

Electronic Supplementary Information

Construction of fused heterocycles by visible-light induced dearomatization of nonactivated arenes

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Table of Contents

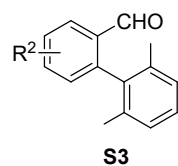
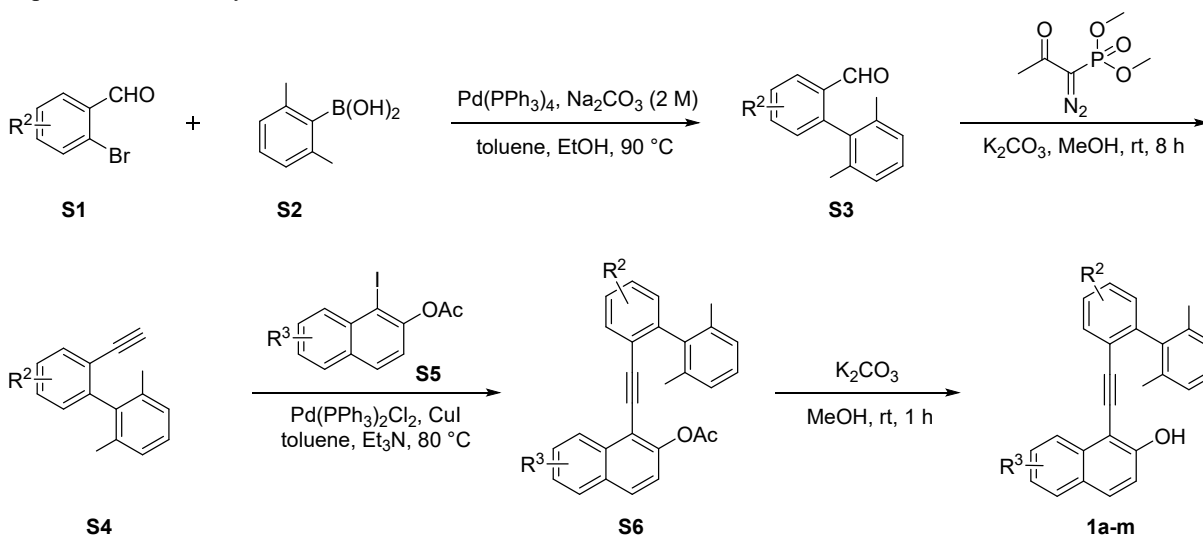
1. General information	S2
2. General procedure for the synthesis of substrates 1	S2
3. Analytical data of compounds 1	S5
4. Reaction conditions screening	S11
5. General procedure for the radical dearomative cyclization of benzene derivatives	S13
6. Analytical data of compounds 2	S13
7. Mechanistic studies	S22
8. Crystallographic details of 2v	S25
9. ¹ H and ¹³ C NMR spectra	S26
10. References	S73

1. General information

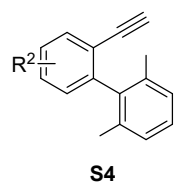
All reagents were obtained from Adamas, Aladin, Accela, or Acros and used without further purification unless otherwise noted. The products were purified by column chromatography with Huanghai Silica Gel 50-75 μm , ultrapure silica gel. ^1H and ^{13}C NMR spectra were recorded on an Agilent 400MR DD2 (400 MHz) or Agilent 600MR DD2 (600 MHz) spectrometer. Chemical shifts were reported in parts per million (ppm), and tetramethylsilane or the residual solvent peak was used as an internal reference. ^1H (tetramethylsilane δ 0.00 ppm, chloroform δ 7.26 ppm), ^{13}C (chloroform δ 77.00 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constants (Hz) and integration. High resolution mass spectra (HRMS) were performed on Bruker Solarix 7.0 T. X-ray crystallography analysis of single crystal was performed on an Agilent SuperNova-CCD X-Ray diffractometer. UV-vis measurements were carried out on Shimadzu UV-vis spectrophotometer UV-2600. Unless otherwise stated, all solvents employed in the reactions were distilled from appropriate drying agents prior to use.

2. General procedure for the synthesis of substrates 1

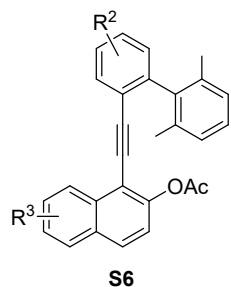
General procedure for the synthesis of substrates **1a-m**



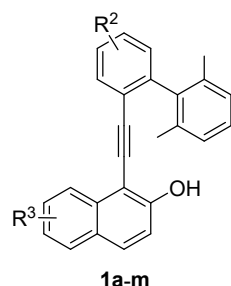
The reactions were carried out according to a literature method with some modifications.¹ To a mixture of **S1** (10.0 mmol, 1.0 equiv), **S2** (10.5 mmol, 1.05 equiv), and 2 M aqueous Na_2CO_3 solution (10 mL) in ethanol (10 mL) and toluene (20 mL) was added $\text{Pd}(\text{PPh}_3)_4$ (577 mg, 0.05 equiv). Then the mixture was heated at 90 °C with stirring under an atmosphere of nitrogen for 3-6 h. After cooling, the crude reaction mixture was quenched with saturated NH_4Cl (20 mL) and was extracted with EtOAc (3×20 mL). The combined organic layers were washed with brine, dried over Na_2SO_4 and filtered. The filtrate was evaporated and the residue was column-chromatographed (PE/EA = 50:1) to afford **S3** (88-96% yields).



The reactions were carried out according to a literature method with some modifications.² In a flame-dried flask under an atmosphere of nitrogen, **S3** (10.0 mmol, 1.0 equiv) was dissolved in methanol (20 mL) and K_2CO_3 (20.0 mmol, 2.0 equiv) was added. After slow addition of 1.2 to 1.5 equiv of dimethyl (1-diazo-2-oxopropyl)phosphonate, the reaction mixture was stirred at room temperature until complete conversion (detected by TLC). Then water was added and the aqueous layer was extracted three times with DCM. The combined organic layers were dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure and the crude product was purified by column chromatography on silica gel (PE/EA = 30:1) to afford **S4** (95-99% yields).

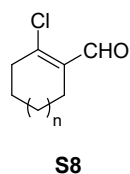
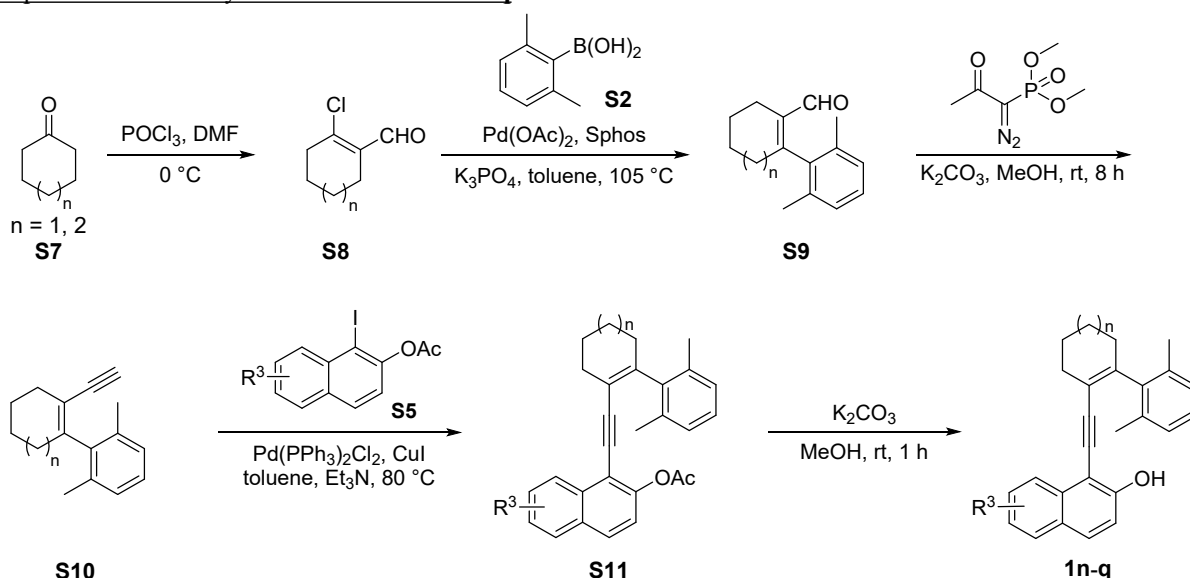


The reactions were carried out according to a literature method with some modifications.³ To a solution of $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (0.5 mmol, 0.05 equiv), CuI (1.0 mmol, 0.1 equiv) and Et_3N (50.0 mmol, 5.0 equiv) in toluene (20 mL) were added **S4** (10.5 mmol, 1.05 equiv) and **S5** (10.0 mmol, 1.0 equiv) at 80 °C. After 2-4 h stirring, the mixture was poured into saturated aqueous NH_4Cl and extracted with EtOAc . The combined organic layers were washed with brine, dried over MgSO_4 , and evaporated to dryness. Removal of the solvent under reduced pressure afforded a residue which was purified by chromatography on silica gel (PE/EA = 10:1) to afford **S6** (58-86% yields).

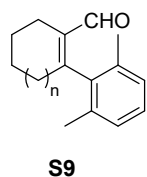


To a stirred solution of **S6** (10.0 mmol, 1.0 equiv) in methanol (5.0 M) was added potassium carbonate (10.0 mmol, 1.0 equiv) at room temperature. The resulted mixture was stirred at room temperature for 1 hour, the mixture was treated with saturated NH_4Cl and extracted with EtOAc , and dried over Na_2SO_4 . Removal of the solvent under reduced pressure afforded a residue which was purified by chromatography on silica gel (PE/EA = 10:1) to afford the compound **1a-m** (89-95% yields).

General procedure for the synthesis of substrates **1n-q**



The reactions were carried out according to a literature method with some modifications.⁴ DMF (7.9 mL, 64.0 mmol) in a 50 mL round-bottomed flask was cooled to 0 °C, POCl_3 (7.7 mL, 82.0 mmol) was added dropwise and stirred for 15 min at room temperature. Cyclic alkene (50.9 mmol) was then added dropwise at 0 °C and stirred for 2 h at room temperature. The reaction mixture was quenched by ice (200 g) and solid NaHCO_3 was slowly added until pH = 7. The organic layer was separated and the aqueous layer was extracted three times with EtOAc (200 mL). The collected organics were dried over anhydrous MgSO_4 , filtered and concentrated in vacuo to provide a yellow oil of **S8** as a crude product.



The reactions were carried out according to a literature method with some modifications.⁵ A mixture of **S2** (150.0 mg, 1.0 mmol), **S8** (1.4 mmol), $\text{Pd}(\text{OAc})_2$ (11.2 mg, 0.05 mmol), 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (41.1 mg, 0.1 mmol), and K_3PO_4 (637 mg, 3.0 mmol) in degassed toluene (2 mL) was stirred at 105 °C under an atmosphere of nitrogen for 2 h. After cooling to room temperature, reaction mixture was poured into 20 mL of H_2O . The organic layer was separated, dried over anhydrous Na_2SO_4 , filtered, and

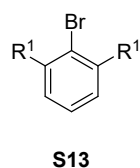
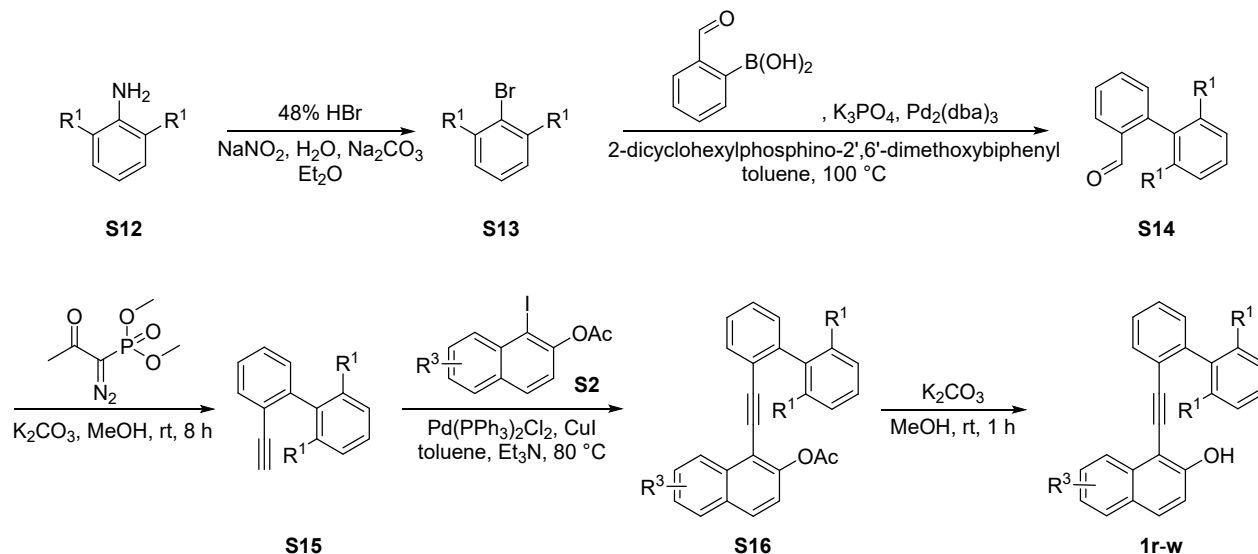
concentrated under reduced pressure. The crude product was purified by flash column chromatography (PE/EA = 95:5) on silica gel to give product **S9** (66-70% yields).

Compounds **S10** were prepared according to the general procedure as described for **S4**.

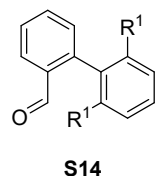
Compounds **S11** were prepared according to the general procedure as described for **S6**.

The deprotection of compounds **S11** were performed according to the general procedure as described for **S6**.

General procedure for the synthesis of substrates **1r-w**



HBr solution (47%, 181 mL, 1.57 mol) was slowly added to substituted aniline (0.2 mol) over 15 min at room temperature. The white suspension was cooled to $-56\text{ }^{\circ}\text{C}$, and sodium nitrite (23.6 g, 0.34 mol) was added portionwise over 10 min and stirring was continued at the same temperature for 1 h. Then, 250 mL of cold diethyl ether was slowly added over 10 min and the temperature was slowly increased over 2 h to $-15\text{ }^{\circ}\text{C}$ until no more gas was produced. The temperature was reduced to $-56\text{ }^{\circ}\text{C}$, 24 mL of water and sodium carbonate decahydrate (118.5 g, 0.41 mol) were added sequentially to give a brown suspension. After 3 h, the temperature was raised to room temperature where gas production started at $-32\text{ }^{\circ}\text{C}$. The resulting orange suspension was further stirred for 16 h at room temperature. The organic layers were washed with water (three times), dried over Na_2SO_4 and concentrated under vacuum. The obtained crude mixture was purified by chromatography on silica gel (heptane) to afford **S13** as a colorless oil (65-80% yields).



The reactions were carried out according to a literature method⁶ with some modifications. A mixture of **S13** (1.0 mmol), 2-formylbenzeneboronic acid (300 mg, 2.0 mmol), K_3PO_4 (637 mg, 3.0 mmol) and 200 μL of a catalyst solution which composed of $\text{Pd}_2(\text{dba})_3$ (4.6 mg, 0.005 mmol), and 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (8.2 mg, 0.02 mmol) in THF (2 mL) was heated at $100\text{ }^{\circ}\text{C}$ in toluene (2 mL) for 24 h. The crude product was purified by flash chromatography on silica gel (hexane) to provide **S14** (50-80% yields).

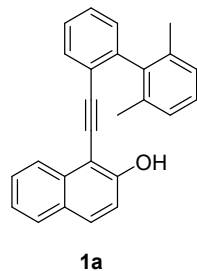
Compounds **S15** were prepared according to the general procedure as described for **S4**.

Compounds **S16** were prepared according to the general procedure as described for **S6**.

The deprotection of compounds **S16** were prepared according to the general procedure as described for **S6**.

3. Analytical data of compounds 1

1-((2',6'-Dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1a)



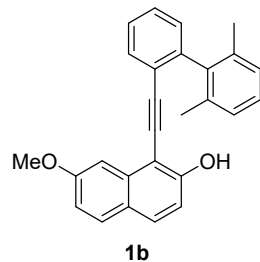
Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (600 MHz, CDCl₃) δ 7.70 (d, *J* = 7.5 Hz, 1H), 7.67 (d, *J* = 8.3 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.57 (d, *J* = 8.8 Hz, 1H), 7.39–7.31 (m, 3H), 7.28–7.20 (m, 2H), 7.18–7.13 (m, 3H), 6.97 (d, *J* = 8.9 Hz, 1H), 5.04 (s, 1H), 2.00 (s, 6H).

¹³C NMR (150 MHz, CDCl₃) δ 155.8, 143.1, 140.5, 135.9, 133.2, 131.5, 130.5, 129.1, 128.8, 128.2, 128.1, 127.9, 127.7, 127.2, 127.2, 124.8, 123.9, 122.5, 116.4, 102.7, 100.2, 84.2, 20.4.

HRMS (ESI) *m/z* calculated for C₂₆H₁₉O⁺ [*M* - H]⁺: 347.1441, found: 347.1452.

1-((2',6'-Dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)-7-methoxynaphthalen-2-ol (1b)



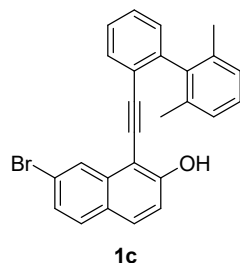
Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.68–7.62 (m, 1H), 7.50–7.42 (m, 2H), 7.38–7.27 (m, 3H), 7.25–7.19 (m, 1H), 7.18–7.09 (m, 3H), 6.87 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.78 (d, *J* = 8.9 Hz, 1H), 4.78 (s, 1H), 3.85 (s, 3H), 1.99 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 159.0, 156.5, 142.8, 140.4, 135.8, 134.7, 131.4, 130.3, 129.7, 129.1, 128.8, 128.0, 127.8, 127.2, 123.5, 122.5, 116.0, 113.8, 103.8, 101.8, 100.1, 84.3, 55.2, 20.4.

HRMS (ESI) *m/z* calculated for C₂₇H₂₁O₂⁺ [*M* - H]⁺: 377.1547, found: 377.1556.

7-Bromo-1-((2',6'-dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1c)



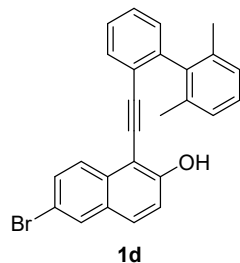
Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 8.03 (s, 1H), 7.75–7.70 (m, 1H), 7.49 (d, *J* = 9.0 Hz, 1H), 7.44 (d, *J* = 8.6 Hz, 1H), 7.41–7.28 (m, 3H), 7.27–7.20 (m, 1H), 7.19–7.12 (m, 3H), 6.94 (d, *J* = 9.0 Hz, 1H), 4.93 (s, 1H), 2.00 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 156.6, 143.1, 140.3, 135.8, 134.3, 131.7, 130.2, 129.7, 129.1, 128.1, 127.8, 127.4, 127.3, 126.9, 126.6, 122.1, 121.9, 116.8, 102.1, 100.5, 83.4, 20.4.

HRMS (ESI) *m/z* calculated for C₂₆H₁₈BrO⁺ [*M* - H]⁺: 425.0547, found: 425.0558.

6-Bromo-1-((2',6'-dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1d)



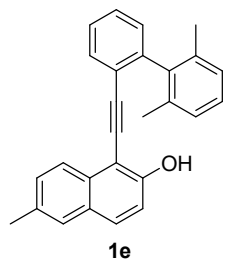
Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.74 (s, 1H), 7.68 (d, *J* = 7.5, 1H), 7.47–7.42 (m, 1H), 7.41–7.37 (m, 2H), 7.37–7.30 (m, 2H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.19–7.12 (m, 3H), 6.98 (d, *J* = 9.0 Hz, 1H), 5.12 (s, 1H), 1.99 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 155.9, 143.2, 140.4, 135.9, 131.8, 131.5, 130.4, 130.0, 129.3, 129.2, 129.1, 127.9, 127.7, 127.2, 126.6, 122.2, 117.6, 117.5, 103.0, 100.5, 83.5, 20.4.

HRMS (ESI) *m/z* calculated for C₂₆H₁₈BrO⁺ [*M* - H]⁺: 425.0547, found: 425.0558.

1-((2',6'-Dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)-6-methylnaphthalen-2-ol (1e)



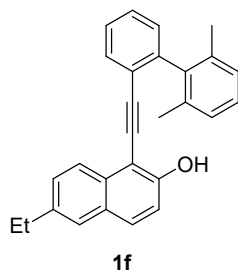
Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (600 MHz, CDCl₃) δ 7.69 (d, *J* = 7.5 Hz, 1H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.48 (d, *J* = 9.1 Hz, 1H), 7.40–7.31 (m, 3H), 7.26 (t, *J* = 7.8 Hz, 1H), 7.22–7.13 (m, 4H), 6.93 (d, *J* = 8.9 Hz, 1H), 4.98 (s, 1H), 2.37 (s, 3H), 2.00 (s, 6H).

¹³C NMR (150 MHz, CDCl₃) δ 155.3, 143.1, 140.5, 135.9, 133.4, 131.5, 131.3, 129.8, 129.4, 129.1, 128.8, 128.4, 127.9, 127.7, 127.2, 124.6, 122.6, 116.3, 102.5, 99.9, 84.4, 21.3, 20.4.

HRMS (ESI) *m/z* calculated for C₂₇H₂₁O⁺ [M - H]⁺: 361.1598, found: 361.1610.

1-((2',6'-Dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)-6-ethylnaphthalen-2-ol (1f)



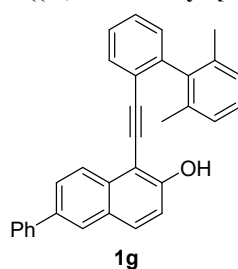
Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (600 MHz, CDCl₃) δ 7.84–7.79 (m, 1H), 7.75–7.69 (m, 1H), 7.62 (d, *J* = 8.7 Hz, 1H), 7.53–7.43 (m, 3H), 7.42–7.33 (m, 2H), 7.31–7.24 (m, 3H), 7.10–7.04 (m, 1H), 5.13–5.09 (m, 1H), 2.83–2.75 (m, 2H), 2.15–2.10 (m, 6H), 1.36–1.30 (m, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 155.3, 143.1, 140.5, 139.8, 135.9, 131.6, 131.5, 130.0, 129.1, 128.7, 128.4, 128.4, 127.9, 127.7, 127.2, 125.9, 124.7, 122.6, 116.3, 102.5, 99.9, 84.4, 28.7, 20.4, 15.5.

HRMS (ESI) *m/z* calculated for C₂₈H₂₃O⁺ [M - H]⁺: 375.1754, found: 375.1740.

1-((2',6'-Dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)-6-phenylnaphthalen-2-ol (1g)



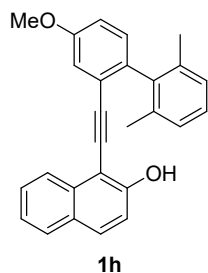
Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.92 (s, 1H), 7.94–7.90 (m, 2H), 7.77–7.68 (m, 4H), 7.54–7.43 (m, 4H), 7.42–7.37 (m, 2H), 7.32–7.24 (m, 3H), 7.11 (d, *J* = 8.9 Hz, 1H), 5.19 (s, 1H), 2.13 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 155.9, 143.1, 140.9, 140.5, 136.7, 136.0, 132.4, 131.5, 130.7, 129.1, 128.9, 128.8, 128.5, 127.9, 127.8, 127.2, 127.2, 126.9, 126.0, 125.3, 122.4, 116.8, 102.6, 100.2, 84.1, 20.4.

HRMS (ESI) *m/z* calculated for C₃₂H₂₃O⁺ [M - H]⁺: 423.1754, found: 423.1759.

1-((4-Methoxy-2',6'-dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1h)

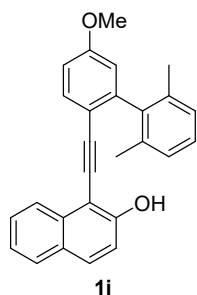


Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.67 (d, *J* = 8.4 Hz, 1H), 7.62 (d, *J* = 8.1 Hz, 1H), 7.57 (d, *J* = 8.9 Hz, 1H), 7.41–7.34 (m, 1H), 7.28–7.19 (m, 3H), 7.18–7.13 (m, 2H), 7.05 (d, *J* = 8.4, 1H), 7.00–6.93 (m, 2H), 5.04 (s, 1H), 3.85 (s, 3H), 2.02 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 158.4, 156.0, 140.2, 136.5, 135.7, 133.2, 130.5, 130.2, 128.2, 128.1, 127.8, 127.7, 127.3, 124.8, 123.9, 123.3, 116.4, 115.9, 115.5, 102.6, 100.2, 84.0, 55.5, 20.5.

HRMS (ESI) *m/z* calculated for C₂₇H₂₁O₂⁺ [M - H]⁺: 377.1547, found: 377.1539.

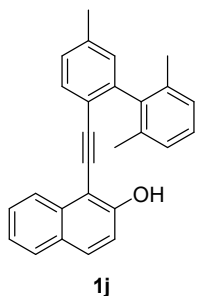
1-((5-Methoxy-2',6'-dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1i)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (600 MHz, CDCl₃) δ 7.66–7.60 (m, 3H), 7.56 (d, *J* = 8.9 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.29–7.22 (m, 2H), 7.19–7.15 (m, 2H), 6.98 (d, *J* = 8.9 Hz, 1H), 6.89 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.71 (s, 1H), 5.03 (s, 1H), 3.80 (s, 3H), 2.04 (s, 6H).

¹³C NMR (150 MHz, CDCl₃) δ 160.0, 155.4, 144.9, 140.4, 135.9, 133.1, 133.0, 129.9, 128.2, 128.0, 127.9, 127.7, 127.1, 124.8, 123.8, 116.3, 114.8, 114.5, 113.2, 103.1, 100.2, 82.8, 55.4, 20.3.

HRMS (ESI) *m/z* calculated for C₂₇H₂₁O₂⁻ [*M* - *H*]⁻: 377.1547, found: 377.1556.

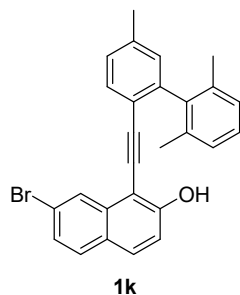
1-((2',5,6'-Trimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1j)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.68–7.64 (m, 1H), 7.62–7.57 (m, 2H), 7.55 (d, *J* = 8.9 Hz, 1H), 7.38–7.32 (m, 1H), 7.28–7.20 (m, 2H), 7.17–7.12 (m, 3H), 6.97 (dd, *J* = 5.3, 3.6 Hz, 2H), 5.05 (s, 1H), 2.35 (s, 3H), 2.01 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 155.6, 143.1, 140.6, 139.1, 135.9, 133.2, 131.4, 130.2, 129.8, 128.2, 128.1, 128.0, 127.8, 127.7, 127.2, 124.8, 123.8, 119.5, 116.4, 103.0, 100.4, 83.5, 21.6, 20.4.

HRMS (ESI) *m/z* calculated for C₂₇H₂₁O⁻ [*M* - *H*]⁻: 361.1598, found: 361.1610.

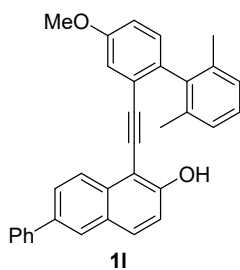
7-Bromo-1-((2',5,6'-trimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1k)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 8.09 (s, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.56 (d, *J* = 8.9 Hz, 1H), 7.52 (d, *J* = 8.5 Hz, 1H), 7.36 (d, *J* = 8.5 Hz, 1H), 7.30–7.25 (m, 1H), 7.23–7.17 (m, 3H), 7.04–6.98 (m, 2H), 4.97 (s, 1H), 2.41 (s, 3H), 2.05 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 156.4, 143.1, 140.4, 139.4, 135.8, 134.3, 131.6, 130.0, 129.7, 129.7, 128.1, 128.0, 127.8, 127.4, 127.0, 126.7, 121.8, 119.1, 116.9, 102.3, 100.7, 82.7, 21.7, 20.4.

HRMS (ESI) *m/z* calculated for C₂₇H₂₀BrO⁻ [*M* - *H*]⁻: 439.0703 found: 439.0712.

1-((4-Methoxy-2',6'-dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)-6-phenylnaphthalen-2-ol (1l)

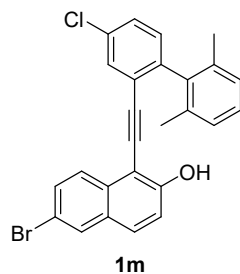
Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.83 (s, 1H), 7.71 (d, *J* = 8.6 Hz, 1H), 7.66–7.58 (m, 4H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.33–7.28 (m, 1H), 7.28–7.24 (m, 1H), 7.23 (d, *J* = 2.7 Hz, 1H), 7.19–7.15 (m, 2H), 7.07 (d, *J* = 8.4 Hz, 1H), 7.01 (d, *J* = 8.9 Hz, 1H), 6.96 (dd, *J* = 8.5, 2.7 Hz, 1H), 5.07 (s, 1H), 3.87 (s, 3H), 2.03 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 158.5, 156.0, 140.9, 140.2, 136.8, 136.5, 135.7, 132.5, 130.8, 130.2, 128.8, 128.5, 127.8, 127.7, 127.2, 126.9, 126.0, 125.3, 123.3, 116.9, 116.0, 115.5, 102.6, 100.2, 83.9,

55.5, 20.5.

HRMS (ESI) *m/z* calculated for C₃₃H₂₅O₂⁻ [*M* - *H*]⁻: 453.1860, found: 453.1868.

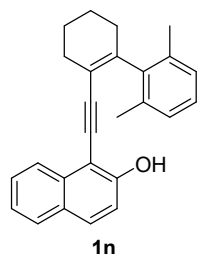
6-Bromo-1-((4-chloro-2',6'-dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1m)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.76 (s, 1H), 7.68 (s, 1H), 7.48 (d, *J* = 9.0 Hz, 1H), 7.41–7.34 (m, 3H), 7.29 (t, *J* = 7.7 Hz, 1H), 7.19–7.13 (m, 2H), 7.09 (d, *J* = 8.2 Hz, 1H), 6.98 (d, *J* = 9.0 Hz, 1H), 5.04 (s, 1H), 1.99 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 156.3, 141.5, 139.2, 135.9, 133.0, 131.7, 131.1, 130.6, 130.5, 130.0, 129.8, 129.3, 129.2, 128.2, 127.9, 126.5, 124.0, 117.7, 117.5, 102.5, 99.1, 84.8, 20.4.

HRMS (ESI) *m/z* calculated for C₂₆H₁₇BrClO⁺ [M - H]⁺: 459.0157, found: 459.0154.

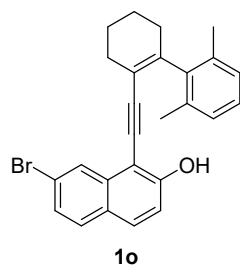
1-((2',6'-Dimethyl-3,4,5,6-tetrahydro-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1n)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.59–7.55 (m, 1H), 7.55–7.52 (m, 1H), 7.49 (d, *J* = 8.9 Hz, 1H), 7.32–7.27 (m, 1H), 7.21–7.17 (m, 1H), 7.15–7.11 (m, 1H), 7.10–7.05 (m, 2H), 6.92 (d, *J* = 8.9 Hz, 1H), 4.92 (s, 1H), 2.52–2.42 (m, 2H), 2.24–2.14 (m, 8H), 1.81–1.72 (m, 4H).

¹³C NMR (100 MHz, CDCl₃) δ 155.3, 145.5, 142.2, 134.6, 133.1, 129.7, 128.2, 128.0, 127.9, 127.2, 127.0, 124.8, 123.7, 117.8, 116.2, 103.2, 102.2, 82.5, 29.9, 29.3, 22.5, 22.4, 19.2.

HRMS (ESI) *m/z* calculated for C₂₆H₂₃O⁺ [M - H]⁺: 351.1754, found: 351.1762.

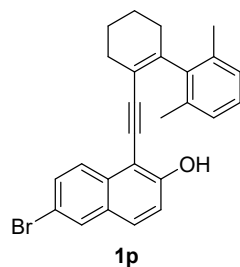
7-Bromo-1-((2',6'-dimethyl-3,4,5,6-tetrahydro-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1o)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.90 (s, 1H), 7.45 (t, *J* = 8.9 Hz, 2H), 7.29 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.15–7.11 (m, 1H), 7.10–7.06 (m, 2H), 6.92 (d, *J* = 8.9 Hz, 1H), 4.84 (s, 1H), 2.53–2.46 (m, 2H), 2.25–2.17 (m, 8H), 1.84–1.75 (m, 4H).

¹³C NMR (100 MHz, CDCl₃) δ 156.1, 146.0, 142.0, 134.5, 134.3, 129.6, 129.6, 128.0, 127.4, 127.2, 126.9, 126.6, 121.7, 117.7, 116.7, 102.6, 102.5, 81.7, 29.9, 29.2, 22.5, 22.3, 19.2.

HRMS (ESI) *m/z* calculated for C₂₆H₂₂BrO⁺ [M - H]⁺: 429.0860, found: 429.0847.

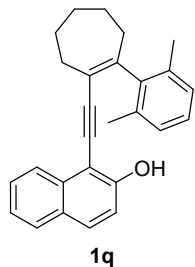
6-Bromo-1-((2',6'-dimethyl-3,4,5,6-tetrahydro-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1p)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.72 (s, 1H), 7.40 (d, *J* = 9.0 Hz, 1H), 7.36–7.27 (m, 2H), 7.16 (dd, *J* = 8.4, 6.6 Hz, 1H), 7.10–7.06 (m, 2H), 6.94 (d, *J* = 9.0 Hz, 1H), 4.98 (s, 1H), 2.51–2.43 (m, 2H), 2.25–2.16 (m, 8H), 1.82–1.74 (m, 4H).

¹³C NMR (100 MHz, CDCl₃) δ 155.4, 146.1, 142.1, 134.6, 131.7, 130.1, 129.9, 129.3, 128.6, 127.9, 127.2, 126.7, 117.7, 117.4, 117.3, 103.6, 102.6, 81.9, 30.0, 29.2, 22.5, 22.3, 19.2.

HRMS (ESI) *m/z* calculated for C₂₆H₂₂BrO⁺ [M - H]⁺: 429.0860, found: 429.0873.

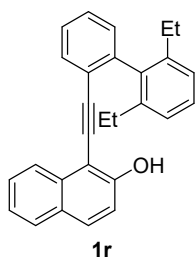
1-((2-(2,6-Dimethylphenyl)cyclohept-1-en-1-yl)ethynyl)naphthalen-2-ol (1q)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.70 (t, *J* = 8.7 Hz, 2H), 7.62 (d, *J* = 9.0 Hz, 1H), 7.49–7.40 (m, 1H), 7.35–7.30 (m, 1H), 7.29–7.23 (m, 1H), 7.23–7.18 (m, 2H), 7.06 (d, *J* = 8.9 Hz, 1H), 4.99 (s, 1H), 2.84–2.76 (m, 2H), 2.61–2.54 (m, 2H), 2.36 (s, 6H), 1.98–1.80 (m, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 155.3, 150.5, 144.9, 134.0, 133.1, 129.7, 128.2, 128.0, 126.9, 126.9, 124.8, 123.7, 123.2, 116.2, 103.9, 103.3, 83.2, 35.4, 34.7, 31.9, 26.8, 26.4, 20.0.

HRMS (ESI) *m/z* calculated for C₂₇H₂₅O⁺ [*M* - H]⁺: 365.1911, found: 365.1920.

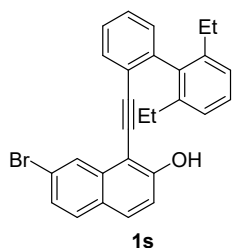
1-((2',6'-Diethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1r)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.72–7.64 (m, 2H), 7.61 (d, *J* = 8.1 Hz, 1H), 7.56 (d, *J* = 8.9 Hz, 1H), 7.40–7.32 (m, 4H), 7.26–7.17 (m, 4H), 6.97 (d, *J* = 9.0 Hz, 1H), 5.01 (s, 1H), 2.40–2.22 (m, 4H), 0.97 (t, *J* = 7.6 Hz, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 155.9, 142.5, 142.0, 139.3, 133.2, 131.3, 130.4, 129.9, 128.4, 128.3, 128.2, 128.1, 127.2, 126.1, 125.4, 124.8, 123.9, 123.3, 116.4, 102.7, 100.6, 84.9, 26.7, 15.3.

HRMS (ESI) *m/z* calculated for C₂₈H₂₃O⁺ [*M* - H]⁺: 375.1754, found: 375.1755.

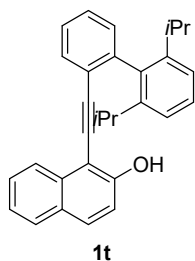
7-Bromo-1-((2',6'-diethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1s)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 8.04 (s, 1H), 7.76–7.69 (m, 1H), 7.50 (d, *J* = 8.9 Hz, 1H), 7.45 (d, *J* = 8.6 Hz, 1H), 7.39–7.29 (m, 4H), 7.25–7.17 (m, 3H), 6.95 (d, *J* = 8.8 Hz, 1H), 4.89 (s, 1H), 2.31 (dq, *J* = 19.9, 7.2 Hz, 4H), 0.98 (t, *J* = 7.5 Hz, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 156.6, 142.5, 141.9, 139.1, 134.3, 131.5, 130.2, 129.9, 129.7, 128.6, 127.4, 127.3, 126.9, 126.6, 126.2, 122.9, 121.9, 116.9, 102.0, 100.9, 84.1, 26.7, 15.3.

HRMS (ESI) *m/z* calculated for C₂₈H₂₂BrO⁺ [*M* - H]⁺: 453.0860, found: 453.0867.

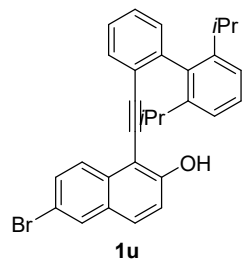
1-((2',6'-Diisopropyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1t)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.72–7.67 (m, 1H), 7.66–7.59 (m, 2H), 7.56 (d, *J* = 8.9 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.39–7.32 (m, 3H), 7.27 (d, *J* = 7.7 Hz, 2H), 7.25–7.21 (m, 1H), 7.20–7.16 (m, 1H), 6.96 (d, *J* = 8.9 Hz, 1H), 4.94 (s, 1H), 2.53 (hept, *J* = 7.0 Hz, 2H), 1.06–0.97 (m, 12H).

¹³C NMR (100 MHz, CDCl₃) δ 155.9, 146.7, 142.8, 137.9, 133.2, 131.1, 130.4, 129.9, 128.7, 128.2, 128.1, 127.2, 127.2, 124.8, 123.9, 123.4, 123.3, 116.5, 102.5, 100.9, 85.4, 30.7, 24.5, 24.0.

HRMS (ESI) *m/z* calculated for C₃₀H₂₇O⁺ [*M* - H]⁺: 403.2067, found: 403.2076.

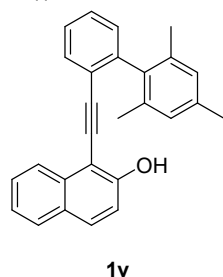
6-Bromo-1-((2',6'-diisopropyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1u)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.74 (s, 1H), 7.70–7.63 (m, 1H), 7.50–7.41 (m, 2H), 7.40–7.31 (m, 4H), 7.29–7.23 (m, 2H), 7.21–7.14 (m, 1H), 6.97 (d, *J* = 9.0 Hz, 1H), 5.06 (s, 1H), 2.60–2.42 (m, 2H), 1.09–0.93 (m, 12H).

¹³C NMR (100 MHz, CDCl₃) δ 155.9, 146.7, 143.0, 137.8, 131.8, 131.1, 130.4, 129.9, 129.9, 129.4, 129.3, 128.7, 128.5, 127.2, 126.7, 123.3, 123.1, 117.6, 117.6, 102.8, 101.2, 84.8, 30.7, 24.5, 24.0.

HRMS (ESI) *m/z* calculated for C₃₀H₂₆BrO⁺ [*M* - H]⁺: 481.1173, found: 481.1167.

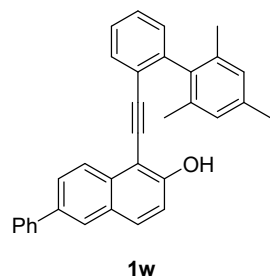
1-((2',4',6'-Trimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1v)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.70–7.63 (m, 2H), 7.61 (d, *J* = 8.1 Hz, 1H), 7.57 (d, *J* = 8.9 Hz, 1H), 7.38–7.29 (m, 3H), 7.25–7.20 (m, 1H), 7.16–7.12 (m, 1H), 6.99–6.96 (m, 3H), 5.12 (s, 1H), 2.34 (s, 3H), 1.97 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 155.9, 143.3, 137.6, 137.5, 135.8, 133.3, 131.5, 130.4, 129.4, 128.8, 128.5, 128.2, 128.1, 127.1, 127.1, 124.8, 123.9, 122.8, 116.5, 102.8, 100.3, 84.1, 21.2, 20.3.

HRMS (ESI) *m/z* calculated for C₂₇H₂₁O⁺ [*M* - H]⁺: 361.1598, found: 361.1583.

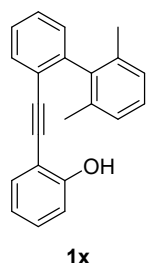
6-Phenyl-1-((2',4',6'-trimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-ol (1w)

Appearance: white solid. The crude mixture was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.83 (s, 1H), 7.73–7.68 (m, 2H), 7.66–7.59 (m, 4H), 7.43–7.27 (m, 5H), 7.18–7.15 (m, 1H), 7.03–6.99 (m, 3H), 5.15 (s, 1H), 2.37 (s, 3H), 1.99 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 156.0, 143.3, 140.9, 137.6, 137.5, 136.7, 135.8, 132.5, 131.5, 130.6, 129.5, 128.9, 128.8, 128.5, 127.2, 127.1, 126.7, 126.0, 125.4, 122.8, 116.9, 102.7, 100.3, 84.0, 21.2, 20.3.

HRMS (ESI) *m/z* calculated for C₃₃H₂₅O⁺ [*M* - H]⁺: 437.1911, found: 437.1889.

2-((2',6'-Dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)phenol (1x)

Compound **1x** was purified by silica gel column chromatography using PE/EA (30:1 to 15:1) as eluent.

Appearance: yellow solid.

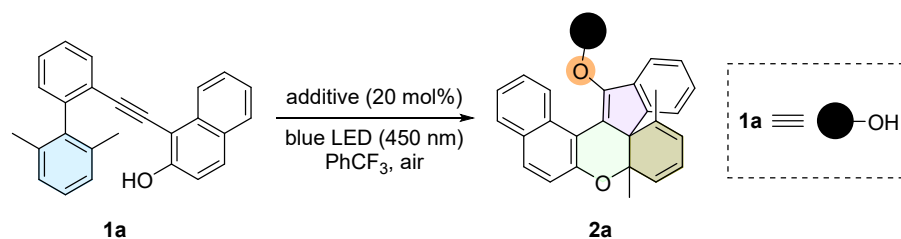
¹H NMR (400 MHz, CDCl₃) δ 7.54 (d, *J* = 7.5 Hz, 1H), 7.30 (t, *J* = 7.0 Hz, 1H), 7.26–7.17 (m, 2H), 7.14–7.05 (m, 4H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.72–6.63 (m, 2H), 4.44 (s, 1H), 1.94 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 156.4, 143.2, 140.3, 135.7, 131.4, 131.1, 130.2, 128.9, 128.8, 128.0, 127.7, 127.1, 122.1, 120.0, 114.7, 109.3, 95.1, 85.7, 20.3.

HRMS (ESI) *m/z* calculated for C₂₂H₁₇O⁺ [*M* - H]⁺: 297.1285, found: 297.1293.

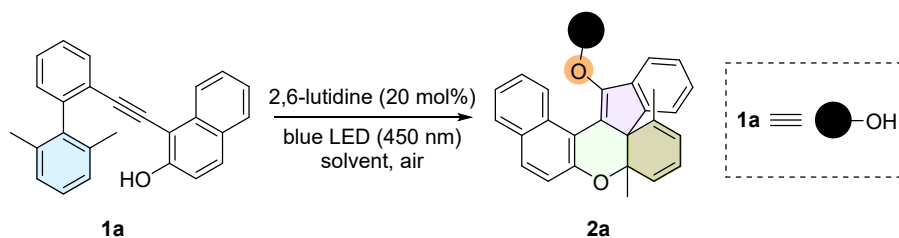
4. Reaction conditions screening

Table S1. Additive screening^a



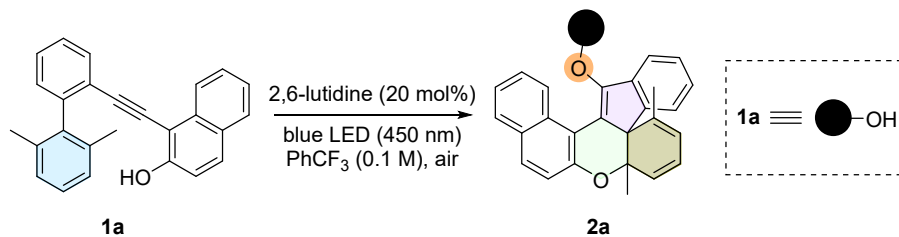
Entry	Additive	Yield (%) ^b
1	PhCOOH	10
2	AcOH	20
3	TFA	6
4	DPP	trace
5	CSA	trace
6	Zn(OTf) ₂	trace
7	DIPEA	3
8	Et ₃ N	3
9	DBU	trace
10	DABCO	9
11	pyridine	trace
12	DMAP	7
13	2,6-lutidine	75
14	Cs ₂ CO ₃	28
15	TMG	trace
16	tetrahydropyrrole	trace
17	imidazole	51
18	2,6-diphenylpyridine	38
19	2,6-di- <i>tert</i> -butyl-4-methylpyridine	49
20	2,6-di- <i>tert</i> -butylpyridine	40

^aReaction conditions: **1a** (0.1 mmol, 1.0 equiv) and additive (0.02 mmol, 0.2 equiv) in PhCF₃ (0.2 M) were stirred for 24 h and irradiated with blue LEDs (λ_{max} = 450 nm) at ambient temperature under air. ^bIsolated yield.

Table S2. Solvent and concentration screening^a

Entry	Solvent	Yield (%) ^b
1	MTBE	15
2	DCM	31
3	toluene	69
4	Et ₂ O	trace
5	THF	49
6	MeCN	30
7	1,4-dioxane	35
8	DMF	17
9 ^c	PhCF ₃	82
10 ^d	PhCF ₃	60
11 ^e	PhCF ₃	45

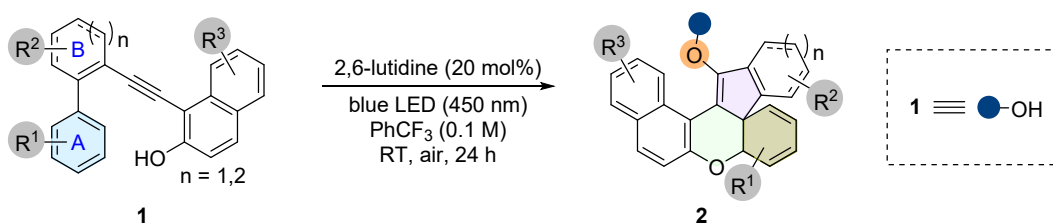
^aReaction conditions: **1a** (0.1 mmol, 1.0 equiv) and 2,6-lutidine (0.02 mmol, 0.2 equiv) in solvent (0.2 M) were stirred for 24 h and irradiated with blue LEDs ($\lambda_{\text{max}} = 450$ nm) at ambient temperature under air. ^bIsolated yield. ^cPhCF₃ 1.0 mL. ^dPhCF₃ 2.0 mL. ^ePhCF₃ 0.33 mL.

Table S3. Control experiments^a

Entry	Deviation from standard conditions	Yield (%) ^b
1	none	82
2	no light	NR
3	no 2,6-lutidine	37
4	O ₂	78
5 ^c	under N ₂ atmosphere	NR

^aReaction conditions: **1a** (0.1 mmol, 1.0 equiv) and 2,6-lutidine (0.02 mmol, 0.2 equiv) in PhCF₃ (0.1 M) were stirred for 24 h and irradiated with blue LEDs ($\lambda_{\text{max}} = 450$ nm) at ambient temperature under air. NR = no reaction. ^bIsolated yield. ^cThe reaction mixture was degassed via freeze pump thaw three times.

5. General procedure for the radical dearomative cyclization of benzene derivatives



In an oven-dried 10 mL Schlenk tube equipped with a magnetic stirrer bar was charged sequentially with the substrate **1** (0.2 mmol, 1.0 equiv), 2,6-lutidine (0.04 mmol, 0.2 equiv), and α,α,α -trifluorotoluene (2.0 mL). The reaction mixture was then stirred under irradiation with blue LEDs (30 W, $\lambda_{\text{max}} = 450$ nm) for 24 h. The crude mixture was purified by flash column chromatography to afford the title compounds **2** in the stated yield.

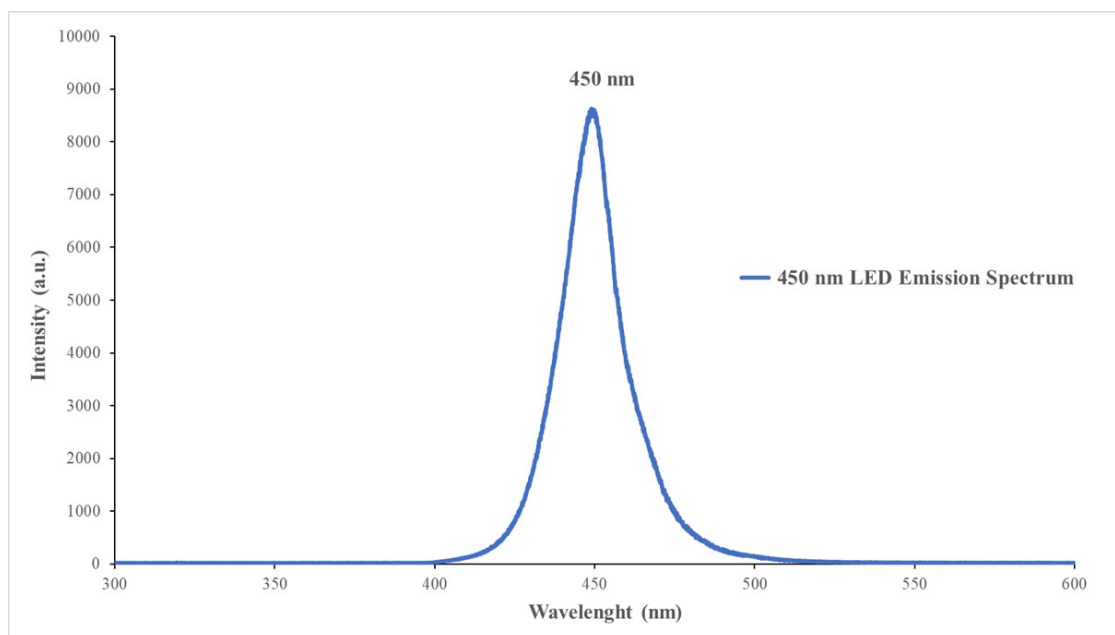
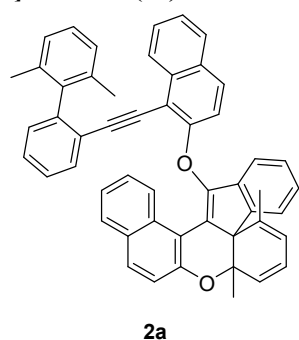


Figure S1. Emission spectrum of the light source (blue LEDs, $\lambda_{\text{max}} = 450$ nm) used in our experiments.

6. Analytical data of compounds **2**

16-((1-((2',6'-Dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-dimethyl-7aH-benzo[a]indeno[1,2-b]xanthene (2a**)**



2a

Compound **2a** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 82%, 56.9 mg.

Appearance: yellow solid.

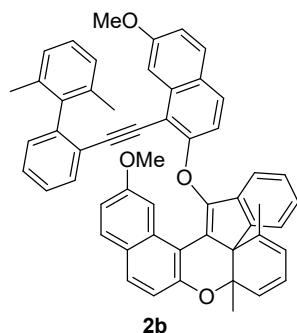
¹H NMR (400 MHz, CDCl₃) δ 8.50 (d, $J = 8.5$ Hz, 1H), 7.86 (d, $J = 7.1$ Hz, 1H), 7.59–7.49 (m, 3H), 7.46–7.33 (m, 4H), 7.28 (t, $J = 7.8$ Hz, 1H), 7.24–7.14 (m, 4H), 7.13–6.96 (m, 7H), 6.90 (d, $J = 9.0$ Hz, 1H), 6.84–6.76 (m, 1H), 6.35 (dd, $J = 9.4, 5.6$ Hz, 1H), 6.00–5.92 (m, 2H), 2.06 (s, 6H), 1.38 (s, 3H), 1.26 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 155.0, 153.9, 146.9, 143.6, 141.9, 141.0, 140.7, 139.5, 136.3, 136.2, 134.2, 132.4, 130.6, 130.2, 129.4, 129.3, 129.2, 128.9, 128.8, 128.6, 128.5, 127.8, 127.7, 127.4, 127.4, 127.1, 126.5, 126.4, 126.2, 125.7, 124.7, 123.6, 123.3, 123.2, 122.4, 120.8, 120.0,

117.7, 115.9, 109.9, 108.2, 98.6, 86.1, 79.8, 56.7, 22.7, 20.6, 20.6, 18.7.

HRMS (APCI) m/z calculated for C₅₂H₃₉O₂⁺, [M + H]⁺: 695.2945, found: 695.2949.

16-((1-((2',6'-Dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)-7-methoxynaphthalen-2-yl)oxy)-2-methoxy-7a,11-dimethyl-7aH-benzo[a]indeno[1,2-*l*]xanthene (2b)



Compound **2b** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 66%, 49.8 mg.

Appearance: light yellow solid.

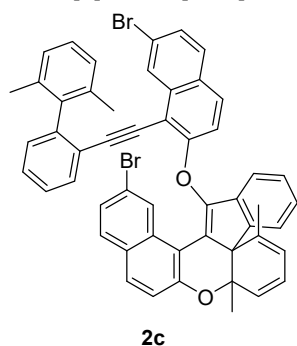
¹H NMR (600 MHz, CDCl₃) δ 7.65 (d, *J* = 7.7 Hz, 1H), 7.59–7.53 (m, 2H), 7.52–7.45 (m, 2H), 7.43–7.39 (m, 1H), 7.36–7.32 (m, 2H), 7.31–7.26 (m, 1H), 7.20–7.15 (m, 2H), 7.09 (d, *J* = 7.7 Hz, 1H), 7.05–7.00 (m, 2H), 6.96–6.88 (m, 3H), 6.86–6.80 (m, 4H), 6.33 (dd, *J* = 9.3, 5.7 Hz, 1H), 5.97–5.93 (m, 2H), 3.75 (s, 3H), 3.46 (s, 3H), 1.99 (s, 6H), 1.38 (s, 3H), 1.17 (s, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 159.1, 158.5, 156.3, 154.9, 147.6, 143.1, 141.6, 140.8, 140.3, 139.9, 135.9, 135.7, 133.1, 132.3, 130.2, 129.7, 129.5, 129.5, 129.3, 128.9, 128.5, 128.2, 128.1, 127.3, 127.2, 127.2, 126.9, 126.3, 124.9, 124.2, 123.4, 122.9, 120.8, 119.9, 117.5, 115.8, 115.3,

114.2, 109.3, 107.7, 105.3, 104.5, 98.8, 85.6, 79.5, 57.0, 55.5, 55.3, 22.8, 20.6, 20.5, 18.6.

HRMS (APCI) *m/z* calculated for C₅₄H₄₃O₄⁺ [*M* + *H*]⁺: 755.3156, found: 755.3153.

2-Bromo-16-((7-bromo-1-((2',6'-dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-dimethyl-7aH-benzo[a]indeno[1,2-*l*]xanthene (2c)



Compound **2c** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 63%, 53.6 mg.

Appearance: yellow solid.

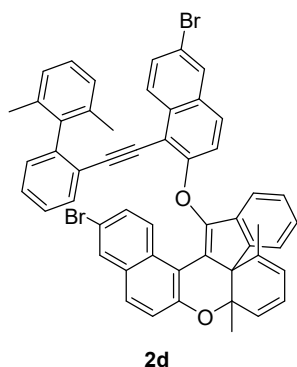
¹H NMR (400 MHz, CDCl₃) δ 8.27 (s, 1H), 7.83 (s, 1H), 7.63 (d, *J* = 7.2 Hz, 1H), 7.54 (d, *J* = 8.7 Hz, 1H), 7.46–7.38 (m, 4H), 7.37–7.29 (m, 2H), 7.27–7.21 (m, 1H), 7.18 (d, *J* = 9.3 Hz, 1H), 7.10 (d, *J* = 7.3 Hz, 1H), 7.08–6.98 (m, 4H), 6.96–6.89 (m, 3H), 6.68 (d, *J* = 6.5 Hz, 1H), 6.38–6.30 (m, 1H), 5.99–5.89 (m, 2H), 2.00 (s, 3H), 1.97 (s, 3H), 1.37 (s, 3H), 1.16 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 155.7, 154.6, 147.4, 143.6, 141.7, 140.5, 140.1, 139.2, 135.9, 135.8, 135.5, 133.0, 131.8, 130.0, 129.4, 129.3, 129.2, 128.7, 128.6, 128.6, 128.5, 128.1, 128.1, 128.0, 127.7, 127.6, 127.4, 127.3, 127.3, 126.7, 126.6, 123.2, 123.1, 122.2, 121.8, 121.1, 121.0,

120.0, 118.3, 116.7, 109.3, 108.4, 99.2, 84.4, 80.3, 56.5, 22.6, 20.6, 20.5, 18.8.

HRMS (APCI) *m/z* calculated for C₅₂H₃₇Br₂O₂⁺ [*M* + *H*]⁺: 853.1134, found: 853.1138.

3-Bromo-16-((6-bromo-1-((2',6'-dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-dimethyl-7aH-benzo[a]indeno[1,2-*l*]xanthene (2d)



Compound **2d** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 65%, 55.3 mg.

Appearance: yellow solid.

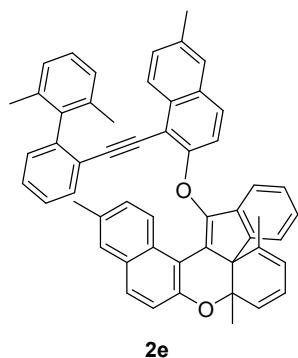
¹H NMR (600 MHz, CDCl₃) δ 8.40 (d, *J* = 9.0 Hz, 1H), 7.91 (d, *J* = 7.5 Hz, 1H), 7.74 (s, 2H), 7.54–7.49 (m, 3H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.38 (d, *J* = 8.9 Hz, 1H), 7.34 (d, *J* = 9.1 Hz, 1H), 7.32–7.28 (m, 3H), 7.22 (d, *J* = 7.5 Hz, 1H), 7.18–7.15 (m, 3H), 7.08 (d, *J* = 8.9 Hz, 1H), 6.98–6.92 (m, 2H), 6.89 (d, *J* = 9.0 Hz, 1H), 6.43 (dd, *J* = 9.4, 5.7 Hz, 1H), 6.06–6.02 (m, 2H), 2.17 (s, 3H), 2.15 (s, 3H), 1.43 (s, 3H), 1.33 (s, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 154.8, 154.1, 147.0, 143.8, 141.8, 140.7, 140.6, 139.2, 136.5, 136.2, 132.8, 132.3, 130.7, 130.2, 130.1, 129.8, 129.5, 129.5, 129.3, 129.3, 129.0, 129.0, 128.6, 128.5, 128.1, 128.1, 128.0, 127.6, 127.5, 127.5, 127.3, 127.2, 126.8, 123.3, 123.1, 121.9, 121.0,

119.8, 118.9, 118.8, 117.0, 116.6, 110.0, 108.6, 99.2, 85.4, 80.1, 56.7, 22.8, 20.7, 20.6, 18.6.

HRMS (APCI) *m/z* calculated for C₅₂H₃₇Br₂O₂⁺ [*M* + *H*]⁺: 853.1134, found: 853.1149.

16-((1-((2',6'-Dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)-6-methylnaphthalen-2-yl)oxy)-3,7a,11-trimethyl-7aH-benzo[a]indeno[1,2-*l*]xanthene (2e)



Compound **2e** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 42%, 30.3 mg.

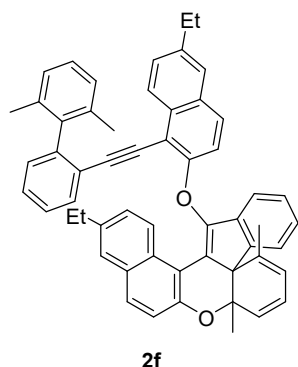
Appearance: yellow solid.

¹H NMR (600 MHz, CDCl₃) δ 8.40 (d, *J* = 8.5 Hz, 1H), 7.84 (d, *J* = 7.3 Hz, 1H), 7.47 (d, *J* = 8.9 Hz, 1H), 7.43–7.34 (m, 3H), 7.32–7.27 (m, 3H), 7.22–7.14 (m, 2H), 7.13–7.09 (m, 2H), 7.06 (d, *J* = 7.4 Hz, 1H), 7.03–6.99 (m, 3H), 6.96 (d, *J* = 8.9 Hz, 1H), 6.91–6.85 (m, 2H), 6.78 (d, *J* = 6.2 Hz, 1H), 6.33 (dd, *J* = 9.1, 5.7 Hz, 1H), 5.96–5.92 (m, 2H), 2.35 (s, 3H), 2.22 (s, 3H), 2.06 (s, 6H), 1.37 (s, 3H), 1.24 (s, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 154.5, 153.4, 147.0, 143.6, 141.9, 141.1, 140.8, 139.6, 136.3, 136.3, 134.3, 132.6, 132.4, 129.6, 129.4, 129.3, 129.1, 128.9, 128.7, 128.6, 128.5, 128.4, 128.4, 127.8, 127.4, 127.4, 127.3, 127.0, 127.0, 126.7, 126.4, 126.3, 125.6, 123.7, 123.2, 122.3, 120.8, 120.0, 117.7, 116.1, 109.9, 108.2, 98.3, 86.3, 79.7, 56.7, 22.7, 21.4, 21.1, 20.6, 20.6, 18.7.

HRMS (APCI) *m/z* calculated for C₅₄H₄₃O₂⁺ [*M* + *H*]⁺: 723.3258, found: 723.3264.

16-((1-((2',6'-Dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)-6-ethylnaphthalen-2-yl)oxy)-3-ethyl-7a,11-dimethyl-7aH-benzo[a]indeno[1,2-*l*]xanthene (2f)



Compound **2f** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 56%, 42.0 mg.

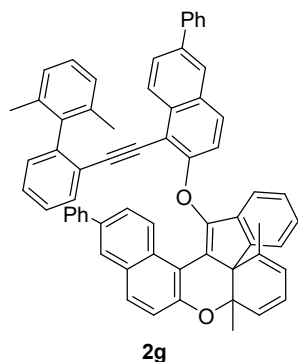
Appearance: yellow solid.

¹H NMR (400 MHz, CDCl₃) δ 8.51 (d, *J* = 8.6 Hz, 1H), 7.95 (d, *J* = 7.3 Hz, 1H), 7.59 (d, *J* = 8.9 Hz, 1H), 7.53–7.39 (m, 6H), 7.30–7.20 (m, 4H), 7.18–6.95 (m, 7H), 6.90–6.85 (m, 1H), 6.43 (dd, *J* = 9.2, 5.6 Hz, 1H), 6.07–6.02 (m, 2H), 2.75 (q, *J* = 7.5 Hz, 2H), 2.62 (q, *J* = 7.5 Hz, 2H), 2.16 (s, 3H), 2.15 (s, 3H), 1.47 (s, 3H), 1.34 (s, 3H), 1.31 (t, *J* = 7.5 Hz, 3H), 1.16 (t, *J* = 7.5 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 154.5, 153.4, 146.9, 143.6, 141.9, 141.2, 140.8, 140.6, 139.6, 138.9, 136.3, 136.2, 132.6, 132.4, 129.7, 129.4, 129.3, 129.1, 129.0, 128.9, 128.7, 128.5, 128.5, 128.4, 127.8, 127.4, 127.3, 127.2, 127.0, 126.4, 126.3, 125.7, 125.4, 123.6, 123.1, 122.1, 120.7, 120.0, 117.6, 116.1, 109.9, 108.2, 98.3, 86.3, 79.7, 56.7, 28.7, 28.4, 22.7, 20.6, 20.5, 18.7, 15.5, 15.1.

HRMS (APCI) *m/z* calculated for C₅₆H₄₇O₂⁺ [*M* + *H*]⁺: 751.3571, found: 751.3579.

16-((1-((2',6'-Dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)-6-phenylnaphthalen-2-yl)oxy)-7a,11-dimethyl-3-phenyl-7aH-benzo[a]indeno[1,2-*l*]xanthene (2g)



Compound **2g** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 60%, 50.8 mg.

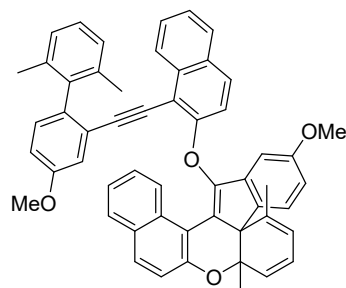
Appearance: yellow solid.

¹H NMR (400 MHz, CDCl₃) δ 8.59 (d, *J* = 8.2 Hz, 1H), 7.94 (d, *J* = 5.8 Hz, 1H), 7.75 (s, 1H), 7.68 (s, 1H), 7.63–7.51 (m, 4H), 7.49–7.31 (m, 9H), 7.30–7.21 (m, 3H), 7.20–7.10 (m, 4H), 7.06 (s, 2H), 7.03–6.83 (m, 5H), 6.40–6.31 (m, 1H), 6.01–5.92 (m, 2H), 2.07 (s, 3H), 1.88 (s, 3H), 1.40 (s, 3H), 1.28 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 155.0, 154.1, 146.8, 143.8, 141.9, 141.0, 140.8, 140.7, 139.5, 137.5, 136.4, 136.2, 135.7, 133.5, 132.4, 130.6, 129.8, 129.5, 129.4, 129.4, 129.2, 128.8, 128.7, 128.7, 128.5, 127.9, 127.5, 127.4, 127.3, 127.1, 127.1, 127.0, 126.9, 126.8, 126.5, 126.3, 125.6, 125.5, 123.5, 123.3, 122.3, 120.9, 120.0, 118.1, 116.2, 109.8, 108.0, 98.7, 86.2, 80.0, 56.7, 22.7, 20.6, 20.4, 18.7.

HRMS (APCI) *m/z* calculated for C₆₄H₄₇O₂⁺ [*M* + *H*]⁺: 847.3571, found: 847.3576.

14-Methoxy-16-((1-((4-methoxy-2',6'-dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-dimethyl-7aH-benzo[a]indeno[1,2-*l*]xanthene (2h)



2h

Compound **2h** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 63%, 47.5 mg.

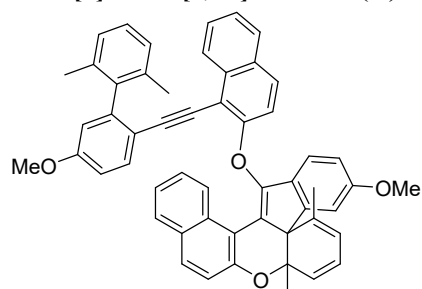
Appearance: white solid.

¹H NMR (600 MHz, CDCl₃) δ 8.57 (d, *J* = 8.2 Hz, 1H), 7.66–7.61 (m, 2H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.50–7.45 (m, 2H), 7.42–7.37 (m, 2H), 7.31–7.24 (m, 3H), 7.21–7.14 (m, 4H), 7.13–7.05 (m, 3H), 7.00 (d, *J* = 8.9 Hz, 1H), 6.70 (d, *J* = 8.1 Hz, 1H), 6.53 (s, 1H), 6.43 (dd, *J* = 9.0, 5.6 Hz, 1H), 6.05–6.00 (m, 2H), 3.89 (s, 3H), 3.60 (s, 3H), 2.18 (s, 6H), 1.48 (s, 3H), 1.36 (s, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 159.8, 158.3, 155.1, 154.0, 146.8, 141.1, 140.4, 136.9, 136.8, 136.2, 134.2, 133.7, 130.5, 130.4, 130.3, 129.4, 129.1, 128.8, 128.6, 128.4, 127.8, 127.7, 127.4, 127.3, 126.4, 126.3, 125.6, 124.7, 124.4, 123.9, 123.7, 123.3, 120.5, 117.7, 116.8, 115.8, 115.2, 112.6, 109.9, 108.1, 105.0, 98.6, 86.0, 80.0, 56.0, 55.4, 55.3, 22.7, 20.6, 18.6.

HRMS (APCI) *m/z* calculated for C₅₄H₄₃O₄⁺ [*M* + *H*]⁺: 755.3156, found: 755.3151.

13-Methoxy-16-((1-((5-methoxy-2',6'-dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-dimethyl-7aH-benzo[a]indeno[1,2-*l*]xanthene (2i)



2i

Compound **2i** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 70%, 52.8 mg.

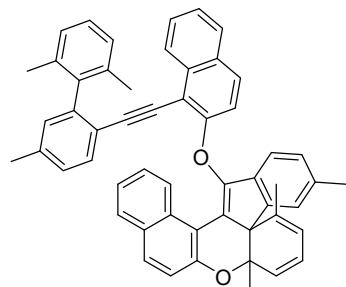
Appearance: yellow solid.

¹H NMR (400 MHz, CDCl₃) δ 8.51 (d, *J* = 8.5 Hz, 1H), 7.78 (d, *J* = 8.5 Hz, 1H), 7.55–7.48 (m, 3H), 7.36 (d, *J* = 9.0 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.25–7.13 (m, 3H), 7.13–7.04 (m, 3H), 7.04–6.94 (m, 3H), 6.92–6.87 (m, 2H), 6.75–6.71 (m, 1H), 6.65 (d, *J* = 8.3 Hz, 1H), 6.55 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.32 (dd, *J* = 9.4, 5.5 Hz, 1H), 5.97–5.89 (m, 2H), 3.79 (s, 3H), 3.67 (s, 3H), 2.08 (s, 6H), 1.39 (s, 3H), 1.27 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 159.8, 158.9, 154.6, 153.6, 146.9, 145.3, 143.9, 141.5, 140.6, 136.3, 136.2, 134.1, 133.8, 132.3, 130.6, 129.7, 129.2, 128.9, 128.7, 128.7, 128.4, 127.8, 127.6, 127.4, 127.4, 127.3, 127.2, 126.6, 126.1, 125.8, 124.6, 123.2, 120.7, 120.7, 120.0, 117.7, 116.3, 115.9, 114.6, 113.1, 112.6, 110.3, 110.2, 108.8, 98.6, 84.8, 79.7, 56.3, 55.4, 55.4, 22.7, 20.5, 18.8.

HRMS (APCI) *m/z* calculated for C₅₄H₄₃O₄⁺ [*M* + *H*]⁺: 755.3156, found: 755.3153.

7a,11,13-Trimethyl-16-((1-((2',5,6'-trimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7aH-benzo[a]indeno[1,2-*l*]xanthene (2j)



2j

Compound **2j** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 56%, 40.4 mg.

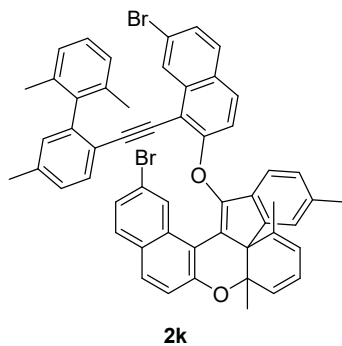
Appearance: yellow solid.

¹H NMR (600 MHz, CDCl₃) δ 8.51 (d, *J* = 8.5 Hz, 1H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.55–7.51 (m, 2H), 7.49 (d, *J* = 7.9 Hz, 1H), 7.35 (d, *J* = 9.0 Hz, 1H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.22–7.13 (m, 5H), 7.11–7.07 (m, 2H), 7.05 (t, *J* = 6.9 Hz, 1H), 7.02–6.95 (m, 3H), 6.89 (d, *J* = 9.0 Hz, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 6.66 (d, *J* = 7.8 Hz, 1H), 6.34 (dd, *J* = 9.4, 5.6 Hz, 1H), 5.98–5.92 (m, 2H), 2.37 (s, 3H), 2.23 (s, 3H), 2.06 (s, 6H), 1.38 (s, 3H), 1.26 (s, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 154.9, 153.8, 147.1, 143.6, 142.2, 141.3, 140.8, 138.7, 136.9, 136.4, 136.3, 136.2, 134.2, 132.2, 130.6, 130.0, 129.9, 129.2, 128.9, 128.9, 128.8, 128.6, 128.5, 127.9, 127.8, 127.6, 127.4, 127.3, 127.3, 126.6, 126.2, 125.8, 124.6, 123.9, 123.3, 121.2, 120.7, 120.6, 119.7, 117.7, 116.1, 110.1, 108.5, 98.8, 85.4, 79.9, 56.5, 22.8, 21.6, 20.6, 20.6, 18.8.

HRMS (APCI) *m/z* calculated for C₅₄H₄₃O₂⁺ [*M* + *H*]⁺: 723.3258, found: 723.3264.

2-Bromo-16-((7-bromo-1-((2',5,6'-trimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11,13-trimethyl-7aH-benzo[a]indeno[1,2-l]xanthene (2k)



Compound **2k** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 50%, 43.9 mg.

Appearance: yellow solid.

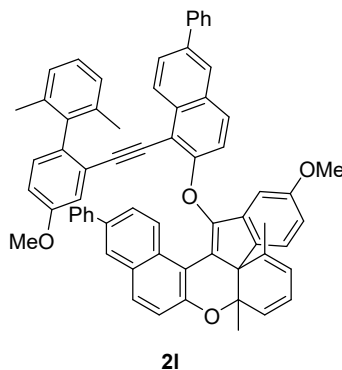
¹H NMR (600 MHz, CDCl₃) δ 8.27 (s, 1H), 7.82 (s, 1H), 7.55–7.48 (m, 2H), 7.46–7.38 (m, 3H), 7.34 (d, *J* = 8.6 Hz, 1H), 7.20–7.15 (m, 2H), 7.06–7.01 (m, 3H), 6.96–6.89 (m, 4H), 6.82 (d, *J* = 7.8 Hz, 1H), 6.55 (d, *J* = 7.8 Hz, 1H), 6.34 (dd, *J* = 9.5, 5.6 Hz, 1H), 5.96–5.92 (m, 2H), 2.31 (s, 3H), 2.24 (s, 3H), 2.00 (s, 3H), 1.97 (s, 3H), 1.37 (s, 3H), 1.17 (s, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 155.6, 154.5, 147.7, 143.5, 142.0, 140.8, 140.2, 138.7, 136.7, 136.6, 135.8, 135.7, 135.6, 132.9, 131.8, 129.9, 129.7, 129.4, 129.0, 128.8, 128.7, 128.6, 128.5, 128.1, 128.0, 127.7, 127.5, 127.5, 127.4, 127.3, 126.6, 123.8, 122.1, 121.0, 120.8,

120.6, 120.2, 119.8, 118.3, 116.8, 109.5, 108.7, 99.4, 83.8, 80.3, 56.3, 22.6, 21.6, 21.6, 20.6, 20.5, 18.9.

HRMS (APCI) *m/z* calculated for C₅₄H₄₁Br₂O₂⁺ [*M* + *H*]⁺: 881.1447, found: 881.1452.

14-Methoxy-16-((1-((4-methoxy-2',6'-dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)-6-phenylnaphthalen-2-yl)oxy)-7a,11-dimethyl-3-phenyl-7aH-benzo[a]indeno[1,2-l]xanthene (2l)



Compound **2l** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 72%, 65.3 mg.

Appearance: yellow solid.

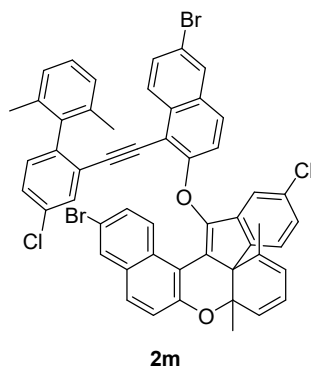
¹H NMR (600 MHz, CDCl₃) δ 8.55 (d, *J* = 8.7 Hz, 1H), 7.73 (s, 1H), 7.68 (s, 1H), 7.63–7.59 (m, 2H), 7.55 (d, *J* = 7.7 Hz, 2H), 7.48–7.36 (m, 7H), 7.33–7.24 (m, 4H), 7.20–7.14 (m, 2H), 7.13–7.06 (m, 2H), 7.06–6.97 (m, 4H), 6.93 (d, *J* = 9.1 Hz, 1H), 6.62 (d, *J* = 8.4 Hz, 1H), 6.47 (s, 1H), 6.34 (dd, *J* = 9.5, 5.5 Hz, 1H), 5.97–5.92 (m, 2H), 3.79 (s, 3H), 3.53 (s, 3H), 2.08 (s, 3H), 1.91 (s, 3H), 1.41 (s, 3H), 1.29 (s, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 159.8, 158.4, 155.1, 154.1, 146.7, 141.1, 140.8, 140.8, 140.4, 137.5, 137.0, 136.7, 136.3, 135.7, 133.7, 133.5, 130.6, 130.5, 129.7, 129.6, 129.4, 129.1, 128.8, 128.6, 128.5, 128.5, 127.4, 127.3, 127.3, 127.2, 127.1, 126.9, 126.8, 126.2,

125.7, 125.6, 125.5, 124.3, 123.9, 123.6, 120.5, 118.2, 116.9, 116.1, 115.2, 112.7, 109.9, 108.0, 105.0, 98.7, 86.0, 80.1, 56.1, 55.5, 55.4, 22.7, 20.7, 20.5, 18.6.

HRMS (APCI) *m/z* calculated for C₆₆H₅₁O₄⁺ [*M* + *H*]⁺: 907.3782, found: 907.3780.

3-Bromo-16-((6-bromo-1-((4-chloro-2',6'-dimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-14-chloro-7a,11-dimethyl-7aH-benzo[a]indeno[1,2-l]xanthene (2m)



Compound **2m** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 55%, 50.5 mg.

Appearance: yellow solid.

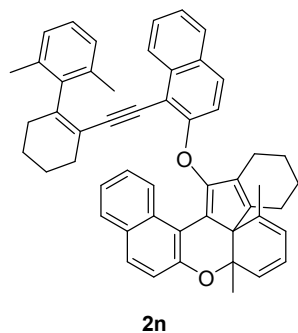
¹H NMR (600 MHz, CDCl₃) δ 8.21 (d, *J* = 8.9 Hz, 1H), 7.88 (s, 1H), 7.75–7.70 (m, 2H), 7.53 (d, *J* = 8.9 Hz, 1H), 7.49 (d, *J* = 8.1 Hz, 1H), 7.42 (d, *J* = 8.1 Hz, 1H), 7.36–7.31 (m, 3H), 7.26–7.26 (m, 1H), 7.22 (d, *J* = 8.2 Hz, 1H), 7.19 (d, *J* = 7.4 Hz, 1H), 7.15 (d, *J* = 7.4 Hz, 2H), 7.07 (d, *J* = 8.9 Hz, 1H), 7.01 (s, 1H), 6.93 (d, *J* = 9.0 Hz, 1H), 6.89 (d, *J* = 9.1 Hz, 1H), 6.42 (dd, *J* = 9.0, 5.8 Hz, 1H), 6.06–6.00 (m, 2H), 2.17 (s, 3H), 2.15 (s, 3H), 1.44 (s, 3H), 1.32 (s, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 154.8, 154.4, 145.8, 142.2, 141.2, 139.9, 139.8, 139.5, 136.5, 136.2, 134.2, 132.9, 132.8, 131.8, 130.9, 130.9, 130.2, 130.0, 129.9, 129.8, 129.6, 129.5, 129.2, 128.8, 128.8, 128.5, 128.5, 127.8, 127.6, 127.4, 127.4, 126.9, 124.8, 124.4, 124.2, 121.3, 119.7,

119.0, 118.9, 117.1, 115.9, 109.4, 107.9, 98.0, 86.4, 79.9, 56.5, 22.9, 20.7, 20.6, 18.6.

HRMS (APCI) *m/z* calculated for C₅₂H₃₅Br₂Cl₂O₂⁺ [*M* + *H*]⁺: 921.0355, found: 921.0354.

16-((1-((2',6'-Dimethyl-3,4,5,6-tetrahydro-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-dimethyl-12,13,14,15-tetrahydro-7aH-benzo[a]indeno[1,2-*l*]xanthene (2n)



Compound **2n** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 38%, 26.7 mg.

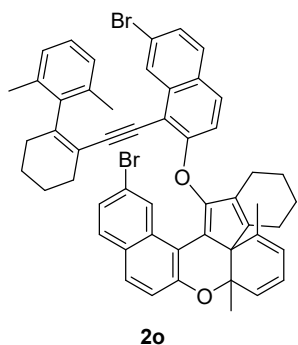
Appearance: yellow solid.

¹H NMR (600 MHz, CDCl₃) δ 8.28 (d, *J* = 8.4 Hz, 1H), 7.53–7.44 (m, 3H), 7.37 (d, *J* = 9.0 Hz, 1H), 7.24 (t, *J* = 7.8 Hz, 1H), 7.18–7.15 (m, 1H), 7.14–7.08 (m, 2H), 7.05 (t, *J* = 7.5 Hz, 1H), 7.03–6.97 (m, 3H), 6.96–6.91 (m, 2H), 6.13 (dd, *J* = 9.5, 5.6 Hz, 1H), 5.89 (d, *J* = 5.4 Hz, 1H), 5.83 (d, *J* = 9.5 Hz, 1H), 2.67–2.55 (m, 2H), 2.30–2.22 (m, 8H), 2.12–2.05 (m, 1H), 2.03–1.95 (m, 1H), 1.93–1.85 (m, 1H), 1.84–1.78 (m, 4H), 1.68–1.60 (m, 1H), 1.58–1.44 (m, 7H), 1.37 (s, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 154.9, 152.6, 149.9, 145.0, 142.5, 141.2, 138.6, 138.5, 135.0, 135.0, 134.3, 130.2, 129.1, 128.9, 128.8, 128.6, 128.4, 127.8, 127.6, 127.6, 127.4, 127.4, 127.0, 126.6, 125.9, 125.7, 124.4, 122.9, 120.9, 120.4, 118.7, 117.6, 115.7, 110.5, 108.7, 100.2, 84.5, 78.8, 59.0, 30.4, 30.0, 22.7, 22.7, 22.7, 22.6, 22.5, 22.4, 19.4, 19.4, 18.2.

HRMS (APCI) *m/z* calculated for C₅₂H₄₇O₂⁺ [*M* + *H*]⁺: 703.3571, found: 703.3577.

2-Bromo-16-((7-bromo-1-((2',6'-dimethyl-3,4,5,6-tetrahydro-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-dimethyl-12,13,14,15-tetrahydro-7aH-benzo[a]indeno[1,2-*l*]xanthene (2o)



Compound **2o** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 34%, 29.2 mg.

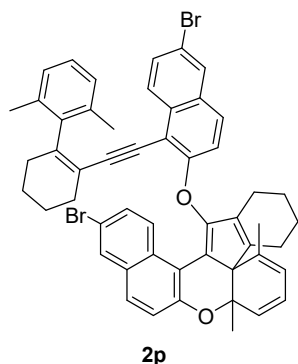
Appearance: yellow solid.

¹H NMR (600 MHz, CDCl₃) δ 8.23 (s, 1H), 7.78 (s, 1H), 7.46 (d, *J* = 8.9 Hz, 1H), 7.43–7.38 (m, 3H), 7.31 (d, *J* = 8.7 Hz, 1H), 7.19–7.15 (m, 1H), 7.02–6.88 (m, 5H), 6.14 (dd, *J* = 9.4, 5.7 Hz, 1H), 5.91 (d, *J* = 5.3 Hz, 1H), 5.83 (d, *J* = 9.5 Hz, 1H), 2.58–2.49 (m, 1H), 2.47–2.38 (m, 1H), 2.25 (s, 3H), 2.23–2.17 (m, 5H), 2.11–2.03 (m, 1H), 1.99–1.91 (m, 1H), 1.74 (s, 4H), 1.70–1.63 (m, 1H), 1.57–1.52 (m, 1H), 1.51–1.42 (m, 7H), 1.32 (s, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 155.5, 153.3, 150.5, 145.1, 142.0, 141.8, 138.5, 138.1, 135.5, 134.8, 134.7, 131.4, 129.3, 128.7, 128.5, 128.3, 128.3, 128.2, 127.8, 127.8, 127.4, 127.3, 126.8, 126.4, 121.8, 121.1, 120.6, 119.8, 118.5, 118.1, 116.6, 109.9, 109.0, 100.8, 83.0, 79.1, 58.8, 30.3, 30.0, 22.7, 22.7, 22.6, 22.5, 22.5, 22.1, 19.5, 19.5, 18.3.

HRMS (APCI) *m/z* calculated for C₅₂H₄₅Br₂O₂⁺ [*M* + *H*]⁺: 861.1760, found: 861.1761.

3-Bromo-16-((6-bromo-1-((2',6'-dimethyl-3,4,5,6-tetrahydro-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-dimethyl-12,13,14,15-tetrahydro-7aH-benzo[a]indeno[1,2-*l*]xanthene (2p)



Compound **2p** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 32%, 27.5 mg.

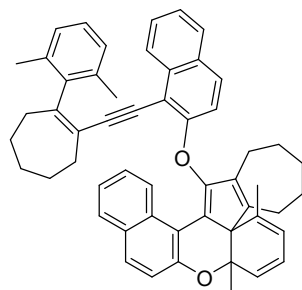
Appearance: yellow solid.

¹H NMR (600 MHz, CDCl₃) δ 8.20 (d, *J* = 8.3 Hz, 1H), 7.71 (s, 2H), 7.43 (d, *J* = 8.7 Hz, 1H), 7.38–7.30 (m, 2H), 7.22 (d, *J* = 8.9 Hz, 1H), 7.19–7.15 (m, 1H), 7.13–7.07 (m, 2H), 7.01 (d, *J* = 8.8 Hz, 1H), 6.96 (d, *J* = 8.5 Hz, 1H), 6.82 (d, *J* = 8.9 Hz, 1H), 6.23–6.19 (m, 1H), 5.98 (s, 1H), 5.90 (d, *J* = 9.3 Hz, 1H), 2.70–2.61 (m, 2H), 2.40–2.30 (m, 8H), 2.20–2.13 (m, 1H), 2.10–2.00 (m, 2H), 1.91 (s, 4H), 1.79–1.72 (m, 1H), 1.67–1.56 (m, 3H), 1.50 (s, 3H), 1.43 (s, 3H), 1.29–1.24 (m, 1H).

¹³C NMR (150 MHz, CDCl₃) δ 154.7, 152.8, 149.8, 146.0, 142.4, 141.8, 138.3, 138.1, 135.2, 134.9, 132.8, 130.3, 130.1, 130.1, 129.5, 129.4, 129.1, 128.6, 128.2, 128.0, 127.9, 127.7, 127.6, 127.5, 127.4, 126.7, 121.2, 119.9, 118.7, 118.5, 118.4, 116.7, 116.2, 110.5, 108.9, 100.9, 83.8, 79.0, 59.0, 30.4, 29.9, 22.7, 22.7, 22.5, 22.4, 22.4, 19.6, 19.4, 18.1.

HRMS (APCI) *m/z* calculated for C₅₂H₄₅Br₂O₂⁺ [*M* + *H*]⁺: 861.1760, found: 861.1761.

17-((1-((2-(2,6-Dimethylphenyl)cyclohept-1-en-1-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-dimethyl-13,14,15,16-tetrahydro-7aH,12H-azuleno[1,2-*l*]benzo[*a*]xanthene (2q)



2q

Compound **2q** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 36%, 26.3 mg.

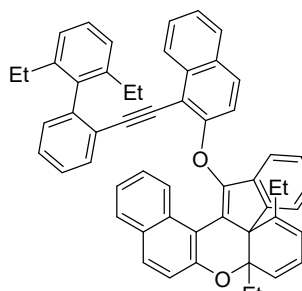
Appearance: yellow solid.

¹H NMR (600 MHz, CDCl₃) δ 8.32 (d, *J* = 8.3 Hz, 1H), 7.54 (d, *J* = 7.9 Hz, 1H), 7.51 (d, *J* = 8.5 Hz, 2H), 7.37 (d, *J* = 9.0 Hz, 1H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.20 (t, *J* = 7.2 Hz, 1H), 7.18–7.06 (m, 5H), 7.01–6.94 (m, 2H), 6.90 (d, *J* = 9.0 Hz, 1H), 6.24–6.18 (m, 1H), 6.03–5.96 (m, 2H), 2.93 (s, 2H), 2.64–2.58 (m, 2H), 2.43–2.33 (m, 8H), 2.26–2.20 (m, 1H), 2.07–2.02 (m, 1H), 1.96 (s, 4H), 1.88–1.80 (m, 3H), 1.68–1.48 (m, 11H).

¹³C NMR (150 MHz, CDCl₃) δ 155.0, 152.7, 150.0, 149.9, 145.0, 145.0, 142.6, 137.7, 134.6, 134.5, 134.3, 130.1, 129.2, 129.0, 128.8, 128.7, 128.5, 127.6, 127.6, 127.5, 127.5, 126.9, 126.4, 126.3, 126.1, 125.7, 124.4, 124.1, 122.9, 121.5, 120.2, 117.3, 114.5, 110.0, 107.9, 102.1, 85.6, 78.8, 59.0, 35.9, 35.4, 32.2, 31.4, 27.2, 27.0, 26.9, 26.5, 25.6, 23.6, 20.3, 20.3, 18.1.

HRMS (APCI) *m/z* calculated for C₅₄H₅₁O₂⁺ [*M* + *H*]⁺: 731.3884, found: 731.3879.

16-((1-((2,6'-Diethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-diethyl-7aH-benzo[*a*]indeno[1,2-*l*]xanthene (2r)



2r

Compound **2r** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 58%, 43.5 mg.

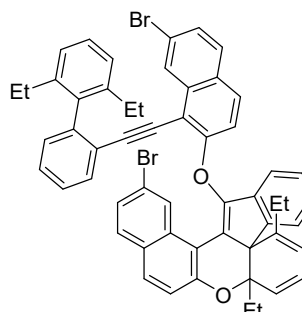
Appearance: yellow solid.

¹H NMR (400 MHz, CDCl₃) δ 8.64 (d, *J* = 8.5 Hz, 1H), 7.97–7.90 (m, 1H), 7.69–7.60 (m, 3H), 7.53–7.37 (m, 6H), 7.36–7.27 (m, 3H), 7.25–7.17 (m, 3H), 7.15–7.00 (m, 5H), 6.84–6.79 (m, 1H), 6.58 (dd, *J* = 9.5, 5.7 Hz, 1H), 6.25 (d, *J* = 9.5 Hz, 1H), 6.07 (d, *J* = 5.5 Hz, 1H), 2.53–2.41 (m, 4H), 1.99–1.86 (m, 2H), 1.82–1.72 (m, 1H), 1.45–1.36 (m, 1H), 1.14–0.97 (m, 9H), 0.78 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 154.9, 153.8, 147.2, 146.5, 143.1, 142.3, 142.3, 142.0, 139.6, 139.5, 134.2, 132.1, 130.7, 130.2, 129.2, 129.0, 128.1, 127.8, 127.7, 127.6, 127.3, 127.1, 126.6, 126.3, 126.1, 125.9, 125.7, 125.7, 124.8, 124.7, 124.2, 123.5, 123.3, 122.2, 120.0, 117.8, 117.8, 116.3, 110.8, 108.5, 99.0, 86.8, 81.4, 57.2, 26.8, 26.0, 23.9, 15.4, 15.3, 11.4, 7.1.

HRMS (APCI) *m/z* calculated for C₅₆H₄₇O₂⁺ [*M* + *H*]⁺: 751.3571, found: 751.3575.

2-Bromo-16-((7-bromo-1-((2,6'-diethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-diethyl-7aH-benzo[*a*]indeno[1,2-*l*]xanthene (2s)



2s

Compound **2s** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 63%, 57.1 mg.

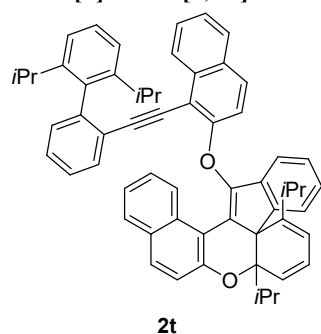
Appearance: yellow solid.

¹H NMR (400 MHz, CDCl₃) δ 8.34 (s, 1H), 7.90 (s, 1H), 7.73–7.60 (m, 2H), 7.60–7.50 (m, 3H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.42–7.36 (m, 1H), 7.35–7.27 (m, 2H), 7.25–7.21 (m, 1H), 7.20–6.98 (m, 7H), 6.66 (d, *J* = 7.2 Hz, 1H), 6.56 (dd, *J* = 9.3, 5.7 Hz, 1H), 6.22 (d, *J* = 9.5 Hz, 1H), 6.06 (d, *J* = 5.2 Hz, 1H), 2.50–2.28 (m, 4H), 1.94–1.84 (m, 1H), 1.82–1.68 (m, 2H), 1.27–1.20 (m, 1H), 1.12–0.88 (m, 9H), 0.79 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 155.7, 154.5, 147.5, 145.9, 143.1, 141.9, 141.8, 141.8, 139.2, 138.9, 135.6, 132.7, 131.9, 130.0, 130.0, 129.4, 129.4, 129.3, 129.0, 128.7, 128.2, 128.1, 128.1, 128.0, 127.9, 127.7, 127.4, 126.7, 126.7, 126.5, 125.8, 125.8, 124.8, 123.9, 123.4, 122.2, 121.8, 120.9, 120.0, 118.4, 117.9, 116.9, 110.1, 108.5, 99.5, 85.0, 81.9, 57.1, 26.8, 26.7, 25.8, 24.0, 15.4, 11.3, 7.0.

HRMS (APCI) *m/z* calculated for C₅₆H₄₅Br₂O₂⁺ [*M* + *H*]⁺: 909.1760, found: 909.1770.

16-((1-((2',6'-Diisopropyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-diisopropyl-7aH-benzo[a]indeno[1,2-*l*]xanthene (2t)



Compound **2t** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 39%, 31.5 mg.

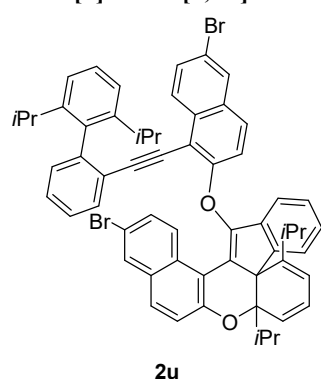
Appearance: yellow solid.

¹H NMR (400 MHz, CDCl₃) δ 8.78 (s, 1H), 8.01–7.94 (m, 1H), 7.68–7.58 (m, 3H), 7.55–7.44 (m, 5H), 7.36–7.28 (m, 4H), 7.23–7.18 (m, 2H), 7.16–6.92 (m, 5H), 6.86 (d, *J* = 8.2 Hz, 1H), 6.81–6.74 (m, 1H), 6.65 (dd, *J* = 9.3, 5.8 Hz, 1H), 6.23–6.14 (m, 2H), 2.79–2.65 (m, 2H), 2.49–2.41 (m, 1H), 2.24–2.15 (m, 1H), 1.14 (s, 9H), 1.11–1.03 (m, 6H), 0.67 (d, *J* = 6.6 Hz, 3H), 0.58 (d, *J* = 6.6 Hz, 3H), 0.41 (d, *J* = 6.5 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 155.0, 153.5, 151.8, 147.4, 147.1, 146.9, 143.5, 141.8, 139.5, 138.4, 134.2, 132.0, 130.8, 130.2, 130.2, 130.1, 129.2, 129.2, 129.1, 128.2, 128.0, 127.8, 127.8, 127.5, 127.3, 127.1, 126.8, 126.0, 126.0, 125.9, 125.1, 124.8, 124.5, 123.3, 123.2, 123.0, 122.9, 122.6, 122.2, 120.1, 117.8, 116.1, 112.0, 108.3, 99.2, 87.4, 85.9, 58.6, 31.7, 30.8, 30.8, 30.0, 25.0, 24.6, 24.5, 24.2, 24.1, 22.7, 20.5, 18.4.

HRMS (APCI) *m/z* calculated for C₆₀H₅₅O₂⁺ [*M* + *H*]⁺: 807.4197, found: 807.4200.

3-Bromo-16-((6-bromo-1-((2',6'-diisopropyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7a,11-diisopropyl-7aH-benzo[a]indeno[1,2-*l*]xanthene (2u)



Compound **2u** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 38%, 36.7 mg.

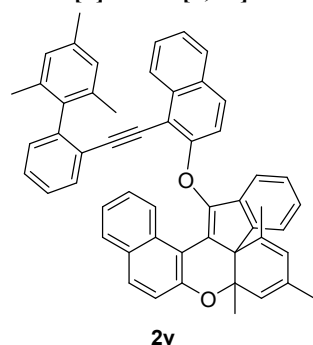
Appearance: yellow solid.

¹H NMR (600 MHz, CDCl₃) δ 8.63 (s, 1H), 7.94 (s, 1H), 7.77 (d, *J* = 14.3 Hz, 2H), 7.59–7.46 (m, 5H), 7.44–7.28 (m, 5H), 7.25–7.21 (m, 1H), 7.12–7.04 (m, 3H), 6.93 (s, 1H), 6.79–6.73 (m, 1H), 6.68–6.60 (m, 2H), 6.21–6.14 (m, 2H), 2.77–2.66 (m, 2H), 2.42–2.35 (m, 1H), 2.14–2.07 (m, 1H), 1.18–1.10 (m, 9H), 1.05 (d, *J* = 6.7 Hz, 3H), 1.01 (d, *J* = 6.7 Hz, 3H), 0.64 (d, *J* = 6.6 Hz, 3H), 0.54 (d, *J* = 6.7 Hz, 3H), 0.39 (d, *J* = 6.2 Hz, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 154.8, 153.7, 151.4, 147.3, 147.3, 146.9, 143.7, 141.8, 138.9, 138.2, 132.7, 131.7, 130.7, 130.3, 130.3, 130.2, 129.8, 129.5, 129.3, 129.2, 129.2, 128.5, 128.4, 128.3, 128.1, 127.9, 127.8, 127.2, 126.3, 125.2, 124.0, 123.2, 123.0, 122.8, 121.9, 120.1, 118.9, 118.0, 117.1, 116.9, 112.0, 108.4, 99.8, 86.7, 86.2, 58.5, 31.8, 30.9, 30.8, 30.0, 25.0, 24.6, 24.4, 24.3, 24.0, 22.7, 20.5, 18.3.

HRMS (APCI) *m/z* calculated for C₆₀H₅₃Br₂O₂⁺ [*M* + *H*]⁺: 965.2386, found: 965.2391.

7a,9,11-Trimethyl-16-((1-((2',4',6'-trimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7aH-benzo[a]indeno[1,2-*l*]xanthene (2v)



Compound **2v** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 51%, 36.8 mg.

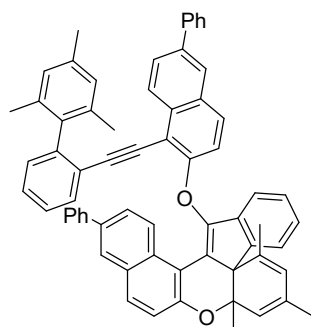
Appearance: yellow solid.

¹H NMR (400 MHz, CDCl₃) δ 8.53 (d, *J* = 8.5 Hz, 1H), 7.88–7.80 (m, 1H), 7.55–7.45 (m, 3H), 7.40–7.23 (m, 5H), 7.23–7.09 (m, 3H), 7.08–6.86 (m, 8H), 6.82–6.75 (m, 1H), 5.81 (s, 1H), 5.66 (s, 1H), 2.28 (s, 3H), 2.02 (s, 6H), 1.94 (s, 3H), 1.37 (s, 3H), 1.23 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 155.0, 154.0, 146.7, 143.7, 142.1, 140.7, 139.6, 138.0, 137.2, 136.7, 136.2, 136.2, 134.2, 132.3, 130.6, 130.2, 129.7, 129.2, 128.9, 128.5, 128.3, 128.1, 127.8, 127.7, 127.0, 127.0, 126.5, 126.3, 126.2, 125.9, 124.9, 124.7, 123.9, 123.8, 123.3, 123.1, 122.8, 119.9, 117.8, 116.0, 110.0, 108.3, 98.8, 86.0, 81.0, 56.8, 22.9, 21.6, 21.3, 20.5, 18.5.

HRMS (APCI) *m/z* calculated for C₅₄H₄₃O₂⁺ [*M* + *H*]⁺: 723.3258, found: 723.3266.

7a,9,11-Trimethyl-3-phenyl-16-((6-phenyl-1-((2',4',6'-trimethyl-[1,1'-biphenyl]-2-yl)ethynyl)naphthalen-2-yl)oxy)-7aH-benzo[*a*]indeno[1,2-*I*]xanthene (2w)



2w

Compound **2w** is an unknown compound and was purified by silica gel column chromatography using PE/DCM (8:1) as eluent. **Yield:** 51%, 44.6 mg.

Appearance: yellow solid.

¹H NMR (400 MHz, CDCl₃) δ 8.78 (d, *J* = 8.7 Hz, 1H), 8.08 (d, *J* = 7.0 Hz, 1H), 7.89 (s, 1H), 7.84 (s, 1H), 7.78–7.67 (m, 4H), 7.57–7.46 (m, 9H), 7.43–7.35 (m, 3H), 7.31 (d, *J* = 7.3 Hz, 2H), 7.22–7.07 (m, 6H), 7.04–6.99 (m, 2H), 5.98 (s, 1H), 5.84 (s, 1H), 2.45 (s, 3H), 2.19 (s, 3H), 2.10 (s, 3H), 2.02 (s, 3H), 1.56 (s, 3H), 1.42 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 155.0, 154.2, 146.6, 143.9, 142.1, 140.8, 140.8, 140.6, 139.6, 138.0, 137.4, 137.3, 136.7, 136.4, 136.2, 135.6, 133.5, 132.4, 130.6, 129.8, 129.7, 129.4, 129.2, 128.8, 128.6, 128.5, 128.3, 128.1, 127.9, 127.3, 127.1, 127.0, 126.9, 126.7, 126.4, 125.6, 125.5,

125.5, 124.9, 123.8, 123.7, 123.2, 122.7, 119.9, 118.2, 116.3, 109.9, 108.2, 98.8, 86.2, 81.2, 56.8, 22.9, 21.6, 21.4, 20.5, 20.3, 18.6.

HRMS (APCI) *m/z* calculated for C₆₆H₅₁O₂⁺ [*M* + *H*]⁺: 875.3884, found: 875.3886.

7. Mechanistic studies

7.1 UV/Vis absorption spectroscopy

UV/Vis absorption spectra were recorded on Shimadzu UV-vis spectrophotometer UV-2600, equipped with a temperature control unit at 25 °C. The solutions of **1a** and 2,6-lutidine were prepared by directly dissolving in PhCF₃ ($c = 1 \times 10^{-5}$ M) for the spectroscopic determination.

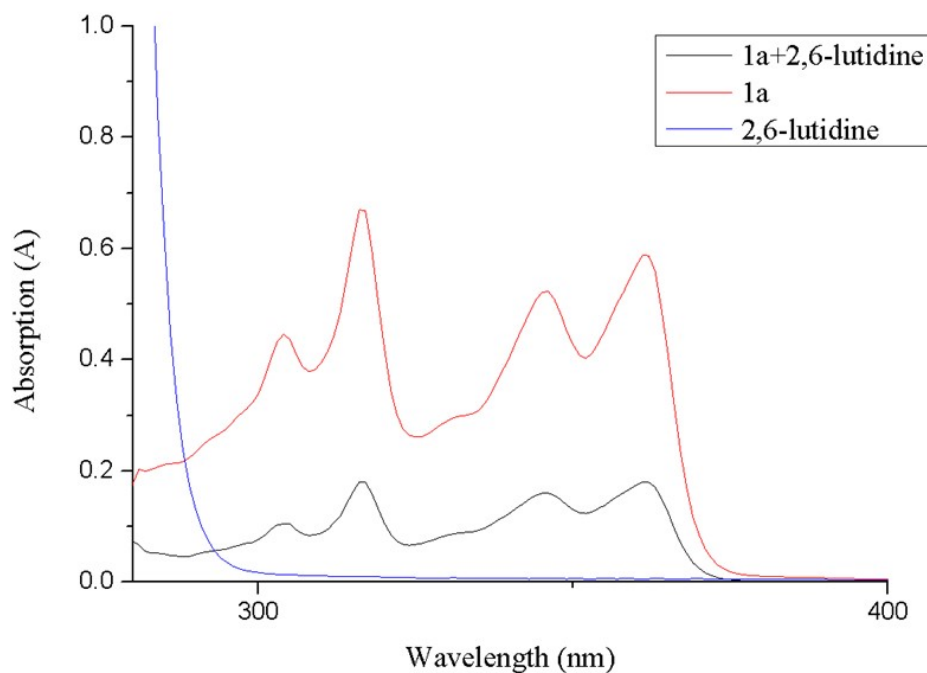
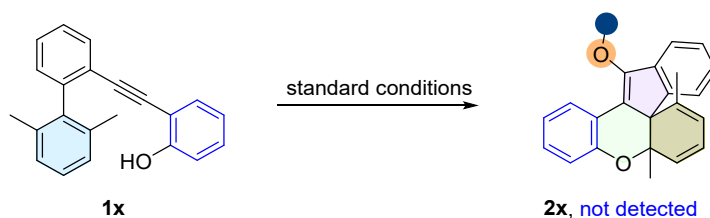


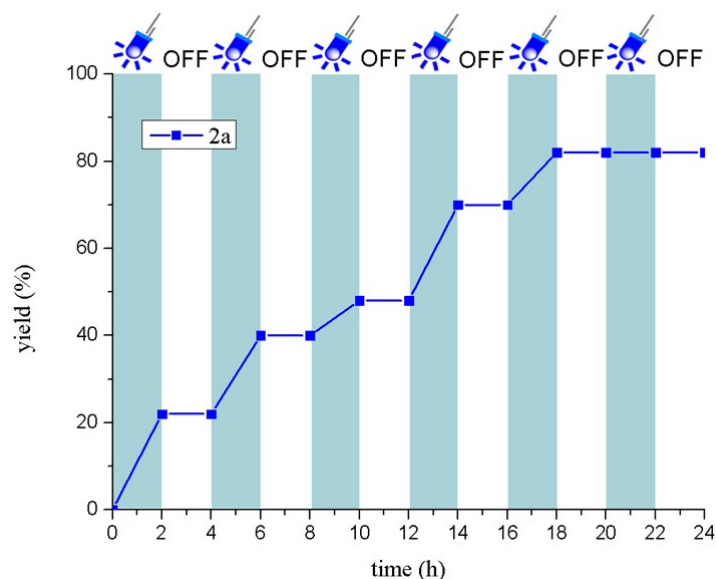
Figure S2. UV/Vis absorption spectra of **1a**, 2,6-lutidine (1×10^{-5} M in PhCF₃), and the mixture of **1a** and 2,6-lutidine (1×10^{-5} M in PhCF₃)

7.2 Control experiments



Substrate **1x** was prepared according to the general procedure for synthesis of **1a-m**. No desired dearomatized product **2x** was observed under standard reaction conditions.

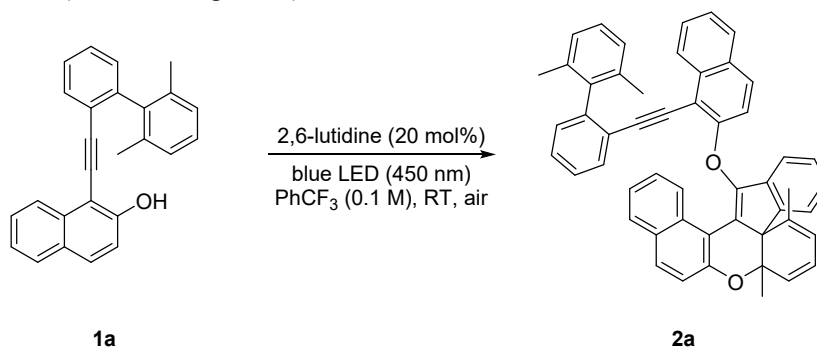
7.3 Light on/off experiments



The reaction of **1a** in the presence of 2,6-lutidine was performed according to the general procedure described above, similar successive intervals of irradiation and dark periods were performed for 2 h. The yields of product **2a** were determined by means of ^1H NMR analysis from an aliquot from the reaction mixture using 1,3,5-trimethoxybenzene as an internal standard.

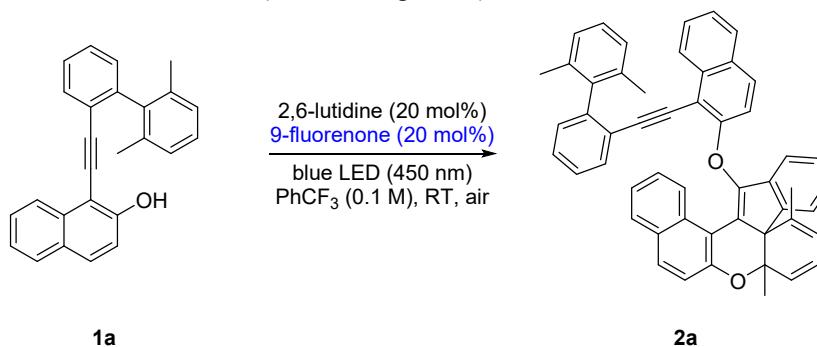
7.4 Initial rate investigation for the photochemical reaction.

Standard reaction conditions (blue trace, Figure S3)



In an oven-dried 10 mL Schlenk tube equipped with a magnetic stirrer bar was charged sequentially with the substrate **1a** (0.2 mmol, 1.0 equiv), 2,6-lutidine (0.04 mmol, 0.2 equiv), and α,α,α -trifluorotoluene (2 mL). The reaction mixture was then stirred under irradiation with blue LEDs (30 W, $\lambda_{\text{max}} = 450$ nm). Time points were taken every 18 minutes. The yields of product **2a** were determined by means of ^1H NMR analysis from an aliquot from the reaction mixture using 1,3,5-trimethoxybenzene as an internal standard.

Standard reaction conditions with 9-fluorenone (red trace, Figure S3)



In an oven-dried 10 mL Schlenk tube equipped with a magnetic stirrer bar was charged sequentially with the substrate **1a** (0.2 mmol, 1.0 equiv), 2,6-lutidine (0.04 mmol, 0.2 equiv), 9-fluorenone (0.04 mmol, 0.2 equiv), and α,α,α -trifluorotoluene (2 mL). The reaction mixture was then stirred under irradiation with blue LEDs (30 W, $\lambda_{\text{max}} = 450$ nm). Time points were taken every 18 minutes. The yields of product **2a** were determined by means of ^1H NMR analysis from an aliquot from the reaction mixture using 1,3,5-trimethoxybenzene as an internal standard.

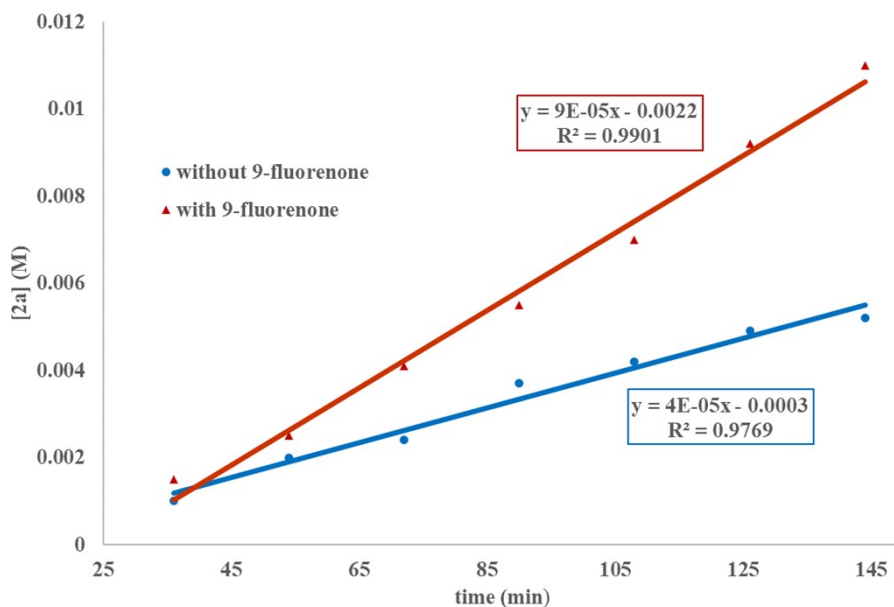
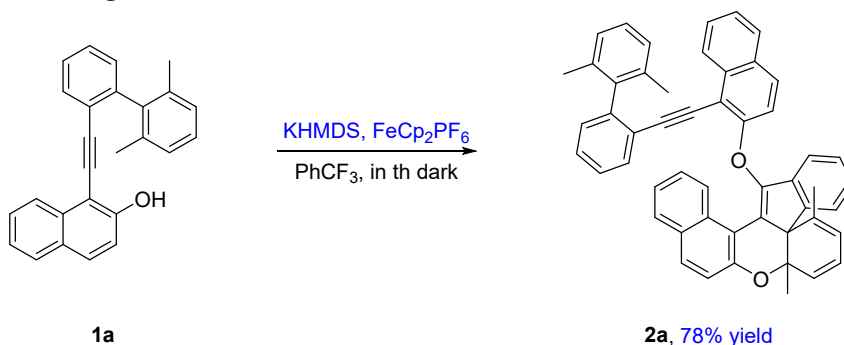


Figure S3. Reaction profile for the dearomatization of the substrate **1a**. An increase in initial rate was observed when 9-fluorenone was added to the reaction mixture.

7.5 The preparation of **2a** using chemical oxidant



Stephenson and coworkers developed a facial pathway to generate the phenoxyl radicals using potassium bis(trimethylsilyl)amide (KHMDS) and FeCp_2PF_6 .⁷ To verify that our strategy may proceed through a phenoxyl radical intermediate, we performed the dearomatization of **1a** under the reaction conditions developed by Stephenson.

A solution of substrate **1a** (0.05 mmol, 1.0 equiv) was prepared in PhCF_3 (1 mL) at room temperature, then potassium bis(trimethylsilyl)amide (0.05 mmol, 1.0 equiv) was added slowly. The reaction mixture was stirred for 5 min in the dark, at which point FeCp_2PF_6 (0.05 mmol, 1.0 equiv) was added in a single portion. At 1 h, an additional FeCp_2PF_6 (0.0125 mmol) was added. After stirring for 24 h, the reaction was quenched by the addition of sat. aq. NH_4Cl . The mixture was then diluted with EtOAc and transferred to a separatory funnel where the phases were separated. The aqueous layer was extracted with additional portions of EtOAc. The combined organic layers were then washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The obtained crude mixture was purified by chromatography (silica gel, PE/EA = 10:1) to afford **2a** as a yellow solid (78% yield).

8. Crystallographic details of 2v

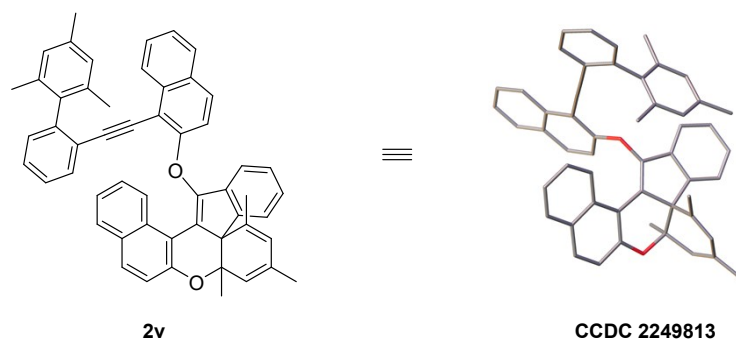
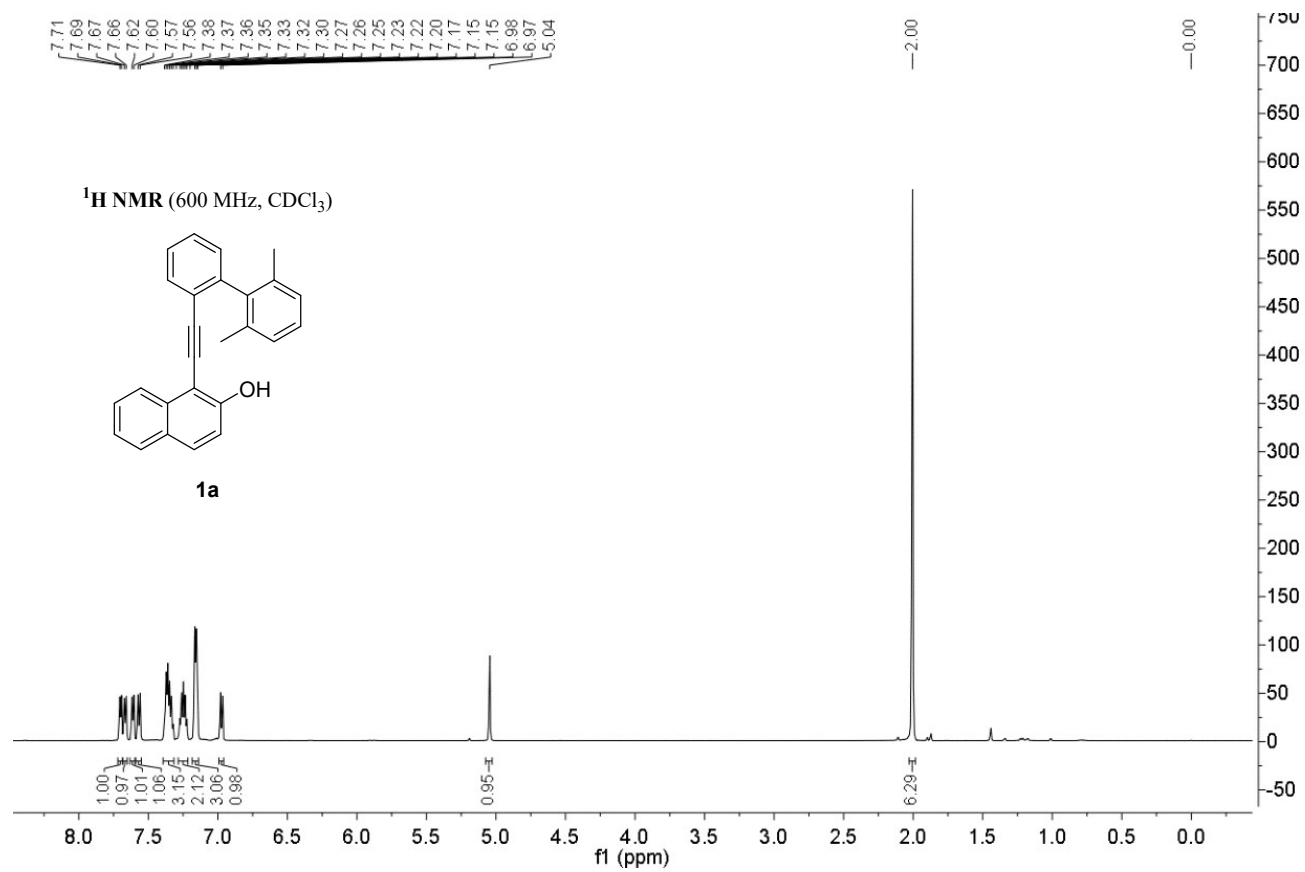


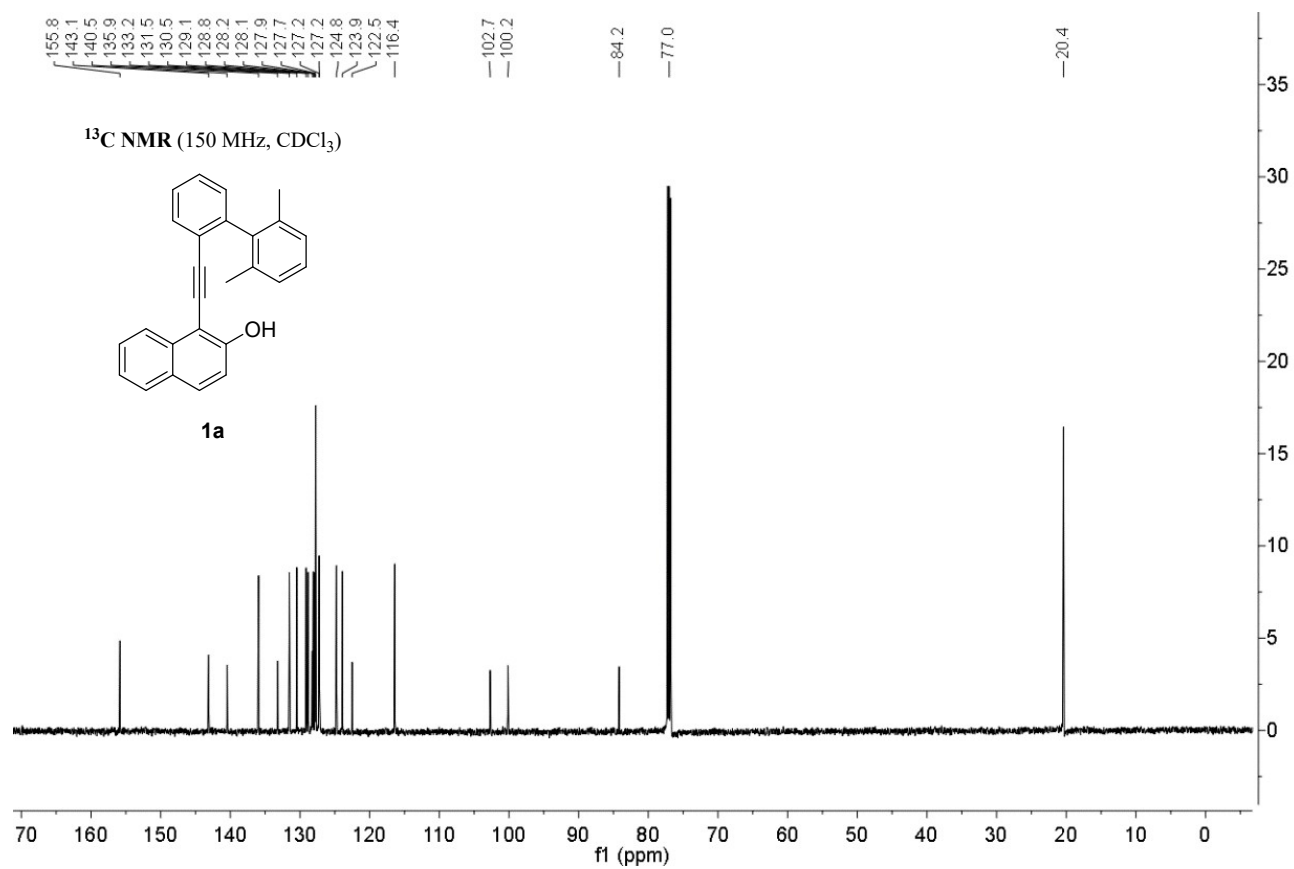
Figure S4. Single crystal X-ray structure of **2v**.

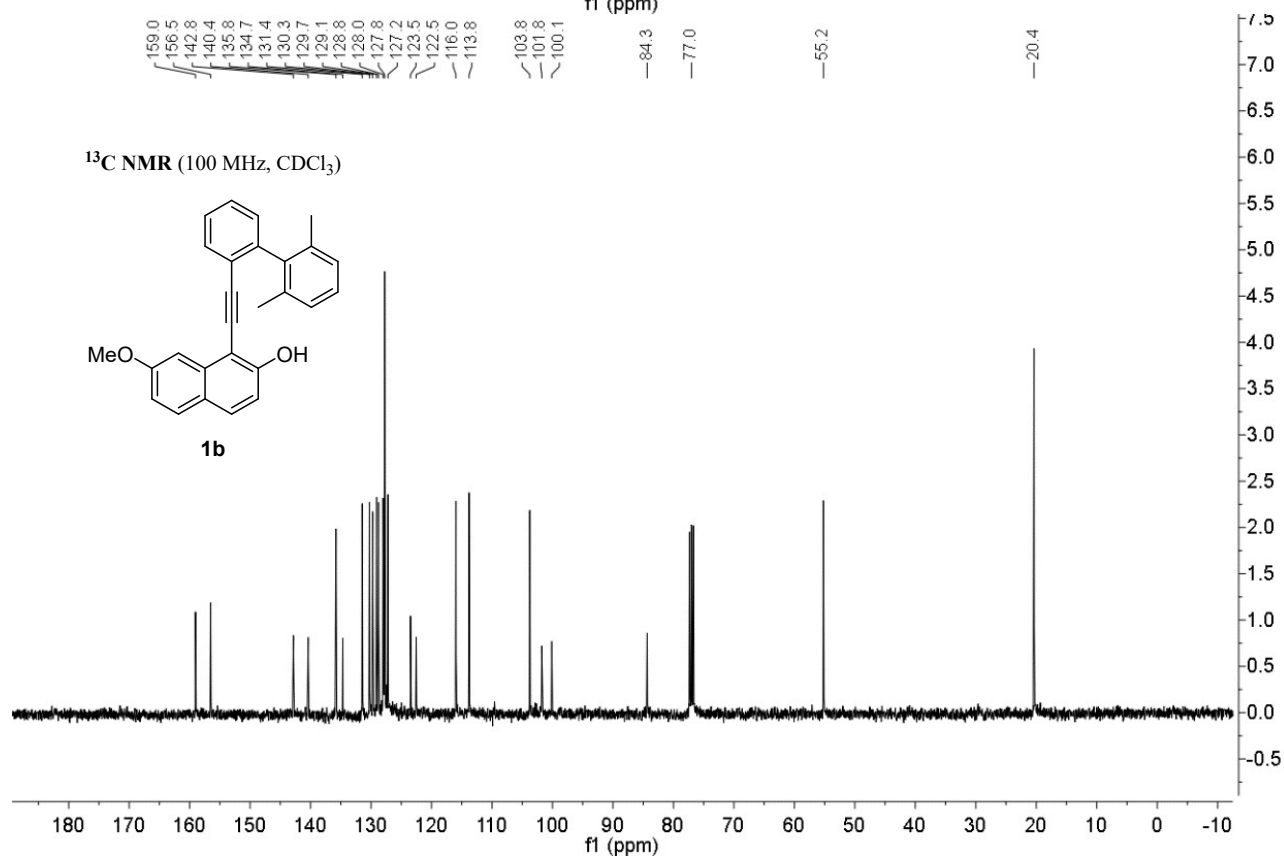
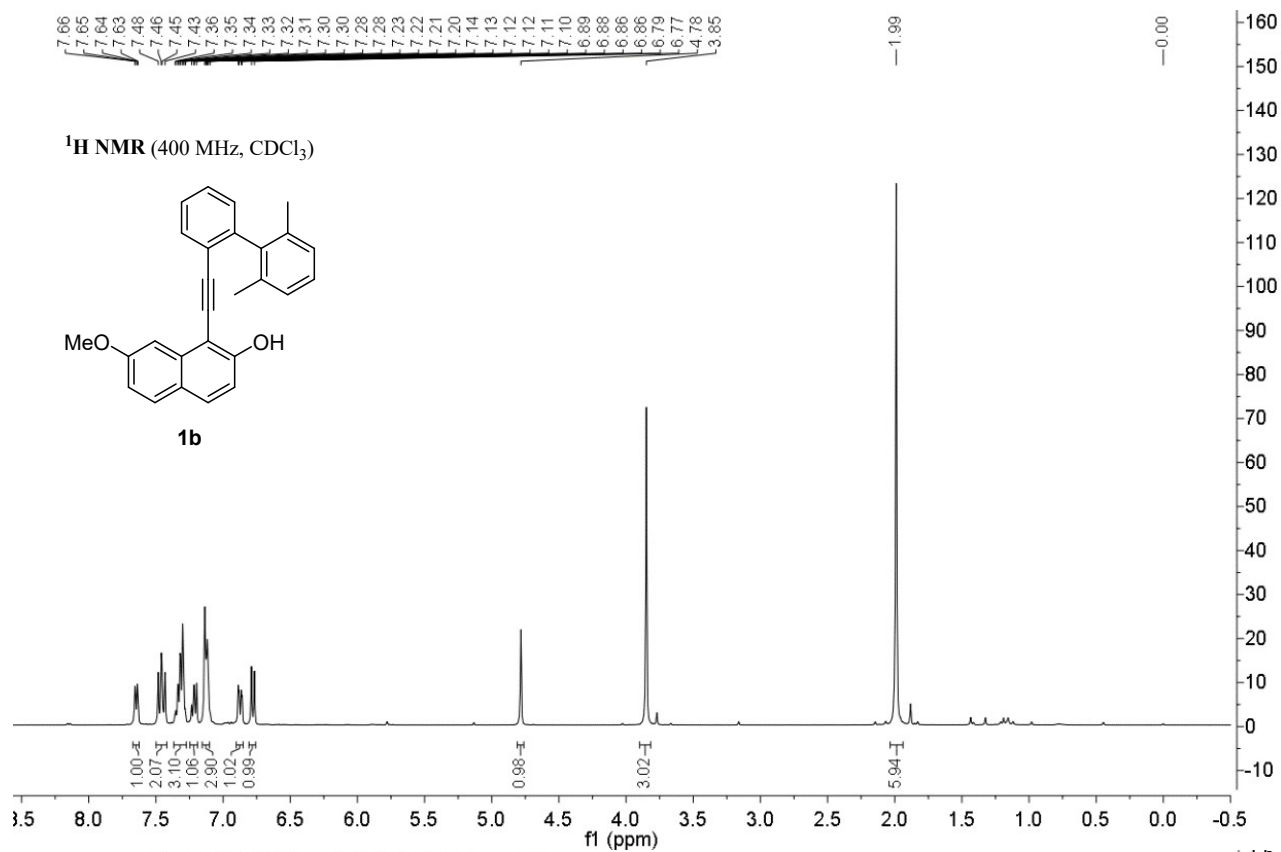
Table S4. Crystal data and structure refinement for **2v**

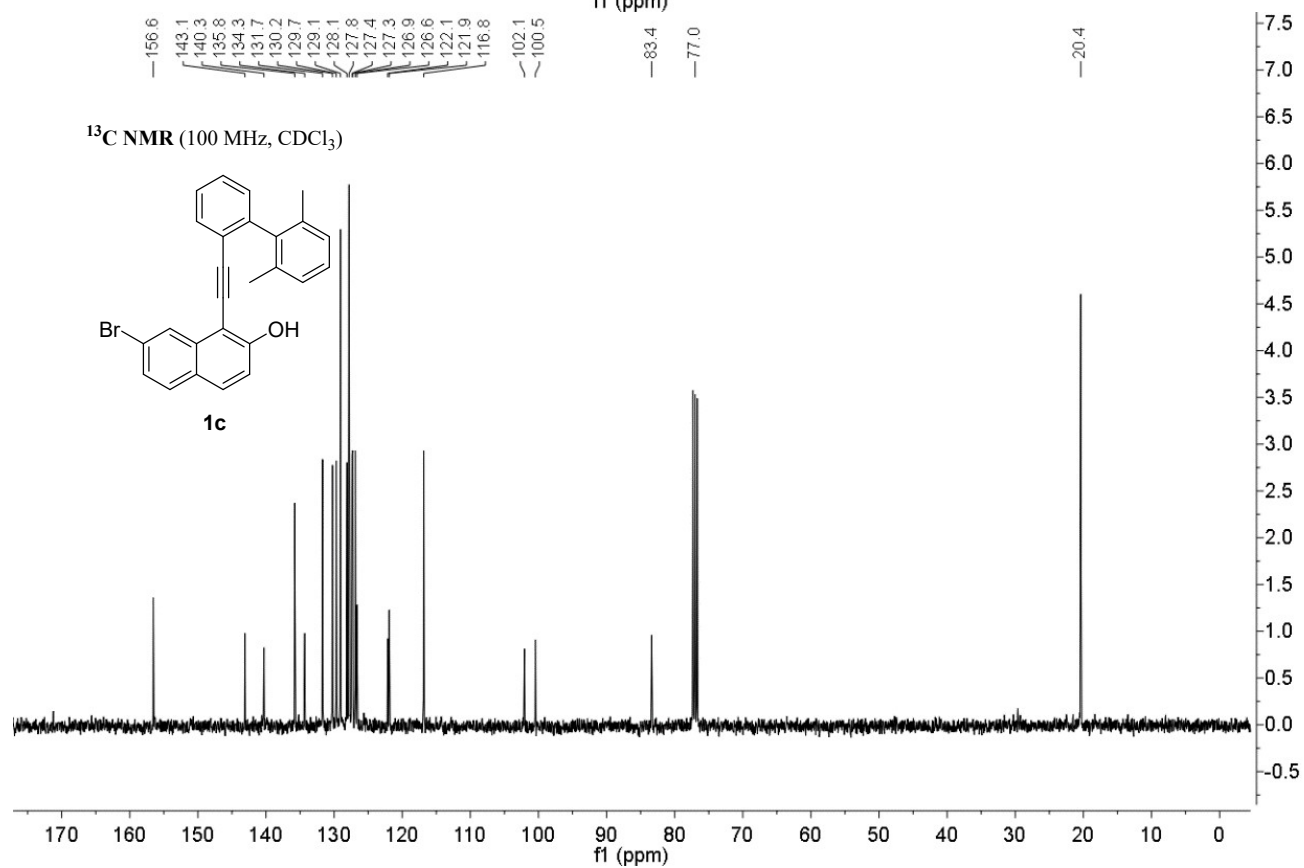
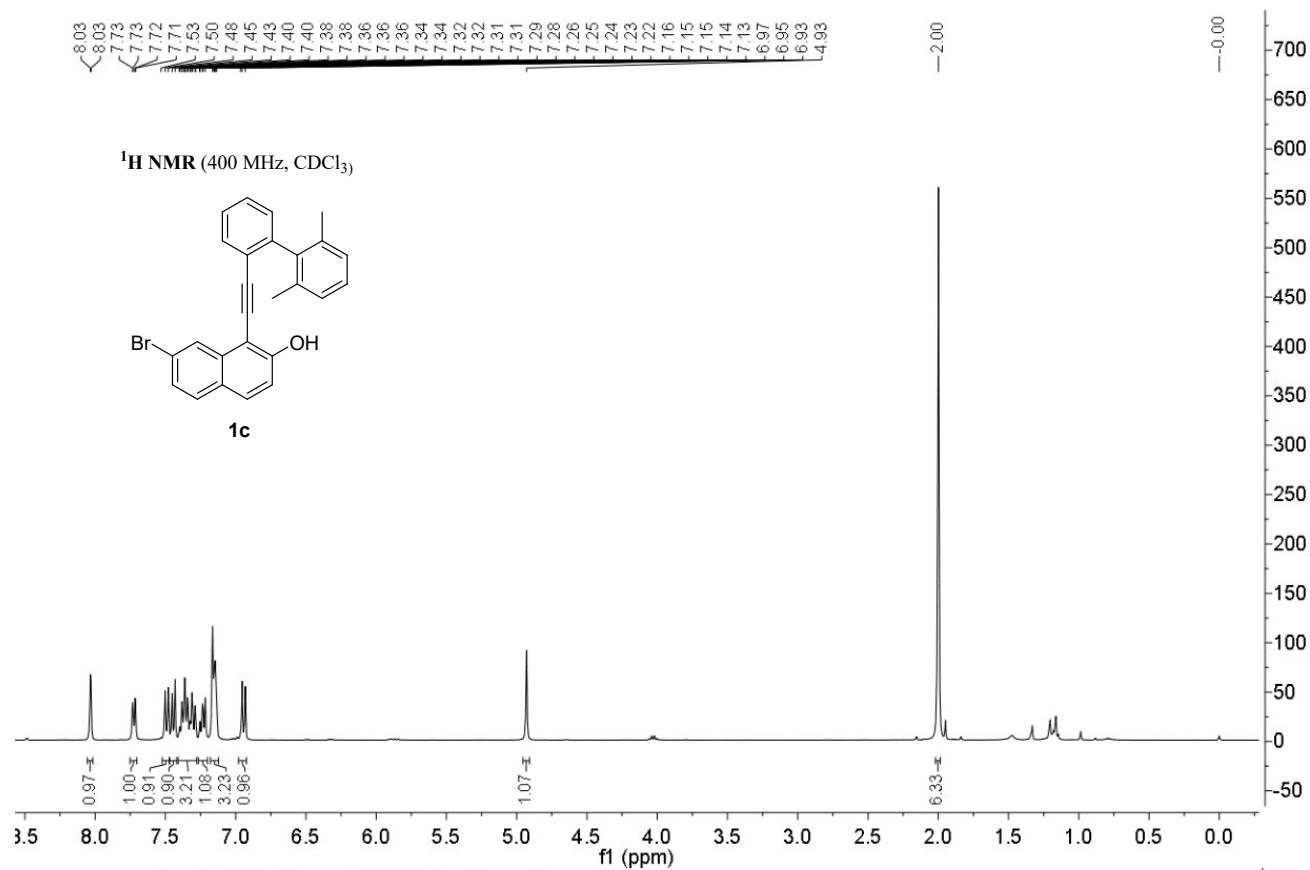
Bond precision: C-C = 0.0036 Å		Wavelength=1.54184	
Cell:	a=11.1157(4)	b=12.0628(5)	c=16.2649(4)
	alpha=94.895(2)	beta=102.914(2)	gamma=109.561(3)
Temperature:	293 K		
	Calculated	Reported	
Volume	1972.37(13)	1972.36(12)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C54 H42 O2	C54 H42 O2	
Sum formula	C54 H42 O2	C54 H42 O2	
Mr	722.88	722.87	
Dx, g cm-3	1.217	1.217	
Z	2	2	
Mu (mm-1)	0.557	0.557	
F000	764.0	764.0	
F000'	766.06		
h, k, lmax	13, 14, 19	13, 14, 19	
Nref	7586	7545	
Tmin, Tmax	0.827, 0.900	0.836, 1.000	
Tmin'	0.827		
Correction method= # Reported T Limits: Tmin=0.836 Tmax=1.000			
AbsCorr = MULTI-SCAN			
Data completeness= 0.995		Theta(max)= 70.700	
R(reflections)= 0.0566(6281)		wR2(reflections)=	
		0.1840(7545)	
S = 1.123	Npar= 512		

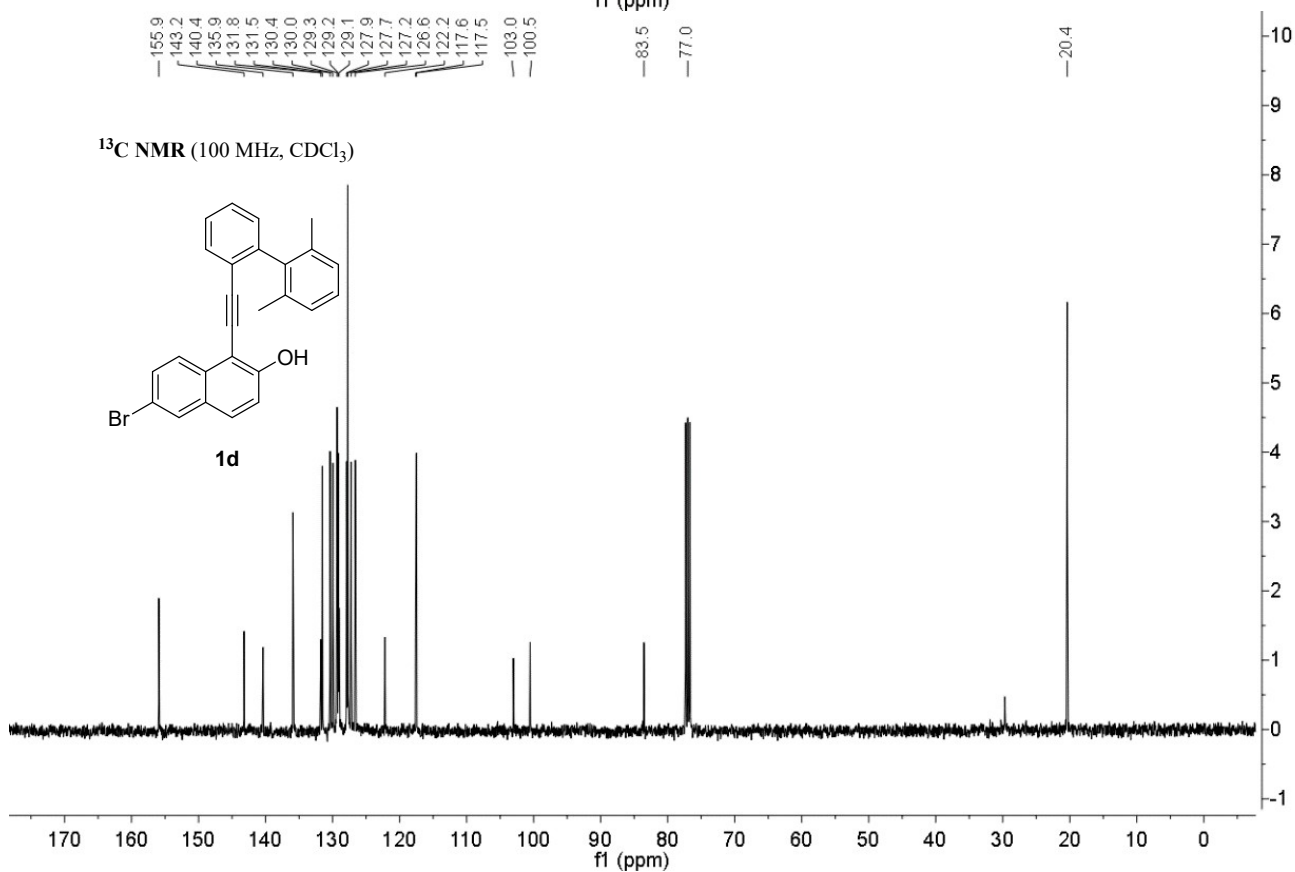
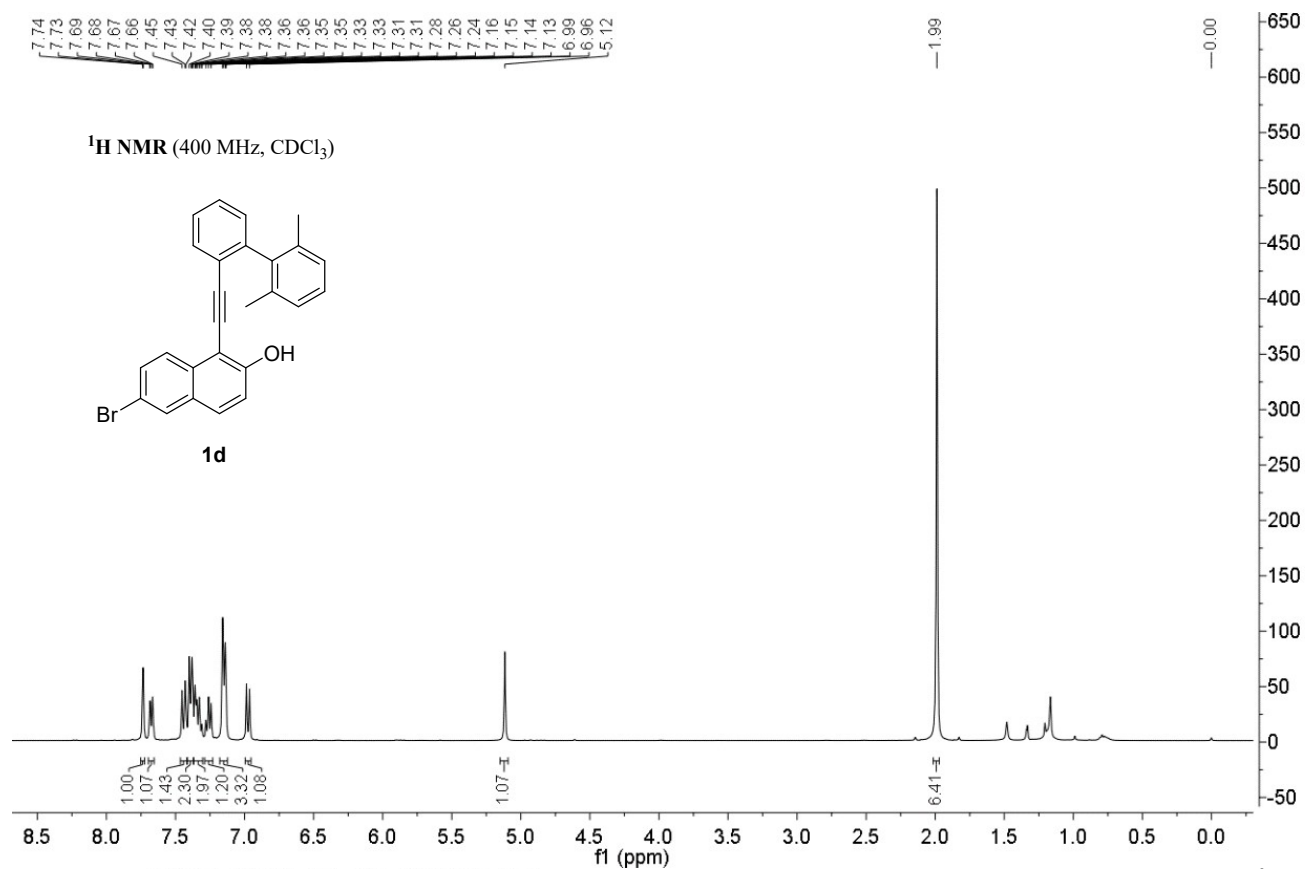
9. ^1H and ^{13}C NMR spectra

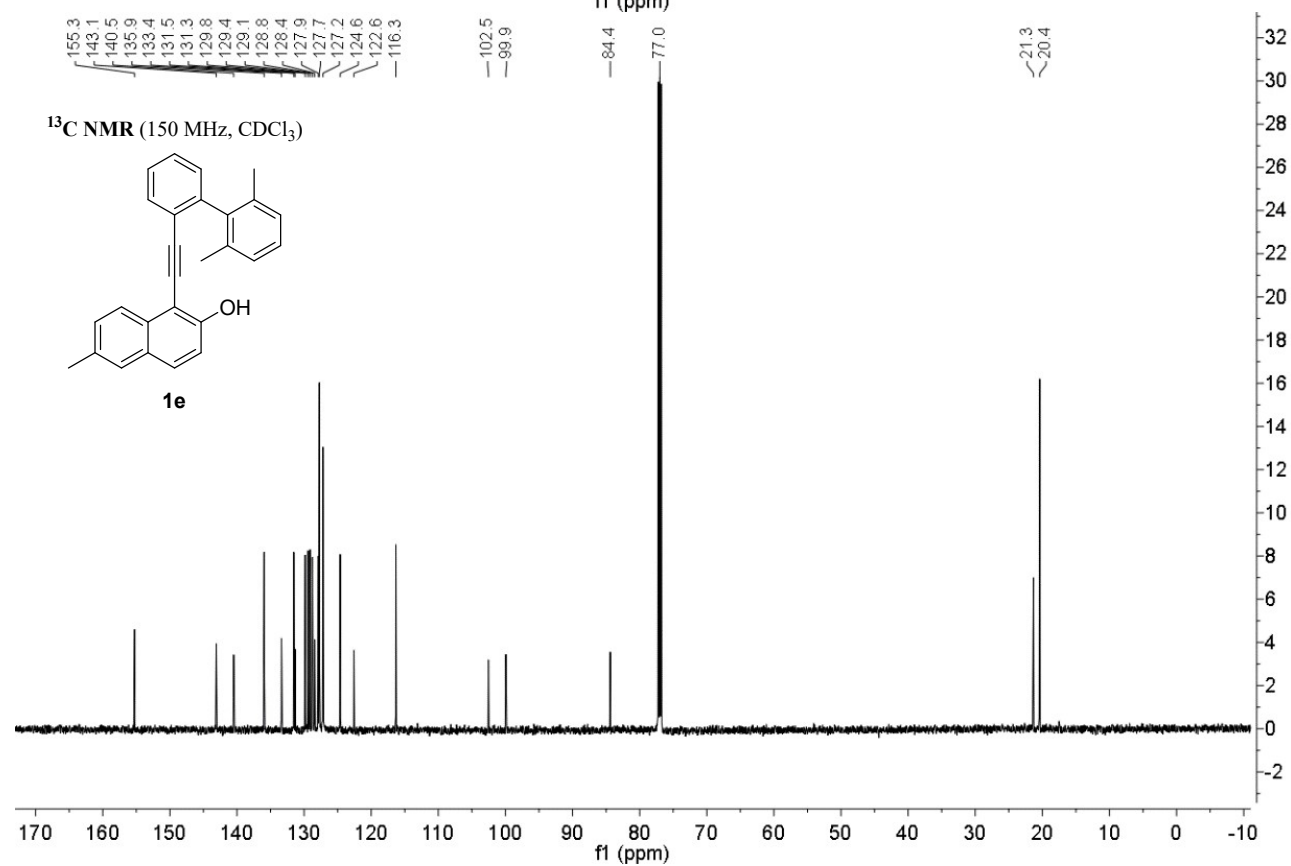
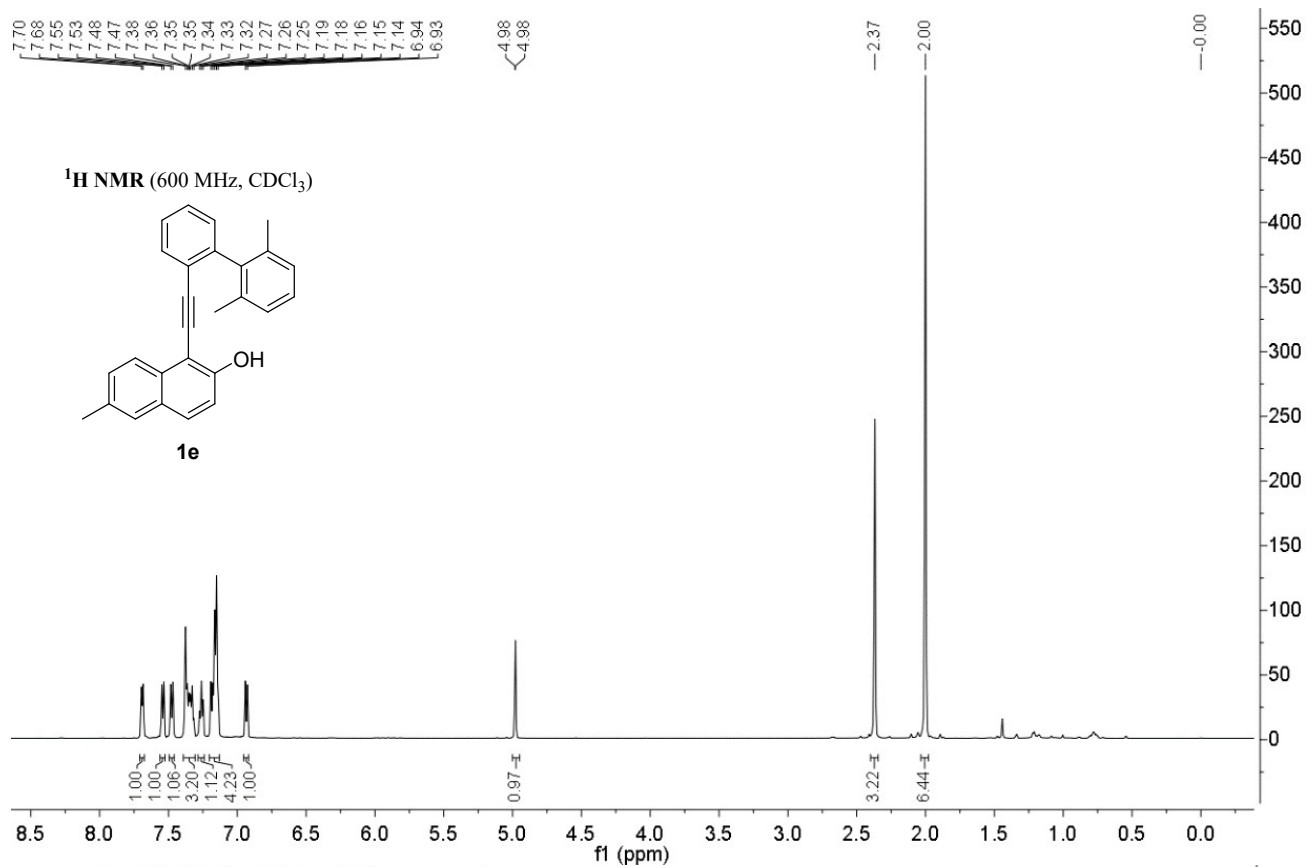


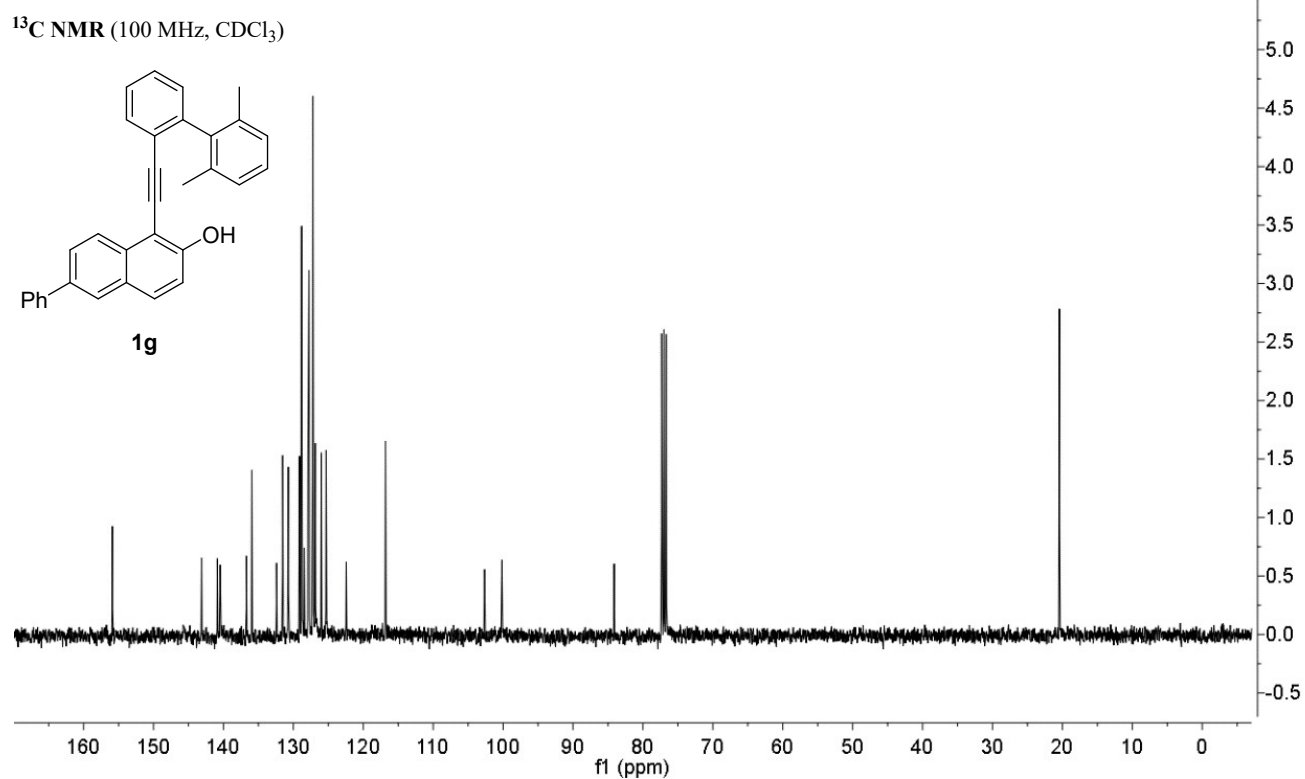
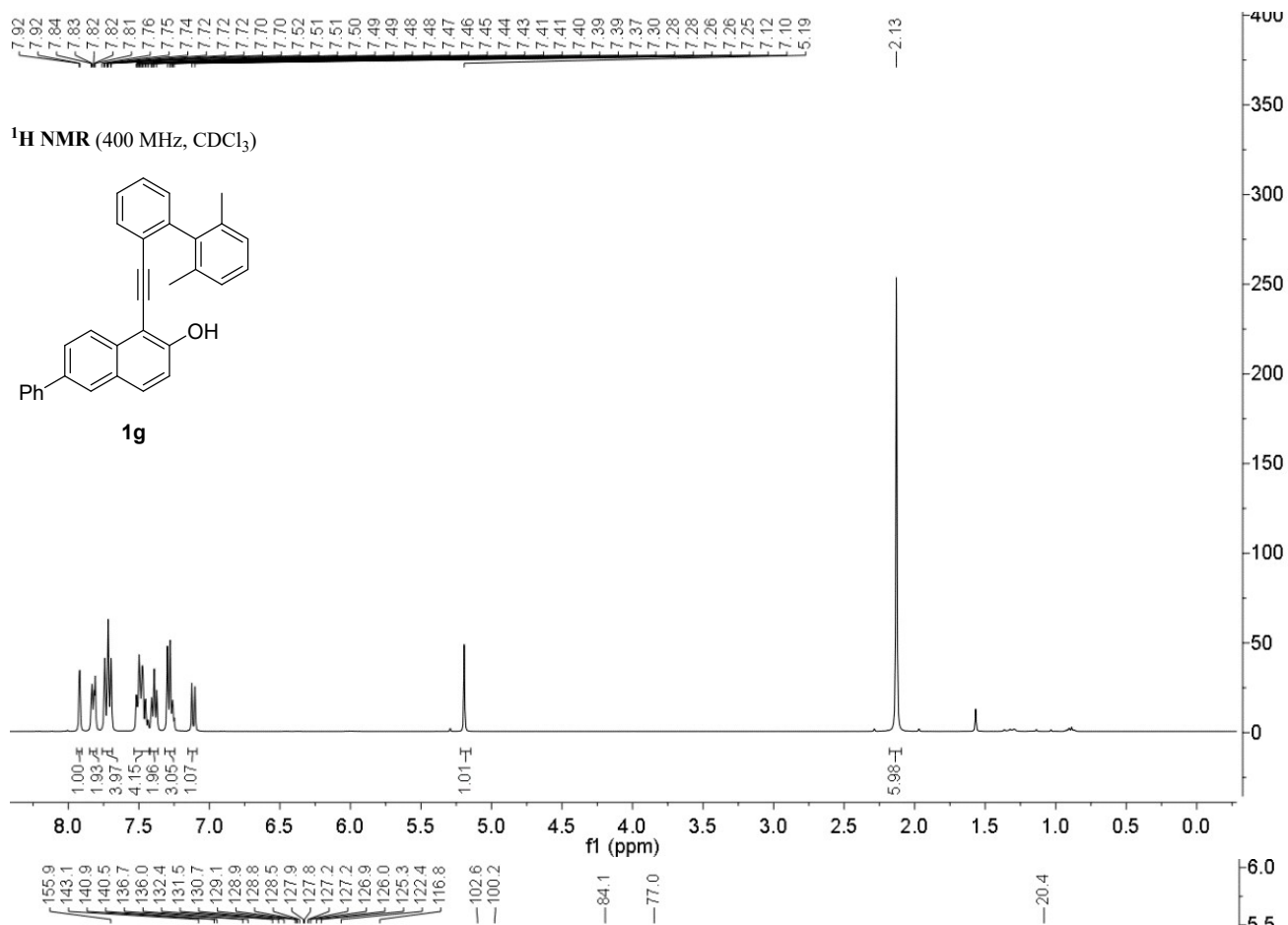


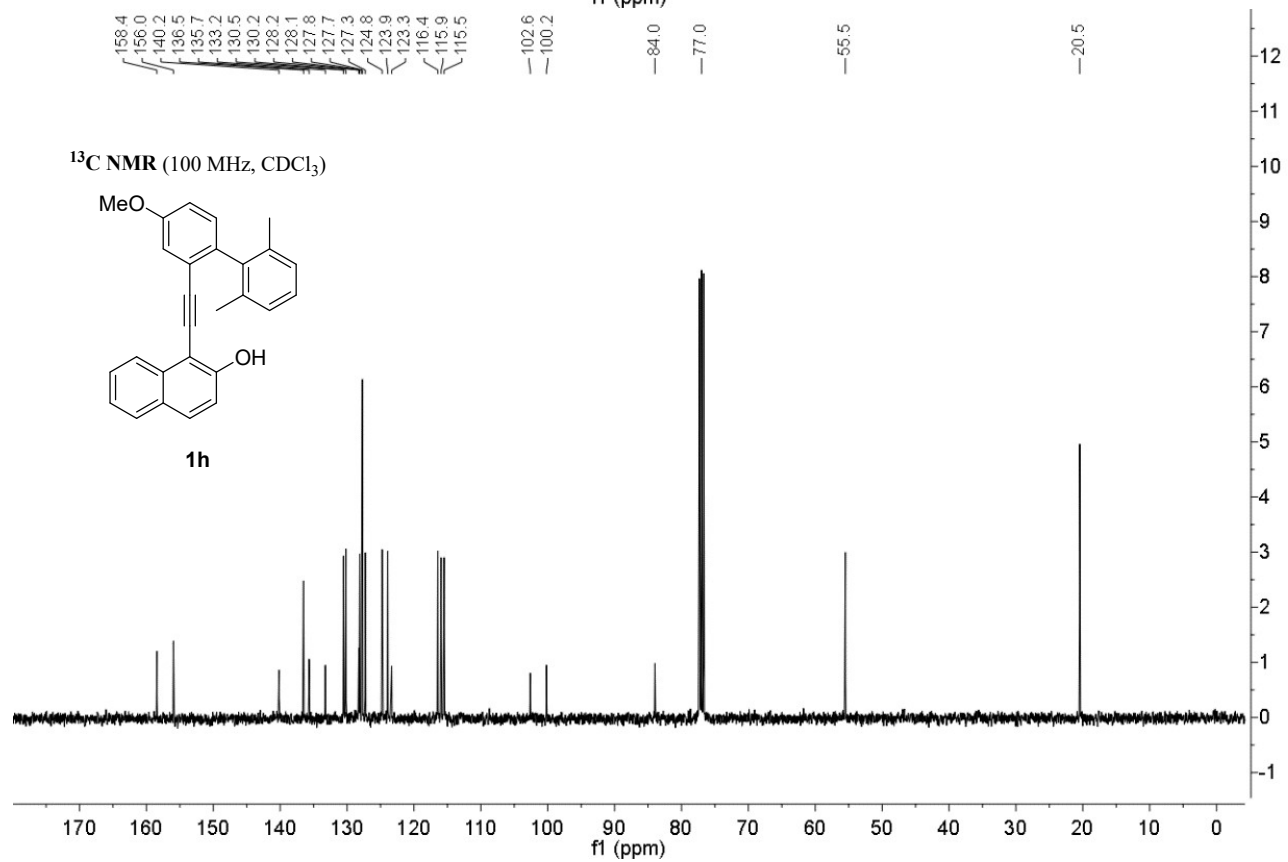
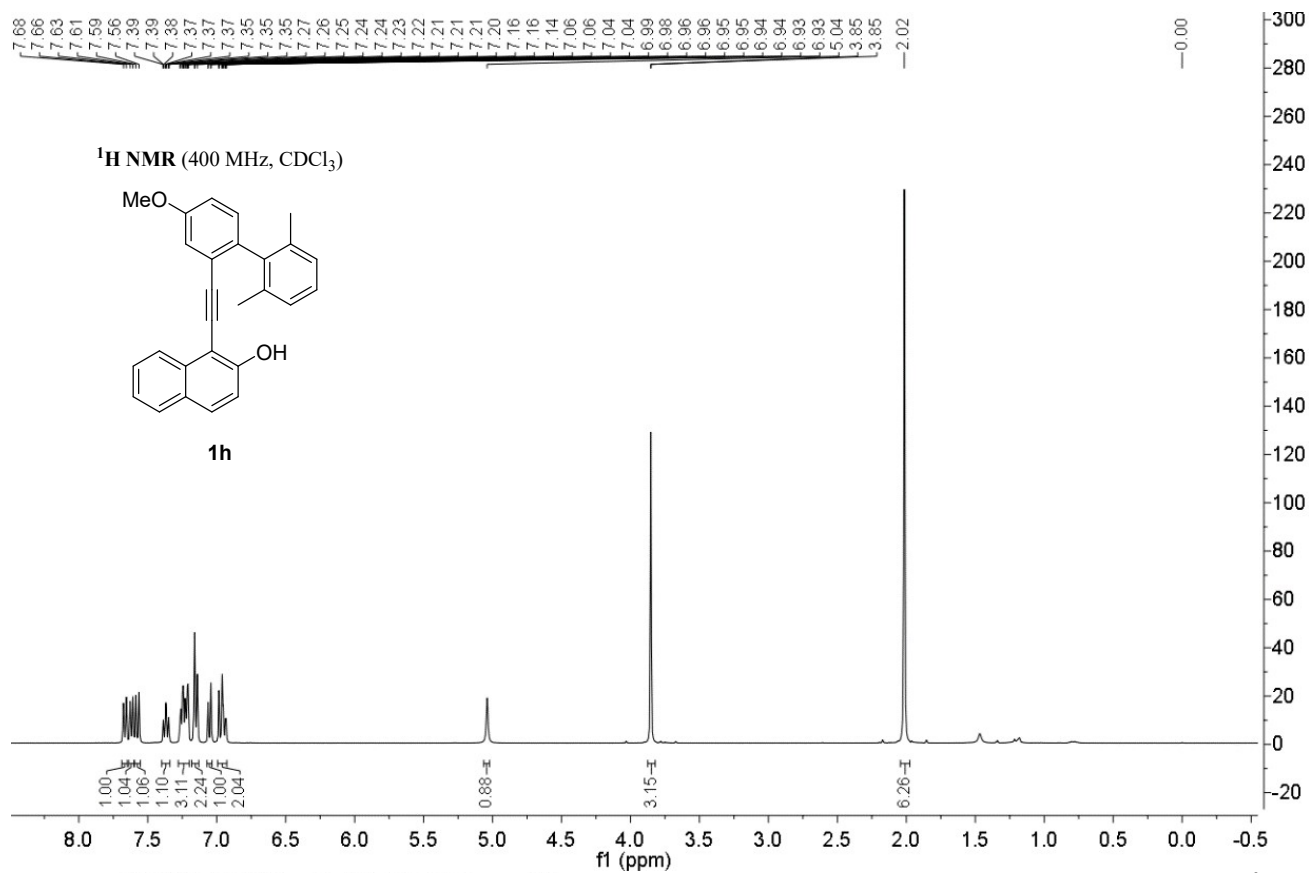


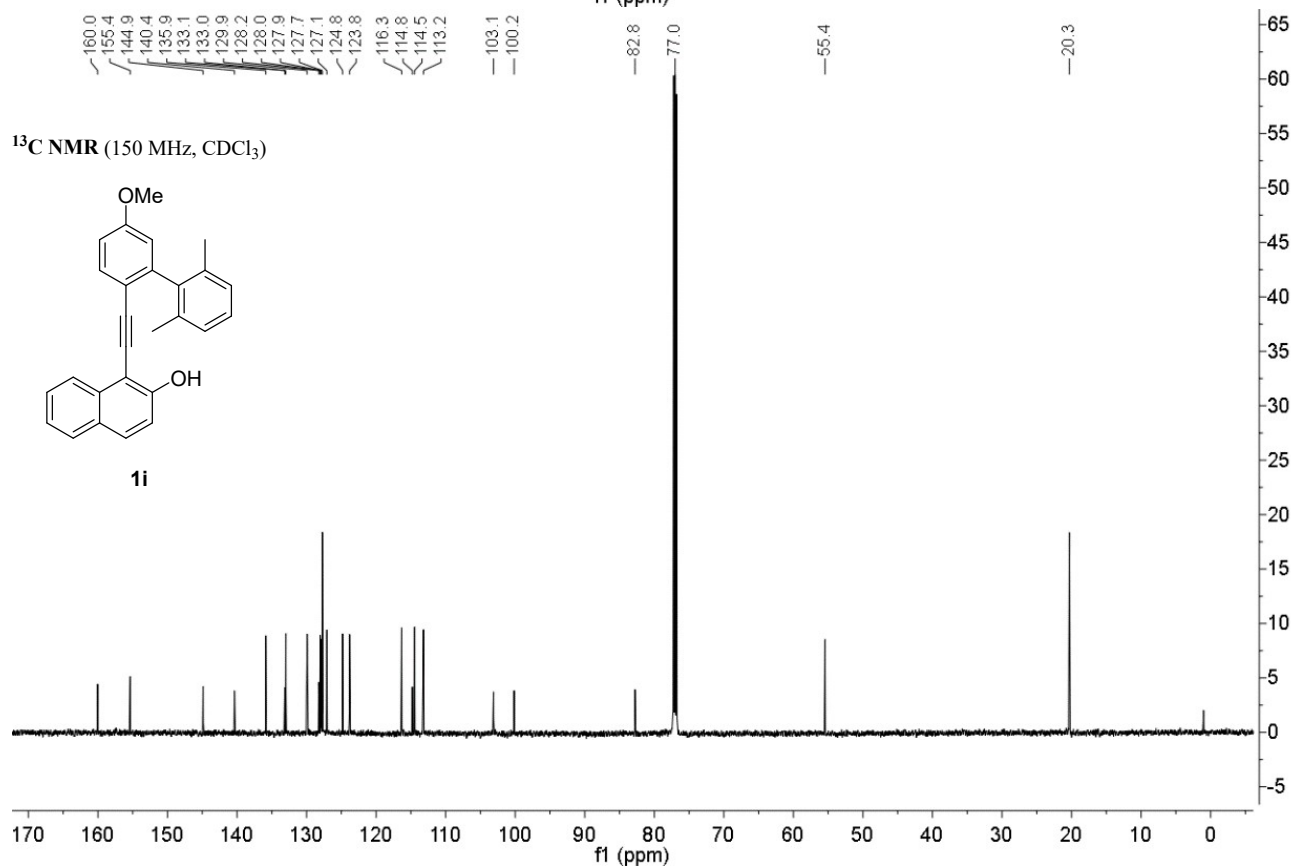
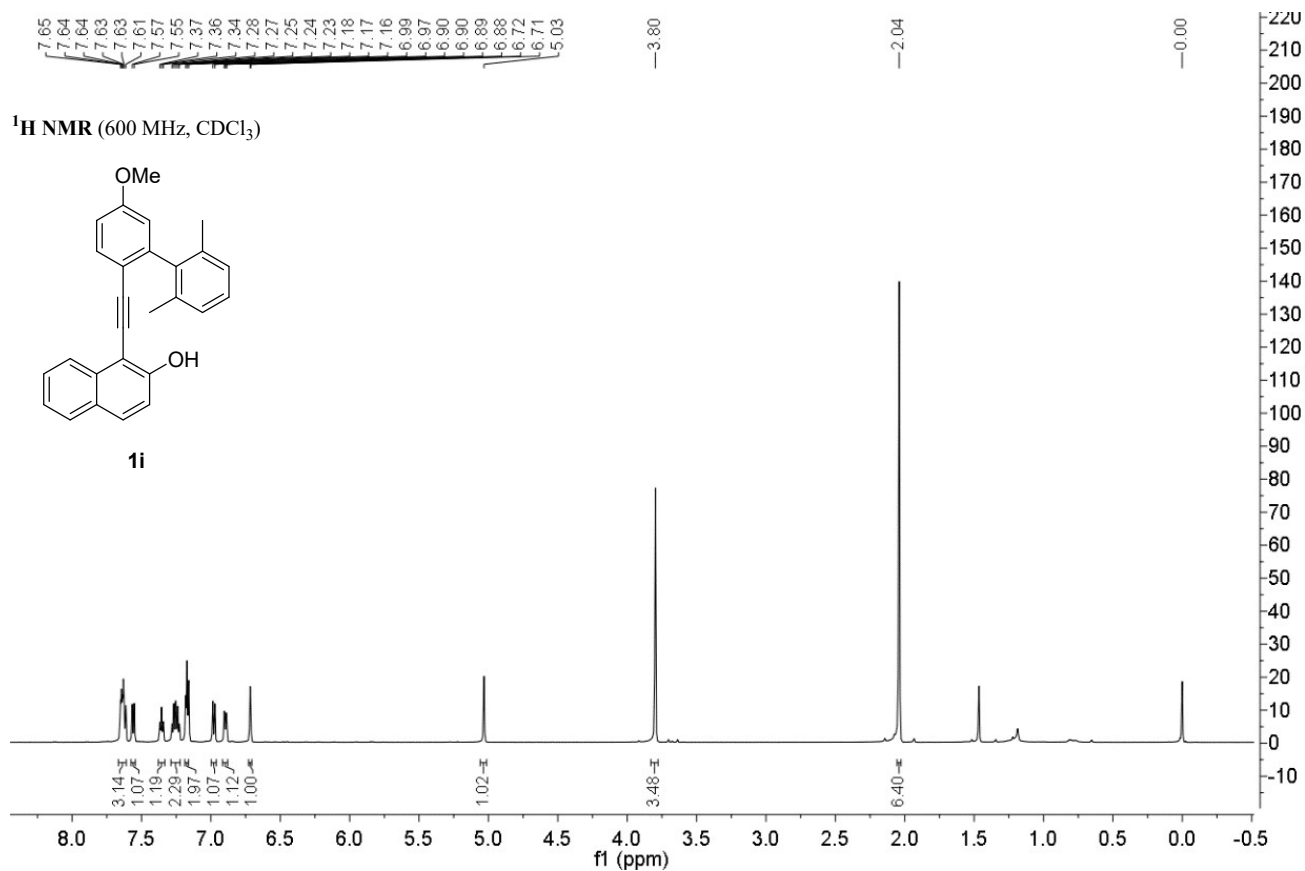


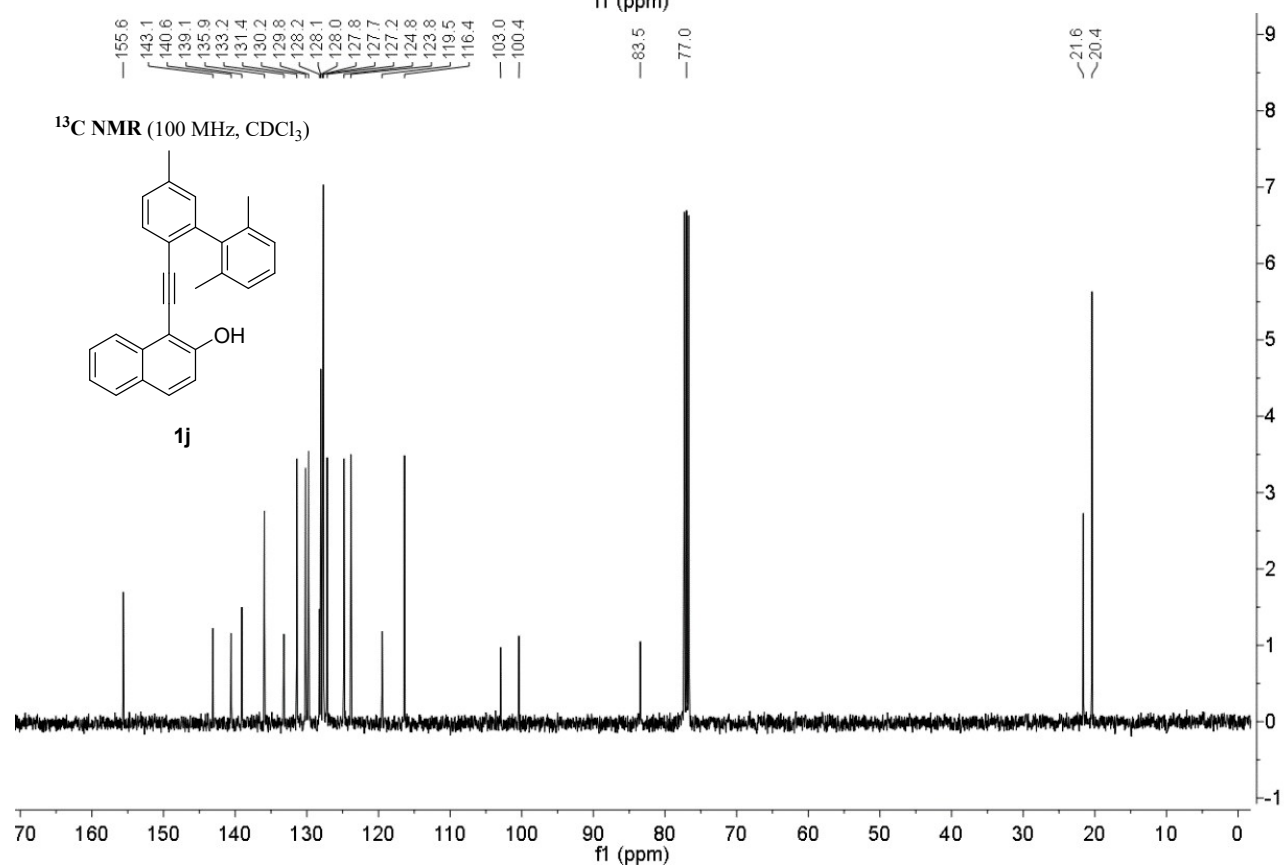
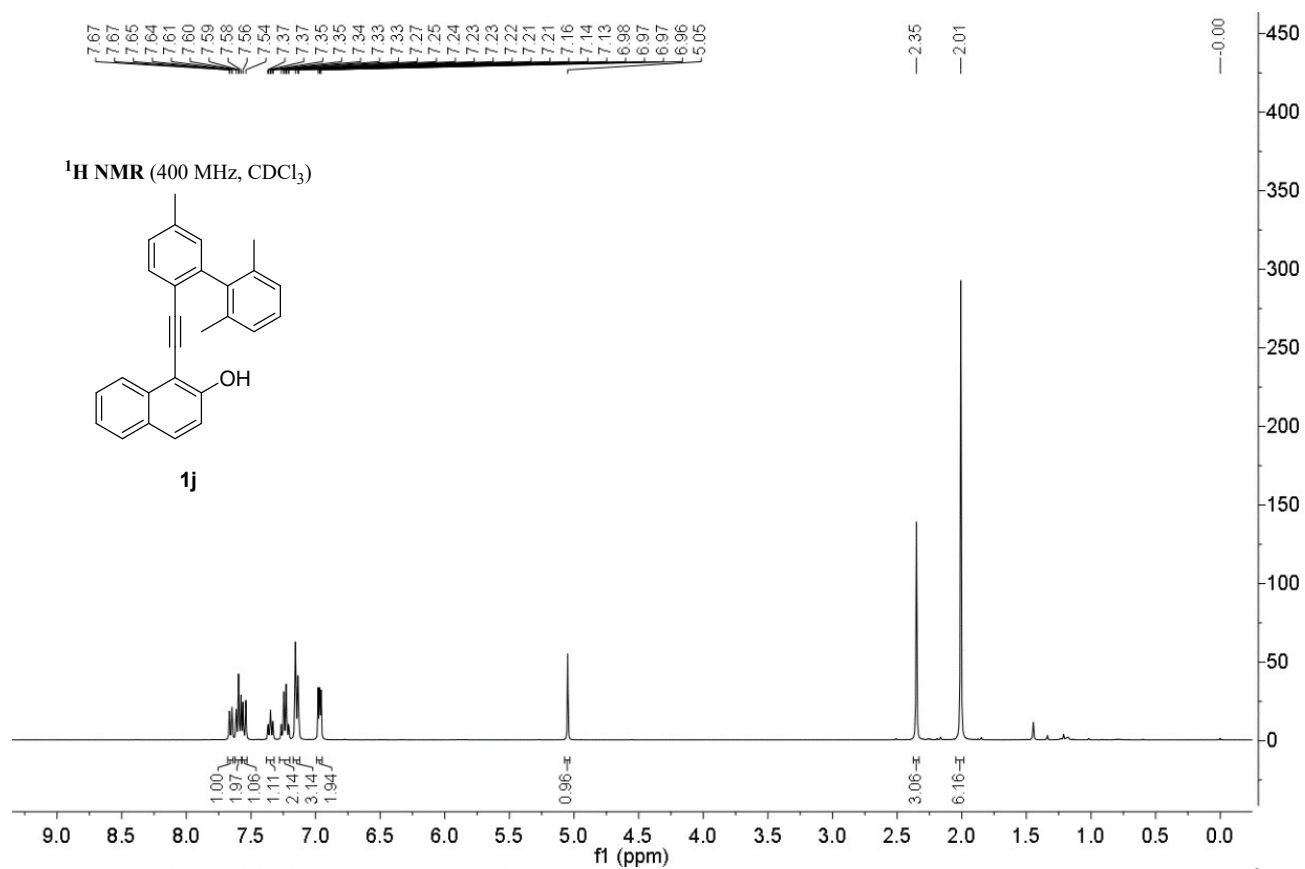


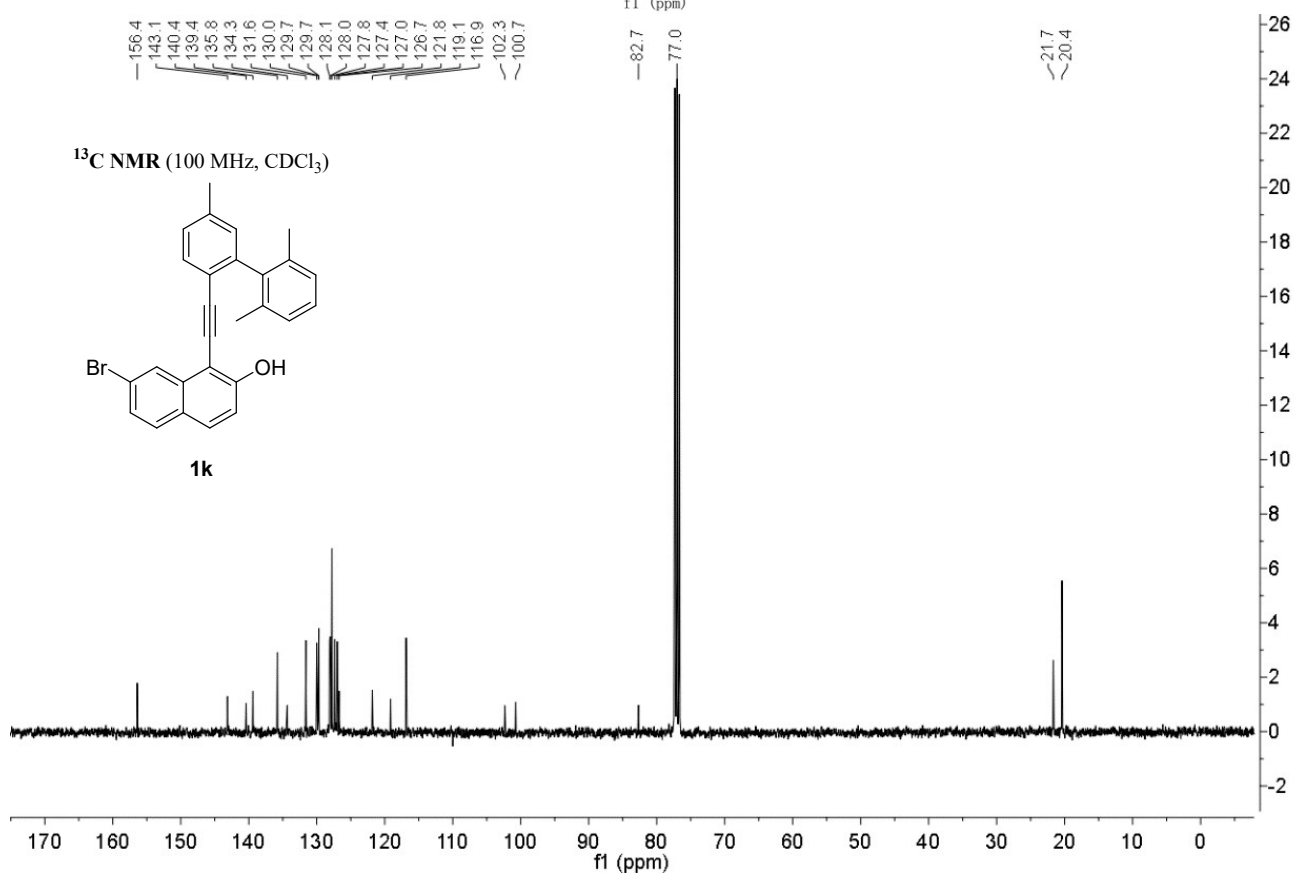
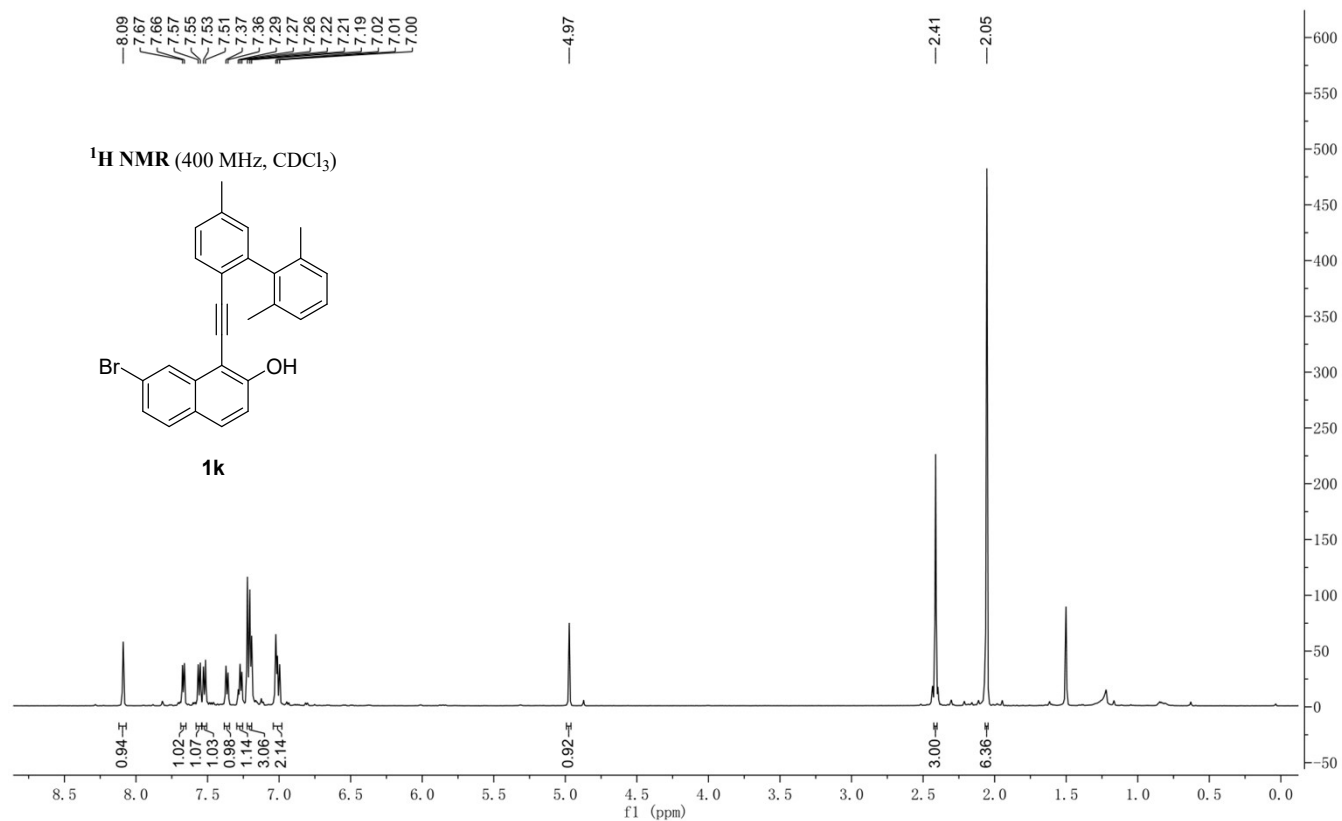


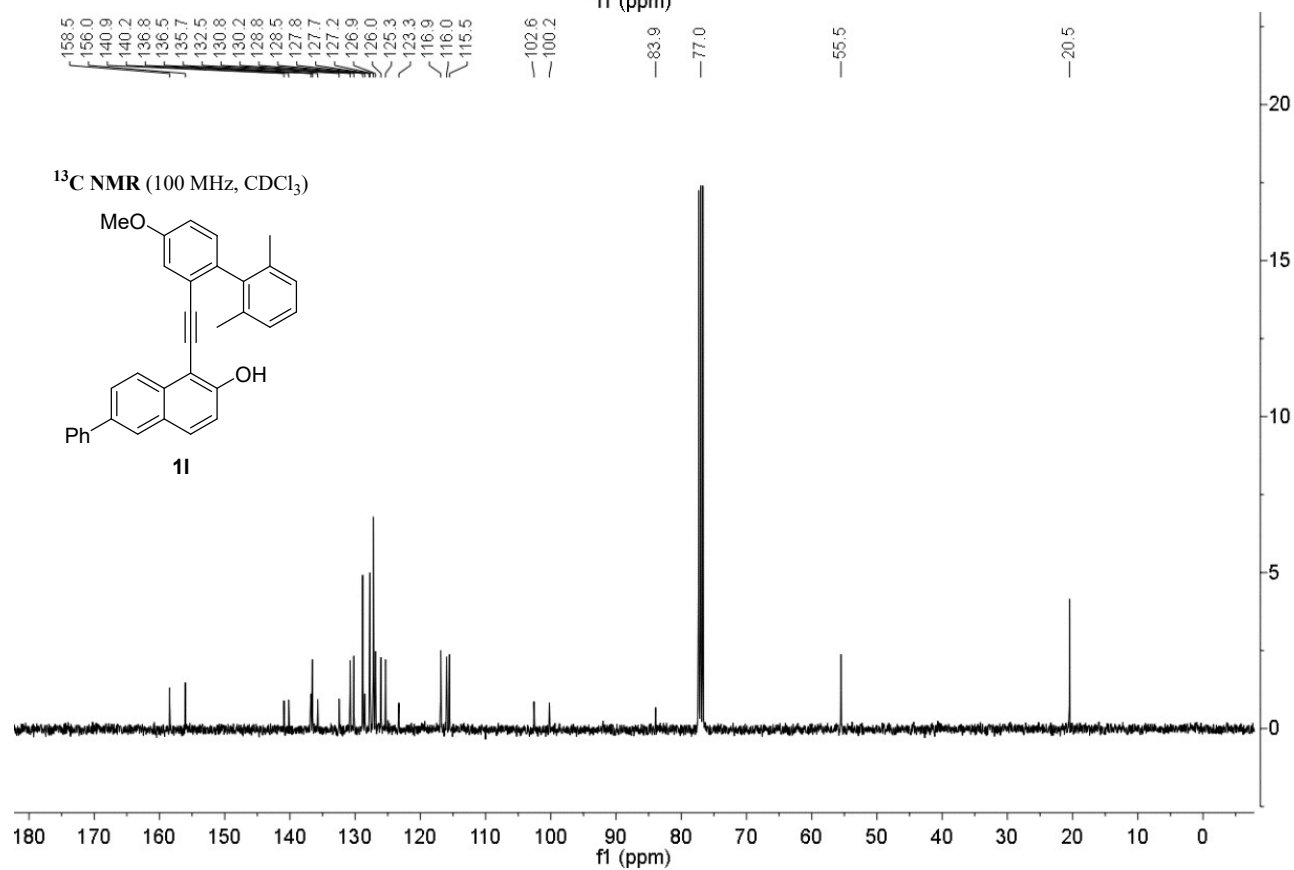
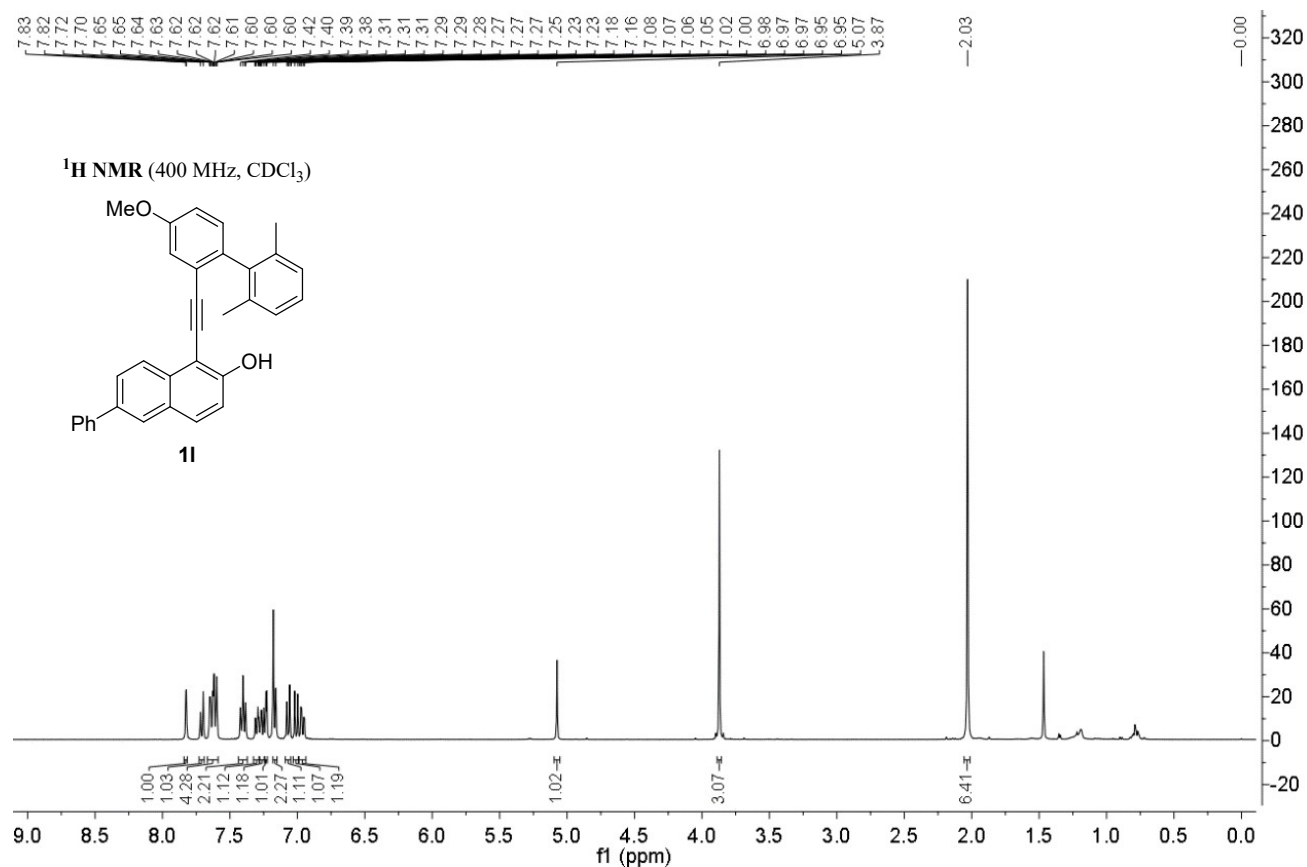


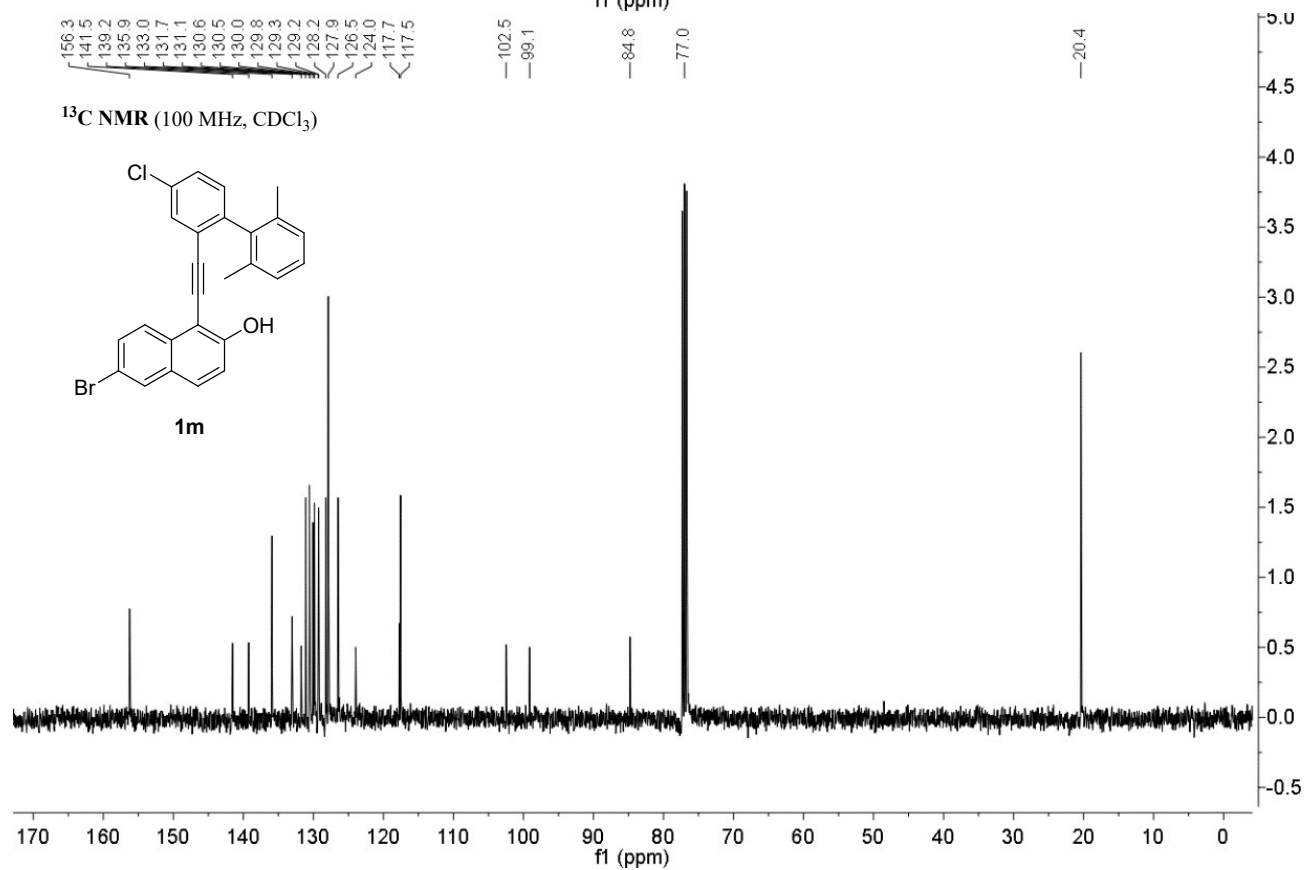
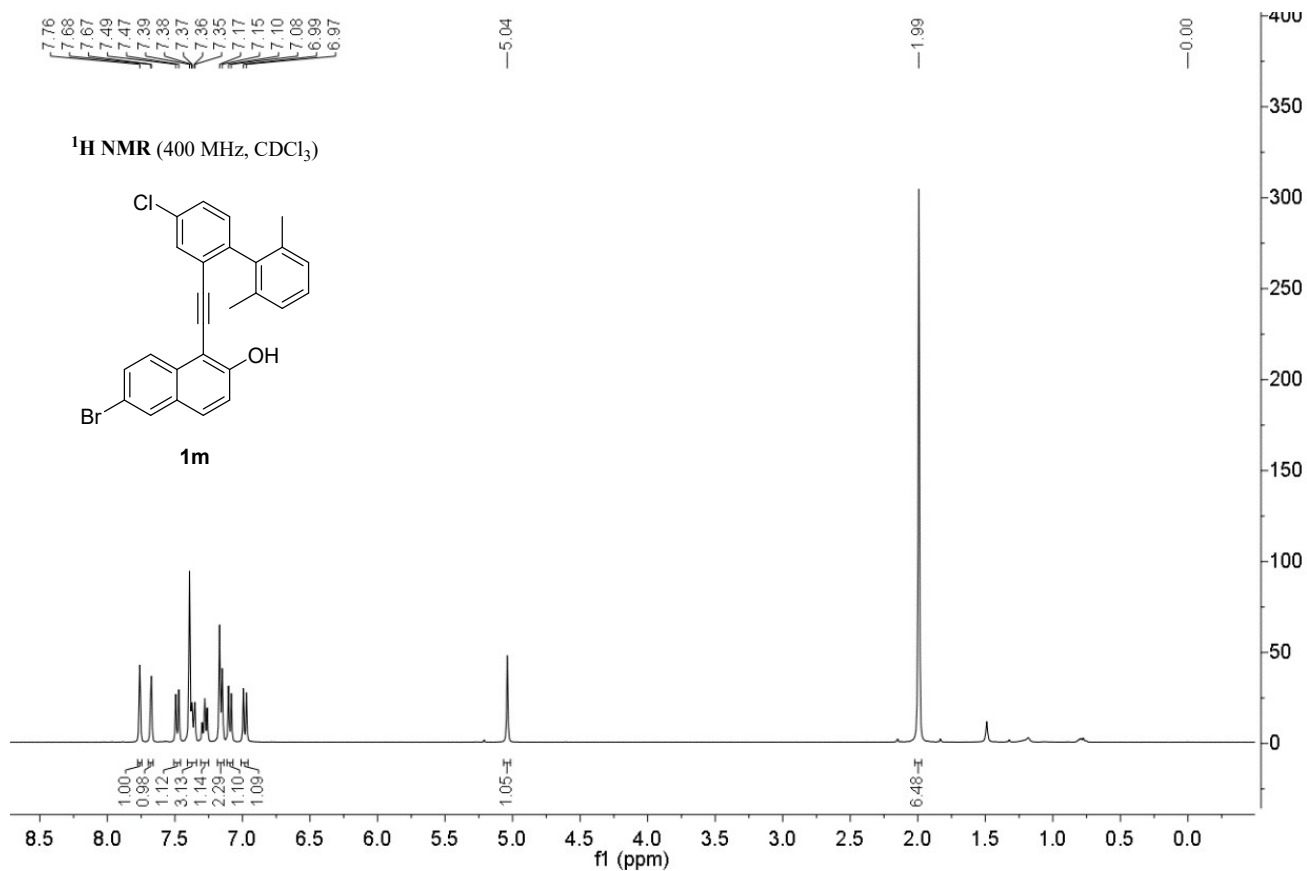


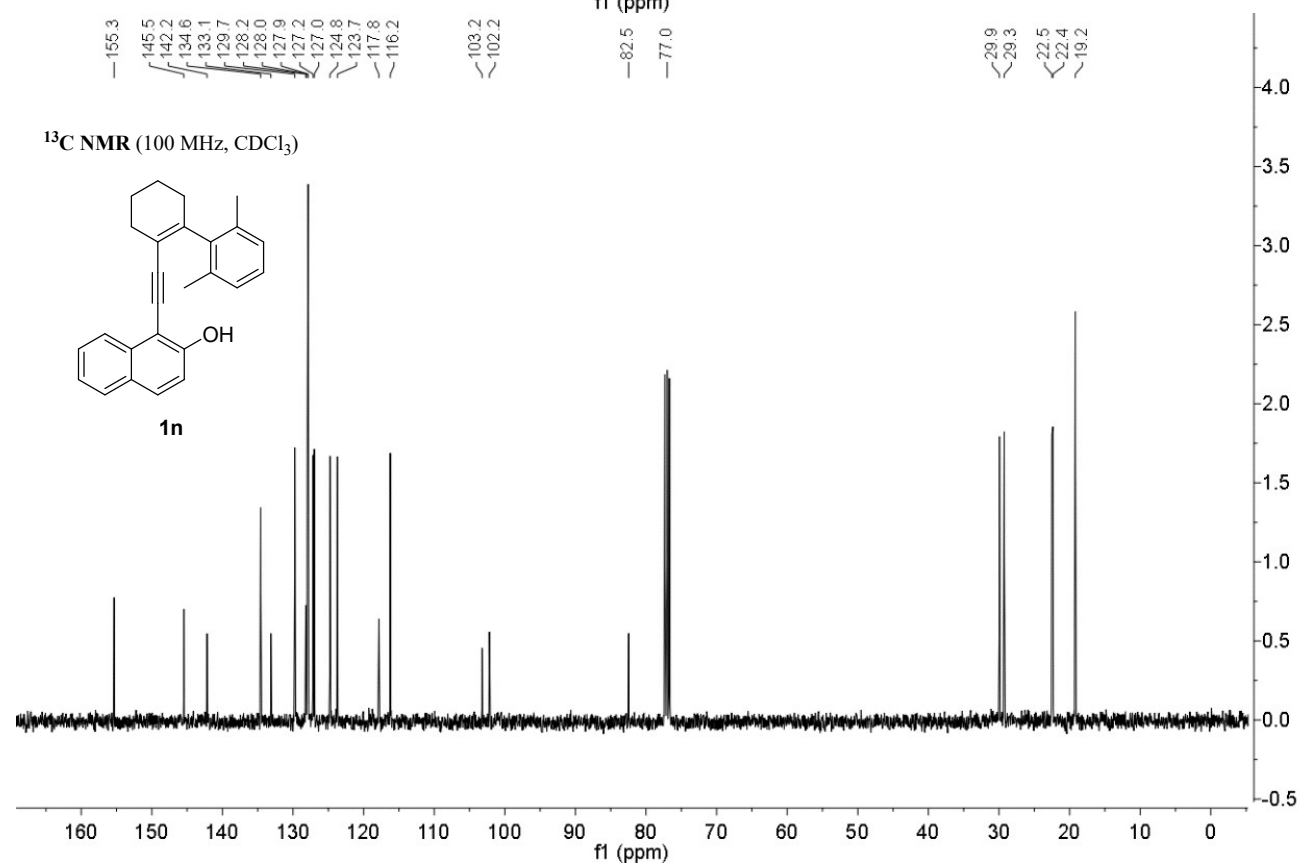
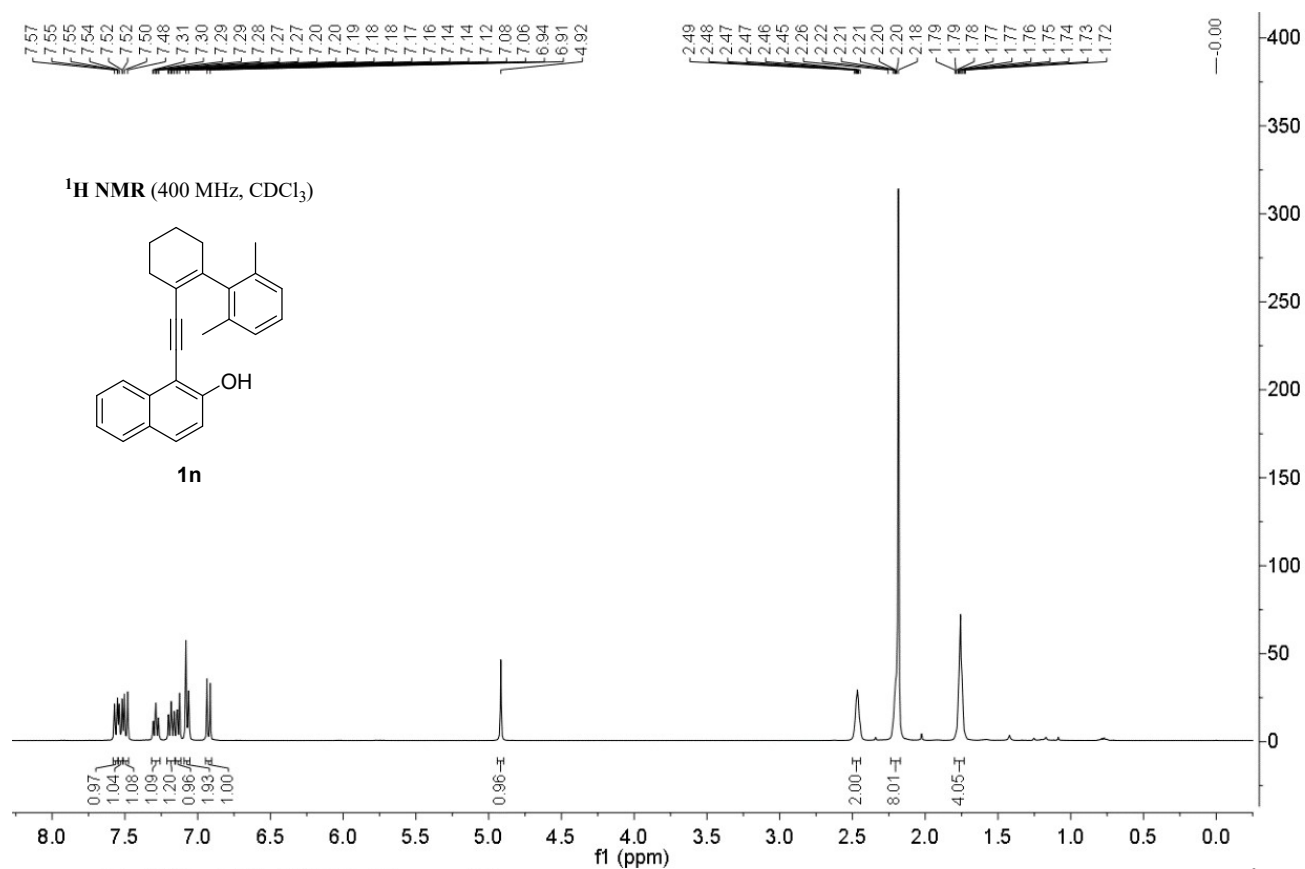


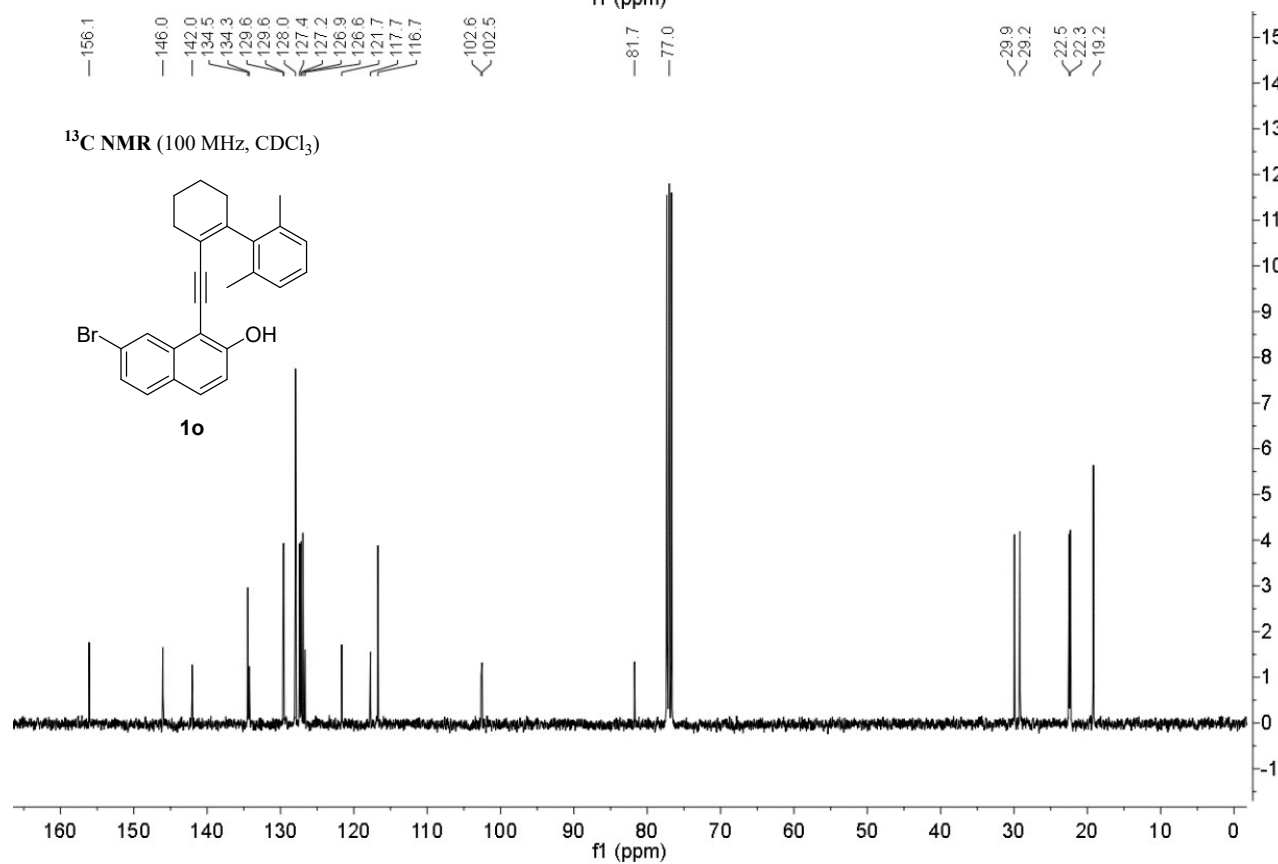
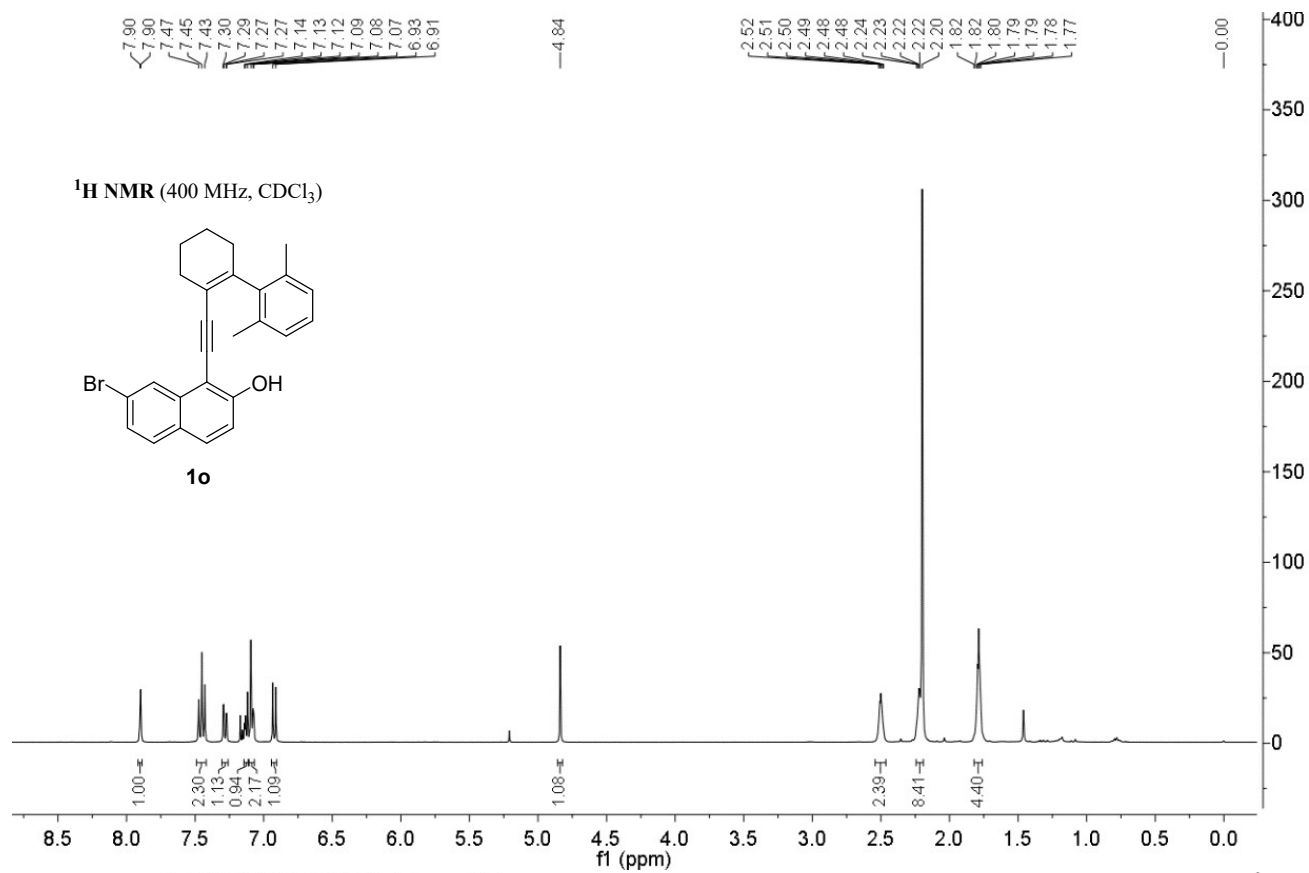


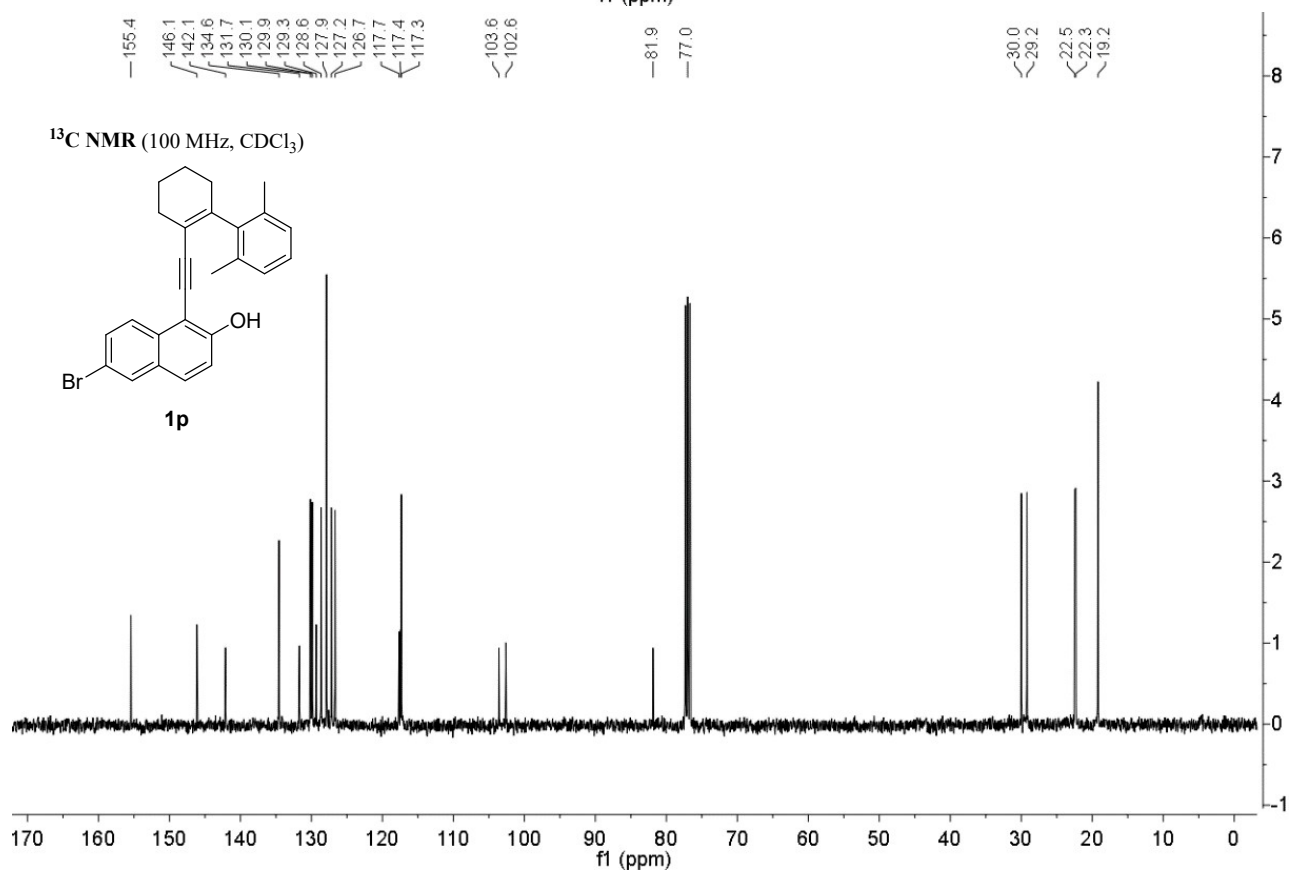
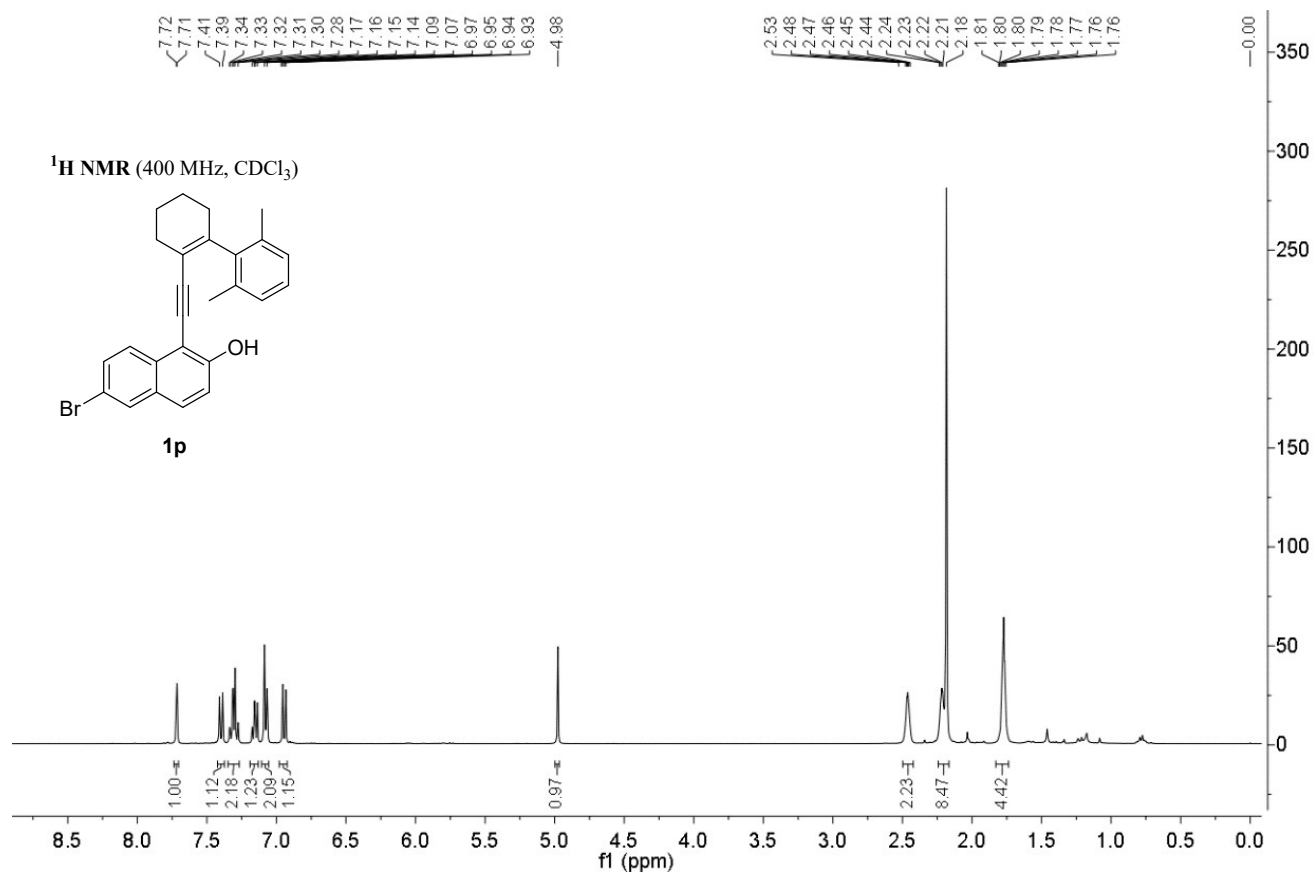


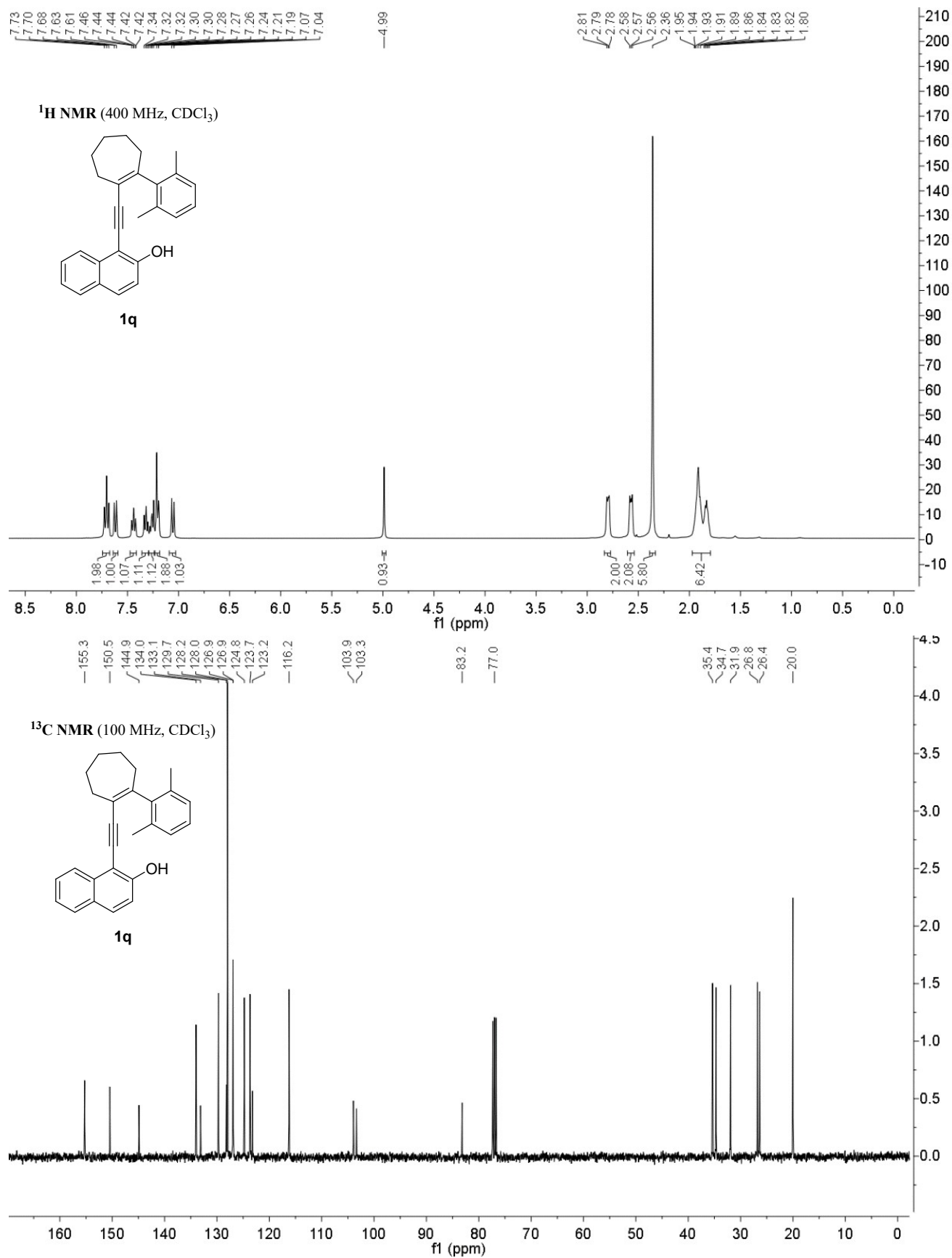


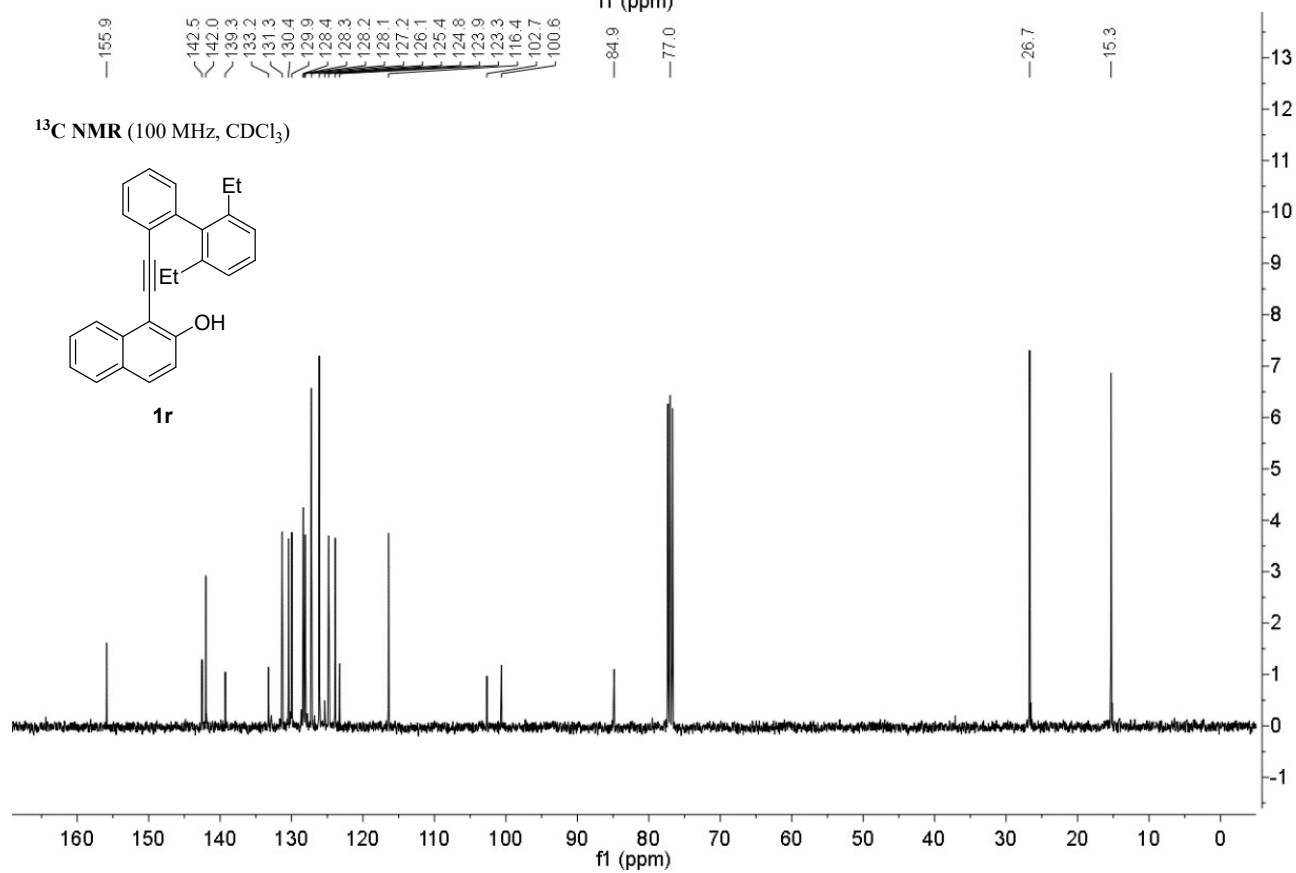
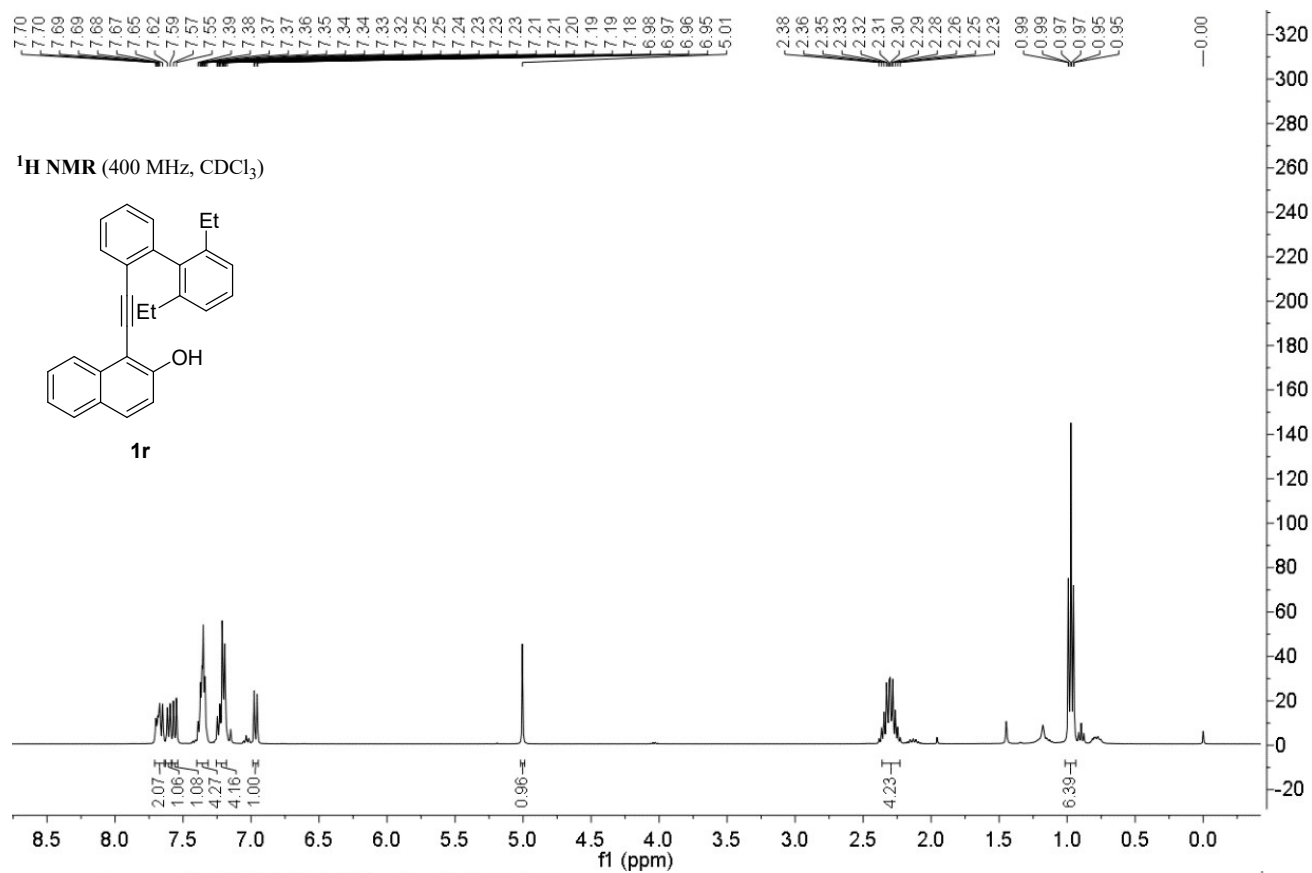


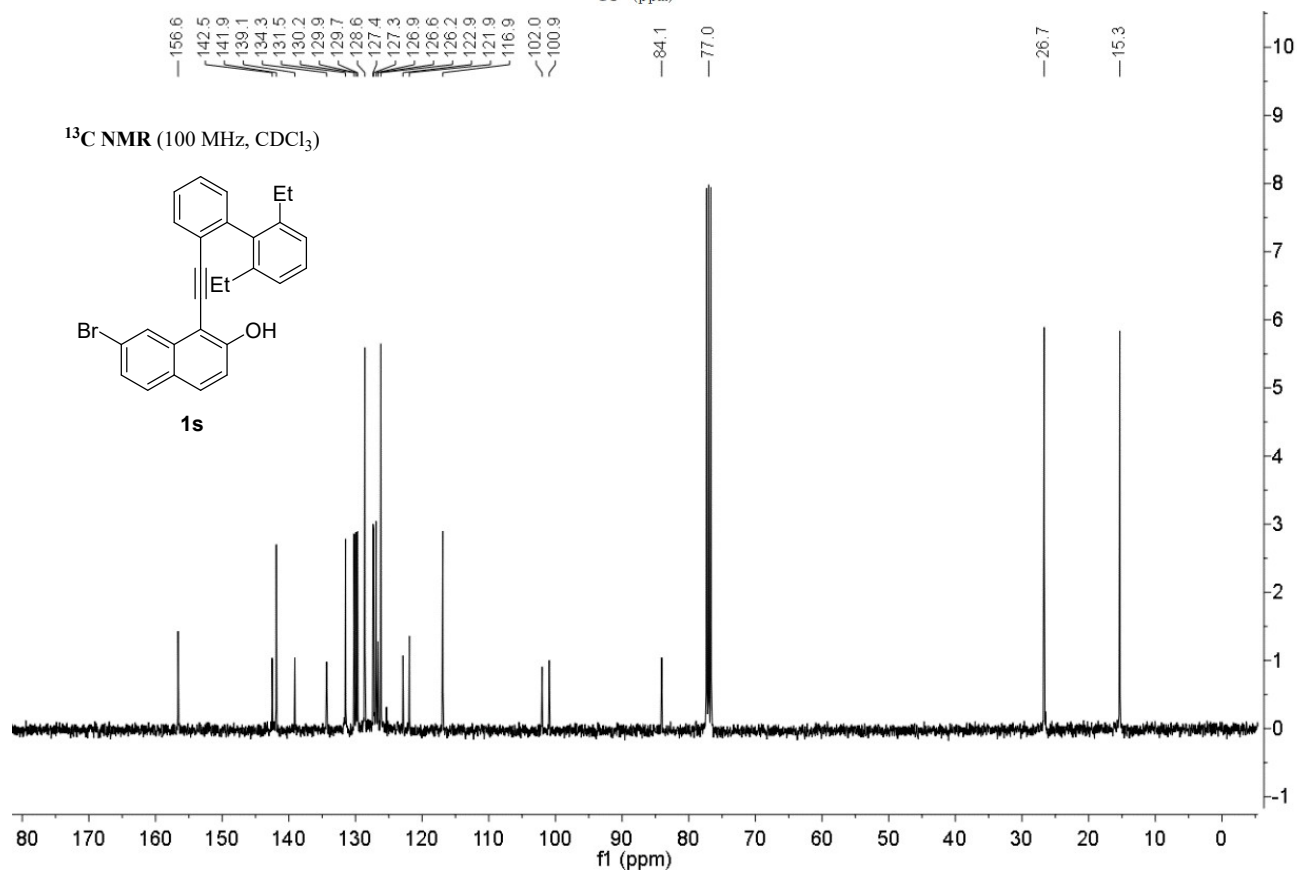
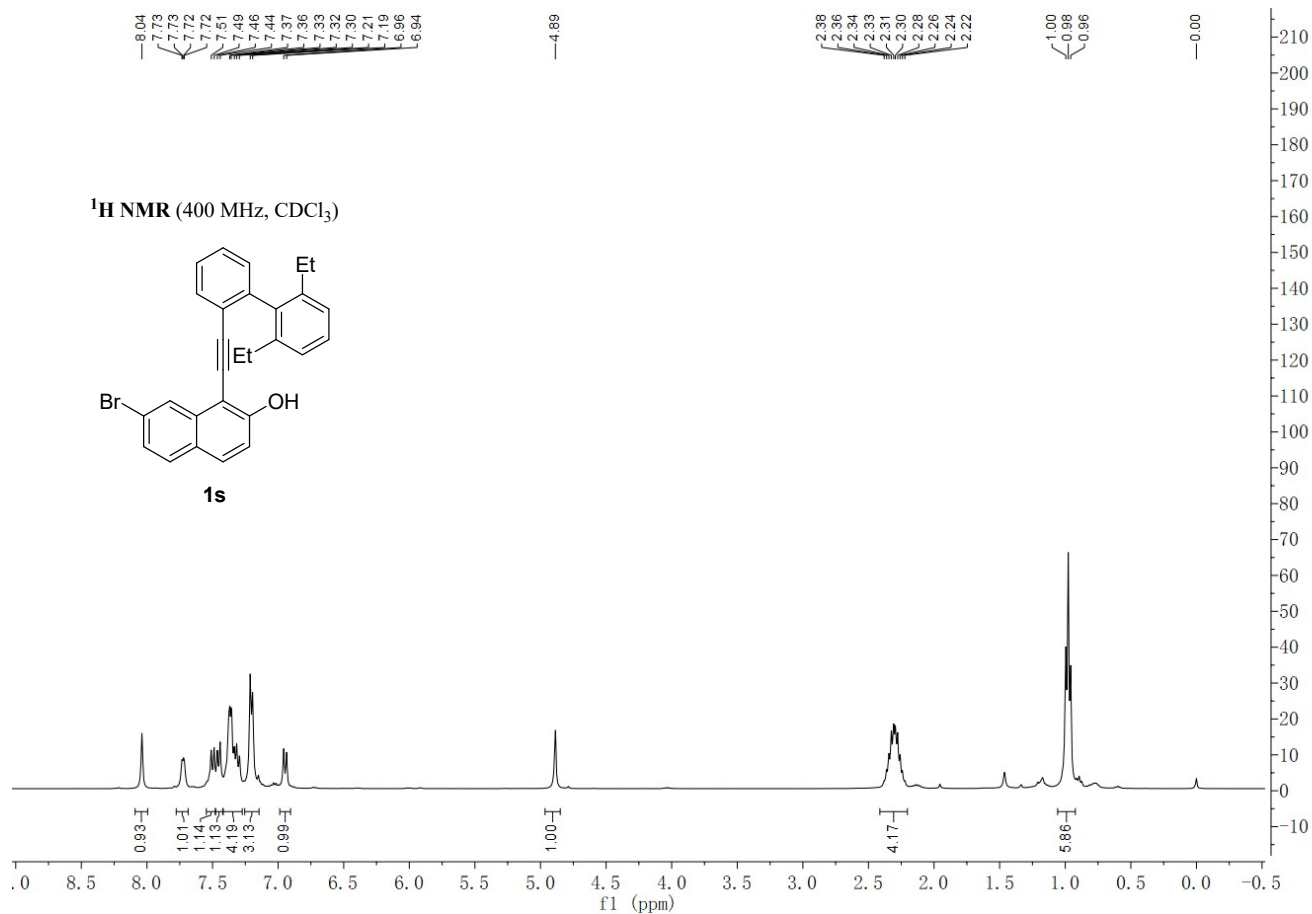


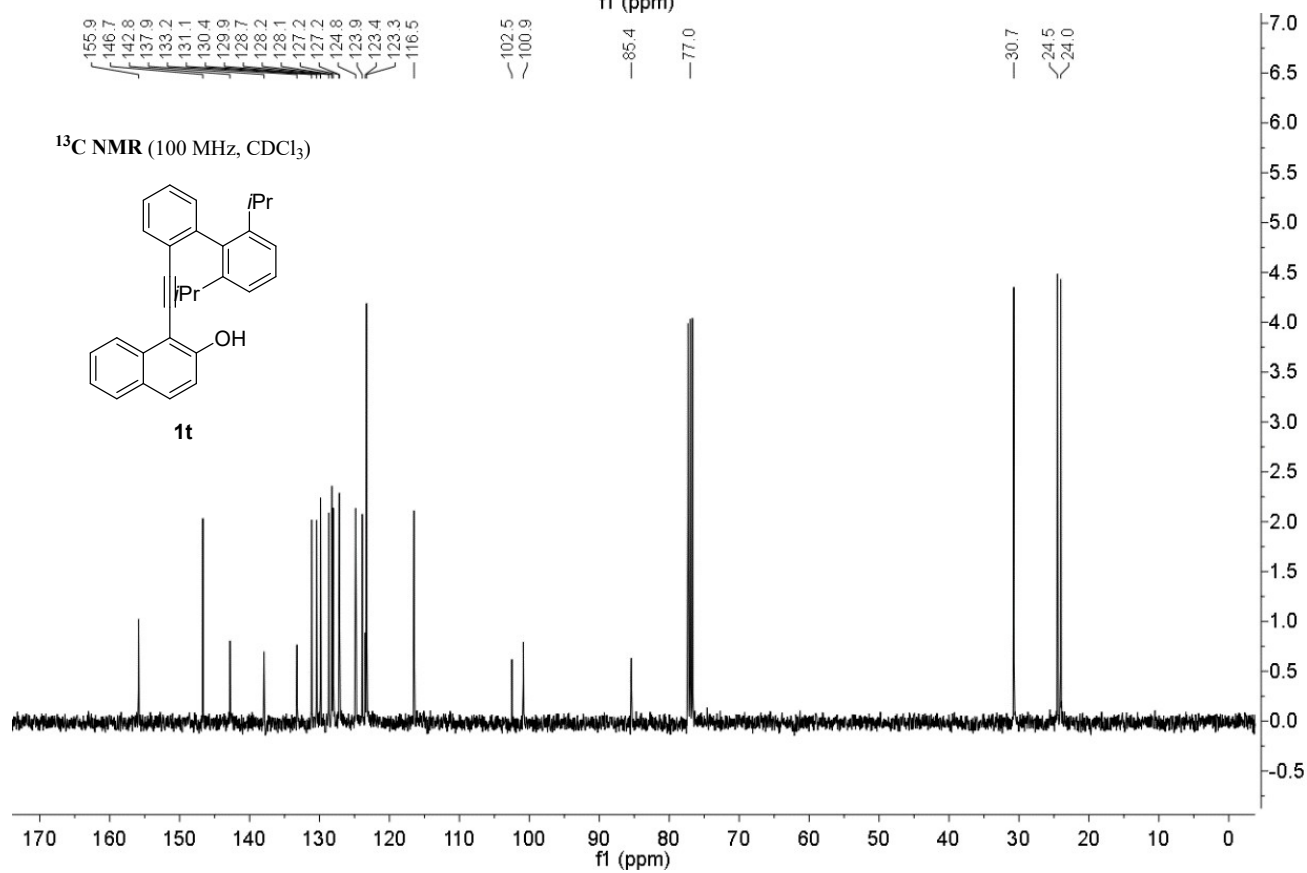
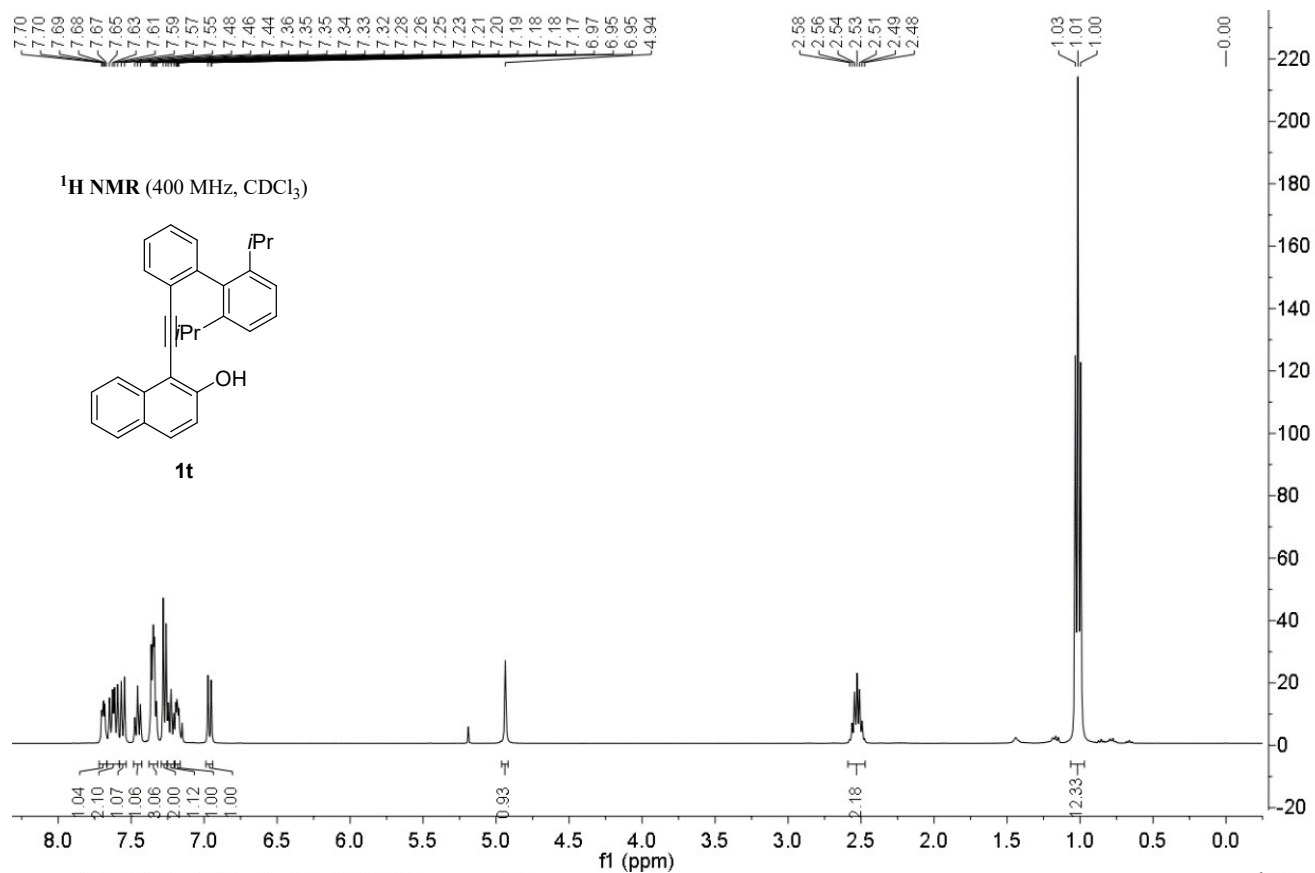


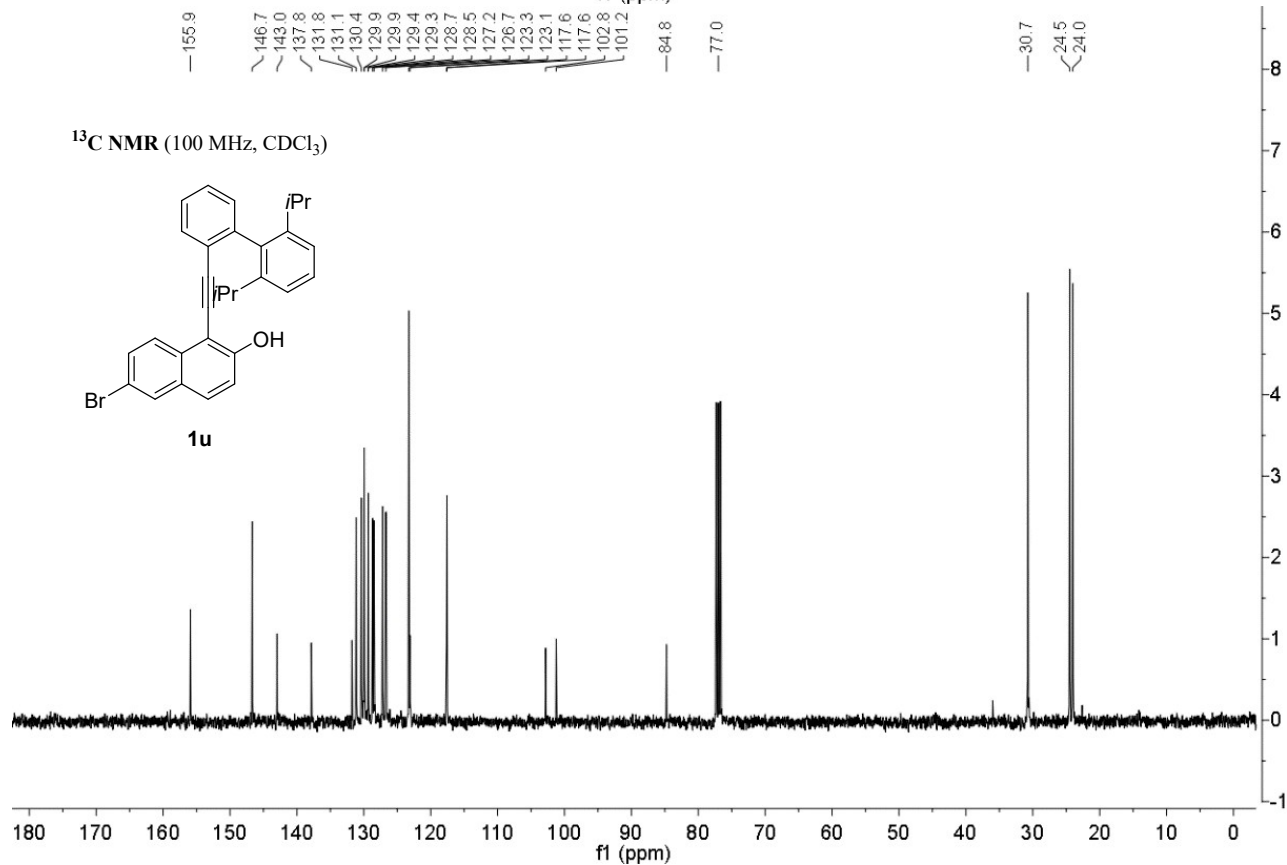
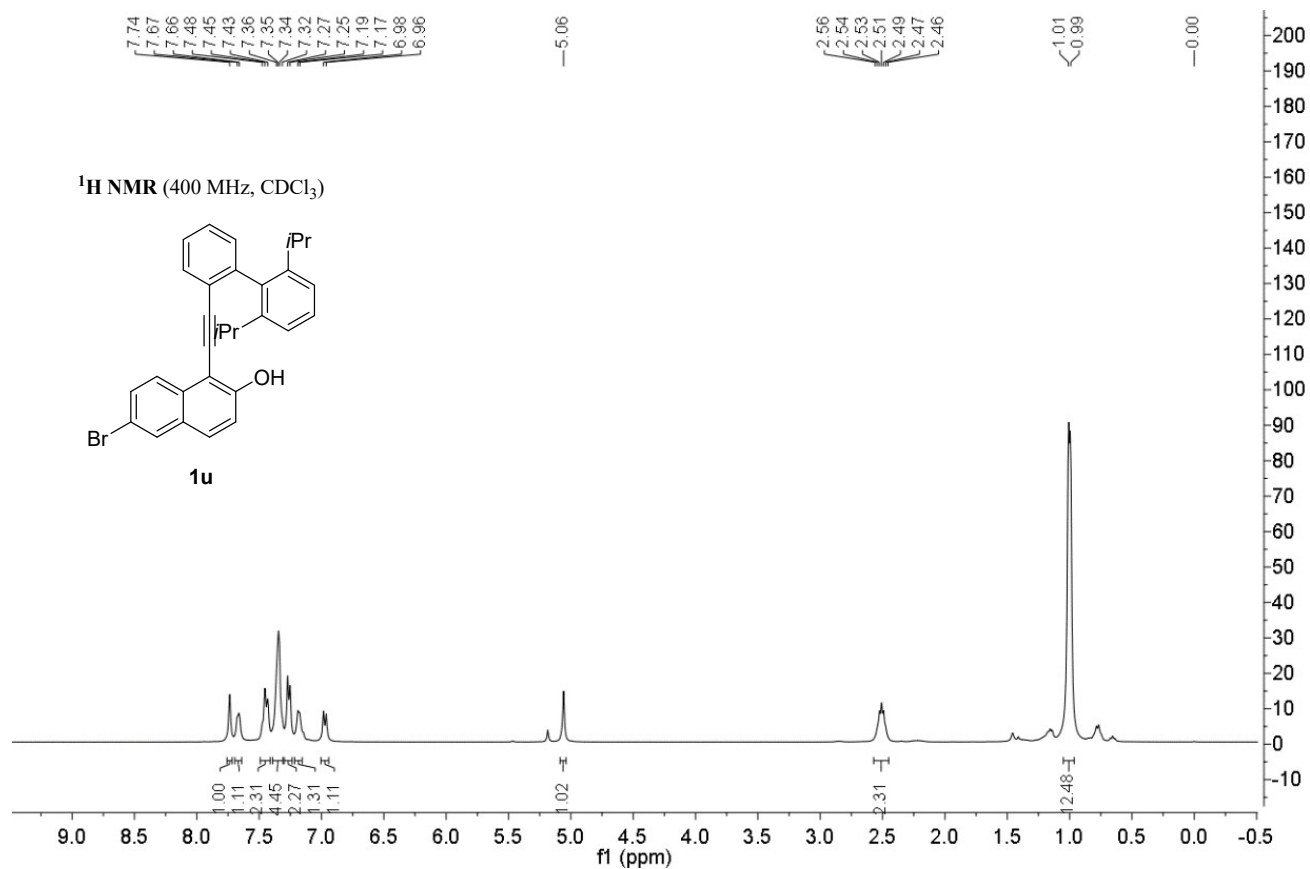


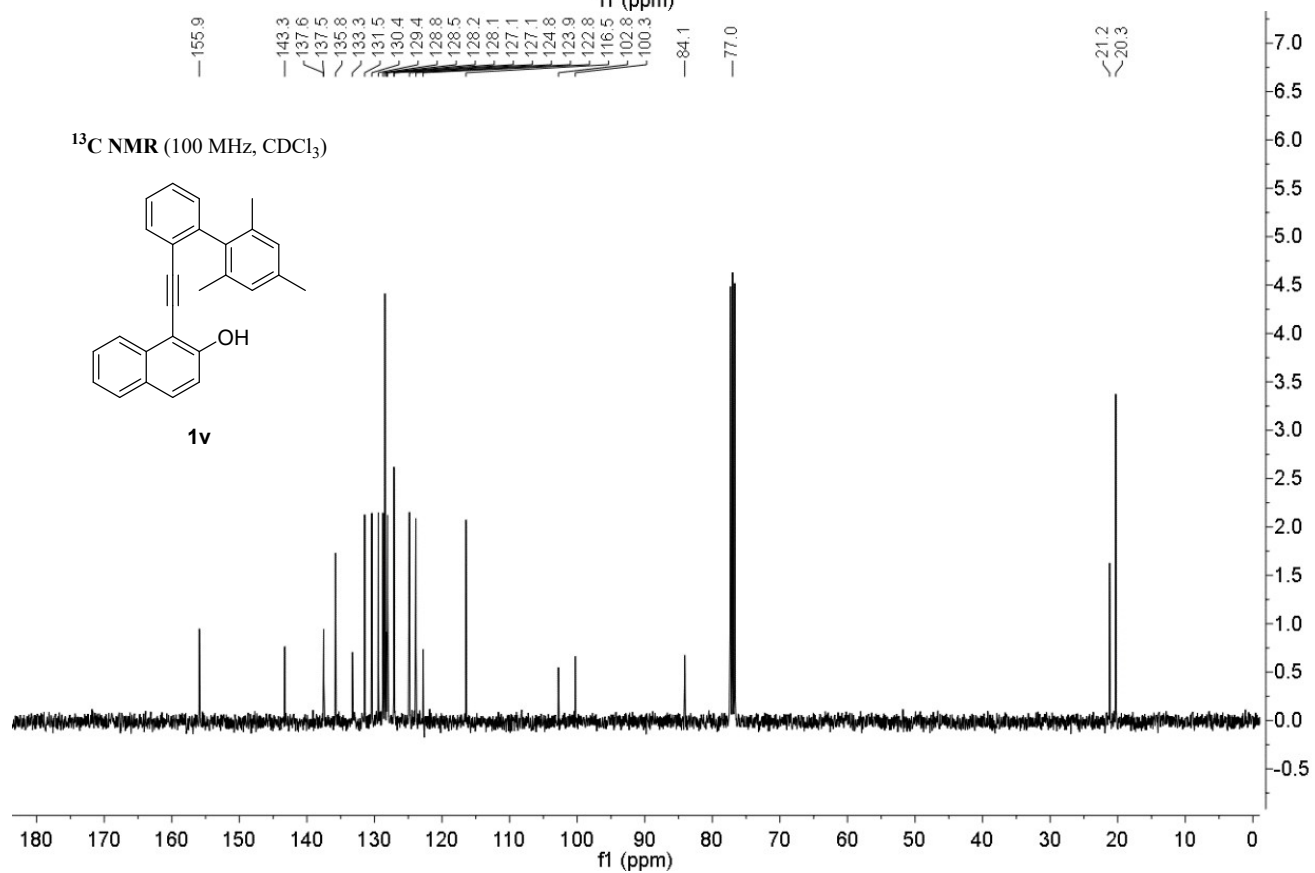
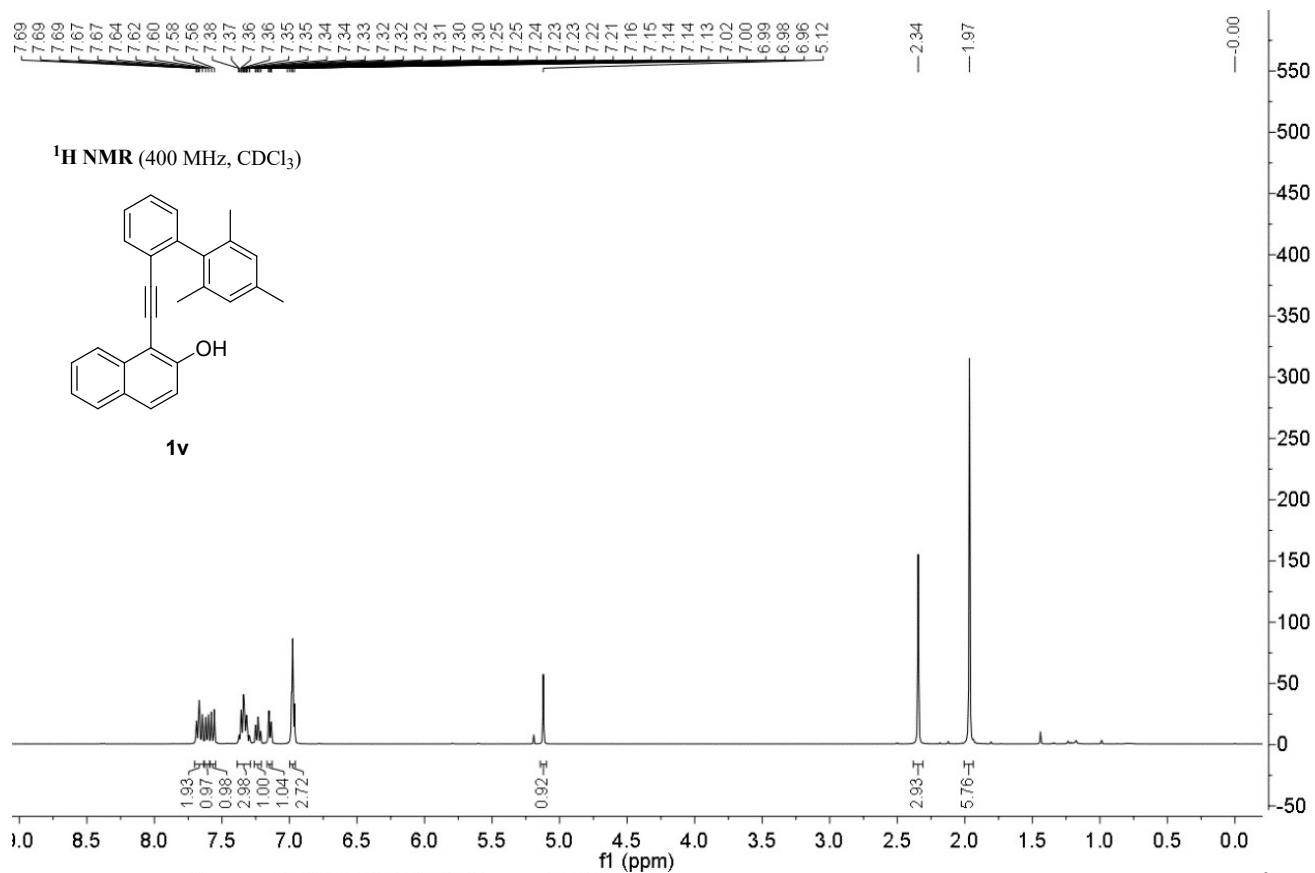


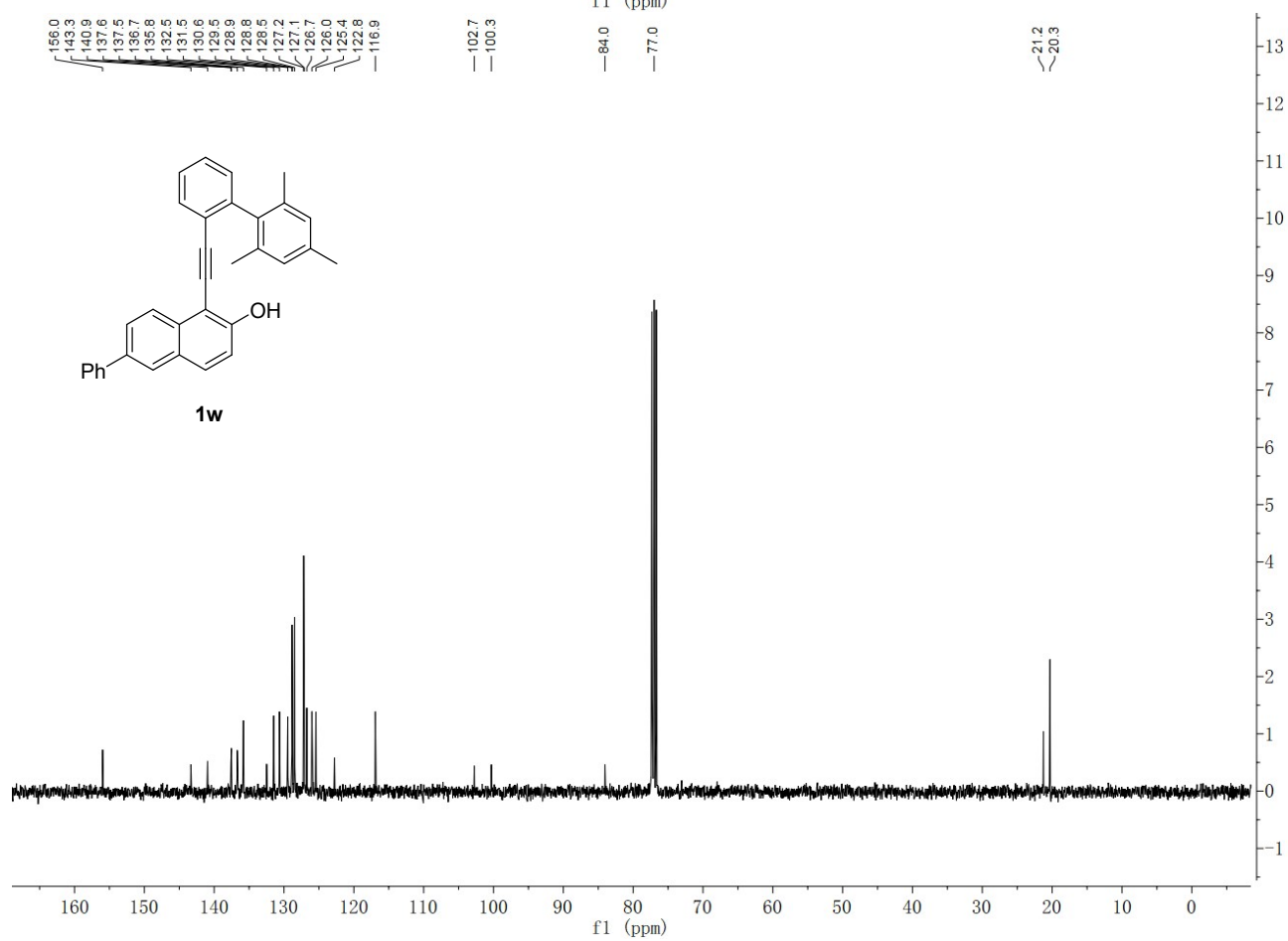
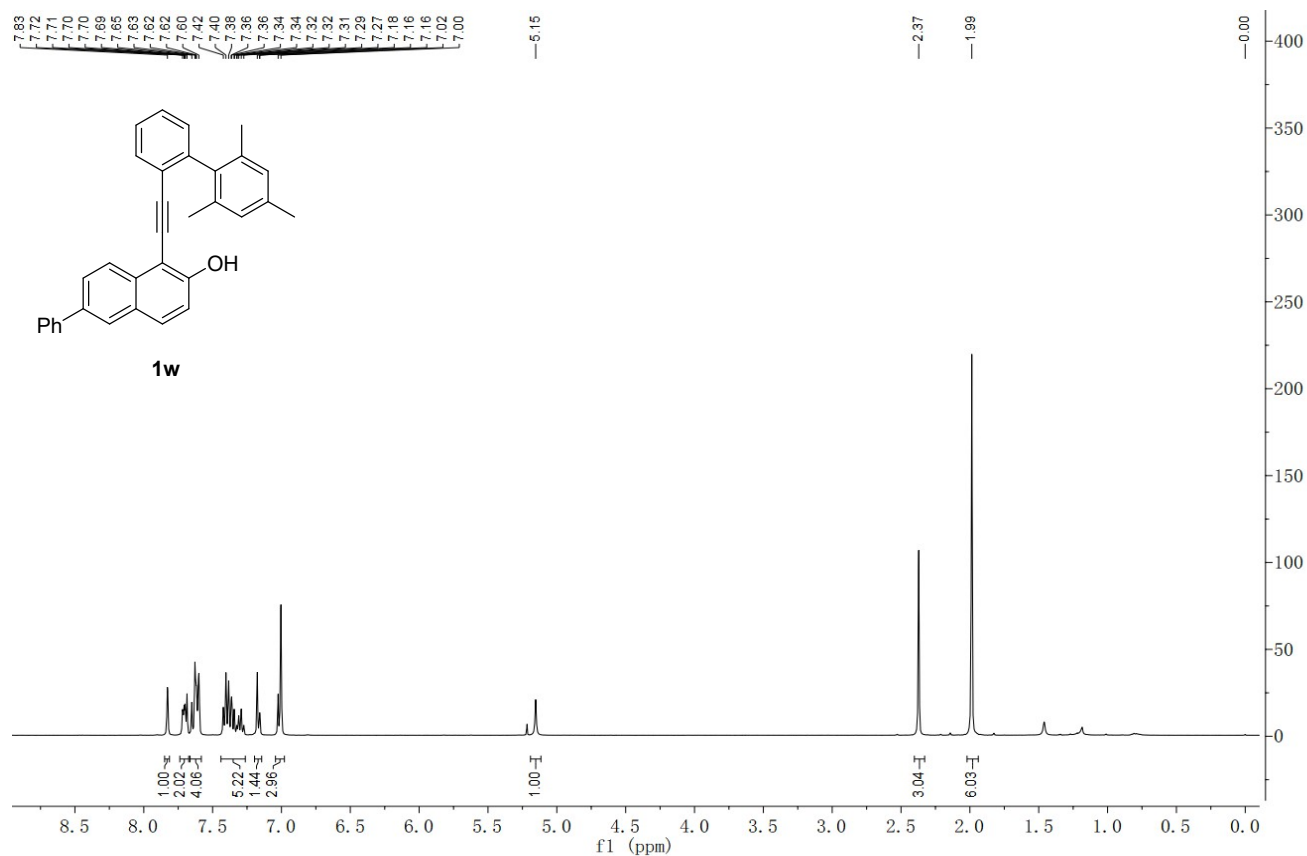


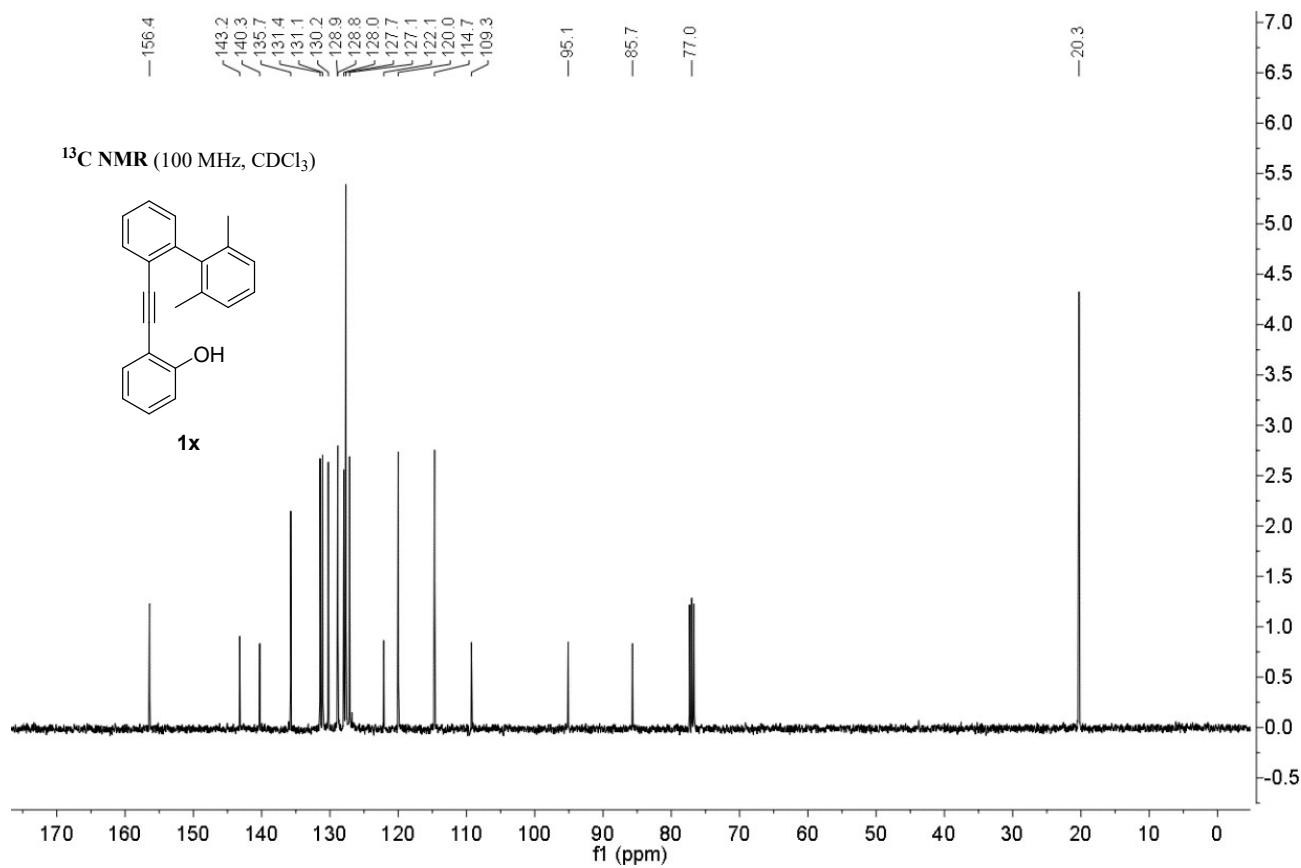
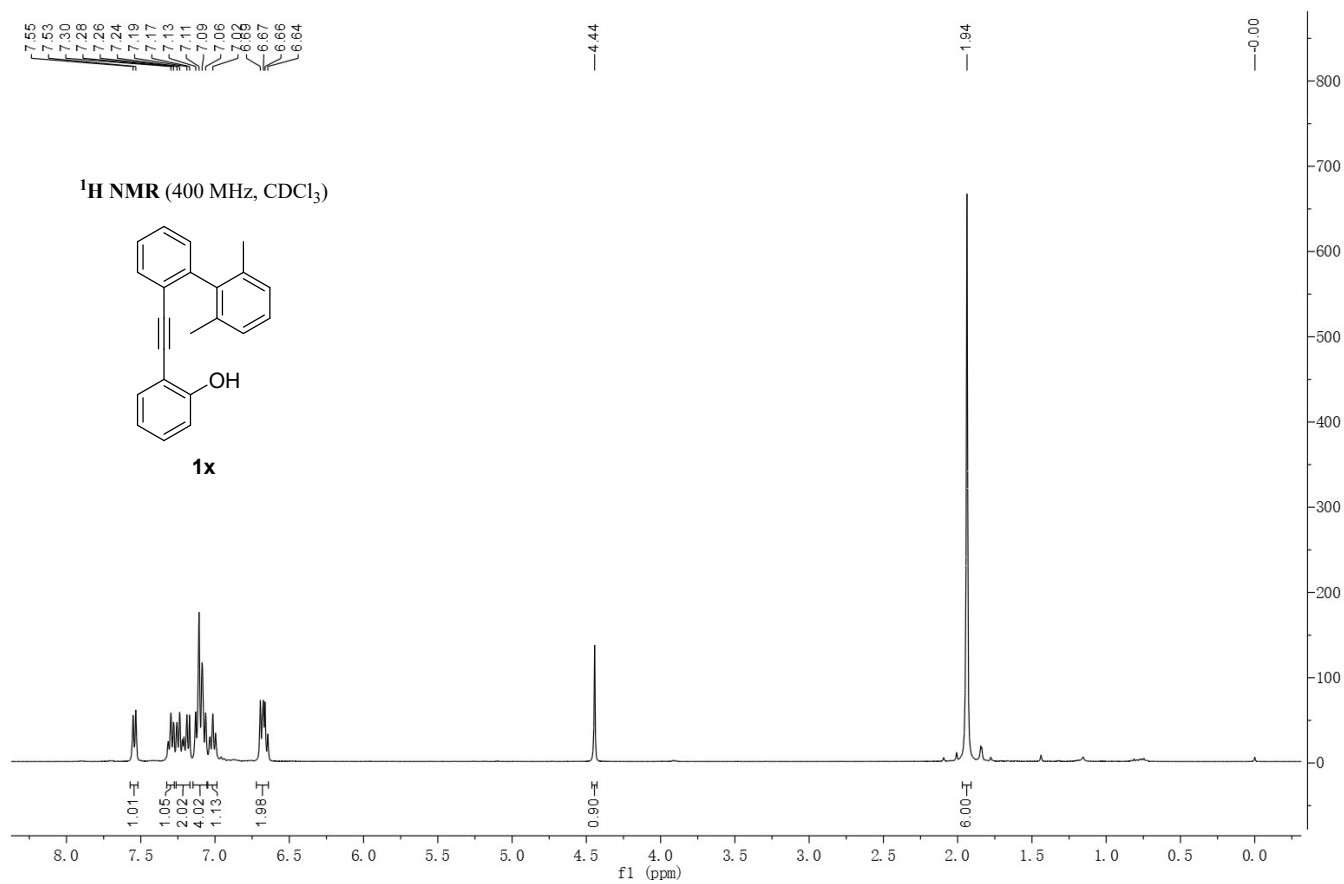


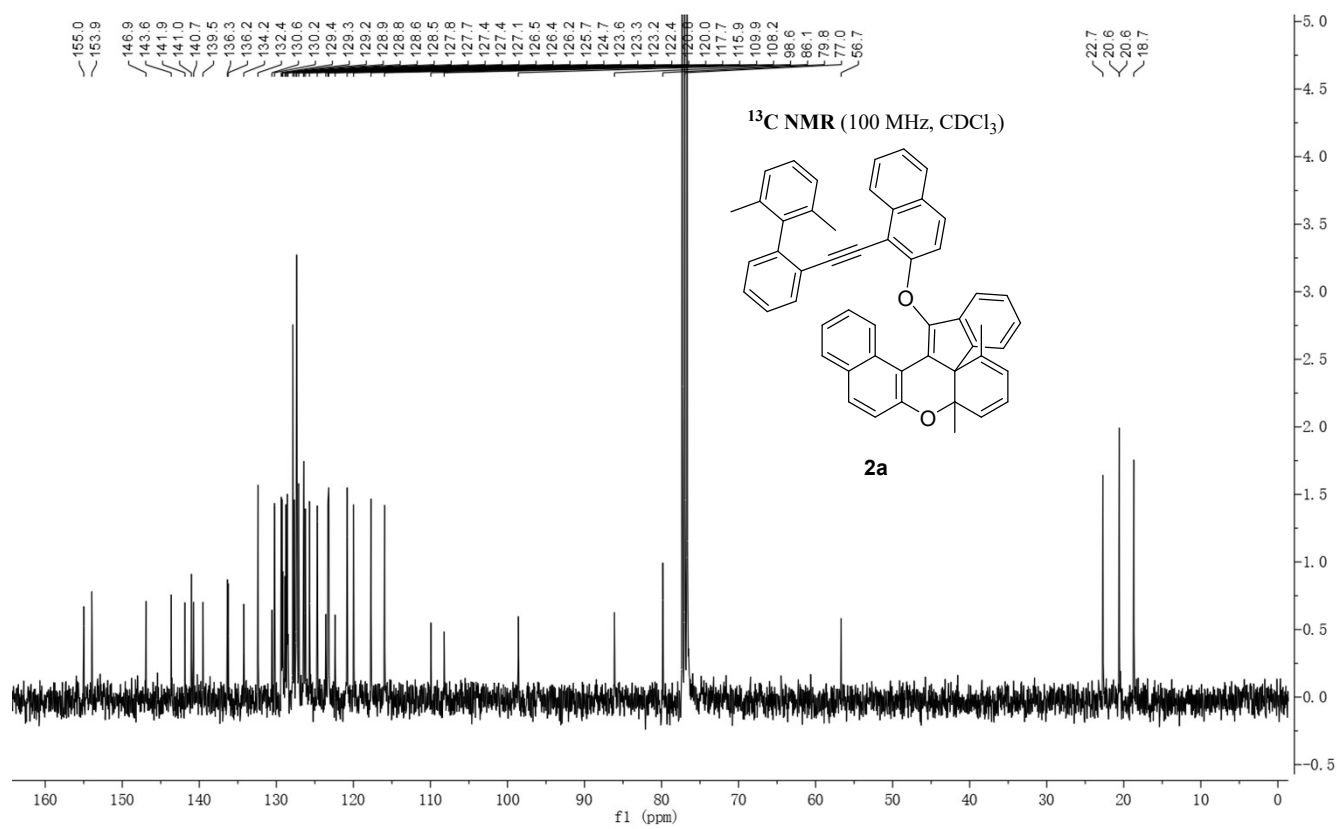
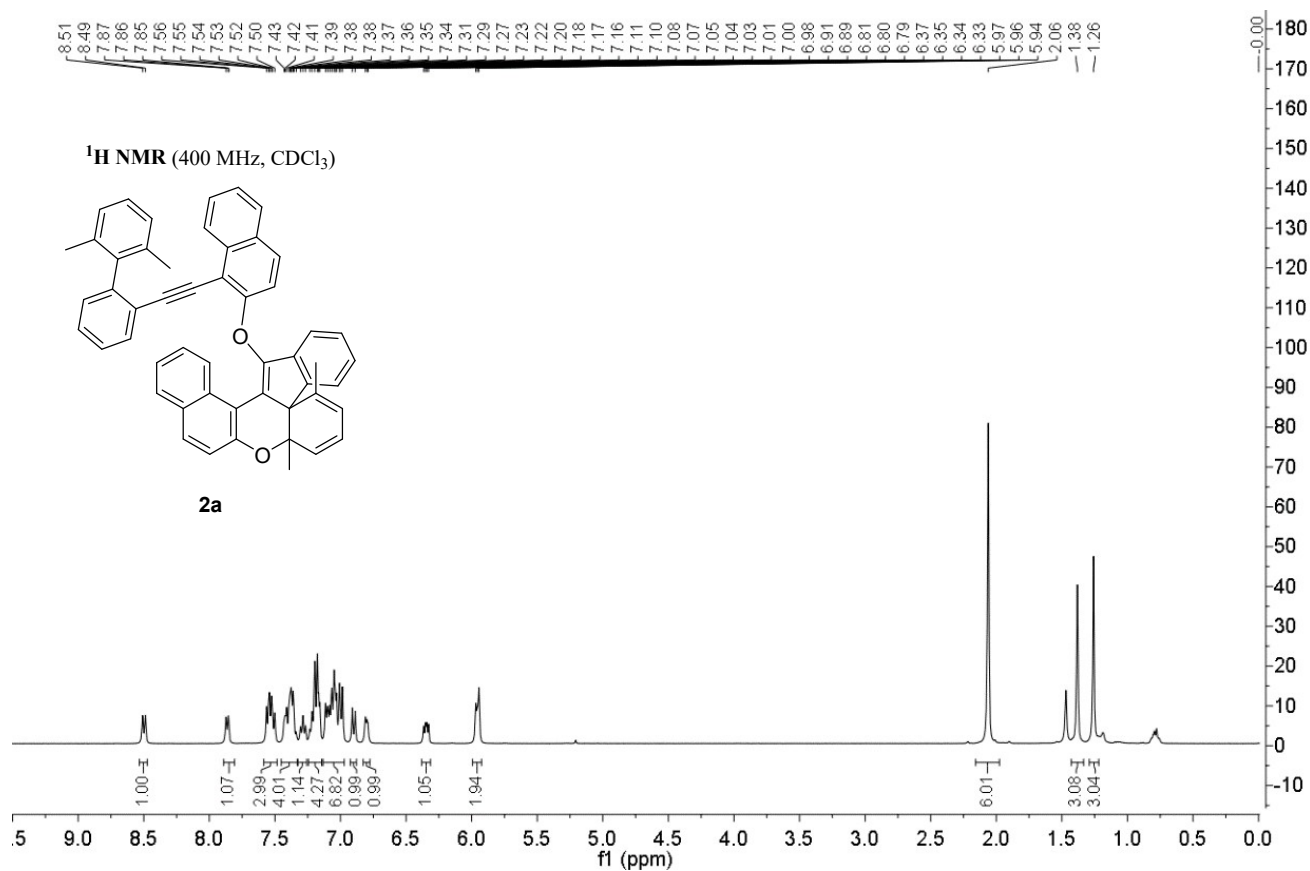


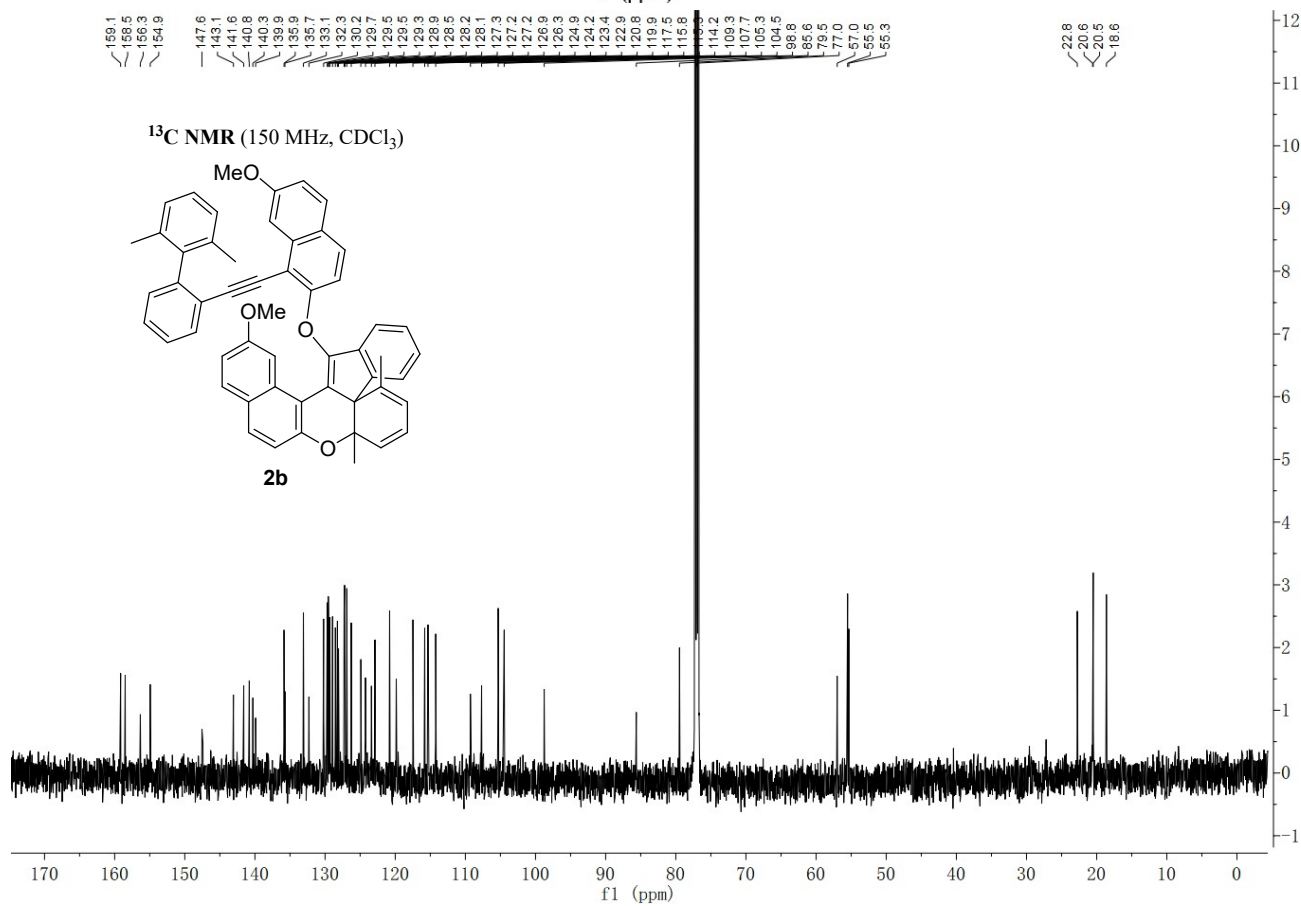
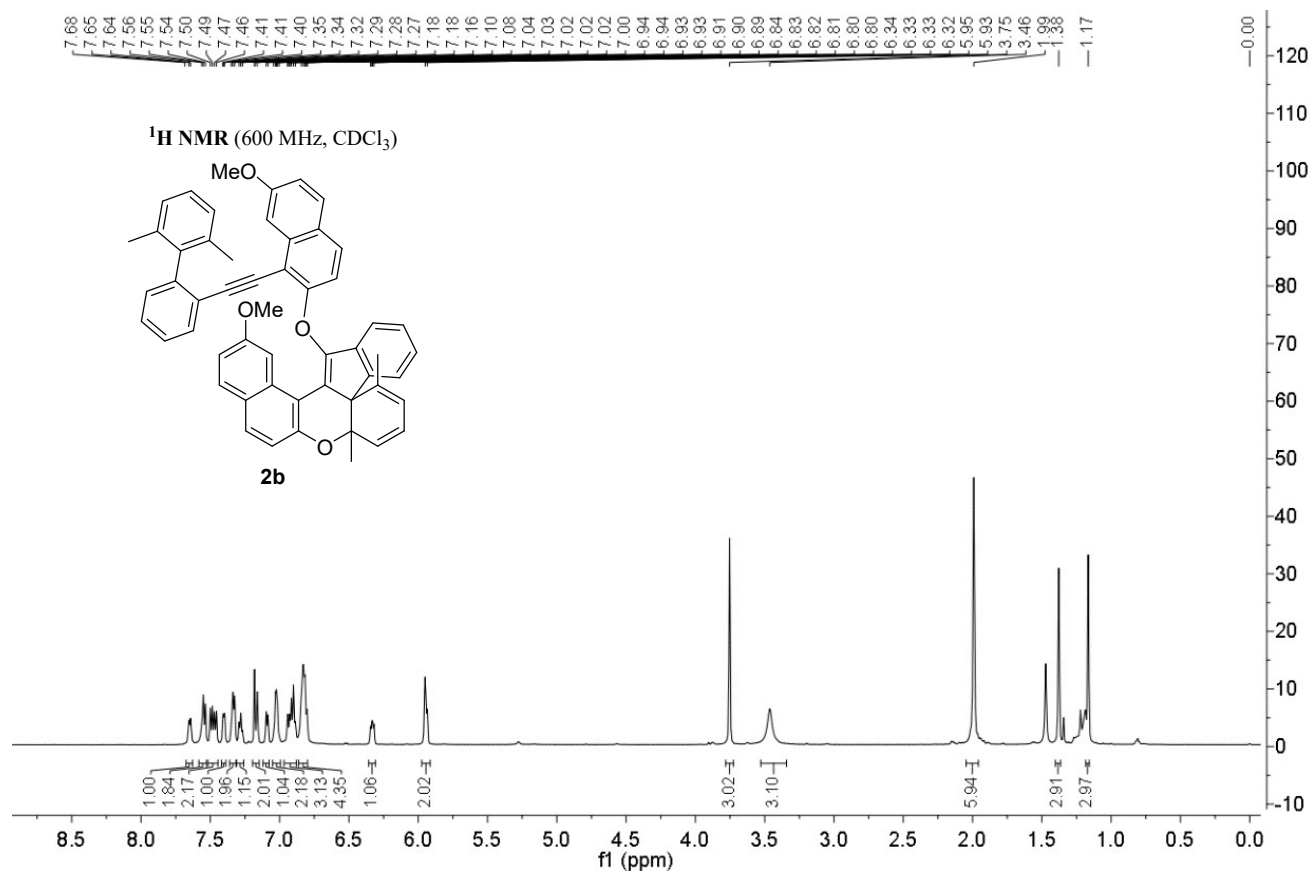


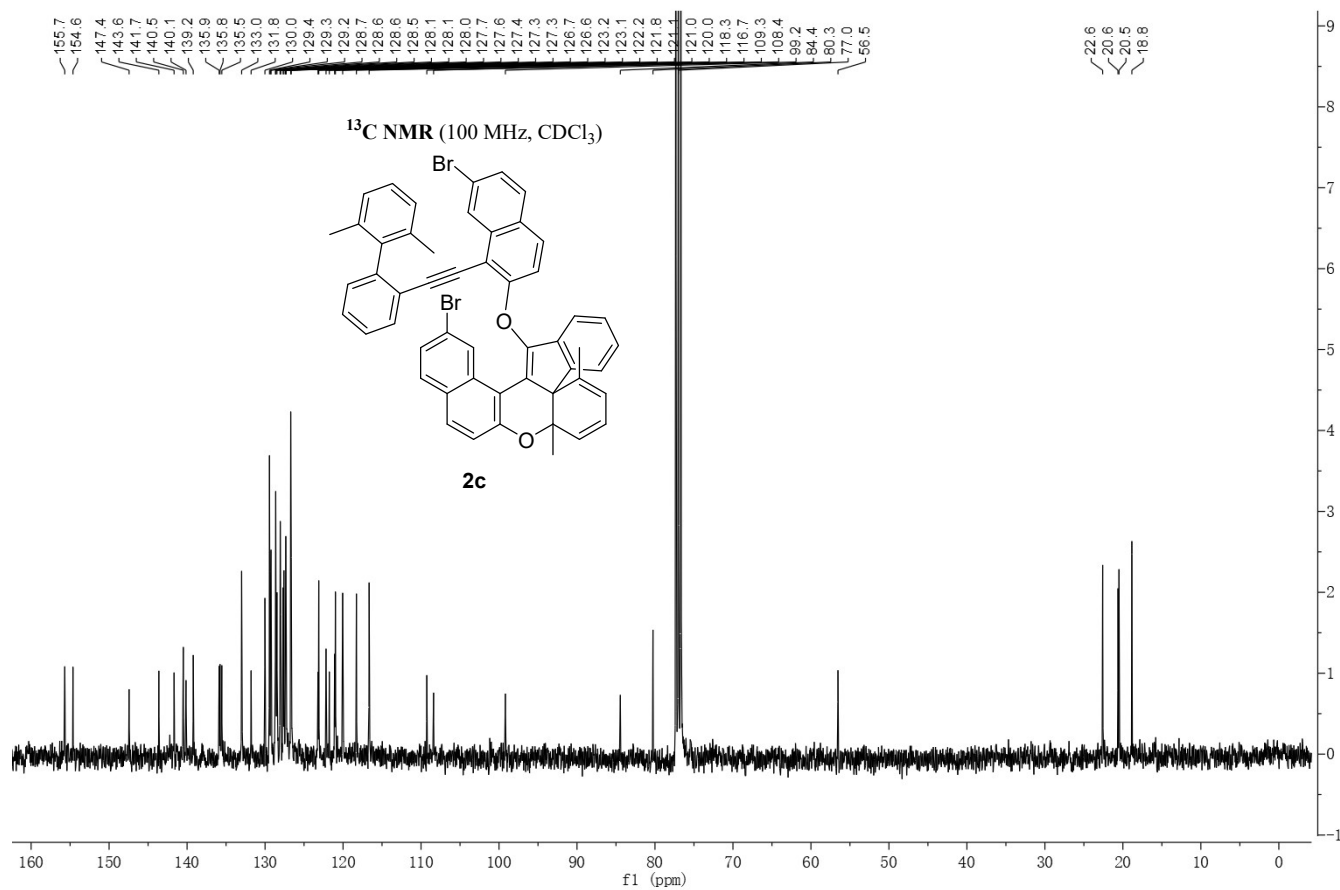
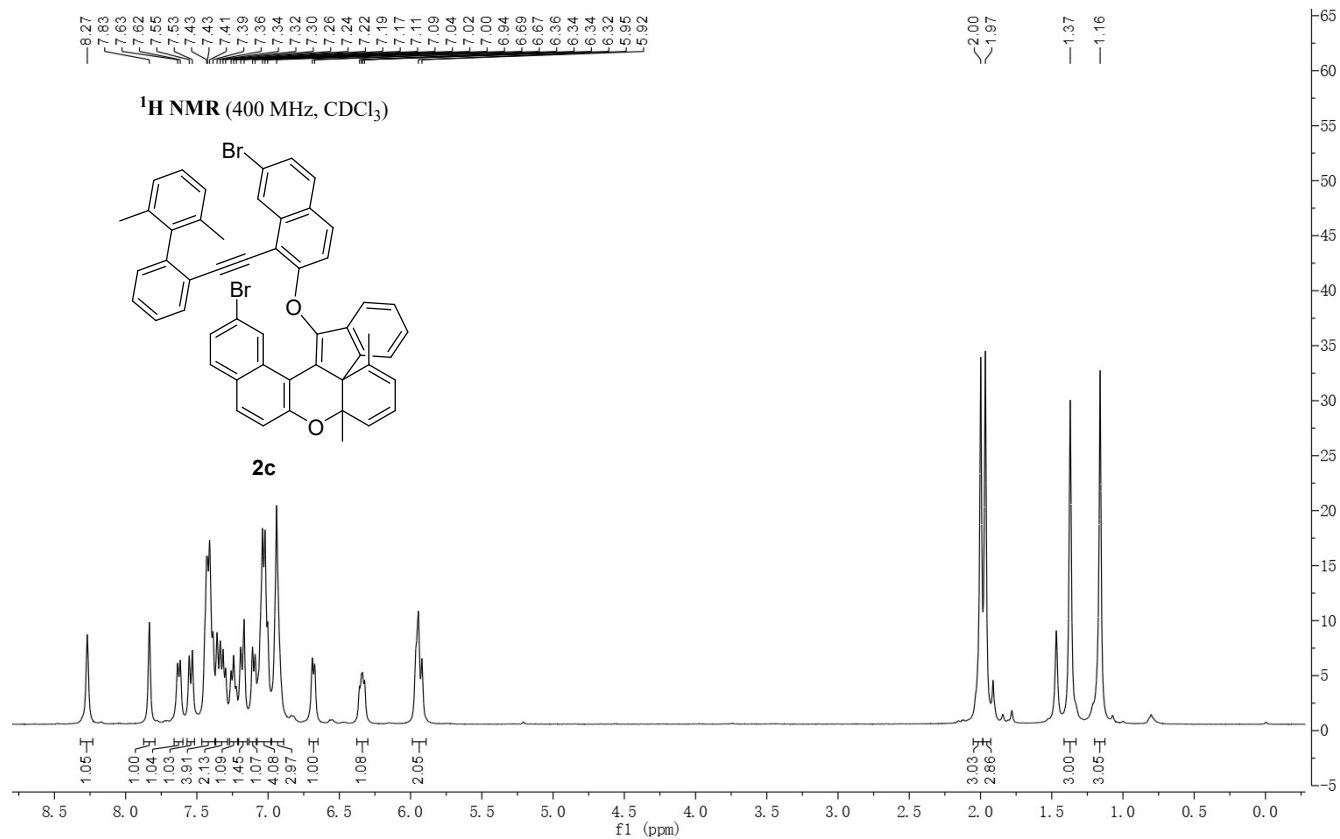


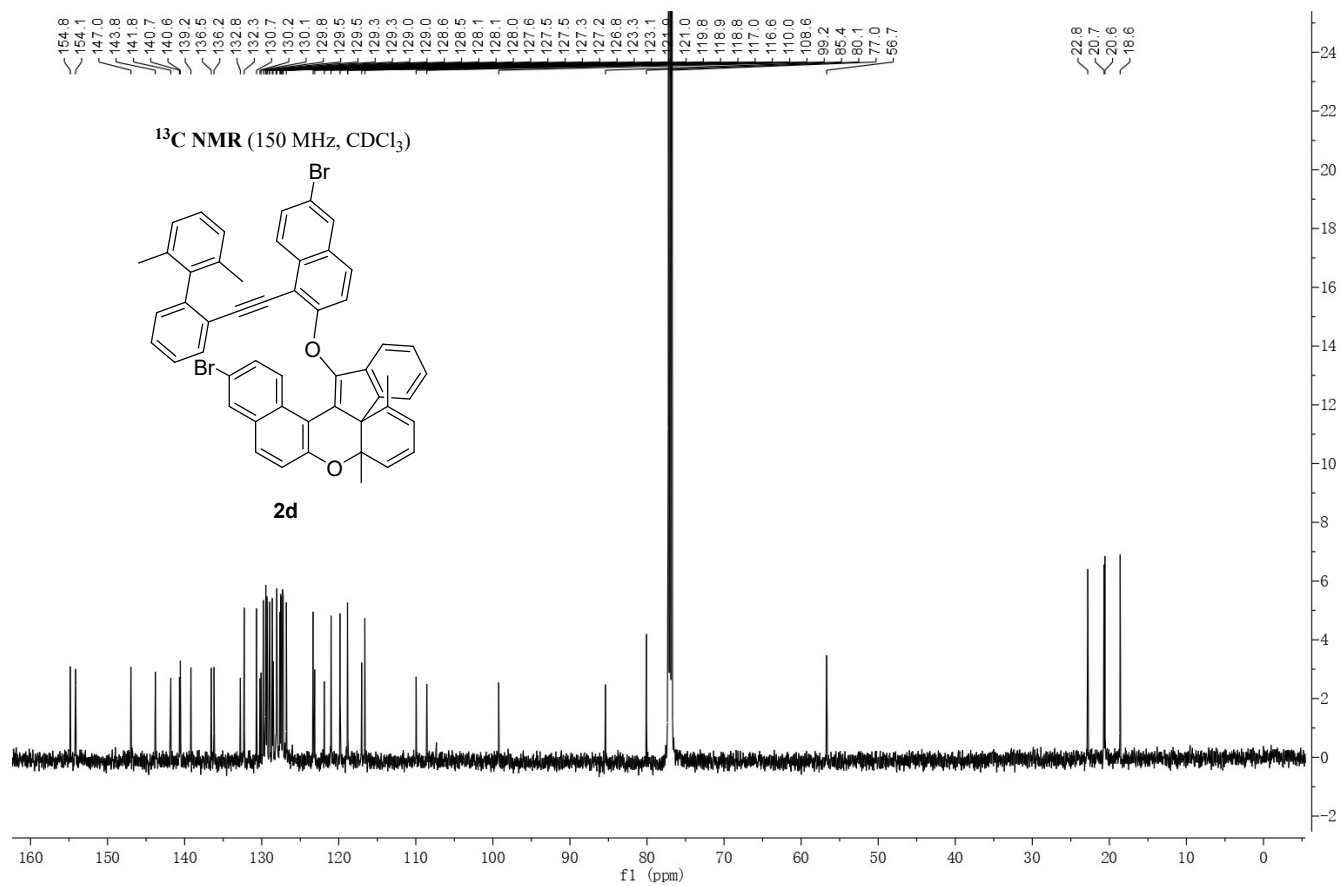
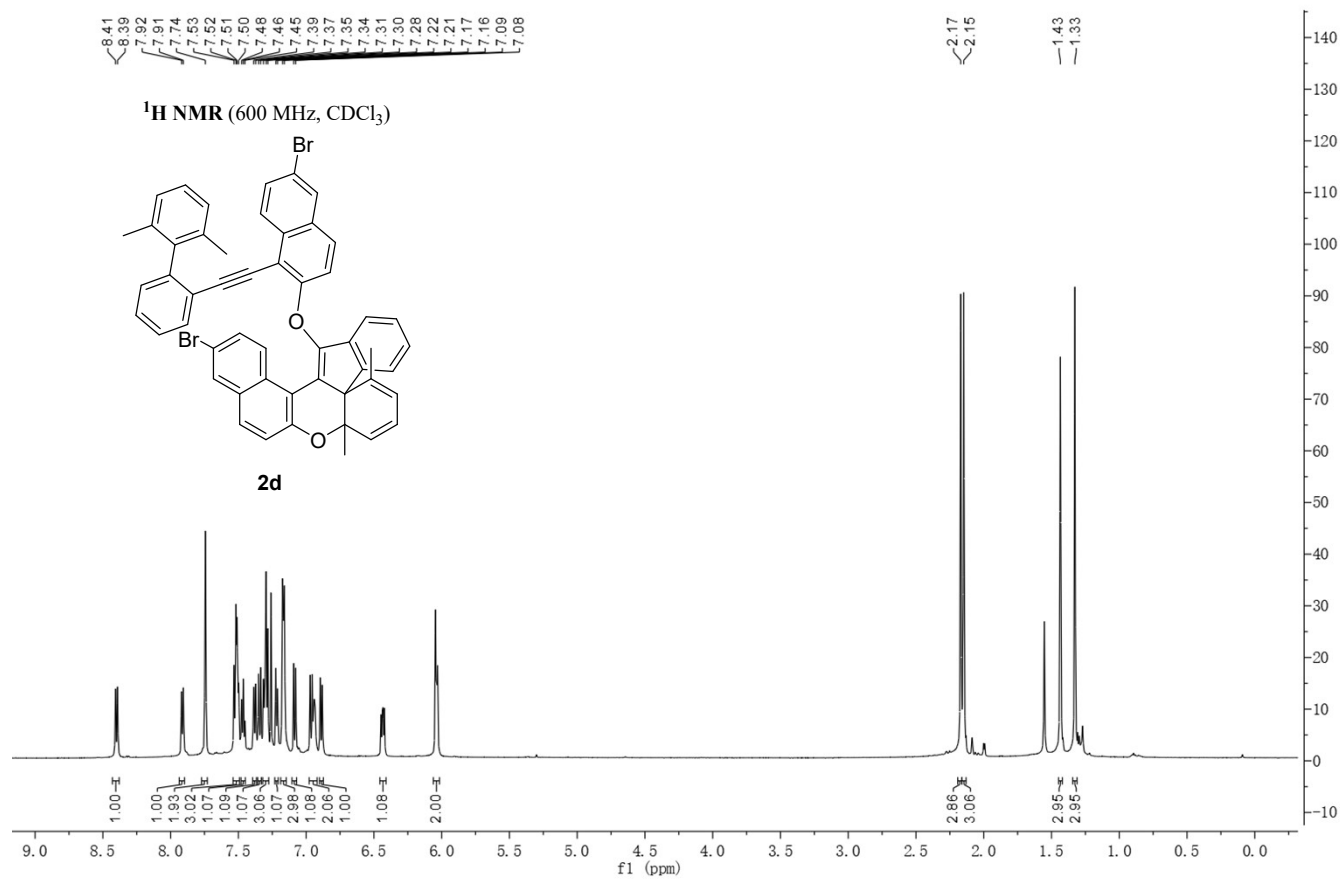


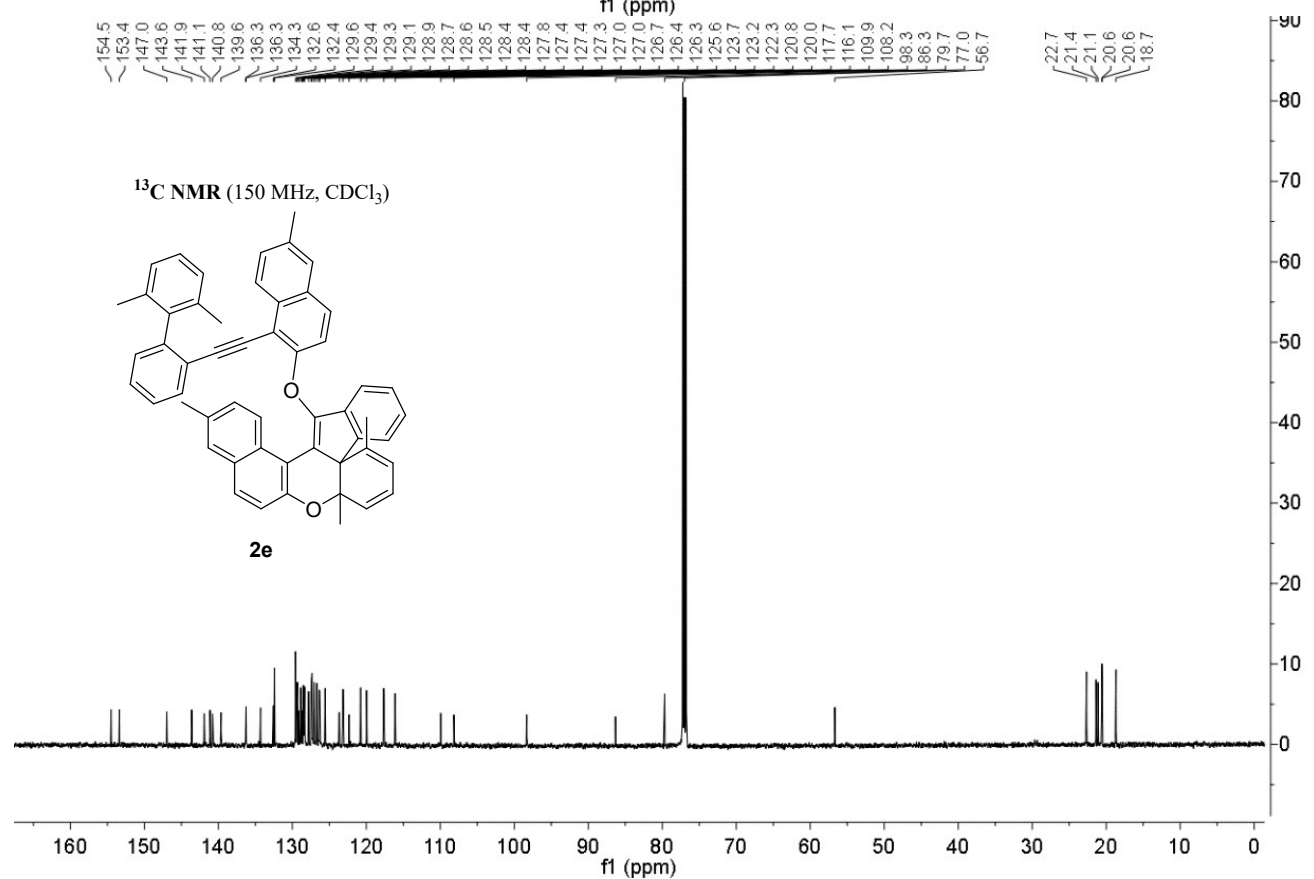
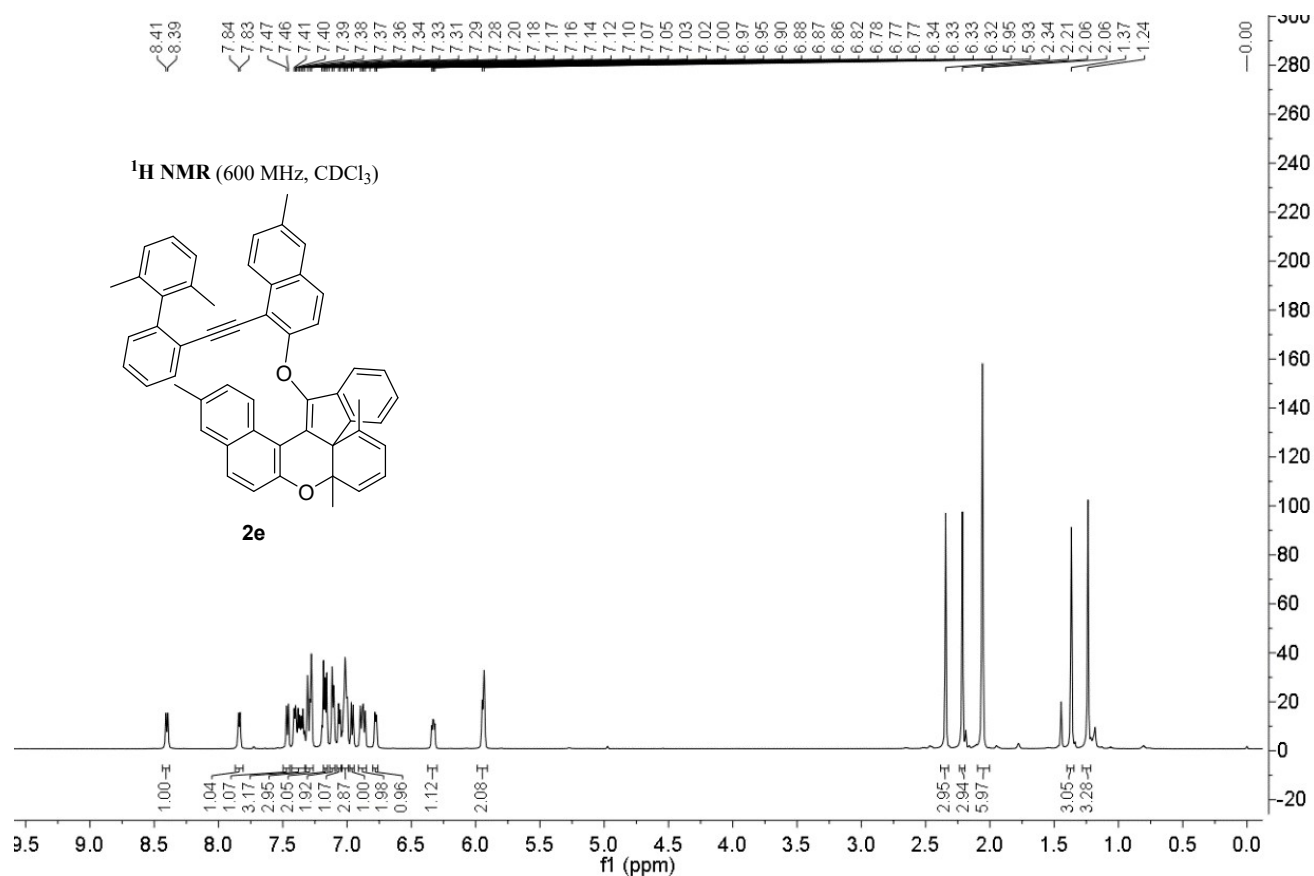


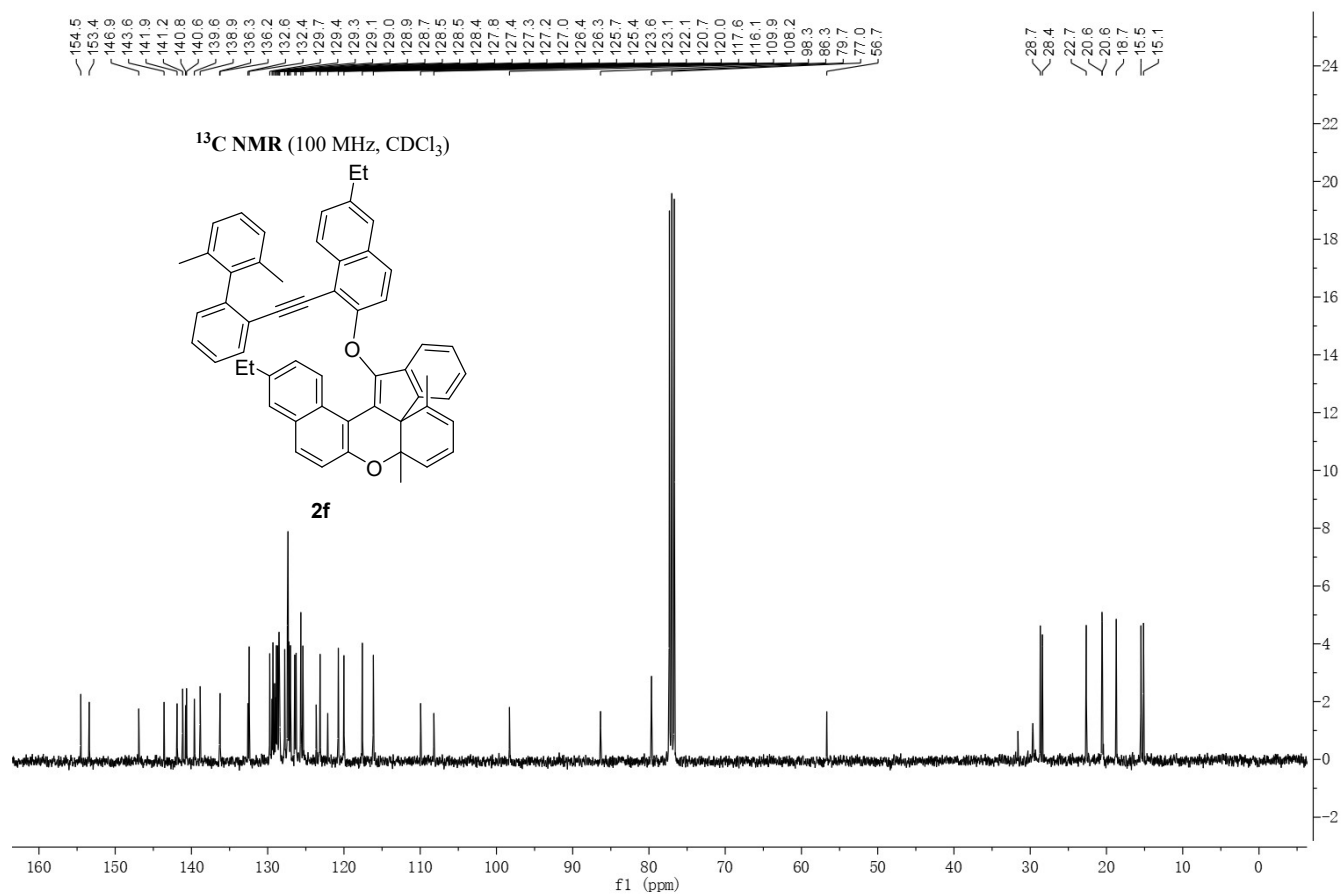
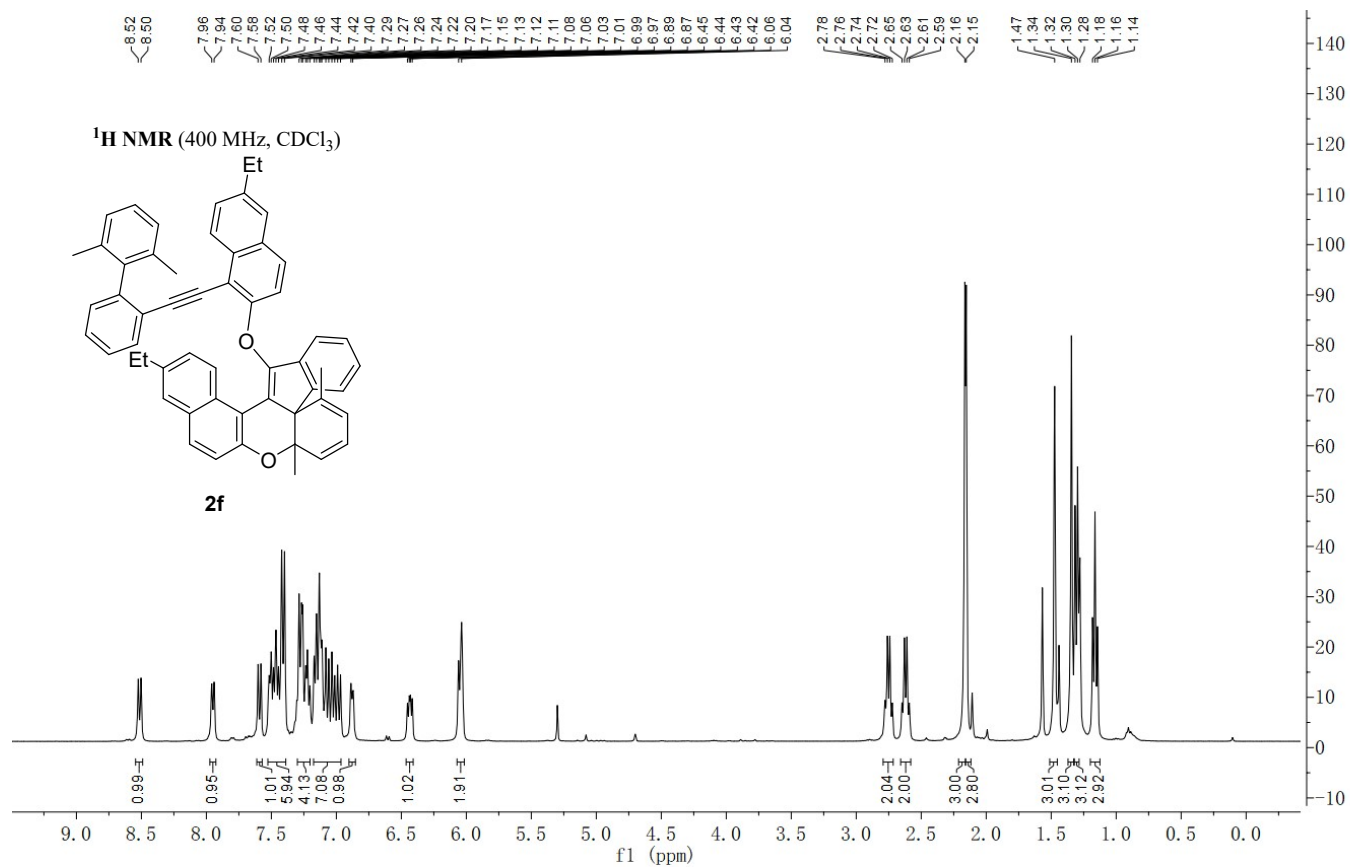


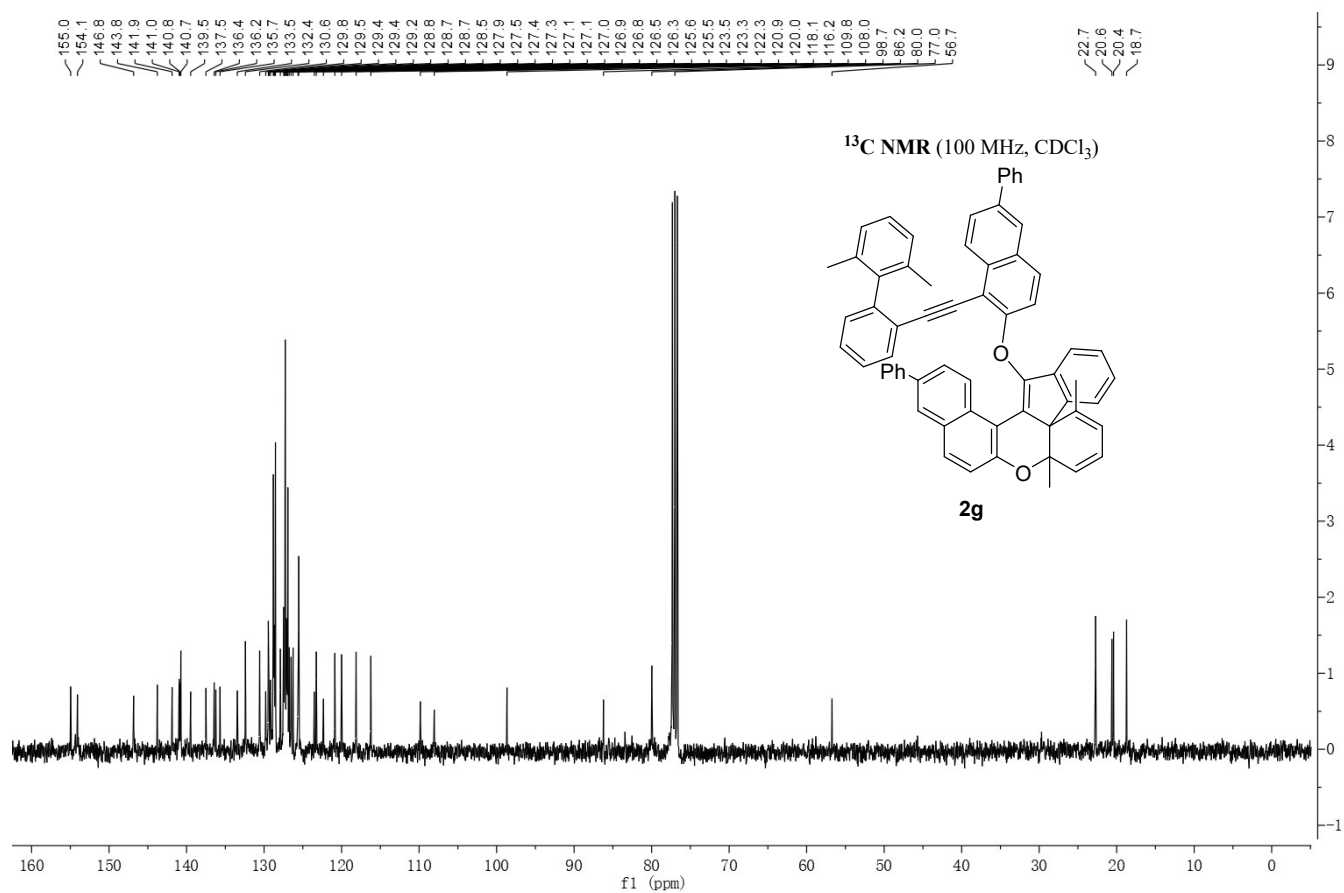
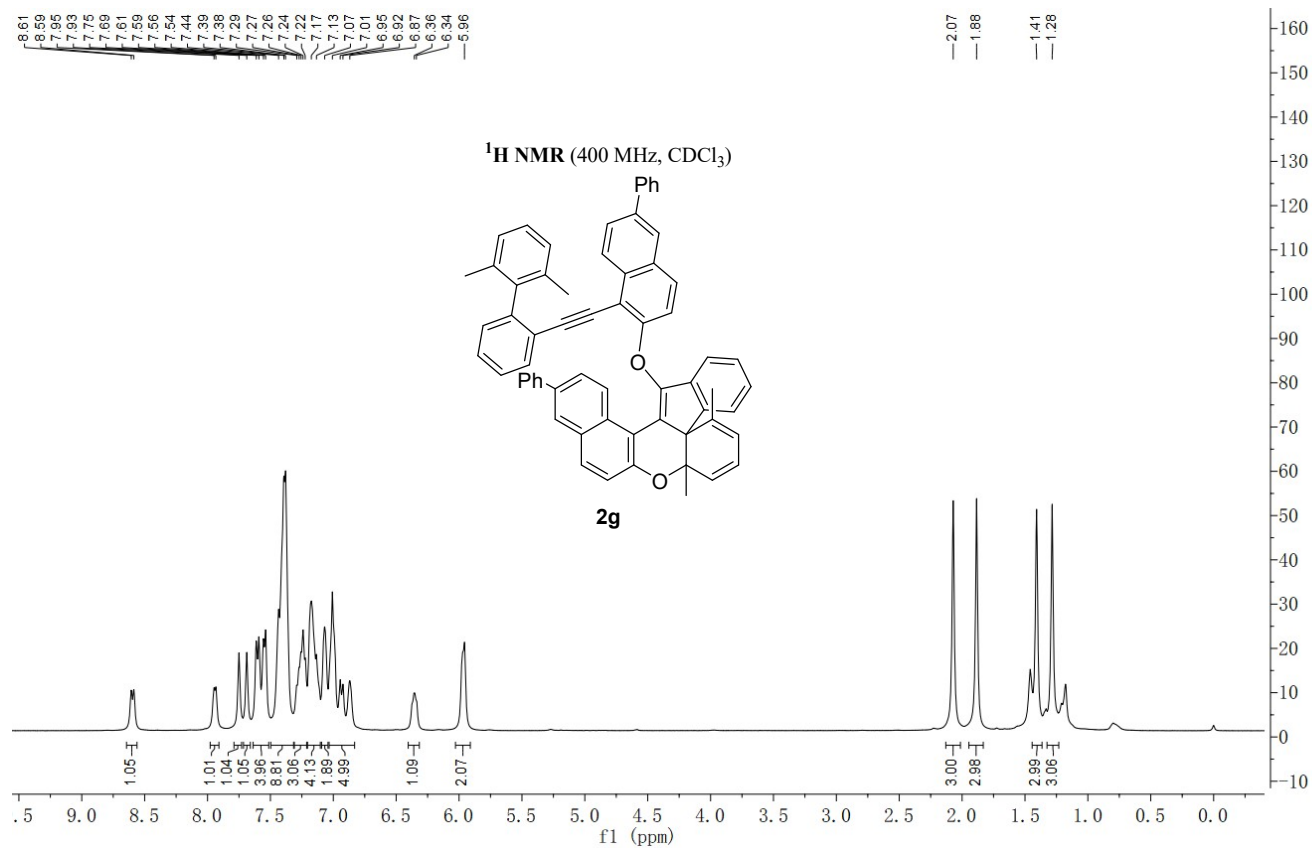


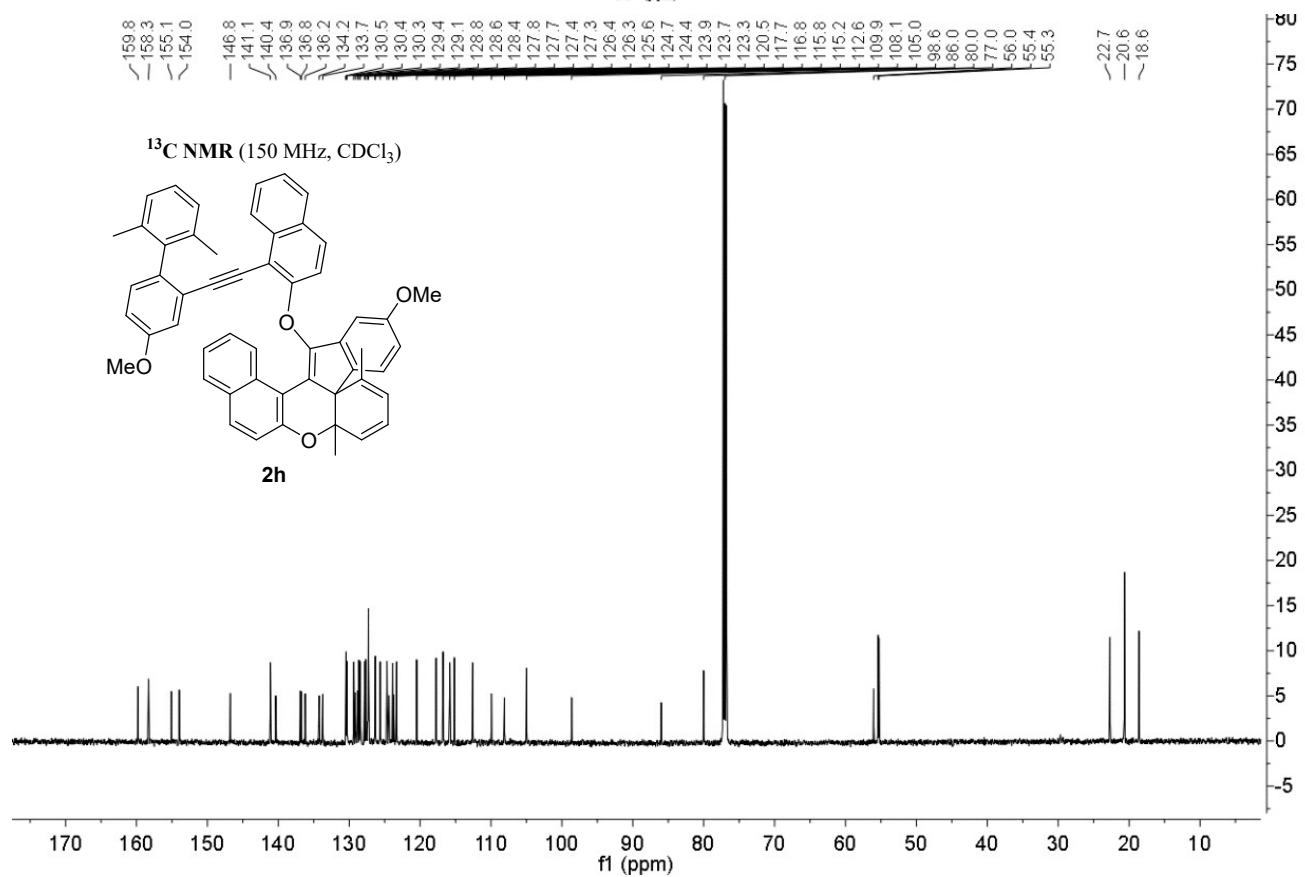
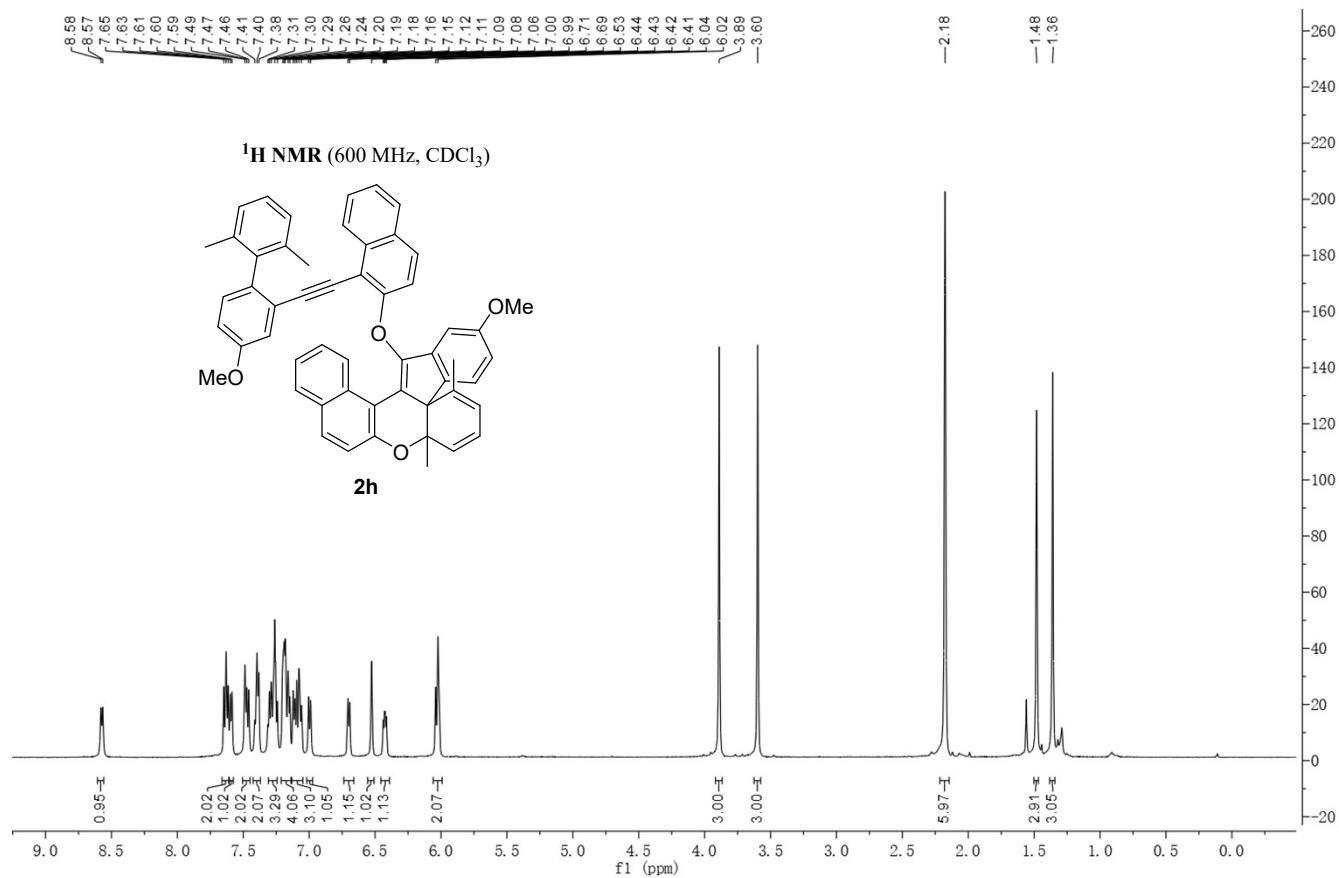


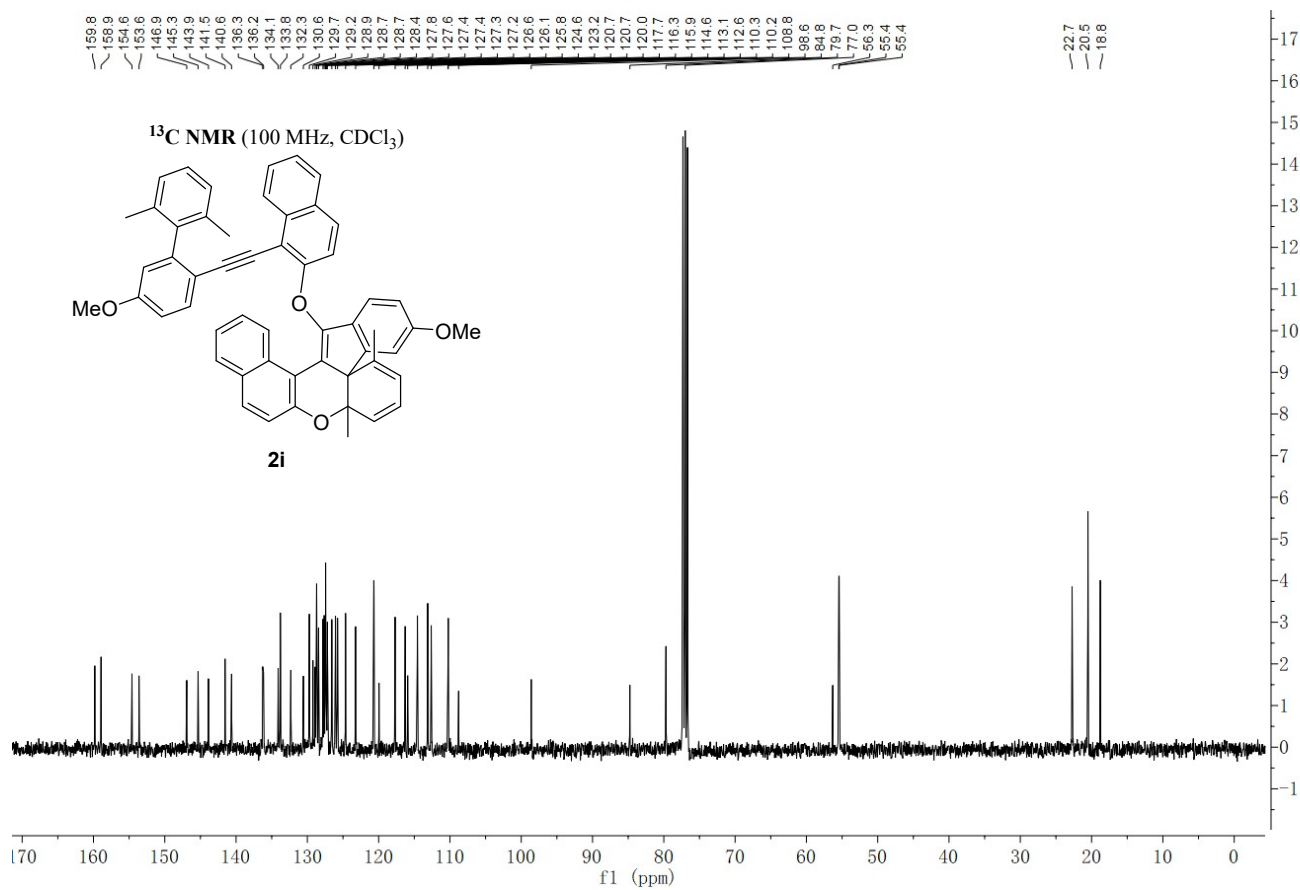
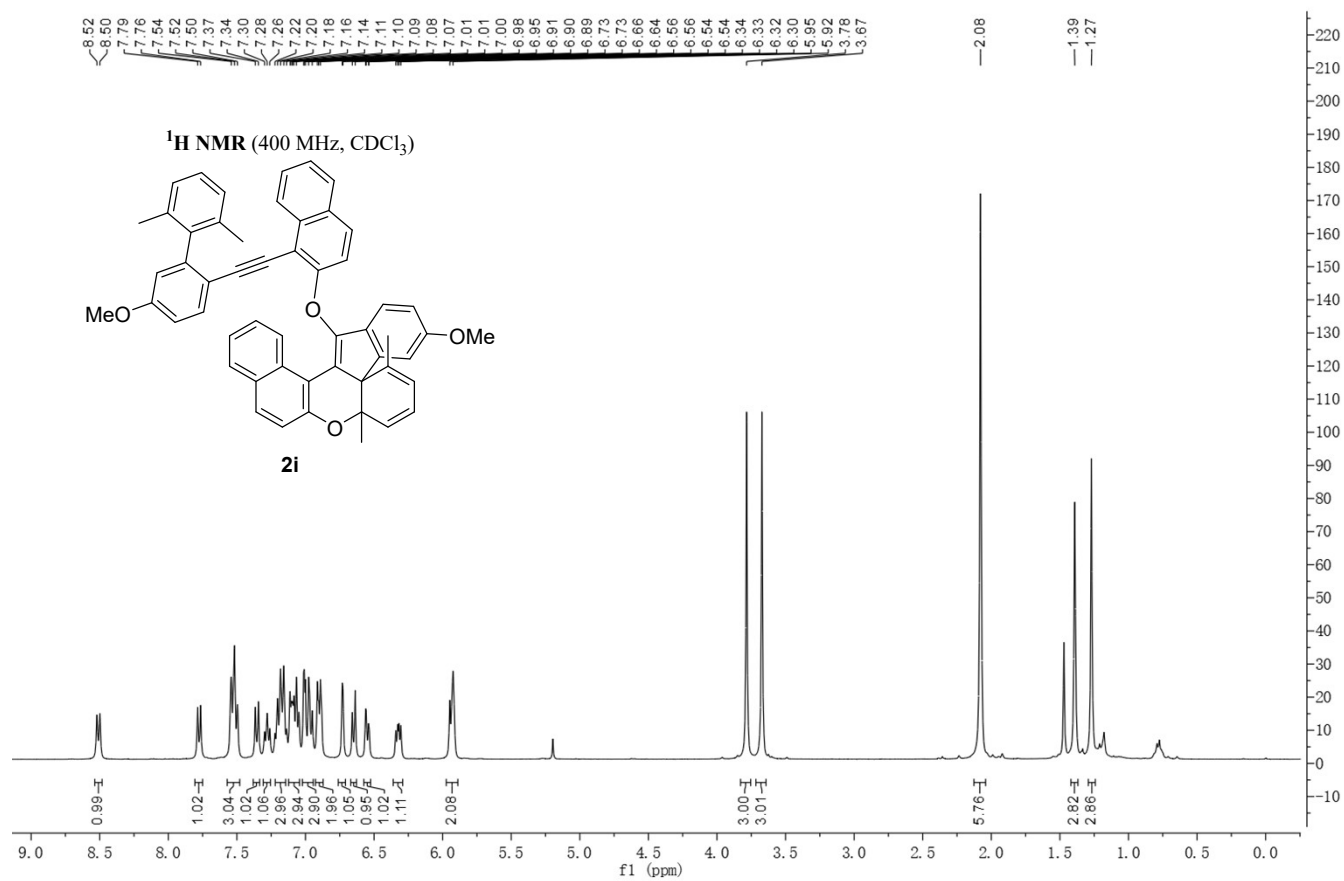


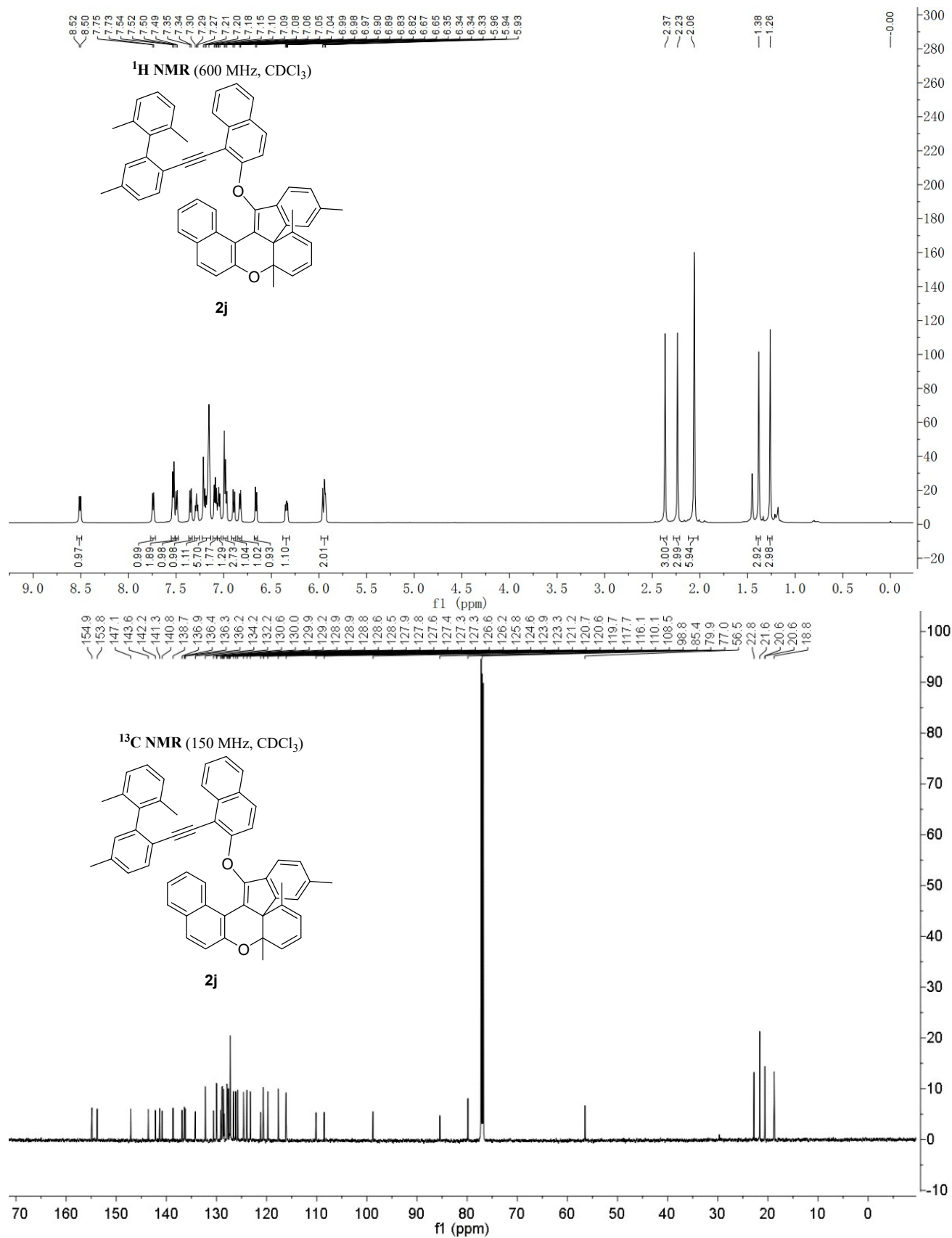


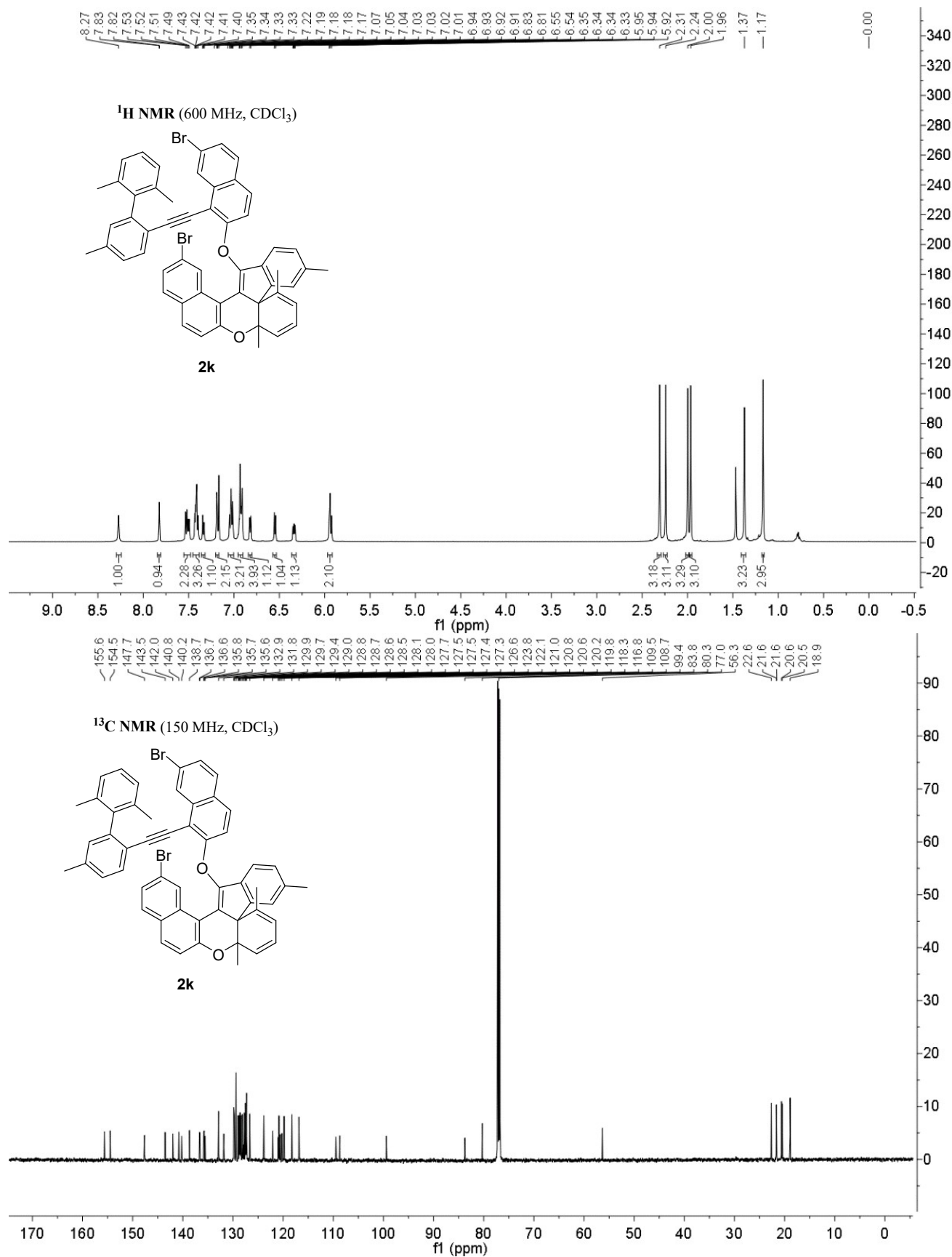


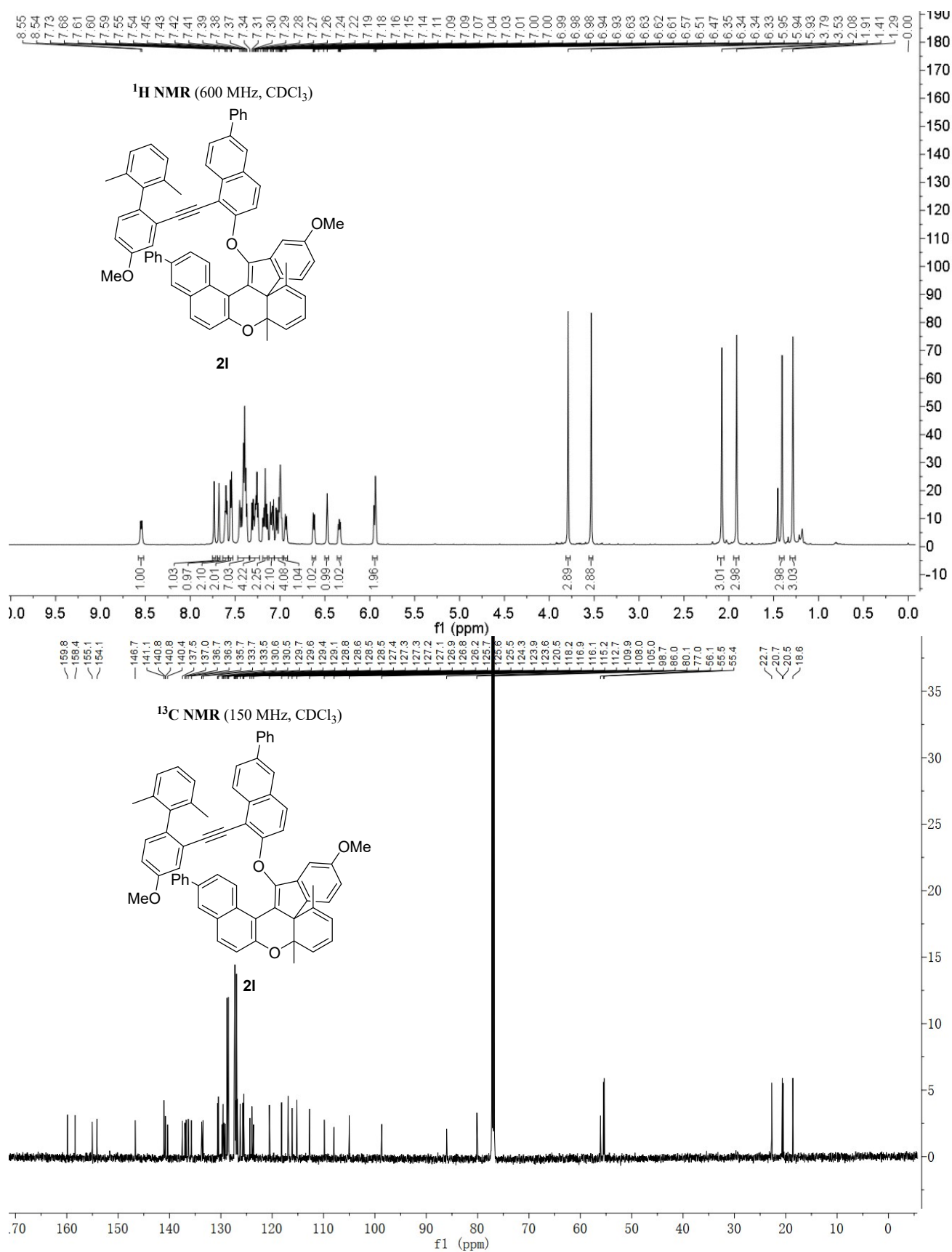


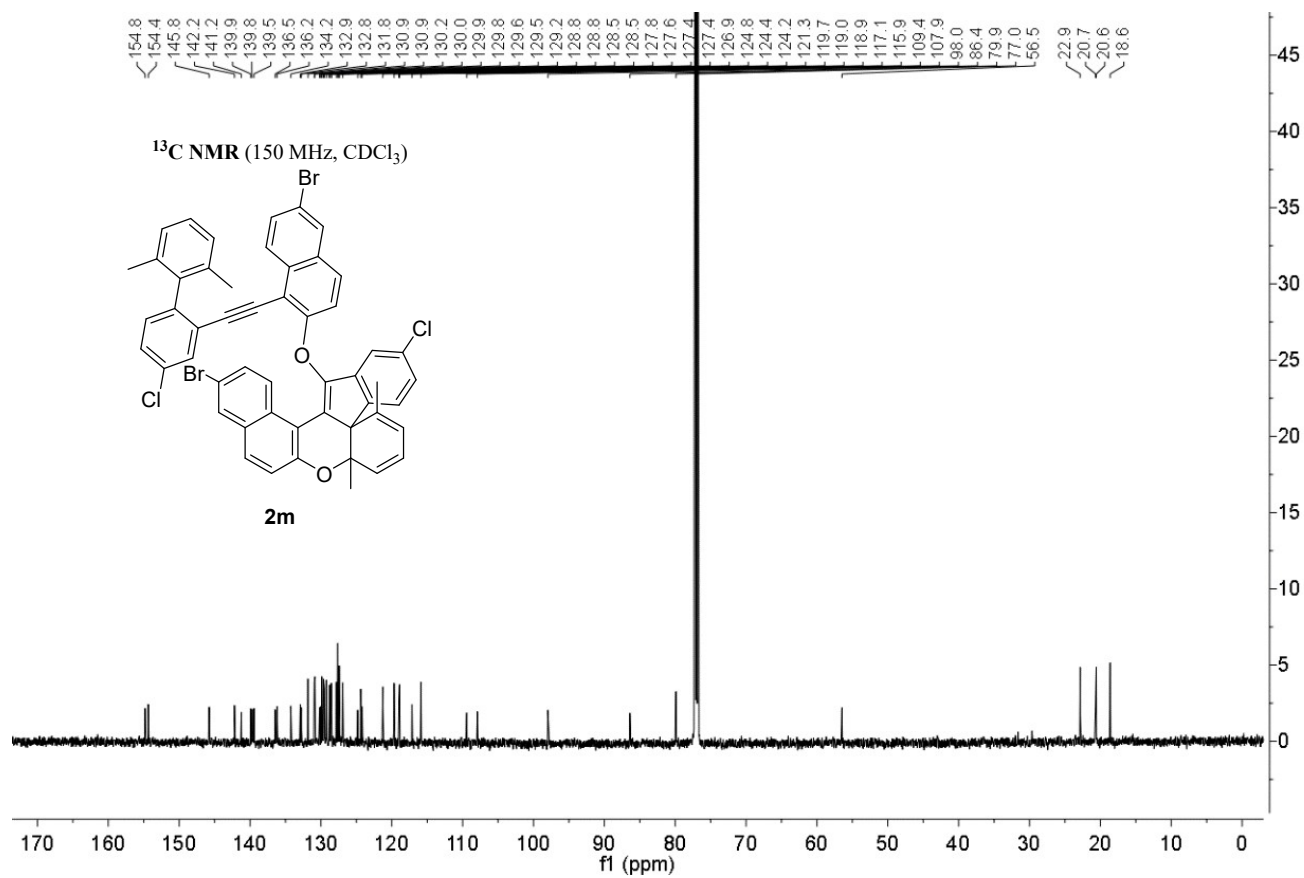
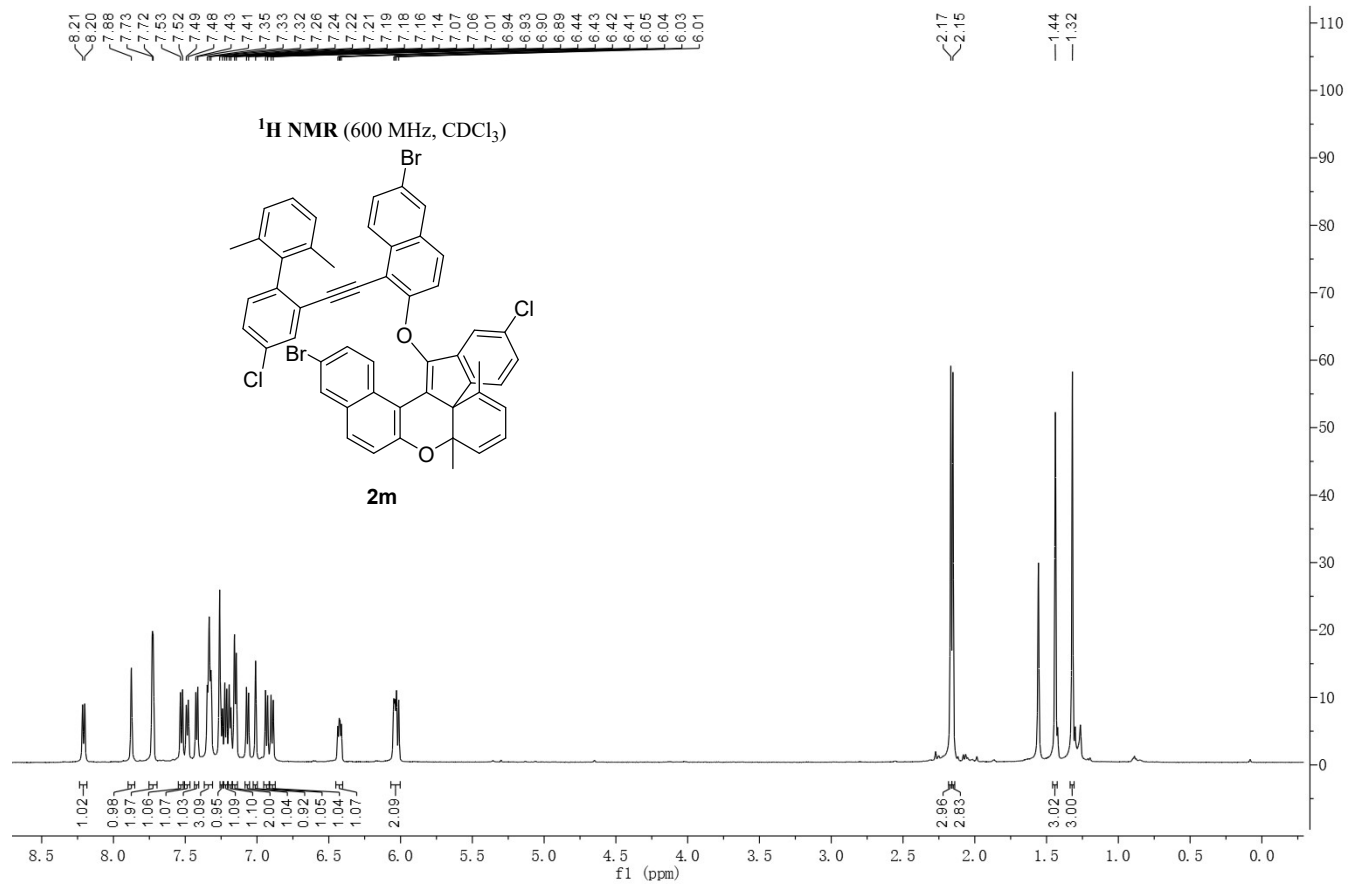


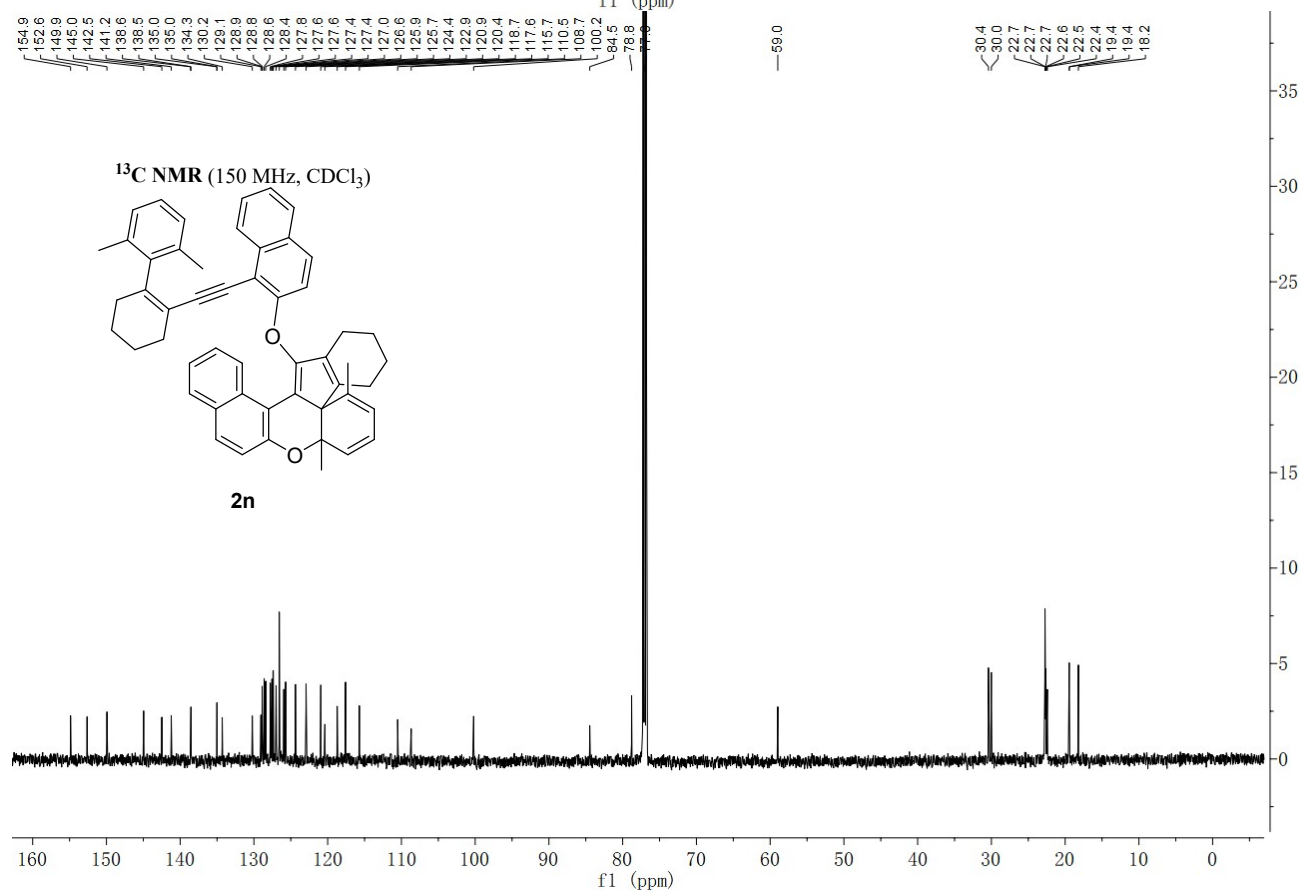
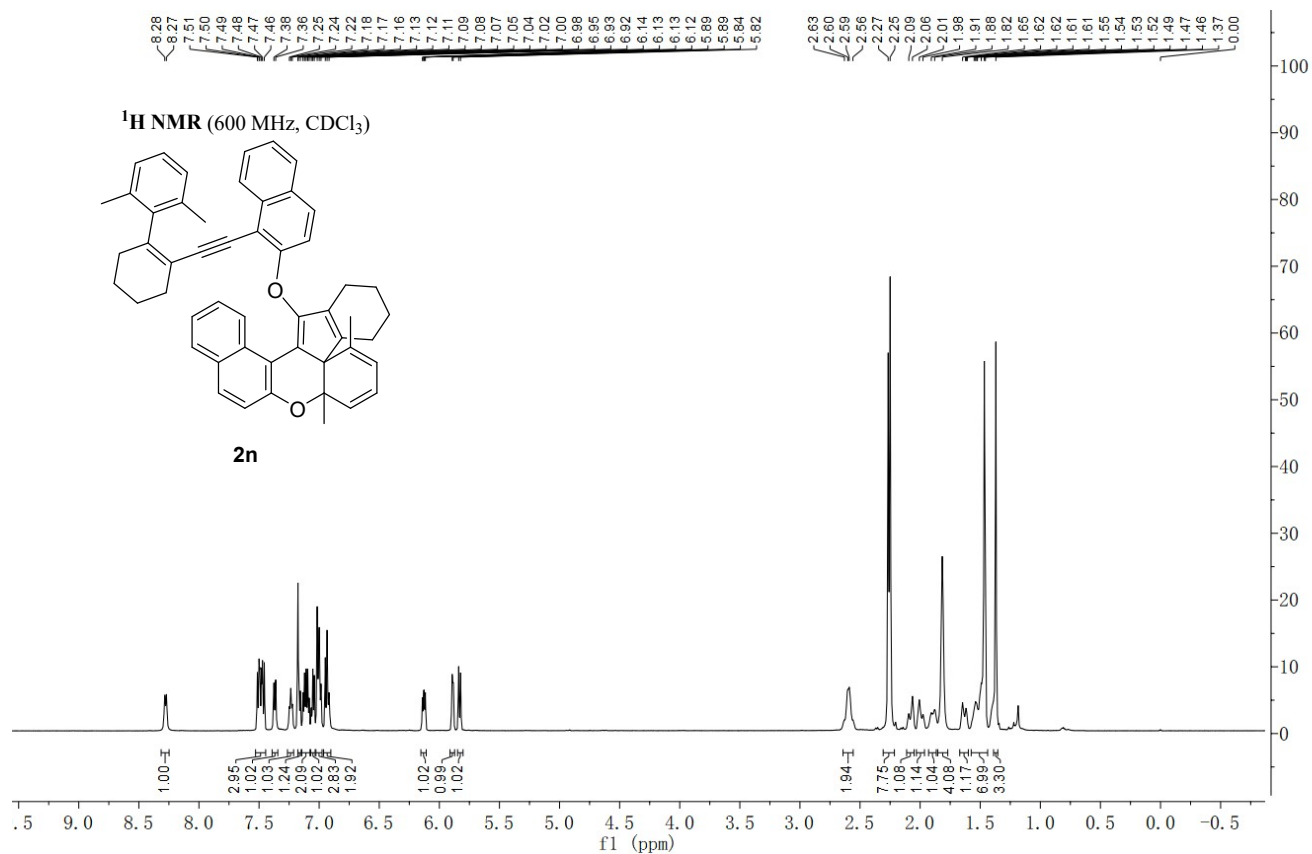


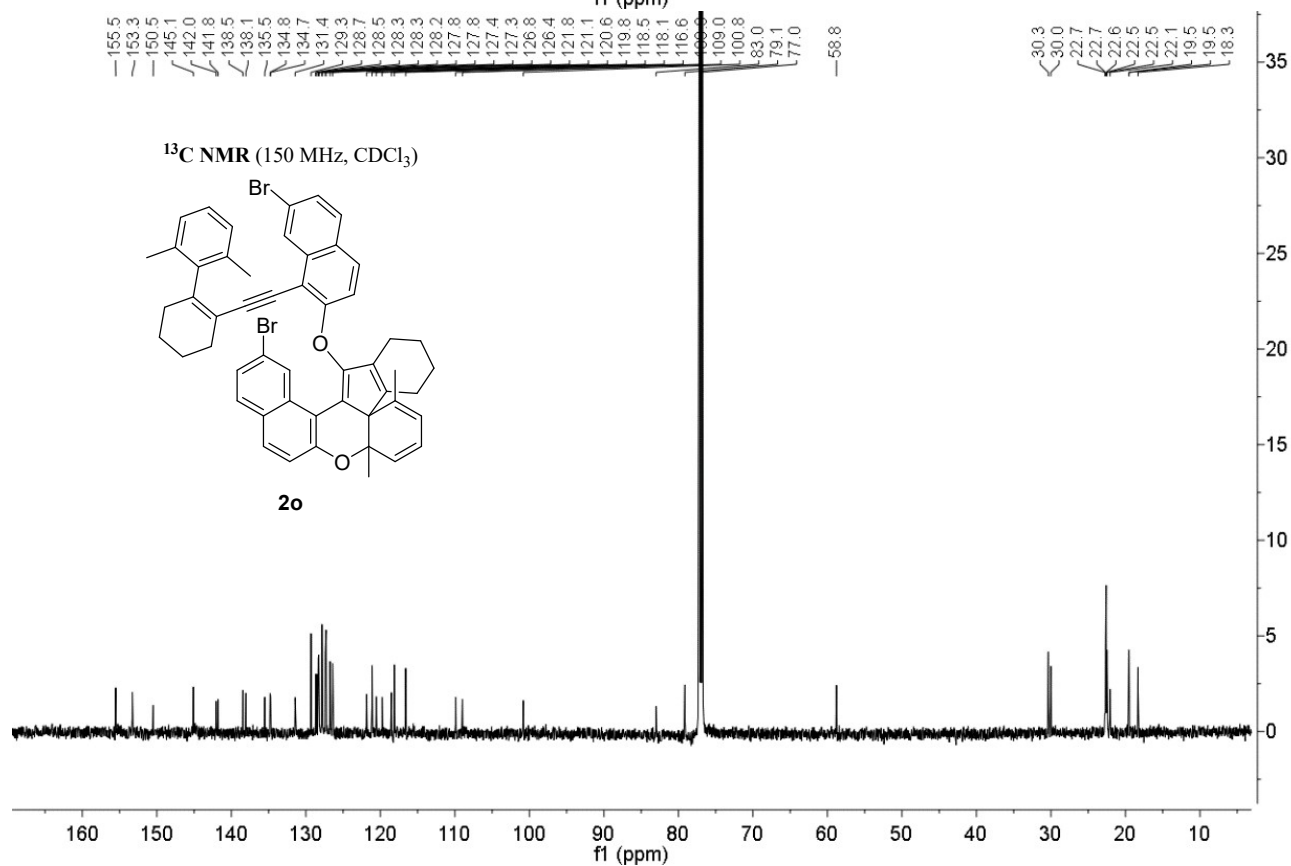
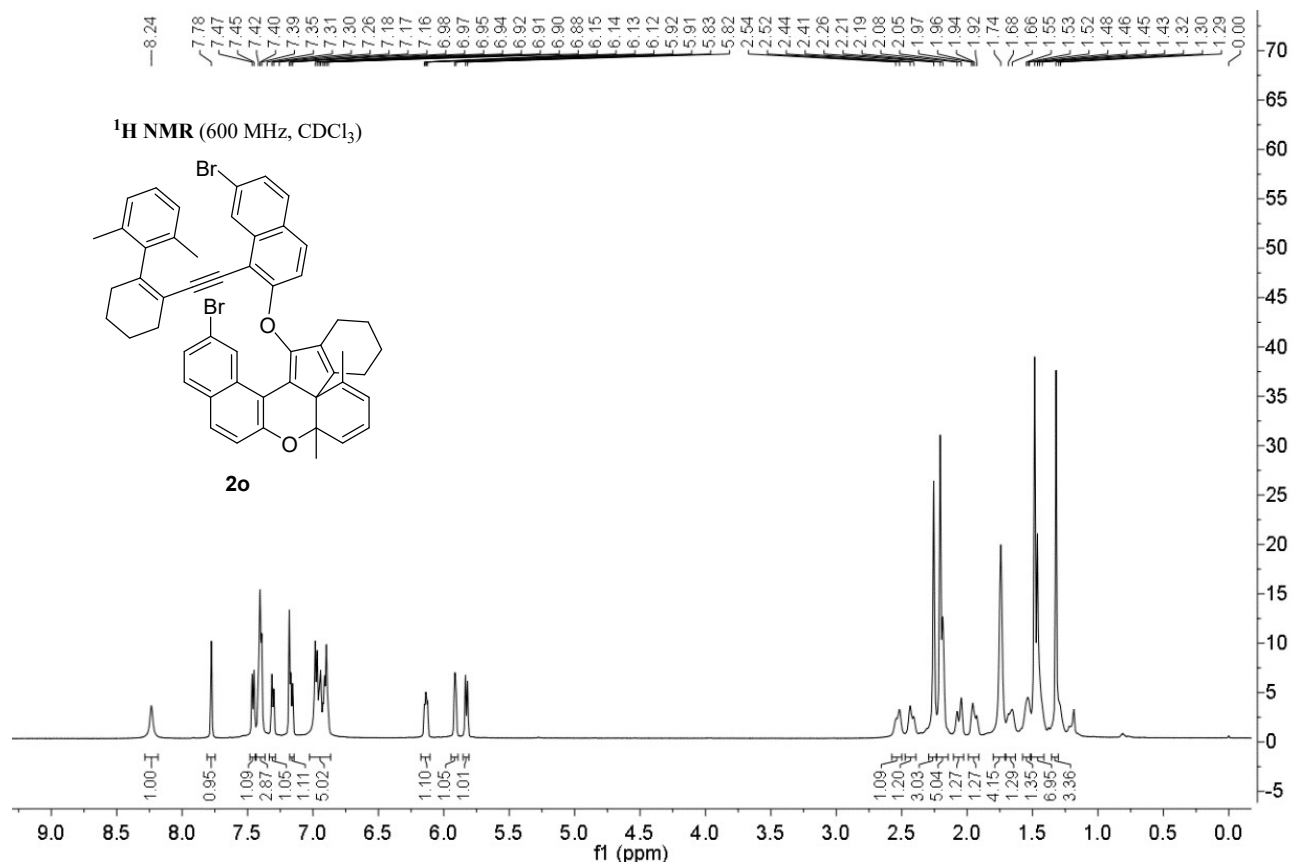


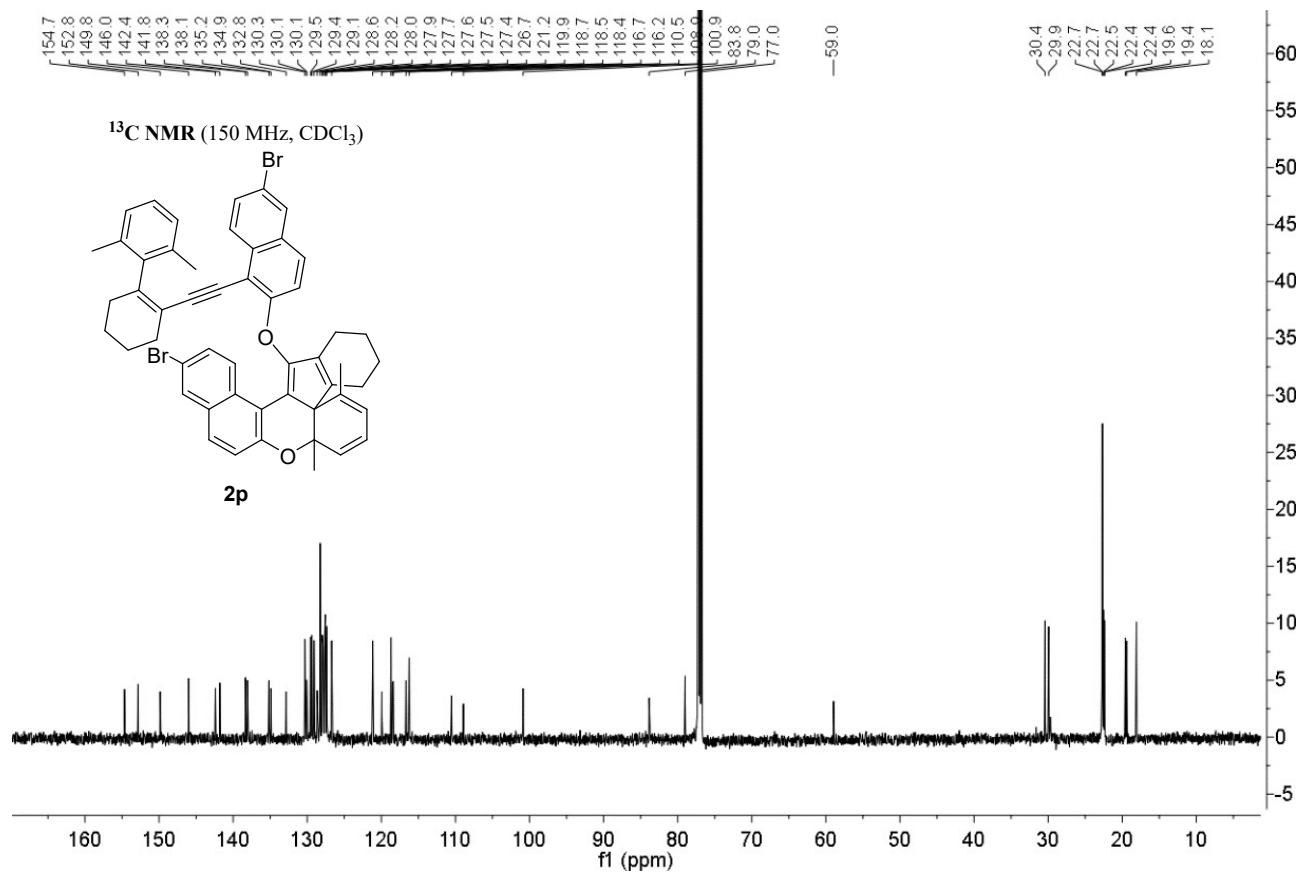
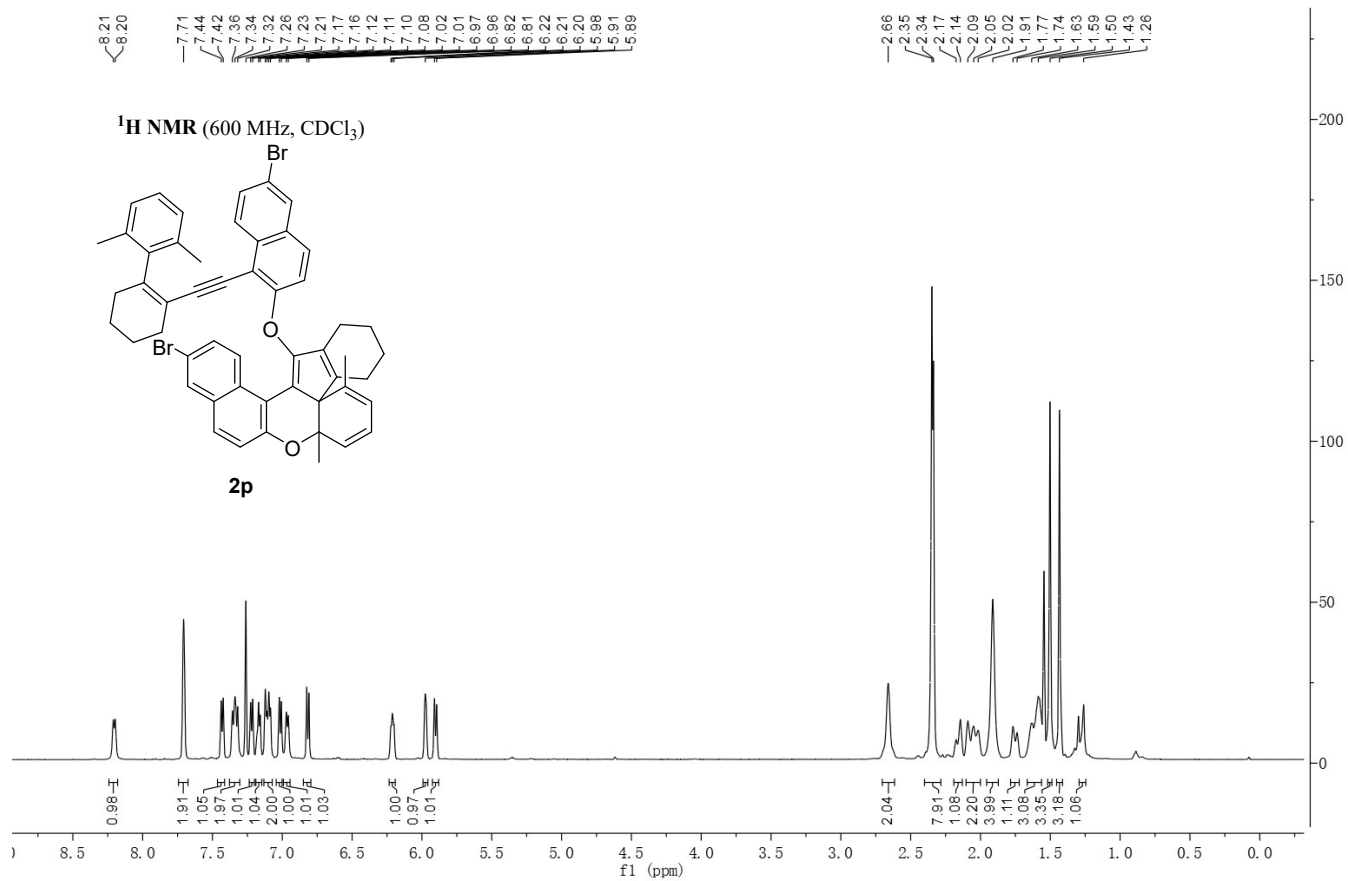


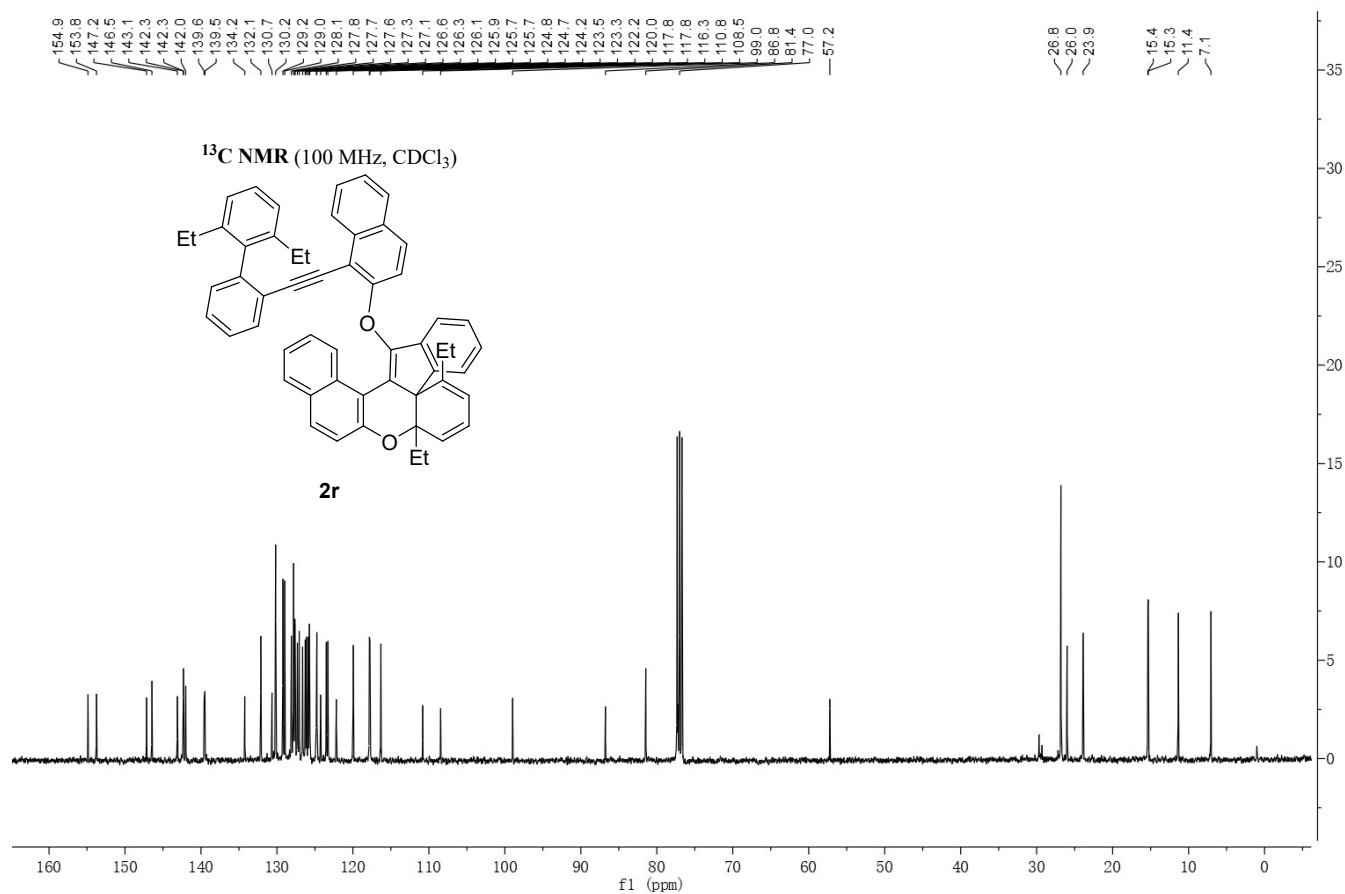
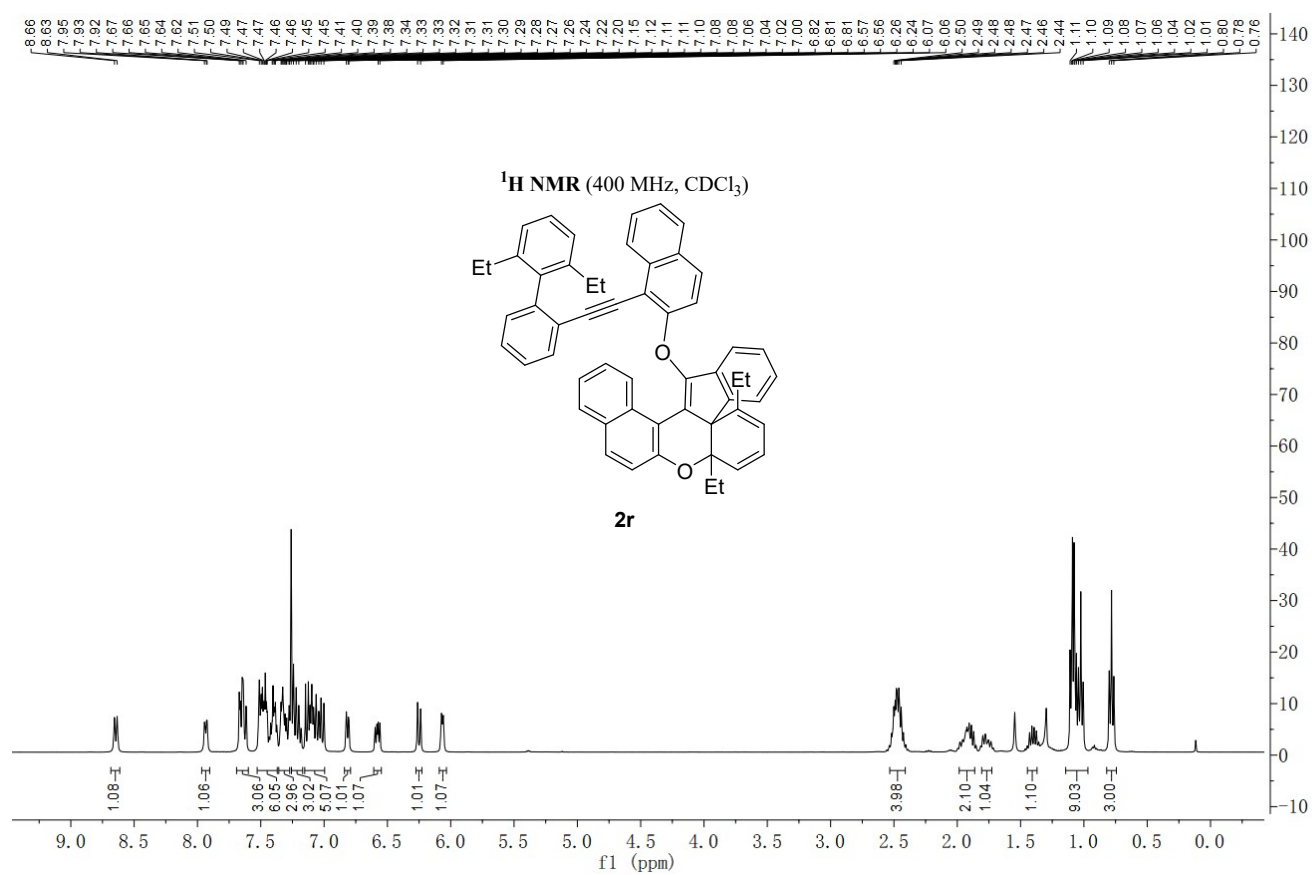


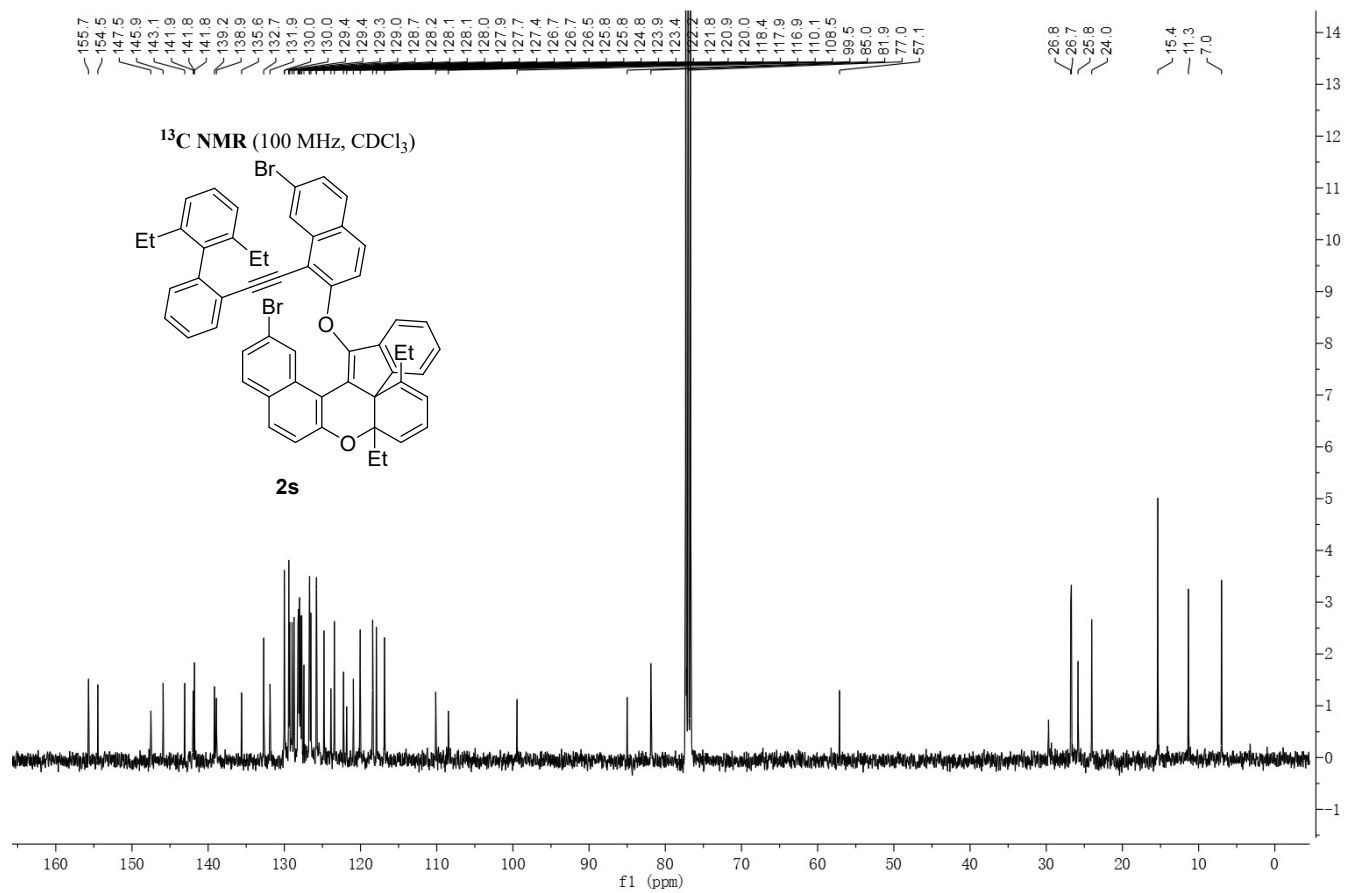
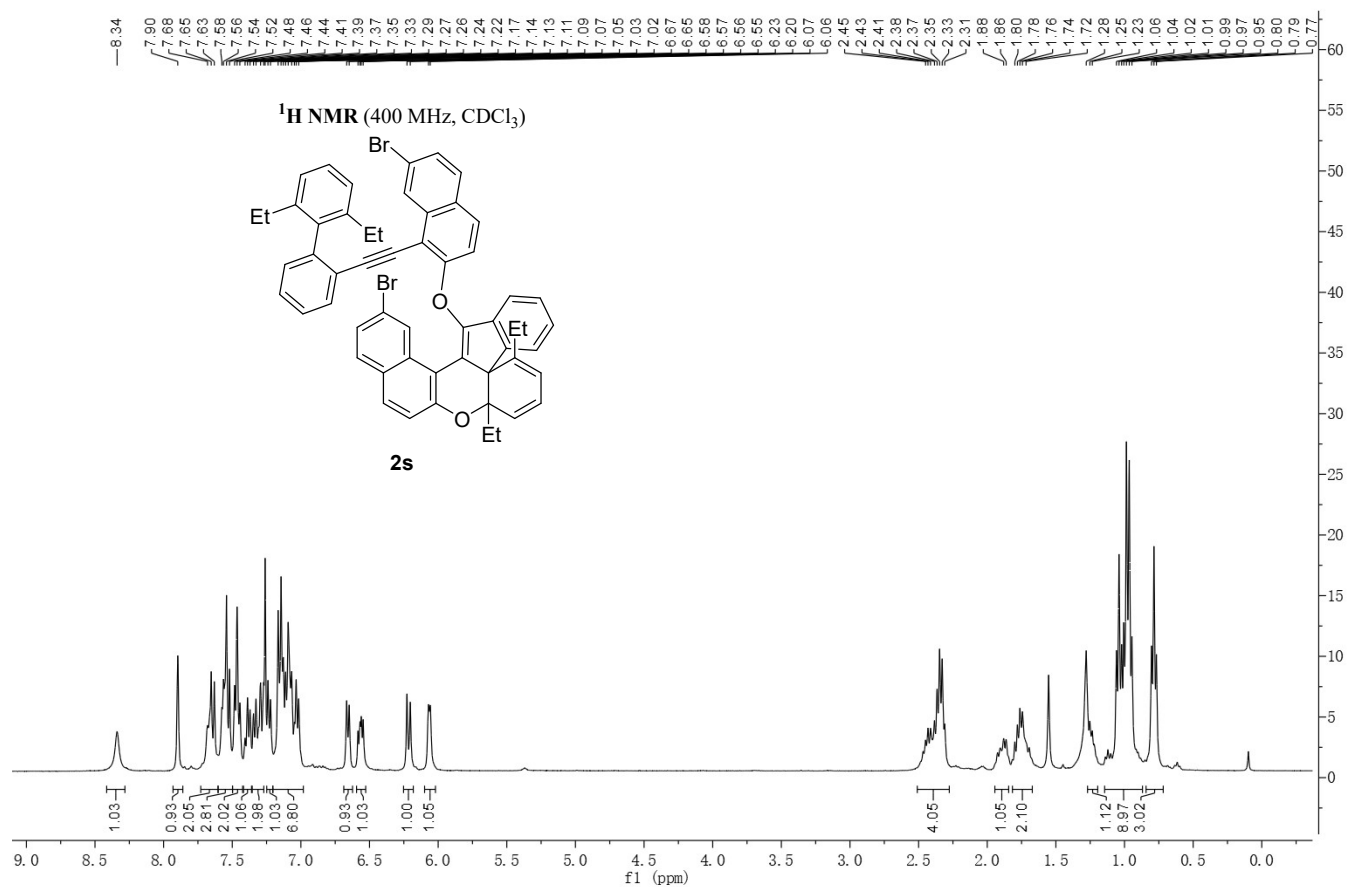


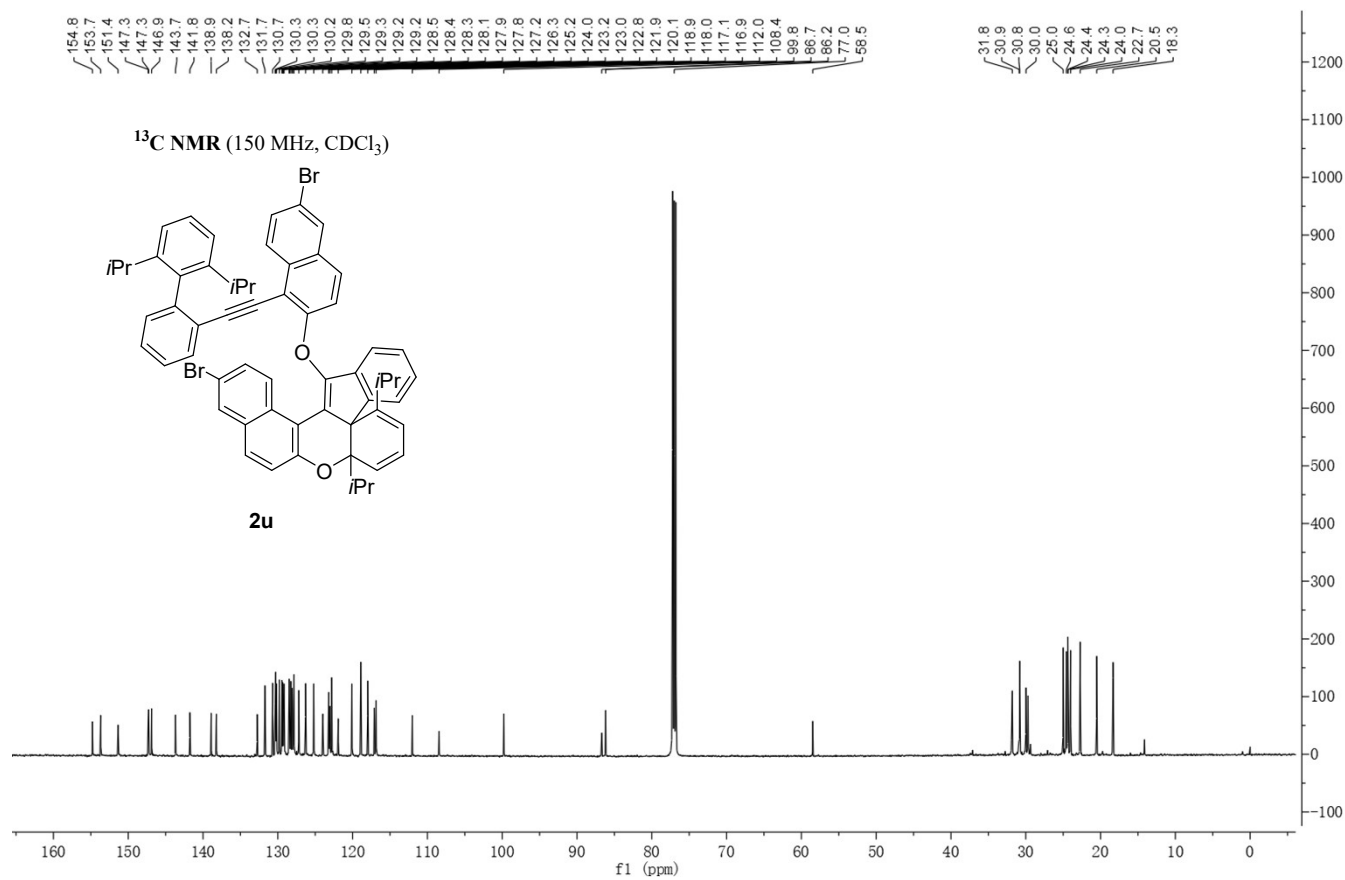
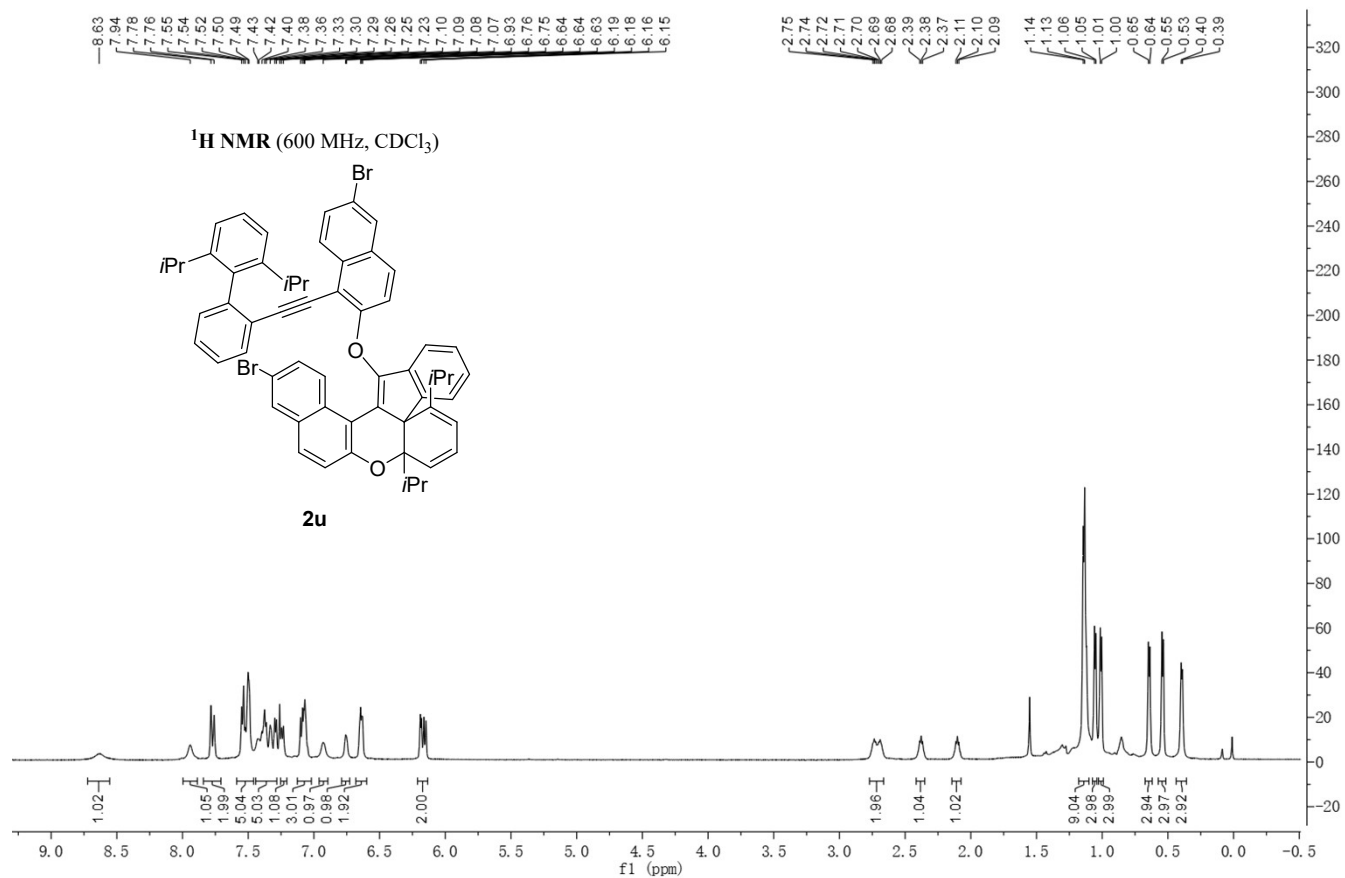


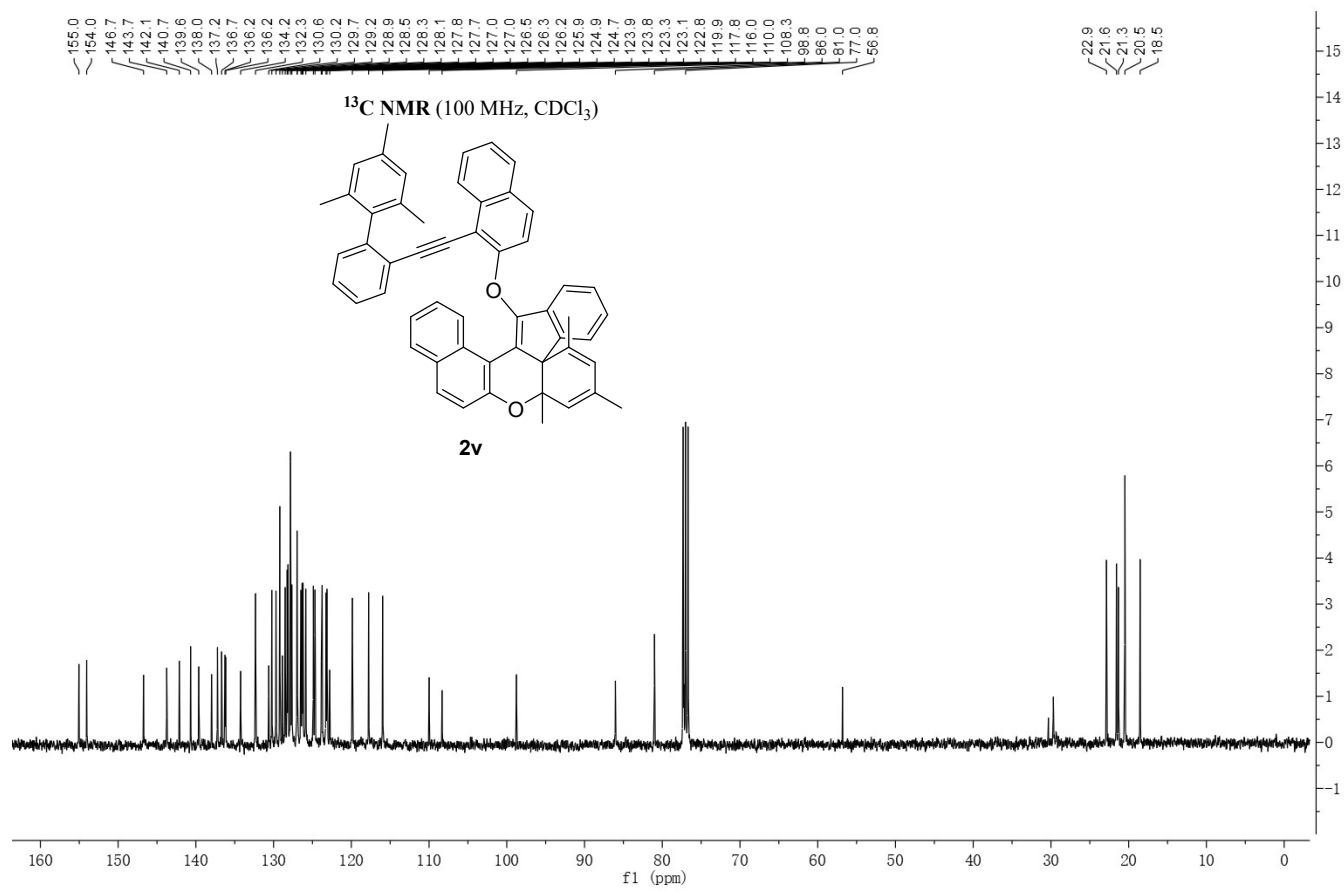
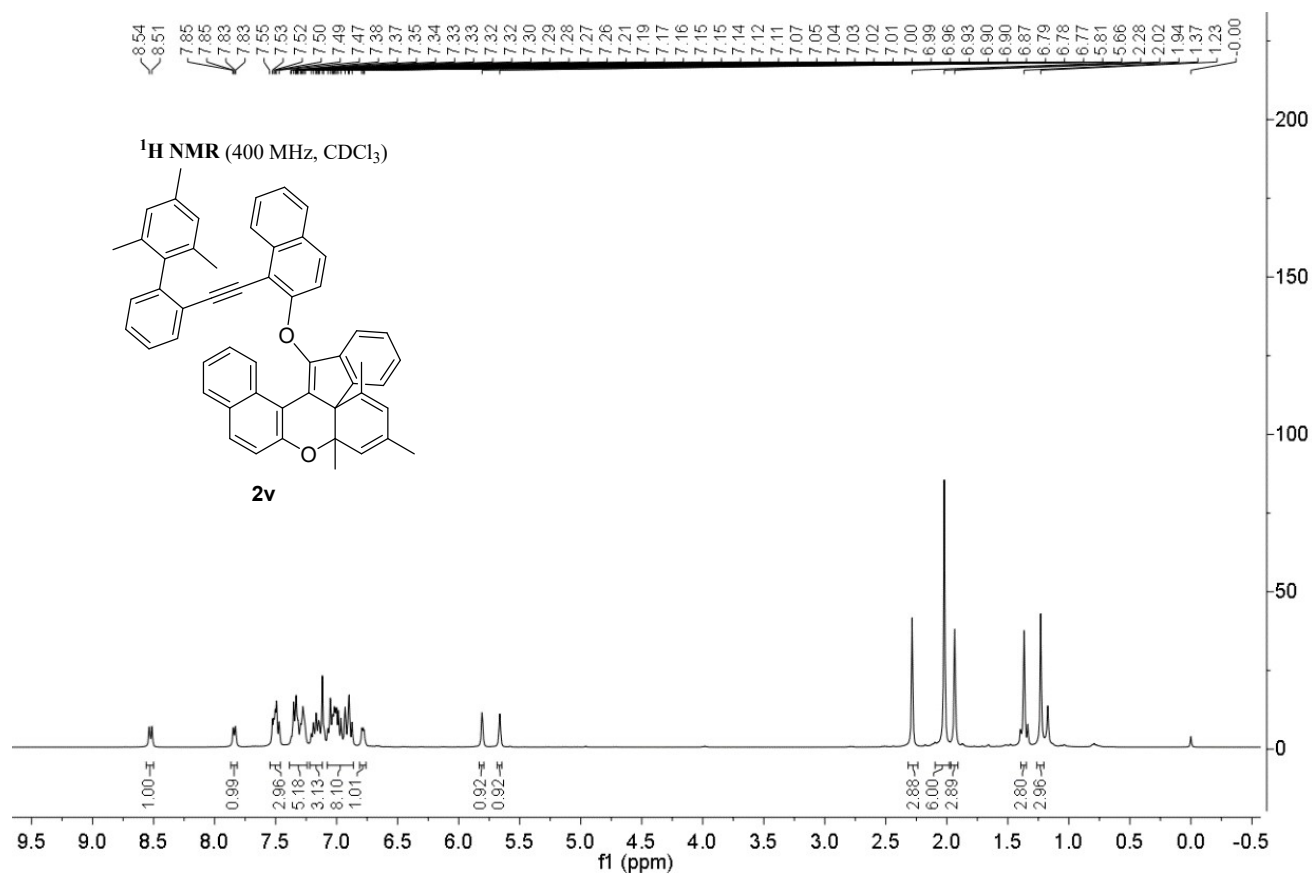


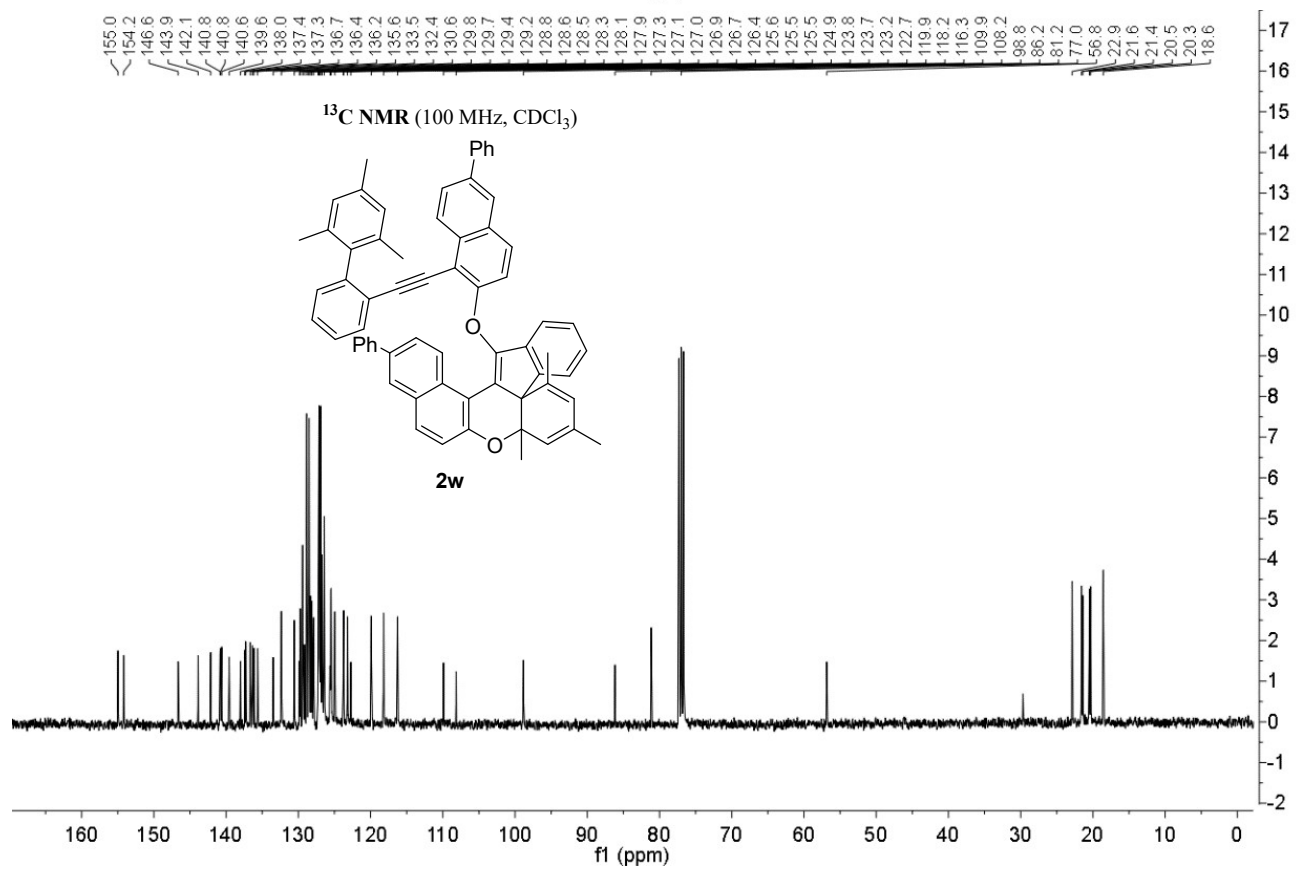
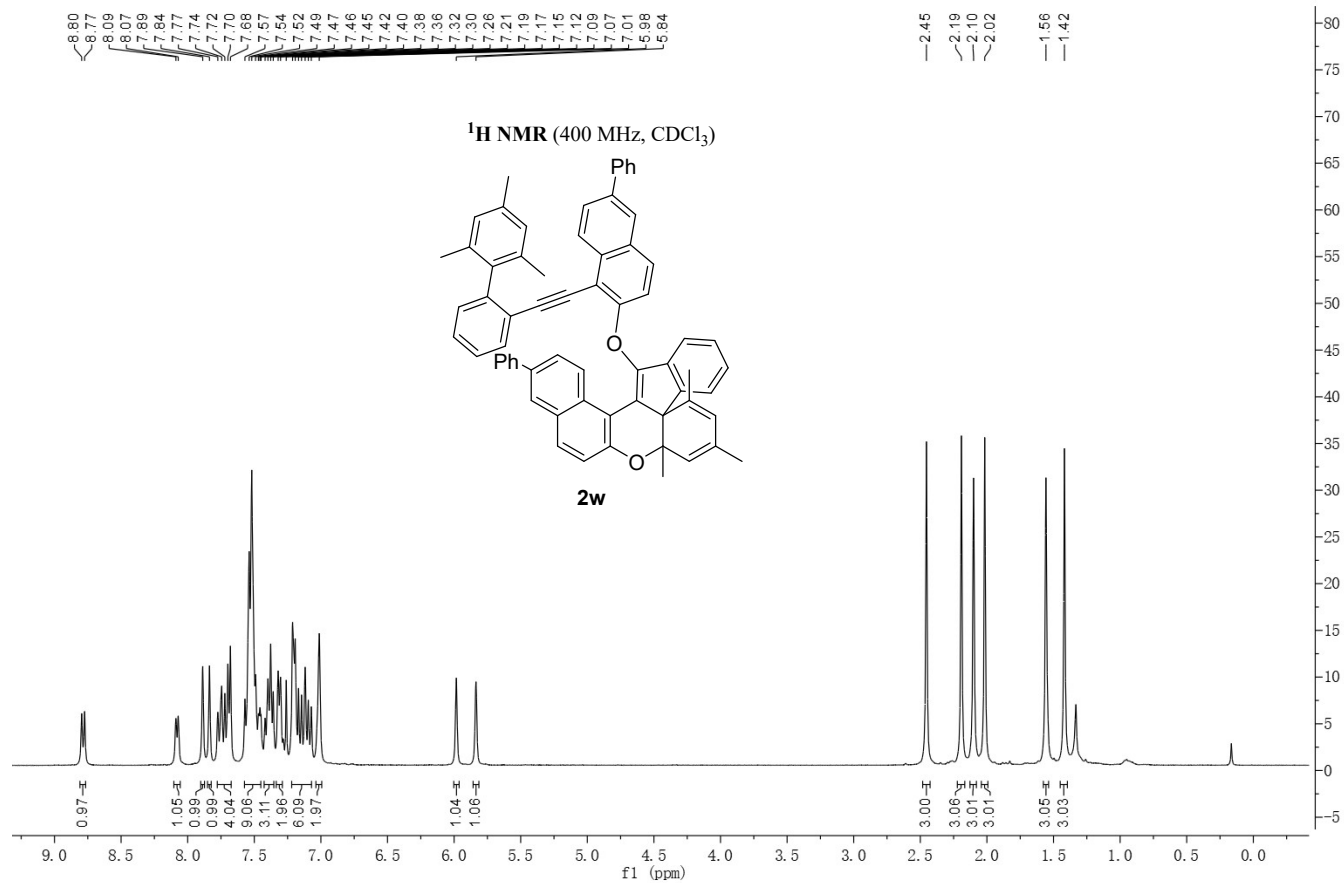












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