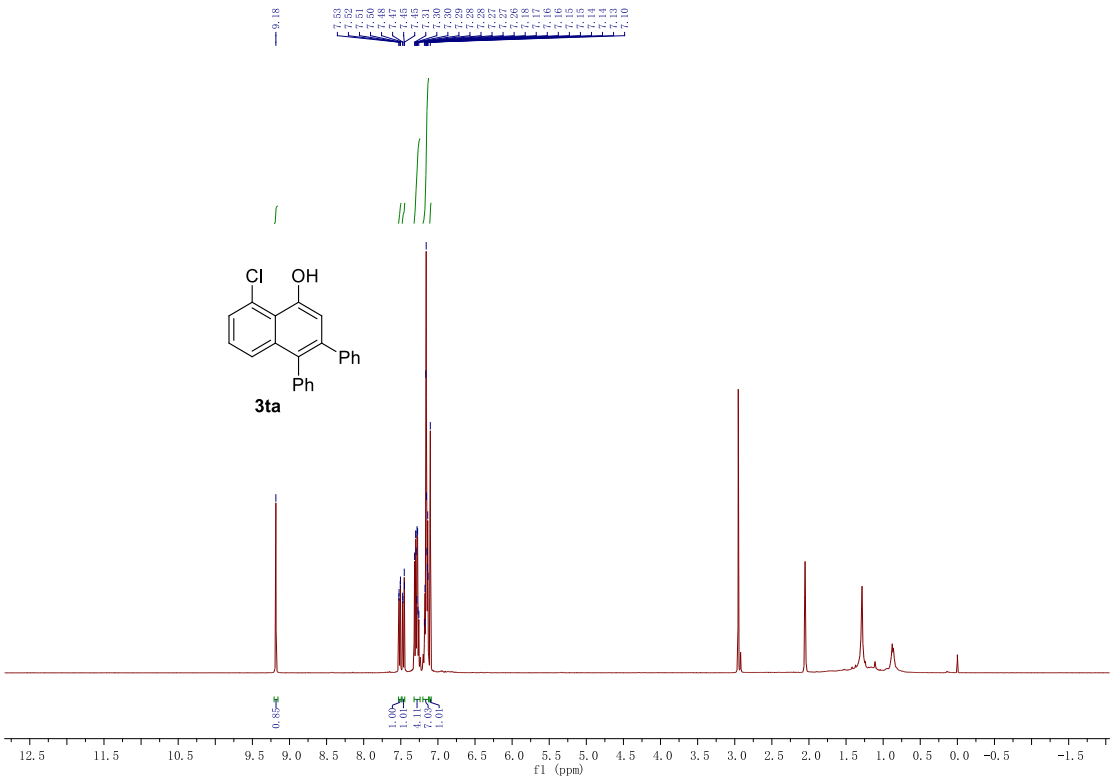

-108.26
-108.28
-112.82
-112.87
F
OH
F
Ph
Ph
3qa
-82
-86
-90
-94
-98
-102
-106
-110
-114
-118
-122
-126
-130
-134
-138
-142
f1 (ppm)

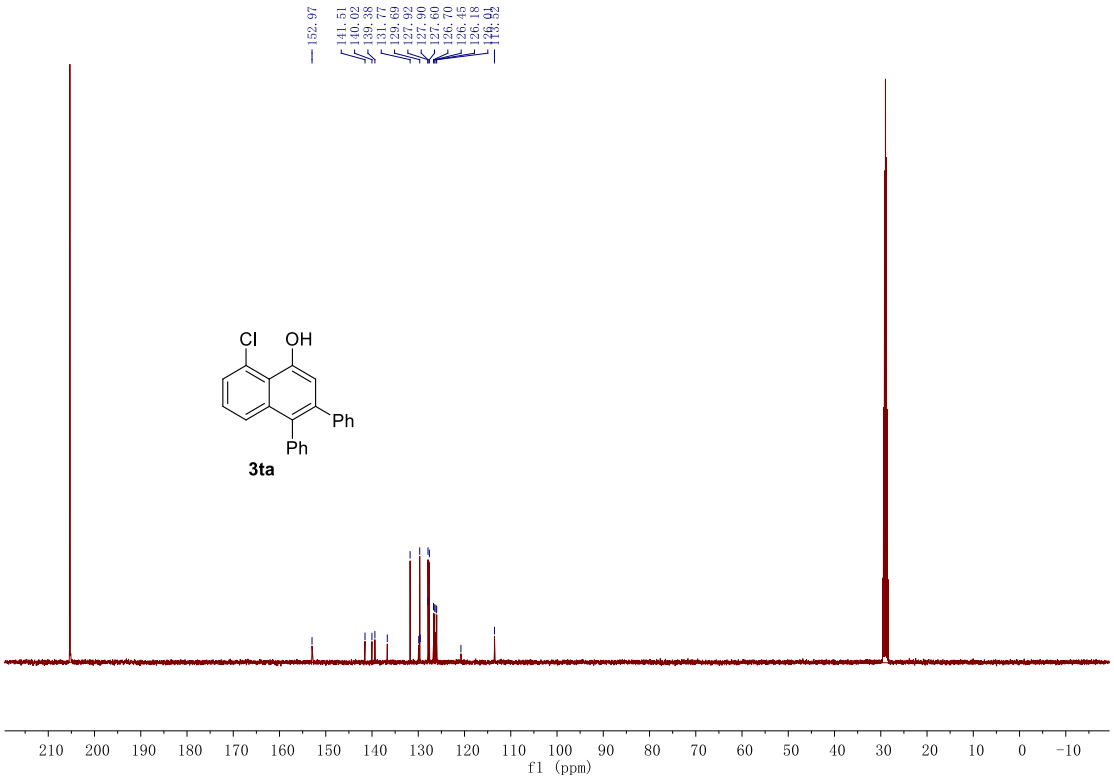

8.95
8.94
7.35
7.33
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.27
7.27
7.27
7.26
7.26
7.25
7.25
7.18
7.17
7.17
7.16
7.16
7.15
7.14
7.14
7.13
7.12
7.12
7.06
F
OH
Ph
Ph
3ra
0.92
5.05
0.85
1.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

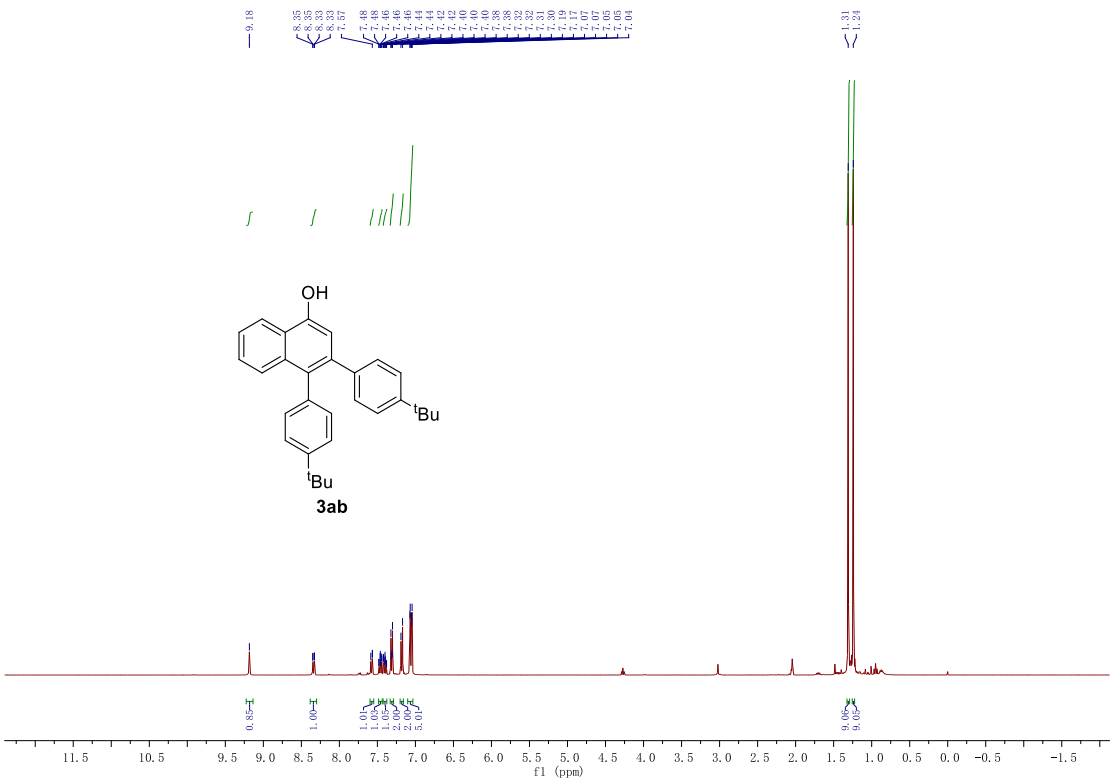

160.68
158.16
152.07
152.04
131.73
129.74
127.87
127.60
126.66
126.42
126.37
126.28
122.68
114.01
112.64
109.93
109.71
F
OH
Ph
Ph
3ra
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

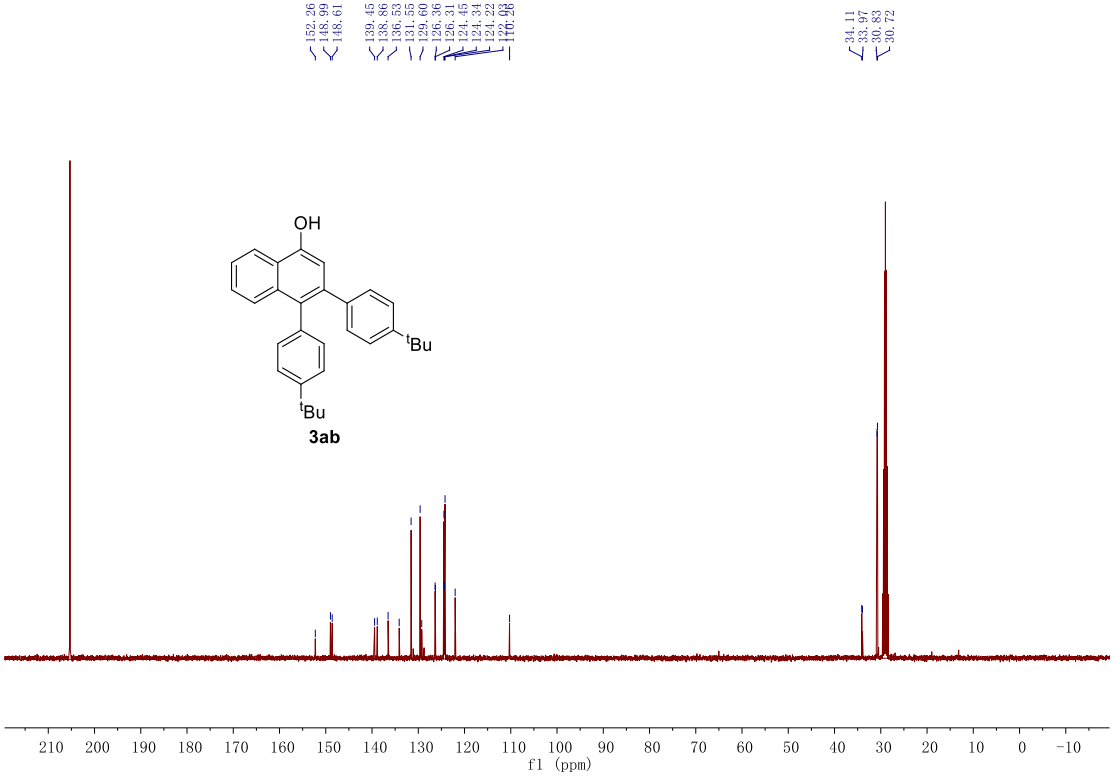

-114.62
F
OH
Ph
Ph
3ra
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

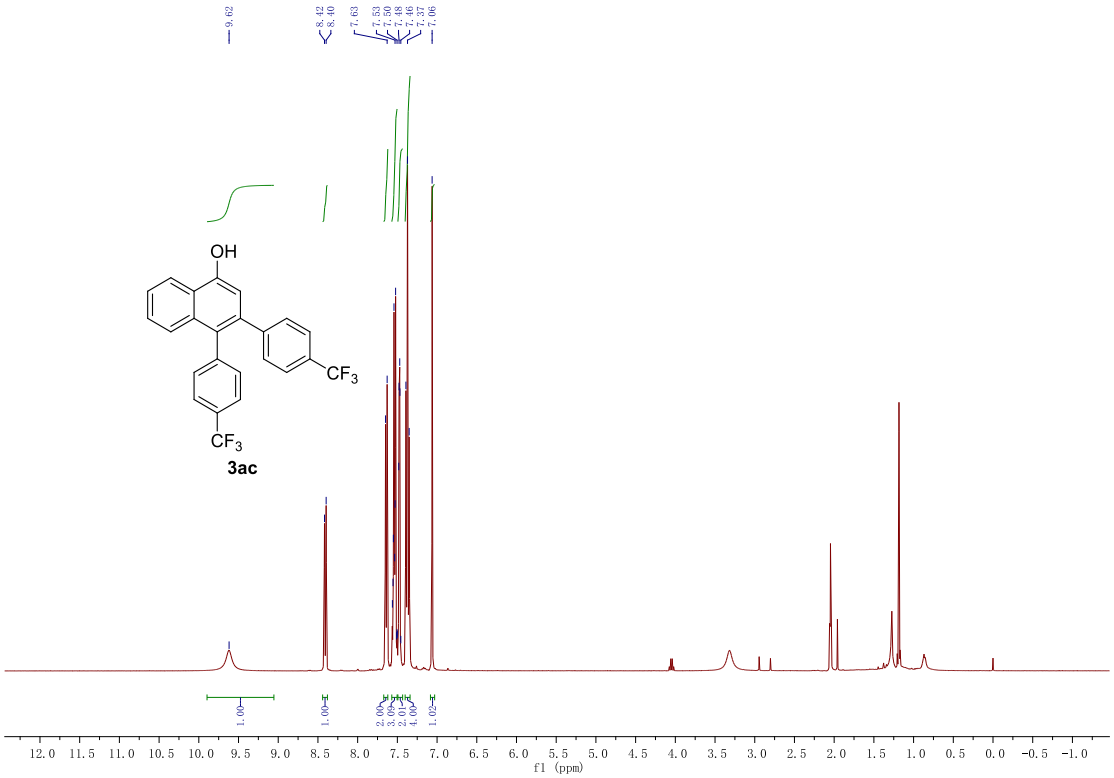

9.08
7.32
7.28
7.27
7.26
7.25
7.24
7.23
7.21
7.20
7.19
7.16
7.15
7.14
7.13
7.13
7.12
7.12
6.99
3.01
Me
OH
Ph
Ph
3sa
0.89
1.00
2.05
1.01
1.98
6.95
1.00
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
154.84
142.18
140.18
138.65
135.73
135.26
131.86
129.77
129.66
127.73
127.49
126.33
126.11
125.89
111.82
24.51
Me
OH
Ph
Ph
3sa
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)

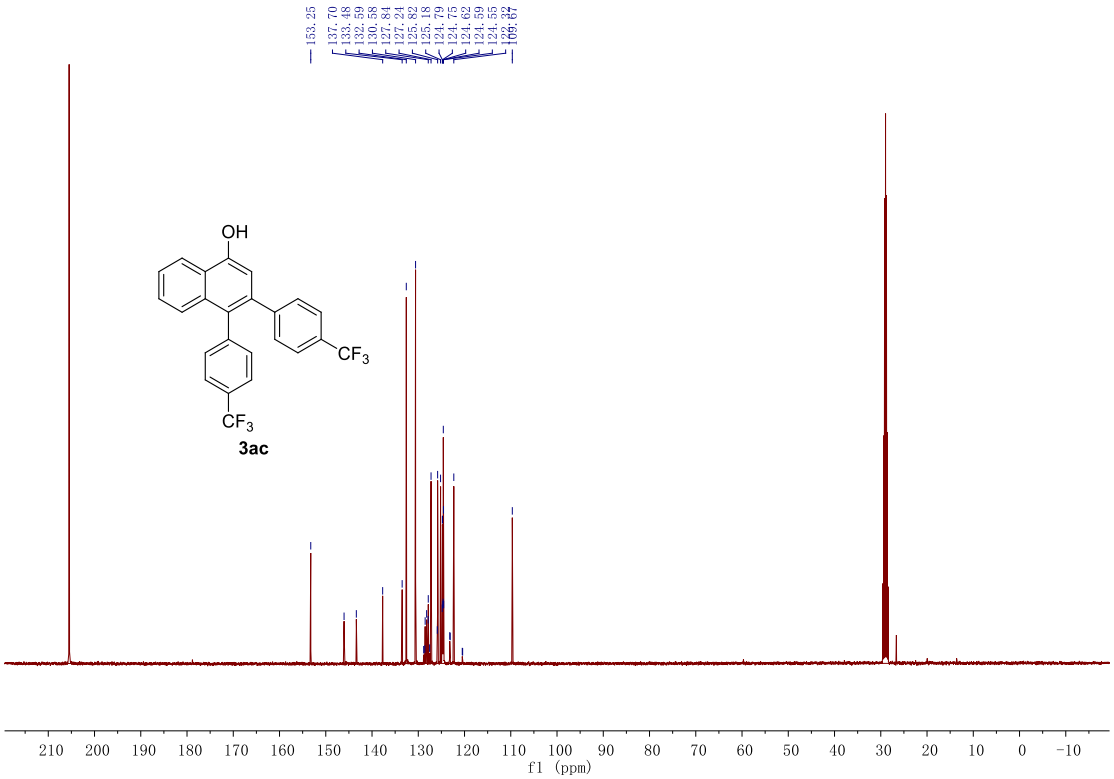

Cl
OH
Ph
Ph
3ta
f1 (ppm)

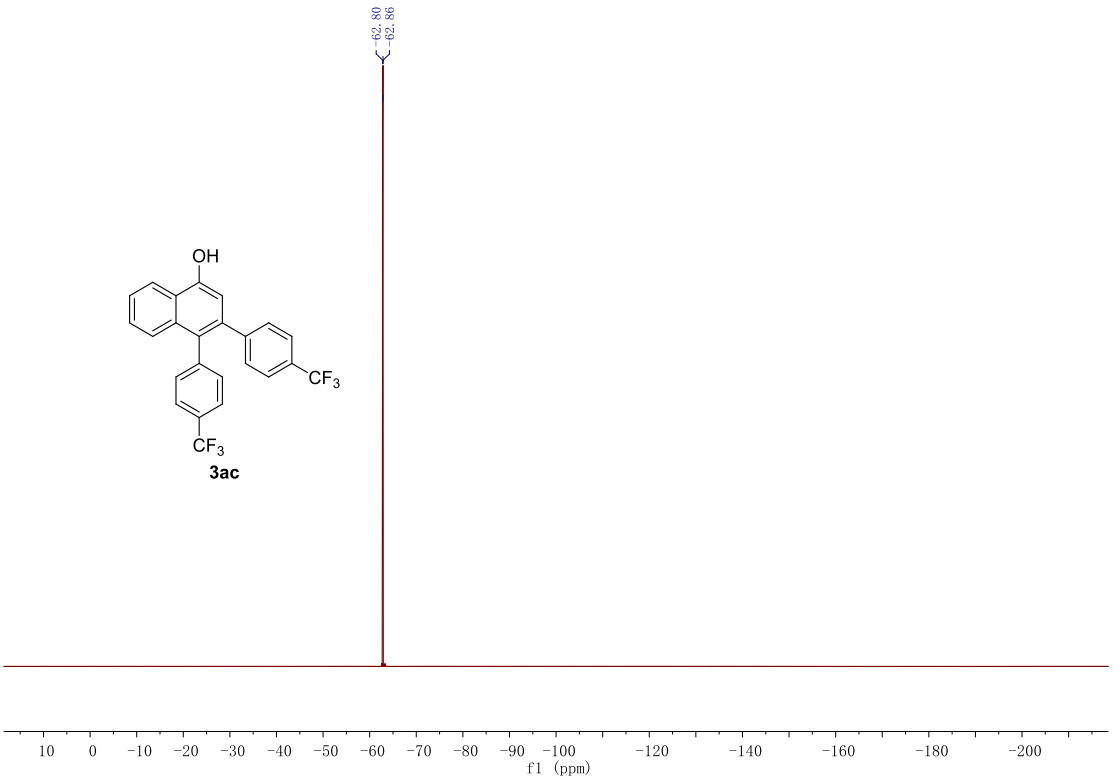

Cl
OH
Ph
Ph
3ta
f1 (ppm)

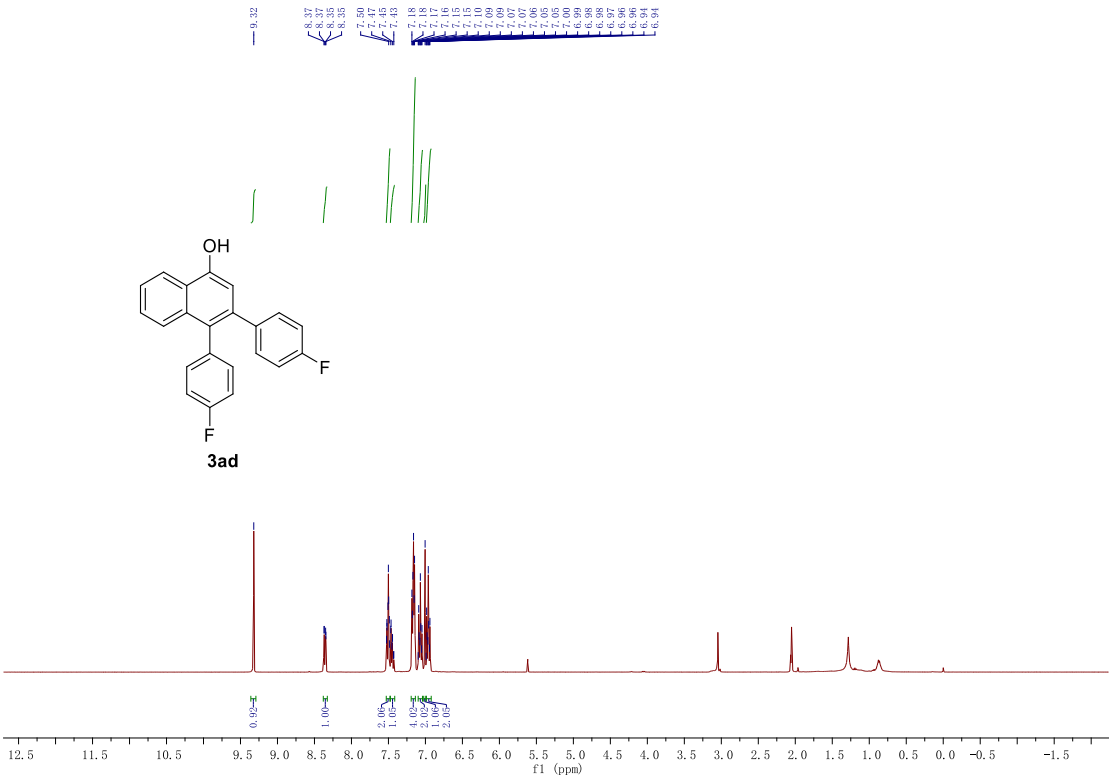

OH
tBu
tBu
3ab
f1 (ppm)

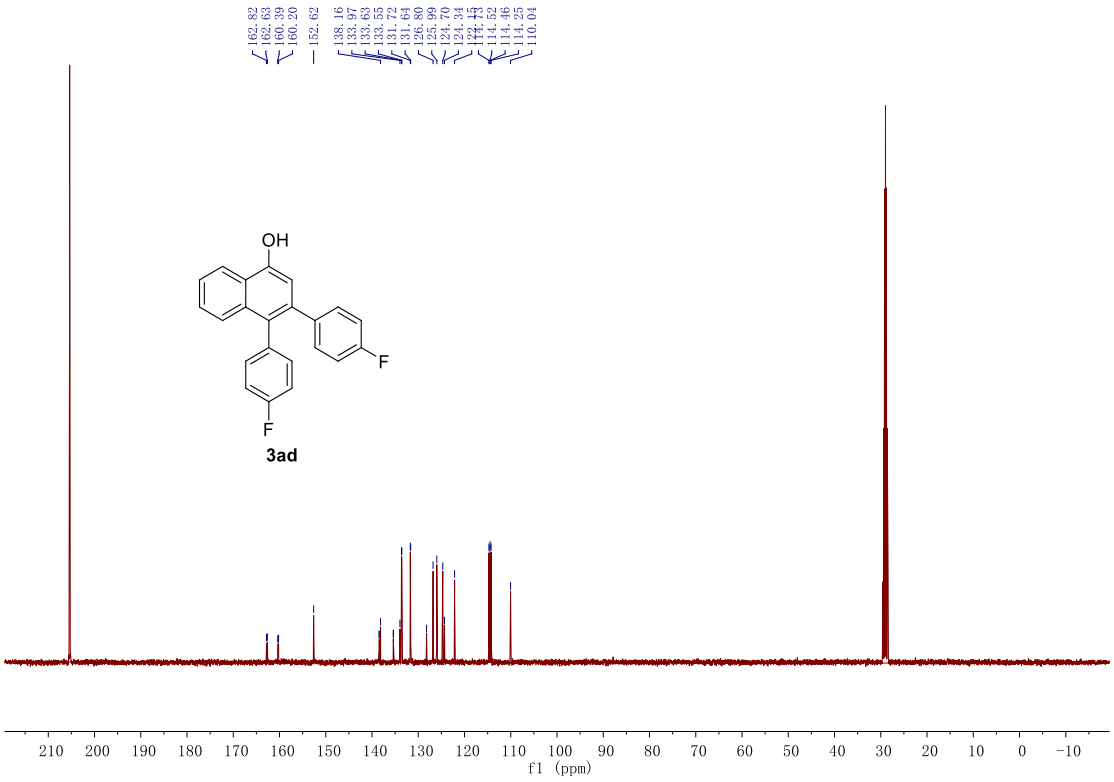

OH
tBu
tBu
3ab
f1 (ppm)

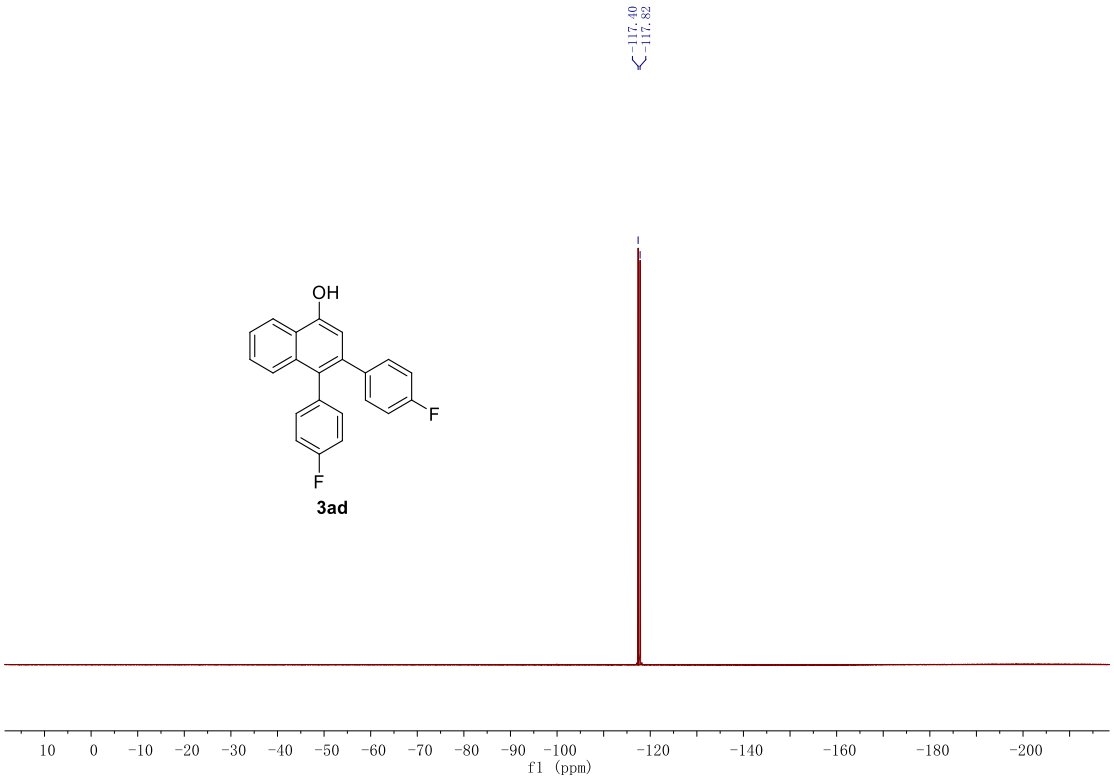

9.62
8.42
8.40
7.63
7.53
7.50
7.48
7.46
7.37
7.06
OH
CF3
CF3
3ac
1.00
1.00
2.00
3.08
2.01
4.00
1.02
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

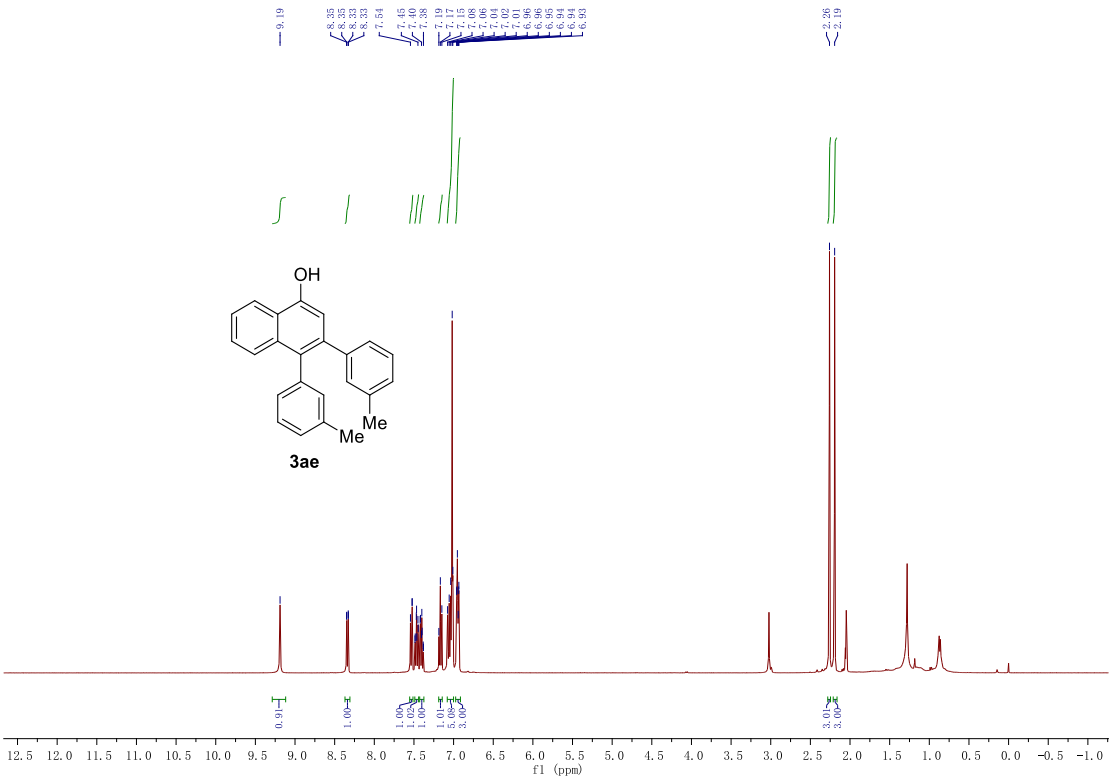

153.25
137.70
133.48
132.59
130.58
127.84
127.24
125.82
125.18
124.79
124.75
124.62
124.59
124.55
OH
CF3
CF3
3ac
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

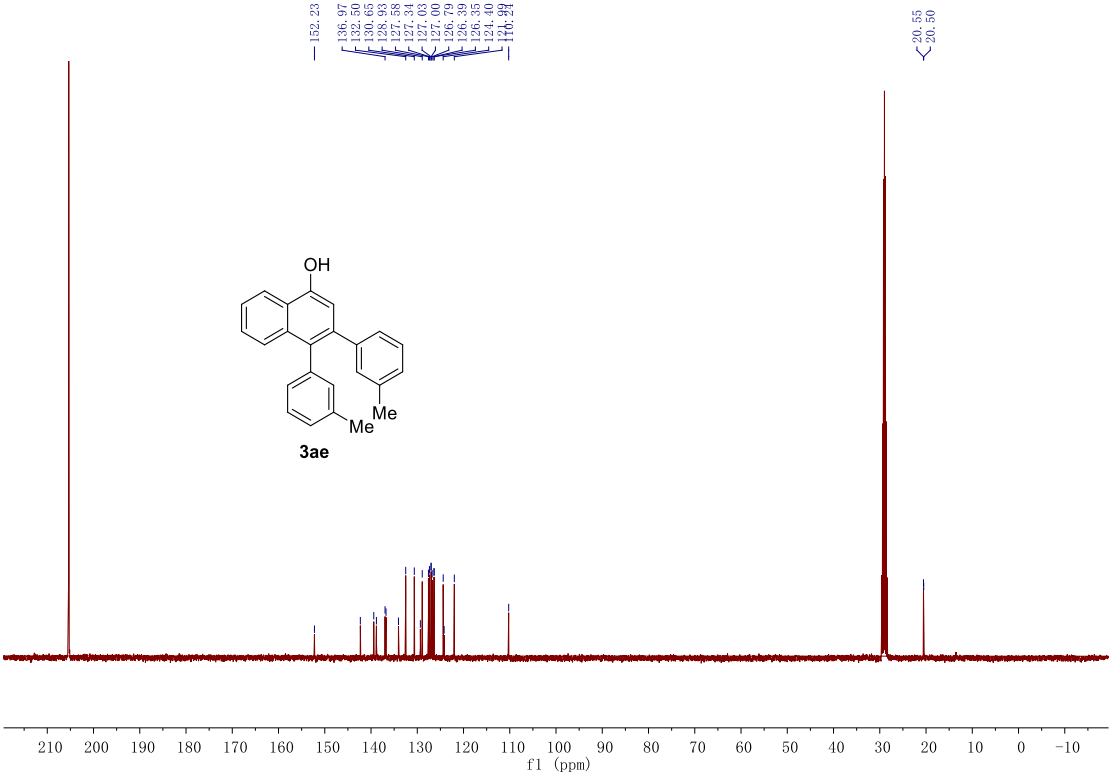

-62.80
-62.86
OH
CF3
CF3
3ac
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

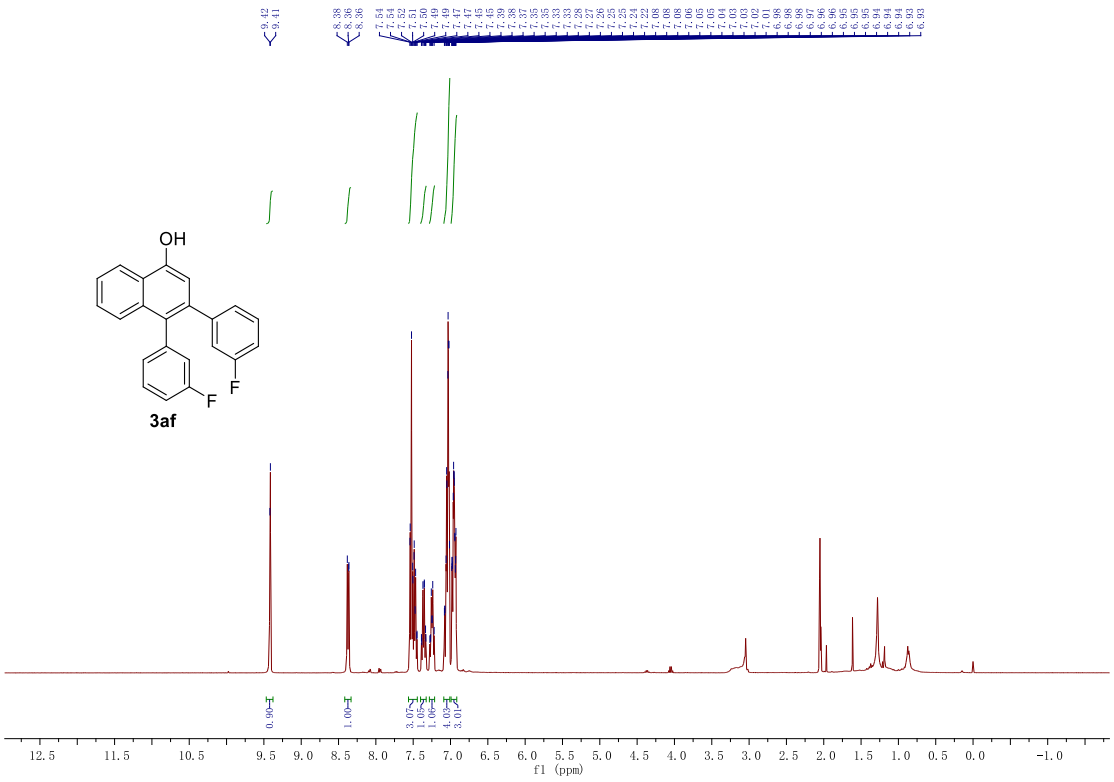

9.32
8.37
8.37
8.35
8.35
7.50
7.47
7.45
7.43
7.18
7.18
7.17
7.16
7.15
7.15
7.10
7.09
7.09
7.07
7.07
7.06
7.05
7.00
6.99
6.98
6.98
6.97
6.96
6.96
6.94
6.94
OH
F
F
3ad
0.92
1.00
2.06
1.05
4.02
2.02
1.07
2.08
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.5
f1 (ppm)

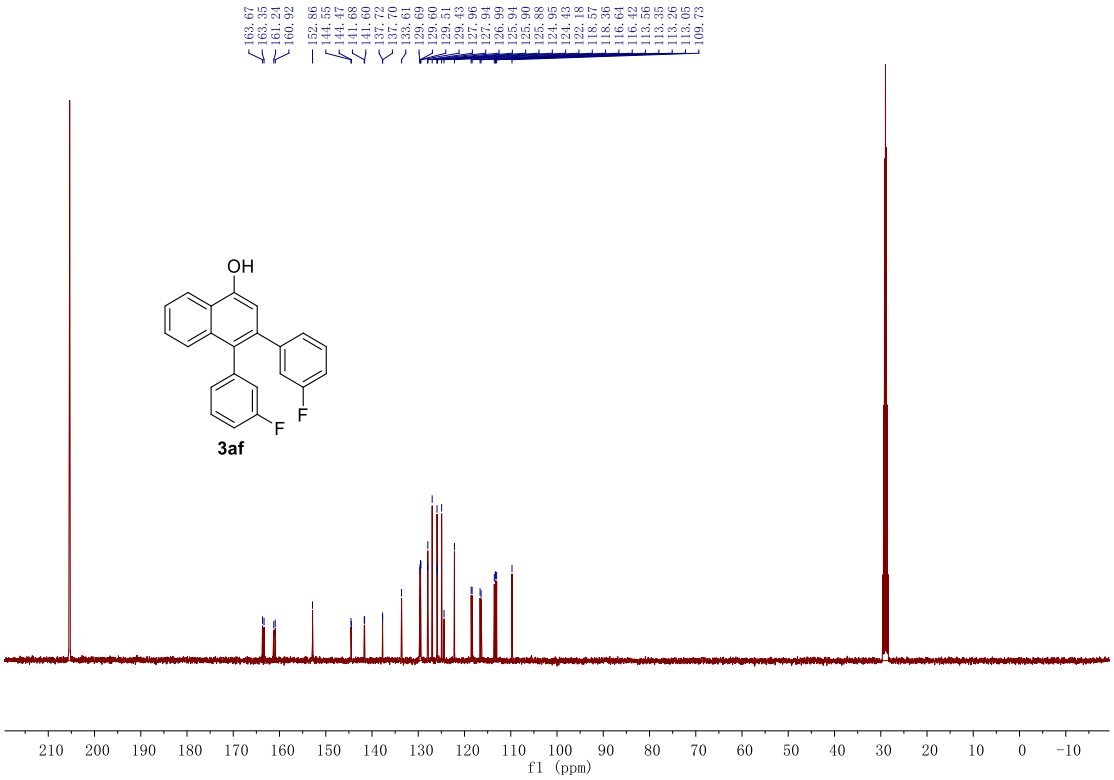

162.82
162.63
160.39
160.20
152.62
138.16
133.97
133.63
133.55
131.72
131.64
126.80
125.99
124.70
124.34
122.13
114.52
114.46
114.25
110.04
OH
F
F
3ad
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

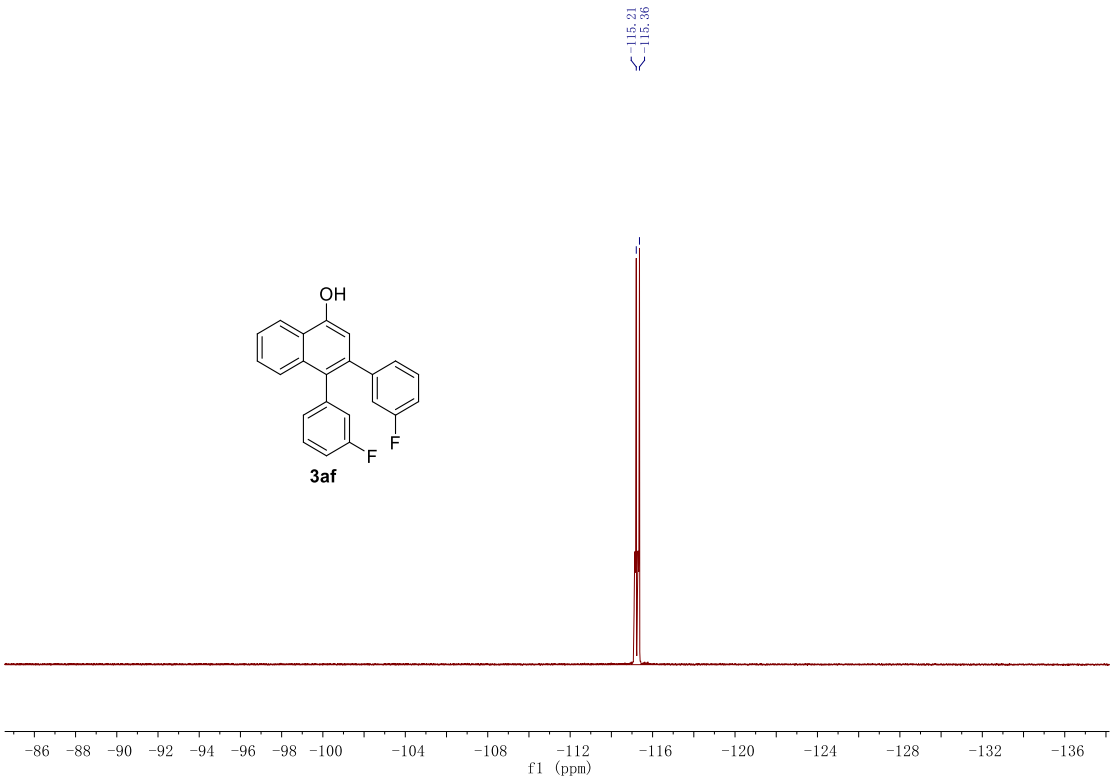

117.40
117.82
OH
F
F
3ad
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

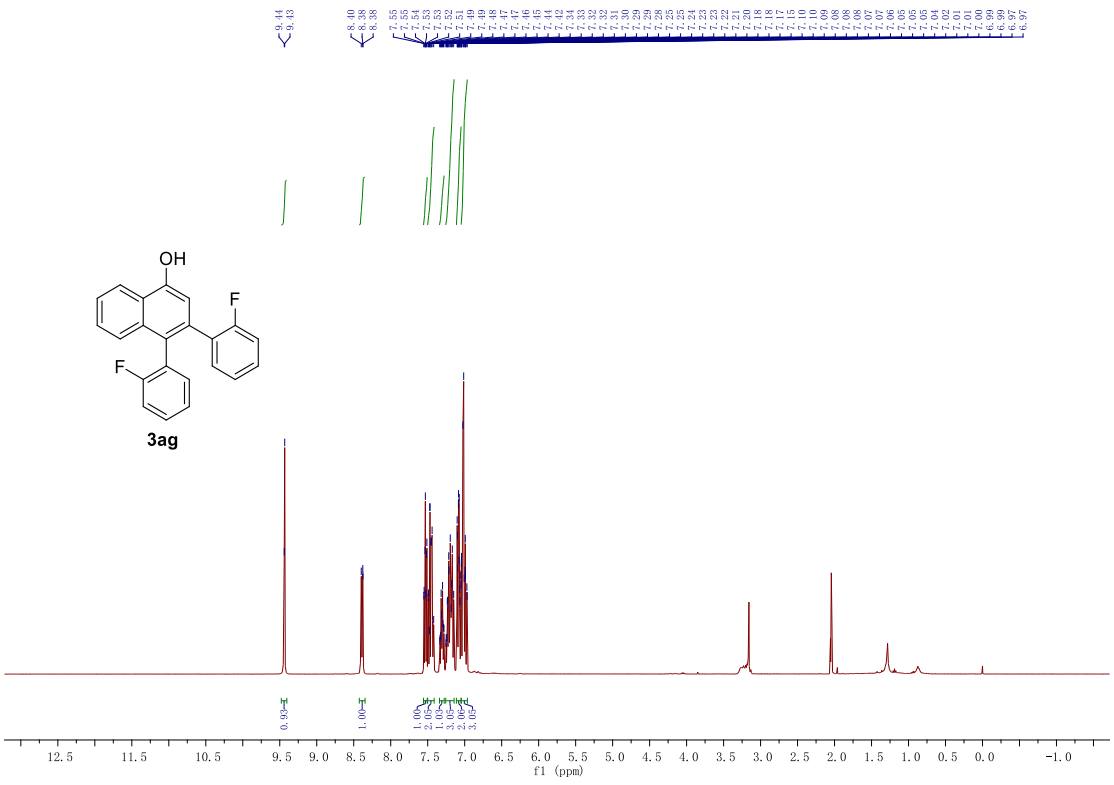

8.19
8.35
8.35
8.33
8.33
7.54
7.45
7.40
7.38
7.19
7.17
7.15
7.08
7.06
7.04
7.02
7.01
6.96
6.96
6.95
6.94
6.94
6.93
2.26
2.19
OH
Me
Me
3ae
0.91
1.00
1.06
1.05
1.00
1.01
5.08
3.00
3.01
3.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

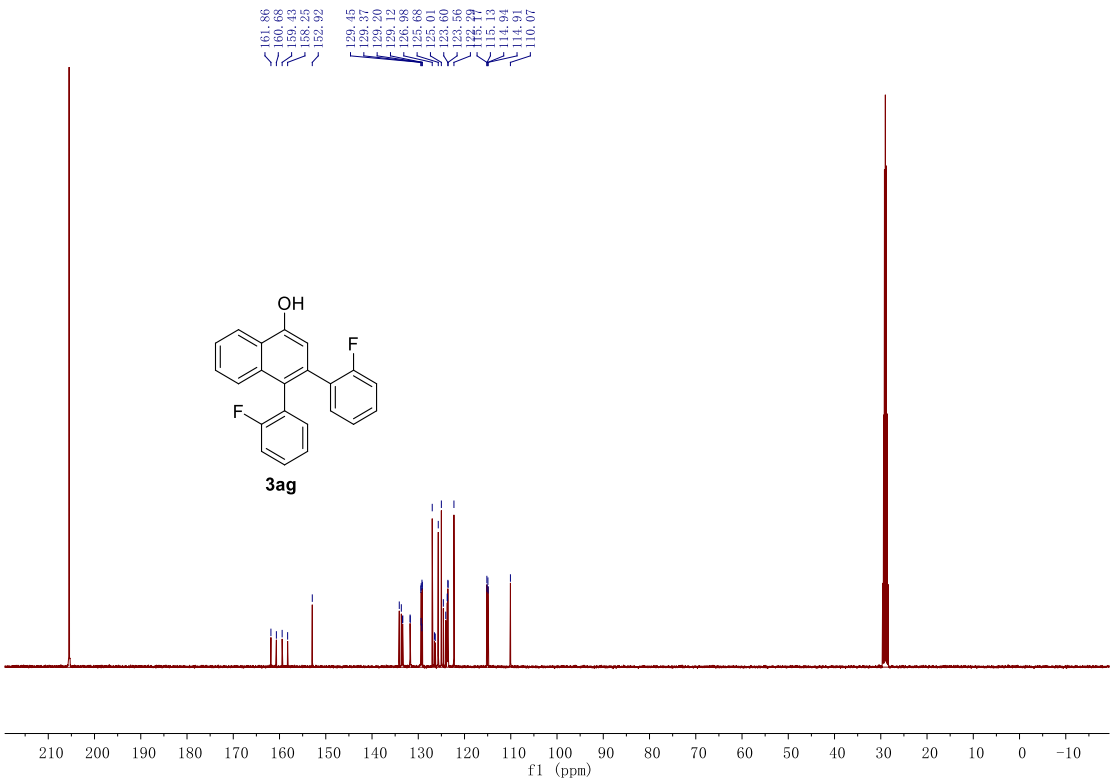

152.23
136.97
132.50
130.65
128.93
127.38
127.34
127.03
127.00
126.79
126.39
126.35
124.40
121.99
116.24
20.55
20.50
OH
Me
Me
3ae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

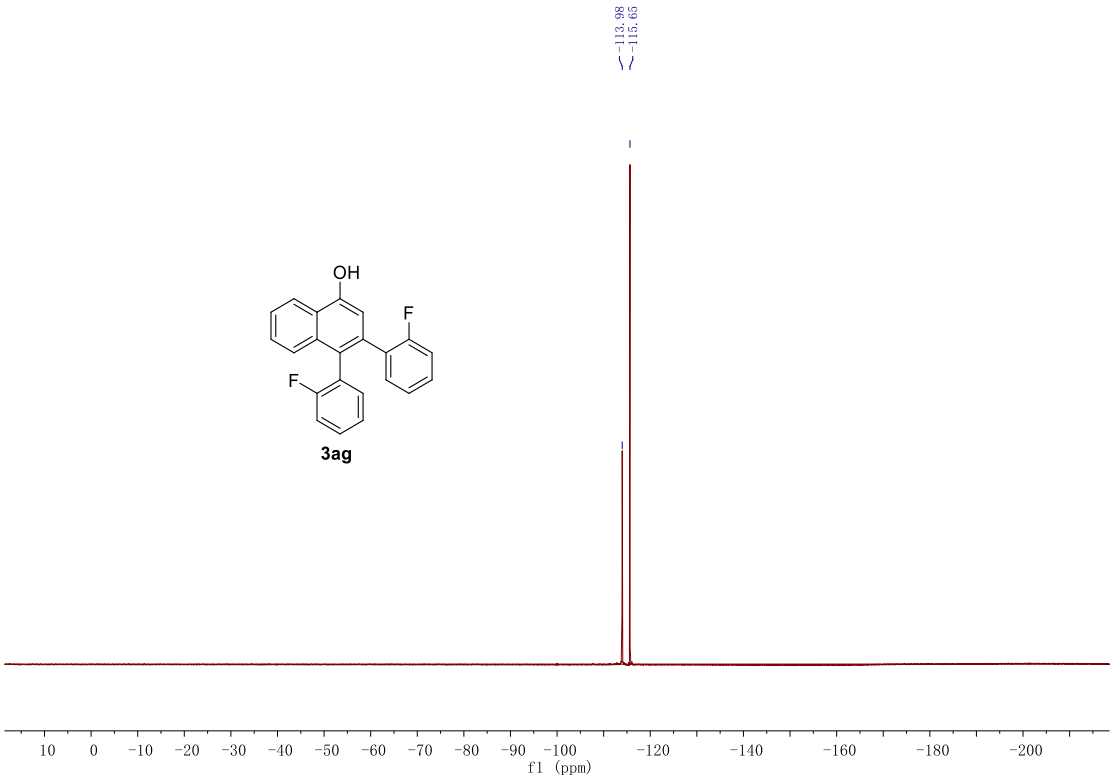

OH
F
F
3af
f1 (ppm)

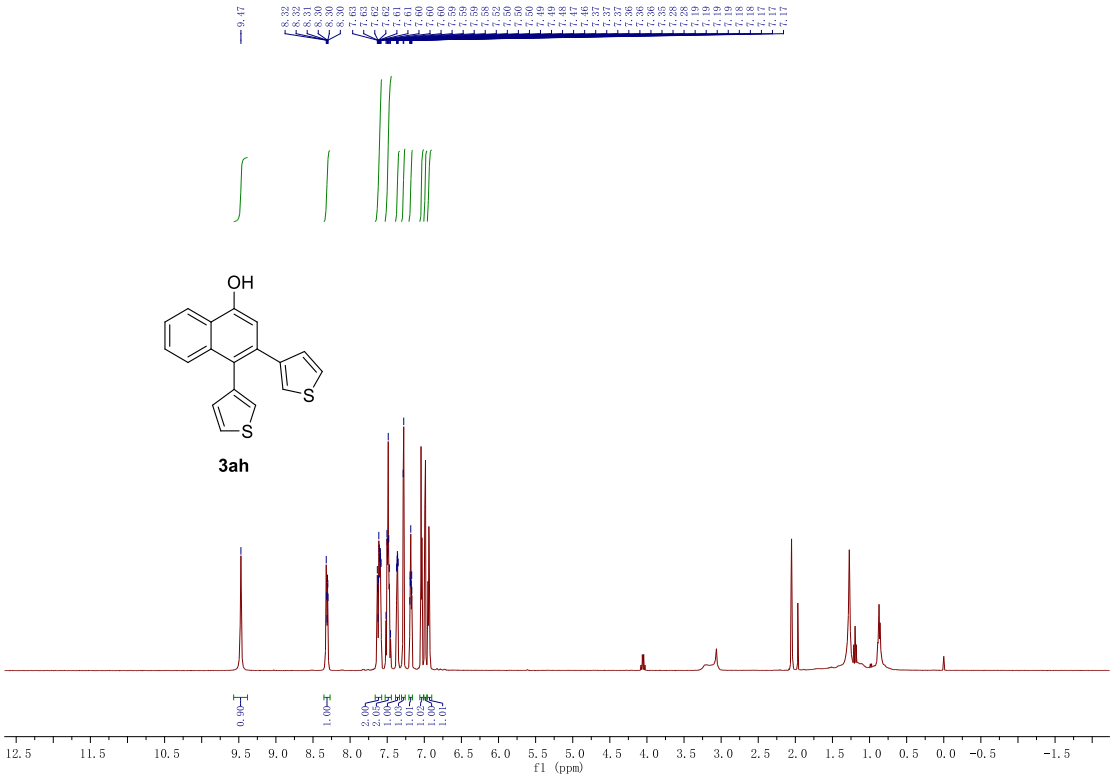

OH
F
F
3af
f1 (ppm)

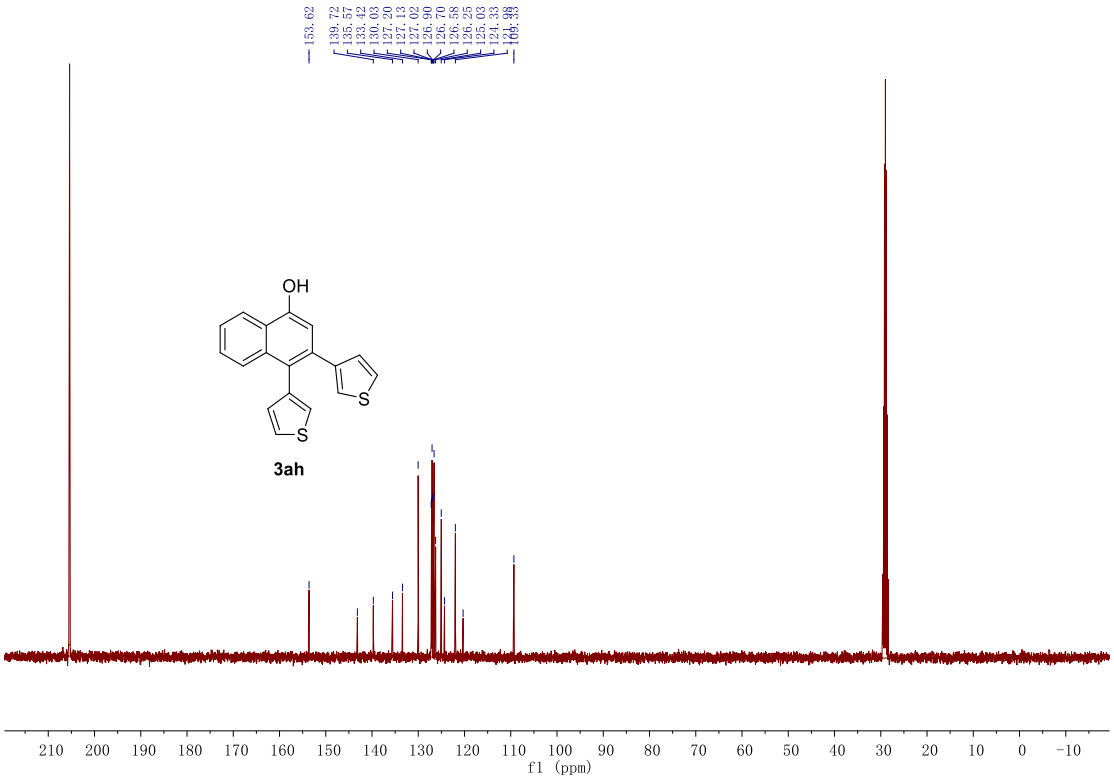

-115.21
-115.36
OH
F
F
3af
-86 -88 -90 -92 -94 -96 -98 -100 -104 -108 -112 -116 -120 -124 -128 -132 -136
f1 (ppm)

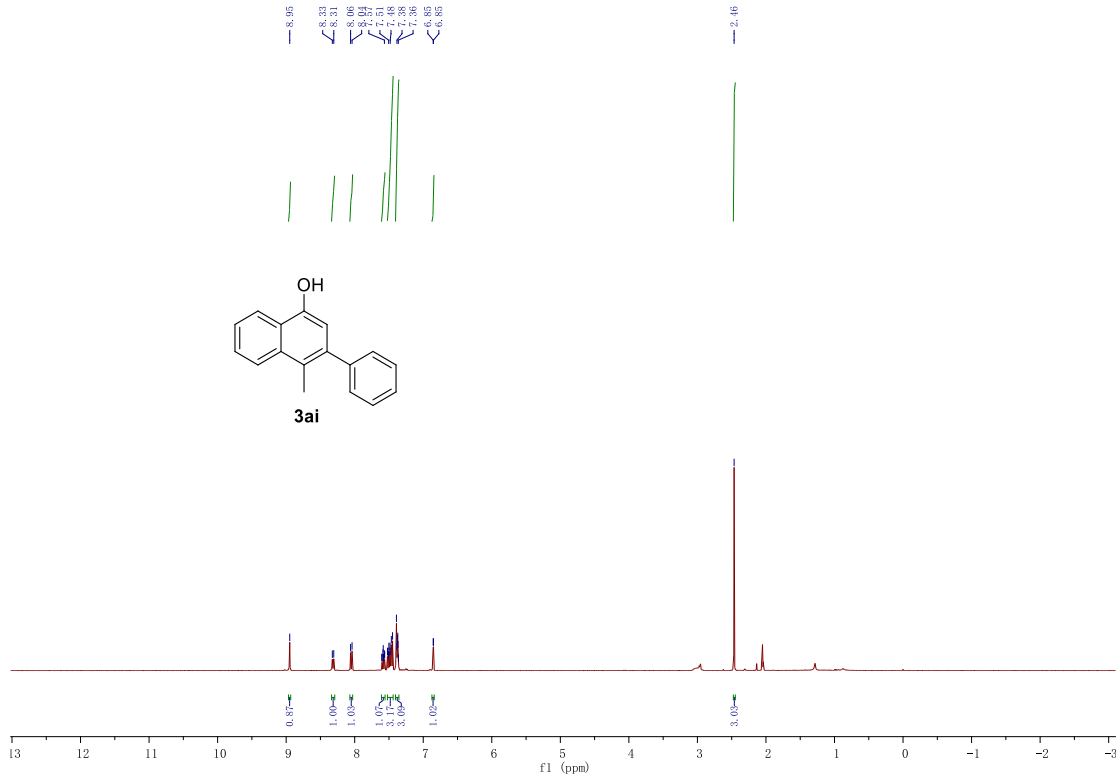

9.44
9.43
8.40
8.38
8.38
OH
F
F
3ag
0.93
1.00
1.00
2.05
1.05
2.06
3.05
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)

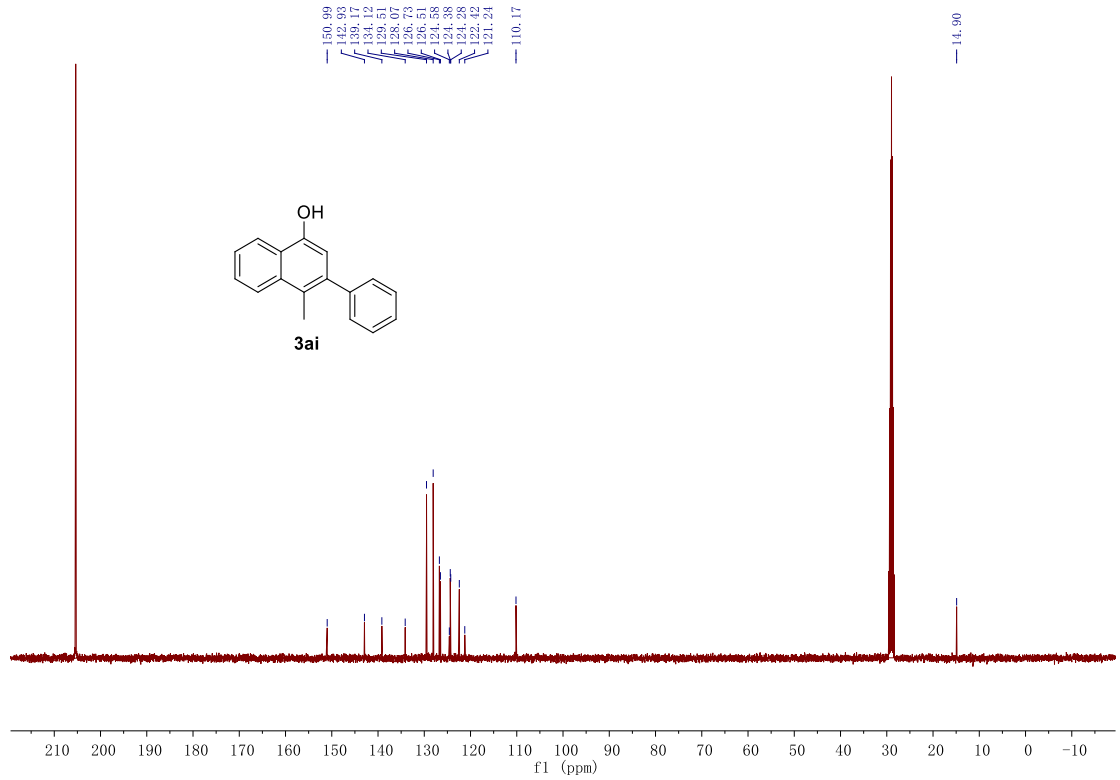

161.86
160.68
159.43
158.25
152.92
129.45
129.37
129.20
129.12
126.98
125.68
125.01
123.60
123.56
115.13
114.94
114.91
110.07
OH
F
F
3ag
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

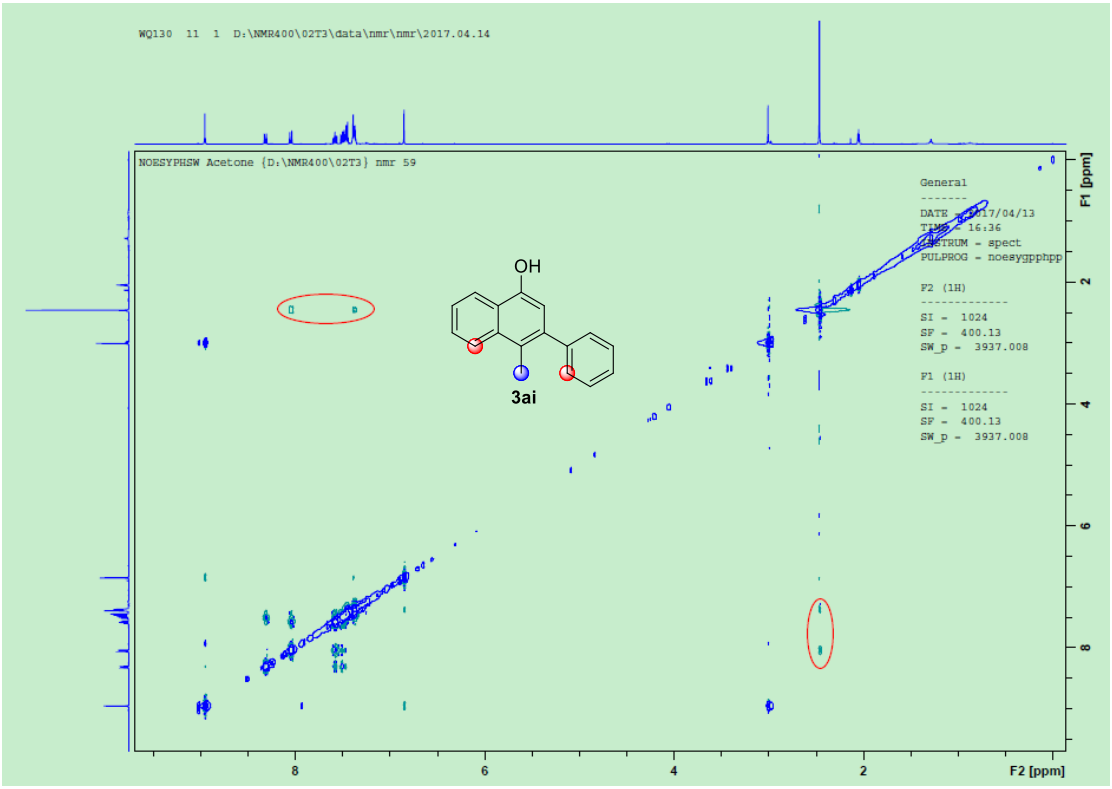

-113.98
-115.65
OH
F
F
3ag
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

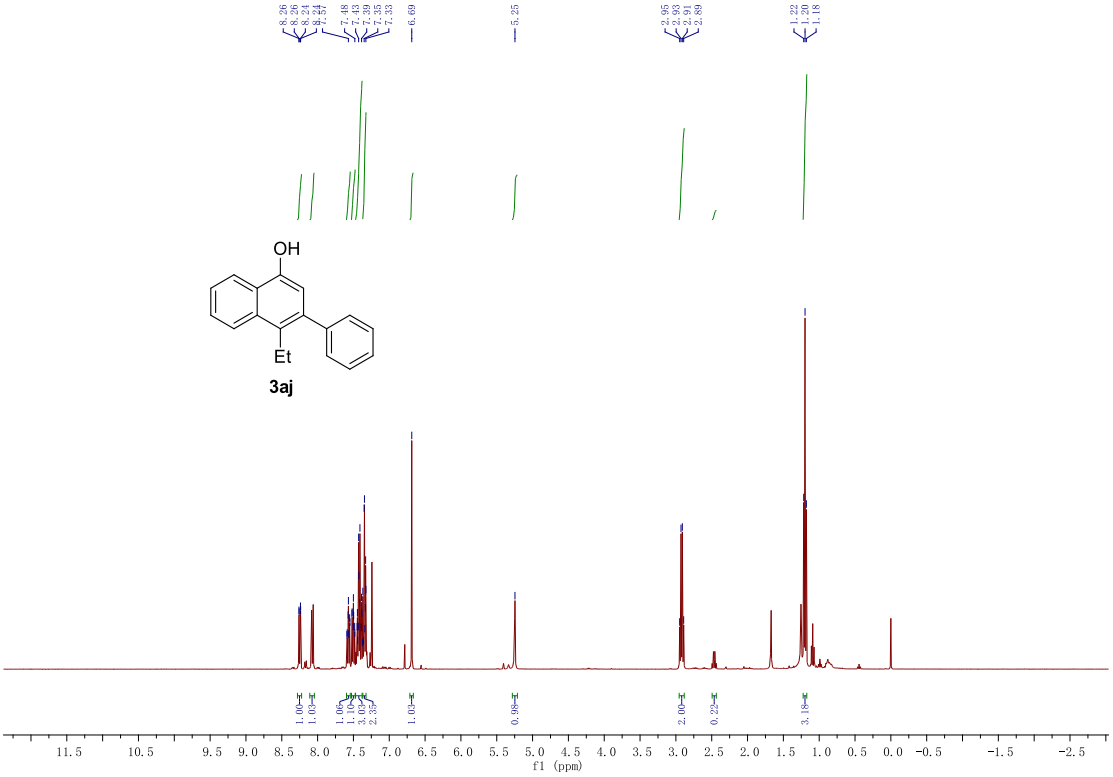

OH
S
S
3ah
f1 (ppm)

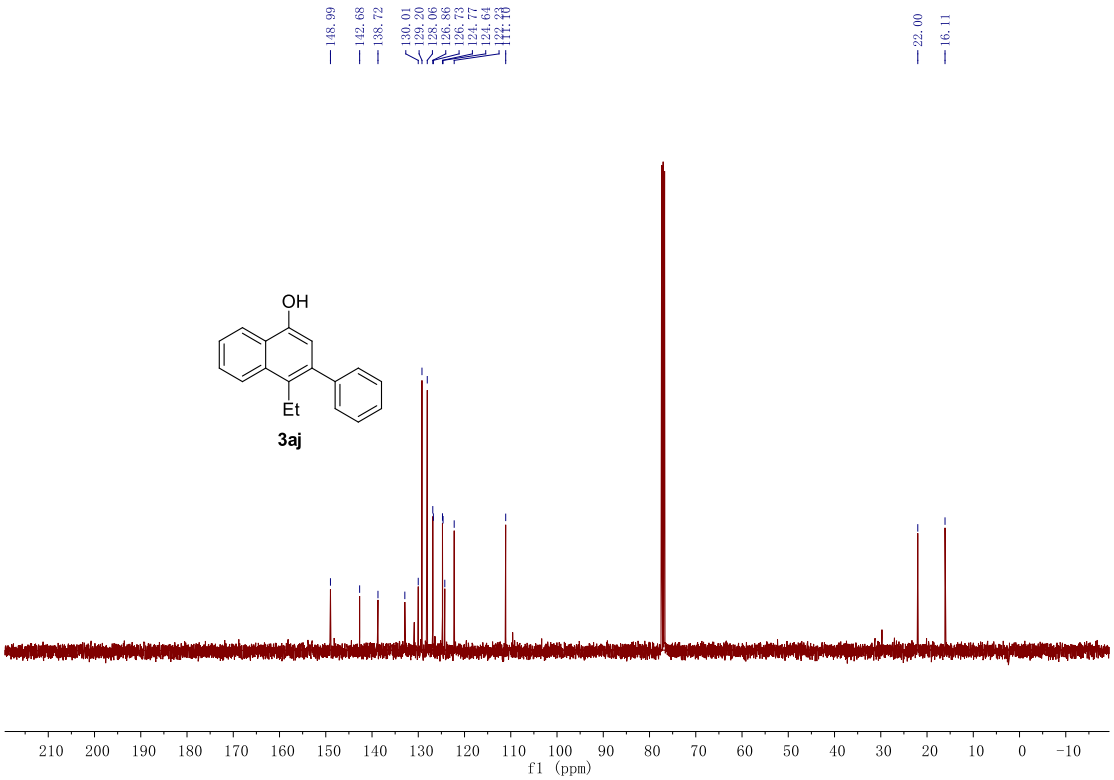

OH
S
S
3ah
f1 (ppm)

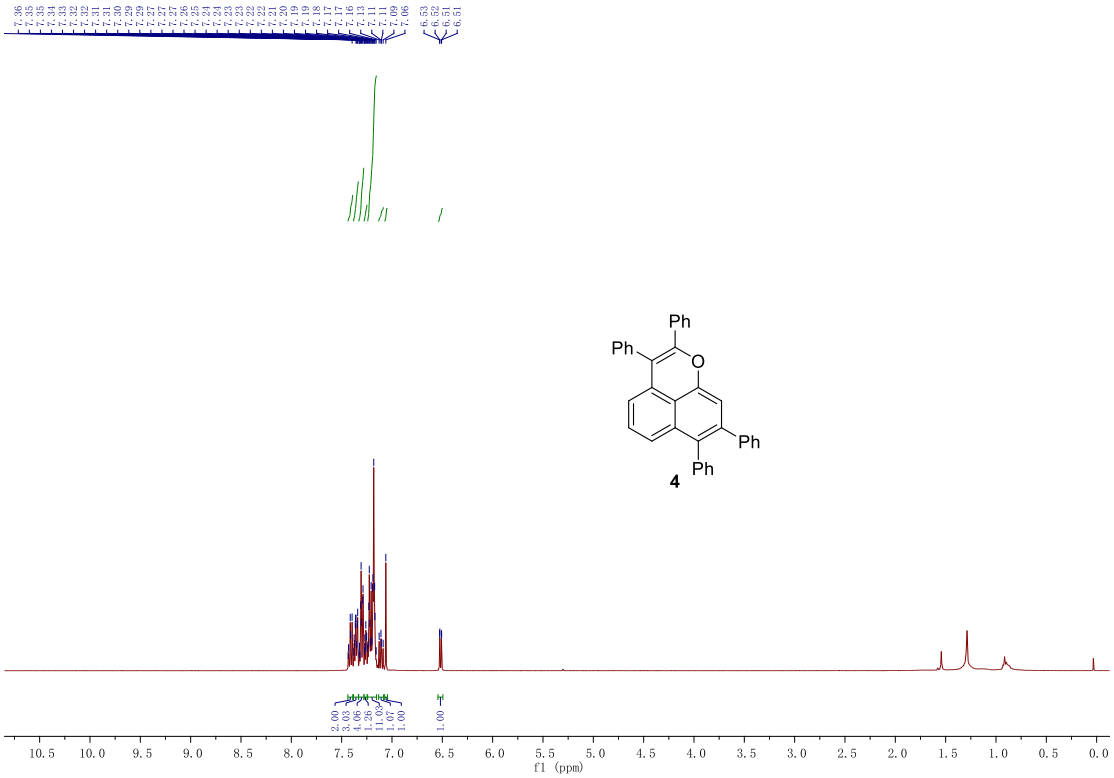

8.95
8.33
8.31
8.06
8.04
7.52
7.51
7.48
7.38
7.36
6.85
6.83
2.46
OH
3ai
0.87
1.00
1.03
1.07
3.17
3.08
1.02
3.03
f1 (ppm)

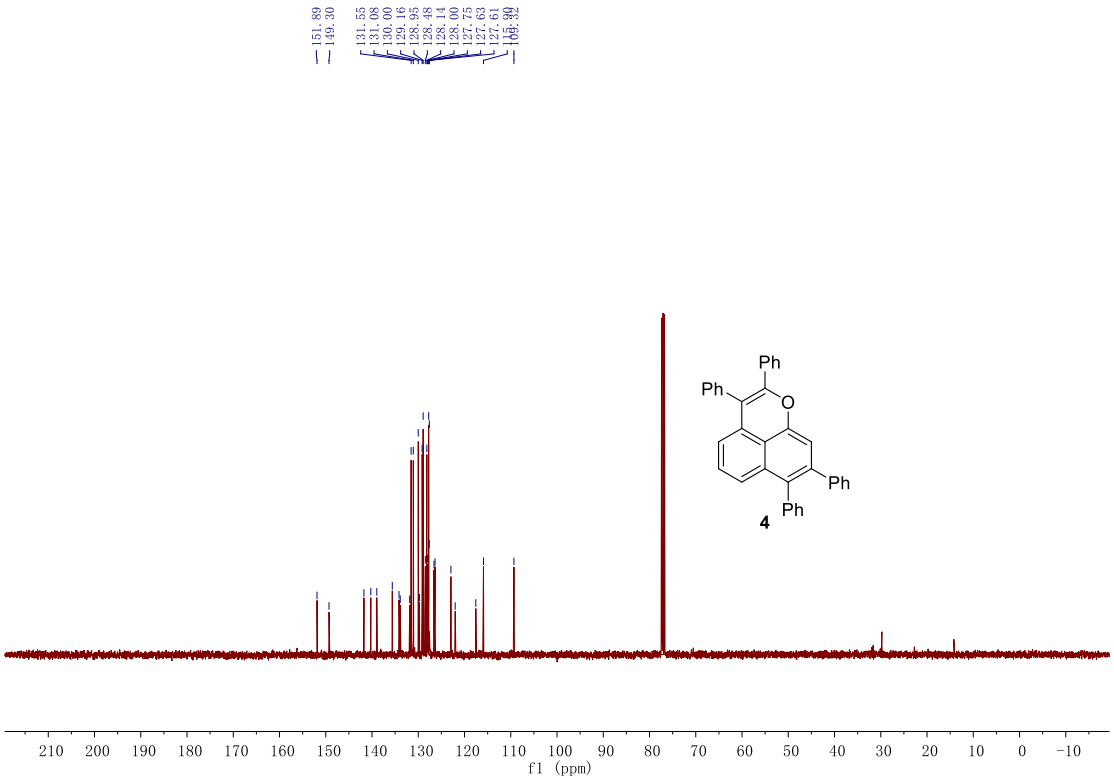

150.99
142.93
139.17
134.12
129.51
128.07
126.73
126.51
124.58
124.38
124.28
122.42
121.24
110.17
14.90
OH
3ai
f1 (ppm)

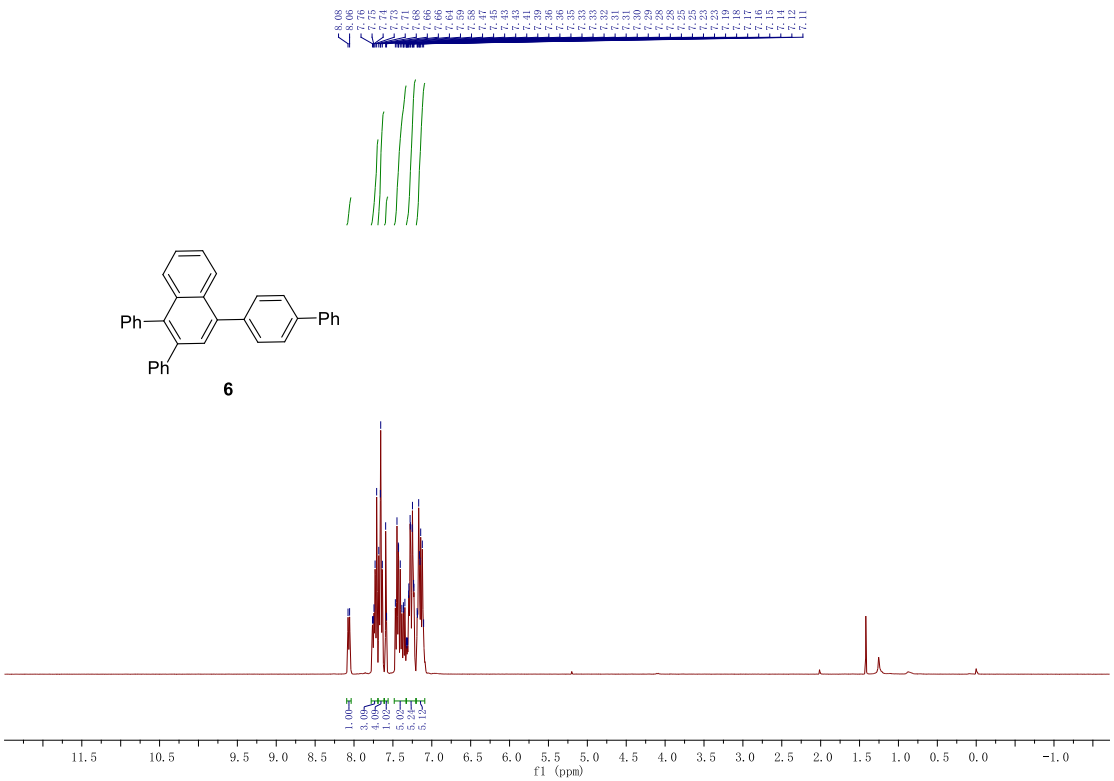

WQ130 11 1 D:\NMR400\02T3\data\nmr\nmr\2017.04.14
NOESYPHSW Acetone {D:\NMR400\02T3} nmr 59
OH
3ai
General
PULPROG = noesygpphpp
F2 (1H)
SI = 1024
SF = 400.13
SW_p = 3937.008
F1 (1H)
SI = 1024
SF = 400.13
SW_p = 3937.008
F1 [ppm]
F2 [ppm]

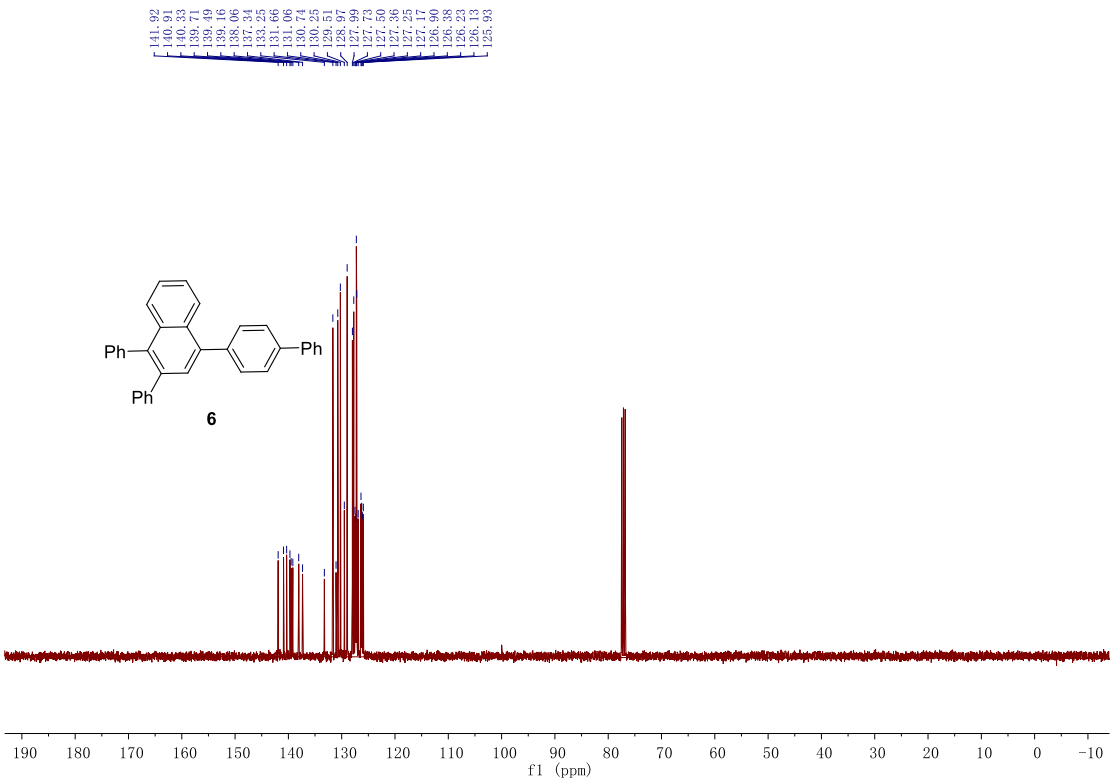

OH
Et
3aj
f1 (ppm)


148.99
142.68
138.72
130.01
129.20
128.06
126.86
126.73
124.77
124.64
22.00
16.11
OH
Et
3aj
f1 (ppm)


Ph
Ph
O
Ph
Ph
4
f1 (ppm)


151.89
149.30
131.55
131.08
130.00
129.16
128.95
128.48
128.14
128.00
127.75
127.63
127.61
Ph
Ph
O
Ph
Ph
4
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)


8.08
8.06
7.76
7.75
7.74
7.73
7.71
7.68
7.66
7.66
7.64
7.59
7.58
7.47
7.45
7.43
7.43
7.41
7.39
7.36
7.36
7.35
7.33
7.32
7.32
7.31
7.31
7.30
7.29
7.28
7.28
7.25
7.25
7.23
7.23
7.21
7.19
7.18
7.17
7.16
7.15
7.14
7.12
7.11
Ph
Ph
Ph
6
1.00
3.09
4.09
1.02
5.02
5.24
5.12
11.5 10.5 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 −1.0
f1 (ppm)


141.92
140.91
140.33
139.71
139.49
139.16
138.06
137.34
133.25
131.66
131.06
130.74
130.25
129.51
128.97
127.99
127.73
127.50
127.36
127.25
127.17
126.90
126.38
126.23
126.13
125.93
Ph
Ph
Ph
6
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)