Supporting Information

Palladium-catalyzed cascade decarboxylative cyclization of alkyne-tethered aryl iodides with *o*-bromobenzoic acids for the synthesis of fused isoquinolinones

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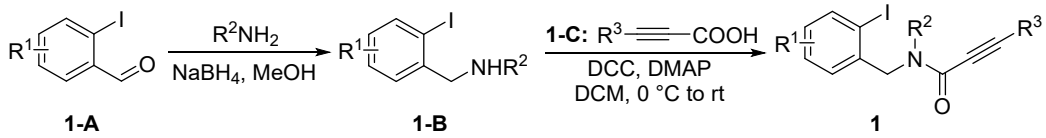
Contents

1. General Information

Unless otherwise noted, all reactions were carried out under N_2 atmosphere. All reagents were from commercial sources and used as received without further purification. All solvents were dried by standard techniques and distilled prior to use. Column chromatography was performed on silica gel (200-300 meshes) using petroleum ether (bp. 60~90 °C) and ethyl acetate as eluent. NMR spectra were recorded on a Bruker Avance operating at for 1H NMR at 400 MHz, 13C NMR at 100 MHz and spectral data were reported in ppm relative to tetramethylsilane (TMS) as internal standard and $CDCl_3$ (1H NMR δ 7.26, 13C NMR δ 77.16) or DMSO-D_6 (1H NMR δ 2.50, 13C NMR δ 39.52) as solvent. All coupling constants (*J*) are reported in Hz. The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, dd = double doublet, ddd = double doublet of doublets, t = triplet, dt = double triplet, q = quatriplet, m = multiplet, br = broad. Mass spectroscopy data of the products were collected on an HRMS-TOF instrument or Waters TOFMS GCT Premier using EI or ESI ionization. Melting points were measured with WRR digital point apparatus and not corrected.

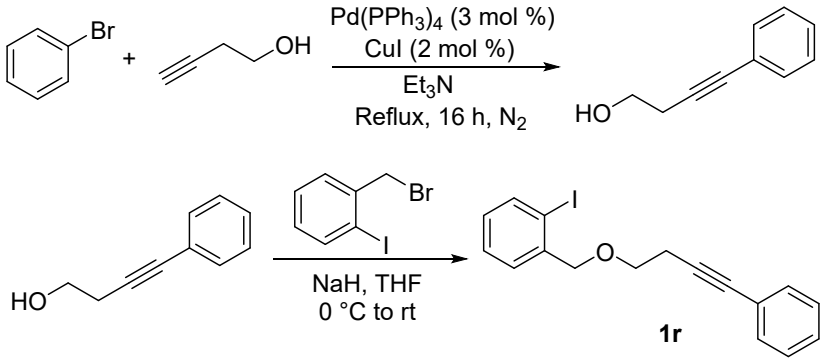
1.1 Preparation of Alkyne-Tethered Aryl Iodides 1



Step 1[1]: To a solution of *o*-iodobenzaldehyde **1-A** (5.0 mmol) in MeOH (40 mL) at 0 °C was added amines (5.0 mmol, 1.0 equiv) slowly, and the reaction mixture was stirred at room temperature for 3 h. The reaction mixture was again cooled to 0 °C, and $NaBH_4$ (7.5 mmol, 1.5 equiv) was added slowly in three portions. Then the resulting mixture was stirred at room temperature for 2 h, and the solvent was evaporated to 1/3 of its original volume under reduced pressure. The reaction was quenched with saturated aqueous $NaHCO_3$ solution and extracted with CH_2Cl_2 for three times. The combined organic phase was washed with brine, dried over Na_2SO_4, filtered and concentrated in vacuo. The obtained residue was purified via flash column chromatography on silica gel (petroleum ether/ethyl acetate = 3/1) to afford compound **1-B.**

Step 2[2]: To a solution of propiolic acid **1-C** (5.0 mmol) in CH_2Cl_2 (10 mL) was added dropwise a solution of DCC (5.0 mmol, 1.0 equiv) and DMAP (0.5 mmol, 0.1 equiv) in CH_2Cl_2 (10 mL) at 0 °C. Then **1-B** (5.0 mmol, 1.0 equiv) in CH_2Cl_2 (5 mL) was added and the mixture was stirred overnight at room temperature. The solid was filtered off and the filtrate was washed with 0.1 N HCl (10 mL), dried over Na_2SO_4, filtered and concentrated in vacuo. The obtained residue was purified via flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5/1) to afford alkyne-tethered aryl iodides **1** as white or yellow solid.

1.2 Preparation of Alkyne-Tethered Ether 1r



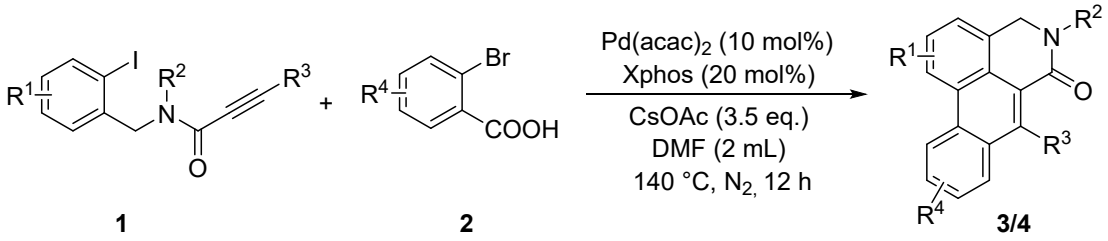
Step 1[3]: Iodobenzene (0.55 mL, 5 mmol, 1 equiv) was dissolved under N_2 atmosphere in triethylamine (20 mL). CuI (19 mg, 0.1 mmol, 0.02 equiv), $Pd(PPh_3)_4$ (173 mg, 0.15 mmol, 0.03 equiv) and but-3-yn-1-ol (0.55 mL, 7.5 mmol, 1.5 equiv) were added and the solution was heated to reflux for 16 h. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography (petroleum ether/ethyl acetate = 2/1) to afford the 4-phenylbut-3-yn-1-ol as an orange oil in almost quantitative yield (730 mg).

Step 2[4]: To a suspension of sodium hydride (60% in mineral oil, 10.0 mmol, 2.0 equiv) in anhydrous THF (10 mL) under a nitrogen atmosphere was added a solution of alcohol 4-phenylbut-3-yn-1-ol (5.0 mmol, 1.0 equiv) in anhydrous THF (10 mL) at 0 ℃. After 30 minutes, 2-iodobenzyl bromide (5.0 mmol, 1.0 equiv) in THF (5 mL) was added and the resulting mixture was stirred at room temperature overnight. The reaction was quenched with H_2O and extracted with ethyl acetate for three times. The combined organic phase was washed with brine, and dried over Na_2SO_4, filtered and concentrated

in vacuo. The obtained residue was purified via flash column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1) to afford compound **1r**.

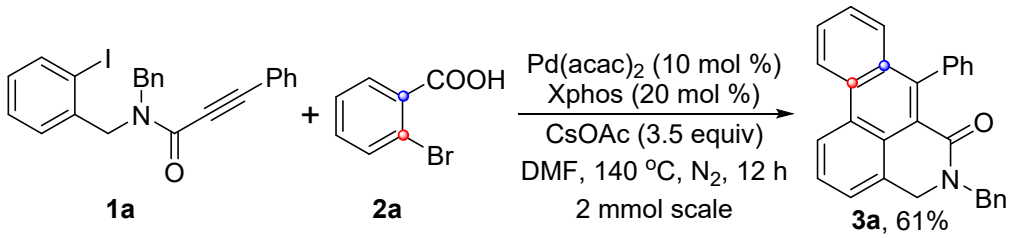
2. Experimental Procedures

2.1. General Procedure for the Synthesis of Fused Isoquinolinones 3/4



Under nitrogen atmosphere, a 25 mL Schlenk-type tube (with a Teflon screw cap and a side arm) equipped with a magnetic stir bar was charged with **1** (1.0 equiv, 0.2 mmol), **2** (1.5 equiv, 0.3 mmol), $Pd(acac)_2$ (10 mol%, 0.02 mmol, 6.1 mg), Xphos (20 mol%, 0.04 mmol, 19.1 mg), CsOAc (3.5 equiv, 0.7 mmol, 134.4 mg) and DMF (2 mL). The mixture was stirred at 140 °C (oil bath heating) for 12 hours. After cooling to room temperature slowly, the reaction mixture was extracted with EtOAc (3 X 10 mL). The combined organic phase was washed with brine, dried over Na_2SO_4, filtered and concentrated in vacuo. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate) to give the fused isoquinolinone products **3/4**.

2.2. Scale-up Reaction

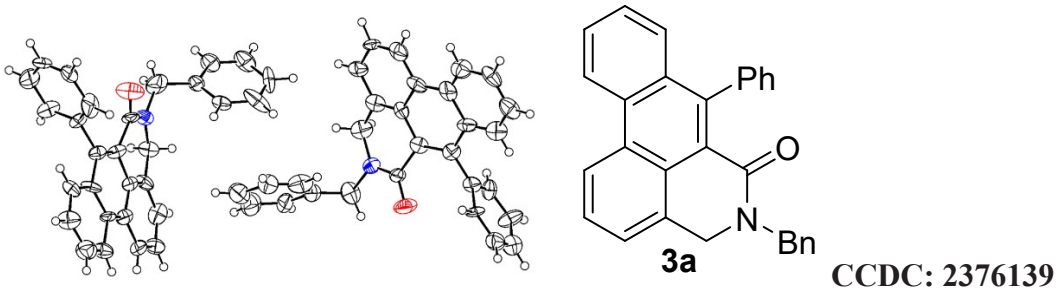


Under nitrogen atmosphere, a 250 mL Schlenk-type tube (with a Teflon screw cap and a side arm) equipped with a magnetic stir bar was charged with **1a** (1.0 equiv, 2 mmol, 902 mg), **2a** (1.5 equiv, 3 mmol, 603 mg), $Pd(acac)_2$ (10 mol%, 0.2 mmol, 61 mg), Xphos (20 mol%, 0.4 mmol, 191 mg), CsOAc (3.5 equiv, 7 mmol, 1344 mg) and DMF (20 mL). The mixture was stirred at 140 °C (oil bath heating) for 12 hours. After cooling to room temperature slowly, the reaction mixture was extracted with EtOAc (3

X 50 mL). The combined organic phase was washed with brine, dried over Na_2SO_4, filtered and concentrated in vacuo. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate) to give the fused isoquinolinone product **3a** as a white solid in 61% yield (486.8 mg).

3. The Crystal Structure of Product 3a

Figure S1. ORTEP drawing of compound **3a** with ellipsoid contour at 30% probability level



CCDC: 2376139

(a) Method for crystal growth of 3a:

0.05 mmol of **3a** was dissolved in 2.0 mL of solvent (Petroleum ether/EtOAc/DCM = 3/1/1) in 3.0 mL sample bottle. After about 12 hours of natural volatilization at room temperature, single crystal could be obtained.

(b) Crystallographic structure analysis of 3a:

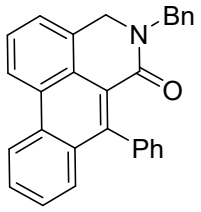
A suitable single crystal was mounted on a Xcalibur, Atlas, Gemini ultra at 296(2), 100.01(10), 296(2) and 296 K, using Mo Kα radiation (λ = 0.71073 Å). The intensity data were collected with CrysAlisPro program and reduced by CrysAlisPro program. The structure was solved by direct methods, expended by difference Fourier syntheses and refined by Full-matrix squares on F2 using SHELXL program packages. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in ideal positions and refined as riding atoms. Details of the X-Ray experiments and crystal data are summarized in **Table S1**.

Table S1. Crystal data and structure refinement for **3a**

Empirical formula	$C_{58}H_{42}N_2O_2$
Formula weight	798.93

Temperature/K	296(2)
Crystal system	orthorhombic
Space group	$Pca2_1$
a/Å	38.74(3)
b/Å	5.644(4)
c/Å	18.394(12)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4022(5)
Z	4
ρ_{calc}g/cm^3	1.319
μ/mm^{-1}	0.079
F(000)	1680.0
Crystal size/mm^3	0.16 × 0.15 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.102 to 51.5
Index ranges	$-42 \leq h \leq 47$, $-6 \leq k \leq 5$, $-16 \leq l \leq 22$
Reflections collected	20285
Independent reflections	6970 [R_{int} = 0.1888, R_{sigma} = 0.2759]
Data/restraints/parameters	6970/52/560
Goodness-of-fit on F^2	1.199
Final R indexes [I>=2σ (I)]	R_1 = 0.1588, wR_2 = 0.3393
Final R indexes [all data]	R_1 = 0.2878, wR_2 = 0.4210
Largest diff. peak/hole / e Å^{-3}	0.79/-0.47
Flack parameter	2(10)

4 Characterization Data of the Corresponding Products



5-benzyl-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**3a**)

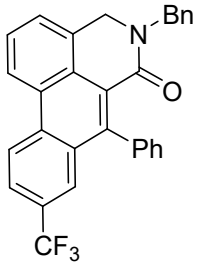
White solid, 71 % yield, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 M Hz, $CDCl_3$) δ 8.70 (d, *J* = 8.4 Hz, 1H), 8.63 (d, *J* = 8.3 Hz, 1H), 7.69 (ddd, *J* = 8.3, 5.7, 2.5 Hz, 1H), 7.64 (t, *J* = 7.7 Hz, 1H), 7.56 – 7.53 (m, 2H), 7.49 – 7.46 (m, 3H), 7.37 – 7.27 (m, 8H), 4.84 (s, 2H), 4.83 (s, 2H).

^{13}C NMR (101 M Hz, $CDCl_3$) δ 162.9, 142.9, 141.8, 137.1, 133.2, 131.4, 129.7, 129.6, 129.4, 128.9, 128.7, 128.31, 128.27, 128.0, 127.5, 127.3, 127.1, 126.7, 126.5, 123.8, 122.5, 121.3, 120.1, 50.2, 49.9.

M. p. = 202.9-203.3 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{29}H_{21}NONa^+$ 422.1521; found 422.1525.



5-benzyl-7-phenyl-9-(trifluoromethyl)-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**3b**)

White solid, yield 56%, (petroleum ether/ethyl acetate = 5:1, Rf = 0.3).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 8.7 Hz, 1H), 8.65 (d, *J* = 8.3 Hz, 1H), 7.87 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.78 (s, 1H), 7.70 (t, *J* = 7.8 Hz, 1H), 7.54 (dt, *J* = 14.1, 7.1 Hz, 3H), 7.44 (d, *J* = 7.3 Hz, 1H), 7.32 (d, *J* = 7.5 Hz, 7H), 4.85 (s, 2H), 4.85 (s, 2H).

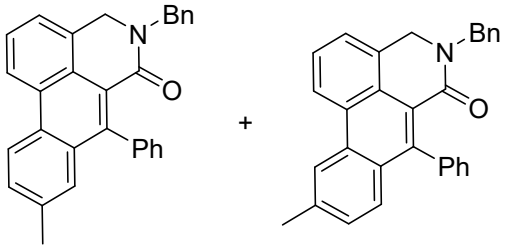
^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 142.6, 140.6, 136.9, 133.4, 132.9, 129.7, 128.9 (q, $J_{(C-F)}$ = 32.1 Hz), 129.0, 128.8, 128.8, 128.4, 128.2, 128.0, 127.7, 127.3, 127.1, 126.7

(q, $J_{(C-F)}$ = 3.7 Hz), 124.9, 124.2 (q, $J_{(C-F)}$ = 272.3 Hz), 124.0 (q, $J_{(C-F)}$ = 3.0 Hz), 123.5, 121.8, 121.4, 50.4, 49.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.3.

M. p. = 190.1-190.9 ℃.

HRMS (ESI) m/z: [M + H]+ calcd for $C_{30}H_{21}NOF_3^+$ 468.1575; found 468.1568.



Mixture of 5-benzyl-9-methyl-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de*,*g*]isoquinolin-6-one (**3c**) and 5-benzyl-10-methyl-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de*,*g*]isoquinolin-6-one (**3c′**)

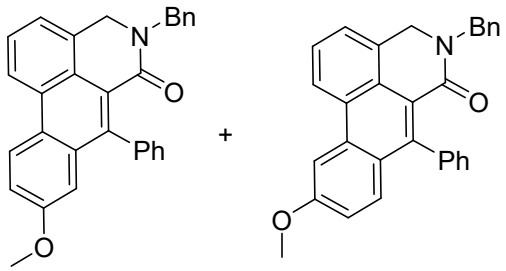
White solid, yield 80% [**3c**/**3c′**=2/1], (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 – 8.56 (m, 1.69H), 8.49 (s, 0.3H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.57 – 7.44 (m, 4H), 7.40 – 7.28 (m, 9H), 4.84 (s, 2H), 4.82 (s, 2H), 2.61 (s, 0.97H), 2.40 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 142.9, 142.7, 142.0, 141.9, 138.4, 137.1, 137.0, 133.3, 131.2, 130.1, 129.8, 129.5, 129.3, 129.1, 128.9, 128.9, 128.7, 128.3, 127.9, 127.5, 126.9, 126.7, 126.6, 126.5, 126.3, 123.7, 123.3, 122.4, 122.3, 121.3, 121.0, 120.1, 50.2, 50.2, 49.9, 22.2, 21.9.

M. p. = 213.9-214.8 ℃.

HRMS (ESI) m/z: [M + H]+ calcd for $C_{30}H_{24}NO^+$ 414.1858; found 414.1862.



Mixture of 5-benzyl-9-methoxy-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**3d**) and 5-benzyl-10-methoxy-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**3d′**)

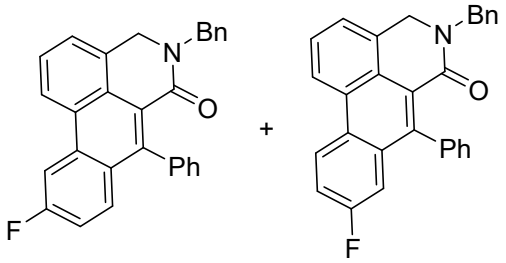
Yellow solid, yield 73% [**3d**/**3d′**=2/1], (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, *J* = 9.1 Hz, 0.64H), 8.57 – 8.45 (m, 0.97H), 8.05 (d, *J* = 2.6 Hz, 0.3H), 7.66 – 7.27 (m, 13H), 7.11 (dd, *J* = 9.2, 2.6 Hz, 0.35H), 6.86 (d, *J* = 2.7 Hz, 0.64H), 4.85 – 4.83 (m, 2H), 4.82 (s, 2H), 4.02 (s, 1H), 3.68 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1, 162.9, 159.7, 158.5, 142.9, 142.2, 142.0, 141.9, 137.2, 137.1, 134.8, 133.1, 131.4, 129.8, 129.4, 129.3, 129.0, 128.8, 128.7, 128.7, 128.3, 128.0, 127.9, 127.5, 127.5, 126.7, 126.6, 126.6, 126.3, 126.1, 125.8, 124.1, 123.9, 122.7, 121.3, 120.6, 120.5, 118.4, 117.9, 116.8, 110.2, 104.0, 55.6, 55.1, 50.2, 50.1, 49.9.

M. p. = 149.6-150.1 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{30}H_{23}NO_2Na^+$ 452.1626; found 452.1631.



Mixture of 5-benzyl-10-fluoro-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**3e**) and 5-benzyl-9-fluoro-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**3e′**)

White solid, yield 51% [**3e**/**3e′**=3/1], (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (dd, *J* = 9.1, 5.5 Hz, 0.24H), 8.54 (d, *J* = 8.3 Hz, 0.24H), 8.48 (d, *J* = 8.3 Hz, 0.74H), 8.29 (dd, *J* = 10.8, 2.6 Hz, 0.73H), 7.64 (t, *J* = 7.8 Hz, 1H), 7.59 – 7.45 (m, 4H), 7.41 – 7.27 (m, 7.85H), 7.24 – 7.17 (m, 0.83H), 7.14 (d, *J* = 2.7 Hz, 0.13H), 7.11 (d, *J* = 2.7 Hz, 0.14H), 4.84 (s, 2H), 4.83 (s, 2H).

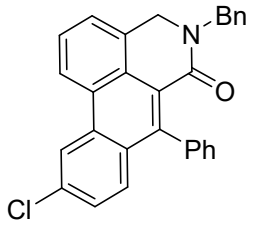
^{13}C NMR (101 MHz, $CDCl_3$) δ 163.9, 162.7, 161.4, 142.5, 141.6, 141.2, 137.0, 137.0, 133.4, 133.3, 132.3 (d, $J_{(C-F)}$ = 8.8 Hz), 130.0, 129.5, 129.0 (d, $J_{(C-F)}$ = 4.2 Hz), 128.8,

128.7, 128.3, 128.2, 128.0, 127.6, 127.6, 127.0, 126.9, 126.6, 124.8 (d, $J_{(C-F)}$ = 8.6 Hz), 124.4, 122.3 (d, $J_{(C-F)}$ = 252.9 Hz), 121.5, 119.5, 117.2 (d, $J_{(C-F)}$ = 24.0 Hz), 116.0 (d, $J_{(C-F)}$ = 23.2 Hz), 114.1 (d, $J_{(C-F)}$ = 22.7 Hz), 107.7 (d, $J_{(C-F)}$ = 22.5 Hz), 50.3, 50.2, 49.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ -111.2, -112.7.

M. p. = 223.6-224.2 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{29}H_{20}NONaF^+$ 440.1427; found 440.1428.



5-benzyl-10-chloro-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**3f**)

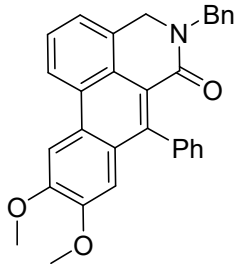
Yellow solid, yield 34 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (s, 1H), 8.53 (d, *J* = 8.3 Hz, 1H), 7.65 (t, *J* = 7.8 Hz, 1H), 7.58 – 7.51 (m, 2H), 7.49 (d, *J* = 7.2 Hz, 1H), 7.44 – 7.36 (m, 3H), 7.35 – 7.27 (m, 7H), 4.83 (s, 2H), 4.83 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1, 142.2, 140.2, 139.9, 139.7, 137.1, 130.1, 128.7, 128.3, 128.2, 128.0, 127.8, 127.5, 126.9, 126.8, 126.6, 125.1, 122.9, 122.1, 118.7, 50.1.

M. p. = 183.9-184.5 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{29}H_{20}NONaCl^+$ 456.1131; found 456.1131.



5-benzyl-9,10-dimethoxy-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**3g**)

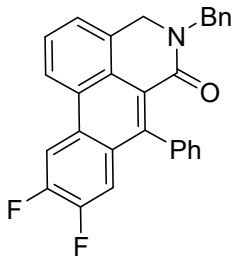
Pale yellow solid, yield 73 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 8.4 Hz, 1H), 8.00 (s, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.47 (d, *J* = 7.5 Hz, 1H), 7.37 – 7.25 (m, 8H), 6.82 (s, 1H), 4.84 (s, 2H), 4.82 (s, 2H), 4.13 (s, 3H), 3.68 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1, 150.7, 149.3, 142.2, 142.1, 137.2, 129.5, 128.9, 128.7, 128.3, 128.3, 128.0, 127.4, 126.8, 126.7, 126.7, 126.1, 122.7, 120.7, 118.5, 109.5, 102.9, 56.2, 55.6, 50.1, 50.0.

M. p. = 168.8-169.5 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{31}H_{25}NO_3Na^+$ 482.1732; found 482.1735.



5-benzyl-9,10-difluoro-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**3h**)

Yellow solid, yield 52 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

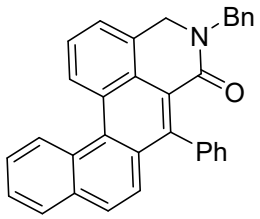
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 – 8.36 (m, 2H), 7.65 (t, *J* = 7.8 Hz, 1H), 7.59 – 7.46 (m, 3H), 7.39 (d, *J* = 7.3 Hz, 1H), 7.34 – 7.27 (m, 7H), 7.25 – 7.20 (m, 1H), 4.83 (s, 2H), 4.83 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 151.2 (dd, $J_{(C-F)}$ = 253.1, 14.8 Hz), 150.0 (dd, $J_{(C-F)}$ = 249.7, 14.3 Hz), 141.6, 141.1, 136.9, 130.8 (dd, $J_{(C-F)}$ = 6.3, 1.8 Hz), 129.7, 129.0, 128.9, 128.8, 128.7, 128.3, 128.3, 127.6, 127.2, 127.2, 126.9, 124.2, 121.7, 120.7 (d, $J_{(C-F)}$ = 2.3 Hz), 116.8 (d, $J_{(C-F)}$ = 18.7 Hz), 110.2 (d, $J_{(C-F)}$ = 18.7 Hz), 50.3, 49.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ -134.50 (ddd, *J* = 21.1, 11.8, 8.5 Hz), -135.33 – -137.13 (m).

M. p. = 234.7-235.1 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{29}H_{19}NONaF_2^+$ 458.1332; found 458.1335.



5-benzyl-7-phenyl-4,5-dihydro-6*H*-benzo[*de*]naphtho[1,2-*g*]isoquinolin-6-one (**3i**)

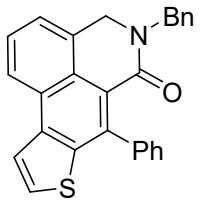
Pale yellow solid, yield 52 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 M Hz, $CDCl_3$) δ 9.05 (d, *J* = 7.7 Hz, 1H), 8.95 (d, *J* = 8.5 Hz, 1H), 7.99 (dd, *J* = 7.6, 1.9 Hz, 1H), 7.75 (d, *J* = 9.0 Hz, 1H), 7.74 – 7.65 (m, 2H), 7.68 – 7.60 (m, 1H), 7.55 (ddd, *J* = 13.4, 7.8, 6.1 Hz, 3H), 7.46 (d, *J* = 8.9 Hz, 1H), 7.39 (d, *J* = 6.5 Hz, 2H), 7.35 – 7.31 (m, 4H), 7.29 (dd, *J* = 8.0, 4.2 Hz, 1H), 4.92 (s, 2H), 4.87 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 142.1, 141.6, 137.1, 133.8, 131.6, 130.2, 129.5, 129.4, 129.2, 128.8, 128.7, 128.6, 128.3, 128.0, 127.5, 127.3, 127.2, 127.0, 126.9, 126.4, 125.9, 125.7, 123.0, 120.8, 50.1, 50.0.

M. p. = 198.7-199.6 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{33}H_{23}NONa^+$ 472.1677; found 472.1681.



5-benzyl-7-phenyl-4,5-dihydro-6*H*-benzo[*de*]thieno[3,2-*g*]isoquinolin-6-one (**3j**)

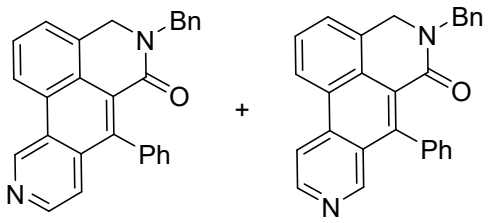
Yellow solid, yield 31 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.2 Hz, 1H), 8.02 (d, *J* = 5.4 Hz, 1H), 7.71 (d, *J* = 5.4 Hz, 1H), 7.59 (t, *J* = 7.7 Hz, 1H), 7.53 (d, *J* = 7.3 Hz, 2H), 7.49 (d, *J* = 6.6 Hz, 1H), 7.47 – 7,42 (m, 2H), 7.35 – 7.27 (m, 6H), 4.87 (s, 2H), 4.85 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 142.8, 142.2, 139.1, 137.5, 137.0, 130.7, 129.6, 128.7, 128.3, 128.2, 128.1, 128.0, 127.6, 127.5, 127.4, 126.2, 122.5, 122.4, 122.1, 50.1, 50.0.

M. p. = 193.6-194.3 ℃.

HRMS (ESI) m/z: [M + H]+ calcd for $C_{27}H_{20}NOS^+$ 406.1266; found 406.1268.



Mixture of 5-benzyl-7-phenyl-4,5-dihydro-6*H*-benzo[*de*]pyrido[3,4-*g*]isoquinolin-6-one (**3k**) and 5-benzyl-7-phenyl-4,5-dihydro-6*H*-benzo[*de*]pyrido[4,3-*g*]isoquinolin-6-one (**3k′**)

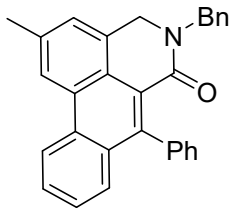
Brown solid, yield 73%[**3e**/**3e′**=4.5/1], (petroleum ether/ethyl acetate = 2:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (s, 0.82H), 7.70 (d, *J* = 7.5 Hz, 0.33H), 7.64 (d, *J* = 7.6 Hz, 0.21H), 7.46 – 7.39 (m, 2H), 7.40 – 7.25 (m, 10H), 7.22 – 7.12 (m, 1.50H), 7.12 – 7.08 (m, 1H), 7.06 – 6.99 (m, 1H), 4.84 (s, 1.68H), 4.82 (s, 0.35H), 4.42 (s, 0.37H), 4.41 (s, 1.63H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 136.9, 136.8, 136.0, 135.3, 132.4, 131.2, 130.2, 129.4, 129.1, 128.9, 128.6, 128.5, 128.2, 128.1, 128.1, 127.8, 127.7, 127.7, 126.9, 125.9, 125.1, 123.9, 50.9, 50.2, 50.0.

M. p. = 190.7-191.7 ℃.

HRMS (ESI) m/z: [M + H]+ calcd for $C_{28}H_{21}N_2O^+$ 401.1654; found 401.1639.



5-benzyl-2-methyl-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4a**)

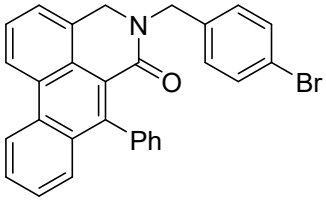
White solid, yield 32%, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, J = 8.3 Hz, 1H), 8.42 (s, 1H), 7.71 – 7.62 (m, 1H), 7.57 – 7.49 (m, 2H), 7.51 – 7.43 (m, 3H), 7.34 – 7.26 (m, 7H), 7.20 (s, 1H), 4.83 (s, 2H), 4.79 (s, 2H), 2.60 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 141.9, 137.2, 136.4, 133.4, 131.2, 129.9, 129.6, 129.2, 129.0, 128.7, 128.3, 128.1, 128.0, 127.5, 127.0, 126.6, 125.3, 122.5, 121.2, 50.2, 49.8, 22.1.

M. p. = 194.6-195.3 ℃.

HRMS (ESI) m/z: [M + H]+ calcd for $C_{30}H_{24}NO^+$ 414.1858; found 414.1859.



5-(4-bromobenzyl)-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4b**)

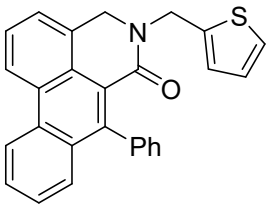
White solid, yield 39 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 8.3 Hz, 1H), 8.64 (d, *J* = 8.4 Hz, 1H), 7.73 – 7.61 (m, 2H), 7.58 – 7.50 (m, 2H), 7.48 (d, *J* = 4.0 Hz, 3H), 7.43 (d, *J* = 8.3 Hz, 2H), 7.37 (d, *J* = 7.2 Hz, 1H), 7.31 (d, *J* = 6.7 Hz, 2H), 7.17 (d, *J* = 8.3 Hz, 2H), 4.82 (s, 2H), 4.78 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 143.1, 141.7, 136.2, 133.2, 131.9, 131.4, 130.0, 129.8, 129.7, 129.1, 128.8, 128.4, 128.0, 127.2, 126.8, 126.6, 123.8, 122.5, 121.5, 121.4, 119.8, 50.0, 49.7.

M. p. = 197.3-198.1 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{29}H_{20}NONaBr^+$ 500.0626; found 500.0627.



7-phenyl-5-(thiophen-2-ylmethyl)-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4c**)

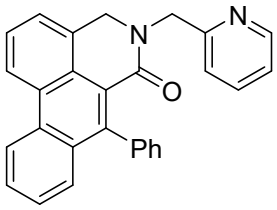
White solid, yield 56 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 8.3 Hz, 1H), 8.62 (d, *J* = 8.3 Hz, 1H), 7.72 – 7.60 (m, 2H), 7.57 – 7.52 (m, 2H), 7.51 – 7.46 (m, 3H), 7.41 (d, *J* = 7.2 Hz, 1H), 7.34 – 7.29 (m, 2H), 7.22 (dd, *J* = 5.1, 1.3 Hz, 1H), 7.04 (d, *J* = 3.2 Hz, 1H), 6.95 (dd, *J* = 5.1, 3.4 Hz, 1H), 4.97 (s, 2H), 4.92 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.5, 142.9, 141.6, 139.5, 133.1, 131.4, 129.7, 129.6, 129.3, 128.9, 128.3, 127.9, 127.1, 126.8, 126.7, 126.5, 125.7, 123.8, 122.5, 121.3, 119.9, 49.8, 45.2.

M. p. = 180.7-181.6 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{27}H_{19}NONaS^+$ 428.1085; found 428.1088.



7-phenyl-5-(pyridin-2-ylmethyl)-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4d**)

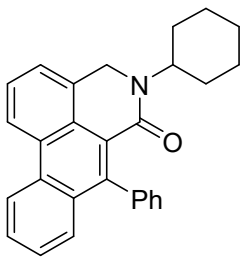
Brown solid, yield 58 %, (petroleum ether/ethyl acetate = 2:1, Rf = 0.4).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.70 (d, *J* = 8.4 Hz, 1H), 8.63 (d, *J* = 8.3 Hz, 1H), 8.54 (d, *J* = 4.5 Hz, 1H), 7.72 – 7.56 (m, 3H), 7.57 – 7.43 (m, 5H), 7.40 (d, *J* = 7.3 Hz, 1H), 7.36 – 7.28 (m, 3H), 7.17 (dd, *J* = 7.1, 5.1 Hz, 1H), 5.01 (s, 2H), 4.96 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 157.4, 149.2, 142.9, 141.7, 137.0, 133.2, 131.4, 129.7, 129.6, 129.3, 128.9, 128.3, 127.9, 127.3, 127.1, 126.7, 126.6, 123.8, 122.5, 122.5, 122.4, 121.3, 119.9, 52.4, 50.8.

M. p. = 196.2-197.0 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{28}H_{20}N_2ONa^+$ 423.1473; found 423.1475.



5-cyclohexyl-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4e**)

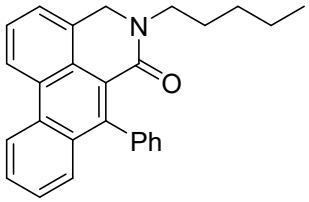
White solid, yield 61 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.70 (d, *J* = 8.3 Hz, 1H), 8.63 (d, *J* = 8.3 Hz, 1H), 7.74 – 7.59 (m, 2H), 7.56 – 7.37 (m, 6H), 7.32 – 7.27 (m, 2H), 4.86 (s, 2H), 4.74 (tt, *J* = 12.1, 3.6 Hz, 1H), 1.88 – 1.71 (m, 4H), 1.67 – 1.49 (m, 4H), 1.40 (qt, *J* = 13.9, 3.6 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.1, 142.2, 142.0, 133.4, 131.2, 130.0, 129.6, 129.5, 128.9, 128.0, 127.9, 127.1, 127.0, 126.5, 126.5, 123.6, 122.4, 121.1, 121.0, 51.9, 45.0, 29.8, 25.8, 25.7.

M. p. = 280.1-280.9 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{28}H_{25}NONa^+$ 414.1834; found 414.1834.



5-pentyl-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4f**)

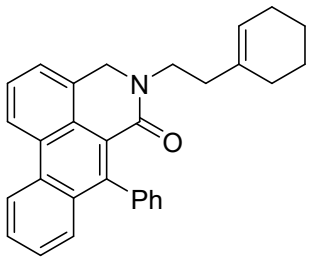
Yellow solid, yield 57 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.3 Hz, 1H), 8.64 (d, *J* = 8.3 Hz, 1H), 7.72 – 7.63 (m, 2H), 7.54 – 7.44 (m, 6H), 7.32 – 7.27 (m, 2H), 4.96 (s, 2H), 3.55 (t, J = 7.8 Hz, 2H), 1.65 (p, *J* = 7.7 Hz, 2H), 1.35 – 1.28 (m, 4H), 0.88 (t, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 142.2, 141.8, 133.3, 131.2, 129.7, 129.5, 128.9, 128.1, 127.9, 127.4, 127.1, 126.6, 126.5, 123.6, 122.4, 121.2, 120.5, 50.7, 47.5, 29.3, 26.8, 22.7, 14.2.

M. p. = 124.2-125.6 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{27}H_{25}NONa^+$ 402.1834; found 402.1836.



5-(2-(cyclohex-1-en-1-yl)ethyl)-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4g**)

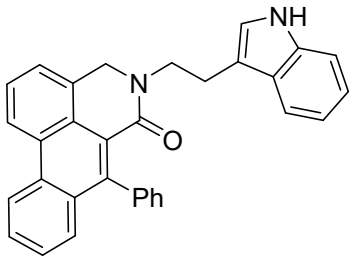
Pale yellow solid, yield 55 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.3 Hz, 1H), 8.63 (d, *J* = 8.3 Hz, 1H), 7.70 – 7.64 (m, 2H), 7.54 – 7.42 (m, 6H), 7.29 (d, *J* = 7.1 Hz, 2H), 5.41 (s, 1H), 4.95 (s, 2H), 3.66 (t, *J* = 7.4 Hz, 2H), 2.26 (t, *J* = 7.4 Hz, 2H), 1.94 (d, *J* = 21.7 Hz, 4H), 1.65 – 1.49 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3, 142.2, 141.8, 135.1, 133.2, 131.3, 129.7, 129.7, 129.5, 129.0, 128.1, 127.9, 127.5, 127.1, 126.6, 126.5, 123.5, 123.0, 122.4, 121.2, 120.6, 51.0, 46.0, 35.3, 28.5, 25.4, 23.1, 22.5.

M. p. = 130.5-131.4 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{30}H_{27}NONa^+$ 440.1990; found 440.1991.



5-(2-(1H-indol-3-yl)ethyl)-7-phenyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4h**)

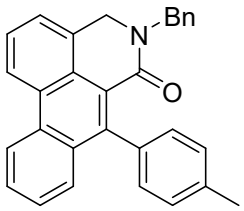
Brown solid, yield 43 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.3 Hz, 1H), 8.62 (d, *J* = 8.3 Hz, 1H), 8.07 (s, 1H), 7.69 (ddd, *J* = 8.3, 5.6, 2.6 Hz, 1H), 7.65 – 7.60 (m, 2H), 7.56 – 7.50 (m, 2H), 7.50 – 7.43 (m, 3H), 7.35 – 7.28 (m, 4H), 7.21 – 7.15 (m, 1H), 7.13 – 7.06 (m, 1H), 6.92 (d, *J* = 2.2 Hz, 1H), 4.82 (s, 2H), 3.87 (t, *J* = 7.4 Hz, 2H), 3.11 (t, *J* = 7.3 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.6, 142.2, 141.7, 136.3, 133.2, 131.3, 129.7, 129.6, 129.5, 129.0, 128.1, 127.9, 127.5, 127.4, 127.1, 126.7, 126.5, 123.5, 122.5, 122.3, 122.0, 121.2, 120.6, 119.3, 118.7, 113.2, 111.3, 51.5, 48.3, 23.1.

M. p. = 206.3-207.1 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{32}H_{24}N_2ONa^+$ 475.1786; found 475.1787.



5-benzyl-7-(p-tolyl)-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4i**)

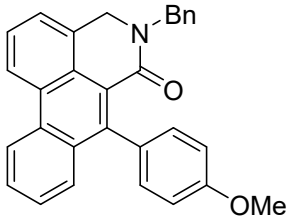
White solid, yield 53 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.3 Hz, 1H), 8.63 (d, *J* = 8.3 Hz, 1H), 7.68 (ddd, *J* = 8.3, 6.7, 1.5 Hz, 1H), 7.63 (t, *J* = 7.8 Hz, 1H), 7.55 – 7.44 (m, 2H), 7.38 – 7.27 (m, 8H), 7.23 (s, 1H), 7.21 (s, 1H), 4.85 (s, 2H), 4.83 (s, 2H), 2.50 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 143.1, 138.7, 137.1, 136.0, 133.4, 131.4, 129.7, 129.7, 129.3, 128.8, 128.7, 128.3, 128.2, 127.5, 127.3, 127.1, 126.5, 123.7, 122.4, 121.3, 120.1, 50.2, 49.9, 21.7.

M. p. = 136.9-137.8 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{30}H_{23}NONa^+$ 436.1677; found 436.1681.



5-benzyl-7-(4-methoxyphenyl)-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4j**)

White solid, yield 58 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

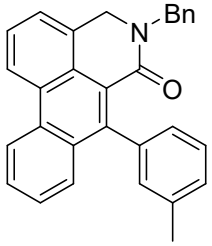
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.3 Hz, 1H), 8.63 (d, *J* = 8.3 Hz, 1H), 7.69 (ddd, *J* = 8.3, 6.8, 1.5 Hz, 1H), 7.66 – 7.61 (m, 1H), 7.58 – 7.53 (m, 1H), 7.52 – 7.45

(m, 1H), 7.36 (dd, *J* = 7.2, 1.3 Hz, 1H), 7.32 – 7.28 (m, 4H), 7.25 – 7.21 (m, 3H), 4.85 (s, 2H), 4.83 (s, 2H), 3.92 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 158.4, 142.8, 137.1, 133.9, 133.6, 131.4, 130.0, 129.7, 128.8, 128.3, 128.2, 127.5, 127.4, 127.1, 126.5, 123.7, 122.5, 121.3, 120.3, 113.5, 55.3, 50.3, 49.9.

M. p. = 161.3-162.4 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{30}H_{23}NO_2Na^+$ 452.1626; found 452.1630.



5-benzyl-7-(m-tolyl)-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one(**4k**)

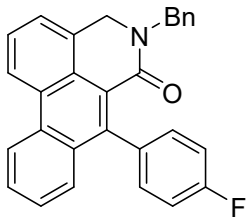
White solid, yield 54 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.3 Hz, 1H), 8.62 (d, *J* = 8.3 Hz, 1H), 7.69 (ddd, *J* = 8.3, 6.5, 1.7 Hz, 1H), 7.63 (t, *J* = 7.8 Hz, 1H), 7.54 – 7.47 (m, 2H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.36 (d, *J* = 7.3 Hz, 1H), 7.33 – 7.27 (m, 6H), 7.17 – 7.12 (m, 2H), 4.85 (d, *J* = 5.0 Hz, 2H), 4.83 (s, 2H), 2.47 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 143.1, 141.7, 137.2, 137.2, 133.3, 131.4, 129.7, 129.7, 129.6, 1294, 128.7, 128.3, 128.2, 127.8, 127.6, 127.5, 127.3, 127.1, 126.5, 126.1, 123.7, 122.4, 121.3, 120.1, 50.3, 50.0, 21.9.

M. p. = 146.2-147.1 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{30}H_{23}NONa^+$ 436.1677; found 436.1681.



5-benzyl-7-(4-fluorophenyl)-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4l**)

White solid, yield 60 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

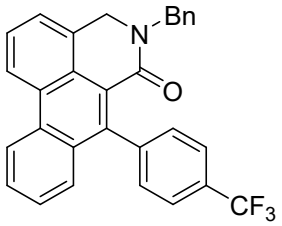
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 8.3 Hz, 1H), 8.63 (d, *J* = 8.3 Hz, 1H), 7.70 (t, *J* = 7.3 Hz, 1H), 7.65 (t, *J* = 7.8 Hz, 1H), 7.55 – 7.43 (m, 2H), 7.37 (d, *J* = 7.2 Hz, 1H), 7.35 – 7.26 (m, 6H), 7.25 – 7.18 (m, 3H), 4.84 (s, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 161.9 (d, $J_{(C-F)}$ = 244.5 Hz), 141.8, 137.5 (d, $J_{(C-F)}$ = 3.5 Hz), 137.0, 133.2, 131.4, 130.3 (d, $J_{(C-F)}$ = 7.9 Hz), 129.8, 129.4, 129.4, 128.8, 128.4, 128.3, 127.6, 127.2, 127.2, 126.7, 123.9, 122.6, 121.3, 120.4, 120.4, 115.1 (d, $J_{(C-F)}$ = 21.2 Hz), 50.3, 49.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ -116.6.

M. p. = 208.2-209.1 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{29}H_{20}NONaF^+$ 440.1427; found 440.1431.



5-benzyl-7-(4-(trifluoromethyl)phenyl)-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4m**)

White solid, yield 60 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

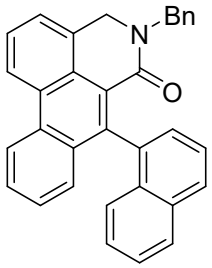
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (d, *J* = 8.3 Hz, 1H), 8.64 (d, *J* = 8.3 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 2H), 7.69 (dt, *J* = 15.8, 7.7 Hz, 2H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 7.3 Hz, 1H), 7.37 – 7.27 (m, 6H), 4.86 (s, 2H), 4.84 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7, 146.0, 141.1, 136.7, 132.6, 131.4, 129.9, 129.3, 129.2, 129.1, 128.8, 128.5, 128.3 (q, $J_{(C-F)}$ = 31.8 Hz), 128.2, 127.7, 127.4, 126.9, 126.9, 125.01 (q, $J_{(C-F)}$ = 3.6 Hz), 124.7 (q, $J_{(C-F)}$ = 272.0 Hz), 124.0, 122.7, 121.3, 120.1, 50.2, 49.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.5.

M. p. = 193.5-194.3 ℃.

HRMS (ESI) m/z: [M + H]+ calcd for $C_{30}H_{21}NOF_3^+$ 468.1575; found 468.1573.



5-benzyl-7-(naphthalen-1-yl)-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4n**)

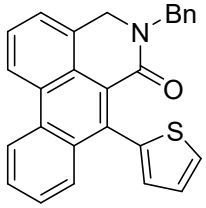
Yellow solid, yield 52 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 8.3 Hz, 1H), 8.69 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 4.1 Hz, 1H), 7.96 (d, *J* = 4.1 Hz, 1H), 7.75 – 7.59 (m, 3H), 7.50 – 7.41 (m, 2H), 7.39 – 7.31 (m, 3H), 7.30 – 7.26 (m, 2H), 7.25 – 7.19 (m, 5H), 4.86 (d, *J* = 4.7 Hz, 2H), 4.73 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3, 141.0, 139.8, 137.1, 133.4, 133.3, 133.0, 131.5, 130.0, 129.7, 129.5, 128.7, 128.6, 128.4, 128.3, 127.5, 127.3, 127.1, 126.7, 126.1, 125.9, 125.8, 125.6, 125.6, 123.8, 122.5, 121.5, 121.3, 50.3, 50.1.

M. p. = 180.2-180.9 ℃.

HRMS (ESI) m/z: [M + H]+ calcd for $C_{33}H_{24}NO^+$ 450.1858; found 450.1861.



5-benzyl-7-(thiophen-2-yl)-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4o**)

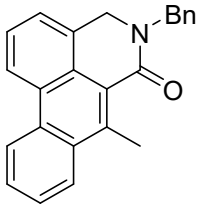
Yellow solid, yield 57 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 8.3 Hz, 1H), 8.62 (d, *J* = 8.3 Hz, 1H), 7.78 (d, *J* = 8.3 Hz, 1H), 7.71 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.68 – 7.61 (m, 1H), 7.60 – 7.50 (m, 2H), 7.37 (dd, *J* = 7.3, 1.3 Hz, 1H), 7.36 – 7.29 (m, 4H), 7.25 – 7.22 (m, 2H), 7.04 (dd, *J* = 3.4, 1.2 Hz, 1H), 4.88 (s, 2H), 4.83 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 137.0, 134.9, 133.6, 131.2, 130.1, 129.6, 129.2, 128.8, 128.5, 128.4, 127.6, 127.5, 127.2, 127.0, 126.9, 126.8, 125.5, 123.8, 122.6, 122.4, 121.3, 50.4, 49.9.

M. p. = 164.9-165.8 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{24}H_{19}NONaS^+$ 428.1085; found 450.1090.



5-benzyl-7-methyl-4,5-dihydro-6*H*-dibenzo[*de,g*]isoquinolin-6-one (**4p**)

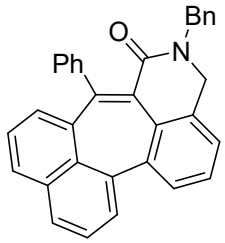
White solid, yield 41 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.43 (d, *J* = 8.3 Hz, 1H), 8.27 (dd, *J* = 7.4, 2.4 Hz, 1H), 7.66 – 7.54 (m, 2H), 7.44 (t, *J* = 8.3 Hz, 1H), 7.36 – 7.29 (m, 2H), 7.25 (t, *J* = 7.3 Hz, 2H), 7.22 – 7.17 (m, 2H), 4.85 (s, 2H), 4.73 (s, 2H), 3.21 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.8, 137.3, 133.2, 131.2, 128.9, 128.4, 128.3, 128.1, 127.9, 127.6, 127.4, 126.5, 125.8, 123.4, 123.0, 121.3, 121.2, 50.8, 50.3, 17.7.

M. p. = 164.3-164.9 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{24}H_{19}NONa^+$ 360.1368; found 360.1364.



2-benzyl-13-phenyl-2,3-dihydro-1*H*-naphtho[1',8':4,5,6]cyclohepta[1,2,3-*de*]isoquinolin-1-one (**5**)

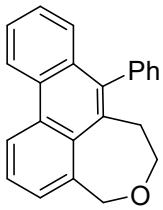
Yellow solid, yield 54 %, (petroleum ether/ethyl acetate = 5:1, Rf = 0.4).

^{1}H NMR (400 M Hz, $CDCl_3$) δ 7.73 (d, *J* = 7.7 Hz, 1H), 7.65 (t, *J* = 6.7 Hz, 2H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.42 – 7.27 (m, 9H), 7.24 (s, 1H), 7.19 (t, *J* = 7.7 Hz, 1H), 7.08 (d, *J* = 7.4 Hz, 1H), 6.99 (d, *J* = 7.9 Hz, 1H), 6.92 (d, *J* = 7.3 Hz, 1H), 6.74 (d, *J* = 7.6 Hz, 1H), 4.66 (dd, *J* = 270.3, 14.7 Hz, 2H), 4.42 (dd, *J* = 216.2, 15.2 Hz, 2H).

^{13}C NMR (101 M Hz, $CDCl_3$) δ 167.2, 151.3, 146.2, 140.7, 140.5, 137.6, 137.3, 136.9, 134.0, 133.5, 133.4, 133.2, 132.6, 131.3, 130.7, 129.6, 129.0, 128.9, 128.7, 128.4, 128.3, 128.0, 127.9, 127.7, 127.6, 126.4, 124.8, 124.3, 50.4, 49.9.

M. p. = 218.3-218.8 ℃.

HRMS (ESI) m/z: [M + Na]+ calcd for $C_{33}H_{23}NONa^+$ 472.1677; found 472.1679.



8-phenyl-6,7-dihydro-4*H*-phenanthro[1,10-*cd*]oxepine (**6**)

Yellow sticky oil, yield 42 %, (petroleum ether/ethyl acetate = 10:1, Rf = 0.65).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.4 Hz, 2H), 7.61 – 7.51 (m, 4H), 7.48 (d, *J* = 7.3 Hz, 1H), 7.45 – 7.37 (m, 2H), 7.37 – 7.29 (m, 3H), 5.17 (s, 2H), 4.11 (t, *J* = 6.0 Hz, 2H), 3.19 (t, *J* = 6.0 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.4, 139.7, 137.9, 132.7, 132.3, 132.3, 131.6, 130.5, 129.9, 128.8, 127.7, 127.6, 127.5, 126.6, 126.1, 125.8, 122.8, 122.6, 70.6, 70.3, 32.5.

HRMS (ESI) m/z: [M + H]+ calcd for $C_{23}H_{19}O^+$ 311.1430; found 311.1427.

5 References

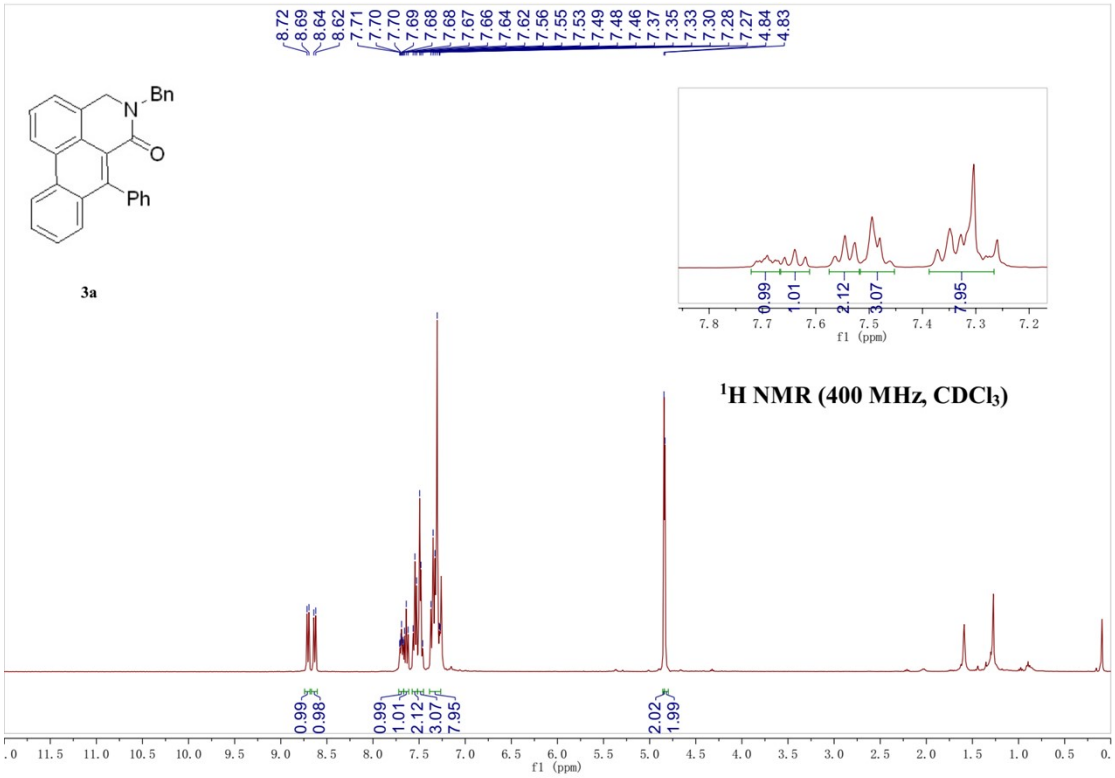
[1] Konishi, H.; Tanaka, H.; Manabe, K. *Org. Lett*., **2017**, *19*, 1578-1581.

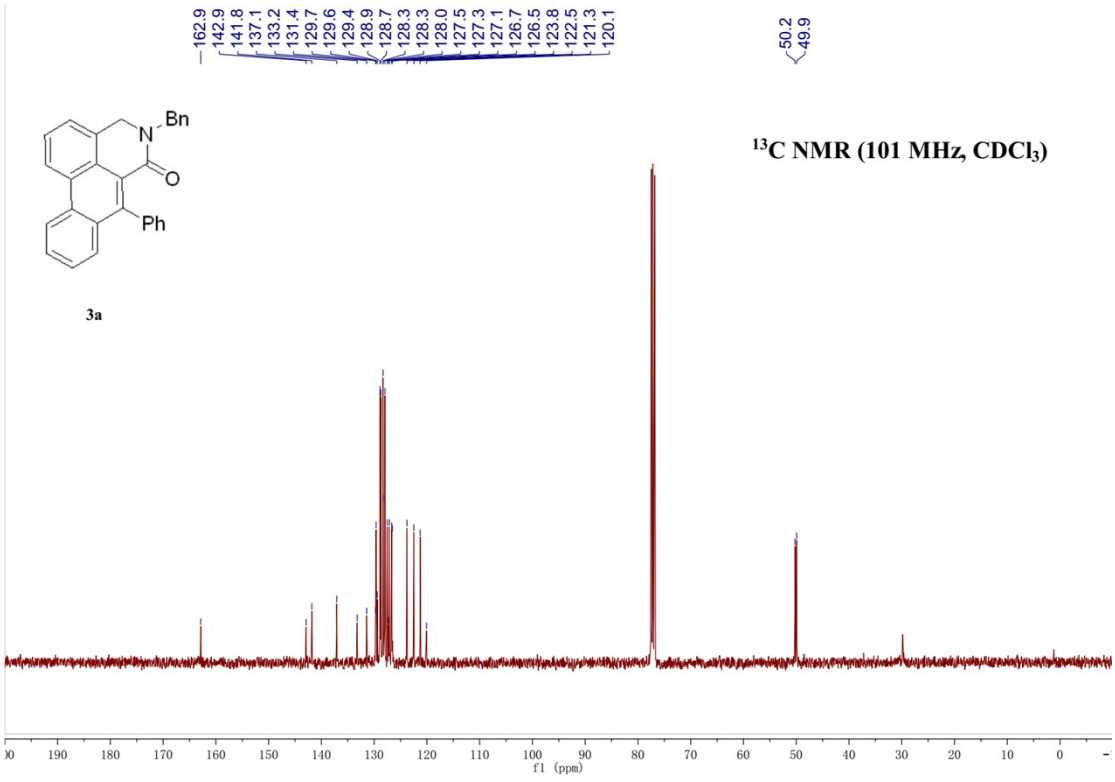
[2] Rodríguez, J. F.; Burton, K. I.; Franzoni, I.; Petrone, D. A.; Scheipers, I.; Lautens, M. *Org. Lett*., **2018**, *20*, 6915-6919.

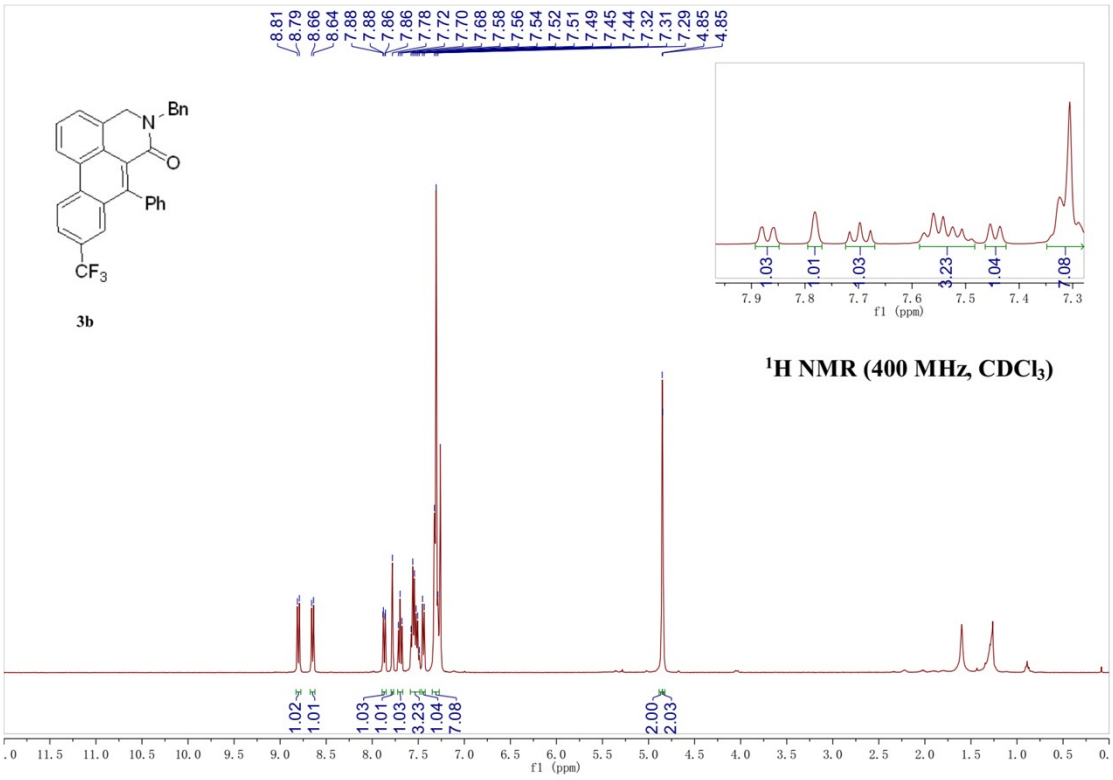
[3] Marina W.; Dirk S.; Simon M. A.; Bernhard W. *Bioorg. Med. Chem.*, **2019**, 27, 3559–3567.

[4] Strat, F. L.; Harrowven, D. C.; Maddaluno, J. *J. Org. Chem*., **2005**, *70*, 489-498.

6 Copy of ^{1}H, ^{13}C and ^{19}F NMR Spectra of Products



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7.54
7.52
7.51
7.49
7.45
7.44
7.32
7.31
7.29
4.85
4.85
Bn
N
O
Ph
CF3
3b
1.03
1.01
1.03
3.23
1.04
7.08
f1 (ppm)
1H NMR (400 MHz, CDCl3)
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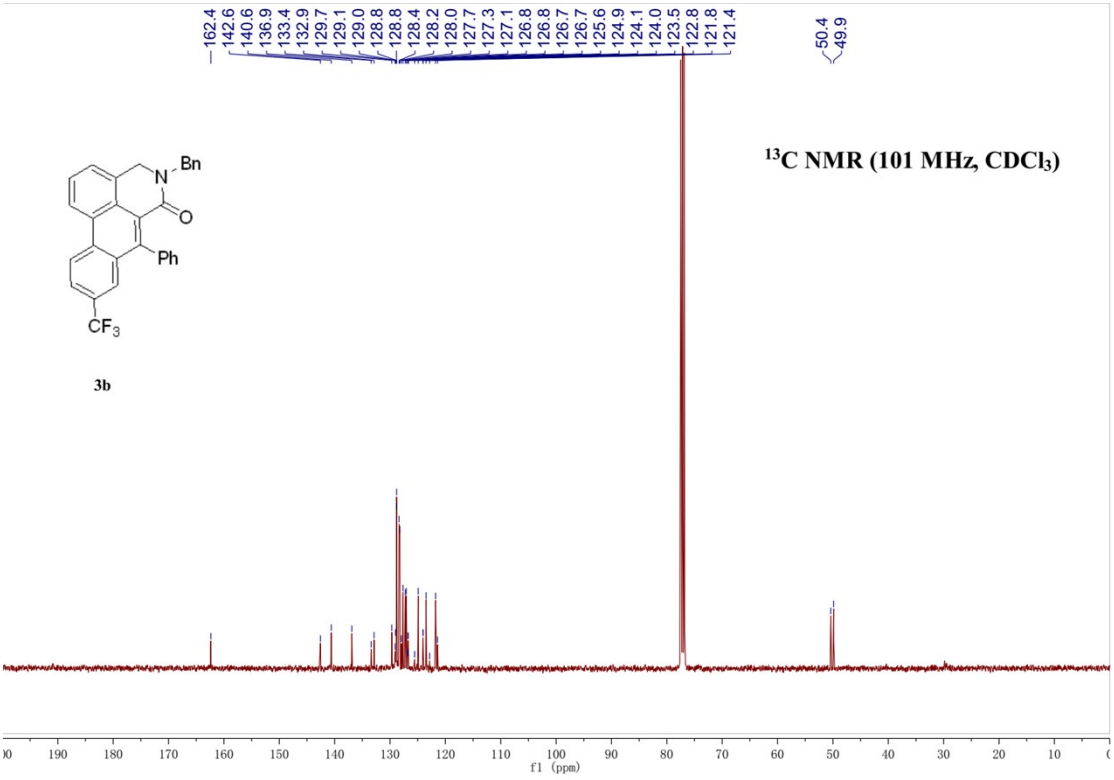
1.03
1.01
1.03
3.23
1.04
7.08
2.00
2.03
f1 (ppm)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140.6
136.9
133.4
132.9
129.7
129.1
129.0
128.8
128.8
128.4
128.2
128.0
127.7
127.3
127.1
126.8
126.8
126.7
125.6
124.9
124.1
124.0
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122.8
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N
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Ph
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3b
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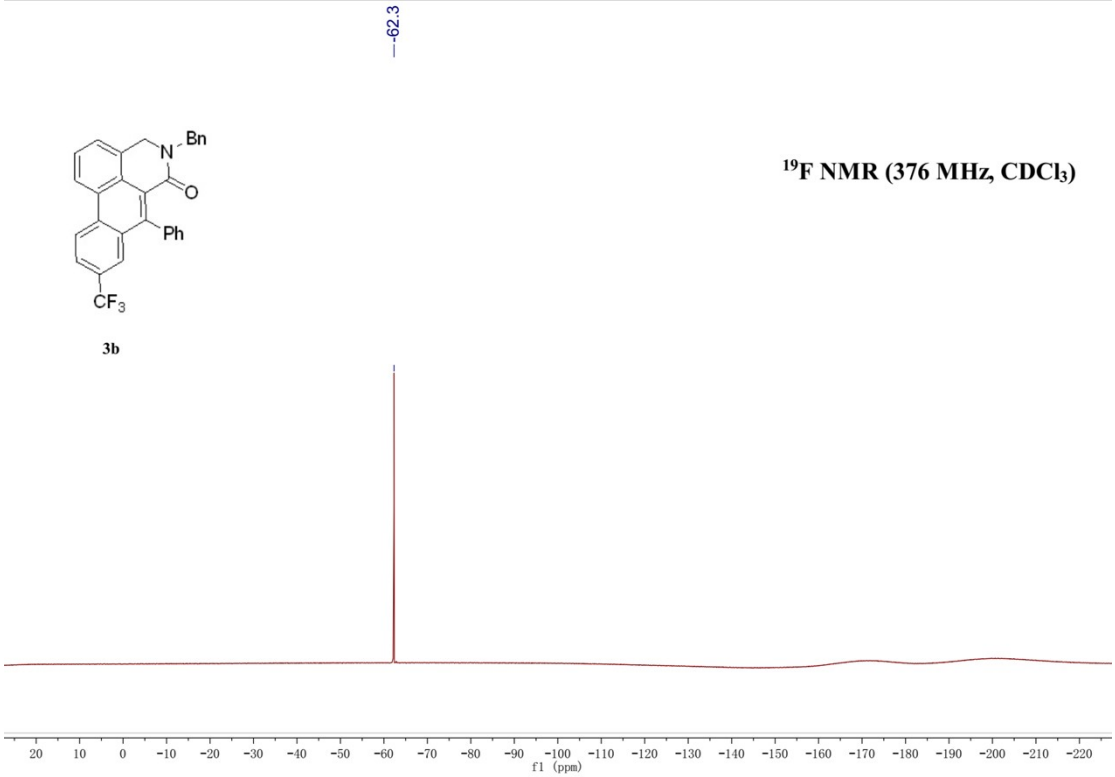
f1 (ppm)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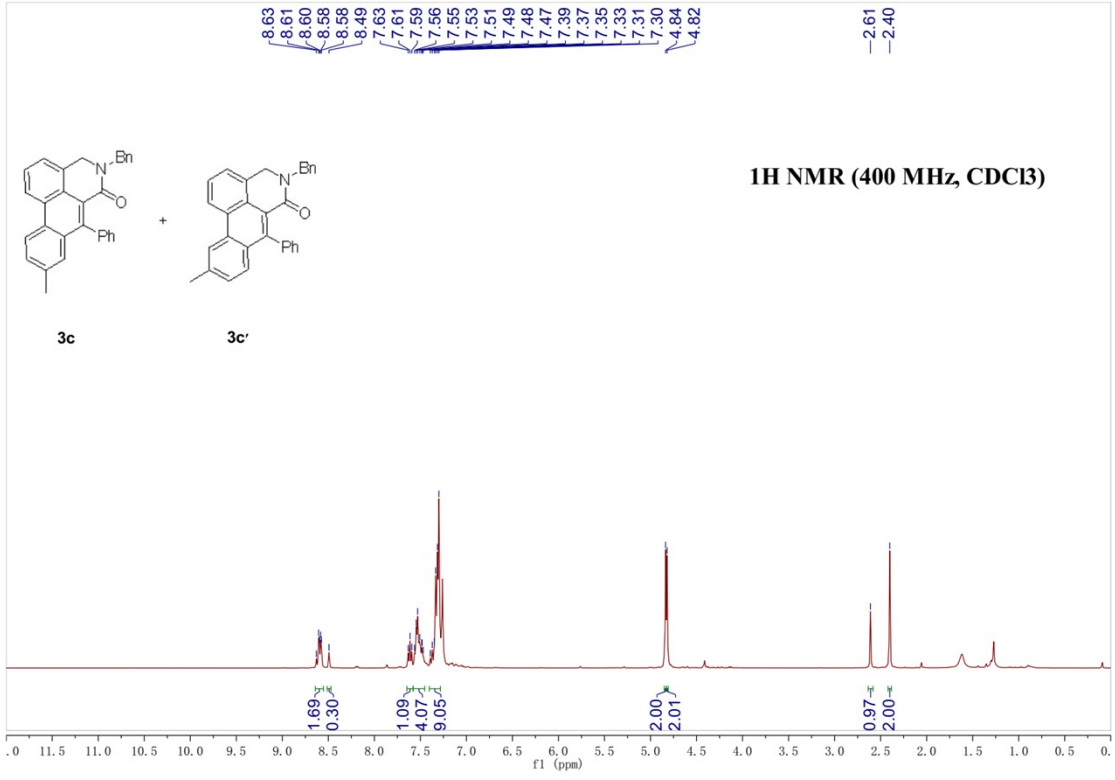
f1 (ppm)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4.82
2.61
2.40
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N
O
Ph
+
3c
3c'
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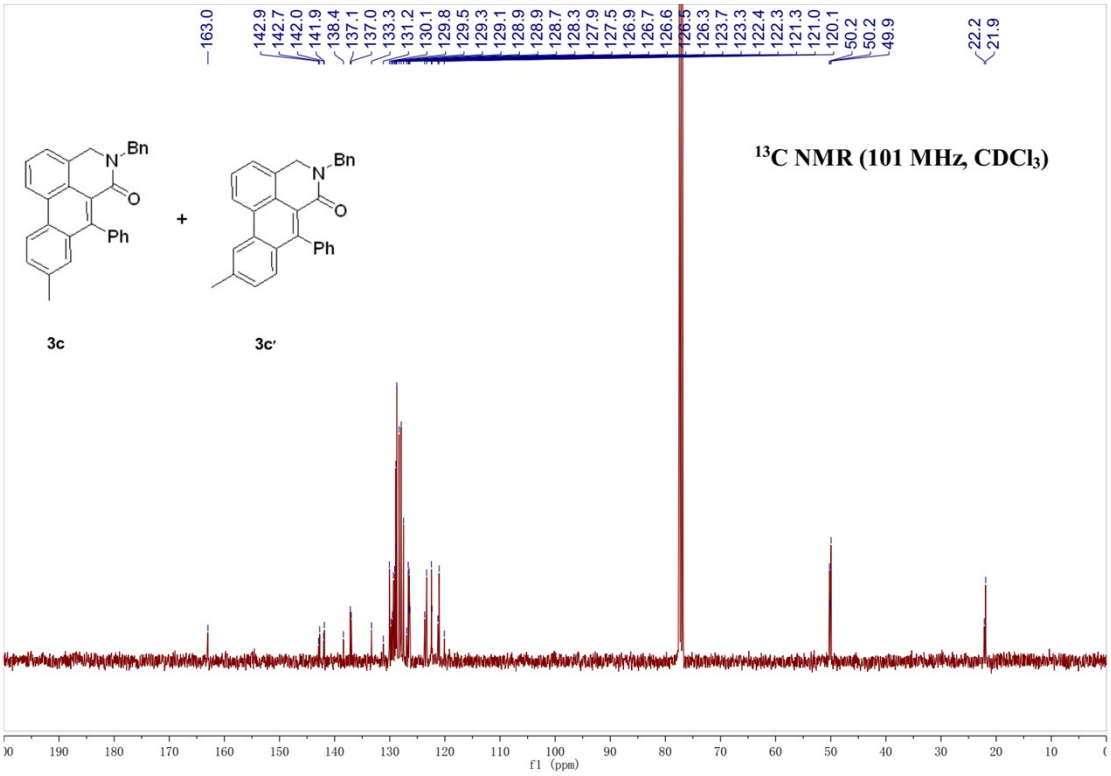
f1 (ppm)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129.1
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121.3
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120.1
50.2
50.2
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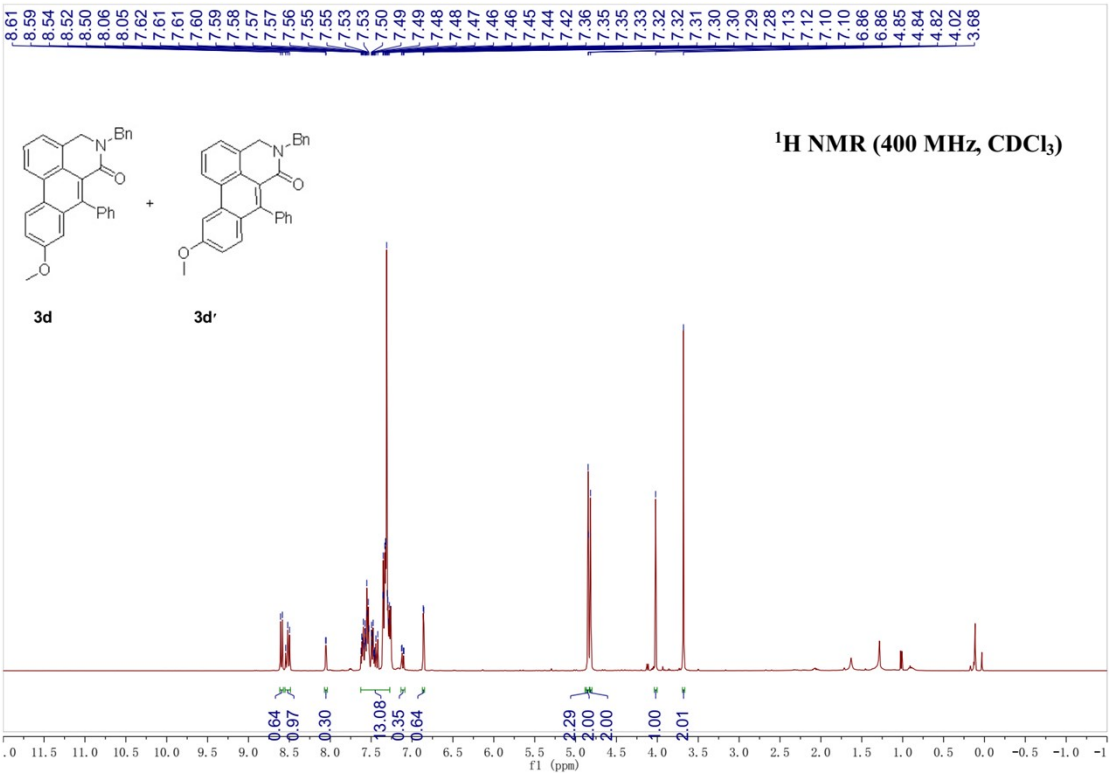
N
O
Ph
+
3c
3c′
13C NMR (101 MHz, CDCl3)
f1 (ppm)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Ph
+
O
3d
3d′
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2.00
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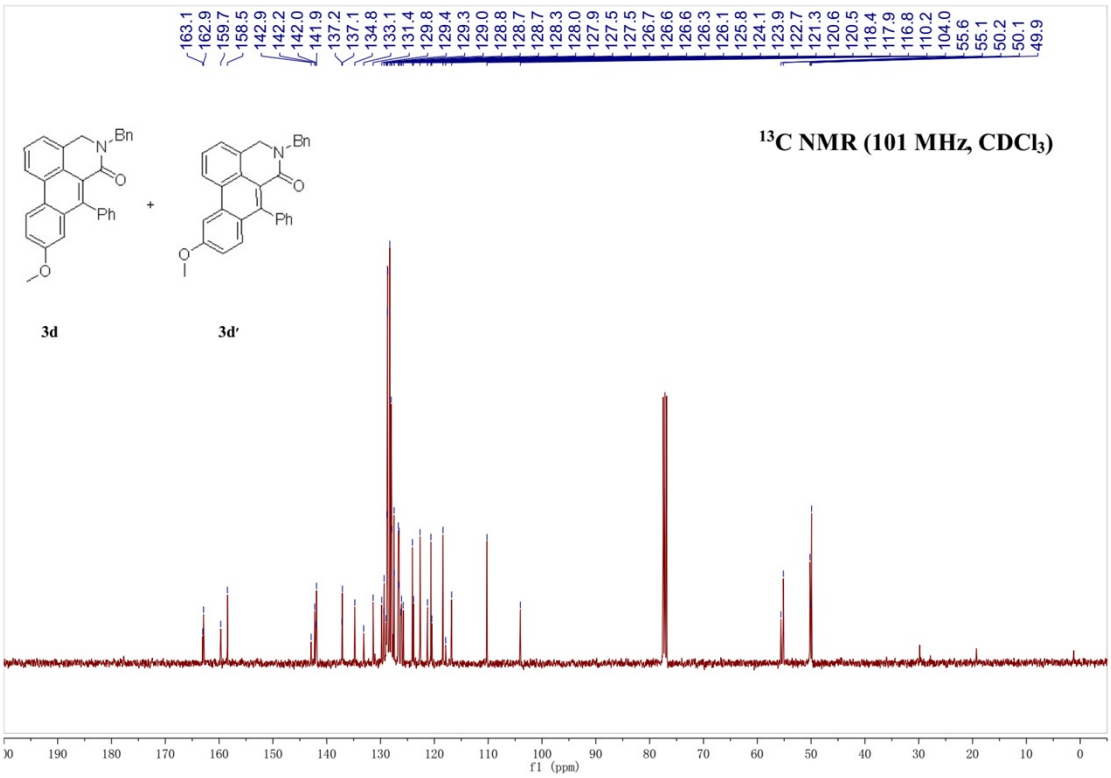
f1 (ppm)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49.9
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O
Ph
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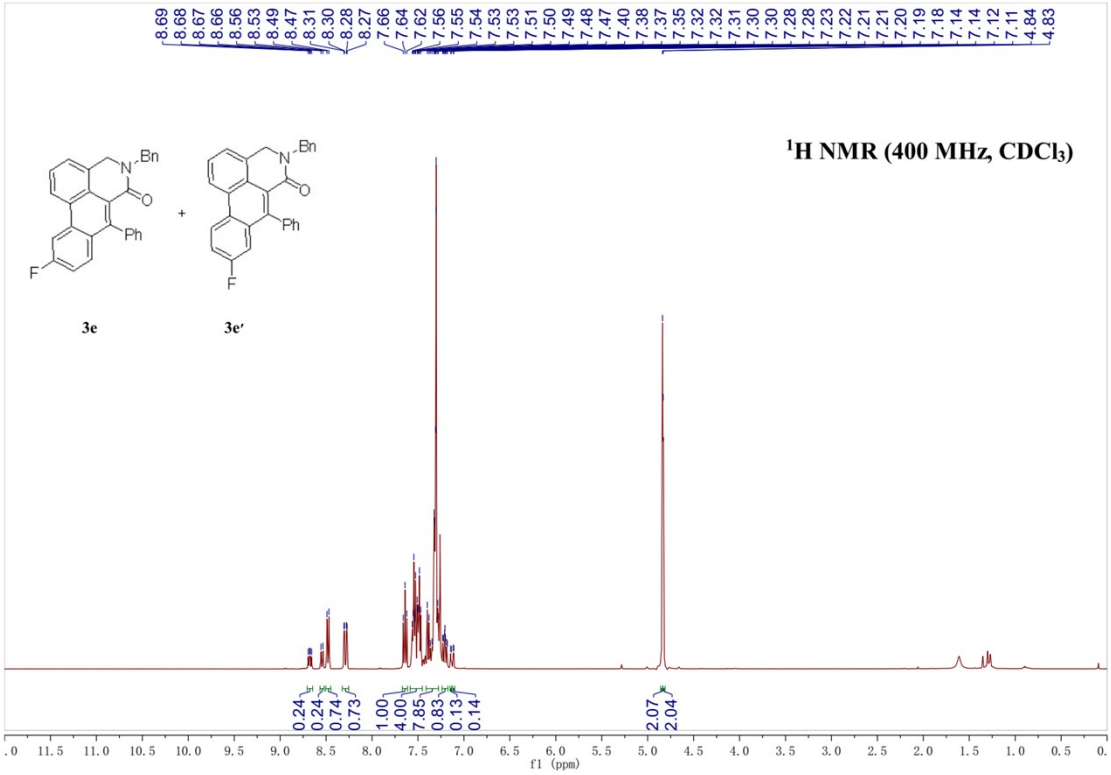
3d
3d′
f1 (ppm)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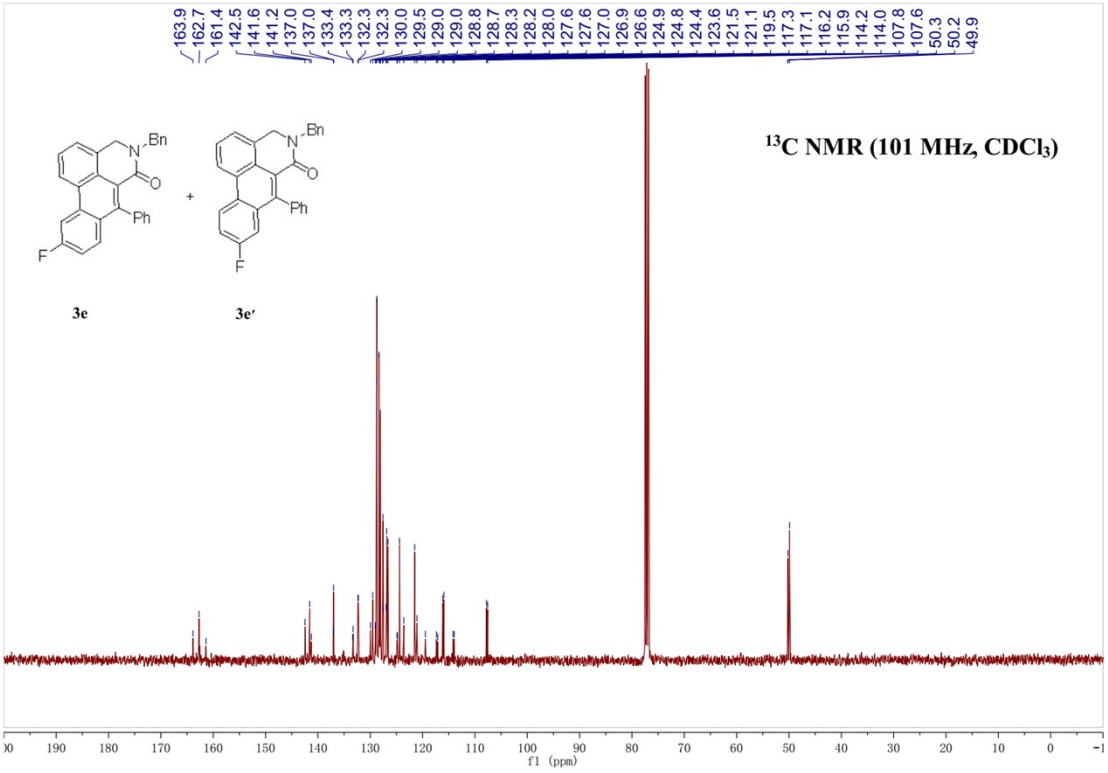
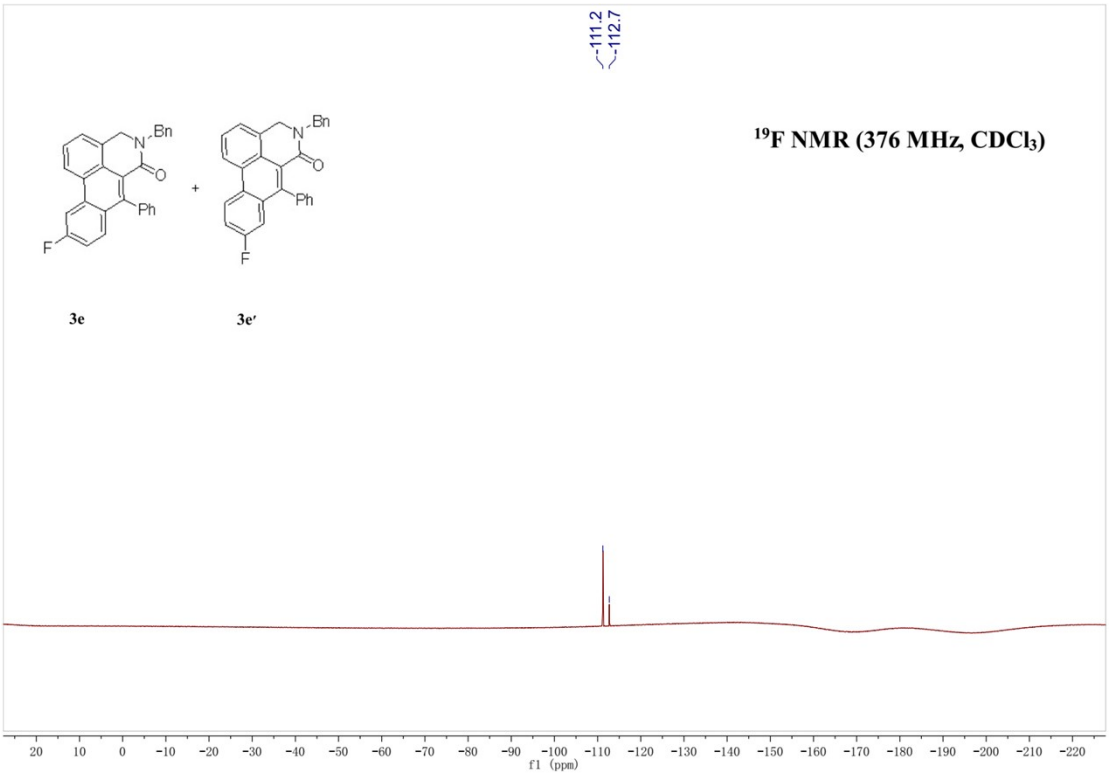
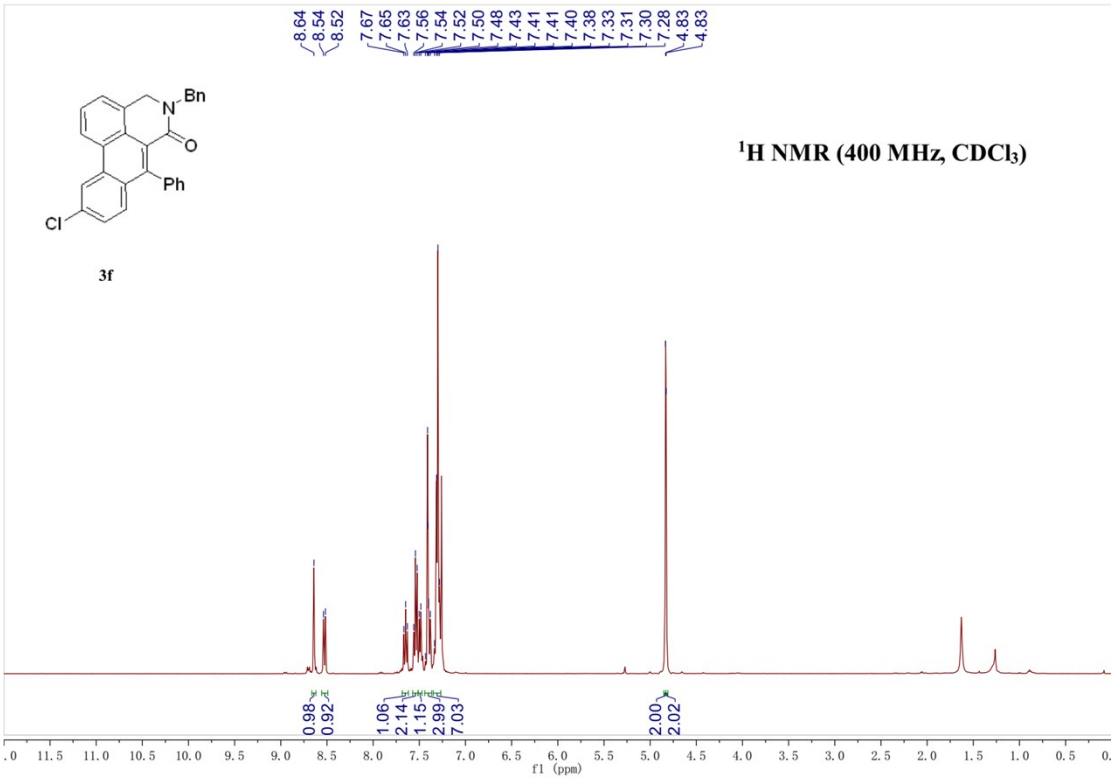
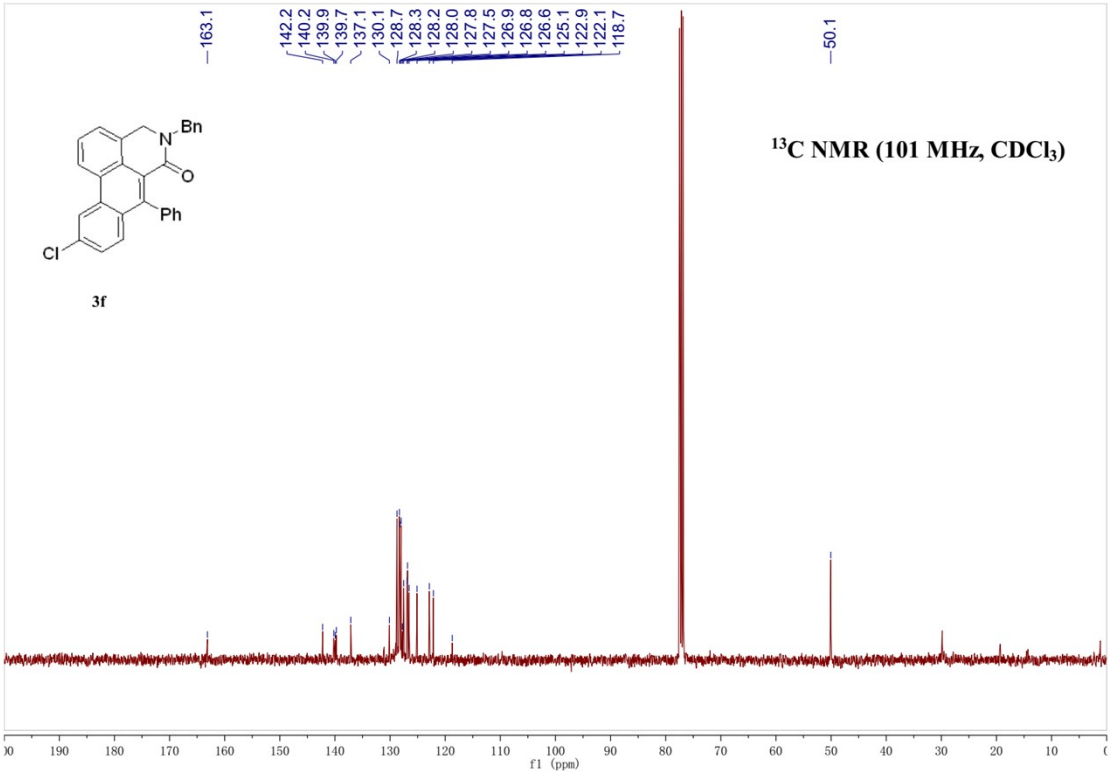
7.11
4.84
4.83
1H NMR (400 MHz, CDCl3)
Bn
N
O
Ph
F
3e
3e′
0.24
0.24
0.74
0.73
1.00
4.00
7.85
0.83
0.13
0.14
2.07
2.04
f1 (ppm)


163.9
162.7
161.4
142.5
141.6
141.2
137.0
137.0
133.4
133.3
132.3
132.3
130.0
129.5
129.0
129.0
128.8
128.7
128.3
128.2
128.0
127.6
127.6
127.0
126.9
126.6
124.9
124.8
124.4
123.6
121.5
121.1
119.5
117.3
117.1
116.2
115.9
114.2
114.0
107.8
107.6
50.3
50.2
49.9
Bn
N
O
Ph
F
3e
3e′
13C NMR (101 MHz, CDCl3)
f1 (ppm)


-111.2
-112.7
Bn
N
O
Ph
F
3e
3e′
19F NMR (376 MHz, CDCl3)
f1 (ppm)


8.64
8.54
8.52
7.67
7.65
7.63
7.56
7.54
7.52
7.50
7.48
7.43
7.41
7.41
7.40
7.38
7.33
7.31
7.30
7.28
4.83
4.83
N
Bn
O
Ph
Cl
3f
^{1}H NMR (400 MHz, CDCl$_3$)
0.98
0.92
1.06
2.14
1.15
2.99
7.03
2.00
2.02
f1 (ppm)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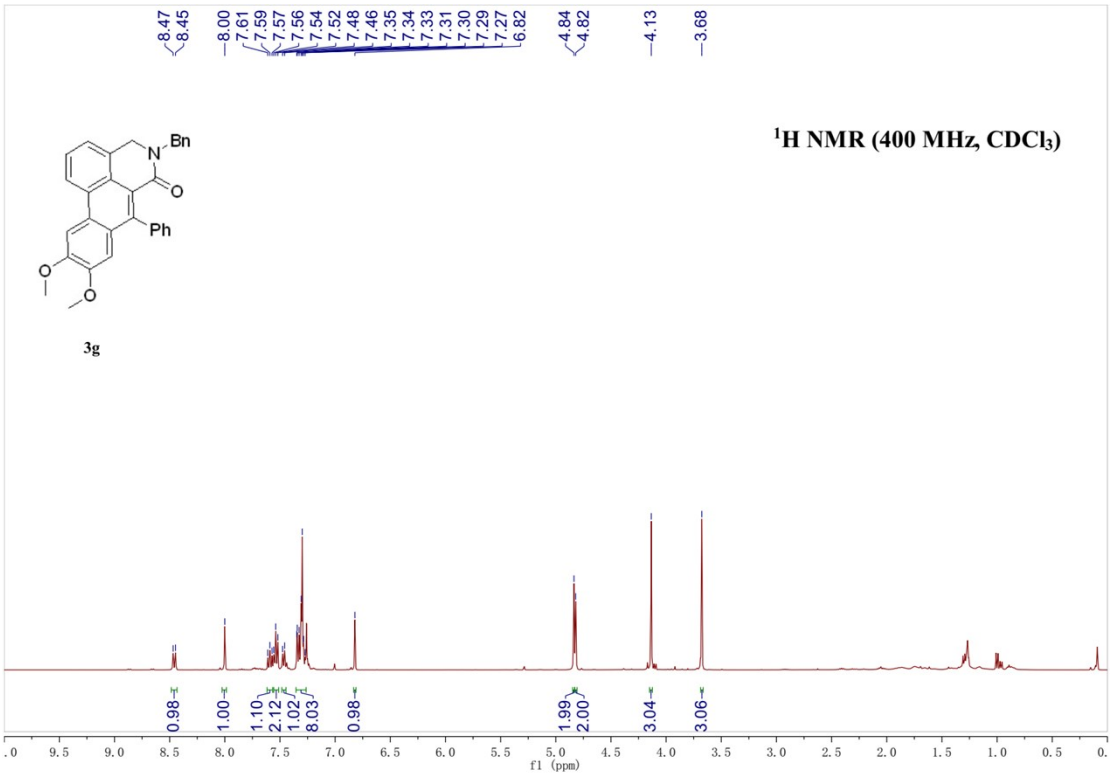
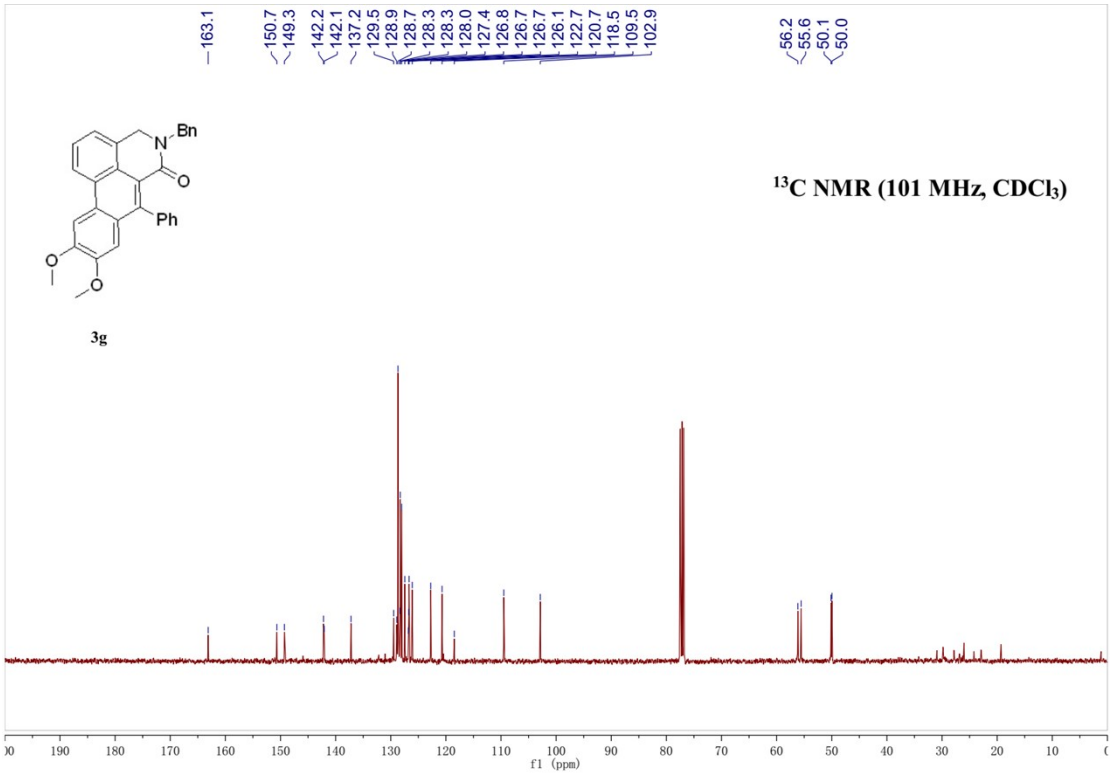
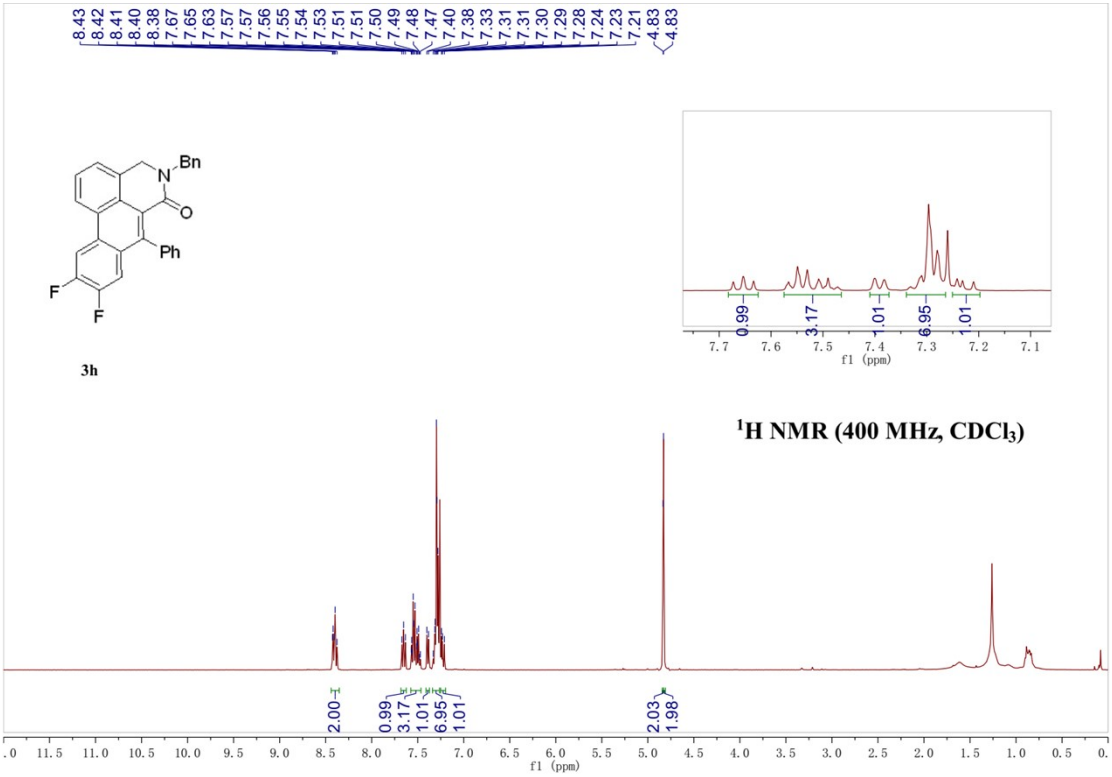
142.2
140.2
139.9
139.7
137.1
130.1
128.7
128.3
128.2
128.0
127.8
127.5
126.9
126.8
126.6
125.1
122.9
122.1
118.7
50.1
N
Bn
O
Ph
Cl
3f
^{13}C NMR (101 MHz, CDCl$_3$)
f1 (ppm)

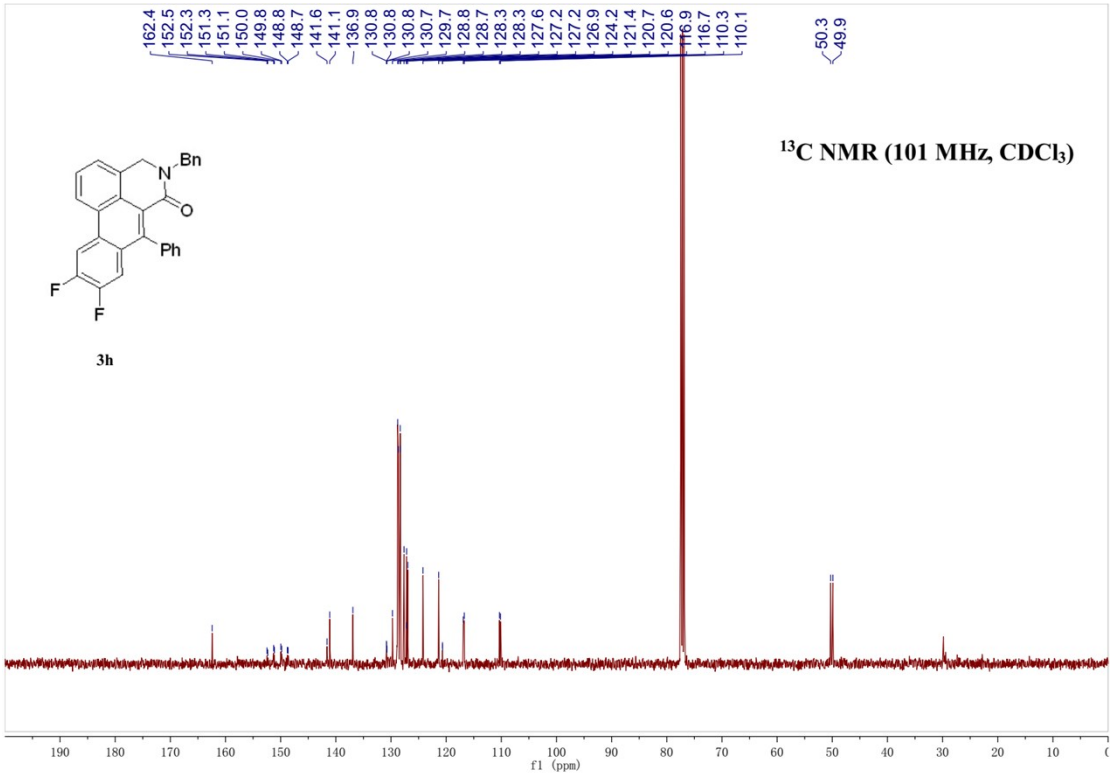


^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)


8.43
8.42
8.41
8.40
8.38
7.67
7.65
7.63
7.57
7.57
7.56
7.55
7.54
7.53
7.51
7.51
7.50
7.49
7.48
7.47
7.40
7.38
7.33
7.31
7.31
7.30
7.29
7.28
7.24
7.23
7.21
4.83
4.83
N
Bn
O
Ph
F
F
3h
0.99
3.17
1.01
6.95
1.01
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
^{1}H NMR (400 MHz, CDCl$_3$)
2.00
0.99
3.17
1.01
6.95
1.01
2.03
1.98
f1 (ppm)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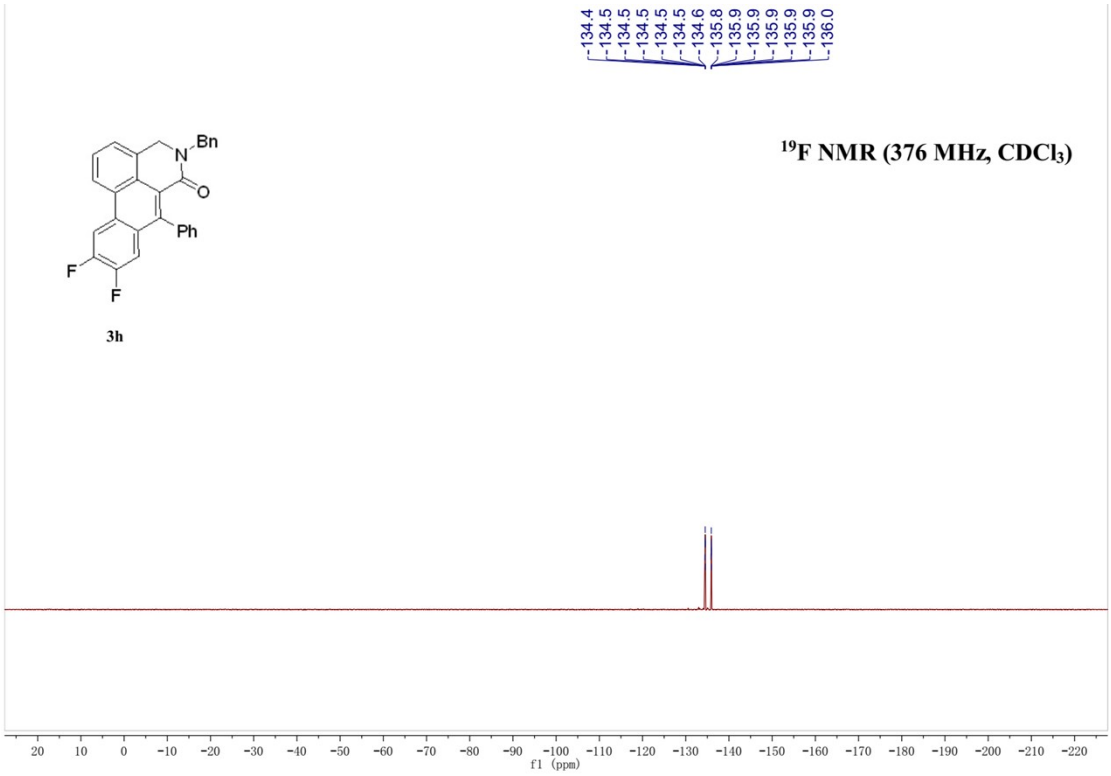
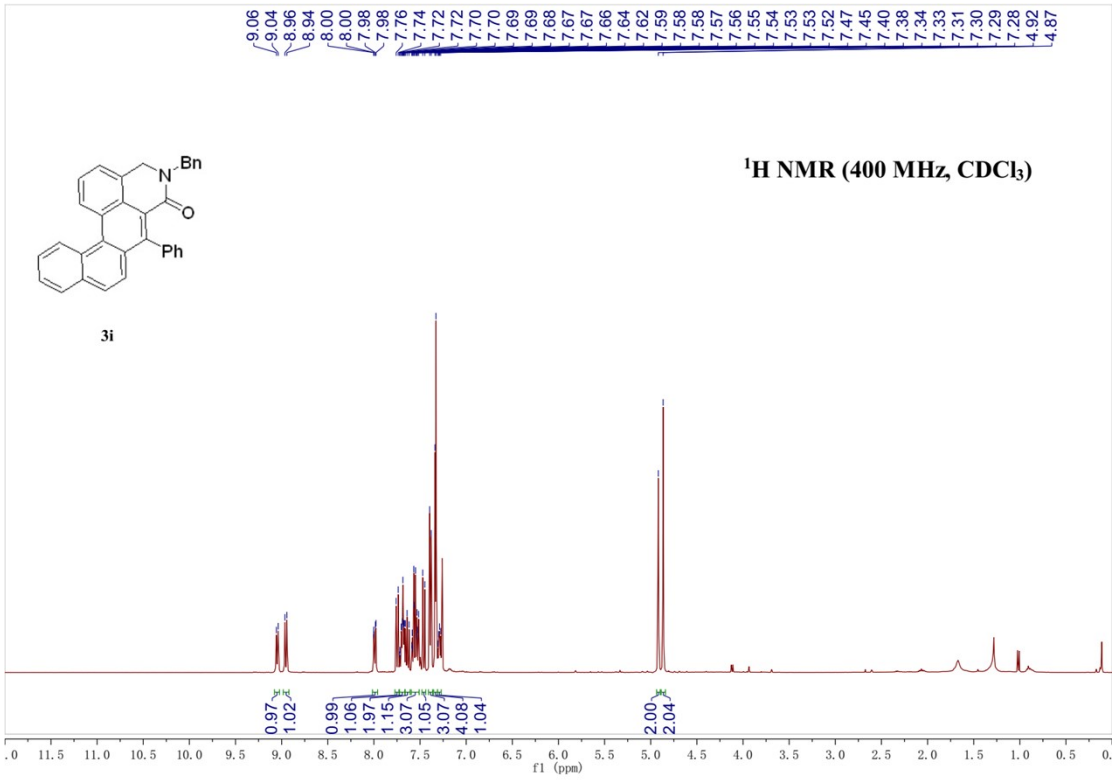
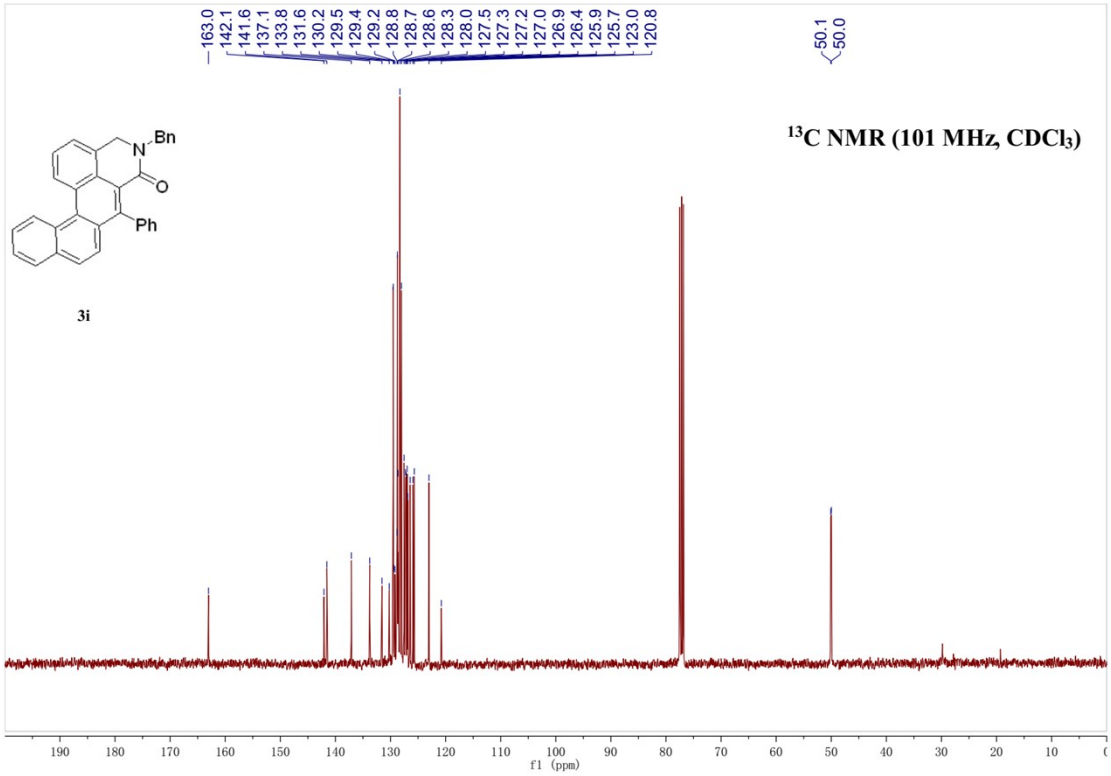
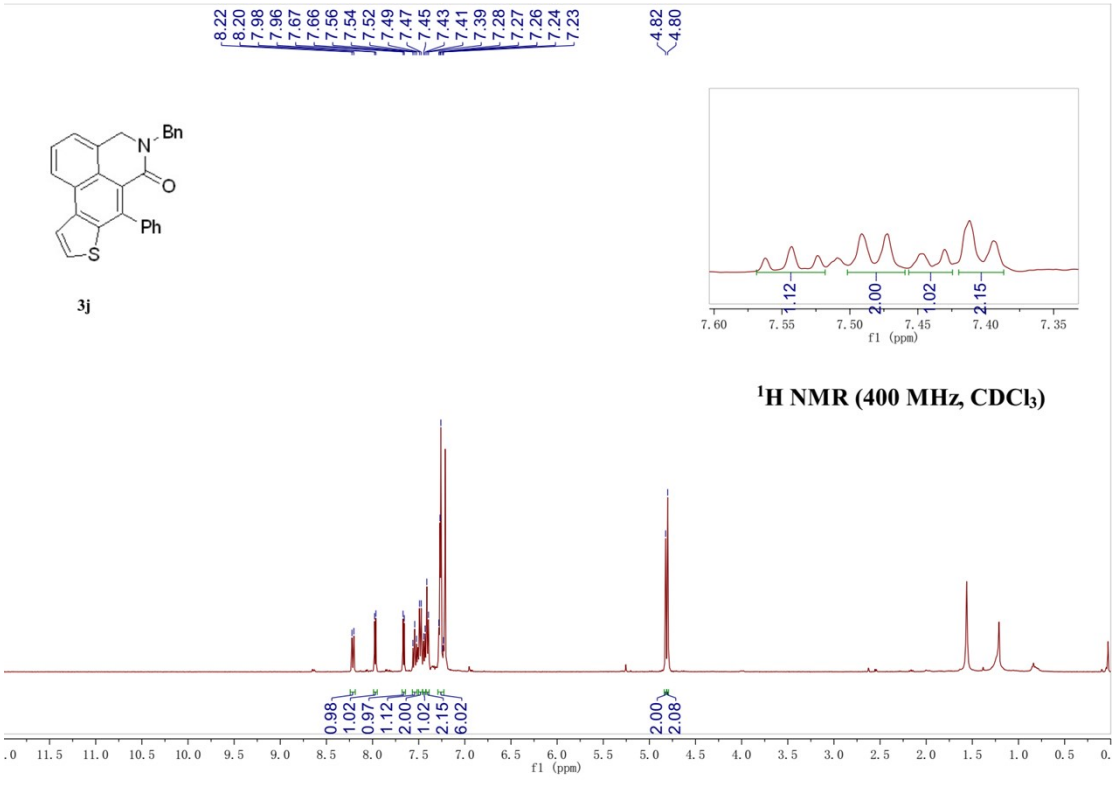
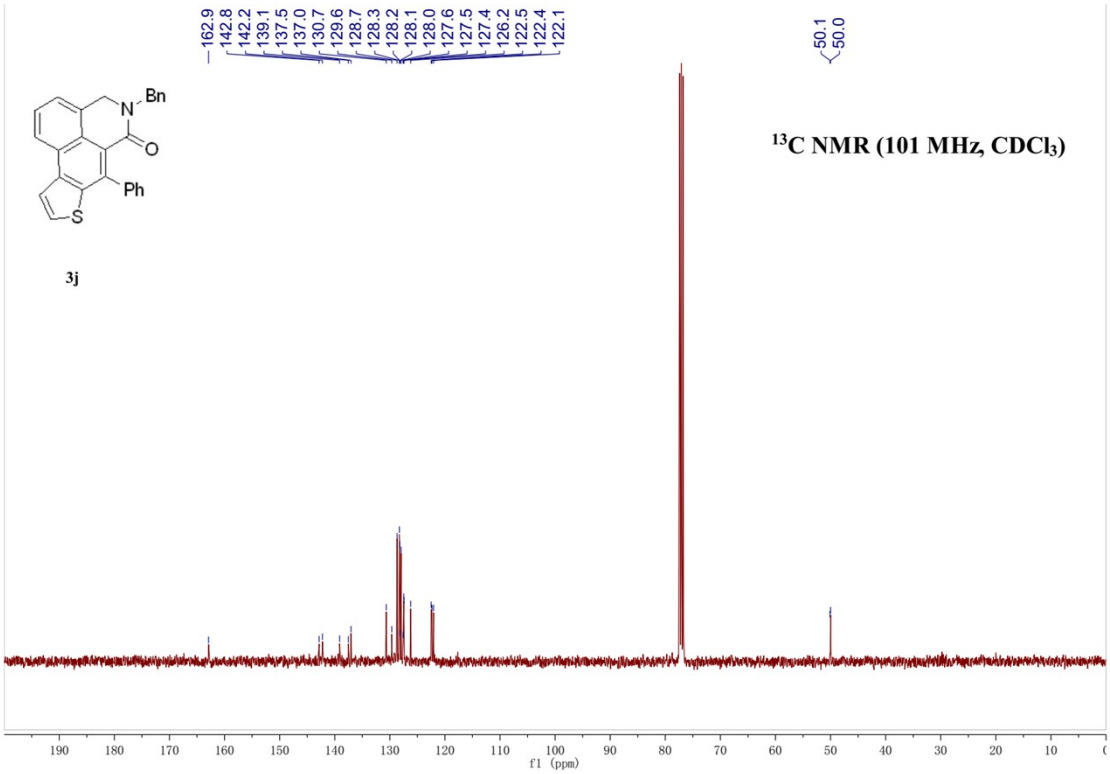
152.5
152.3
151.3
151.1
150.0
149.8
148.8
148.7
141.6
141.1
136.9
130.8
130.8
130.8
130.7
129.7
128.8
128.7
128.3
128.3
127.6
127.2
127.2
126.9
124.2
121.4
120.7
120.6
116.9
116.7
110.3
110.1
50.3
49.9
N
Bn
O
Ph
F
F
3h
^{13}C NMR (101 MHz, CDCl$_3$)
f1 (ppm)

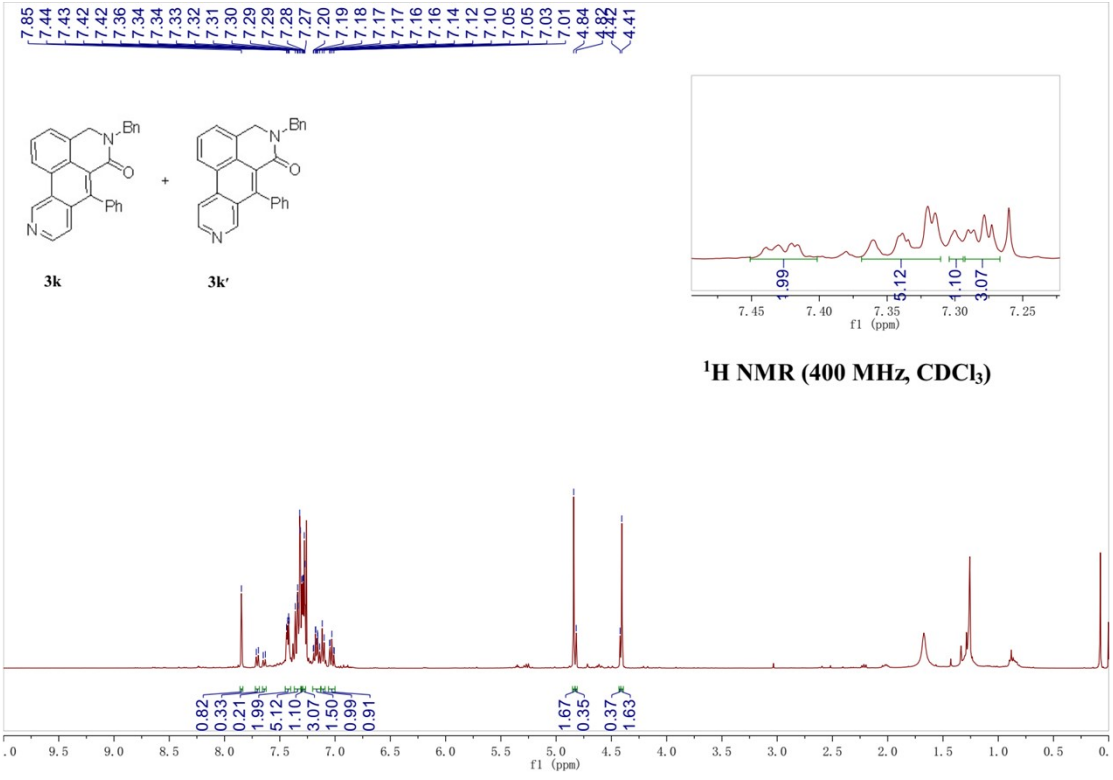

134.4
134.5
134.5
134.5
134.5
134.5
134.6
135.8
135.9
135.9
135.9
135.9
135.9
136.0
Bn
N
O
Ph
F
F
3h
19F NMR (376 MHz, CDCl3)
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

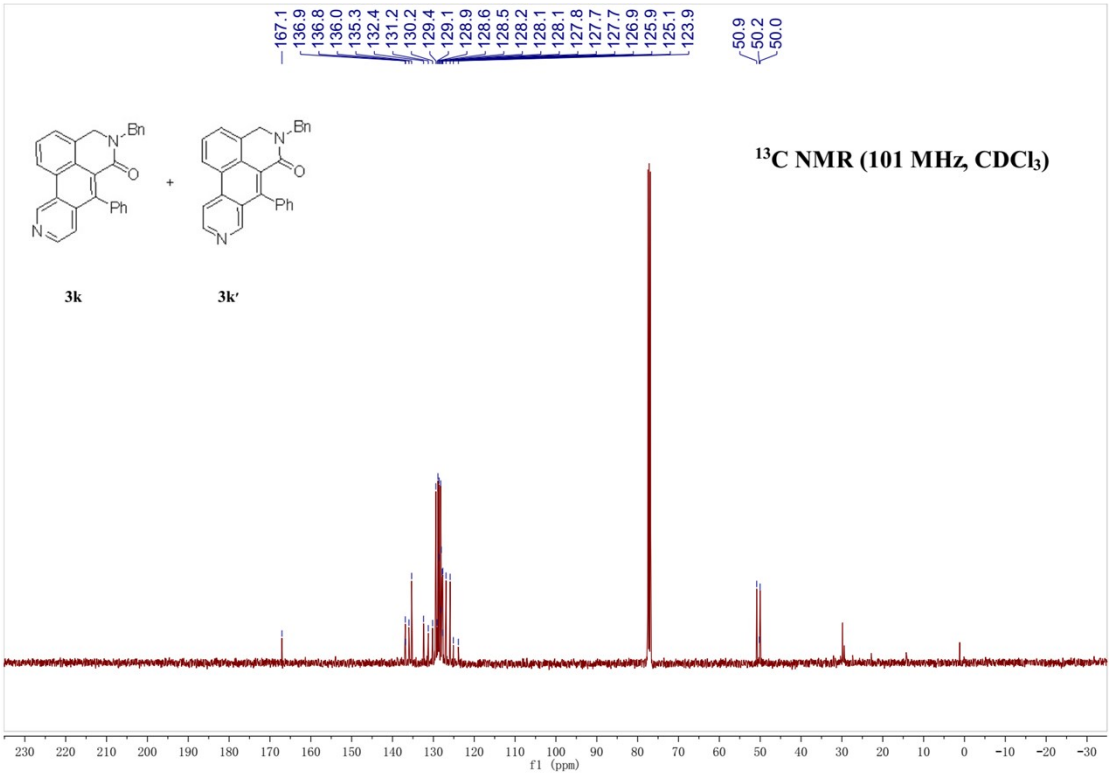

9.06
9.04
8.96
8.94
8.00
8.00
7.98
7.98
7.76
7.74
7.72
7.72
7.70
7.70
7.69
7.69
7.68
7.67
7.67
7.66
7.64
7.62
7.59
7.58
7.58
7.57
7.56
7.55
7.54
7.53
7.53
7.52
7.47
7.45
7.40
7.38
7.34
7.33
7.31
7.30
7.29
7.28
4.92
4.87
Bn
N
O
Ph
3i
1H NMR (400 MHz, CDCl3)
0.97
1.02
0.99
1.06
1.97
1.15
3.07
1.05
3.07
4.08
1.04
2.00
2.04
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
f1 (ppm)

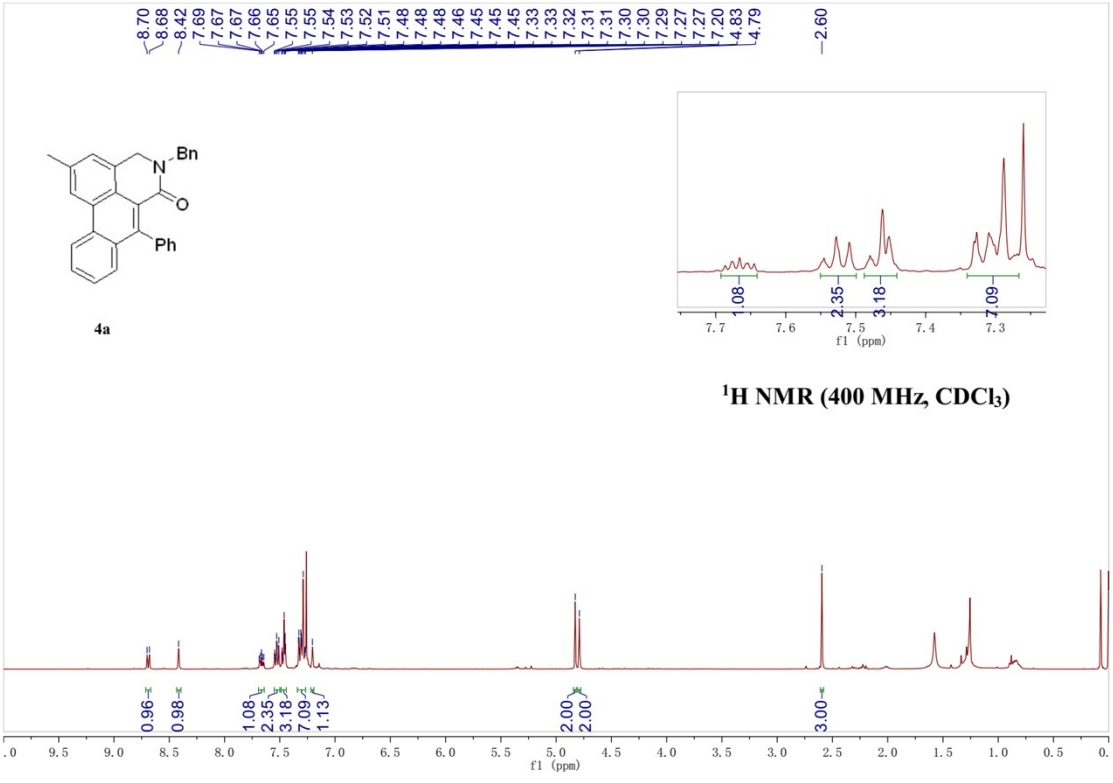

163.0
142.1
141.6
137.1
133.8
131.6
130.2
129.5
129.4
129.2
128.8
128.7
128.6
128.3
128.0
127.5
127.3
127.2
127.0
126.9
126.4
125.9
125.7
123.0
120.8
50.1
50.0
Bn
N
O
Ph
3i
^{13}C NMR (101 MHz, CDCl$_3$)
f1 (ppm)


8.22
8.20
7.98
7.96
7.67
7.66
7.56
7.54
7.52
7.49
7.47
7.45
7.43
7.41
7.39
7.28
7.27
7.26
7.24
7.23
4.82
4.80
Bn
N
O
Ph
S
3j
1.12
2.00
1.02
2.15
^{1}H NMR (400 MHz, CDCl$_3$)
0.98
1.02
0.97
1.12
2.00
1.02
2.15
6.02
2.00
2.08
f1 (ppm)


162.9
142.8
142.2
139.1
137.5
137.0
130.7
129.6
128.7
128.3
128.2
128.1
128.0
127.6
127.5
127.4
126.2
122.5
122.4
122.1
50.1
50.0
N
Bn
O
Ph
S
3j
13C NMR (101 MHz, CDCl3)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


7.85
7.44
7.43
7.42
7.42
7.36
7.34
7.34
7.33
7.32
7.31
7.30
7.29
7.29
7.28
7.27
7.20
7.19
7.18
7.17
7.17
7.16
7.16
7.14
7.12
7.10
7.05
7.05
7.03
7.01
4.84
4.82
4.41
N
Bn
O
Ph
3k
3k′
1.99
5.12
1.10
3.07
7.45 7.40 7.35 7.30 7.25
f1 (ppm)
1H NMR (400 MHz, CDCl3)
0.82
0.33
0.21
1.99
5.12
1.10
3.07
1.50
0.99
0.91
1.67
0.35
0.37
1.63
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


167.1
136.9
136.8
136.0
135.3
132.4
131.2
130.2
129.4
129.1
128.9
128.6
128.5
128.2
128.1
128.1
127.8
127.7
127.7
126.9
125.9
125.1
123.9
50.9
50.2
50.0
Bn
N
O
Ph
N
+
Bn
N
O
Ph
N
3k
3k′
13C NMR (101 MHz, CDCl3)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)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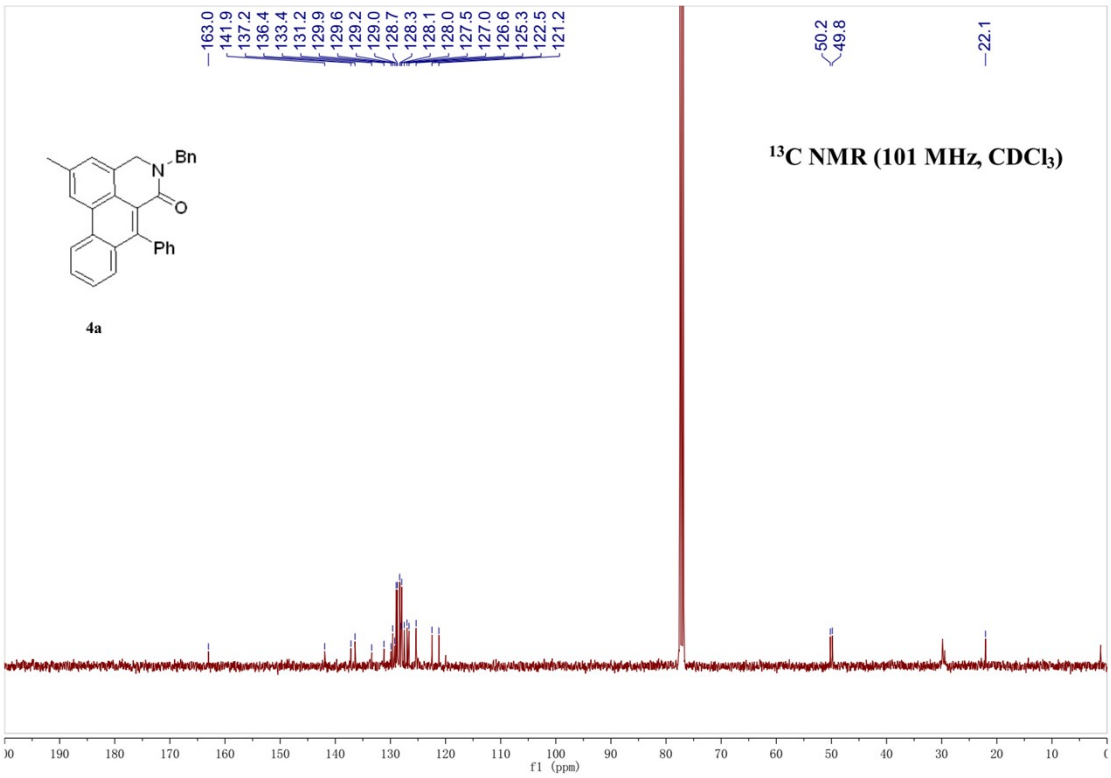
8.68
8.42
7.69
7.67
7.67
7.66
7.65
7.55
7.55
7.54
7.53
7.52
7.51
7.48
7.48
7.48
7.46
7.45
7.45
7.45
7.33
7.33
7.32
7.31
7.31
7.30
7.30
7.29
7.27
7.27
7.20
4.83
4.79
2.60
Bn
N
O
Ph
4a
1.08
2.35
3.18
7.09
7.7 7.6 7.5 7.4 7.3
f1 (ppm)
1H NMR (400 MHz, CDCl3)
0.96
0.98
1.08
2.35
3.18
7.09
1.13
2.00
2.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)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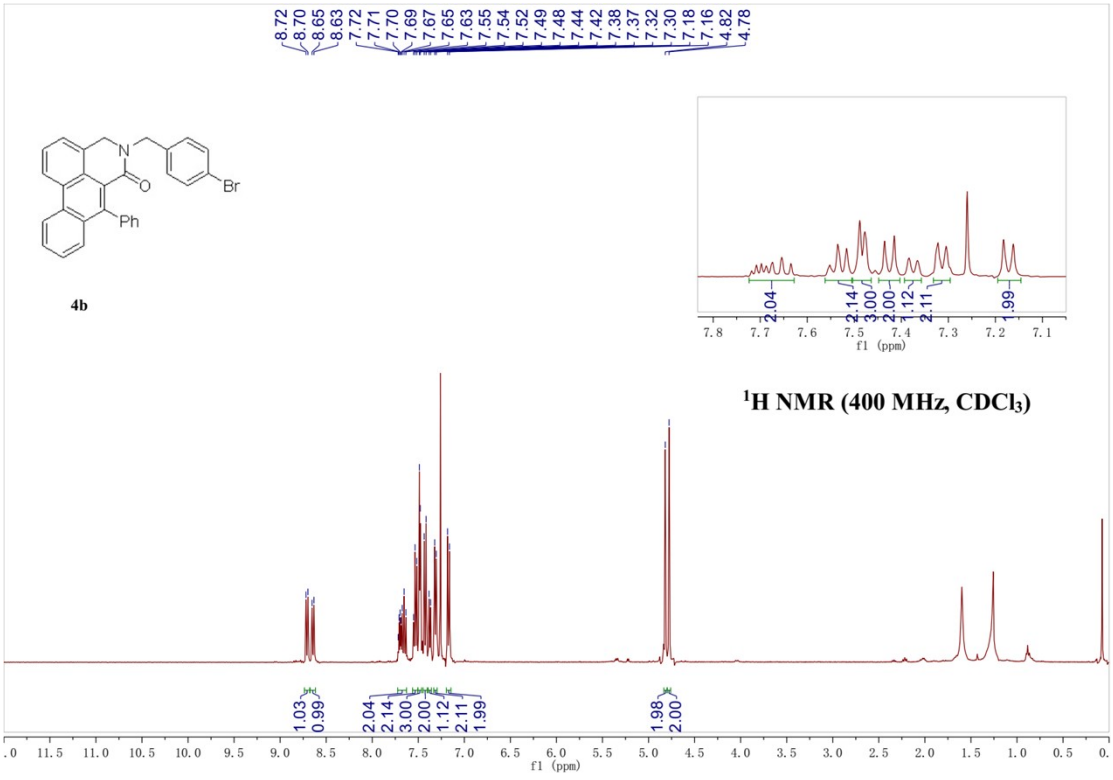
137.2
136.4
133.4
131.2
129.9
129.6
129.2
129.0
128.7
128.3
128.1
128.0
127.5
127.0
126.6
125.3
122.5
121.2
50.2
49.8
22.1
Bn
N
O
Ph
4a
13C NMR (101 MHz, CDCl3)
f1 (ppm)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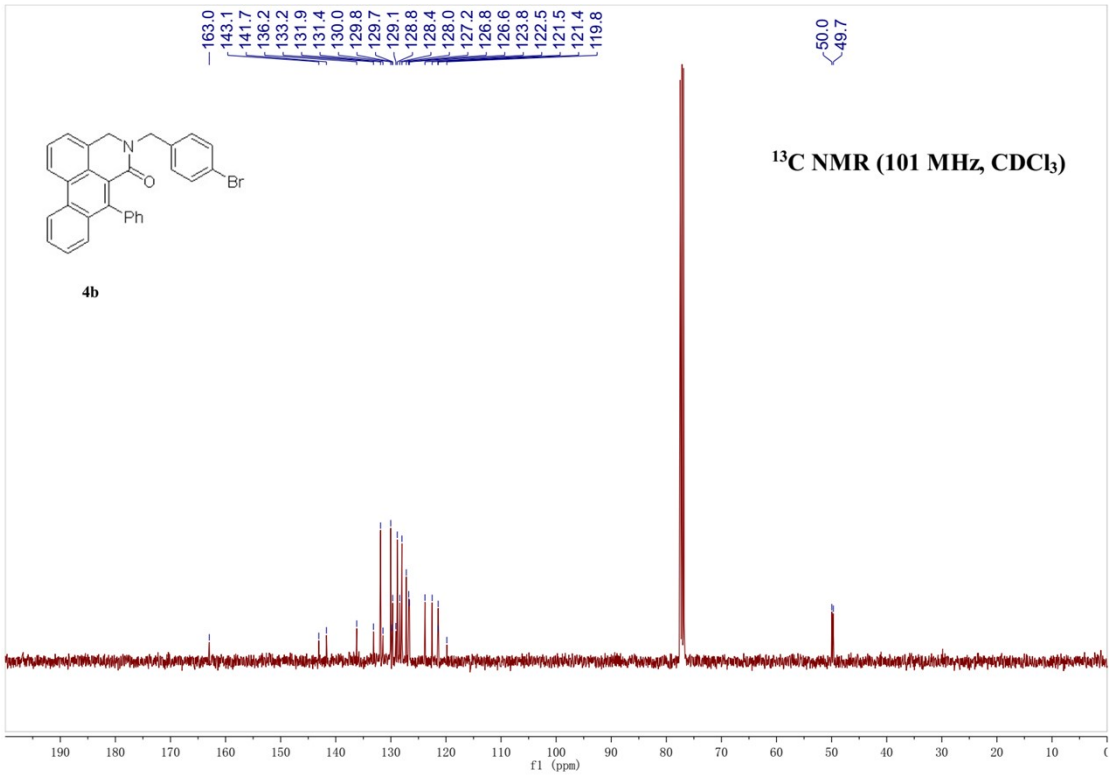
7.70
7.69
7.67
7.65
7.63
7.55
7.54
7.52
7.49
7.48
7.44
7.42
7.38
7.37
7.32
7.30
7.18
7.16
4.82
4.78
N
O
Br
Ph
4b
2.04
2.14
3.00
2.00
1.12
2.11
1.99
1.03
0.99
1.98
2.00
1H NMR (400 MHz, CDCl3)
f1 (ppm)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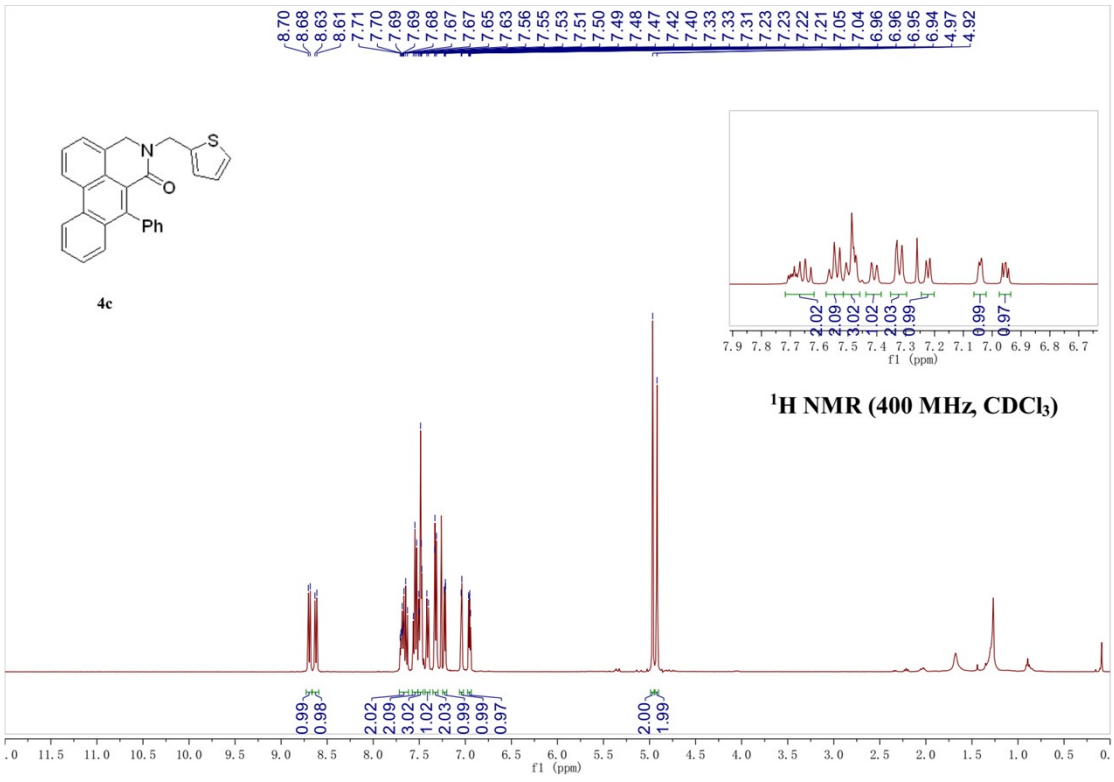
143.1
141.7
136.2
133.2
131.9
131.4
130.0
129.8
129.7
129.1
128.8
128.4
128.0
127.2
126.8
126.6
123.8
122.5
121.5
121.4
119.8
50.0
49.7
N
O
Br
Ph
4b
13C NMR (101 MHz, CDCl3)
f1 (ppm)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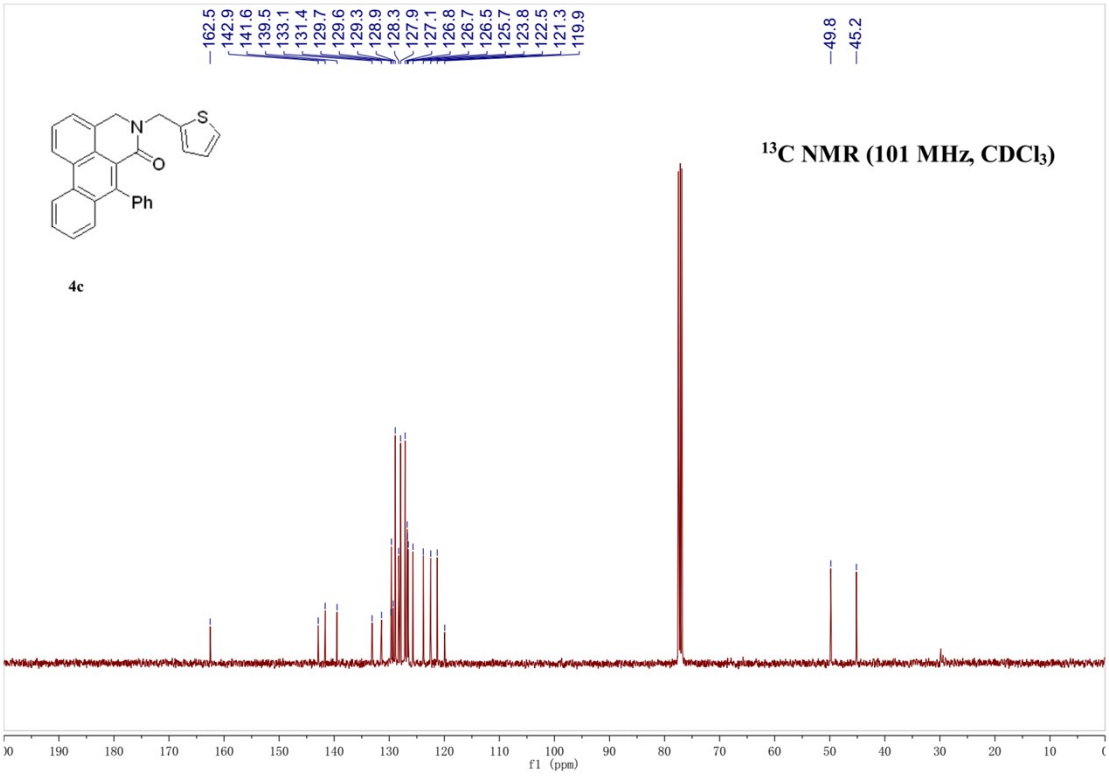
7.70
7.69
7.69
7.68
7.67
7.67
7.65
7.63
7.56
7.55
7.53
7.51
7.50
7.49
7.48
7.47
7.42
7.40
7.33
7.33
7.31
7.23
7.23
7.22
7.21
7.05
7.04
6.96
6.96
6.95
6.94
4.97
4.92
N
S
O
Ph
4c
0.99
0.98
2.02
2.09
3.02
1.02
2.03
0.99
0.99
0.97
2.00
1.99
f1 (ppm)
1H NMR (400 MHz, CDCl3)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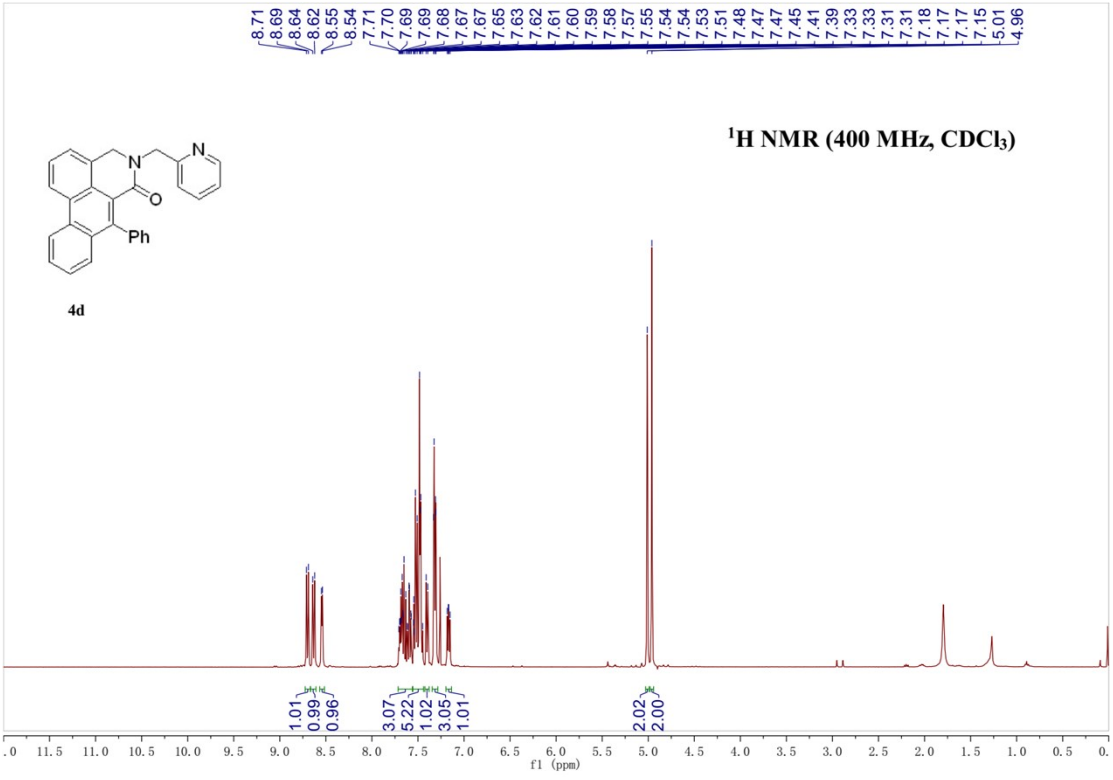
142.9
141.6
139.5
133.1
131.4
129.7
129.6
129.3
128.9
128.3
127.9
127.1
126.8
126.7
126.5
125.7
123.8
122.5
121.3
119.9
49.8
45.2
13C NMR (101 MHz, CDCl3)
N
S
O
Ph
4c
f1 (ppm)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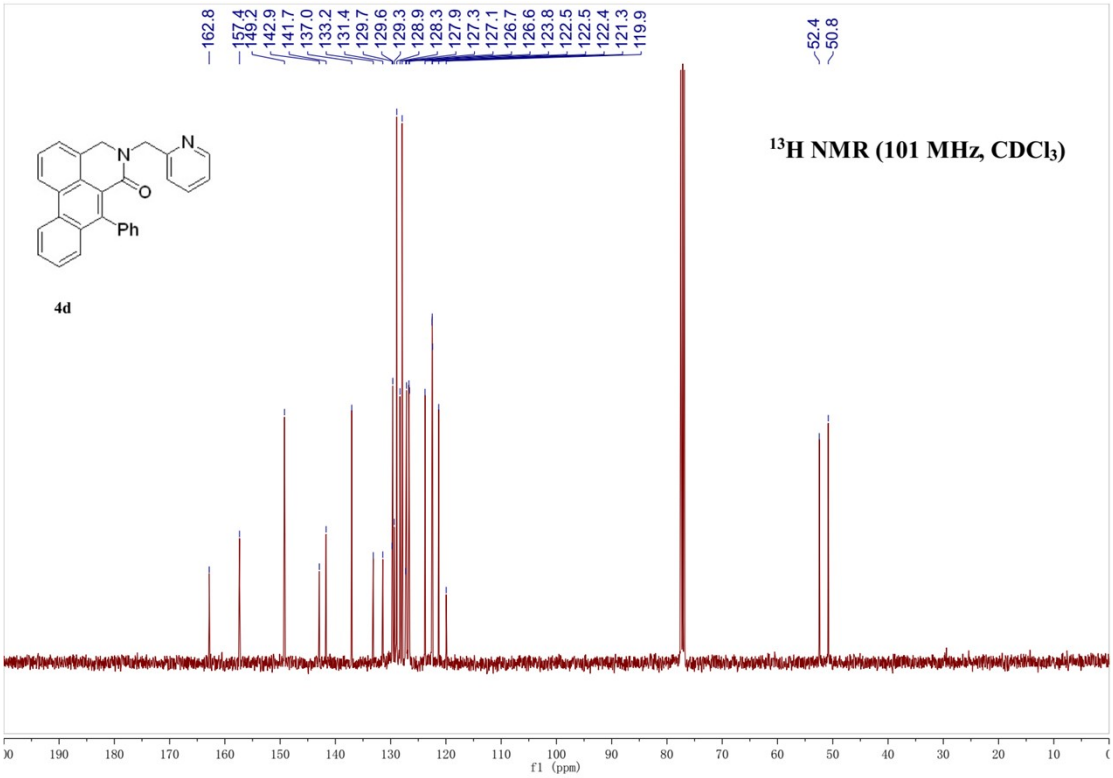
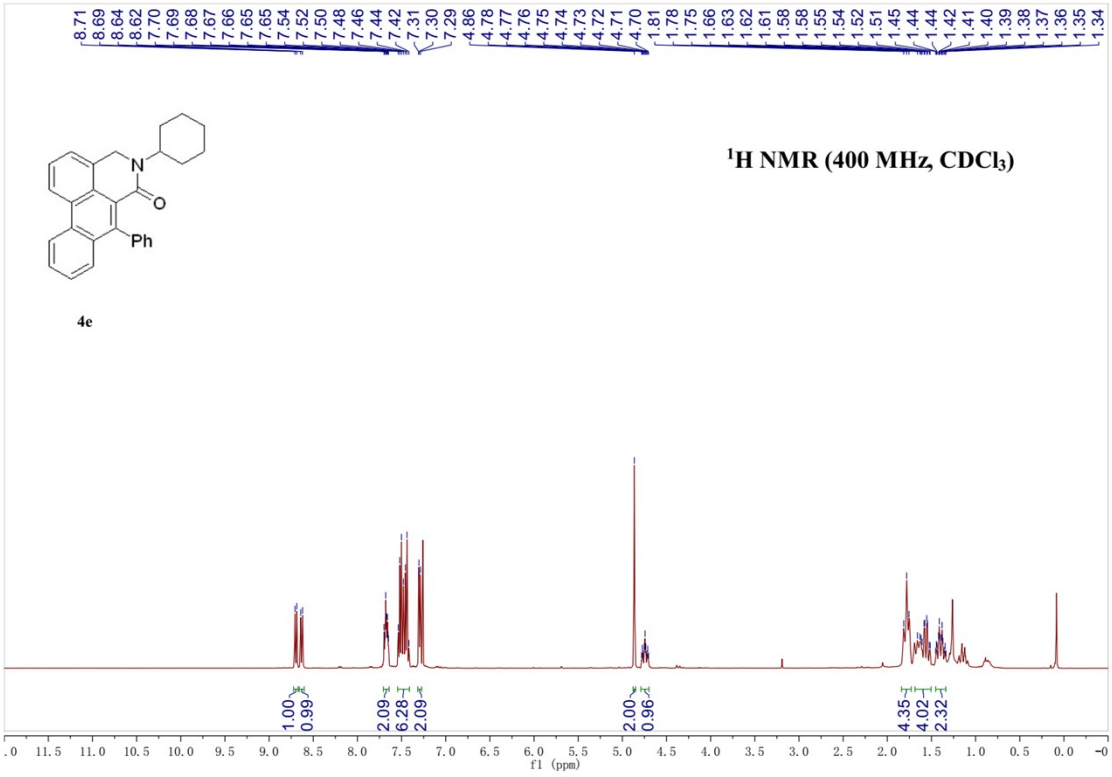
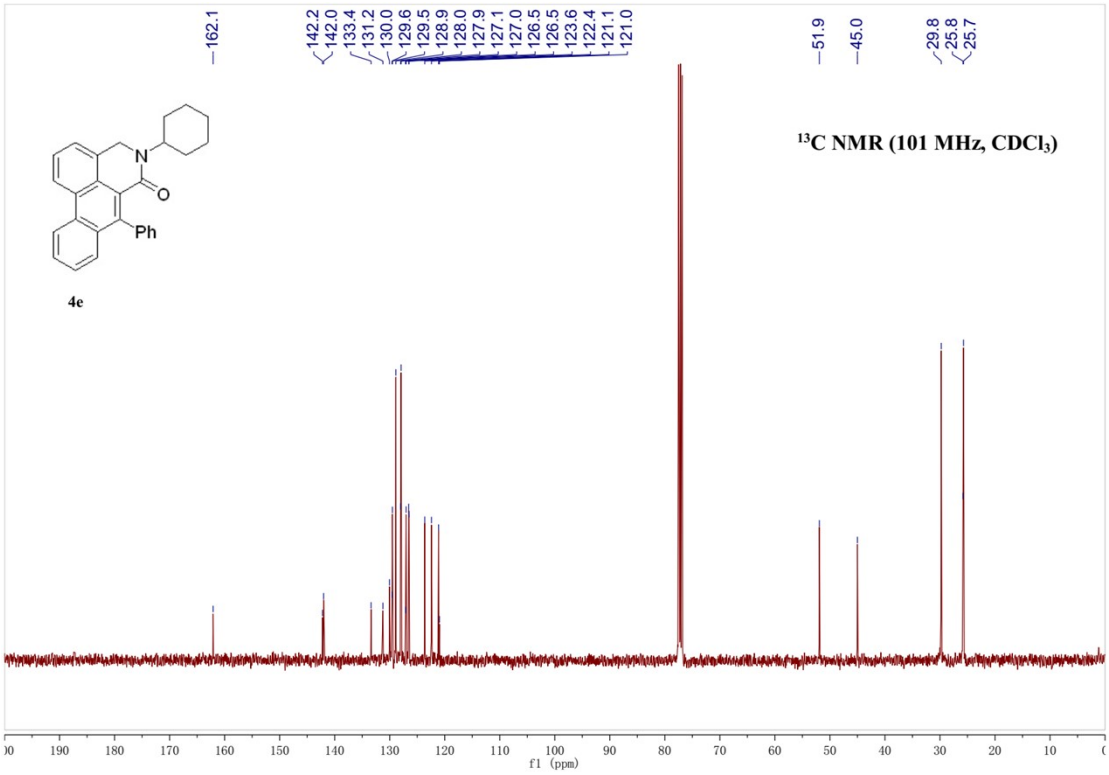
8.54
7.71
7.70
7.69
7.69
7.68
7.67
7.67
7.65
7.63
7.62
7.61
7.60
7.59
7.58
7.57
7.55
7.54
7.54
7.53
7.51
7.48
7.47
7.47
7.45
7.41
7.39
7.33
7.33
7.31
7.18
7.17
7.17
7.15
5.01
4.96
1H NMR (400 MHz, CDCl3)
N
N
O
Ph
4d
1.01
0.99
0.96
3.07
5.22
1.02
3.05
1.01
2.02
2.00
f1 (ppm)


162.8
157.4
149.2
142.9
141.7
137.0
133.2
131.4
129.7
129.6
129.3
128.9
128.3
127.9
127.3
127.1
126.7
126.6
123.8
122.5
122.5
122.4
121.3
119.9
52.4
50.8
N
N
O
Ph
4d
13H NMR (101 MHz, CDCl3)
f1 (ppm)


8.71
8.69
8.64
8.62
7.70
7.69
7.68
7.67
7.66
7.65
7.65
7.54
7.52
7.50
7.48
7.46
7.44
7.42
7.31
7.30
7.29
4.86
4.78
4.77
4.76
4.75
4.74
4.73
4.72
4.71
4.70
1.81
1.78
1.75
1.66
1.63
1.62
1.61
1.58
1.58
1.55
1.54
1.52
1.51
1.45
1.44
1.44
1.42
1.41
1.40
1.39
1.38
1.37
1.36
1.35
1.34
N
O
Ph
4e
1H NMR (400 MHz, CDCl3)
1.00
0.99
2.09
6.28
2.09
2.00
0.96
4.35
4.02
2.32
f1 (ppm)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142.2
142.0
133.4
131.2
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129.6
129.5
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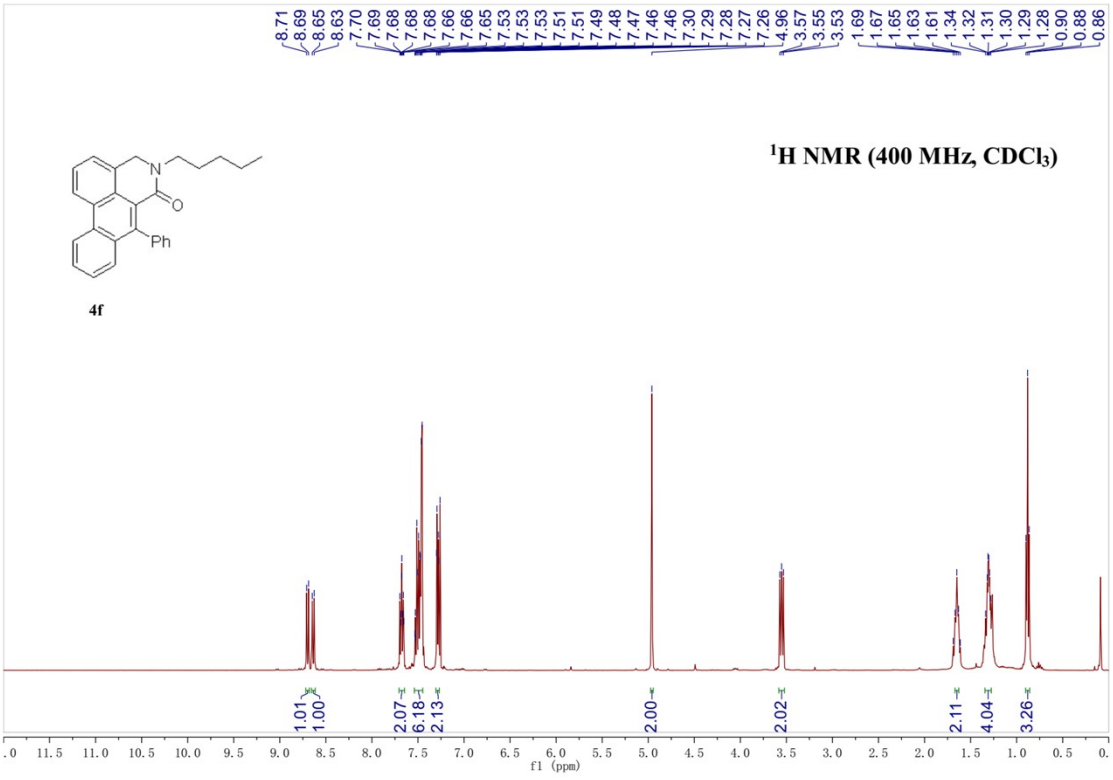
128.0
127.9
127.1
127.0
126.5
126.5
123.6
122.4
121.1
121.0
51.9
45.0
29.8
25.8
25.7
13C NMR (101 MHz, CDCl3)
N
O
Ph
4e
f1 (ppm)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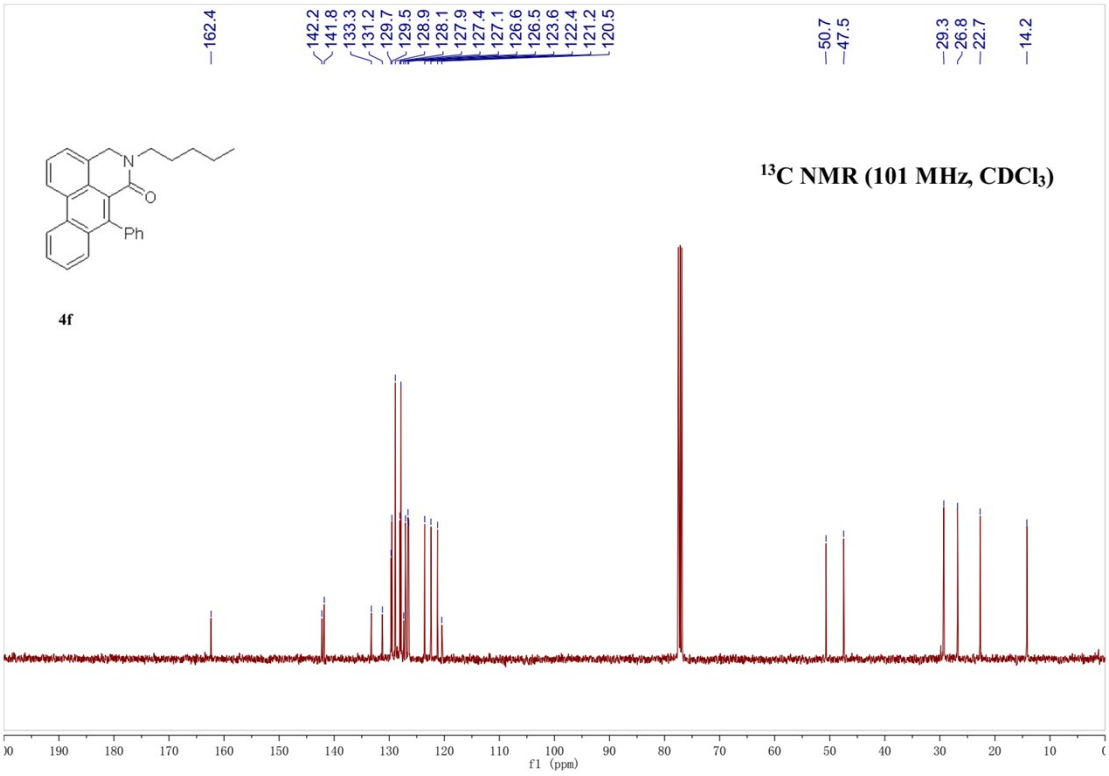
7.66
7.65
7.53
7.53
7.51
7.51
7.49
7.48
7.47
7.46
7.46
7.30
7.29
7.28
7.27
7.26
4.96
3.57
3.55
3.53
1.69
1.67
1.65
1.63
1.61
1.34
1.32
1.31
1.30
1.29
1.28
0.90
0.88
0.86
1H NMR (400 MHz, CDCl3)
N
O
Ph
4f
1.01
1.00
2.07
6.18
2.13
2.00
2.02
2.11
4.04
3.26
f1 (ppm)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141.8
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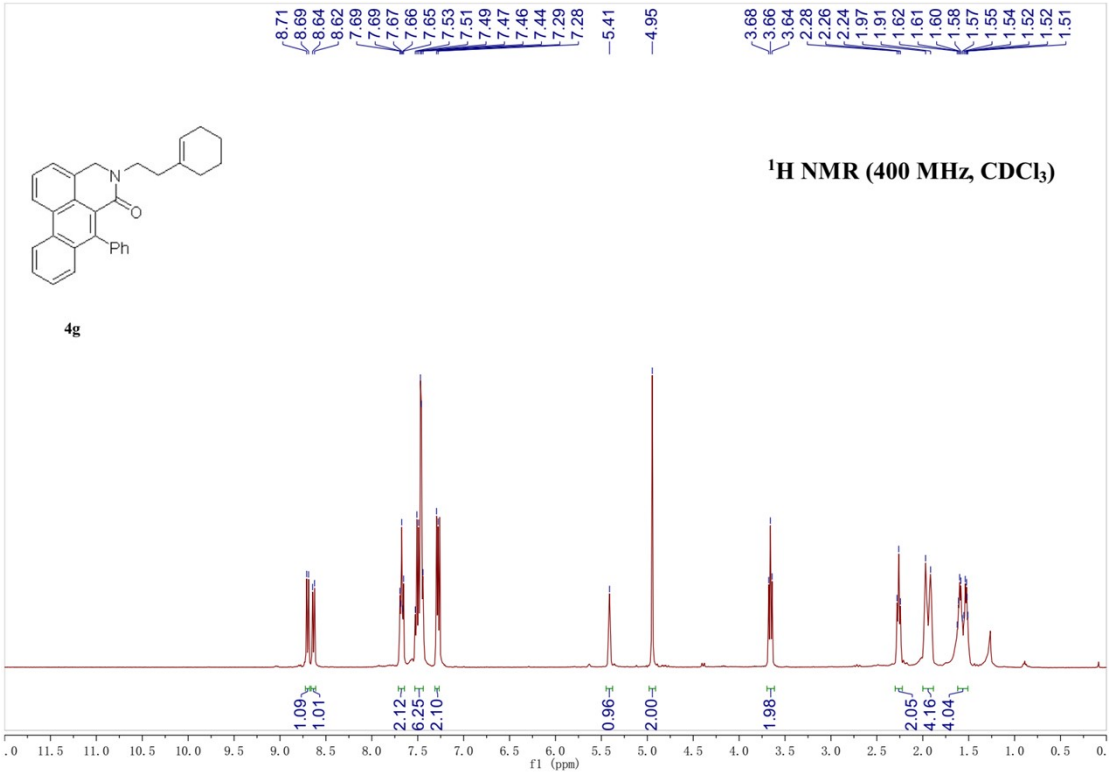
131.2
129.7
129.5
128.9
128.1
127.9
127.4
127.1
126.6
126.5
123.6
122.4
121.2
120.5
50.7
47.5
29.3
26.8
22.7
14.2
N
O
Ph
4f
13C NMR (101 MHz, CDCl3)
f1 (ppm)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7.66
7.65
7.53
7.51
7.49
7.47
7.46
7.44
7.29
7.28
5.41
4.95
3.68
3.66
3.64
2.28
2.26
2.24
1.97
1.91
1.62
1.61
1.60
1.58
1.57
1.55
1.54
1.52
1.52
1.51
1.09
1.01
2.12
6.25
2.10
0.96
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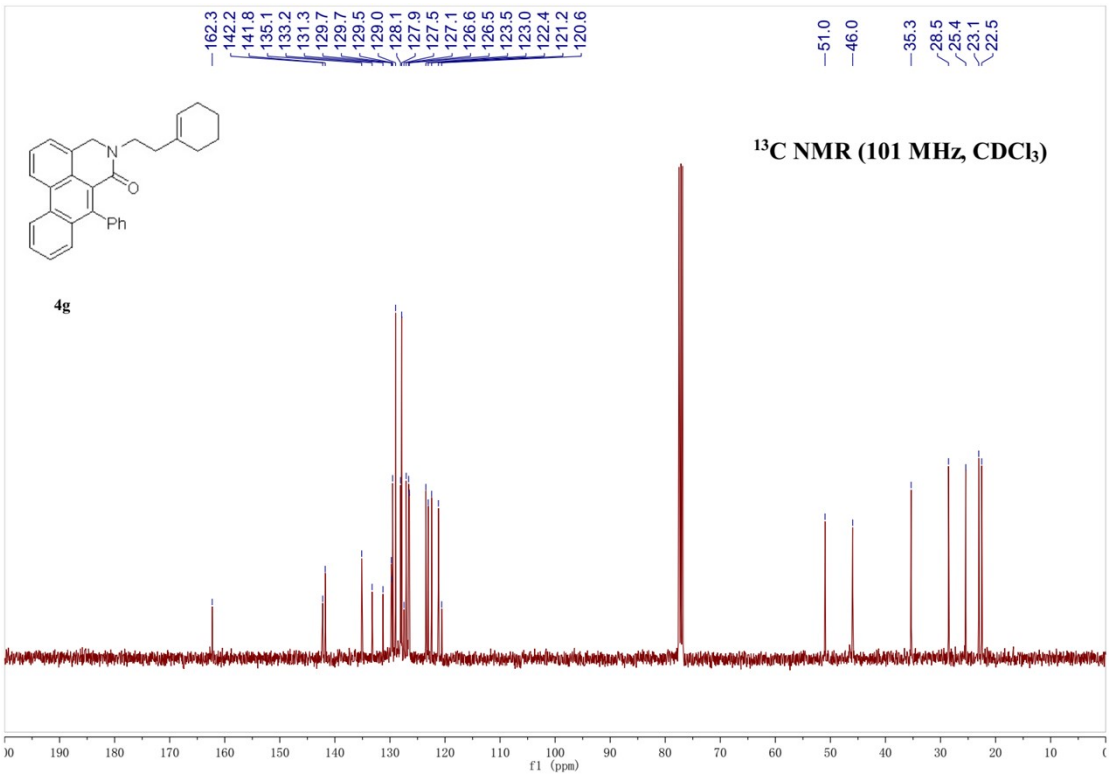
1.98
2.05
4.16
4.04
N
O
Ph
4g
1H NMR (400 MHz, CDCl3)
f1 (ppm)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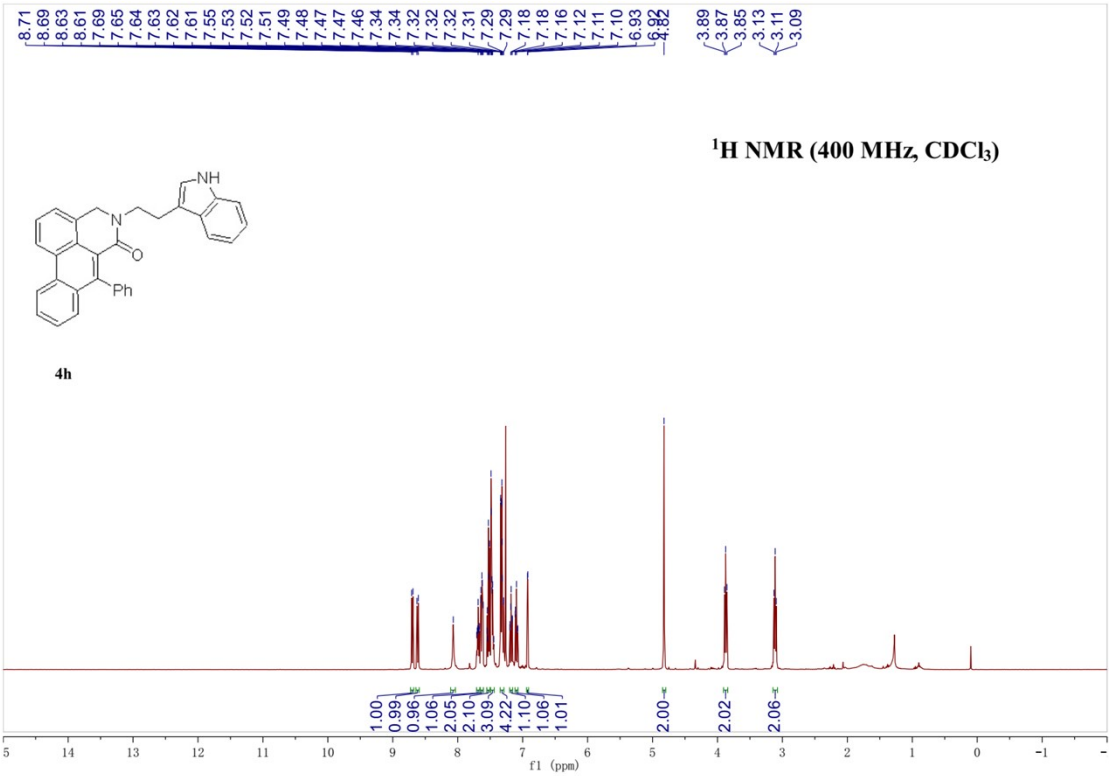
142.2
141.8
135.1
133.2
131.3
129.7
129.7
129.5
129.0
128.1
127.9
127.5
127.1
126.6
126.5
123.5
123.0
122.4
121.2
120.6
51.0
46.0
35.3
28.5
25.4
23.1
22.5
13C NMR (101 MHz, CDCl3)
N
O
Ph
4g
f1 (ppm)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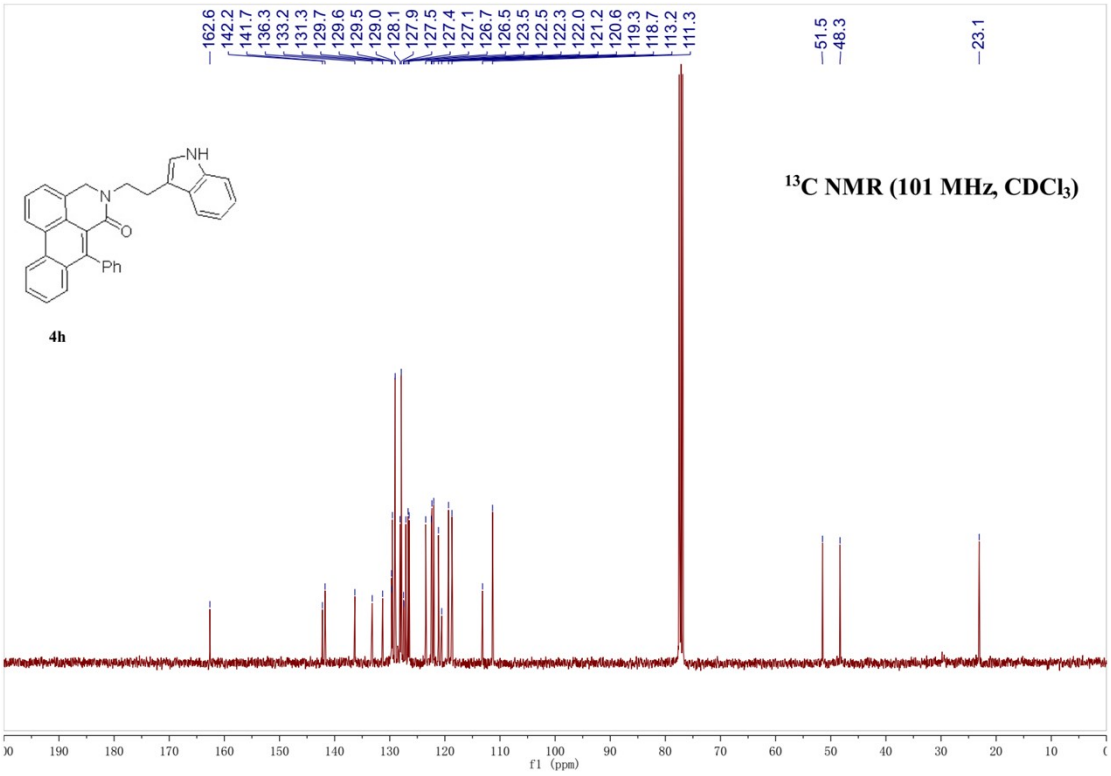
7.63
7.62
7.61
7.55
7.53
7.52
7.51
7.49
7.48
7.47
7.47
7.46
7.34
7.34
7.32
7.32
7.32
7.31
7.29
7.29
7.18
7.16
7.12
7.11
7.10
6.93
4.82
3.89
3.87
3.85
3.13
3.11
3.09
1H NMR (400 MHz, CDCl3)
NH
N
O
Ph
4h
1.00
0.99
0.96
1.06
2.05
2.10
3.09
4.22
1.10
1.06
1.01
2.00
2.02
2.06
f1 (ppm)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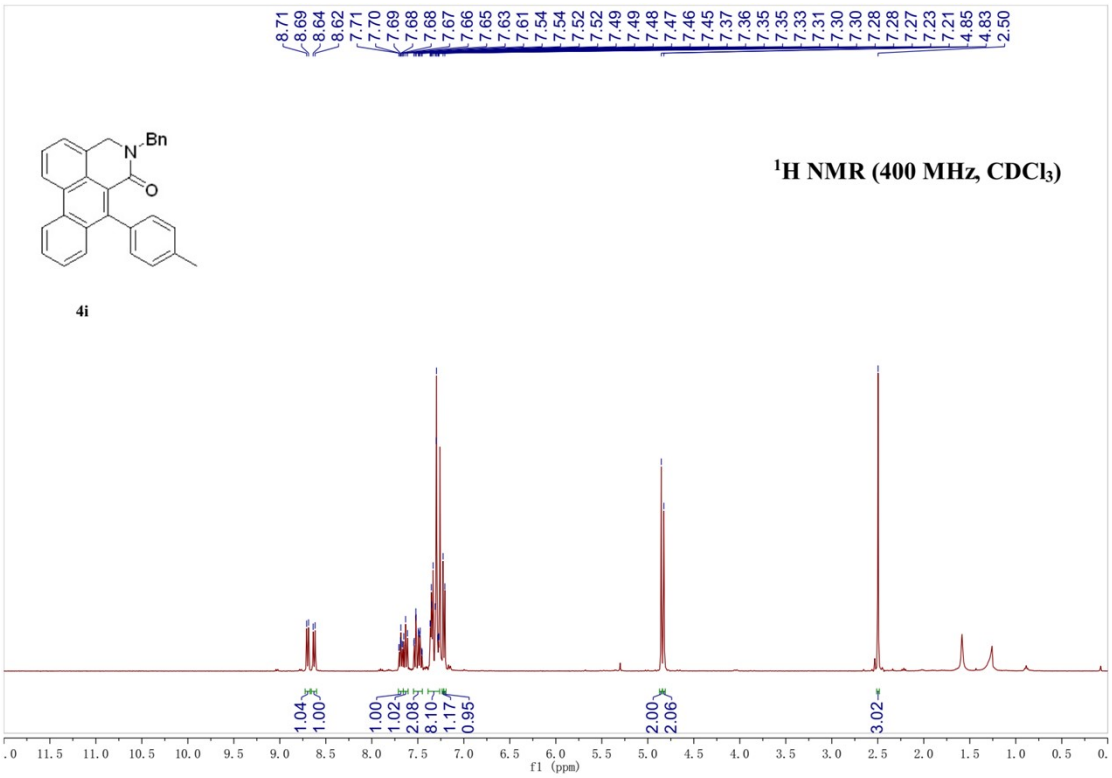
142.2
141.7
136.3
133.2
131.3
129.7
129.6
129.5
129.0
128.1
127.9
127.5
127.4
127.1
126.7
126.5
123.5
122.5
122.3
122.0
121.2
120.6
119.3
118.7
113.2
111.3
51.5
48.3
23.1
NH
N
O
Ph
4h
13C NMR (101 MHz, CDCl3)
f1 (ppm)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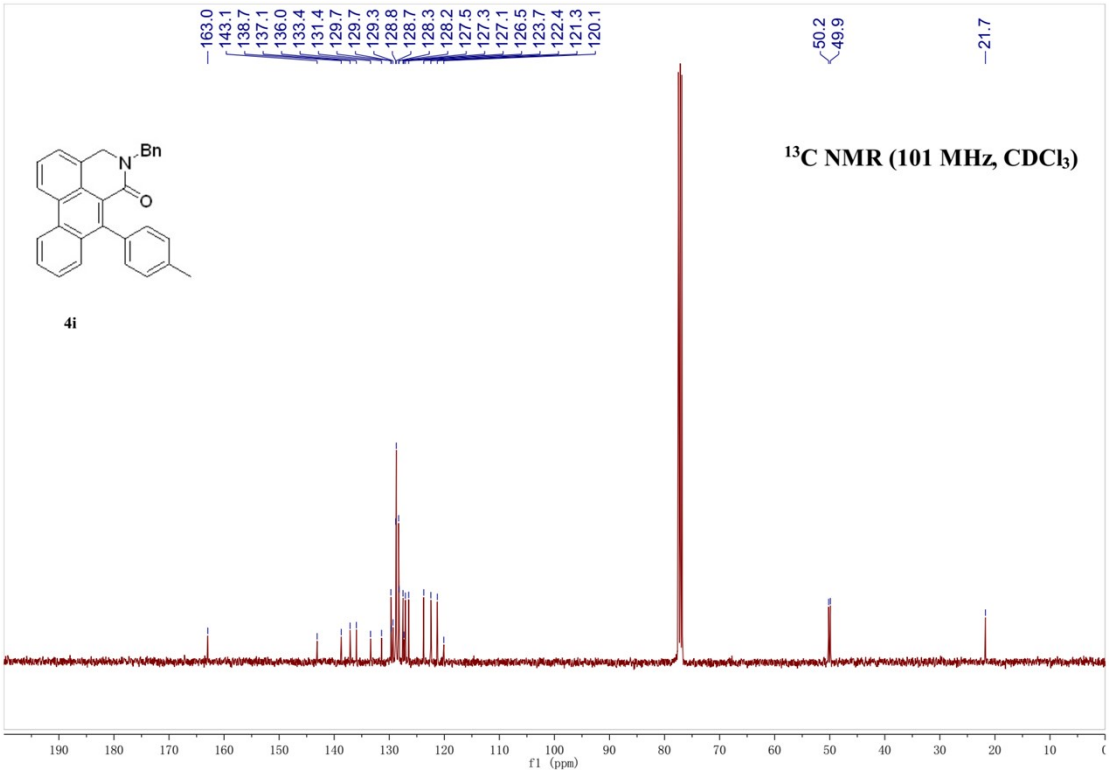
7.67
7.66
7.65
7.63
7.61
7.54
7.54
7.52
7.52
7.49
7.49
7.48
7.47
7.46
7.45
7.37
7.36
7.35
7.35
7.33
7.31
7.30
7.30
7.28
7.28
7.27
7.23
7.21
4.85
4.83
2.50
N
Bn
O
4i
1H NMR (400 MHz, CDCl3)
1.04
1.00
1.00
1.02
2.08
8.10
1.17
0.95
2.00
2.06
3.02
f1 (ppm)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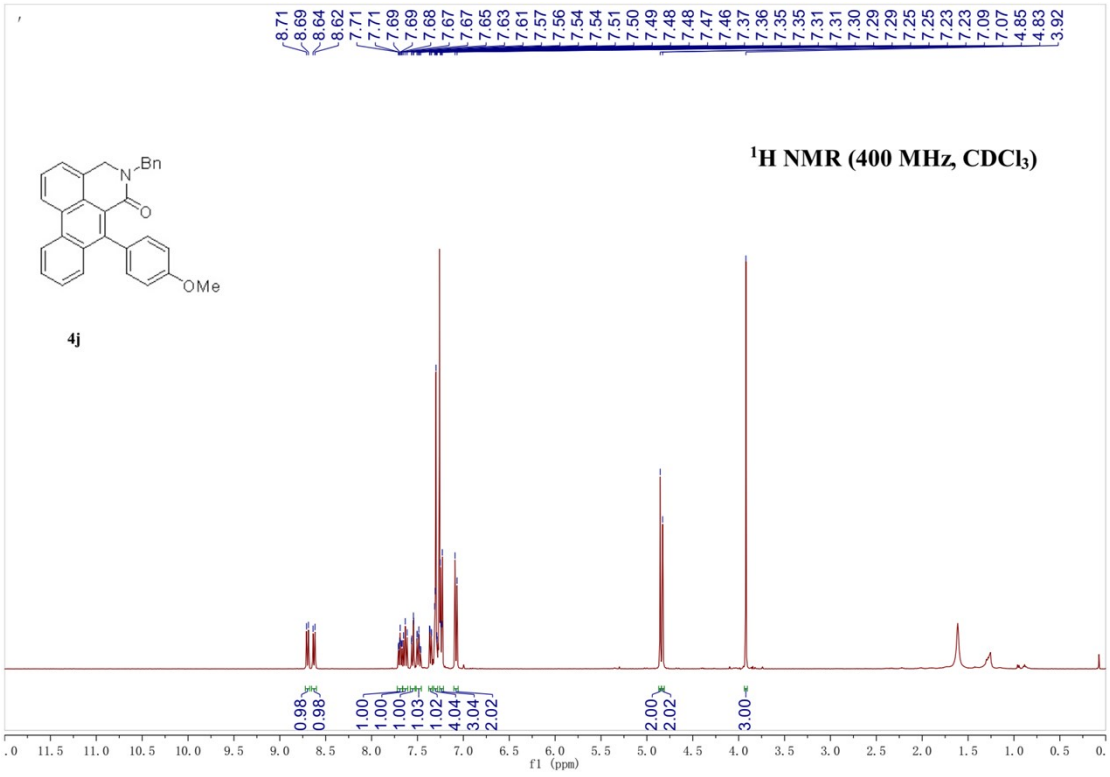
143.1
138.7
137.1
136.0
133.4
131.4
129.7
129.7
129.3
128.8
128.7
128.3
128.2
127.5
127.3
127.1
126.5
123.7
122.4
121.3
120.1
50.2
49.9
21.7
Bn
N
O
4i
13C NMR (101 MHz, CDCl3)
f1 (ppm)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8.69
8.64
8.62
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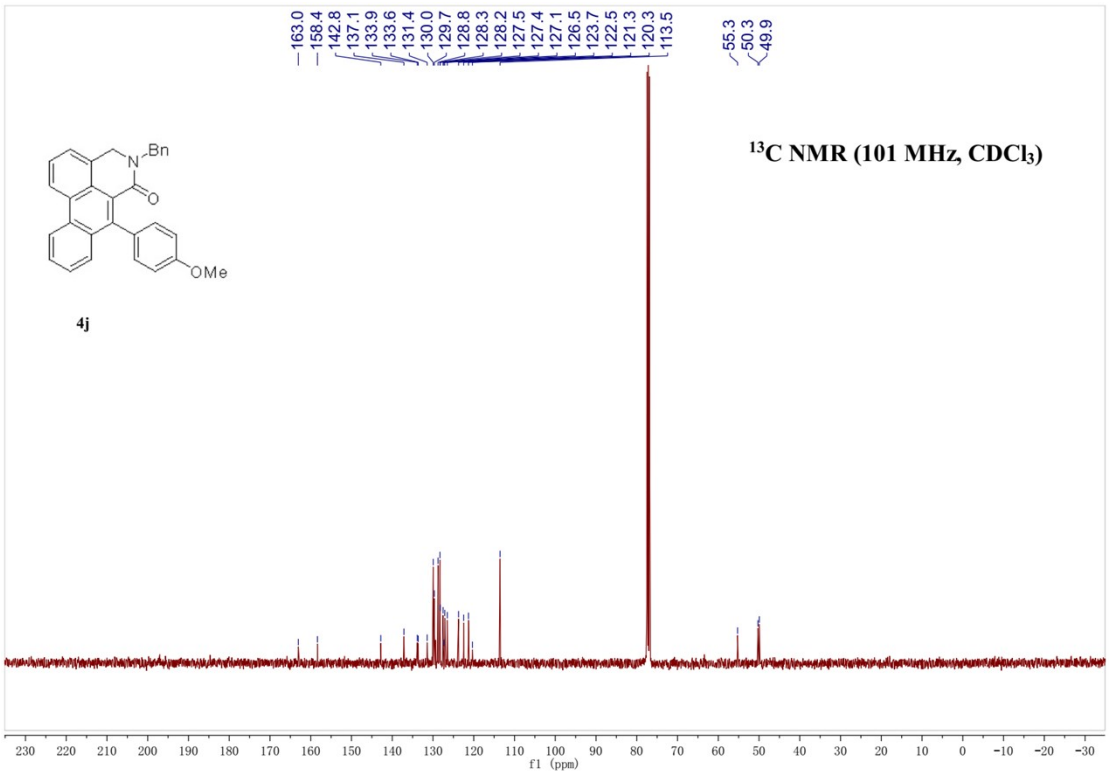
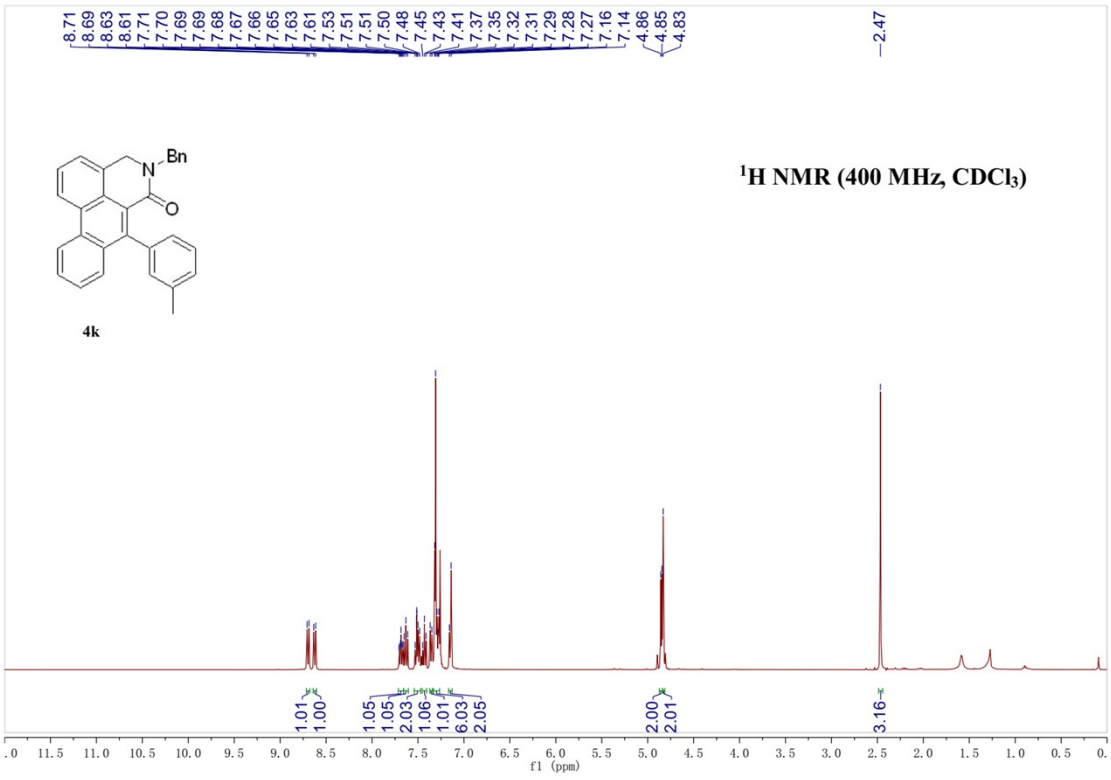
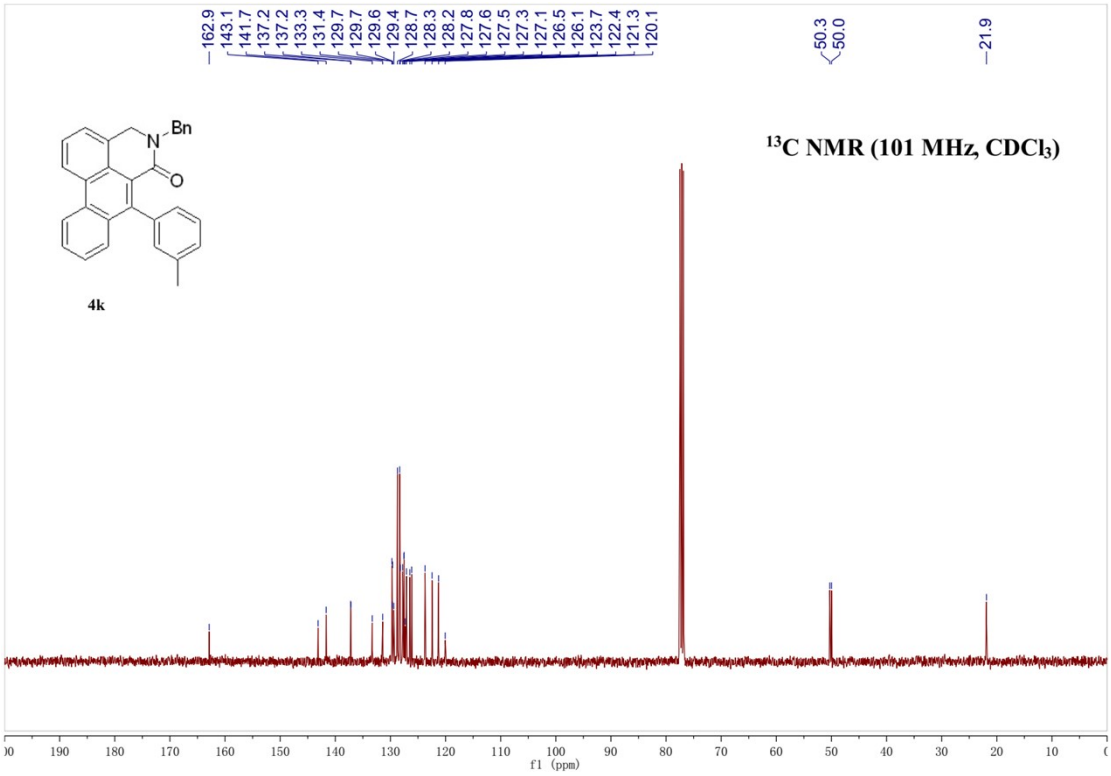
7.71
7.69
7.69
7.68
7.67
7.67
7.65
7.63
7.61
7.57
7.56
7.54
7.54
7.51
7.50
7.49
7.48
7.48
7.47
7.46
7.37
7.36
7.35
7.35
7.31
7.31
7.30
7.29
7.29
7.25
7.25
7.23
7.23
7.09
7.07
4.85
4.83
3.92
Bn
N
O
OMe
4j
1H NMR (400 MHz, CDCl3)
0.98
0.98
1.00
1.00
1.03
1.02
4.04
3.04
2.02
2.00
2.02
3.00
f1 (ppm)


163.0
158.4
142.8
137.1
133.9
133.6
131.4
130.0
129.7
128.8
128.3
128.2
127.5
127.4
127.1
126.5
123.7
122.5
121.3
120.3
113.5
55.3
50.3
49.9
N
Bn
O
OMe
4j
^{13}C NMR (101 MHz, CDCl$_3$)
f1 (ppm)


8.71
8.69
8.63
8.61
7.71
7.70
7.69
7.69
7.68
7.67
7.66
7.65
7.63
7.61
7.53
7.51
7.51
7.50
7.48
7.45
7.43
7.41
7.37
7.35
7.32
7.31
7.29
7.28
7.27
7.16
7.14
4.86
4.85
4.83
2.47
N
Bn
O
4k
^{1}H NMR (400 MHz, CDCl$_3$)
1.01
1.00
1.05
1.05
2.03
1.06
1.01
6.03
2.05
2.00
2.01
3.16
f1 (ppm)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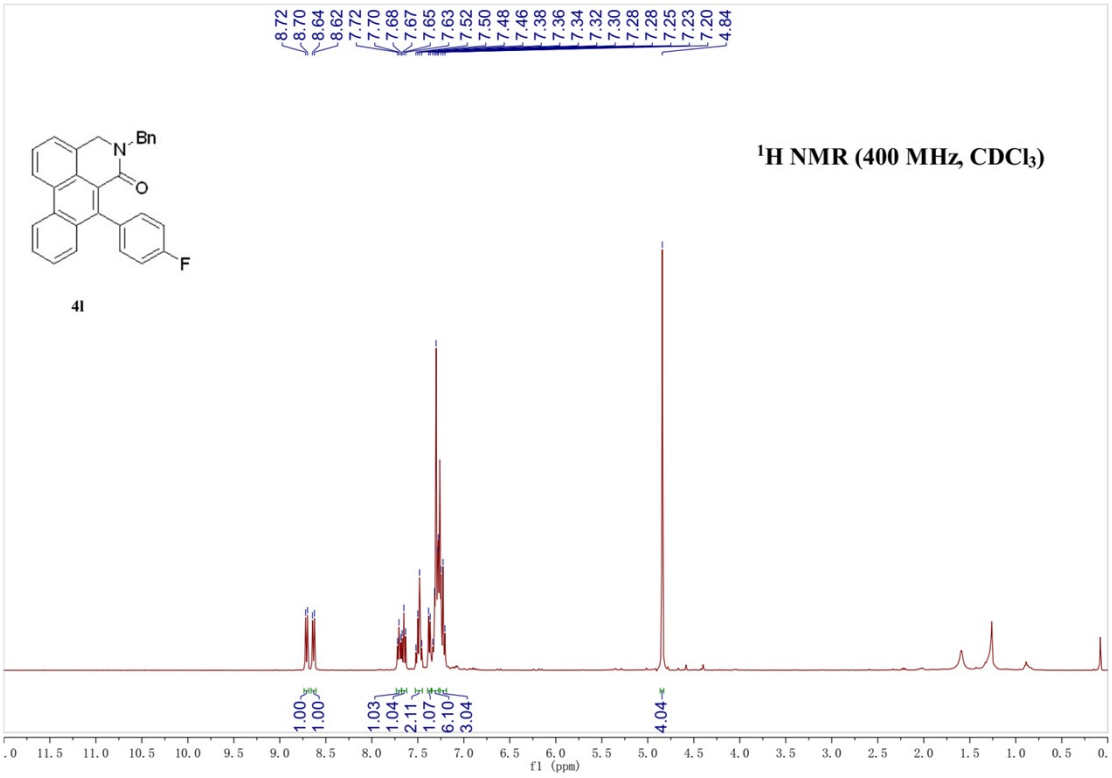
143.1
141.7
137.2
137.2
133.3
131.4
129.7
129.7
129.6
129.4
128.7
128.3
128.2
127.8
127.6
127.5
127.3
127.1
126.5
126.1
123.7
122.4
121.3
120.1
50.3
50.0
21.9
N
Bn
O
4k
13C NMR (101 MHz, CDCl3)
f1 (ppm)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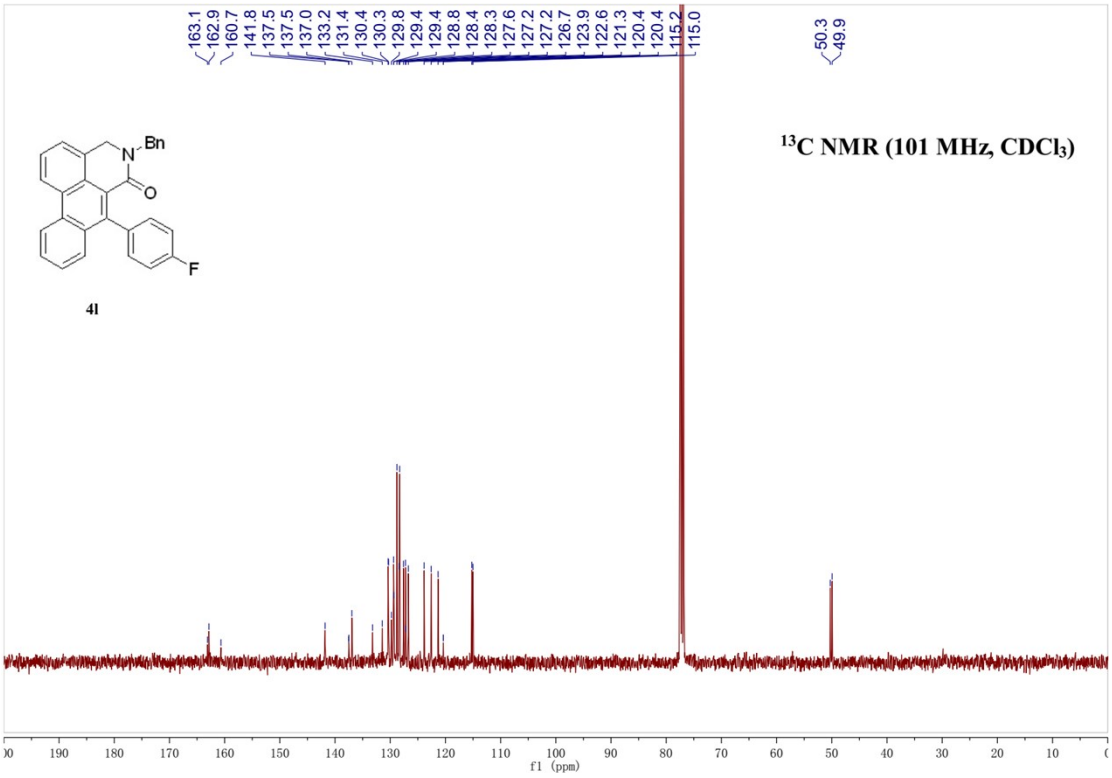
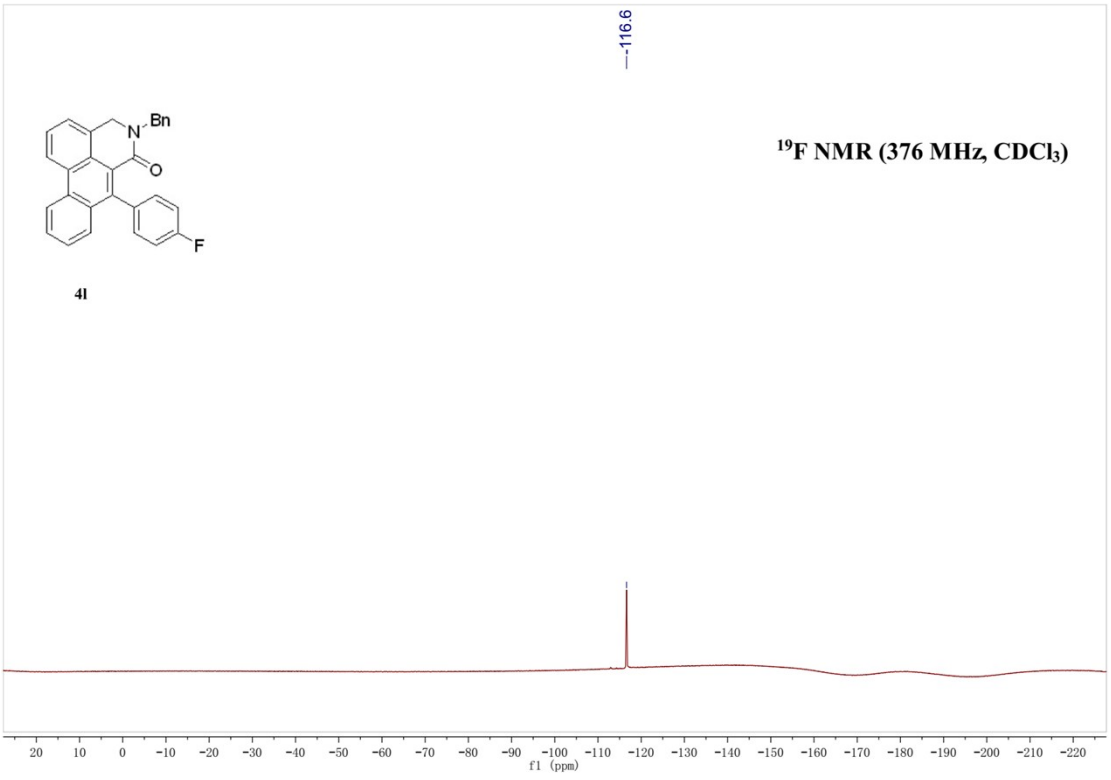
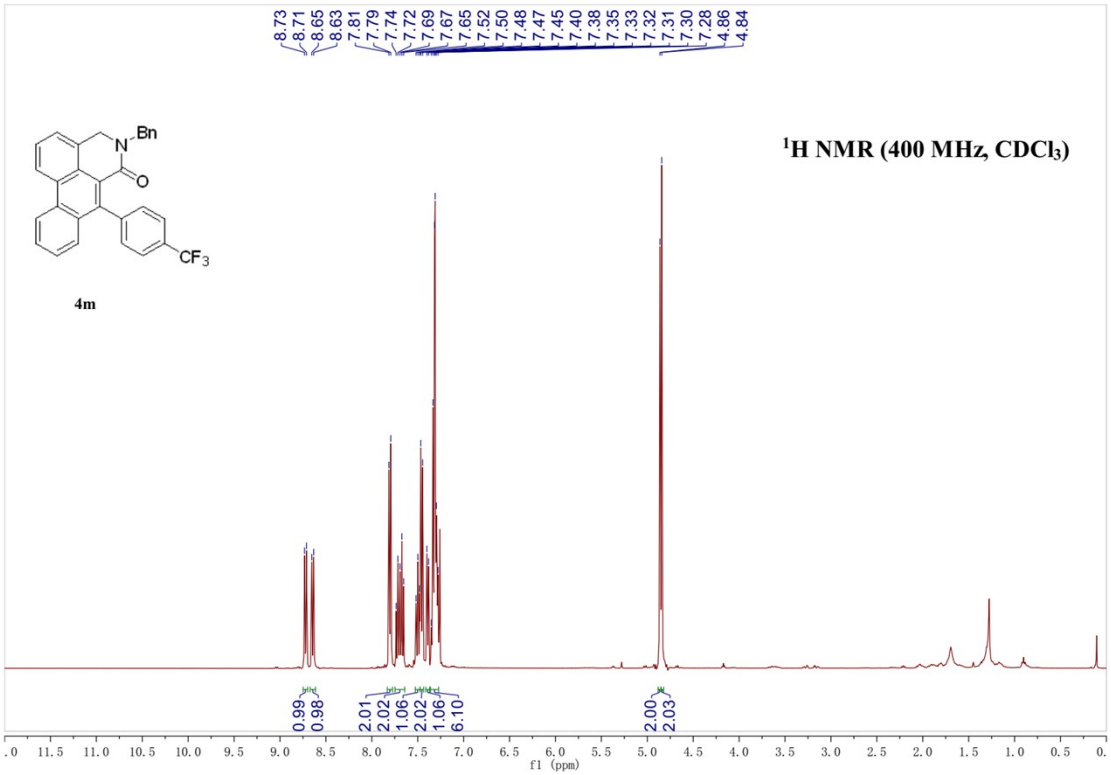
8.64
8.62
7.72
7.70
7.68
7.67
7.65
7.63
7.52
7.50
7.48
7.46
7.38
7.36
7.34
7.32
7.30
7.28
7.28
7.25
7.23
7.20
4.84
N
Bn
O
F
4l
1H NMR (400 MHz, CDCl3)
1.00
1.00
1.03
1.04
2.11
1.07
6.10
3.04
4.04
f1 (ppm)


163.1
162.9
160.7
141.8
137.5
137.5
137.0
133.2
131.4
130.4
130.3
129.8
129.4
129.4
128.8
128.4
128.3
127.6
127.2
127.2
126.7
123.9
122.6
121.3
120.4
120.4
115.2
115.0
50.3
49.9
Bn
N
O
F
41
^{13}C NMR (101 MHz, CDCl$_3$)
f1 (ppm)


-116.6
Bn
N
O
F
41
^{19}F NMR (376 MHz, CDCl$_3$)
f1 (ppm)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7.72
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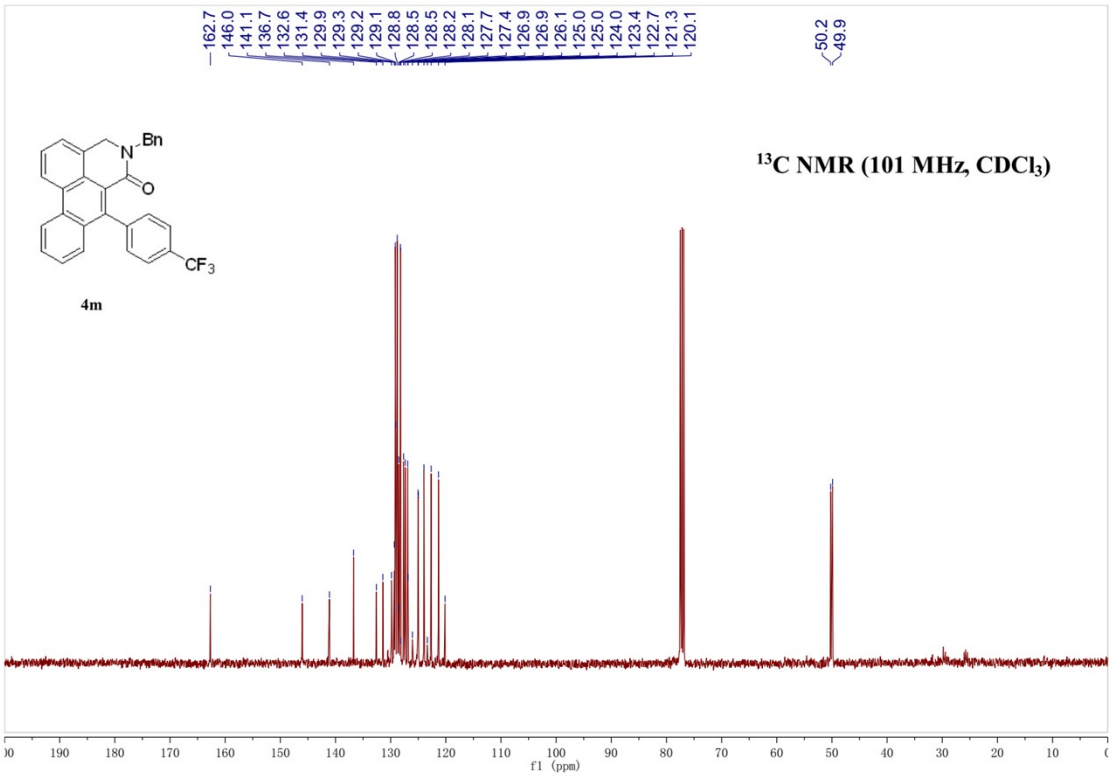
7.67
7.65
7.52
7.50
7.48
7.47
7.45
7.40
7.38
7.35
7.33
7.32
7.31
7.30
7.28
4.86
4.84
Bn
N
O
CF3
4m
1H NMR (400 MHz, CDCl3)
0.99
0.98
2.01
2.02
1.06
2.02
1.06
6.10
2.00
2.03
f1 (ppm)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136.7
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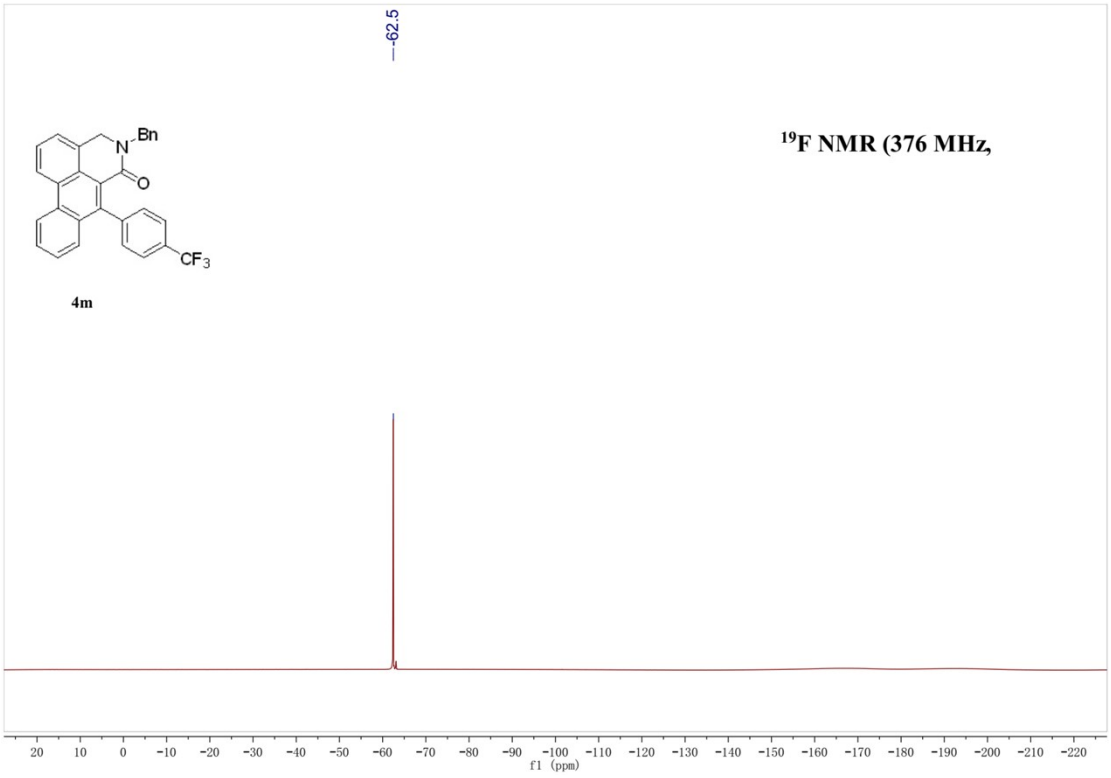
129.9
129.3
129.2
129.1
128.8
128.5
128.5
128.2
128.1
127.7
127.4
126.9
126.9
126.1
125.0
125.0
124.0
123.4
122.7
121.3
120.1
50.2
49.9
Bn
N
O
CF3
4m
13C NMR (101 MHz, CDCl3)
f1 (ppm)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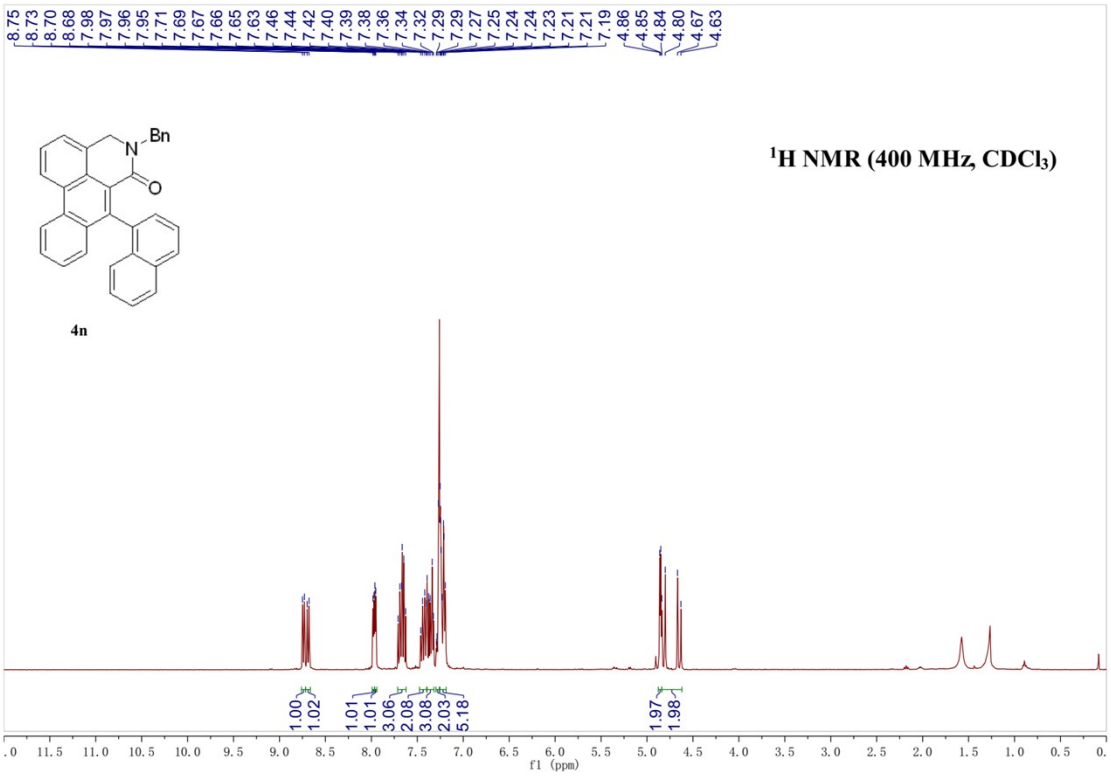
Bn
N
O
CF3
4m
19F NMR (376 MHz,
f1 (ppm)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7.95
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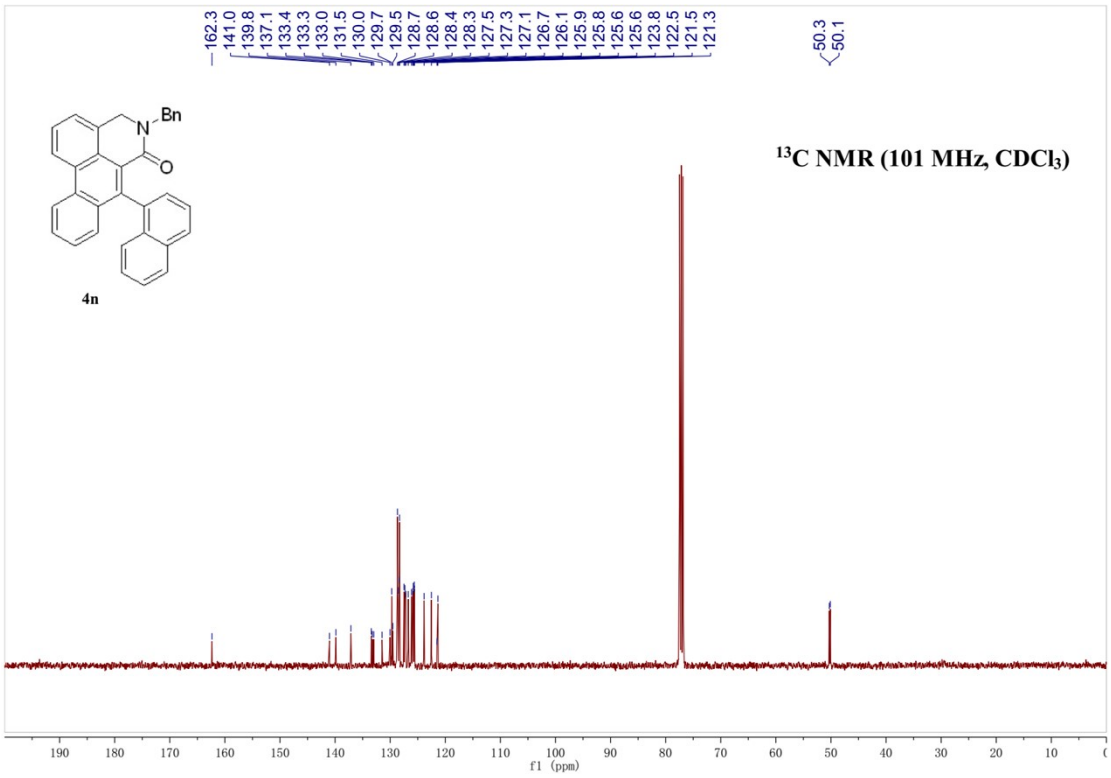
7.69
7.67
7.66
7.65
7.63
7.46
7.44
7.42
7.40
7.39
7.38
7.36
7.34
7.32
7.29
7.29
7.27
7.25
7.24
7.24
7.23
7.21
7.21
7.19
4.86
4.85
4.84
4.80
4.67
4.63
Bn
N
O
4n
1H NMR (400 MHz, CDCl3)
1.00
1.02
1.01
1.01
3.06
2.08
3.08
2.03
5.18
1.97
1.98
f1 (ppm)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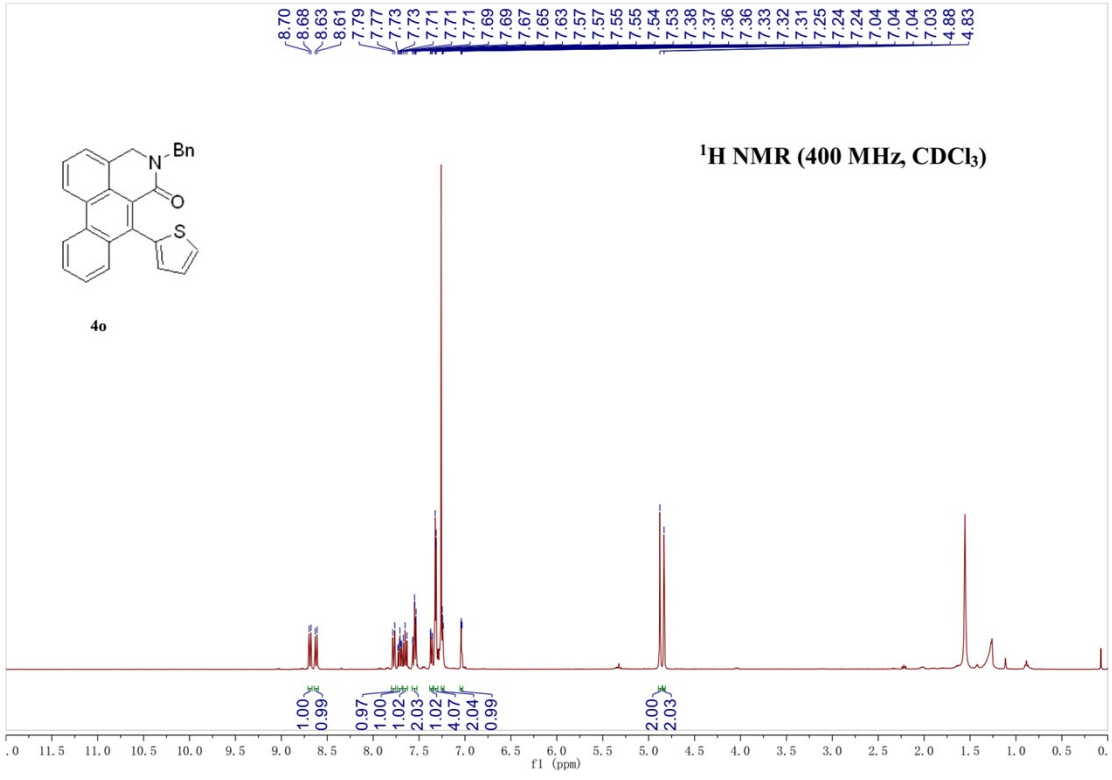
139.8
137.1
133.4
133.3
133.0
131.5
130.0
129.7
129.5
128.7
128.6
128.4
128.3
127.5
127.3
127.1
126.7
126.1
125.9
125.8
125.6
125.6
123.8
122.5
121.5
121.3
50.3
50.1
Bn
N
O
4n
13C NMR (101 MHz, CDCl3)
f1 (ppm)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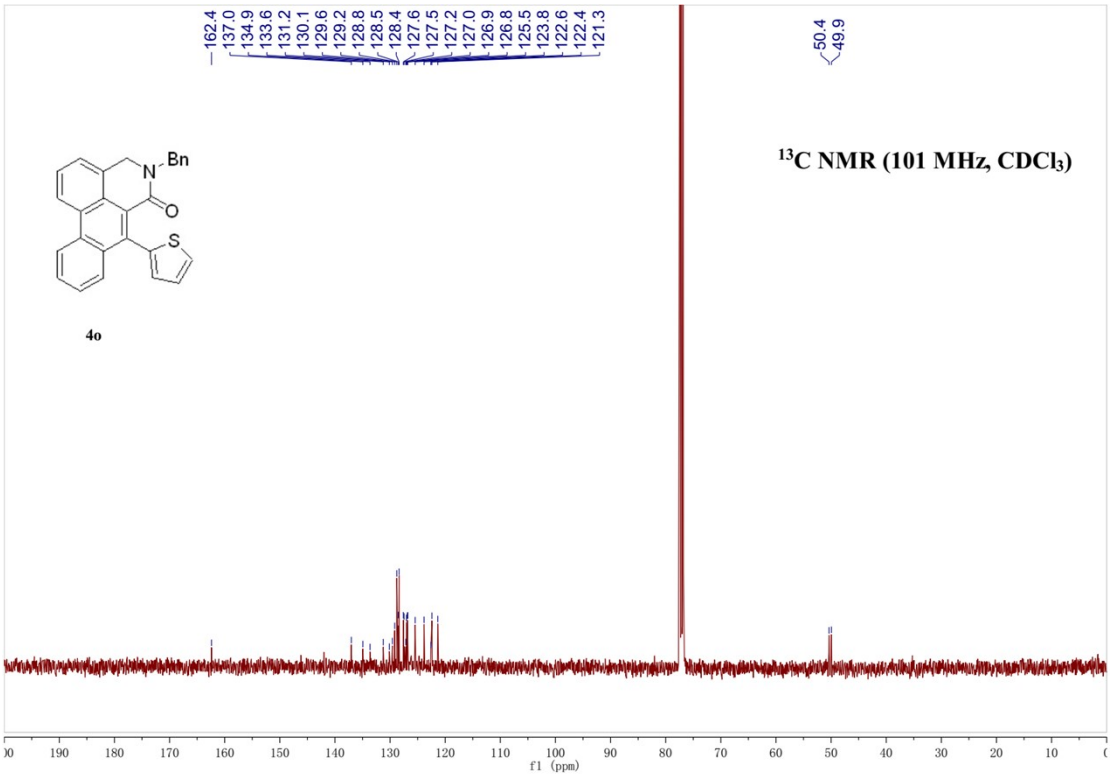
7.77
7.73
7.71
7.71
7.69
7.69
7.67
7.65
7.63
7.57
7.57
7.55
7.55
7.54
7.53
7.38
7.37
7.36
7.36
7.33
7.32
7.31
7.25
7.24
7.24
7.04
7.04
7.04
7.03
4.88
4.83
Bn
N
O
S
4o
1H NMR (400 MHz, CDCl3)
1.00
0.99
0.97
1.00
1.02
2.03
1.02
4.07
2.04
0.99
2.00
2.03
f1 (ppm)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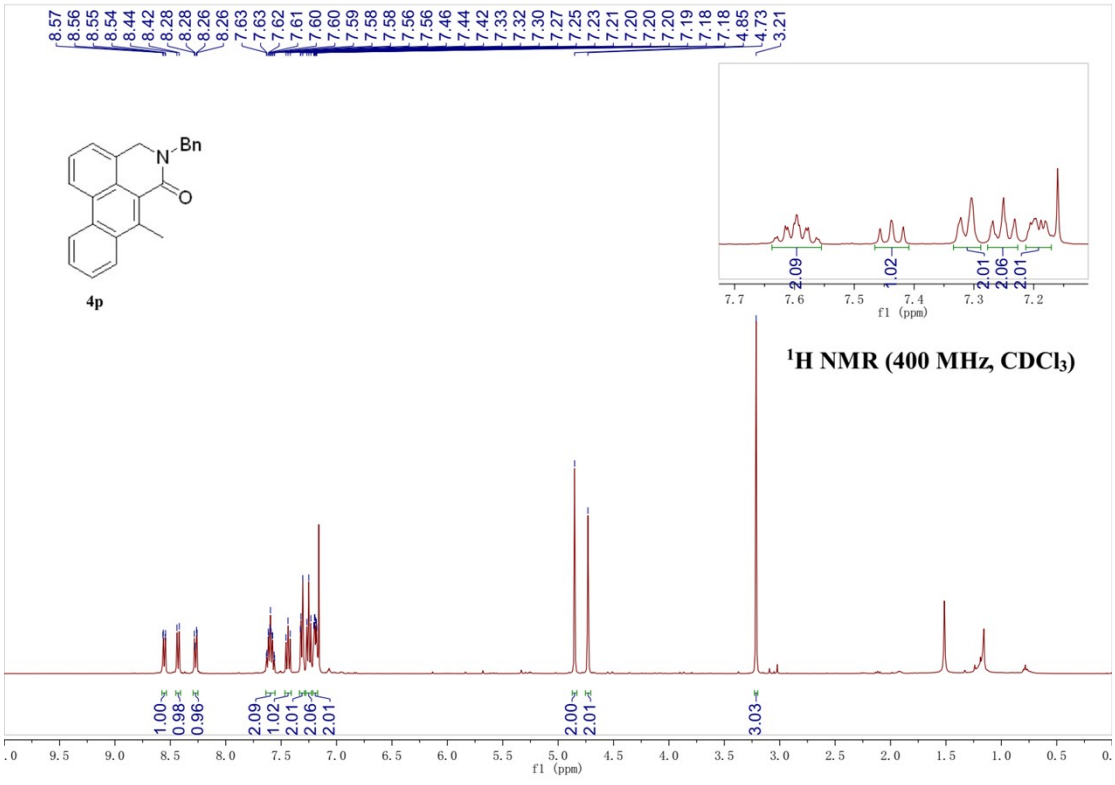
129.2
128.8
128.5
128.4
127.6
127.5
127.2
127.0
126.9
126.8
125.5
123.8
122.6
122.4
121.3
50.4
49.9
Bn
N
O
S
4o
13C NMR (101 MHz, CDCl3)
f1 (ppm)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8.28
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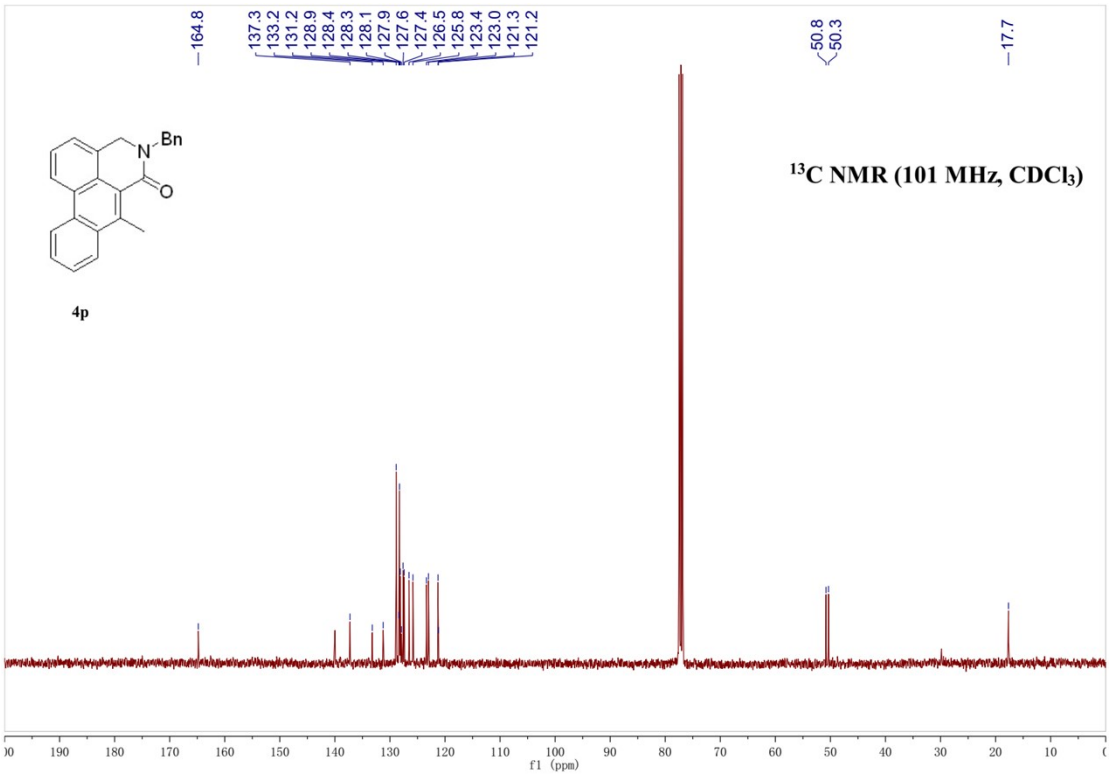
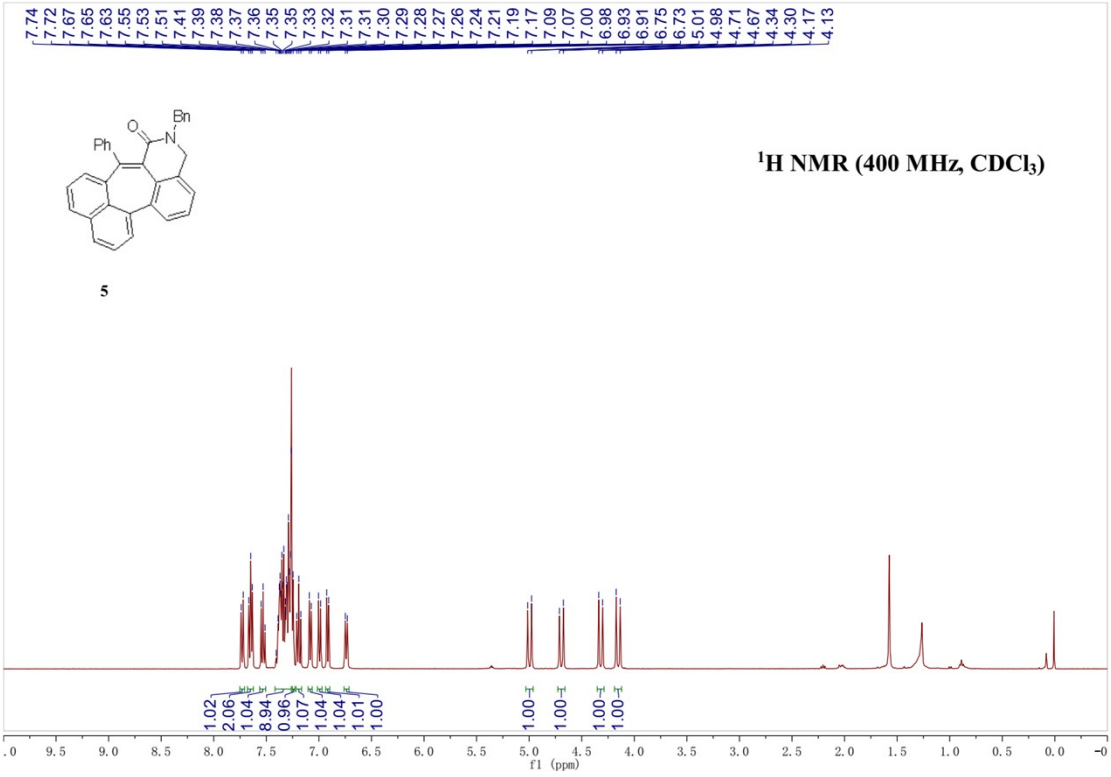
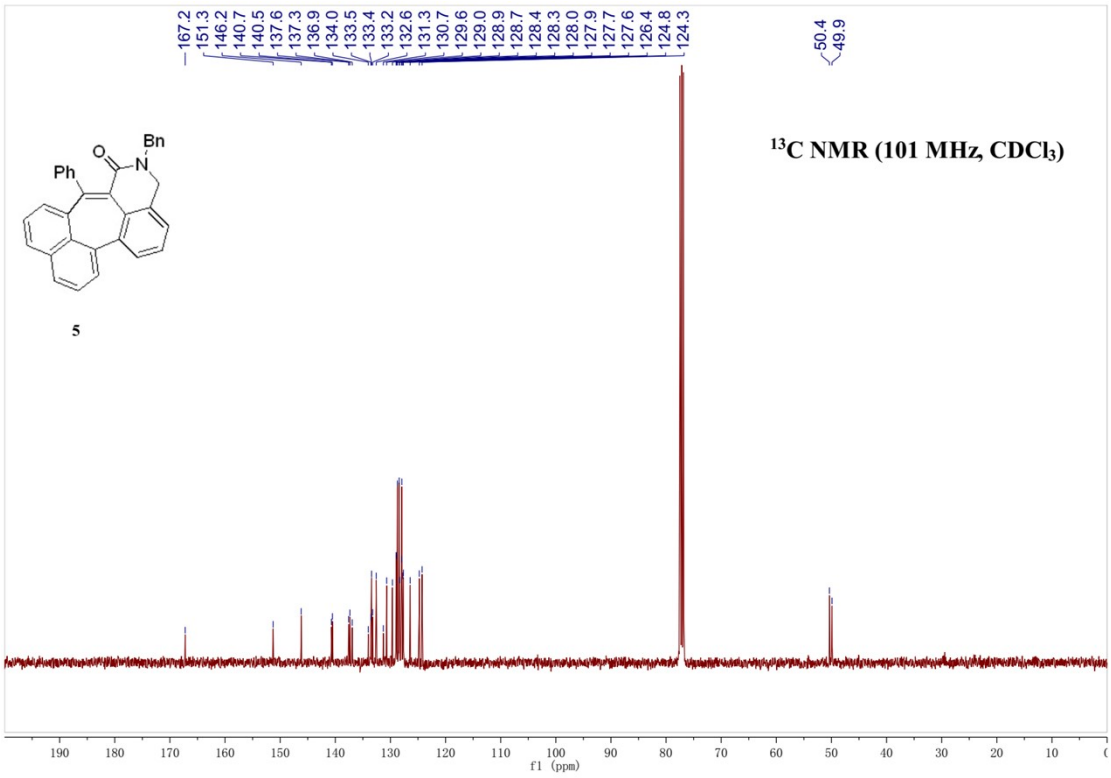
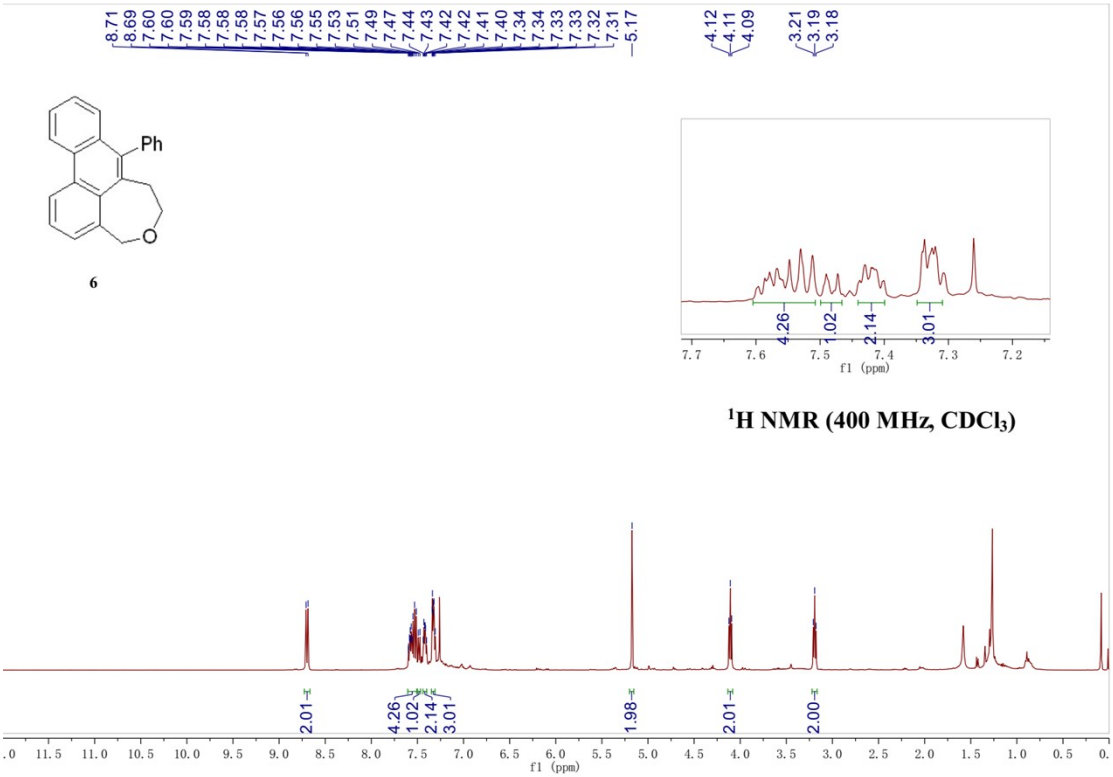
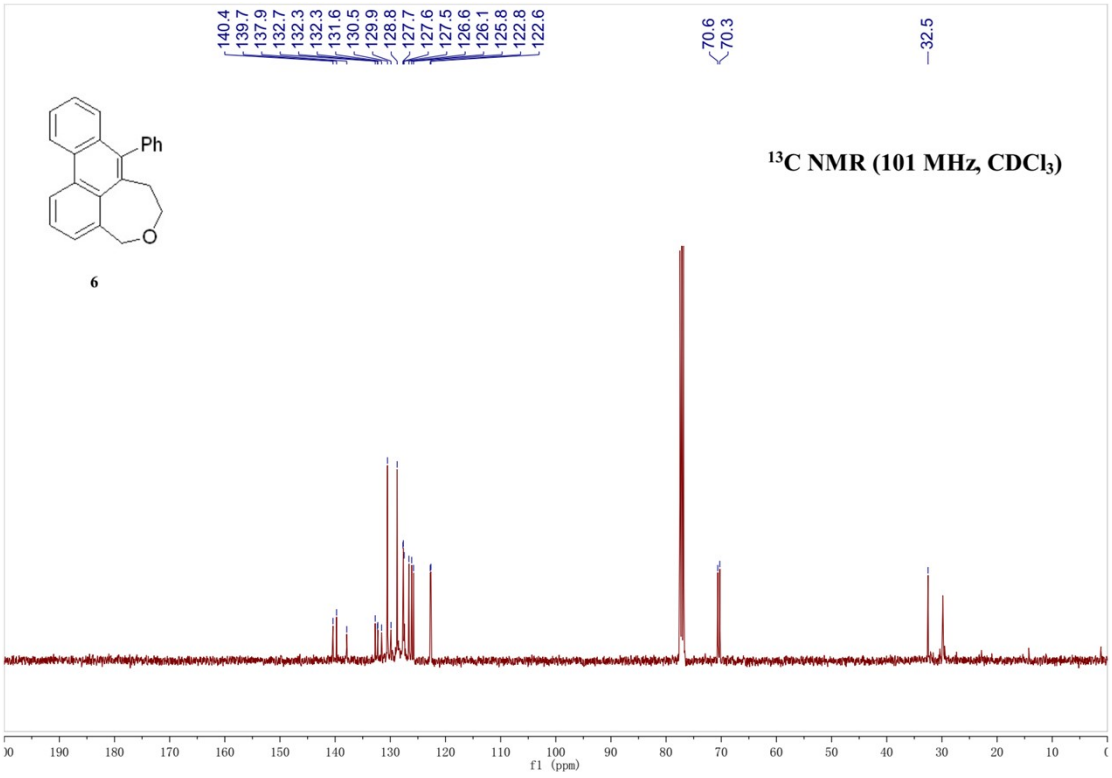
7.63
7.62
7.61
7.60
7.60
7.59
7.58
7.58
7.56
7.56
7.46
7.44
7.42
7.33
7.32
7.30
7.27
7.25
7.23
7.21
7.20
7.20
7.20
7.19
7.18
4.85
4.73
3.21
Bn
N
O
4p
2.09
1.02
2.01
2.06
2.01
f1 (ppm)
1H NMR (400 MHz, CDCl3)
1.00
0.98
0.96
2.09
1.02
2.01
2.06
2.01
2.00
2.01
3.03
f1 (ppm)


164.8
137.3
133.2
131.2
128.9
128.4
128.3
128.1
127.9
127.6
127.4
126.5
125.8
123.4
123.0
121.3
121.2
50.8
50.3
17.7
Bn
N
O
4p
13C NMR (101 MHz, CDCl3)
f1 (ppm)


7.74
7.72
7.67
7.65
7.63
7.55
7.53
7.51
7.41
7.39
7.38
7.37
7.36
7.35
7.35
7.33
7.32
7.31
7.31
7.30
7.29
7.28
7.27
7.26
7.24
7.21
7.19
7.17
7.09
7.07
7.00
6.98
6.93
6.91
6.75
6.73
5.01
4.98
4.71
4.67
4.34
4.30
4.17
4.13
Bn
Ph
O
N
5
1H NMR (400 MHz, CDCl3)
1.02
2.06
1.04
8.94
0.96
1.07
1.04
1.04
1.01
1.00
1.00
1.00
1.00
1.00
f1 (ppm)


167.2
151.3
146.2
140.7
140.5
137.6
137.3
136.9
134.0
133.5
133.4
133.2
132.6
131.3
130.7
129.6
129.0
128.9
128.7
128.4
128.3
128.0
127.9
127.7
127.6
126.4
124.8
124.3
50.4
49.9
O
N
Bn
Ph
5
13C NMR (101 MHz, CDCl3)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


8.71
8.69
7.60
7.60
7.59
7.58
7.58
7.58
7.57
7.56
7.56
7.55
7.53
7.51
7.49
7.47
7.44
7.43
7.42
7.42
7.41
7.40
7.34
7.34
7.33
7.32
7.31
5.17
4.12
4.11
4.09
3.21
3.19
3.18
Ph
O
6
4.26
1.02
2.14
3.01
7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
1H NMR (400 MHz, CDCl3)
2.01
4.26
1.02
2.14
3.01
1.98
2.01
2.00
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
f1 (ppm)


140.4
139.7
137.9
132.7
132.3
131.6
130.5
129.9
128.8
127.7
127.6
127.5
126.6
126.1
125.8
122.8
122.6
70.6
70.3
32.5
Ph
O
6
^{13}C NMR (101 MHz, CDCl$_3$)
f1 (ppm)