Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Formal dual C(sp^2)-H cross-dehydrogenative C-O bond formation to construct highly functionalized diaryl ether with O_2

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1 General Information

Chemicals and solvents were purchased from commercial suppliers and used as received unless noted. All products were purified by flash chromatography on silica gel. The chemical yields referred are isolated products. ^{1}H NMR and ^{13}C NMR spectra were recorded on 400 MHz, 500MHz or 600 MHz Bruker spectrometers. Chemical shifts of ^{1}H NMR were reported in part per million relatives to the $CDCl_3$ residual peak (δ 7.26). Chemical shifts of ^{13}C NMR were reported relative to $CDCl_3$ (δ 77.16) or DMSO-d_6 (δ 39.04). The used abbreviations are as follows: s (singlet), d (doublet), t (triplet), quart (quartet), quint (quintet), m (multiplet), br (broad). Multiplets which arise from accidental equality of coupling constants of magnetically non-equivalent protons are marked as virtual (*virt*). High resolution mass spectra (HRMS) data were measured on a ESI-microTOFII. Melting points were measured on a SGW® X-4B and are not corrected. Reactions were monitored by TLC analysis using silica gel 60 Å F-254 thin layer plates and compounds were visualized with a UV light at 254 nm or 365 nm. Further visualization was achieved by staining with iodine, or $KMnO_4$ followed by heating on a hot plate. Flash column chromatography was performed on silica gel 60 Å, 10-40 μm. The substrates were prepared according to literature methods.[1-6]

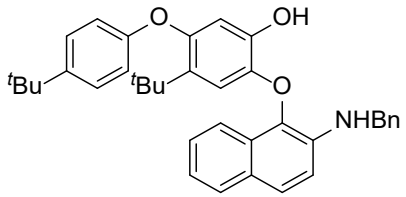
2 Representative procedures

Unless specified otherwise, a flame-dried, 25 mL round bottom flask, backfilled with N_2, equipped with a Teflon-coated stir bar and a rubber septum was charged with phenol **1** (0.45 mmol, 67.5 mg, 2.25 equiv.), **2** (0.2 mmol, 46.6 mg, 1 equiv.) and dry and degassed CH_2Cl_2 (2 mL, 1.0 M in phenol). In a separate, flame-dried 5 mL microwave vial $[Cu(CH_3CN)_4](PF_6)$ (4 mol%, 6.7 mg) and *N*,*N*′-di-*tert*-butylethylenediamine (5 mol%, 5 μL.) were dissolved in dry and degassed CH_2Cl_2 (1.0 mL, 0.04 M) to afford a homogeneous solution. This solution was then added to the round bottom flask *via* syringe to afford a final volume of 3 mL. Under a constant pressure of O_2 (1 atm), the reaction was vented 3 times for 10 s to remove N_2 or air. The reaction mixture was then stirred at rt (20 °C) for 4 h, then TsOH (150 mol%, 58 mg) was added to reaction flask and allow to stir for unless the reaction completed. The reaction was quenched by the addition of $NaHCO_3$ (20 mL, 10% by weight aqueous solution). The phases were then separated, and the aqueous phase was extracted with CH_2Cl_2 (3 x 20 mL). The combined organic phase was evaporated. Purification of crude product was performed by column chromatography using hexane/EtOAc (gradient elution

from100:1 to 100:5) as the eluents to afford **3 and 4**.

3 Analytical data of desired products

2-((2-(Benzylamino)naphthalen-1-yl)oxy)-4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)phenol 3a



A pink solid, 101 mg, 92% yield.

m.p.: 162– 164 °C.

TLC: R_f = 0.58 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

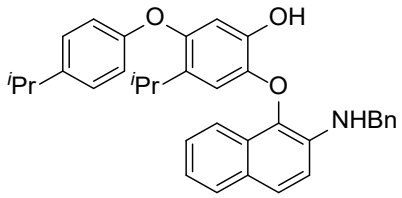
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.1 Hz, 1H), 7.70 – 7.64 (m, 2H), 7.44 – 7.32 (m, 7H), 7.32 – 7.28 (m, 1H), 7.26 (m, 1H), 7.14 (d, *J* = 8.9 Hz, 1H), 6.94 (m, 2H), 6.61 (s, 1H), 6.53 (s, 1H), 4.56 (s, 2H), 1.36 (s, 9H), 1.20 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 151.2, 145.6, 143.6, 139.8, 139.4, 137.9, 132.8, 132.5, 128.8, 128.2, 128.1, 127.8, 127.4, 127.0, 126.9, 126.7, 126.6, 122.6, 119.7, 118.3, 114.5, 112.1, 108.0, 47.7, 34.4, 34.4, 31.7, 30.2.

IR (neat/cm^{-1}) 3506.9, 3407.7, 1628.2, 1506.1, 1258.8, 1175.6, 865.6, 811.5.

HRMS (ESI): $C_{37}H_{40}NO_3^+$ [$(M+H)^+$]: calcd.: 546.3003; found: 546.3000.

2-((2-(benzylamino)naphthalen-1-yl)oxy)-4-*iso*-propyl-5-(4-*iso*-propylphenoxy)phenol 3b



A brown oil, 91 mg, 81% yield.

TLC: R_f = 0.20 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

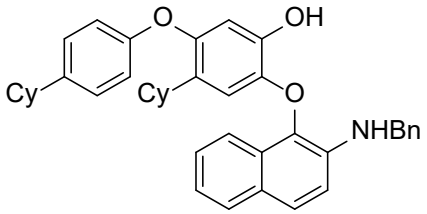
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.1 Hz, 1H), 7.67 (dd, *J* = 8.7, 1.9 Hz, 2H), 7.45 – 7.38 (m, 1H), 7.35 (d, *J* = 4.7 Hz, 4H), 7.32 – 7.25 (m, 2H), 7.23 – 7.13 (m, 3H), 6.92 (d, *J* = 8.6 Hz, 2H), 6.70 (s, 1H), 6.44 (s, 1H), 6.07 (s, 1H), 4.74 (s, 1H), 4.56 (s, 2H), 3.20 – 3.04 (m, 1H), 3.00 – 2.87 (m, 1H), 1.30 (d, *J* = 6.9 Hz, 6H), 1.01 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) 13C NMR (101 MHz, CDCl3) δ 156.3, 148.8, 143.5, 142.9, 140.9, 139.3, 137.8, 132.3, 132.0, 128.7, 128.1, 128.0, 127.7, 127.4, 127.3, 126.9, 126.9, 126.6, 122.5, 119.6, 117.4, 114.5, 111.3, 107.7, 47.6, 33.4, 27.0, 24.2, 22.9.

IR (neat/cm^{-1}) 2958.15, 1630.8, 1494.9, 1373.9, 1217.5, 1181.6, 1107.9, 875.5, 803.9.

HRMS (ESI): $C_{35}H_{36}NO_3^+$ [$(M+H)^+$]: calcd.: 518.2690; found: 518.2698.

2-((2-(Benzylamino)naphthalen-1-yl)oxy)-4-cyclohexyl-5-(4-cyclohexylphenoxy)phenol 3c



A dark brown oil, 97 mg, 79% yield.

TLC: R_f = 0.48 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

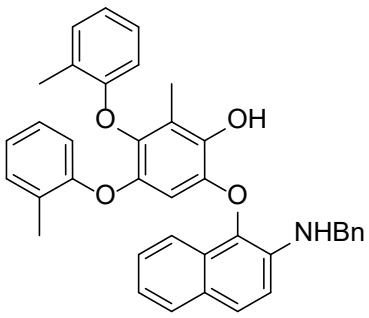
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.1 Hz, 1H), 7.70 – 7.64 (m, 2H), 7.40 (m, 1H), 7.37 – 7.25 (m, 6H), 7.22 – 7.12 (m, 3H), 6.92 (d, *J* = 8.6 Hz, 2H), 6.67 (s, 1H), 6.42 (s, 1H), 6.03 (s, 1H), 4.73 (s, 1H), 4.56 (s, 2H), 2.74 (tt, *J* = 12.1, 2.9 Hz, 1H), 2.60 – 2.43 (m, 1H), 1.98 – 1.87 (m, 4H), 1.85 – 1.75 (m, 2H), 1.73 – 1.56 (m, 4H), 1.53 – 1.35 (m, 4H), 1.35 – 1.18 (m, 3H), 1.17 – 0.98 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.4, 149.3, 143.5, 142.4, 140.8, 139.5, 137.9, 132.3, 131.1, 128.8, 128.2, 128.1, 127.9, 127.7, 127.4, 127.0, 127.0, 126.7, 122.6, 119.6, 117.9, 114.5, 111.8, 107.5, 47.6, 44.0, 37.3, 34.8, 33.3, 27.1, 26.9, 26.3, 26.1.

IR (neat/cm^{-1}) 3415.2, 2850.6, 1494.1, 1281.3, 1121.3, 10554.9, 735.3.

HRMS (ESI): $C_{41}H_{44}NO_3^+$ [$(M+H)^+$]: calcd.: 598.3316; found: 598.3315.

6-((2-(Benzylamino)naphthalen-1-yl)oxy)-2-methyl-3,4-bis(*o*-tolyloxy)phenol 3d



A brown solid, 95 mg, 84% yield.

m.p.: 80–82 °C.

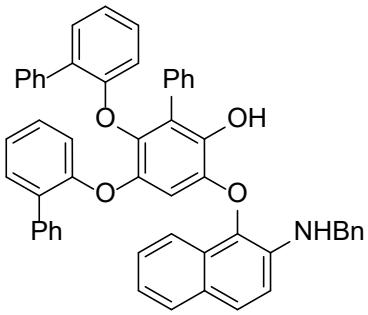
TLC: R_f = 0.39 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.2 Hz, 1H), 7.71 – 7.61 (m, 2H), 7.45 (m, 1H), 7.38 – 7.23 (m, 6H), 7.13 (d, *J* = 8.9 Hz, 1H), 7.07 (d, *J* = 8.9 Hz, 1H), 7.03 – 6.92 (m, 3H), 6.85 (m, 2H), 6.49 (m, 2H), 6.24 (s, 1H), 6.18 (brs, 1H), 4.71 (s, 1H), 4.54 (s, 2H), 2.30 (s, 3H), 1.82 (s, 3H), 1.63 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.2, 156.1, 141.2, 140.6, 140.1, 139.9, 139.2, 137.9, 131.9, 131.0, 130.6, 130.6, 128.8, 128.1, 127.9, 127.7, 127.3, 127.1, 127.0, 126.9, 126.6, 126.4, 126.3, 122.6, 121.5, 121.3, 120.7, 119.3, 114.5, 113.5, 112.5, 105.8, 47.7, 15.4, 15.2, 9.5.

HRMS (ESI): $C_{38}H_{34}NO_4^+$ [$(M+H)^+$]: calcd.: 568.2482; found: 568.2483.

5,6-Bis([1,1'-biphenyl]-2-yloxy)-3-((2-(benzylamino)naphthalen-1-yl)oxy)-[1,1'-biphenyl]-2-ol 3e



A white solid, 128 mg, 85% yield.

m.p.: 65– 67 °C.

TLC: R_f = 0.60 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

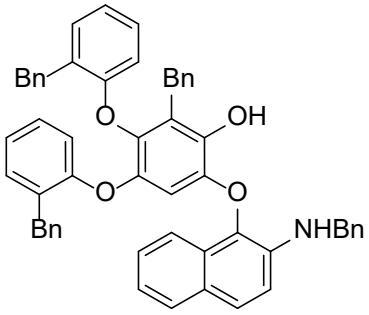
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.1 Hz, 1H), 7.64 (m, 2H), 7.46 – 7.37 (m, 3H), 7.31 (m, 5H), 7.25 (m, 4H), 7.21 – 7.11 (m, 6H), 7.11 – 7.04 (m, 4H), 6.99 (m, 3H), 6.91 (m, 4H), 6.67 – 6.58 (m, 2H), 6.27 (s, 1H), 6.02 (s, 1H), 4.71 (s, 1H), 4.51 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.9, 154.7, 142.2, 140.6, 140.1, 139.2, 138.9, 138.0, 137.9, 137.7, 132.1, 131.9, 131.0, 130.8, 130.5, 130.4, 129.5, 129.4, 128.9, 128.3, 128.2, 128.1, 127.9, 127.9, 127.7, 127.5, 127.5, 127.2, 127.2, 127.1, 126.7, 126.5, 124.7, 122.7, 122.3, 121.7, 119.3, 114.8, 114.5, 113.9, 107.8, 47.8.

IR (neat/cm^{-1}) 3428.52, 3957.0, 1631.8, 117.8, 1202.3, 949.4, 752.6.

HRMS (ESI): $C_{53}H_{40}NO_4^+$ [$(M+H)^+$]: calcd.: 754.2952; found: 754.2956.

2-Benzyl-6-((2-(benzylamino)naphthalen-1-yl)oxy)-3,4-bis(2-benzylphenoxy)phenol 3f



A brown solid, 128 mg, 80 % yield.

m.p.: 61–63 °C.

TLC: R_f = 0.72 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

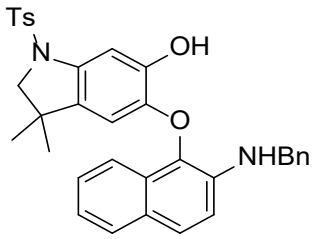
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.1 Hz, 1H), 7.68 – 7.61 (m, 2H), 7.49 – 7.41 (m, 1H), 7.36 – 7.20 (m, 10H), 7.20 – 7.05 (m, 9H), 7.05 – 6.94 (m, 5H), 6.93 – 6.78 (m, 5H), 6.54 (dd, *J* = 8.2, 1.1 Hz, 1H), 6.49 (dd, *J* = 8.1, 1.2 Hz, 1H), 6.23 (s, 1H), 6.17 (s, 1H), 4.53 (s, 2H), 4.00 (s, 2H), 3.46 (s, 2H), 3.24 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.7, 155.6, 141.7, 140.9, 140.6, 140.1, 140.1, 139.9, 139.7, 139.2, 137.9, 131.8, 130.2, 130.0, 129.9, 129.2, 129.1, 129.0, 128.8, 128.2, 128.2, 127.8, 127.7, 127.4, 127.1, 127.0, 127.0, 126.9, 125.9, 125.8, 125.7, 123.8, 122.6, 121.9, 121.7, 119.3, 114.5, 113.7, 113.2, 106.6, 47.6, 35.4, 34.6, 30.2.

IR (neat/cm^{-1}) 3493.7, 2919.9, 1603.1, 1238.3, 1096.9, 998.7.

HRMS (ESI): $C_{56}H_{46}NO_4^+$ [$(M+H)^+$]: calcd.: 796.3421; found: 796.3424.

5-((2-(benzylamino)naphthalen-1-yl)oxy)-3,3-dimethyl-1-tosylindolin-6-ol 3g



A white solid, 93 mg, 82% yield.

m.p.: 222–224 °C.

TLC: R_f = 0.34 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].

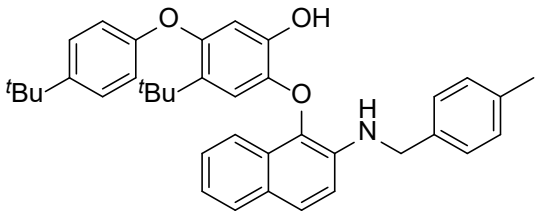
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (m, 3H), 7.63 (d, *J* = 8.9 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 1H), 7.46 (s, 1H), 7.43 – 7.34 (m, 2H), 7.27 (m, 7H), 7.10 (d, *J* = 9.0 Hz, 1H), 6.12 (s, 1H), 6.07 (s, 1H), 4.65 (s, 1H), 4.51 (s, 2H), 3.56 (s, 2H), 2.39 (s, 3H), 0.91 (s, 6H).

^{13}C NMR (101 MHz, DMSO) δ 146.2, 144.1, 142.9, 140.4, 138.1, 134.3, 133.3, 132.6, 130.7, 129.8, 128.2, 127.8, 127.8, 127.1, 126.7, 126.7, 126.6, 126.5, 126.3, 125.7, 121.6, 114.6, 108.4, 103.3, 63.5, 45.7, 39.4, 27.6, 20.9.

IR (neat/cm^{-1}) 2920.0, 1723.2, 1603.3, 1490.0, 1318.5, 1158.9, 1046.6, 663.4, 575.2.

HRMS (ESI): $C_{34}H_{33}N_2OS^+$ [$(M+H)^+$]: calcd.: 565.2156; found: 565.2154.

4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)-2-((2-((4-methylbenzyl)amino)naphthalen-1-yl)oxy)phenol 3h



A brown solid, 104 mg, 93% yield.

m.p.: 80–82 °C.

TLC: R_f = 0.42 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

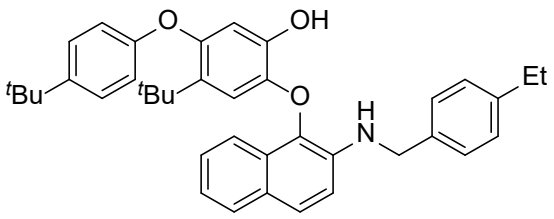
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.2 Hz, 1H), 7.70 – 7.63 (m, 2H), 7.40 (m, 1H), 7.37 (m, 2H), 7.28 (m, 1H), 7.23 (d, *J* = 7.8 Hz, 2H), 7.16 (m, 3H), 6.95 (d, *J* = 7.8 Hz, 2H), 6.61 (s, 1H), 6.53 (s, 1H), 4.51 (s, 2H), 2.36 (s, 3H), 1.37 (s, 9H), 1.20 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 151.1, 145.5, 143.5, 139.7, 138.0, 136.9, 136.3, 132.8, 132.4, 129.4, 128.1, 128.0, 127.7, 127.0, 126.8, 126.6, 126.5, 122.4, 119.6, 118.2, 114.5, 112.0, 107.9, 47.5, 34.3, 34.3, 31.6, 30.1, 21.1.

IR (neat/cm^{-1}) 2957.52, 1603.0, 1496.8, 1389.8, 1264.3, 1196.4, 800.6.

HRMS (ESI): $C_{38}H_{42}NO_3^+$ [$(M+H)^+$]: calcd.: 560.3159; found: 560.3156.

4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)-2-((2-((4-ethylbenzyl)amino)naphthalen-1-yl)oxy)phenol 3i



A brown oil, 102 mg, 89% yield.

TLC: R_f = 0.48 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].

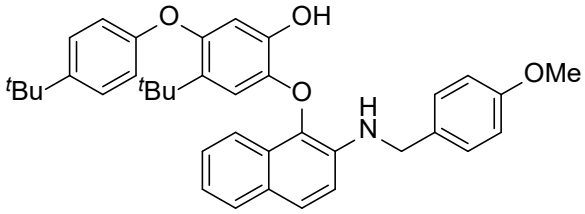
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (m, 1H), 7.67 (m, 2H), 7.45 – 7.32 (m, 3H), 7.31 – 7.24 (m, 3H), 7.22 – 7.15 (m, 3H), 6.95 (d, *J* = 8.9 Hz, 2H), 6.61 (s, 1H), 6.54 (s, 1H), 5.97 (s, 1H), 4.67 (s, 1H), 4.52 (s, 2H), 2.70 – 2.64 (m, 2H), 1.36 (s, 9H), 1.26 (t, *J* = 7.6 Hz, 3H), 1.21 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 151.1, 145.5, 143.5, 143.3, 139.7, 138.1, 136.5, 132.8, 132.3, 128.2, 128.1, 128.0, 127.7, 127.1, 126.8, 126.6, 126.5, 122.4, 119.6, 118.2, 114.5, 112.0, 108.0, 47.5, 34.3, 34.3, 31.6, 30.1, 28.6, 15.7.

IR (neat/cm^{-1}) 2959.5, 1630.7, 1390.2, 1263.4, 1196.1, 886.1, 802.0.

HRMS (ESI): $C_{39}H_{44}NO_3^+$ [$(M+H)^+$]: calcd.: 574.3316; found: 574.3312.

4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)-2-((2-((4-methoxybenzyl)amino)naphthalen-1-yl)oxy)phenol 3j



A dark brown solid, 106 mg, 91% yield.

m.p.: 70–72 °C.

TLC: R_f = 0.56 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

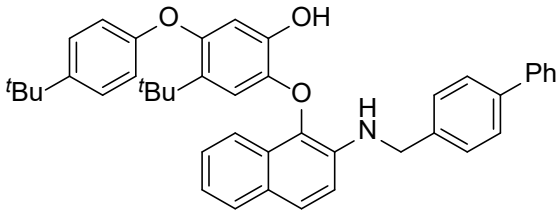
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.2 Hz, 1H), 7.67 (m, 2H), 7.40 (m, 1H), 7.39 – 7.34 (m, 2H), 7.28 – 7.22 (m, 3H), 7.18 (d, *J* = 8.9 Hz, 1H), 6.94 (d, *J* = 8.9 Hz, 2H), 6.87 (d, *J* = 8.1 Hz, 2H), 6.60 (s, 1H), 6.52 (s, 1H), 4.48 (s, 2H), 3.81 (s, 3H), 1.36 (s, 9H), 1.19 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 155.4, 151.1, 145.5, 143.5, 139.7, 138.0, 132.7, 132.4, 131.3, 128.2, 128.1, 128.0, 127.7, 126.8, 126.5, 126.5, 122.4, 119.6, 118.2, 114.5, 114.1, 112.0, 107.9, 55.3, 47.2, 34.3, 34.3, 31.5, 30.1.

IR (neat/cm^{-1}) 2920.0, 1603.4, 1497.7, 1318.2, 1223.3, 1196.8, 885.9.

HRMS (ESI): $C_{38}H_{42}NO_4^+$ [$(M+H)^+$]: calcd.: 576.3108; found: 576.3110.

2-((2-(([1,1'-biphenyl]-4-ylmethyl)amino)naphthalen-1-yl)oxy)-4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)phenol 3k



A brown solid, 112 mg, 90% yield.

m.p.: 90–92 °C.

TLC: R_f = 0.13 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

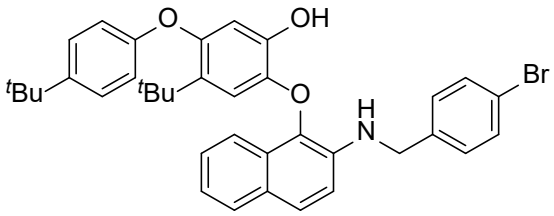
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.1 Hz, 1H), 7.70 (m, 2H), 7.64 – 7.54 (m, 4H), 7.50 – 7.46 (m, 2H), 7.44 – 7.36 (m, 6H), 7.34 – 7.27 (m, 1H), 7.21 (d, *J* = 8.9 Hz, 1H), 7.02 – 6.94 (m, 2H), 6.66 (s, 1H), 6.57 (s, 1H), 4.59 (s, 2H), 1.37 (s, 9H), 1.23 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 151.2, 145.5, 143.6, 140.8, 140.3, 139.7, 138.3, 137.7, 132.8, 132.6, 128.8, 128.2, 128.0, 127.8, 127.5, 127.3, 127.1, 126.9, 126.6, 126.5, 122.6, 119.7, 118.3, 114.5, 112.0, 108.0, 47.5, 34.3, 34.3, 31.6, 30.2.

IR (neat/cm^{-1}) 2956.8, 1629.9, 1497.3, 1390.1, 1195.9, 885.9, 803.2.

HRMS (ESI): $C_{43}H_{44}NO_3^+$ [$(M+H)^+$]: calcd.: 622.3316; found: 622.3313.

2-((2-((4-Bromobenzyl)amino)naphthalen-1-yl)oxy)-4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)phenol 3l



A dark brown solid, 110 mg, 88% yield.

m.p.: 71–73 °C.

TLC: R_f = 0.67 (Hexane/EtOAc = 5:1) [UV, $KMnO_4$].

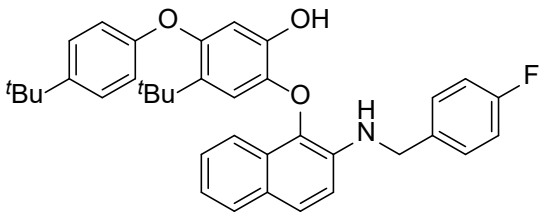
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.2 Hz, 1H), 7.68 – 7.59 (m, 2H), 7.46 – 7.41 (m, 2H), 7.40 – 7.36 (m, 1H), 7.35 – 7.32 (m, 2H), 7.28 – 7.24 (m, 1H), 7.20 – 7.16 (m, 2H), 7.06 – 7.02 (m, 1H), 6.94 – 6.89 (m, 2H), 6.58 (s, 1H), 6.47 (s, 1H), 4.48 (s, 2H), 1.33 (s, 9H), 1.16 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 151.2, 145.6, 143.5, 139.6, 138.5, 137.5, 132.8, 132.5, 131.8, 128.6, 128.1, 128.0, 127.8, 126.9, 126.6, 126.5, 122.6, 121.0, 119.6, 118.2, 114.2, 111.9, 107.9, 47.1, 34.3, 34.3, 31.6, 30.1.

IR (neat/cm^{-1}) 3415.4, 2922.9, 1629.5, 1495.9, 1216.7, 1107.7, 802.5.

HRMS (ESI): $C_{37}H_{39}{}^{79}BrNO_3^+$ [$(M+H)^+$]: calcd.: 624.2108; found: 624.2106.

4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)-2-((2-((4-fluorobenzyl)amino)naphthalen-1-yl)oxy)phenol 3m



A white solid, 93 mg, 82% yield.

m.p.: 144– 146 °C.

TLC: R_f = 0.57 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

^{1}H NMR (600 MHz, $CDCl_3$) 7.78 (d, *J* = 8.1 Hz, 1H), 7.71 – 7.60 (m, 2H), 7.46 – 7.35 (m, 3H), 7.29 (m, 3H), 7.11 (d, *J* = 9.0 Hz, 1H), 7.08 – 7.00 (m, 2H), 6.95 (d, *J* = 8.9 Hz, 2H), 6.63 (s, 1H), 6.52 (s, 1H), 4.69 (s, 1H), 4.51 (s, 2H), 1.37 (s, 9H), 1.21 (s, 9H).

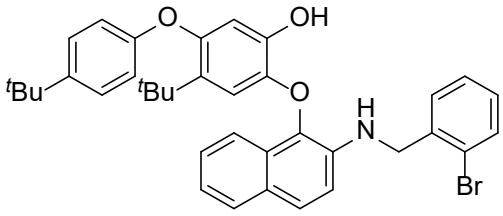
^{13}C NMR (101 MHz, $CDCl_3$) δ 162.1 (d, *J* = 245.3 Hz), 155.3, 151.2, 145.6, 143.5, 139.6, 137.6, 135.0 (d, *J* = 3.1 Hz), 132.8, 132.5, 128.5 (d, *J* = 8.1 Hz), 128.1, 128.0, 127.8, 126.9, 126.6, 126.5, 122.6, 119.6, 118.3, 115.6 (d, *J* = 21.4 Hz), 114.3, 111.9, 107.9, 47.0, 34.3, 34.3, 31.6, 30.1.

^{19}F NMR (376 MHz, $CDCl_3$) δ -115.39.

IR (neat/cm^{-1}) 3405.6, 2960.7, 1602.4, 1392.14, 1258.7, 1223.2, 823.6, 447.1.

HRMS (ESI): $C_{37}H_{39}FNO_3^+$ [$(M+H)^+$]: calcd.: 564.2908; found: 564.2905.

2-((2-((2-Bromobenzyl)amino)naphthalen-1-yl)oxy)-4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)phenol 3n



A brown solid, 107 mg, 88% yield.

m.p.: 130–132 °C.

TLC: R_f = 0.65 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].

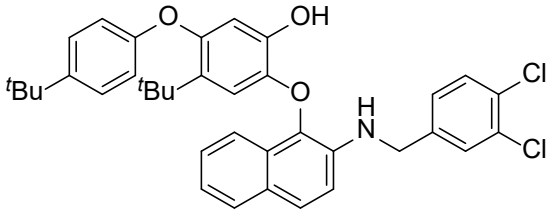
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (d, J = 8.1 Hz, 1H), 7.68 – 7.63 (m, 2H), 7.60 – 7.56 (m, 1H), 7.41 – 7.32 (m, 4H), 7.28 – 7.20 (m, 2H), 7.16 – 7.10 (m, 1H), 7.05 (d, J = 8.9 Hz, 1H), 6.98 – 6.92 (m, 2H), 6.63 (s, 1H), 6.50 (s, 1H), 4.56 (s, 2H), 1.36 (s, 9H), 1.19 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 151.2, 145.5, 143.6, 140.8, 140.3, 139.7, 138.3, 137.7, 132.8, 128.8, 128.2, 128.0, 127.8, 127.5, 127.3, 127.1, 126.9, 126.6, 126.5, 122.6, 119.7, 118.3, 114.5, 112.0, 108.0, 47.5, 34.3, 34.3, 31.6, 30.2.

IR (neat/cm^{-1}) 3512.45, 2960.1, 1603.1, 1495.9, 1372.1, 1176.1, 776.7, 548.3.

HRMS (ESI): $C_{37}H_{39}{}^{79}BrNO_3^+$ [$(M+H)^+$]: calcd.: 624.2108; found: 624.2105.

4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)-2-((2-((3,4-dichlorobenzyl)amino)naphthalen-1-yl)oxy)phenol 3o



A brown solid, 96 mg, 78 % yield.

m.p.: 42– 44 °C.

TLC: R_f = 0.46 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

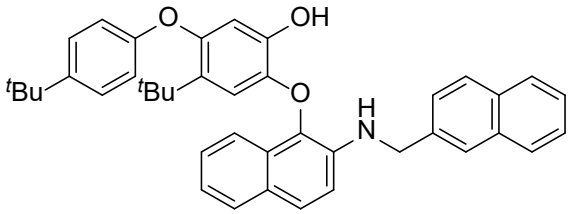
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.1 Hz, 1H), 7.67 (m, 2H), 7.48 – 7.36 (m, 5H), 7.30 (m, 1H), 7.16 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.03 (d, *J* = 8.9 Hz, 1H), 7.01 – 6.94 (m, 2H), 6.65 (s, 1H), 6.52 (s, 1H), 5.98 (s, 1H), 4.75 (s, 1H), 4.48 (s, 2H), 1.38 (s, 9H), 1.22 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 151.3, 145.6, 143.4, 139.9, 139.6, 137.4, 132.9, 132.6, 131.2, 130.7, 128.8, 128.1, 128.0, 127.9, 127.0, 126.7, 126.6, 126.5, 126.0, 122.8, 119.7, 118.3, 114.0, 111.8, 107.9, 46.7, 34.3, 34.3, 31.6, 30.1.

IR (neat/cm^{-1}) 2958.4, 1540.0, 1263.6, 1195.9, 886.1, 760.7, 458.7.

HRMS (ESI): $C_{37}H_{38}Cl_2NO_3^+$ [$(M+H)^+$]: calcd.: 614.2223; found: 614.2222.

4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)-2-((2-((naphthalen-2-ylmethyl)amino)naphthalen-1-yl)oxy)phenol 3p



A brown solid, 89 mg, 71% yield.

m.p.: 58– 60 °C.

TLC: R_f = 0.23 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

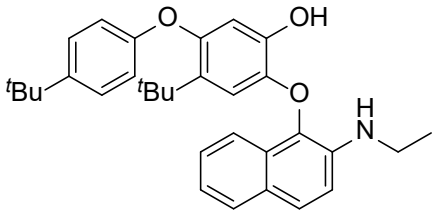
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 – 7.75 (m, 5H), 7.73 – 7.63 (m, 2H), 7.54 – 7.48 (m, 2H), 7.46 – 7.38 (m, 2H), 7.37 (dd, *J* = 9.2, 2.4 Hz, 2H), 7.20 (d, *J* = 8.9 Hz, 1H), 6.96 (dd, *J* = 8.3, 1.7 Hz, 2H), 6.80 (d, *J* = 8.9 Hz, 1H), 6.63 (s, 1H), 6.60 (s, 1H), 4.71 (s, 2H), 1.37 (s, 9H), 1.23 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 153.2, 151.1, 145.5, 143.5, 139.7, 138.0, 136.9, 133.5, 132.8, 132.5, 128.6, 128.1, 128.0, 127.7, 126.8, 126.6, 126.5, 126.4, 126.3, 125.8, 125.6, 125.2, 122.5, 119.6, 118.2, 114.8, 114.5, 112.1, 107.9, 48.0, 34.3, 34.3, 31.6, 30.2.

IR (neat/cm^{-1}) 2957.1630.0, 1362.8, 1262.8, 803.3, 436.4, 421.6.

HRMS (ESI): $C_{41}H_{42}NO_3^+$ [$(M+H)^+$]: calcd.: 596.3159; found: 596.3158.

4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)-2-((2-(ethylamino)naphthalen-1-yl)oxy)phenol 3q



A brown oil, 71 mg, 73% yield.

TLC: R_f = 0.38 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

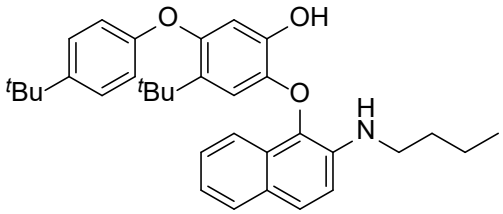
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.1 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.67 – 7.61 (m, 1H), 7.42 – 7.34 (m, 3H), 7.26 – 7.20 (m, 2H), 7.00 – 6.90 (m, 2H), 6.60 (s, 1H), 6.48 (s, 1H), 3.38 (q, *J* = 7.1 Hz, 2H), 1.36 (s, 9H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.17 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 151.2, 145.6, 143.7, 139.8, 138.4, 132.7, 128.2, 128.1, 127.7, 126.8, 126.7, 126.6, 126.5, 122.5, 119.7, 118.4, 114.6, 112.3, 107.9, 38.6, 34.4, 34.3, 31.7, 30.2, 15.6.

IR (neat/cm^{-1}) 2958.9, 1611.4, 1391.8, 1200.6, 1180.8, 1111.1, 852.2.

HRMS (ESI): $C_{32}H_{38}NO_3^+$ [$(M+H)^+$]: calcd.: 484.2846; found: 484.2844.

4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)-2-((2-(butylamino)naphthalen-1-yl)oxy)phenol 3r



A white solid, 90 mg, 86% yield.

m.p.: 56– 58 °C.

TLC: R_f = 0.45 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

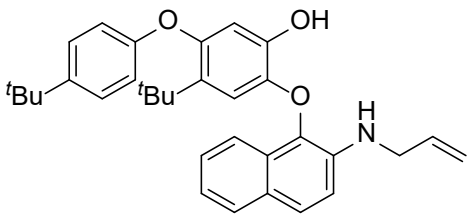
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.1 Hz, 1H), 7.71 (d, *J* = 8.9 Hz, 1H), 7.65 (m, 1H), 7.41 – 7.34 (m, 3H), 7.30 – 7.20 (m, 2H), 6.95 (d, *J* = 8.9 Hz, 2H), 6.61 (s, 1H), 6.48 (s, 1H), 3.32 (t, *J* = 7.1 Hz, 2H), 1.67 – 1.56 (m, 2H), 1.43 – 1.37 (m, 2H), 1.37 (s, 9H), 1.17 (s, 9H), 0.96 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.5, 151.2, 145.6, 143.7, 139.8, 138.4, 132.7, 132.6, 128.3, 128.1, 127.6, 126.8, 126.6, 126.6, 122.4, 119.7, 118.3, 114.6, 112.2, 108.0, 43.7, 34.4, 34.3, 32.2, 31.7, 30.2, 20.2, 14.0.

IR (neat/cm^{-1}) 2956.5, 1603.3, 1497.7, 1420.2, 1222.5, 1175.6, 1043.6, 829.0.

HRMS (ESI): $C_{34}H_{42}NO_3^+$ [$(M+H)^+$]: calcd.: 512.3159; found: 512.3160

2-((2-(Allylamino)naphthalen-1-yl)oxy)-4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)phenol 3s



A white solid, 89 mg, 90% yield.

m.p.: 134– 136 °C.

TLC: R_f = 0.42 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

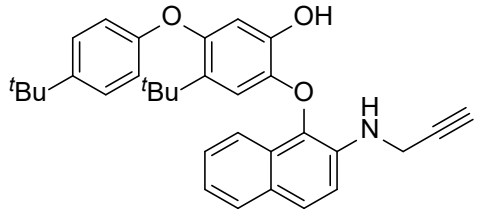
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.1 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.65 (m, 1H), 7.45 – 7.33 (m, 3H), 7.33 – 7.23 (m, 1H), 7.20 (d, *J* = 8.9 Hz, 1H), 6.97 (d, *J* = 8.9 Hz, 2H), 6.63 (s, 1H), 6.49 (s, 1H), 6.05 – 5.88 (m, 1H), 5.27 (dd, *J* = 17.2, 1.6 Hz, 1H), 5.18 (dd, *J* = 10.3, 1.5 Hz, 1H), 4.04 – 3.94 (m, 2H), 1.38 (s, 9H), 1.19 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 151.2, 145.6, 143.6, 139.8, 138.0, 135.4, 132.7, 132.7, 128.2, 128.1, 127.8, 126.8, 126.6, 126.5, 122.6, 119.7, 118.3, 116.3, 114.7, 112.1, 108.0, 46.2, 34.4, 34.3, 31.7, 30.2.

IR (neat/cm^{-1}) 3507.3, 1628.8, 1498.9, 1223.6, 1044.1, 885.5, 799.5, 569.8, 494.8.

HRMS (ESI): $C_{33}H_{38}NO_3^+$ [$(M+H)^+$]: calcd.: 496.2846; found: 496.2844.

4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)-2-((2-(prop-2-yn-1-ylamino)naphthalen-1-yl)oxy)phenol 3t



A white solid, 90 mg, 91 % yield.

m.p.: 158– 160 °C.

TLC: R_f = 0.17 (Hexane/EtOAc = 5:1) [UV, $KMnO_4$].

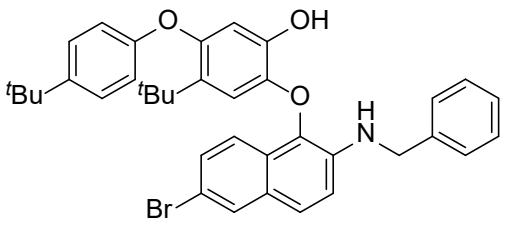
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (m, 2H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.46 – 7.37 (m, 3H), 7.36 – 7.26 (m, 2H), 6.98 (d, *J* = 8.9 Hz, 2H), 6.64 (s, 1H), 6.48 (s, 1H), 6.14 (s, 1H), 4.53 (s, 1H), 4.12 (s, 2H), 2.20 (s, 1H), 1.38 (s, 9H), 1.18 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 151.3, 145.6, 143.5, 139.9, 137.0, 133.7, 132.8, 128.5, 128.1, 128.0, 126.9, 126.6, 126.6, 123.1, 120.0, 118.4, 114.8, 112.1, 107.9, 81.1, 71.5, 34.4, 34.4, 33.5, 31.7, 30.1.

IR (neat/cm^{-1}) 3501.7, 1629.0, 1499.3, 1420.8, 1391.6, 1196.0, 832.8, 438.2.

HRMS (ESI): $C_{33}H_{36}NO_3^+$ [$(M+H)^+$]: calcd.: 494.2690; found: 494.2689.

2-((2-(Benzylamino)-6-bromonaphthalen-1-yl)oxy)-4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)phenol 3u



A brown solid, 101 mg, 82% yield.

m.p.: 76– 78 °C.

TLC: R_f = 0.85 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

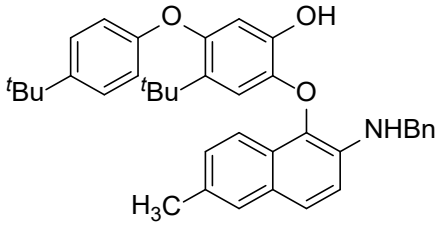
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91 (d, *J* = 1.9 Hz, 1H), 7.54 (m, 2H), 7.47 – 7.41 (m, 1H), 7.39 – 7.36 (m, 2H), 7.34 – 7.32 (m, 2H), 7.15 (d, *J* = 9.0 Hz, 1H), 7.00 – 6.91 (m, 2H), 6.80 (d, *J* = 8.7 Hz, 3H), 6.62 (s, 1H), 6.49 (s, 1H), 4.55 (s, 2H), 1.37 (s, 9H), 1.21 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 153.2, 151.3, 145.6, 143.5, 143.4, 139.5, 139.1, 138.2, 132.9, 132.3, 130.0, 129.9, 128.8, 128.6, 127.4, 126.9, 126.7, 126.5, 126.4, 125.7, 121.5, 118.3, 115.9, 115.4, 114.8, 111.8, 108.0, 47.5, 34.3, 34.1, 31.6, 30.1.

IR (neat/cm^{-1}) 3508.9, 3410.7, 1628.2, 1534.1, 1258.8, 1175.6 860.6 811.5.

HRMS (ESI): $C_{37}H_{39}BrNO_3^+$ [$(M+H)^+$]: calcd.: 624.2108; found: 624.2105.

2-((2-(benzylamino)-6-methylnaphthalen-1-yl)oxy)-4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)phenol 3v



A brown oil, 100 mg, 89% yield.

TLC: R_f = 0.54 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 8.7, 4.8 Hz, 2H), 7.50 (s, 1H), 7.33 (s, 1H), 7.31 – 7.29 (m, 5H), 7.26 – 7.23 (m, 1H), 7.19 (dd, *J* = 8.7, 1.7 Hz, 1H), 7.07 (d, *J* = 8.9 Hz, 1H), 6.91 (d, *J* = 8.7 Hz, 2H), 6.57 (s, 1H), 6.51 (s, 1H), 5.99 (brs, 1H), 4.49 (s, 2H), 2.43 (s, 3H), 1.32 (s, 9H), 1.17 (s, 9H).

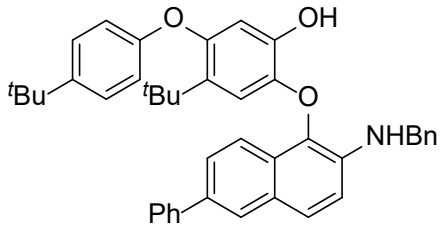
^{13}C NMR (101 MHz, $CDCl_3$) δ 155.5, 151.2, 145.6, 143.6, 139.9, 139.6, 137.3, 132.84, 132.77,

132.0, 129.2, 128.8, 128.2, 127.4, 127.09, 127.07, 126.6, 126.5, 125.9, 119.7, 118.4, 114.7, 112.2, 108.0, 47.9, 34.40, 34.38, 31.7, 30.2, 21.5.

IR (neat/cm^{-1}) 2959.4, 1570.0, 1163.6, 1070.9, 986.1, 760.7, 657.1.

HRMS (ESI): $C_{38}H_{42}NO_3^+$ [$(M+H)^+$]: calcd.: 560.3159; found: 560.3160.

2-((2-(benzylamino)-6-phenylnaphthalen-1-yl)oxy)-4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)phenol 3w



A colorless oil, 107 mg, 86% yield.

TLC: R_f = 0.47 (Hexane/EtOAc = 8:1) [UV, $KMnO_4$].

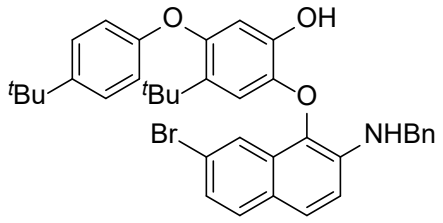
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.76 – 7.66 (m, 5H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.38 – 7.34 (m, 6H), 7.31– 7.28 (m, 2H), 7.16 (d, *J* = 8.9 Hz, 1H), 6.96 (d, *J* = 8.7 Hz, 2H), 6.63 (s, 1H), 6.58 (s, 1H), 6.02 (brs, 1H), 4.75 (brs, 1H), 4.56 (s, 2H), 1.36 (s, 9H), 1.22 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 151.2, 145.5, 143.5, 141.1, 139.7, 139.3, 138.0, 135.1, 132.8, 132.4, 128.9, 128.8, 127.9, 127.3, 127.1, 127.0, 127.0, 126.9, 126.5, 126.5, 125.9, 120.2, 118.3, 114.8, 112.0, 107.9, 47.6, 34.3, 31.6, 30.1.

IR (neat/cm^{-1}) 2956.2, 1640.2, 1510.1, 1240.9, 1195.8, 1072.9, 1090.5, 640.0.

HRMS (ESI): $C_{43}H_{44}NO_3^+$ [$(M+H)^+$]: calcd.: 622.3316; found: 622.3318.

2-((2-(benzylamino)-7-bromonaphthalen-1-yl)oxy)-4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)phenol 3x



A white solid, 104 mg, 83% yield.

m.p.: 71– 73 °C.

TLC: R_f = 0.81 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

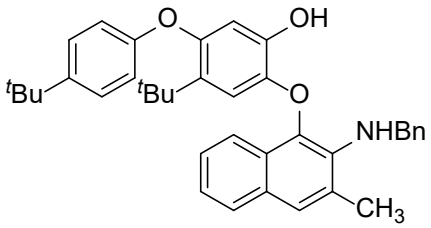
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.57 (dd, *J* = 8.9, 1.8 Hz, 2H), 7.42 – 7.23 (m, 8H), 7.09 (d, *J* = 8.9 Hz, 1H), 6.95 (d, *J* = 8.7 Hz, 2H), 6.60 (s, 1H), 6.48 (s, 1H), 5.99 (brs, 1H), 4.68 (brs, 1H), 4.51 (s, 2H), 1.35 (s, 9H), 1.21 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 151.5, 145.7, 143.6, 139.3, 139.1, 138.6, 132.9, 131.3, 129.8, 129.5, 128.9, 127.5, 127.0, 126.7, 126.6, 126.0, 125.9, 121.9, 121.5, 118.4, 114.8, 111.8, 108.2, 47.6, 34.4, 31.7, 30.2.

IR (neat/cm^{-1}) 2957.2, 1670.2, 1560.1, 1244.9, 1195.8, 1072.9, 640.0, 540.1.

HRMS (ESI): $C_{37}H_{39}BrNO_3^+$ [$(M+H)^+$]: calcd.: 624.2108; found: 624.2105.

2-((2-(benzylamino)-3-methylnaphthalen-1-yl)oxy)-4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)phenol 3y



A colorless oil, 90 mg, 81% yield.

TLC: R_f = 0.55 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

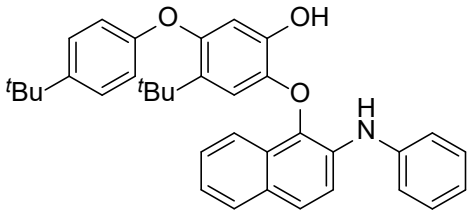
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.2, 1H), 7.73 (d, *J* = 7.8, 1H), 7.54 (s, 1H), 7.40 – 7.24 (m, 10H), 6.93 (d, *J* = 8.7 Hz, 2H), 6.76 (s, 1H), 6.53 (s, 1H), 4.37 (s, 2H), 2.47 (s, 3H), 1.34 (s, 9H), 1.23 (s, 9H).

^{13}C NMR (151 MHz, $CDCl_3$, $CDCl_3$) δ 155.4, 151.5, 145.5, 144.6, 140.9, 139.8, 138.9, 137.6, 132.3, 130.3, 129.9, 128.8, 128.1, 127.6, 127.3, 126.7, 126.6, 125.8, 124.3, 121.1, 118.4, 114.6, 108.3, 52.6, 34.39, 34.35, 31.7, 30.3, 19.2.

IR (neat/cm^{-1}) 2964.4, 1570.0, 1172.6, 909.9, 986.1, 760.7, 657.1.

HRMS (ESI): $C_{38}H_{42}NO_3^+$ [$(M+H)^+$]: calcd.: 560.3159; found: 560.3160.

4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)-2-((2-(phenylamino)naphthalen-1-yl)oxy)phenol 3z



A white solid, 87 mg, 82% yield.

m.p.: 80– 82 °C.

TLC: R_f = 0.68 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

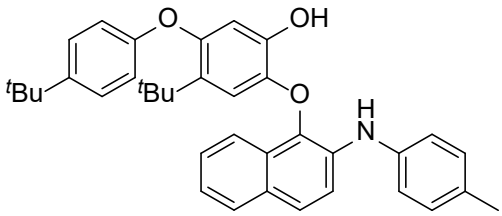
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.1 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.71 (d, *J* = 8.9 Hz, 1H), 7.62 (d, *J* = 8.7 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.39-7.29 (m, 5H), 7.11 (d, *J* = 7.1 Hz, 2H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.90 (d, *J* = 8.2 Hz, 2H), 6.66 (s, 1H), 6.57 (s, 1H), 6.05 (s, 1H), 5.89 (s, 1H), 1.37 (s, 9H), 1.23 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 151.3, 145.6, 143.5, 142.4, 140.0, 136.6, 133.3, 132.9, 130.0, 129.5, 128.6, 128.1, 127.0, 126.6, 126.1, 124.1, 122.1, 120.6, 119.0, 118.9, 118.3, 112.3, 108.0, 34.3, 34.3, 31.6, 30.1.

IR (KBr/cm^{-1}) 2959.3, 1592.3, 1496.2, 1196.0, 762.0, 461.7.

HRMS (ESI): $C_{36}H_{38}NO_3^+$ [$(M+H)^+$]: calcd.: 532.2846; found: 532.2848.

4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)-2-((2-(*p*-tolylamino)naphthalen-1-yl)oxy)phenol 4a



A brown oil, 97 mg, 89% yield.

TLC: R_f = 0.39 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].

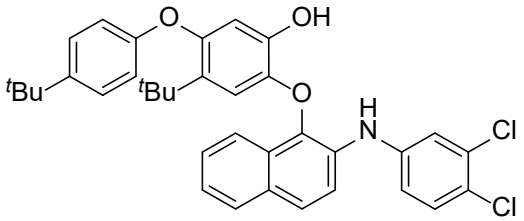
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.9 Hz, 1H), 7.76 (d, *J* = 8.4, 1.1 Hz, 1H), 7.69 (d, *J* = 8.9 Hz, 1H), 7.56 (d, *J* = 8.9 Hz, 1H), 7.48 – 7.42 (m, 1H), 7.36 (m, 3H), 7.15 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.4 Hz, 2H), 6.95 – 6.87 (m, 2H), 6.59 (s, 1H), 6.55 (s, 1H), 5.99 (s, 1H), 5.87 (s, 1H), 2.35 (s, 3H), 1.36 (s, 9H), 1.14 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 151.3, 145.6, 143.6, 139.9, 139.6, 135.6, 134.3, 132.9, 132.2, 130.1, 129.6, 128.6, 128.1, 127.0, 126.6, 126.2, 123.8, 120.4, 120.1, 118.4, 118.3, 112.2, 108.0, 34.4, 34.4, 31.7, 30.1, 20.9.

IR (neat/cm^{-1}) 2958.6, 1631.6, 1496.7, 1390.9, 1195.8, 1072.9, 906.5, 729.0.

HRMS (ESI): $C_{37}H_{40}NO_3^+$ [$(M+H)^+$]: calcd.: 546.3003; found: 546.3002.

4-(*tert*-butyl)-5-(4-(*tert*-butyl)phenoxy)-2-((2-((3,4-dichlorophenyl)amino)naphthalen-1-yl)oxy)phenol 4b



A brown oil, 98 mg, 82% yield.

TLC: R_f = 0.50 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

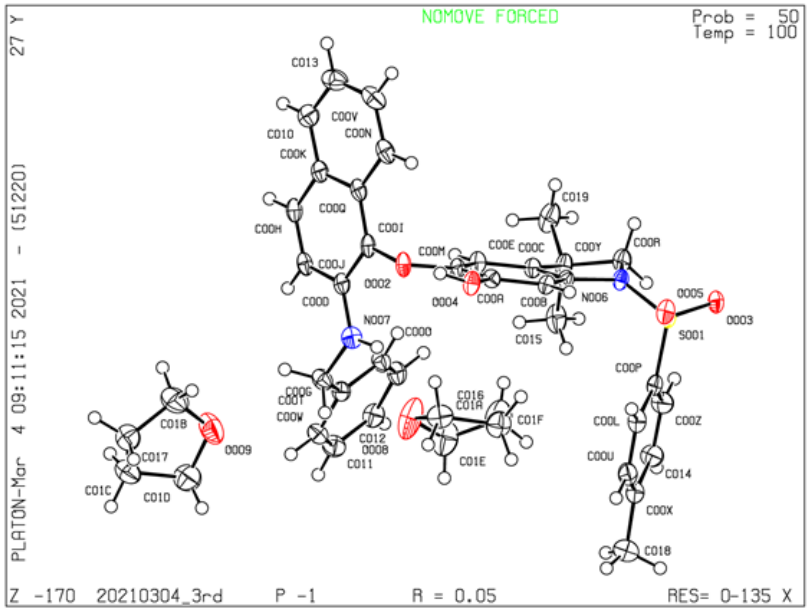
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.83 (m, 2H), 7.77 (d, *J* = 8.9 Hz, 1H), 7.55 (d, *J* = 8.9 Hz, 1H), 7.53 – 7.43 (m, 2H), 7.39 – 7.34 (m, 2H), 7.32 – 7.26 (m, 1H), 7.13 (d, *J* = 2.7 Hz, 1H), 6.90 – 6.82 (m, 3H), 6.58 (s, 1H), 6.48 (s, 1H), 5.99 (s, 1H), 5.86 (s, 1H), 1.36 (s, 9H), 1.12 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 151.6, 145.7, 143.5, 142.8, 140.1, 138.8, 133.2, 133.1, 131.4, 130.9, 130.8, 128.6, 128.2, 127.3, 126.6, 126.3, 125.0, 124.1, 121.0, 120.1, 118.7, 118.3, 116.9, 112.5, 108.2, 34.4, 34.3, 31.7, 30.1.

IR (neat/cm^{-1}) 2959.4, 1550.0, 1263.6, 1010.9, 886.1, 760.7, 657.1, 458.7.

HRMS (ESI): $C_{36}H_{36}Cl_2NO_3^+$ [$(M+H)^+$]: calcd.: 600.2067; found: 600.2069.

4 X-ray crystallographic analysis of 3g



Bond precision	C-C = 0.0027 A	Wavelength =1.54184	
Cell	a=9.7737(1) alpha=75.980(1)	b=12.4725(1) beta=78.674(1)	c=16.1297(2) gamma=74.780(1)
Temperature	100 K		
Volume	**Calculated** 1822.15(3)	**Reported** 1822.15(4)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	$C_{34}H_{32}N_2O_4S$, 2(C_4H_8O)	$C_{34}H_{32}N_2O_4S$, 2(C_4H_8O)	
Sum formula	$C_{42}H_{48}N_2O_6S$	$C_{42}H_{48}N_2O_6S$	
Mr	708.88	708.88	
Dx,g cm^{-3}	1.292	1.292	
Z	2	2	
Mu (mm^{-1})	1.202	1.202	
F000	756.0	756.0	
F000’	758.80		
h,k,lmax	12,15,20	12,15,20	
Nref	7379	7236	
Tmin,Tmax		0.882,1.000	
Tmin’			

Correction method= # Reported T Limits: Tmin=0.882 Tmax = 1.000

AbsCorr = MULTI-SCAN	
Data completeness= 0.981	Theta(max)= 73.911
R(reflections)= 0.0476 (6976)	wR2(reflections)= 0.1270 (7236)
S = 1.068	Npar= 464

5 References

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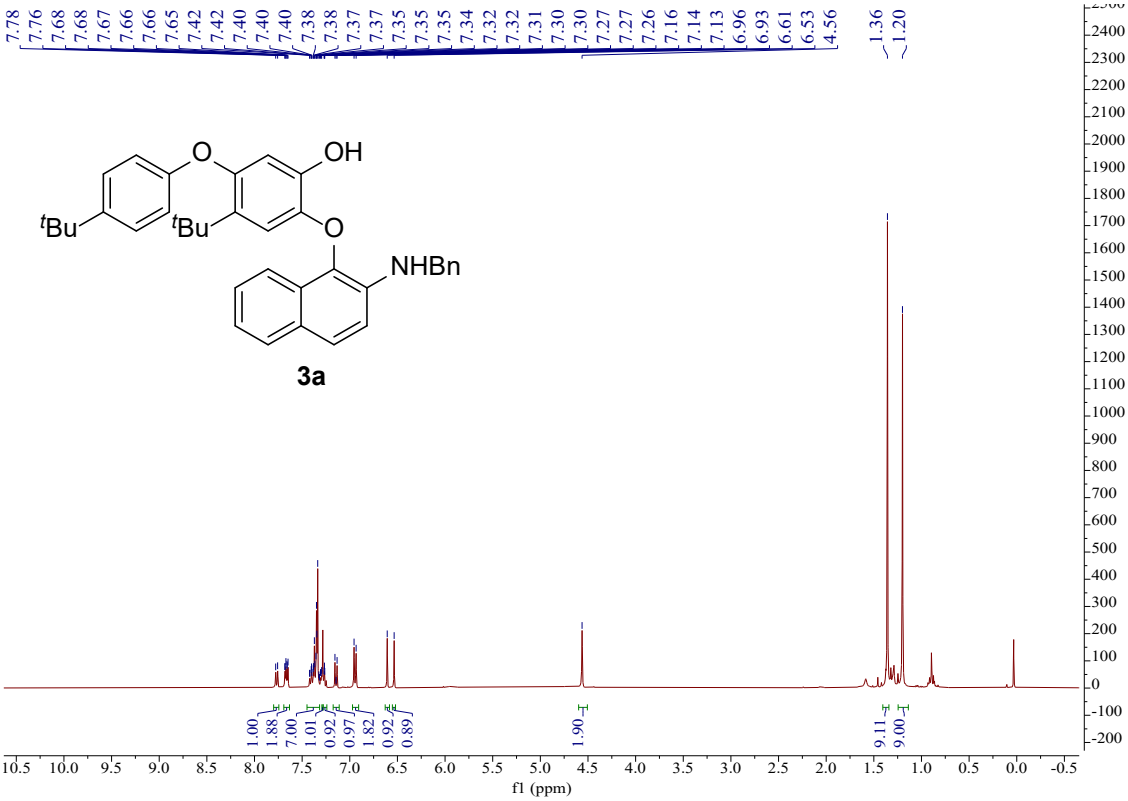
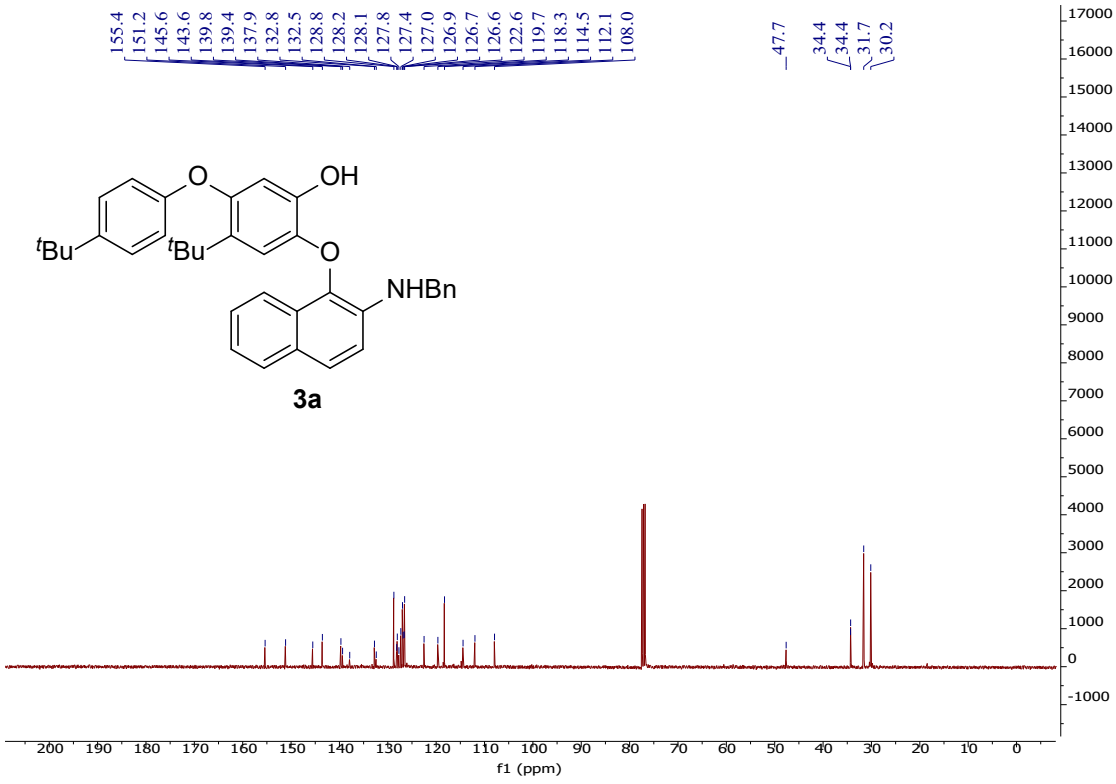
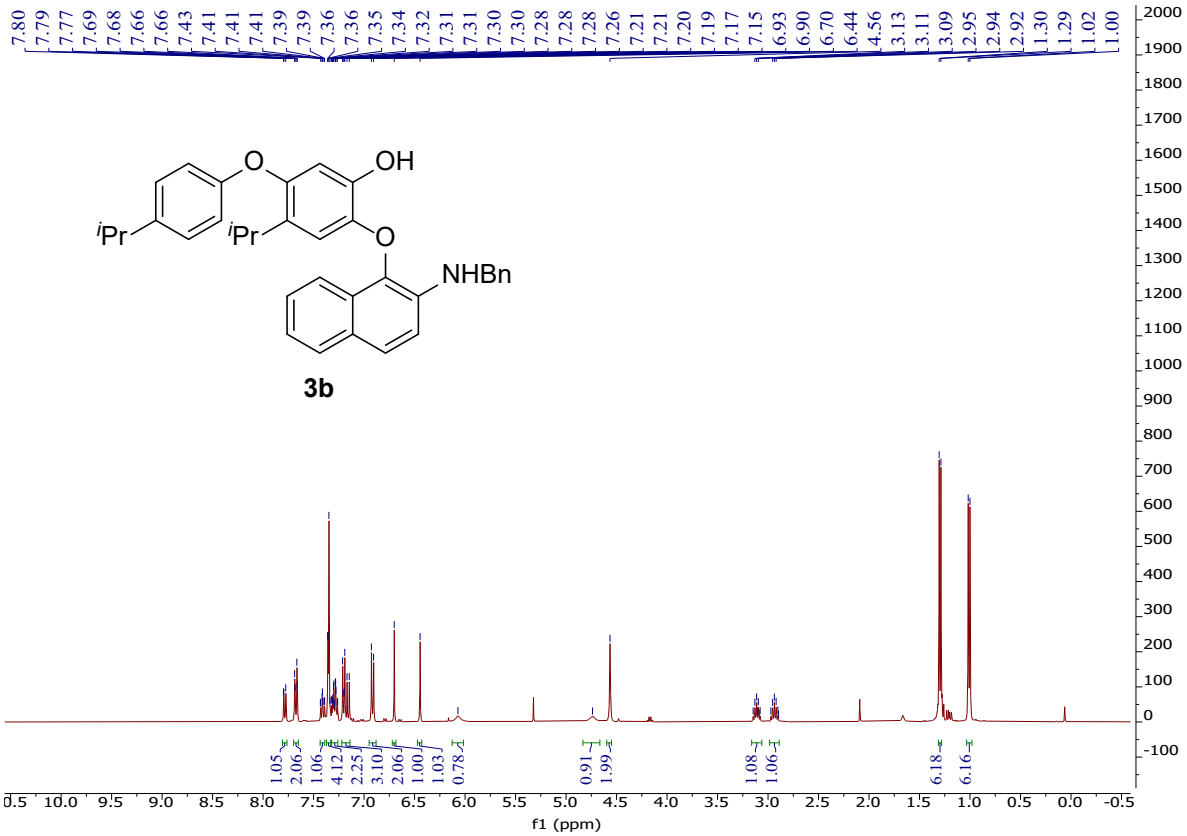
6 Copies of ^{1}H and ^{13}C NMR spectra of products



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O
OH
iPr
iPr
O
NHBn
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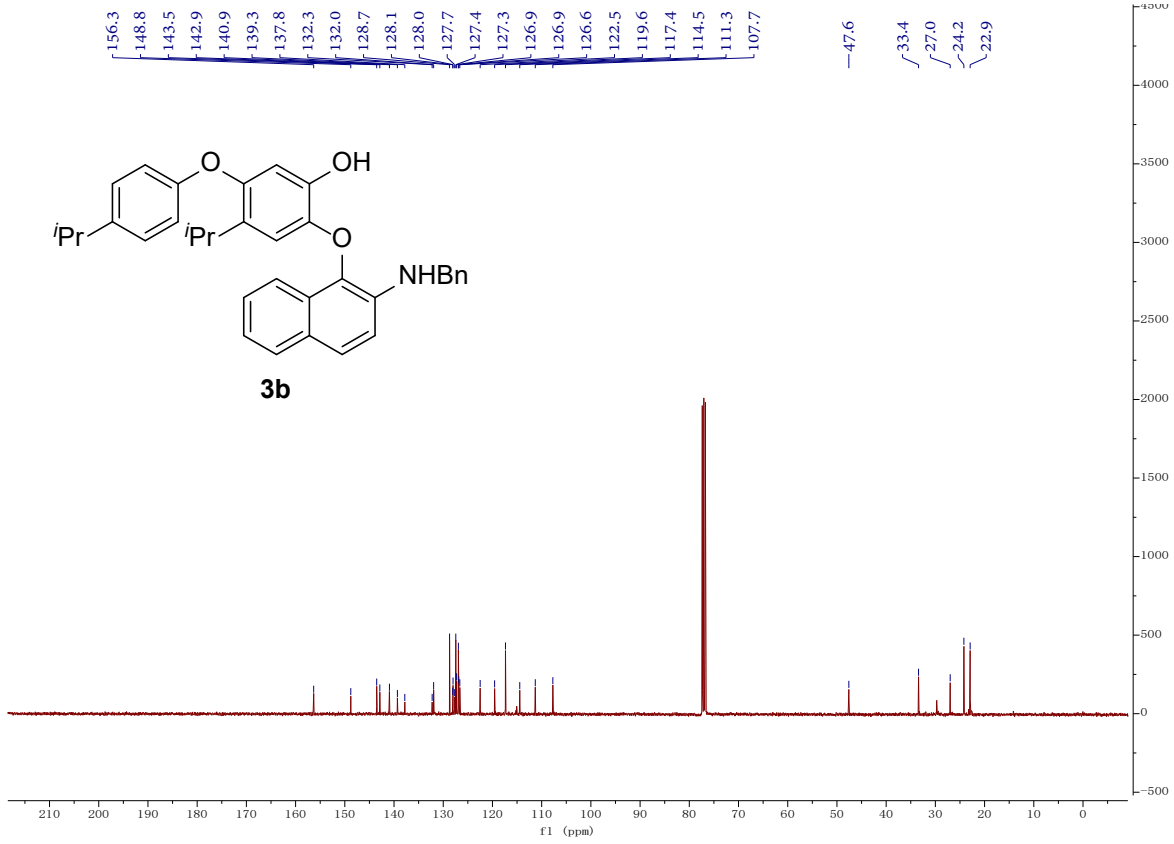
f1 (ppm)

3b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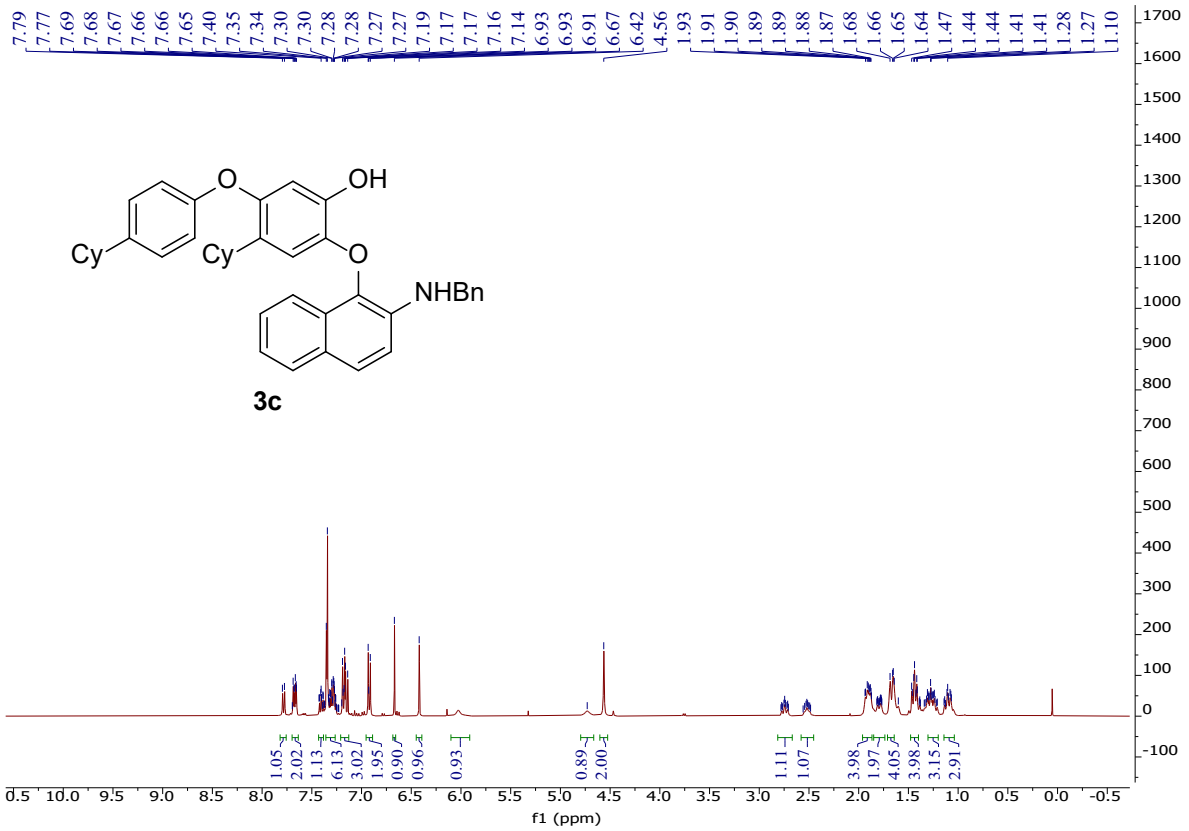
OH
iPr
iPr
O
NHBn
f1 (ppm)

3b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OH
Cy
Cy
O
NHBn
3c
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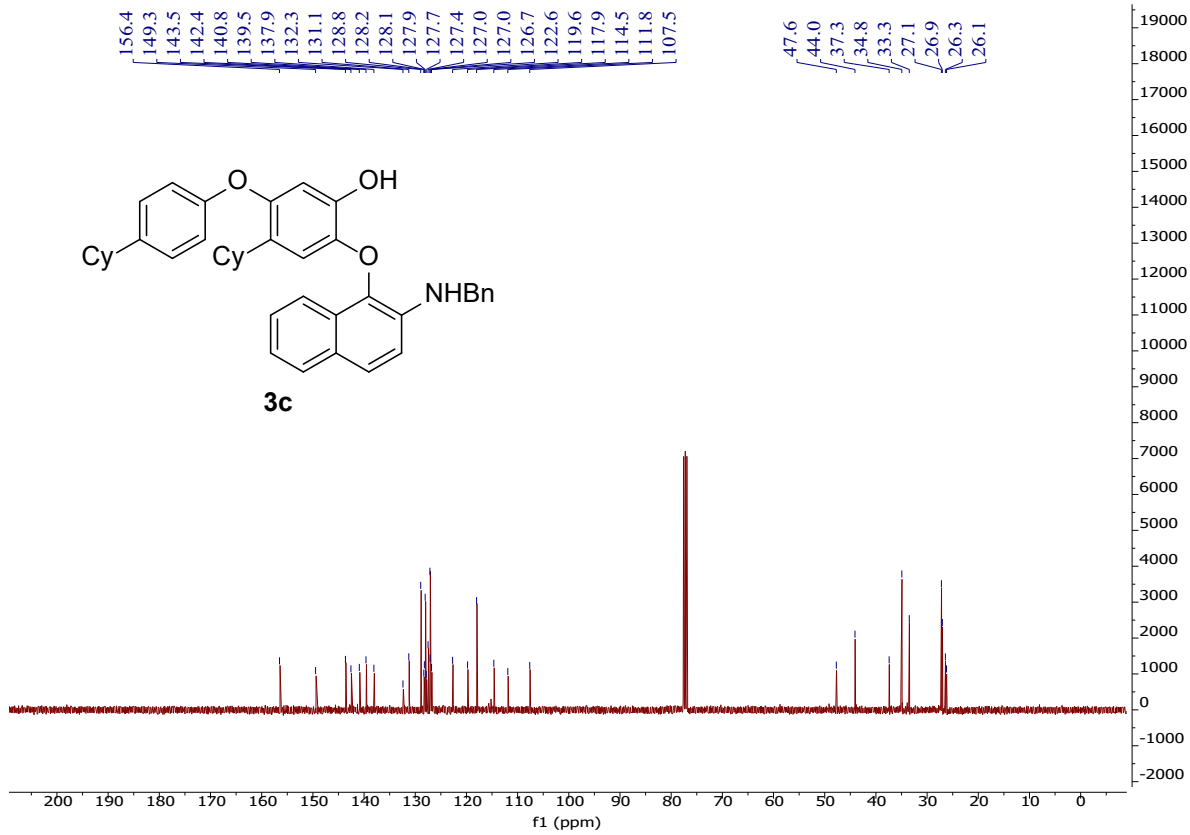
f1 (ppm)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47.6 44.0 37.3 34.8 33.3 27.1 26.9 26.3 26.1
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Cy
Cy
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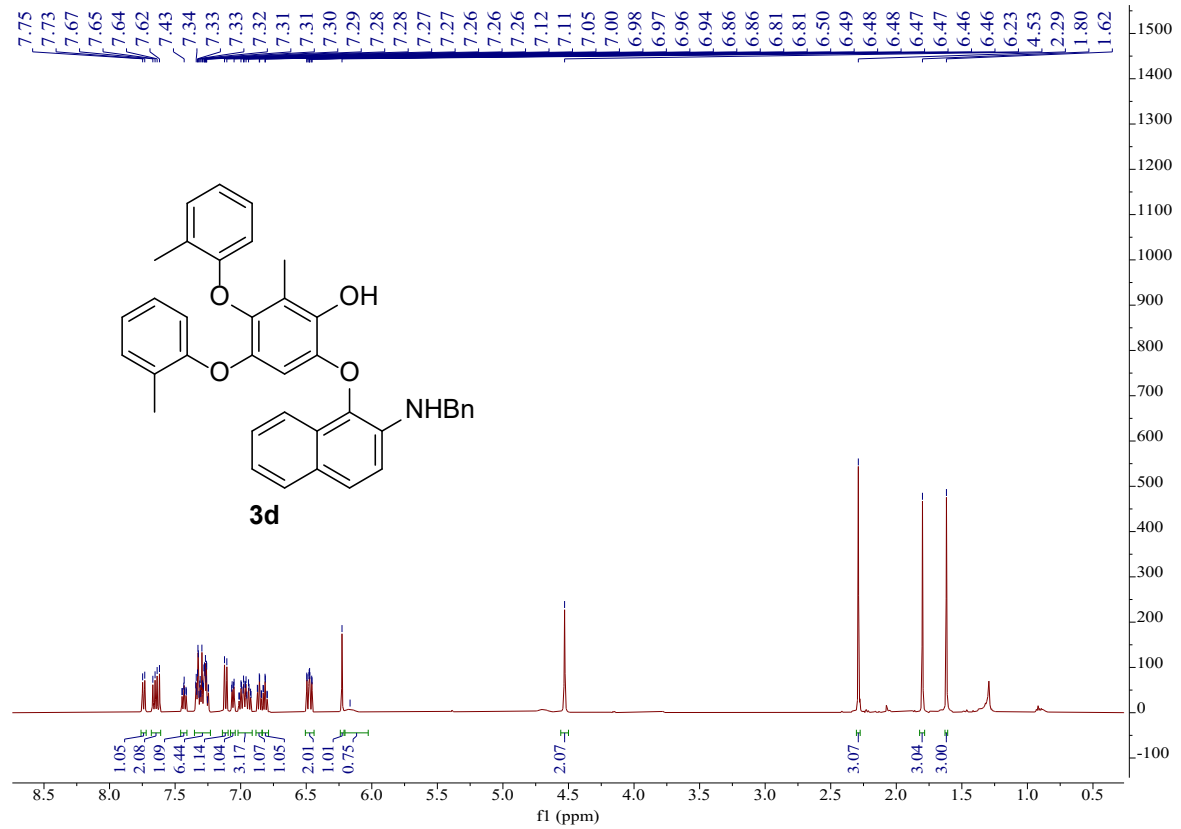
NHBn
3c
f1 (ppm)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O
O
NHBn
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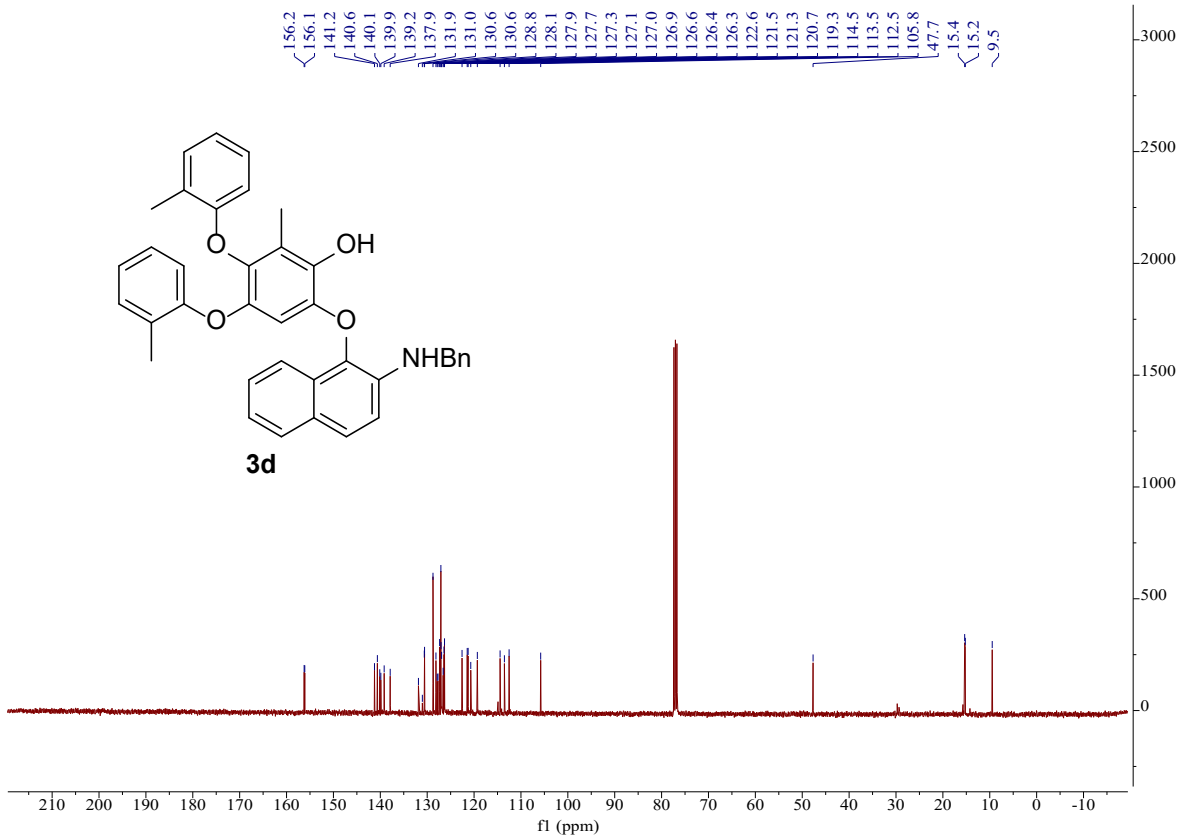
f1 (ppm)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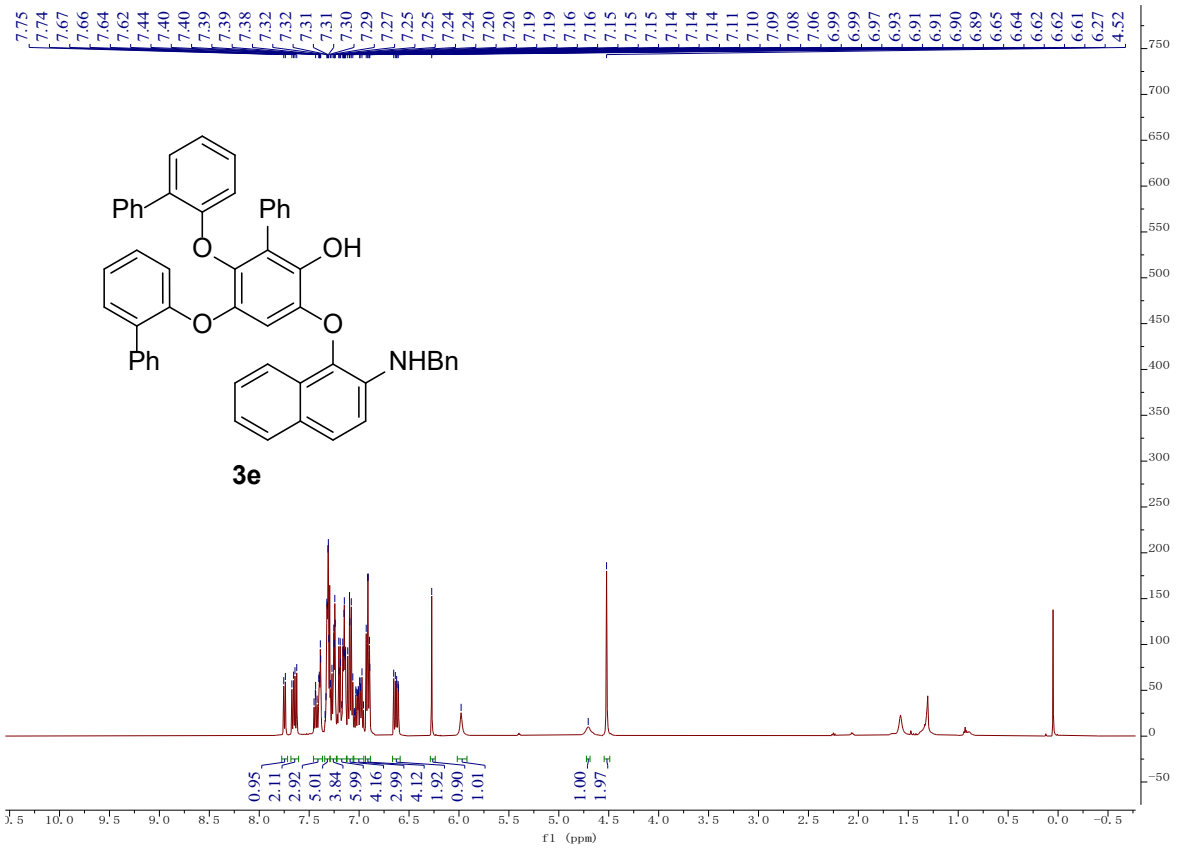
OH
O
O
NHBn
3d
f1 (ppm)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3e

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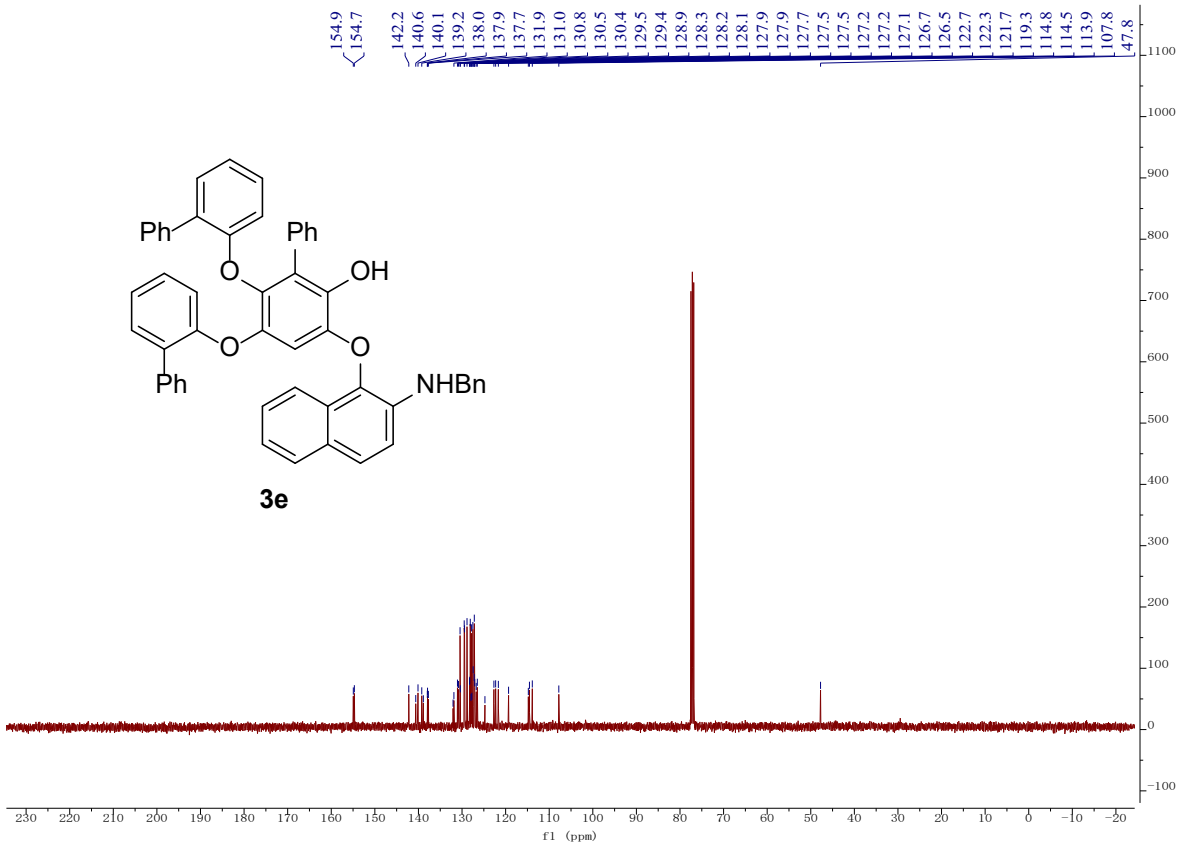
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O
O
Ph
NHBn

3e

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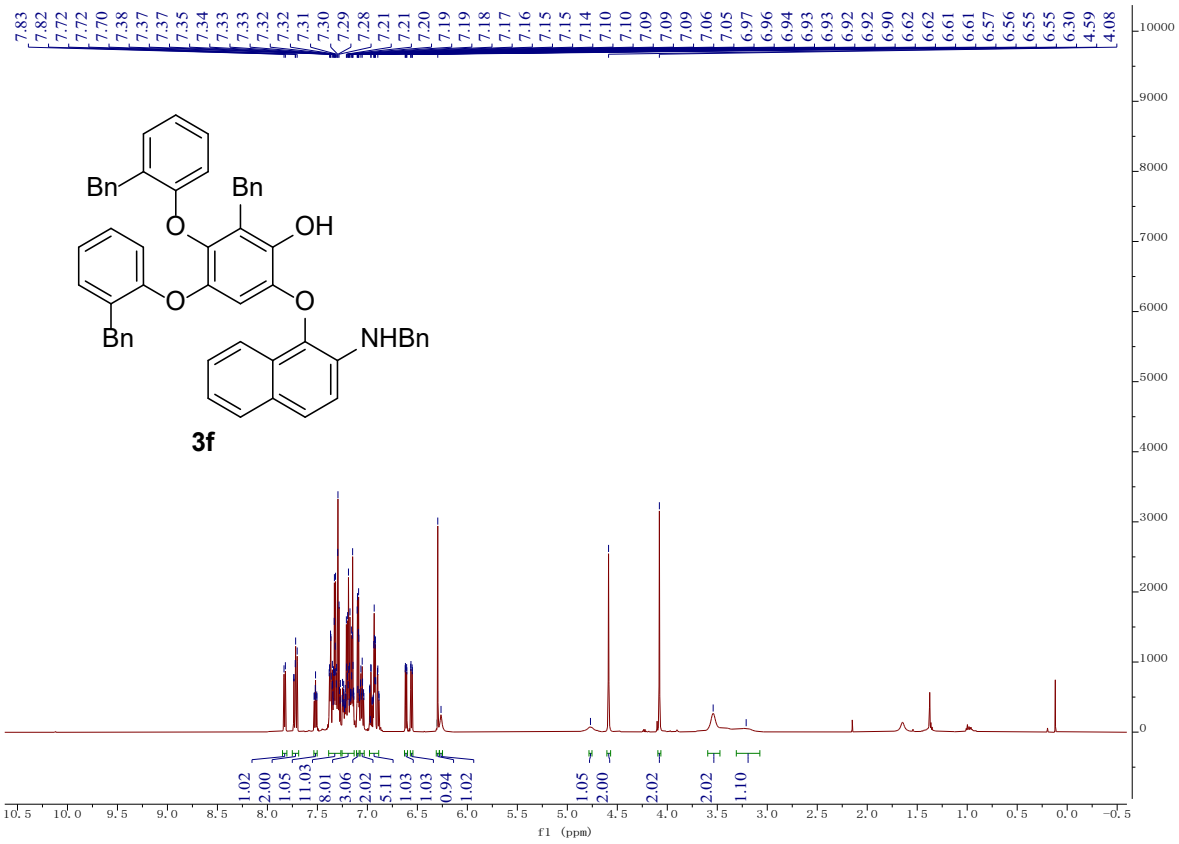
f1 (ppm)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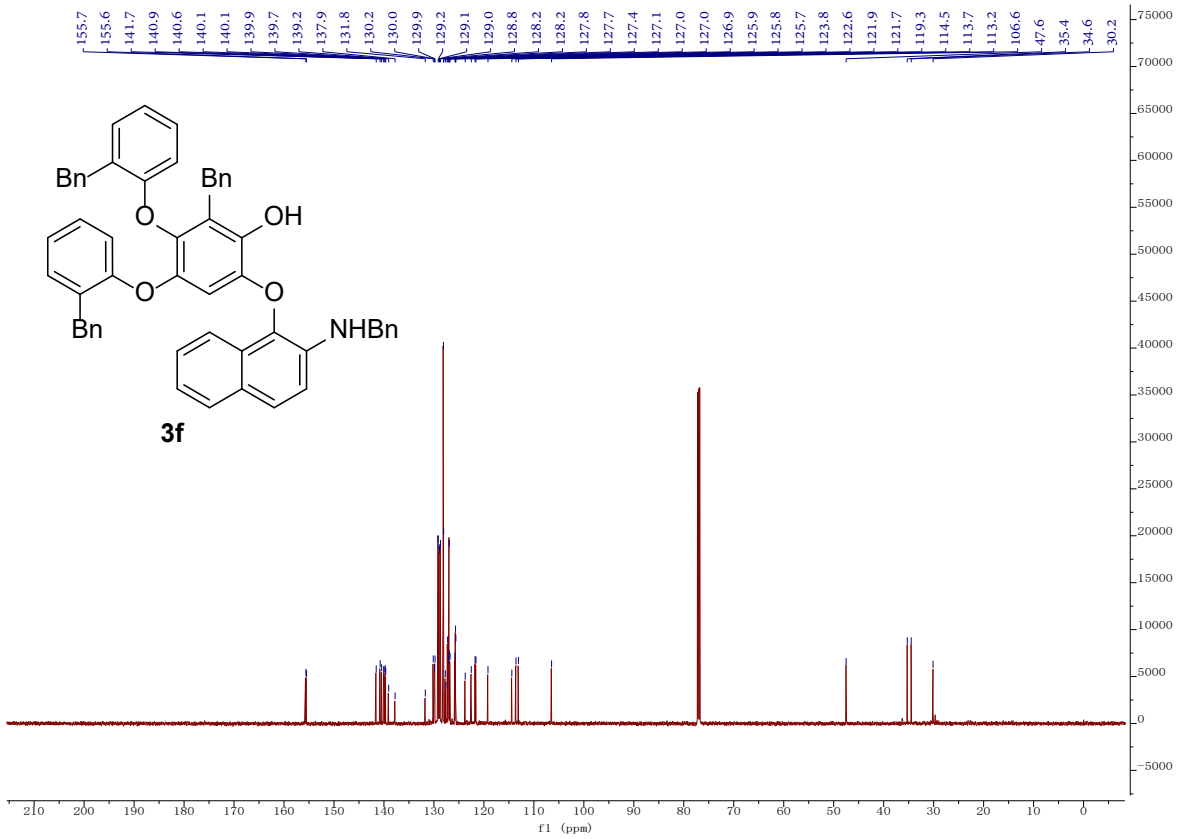
O
Bn
NHBn
3f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Bn
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OH
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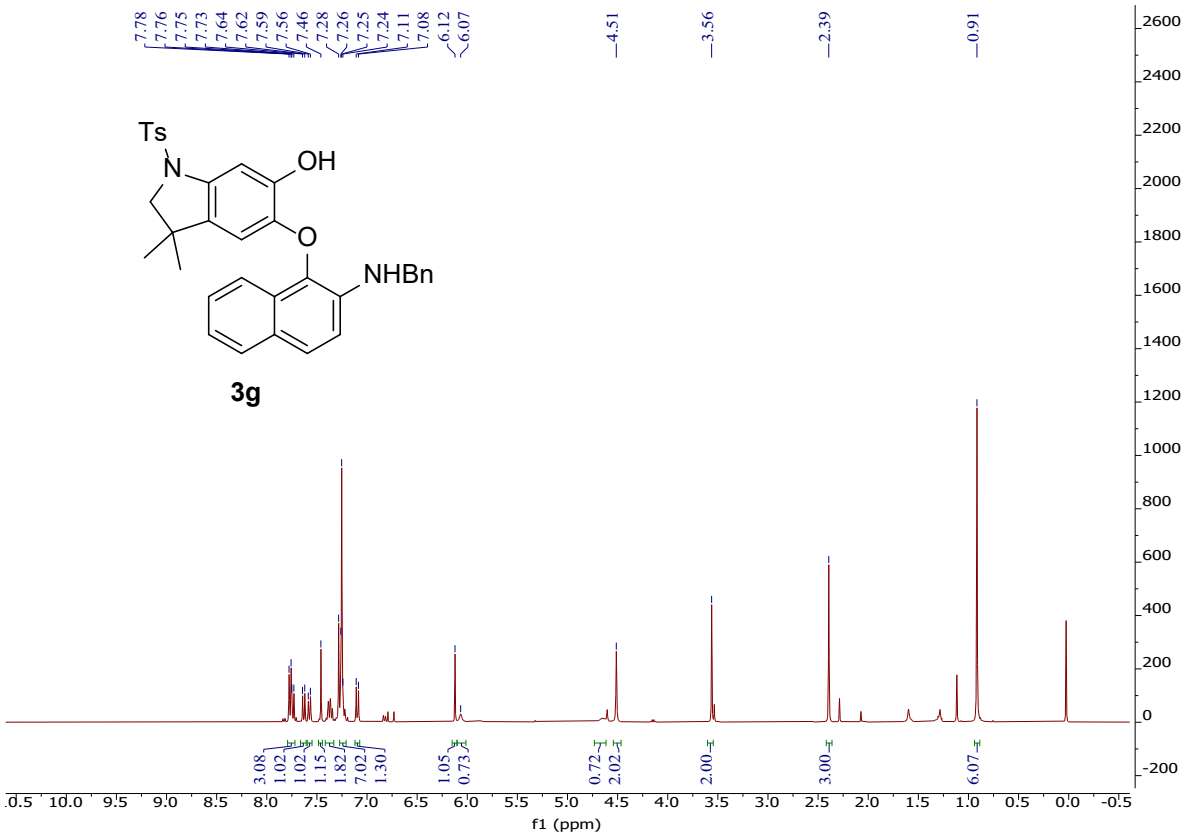
O
Bn
NHBn
3f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7.08
6.12
6.07
4.51
3.56
2.39
0.91
Ts
N
OH
O
NHBn
3g
3.08
1.02
1.02
1.15
1.82
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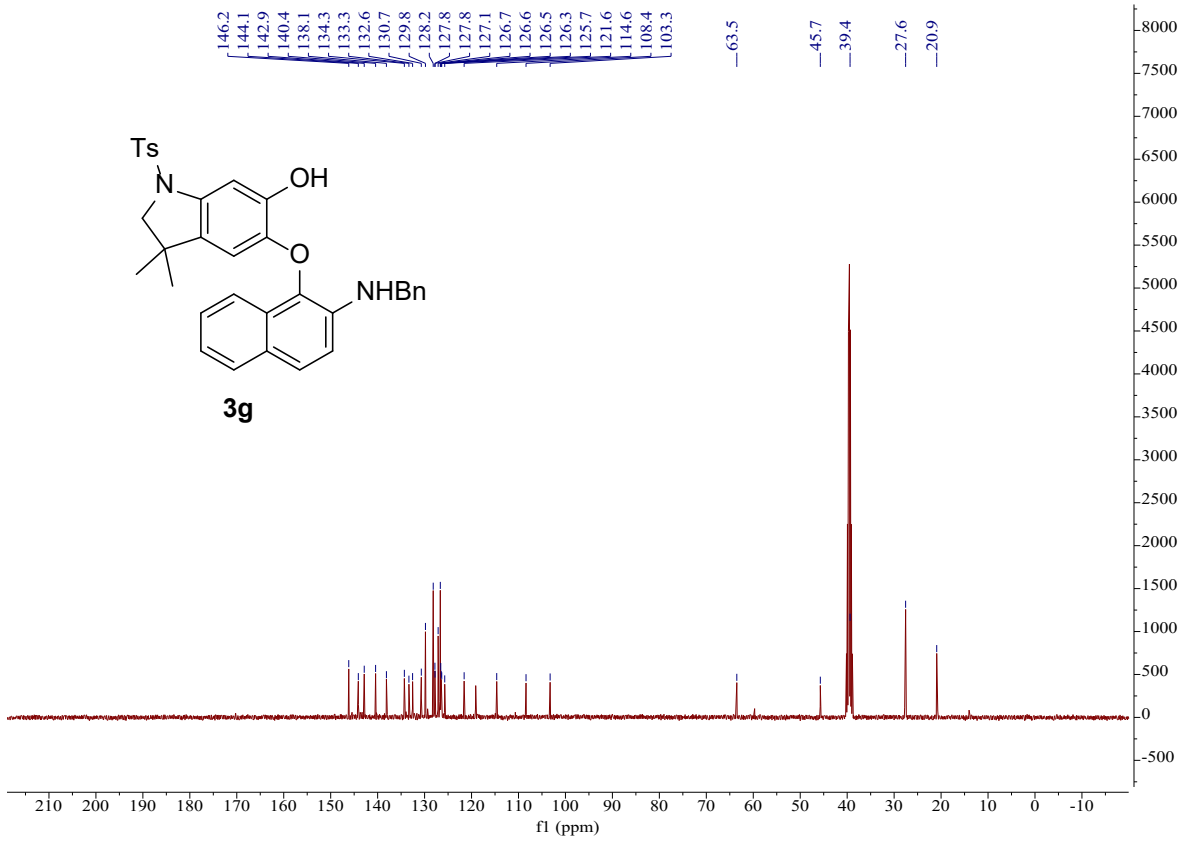
1.30
1.05
0.73
0.72
2.02
2.00
3.00
6.07
f1 (ppm)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127.8
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127.1
126.7
126.6
126.5
126.3
125.7
121.6
114.6
108.4
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39.4
27.6
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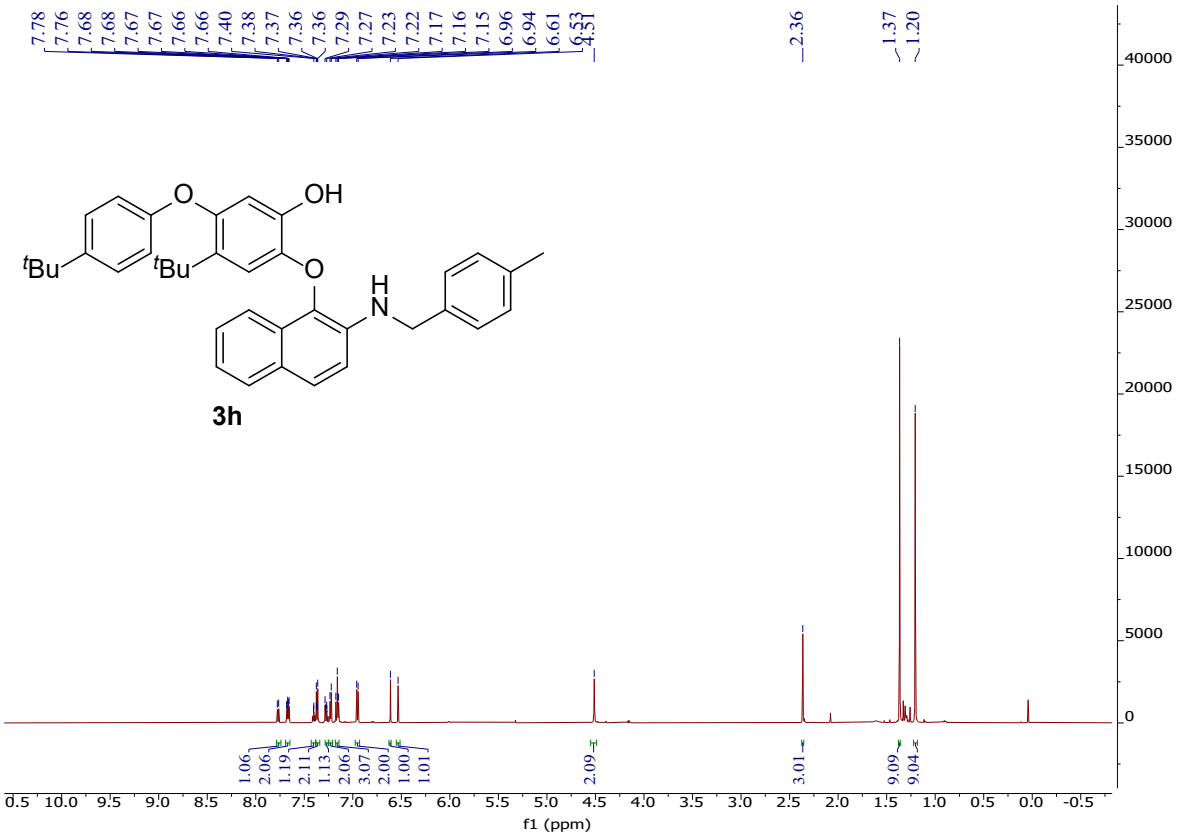
Ts
N
OH
O
NHBn
3g
f1 (ppm)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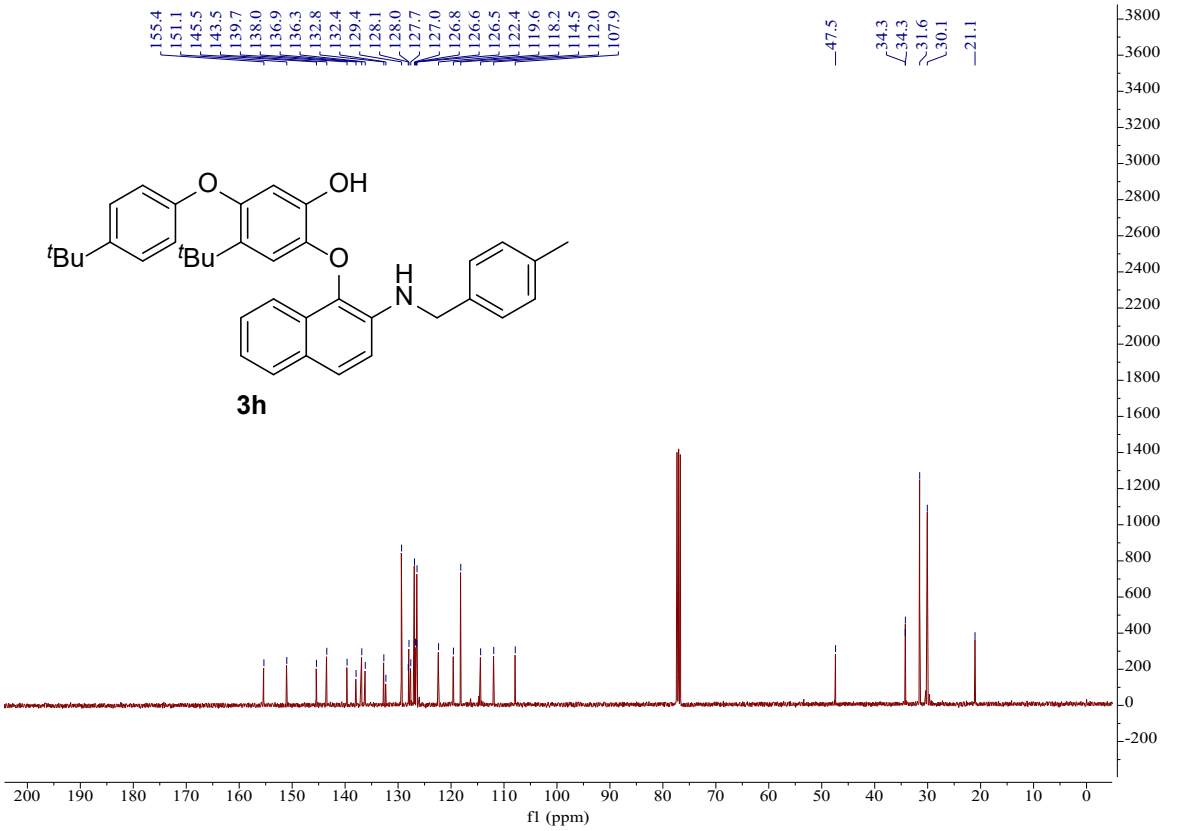
7.29
7.27
7.23
7.22
7.17
7.16
7.15
6.96
6.94
6.61
6.53
4.51
2.36
1.37
1.20
OH
O
O
H
N
tBu
tBu
3h
1.06
2.06
1.19
2.11
1.13
2.06
3.07
2.00
1.00
1.01
2.09
3.01
9.09
9.04
f1 (ppm)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128.0
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127.0
126.8
126.6
126.5
122.4
119.6
118.2
114.5
112.0
107.9
47.5
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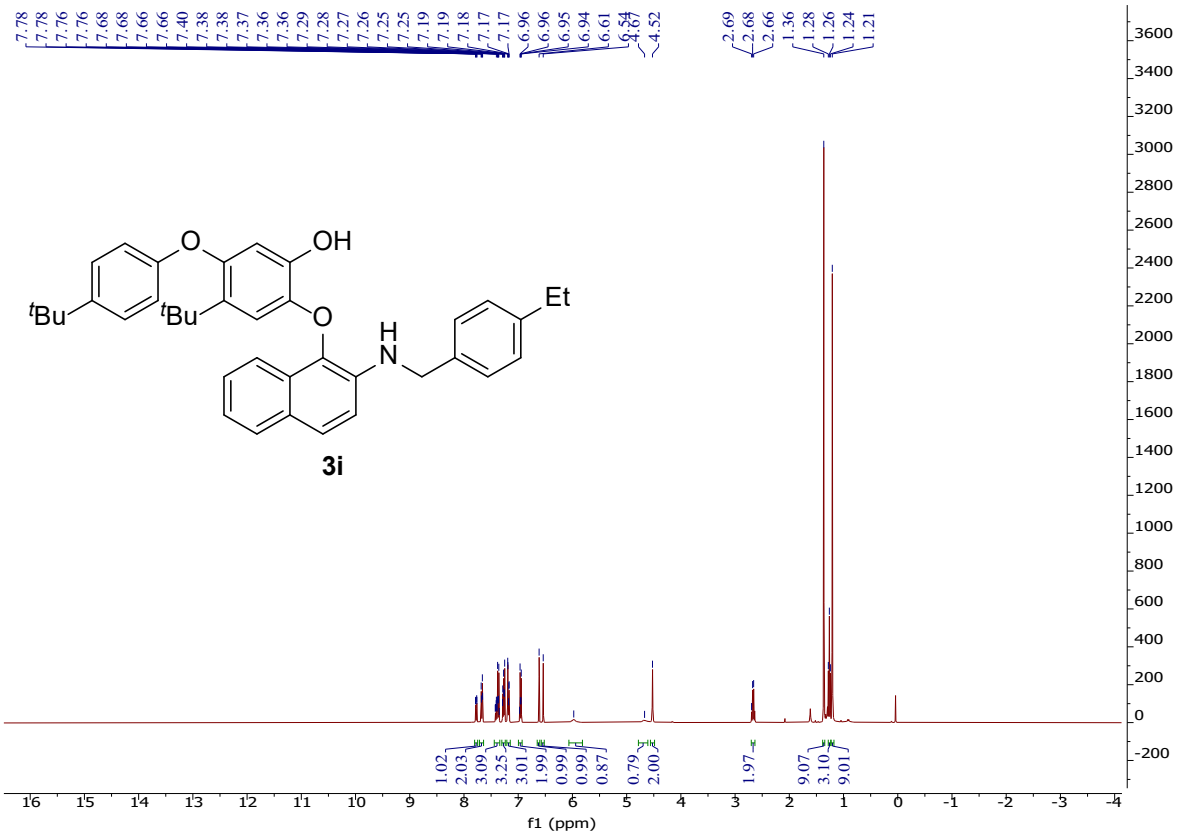
31.6
30.1
21.1
OH
O
O
H
N
tBu
tBu
3h
f1 (ppm)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7.36
7.29
7.28
7.27
7.26
7.25
7.25
7.19
7.19
7.18
7.17
7.17
6.96
6.96
6.95
6.94
6.61
6.54
4.67
4.52
2.69
2.68
2.66
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1.28
1.26
1.24
1.21
OH
O
tBu
tBu
O
H
N
Et
3i
1.02
2.03
3.09
3.25
3.01
1.99
0.99
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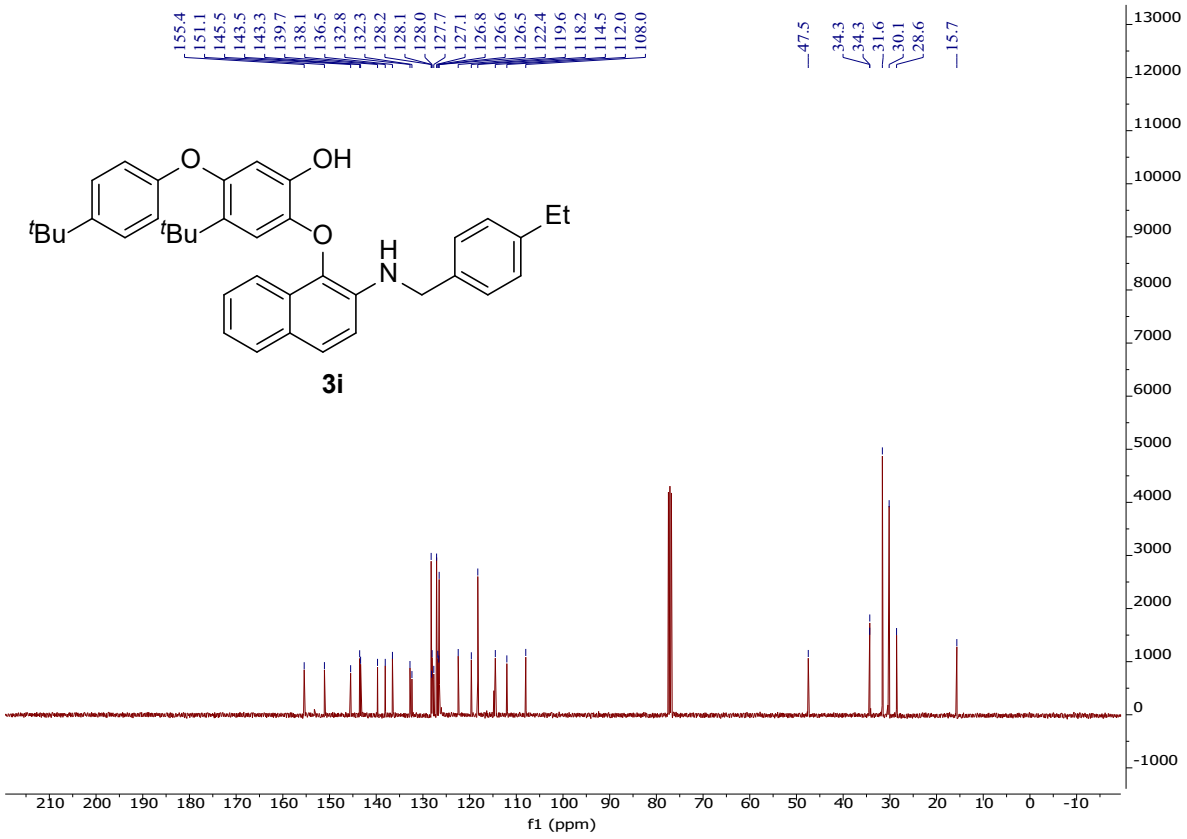
0.87
0.79
2.00
1.97
9.07
3.10
9.01
f1 (ppm)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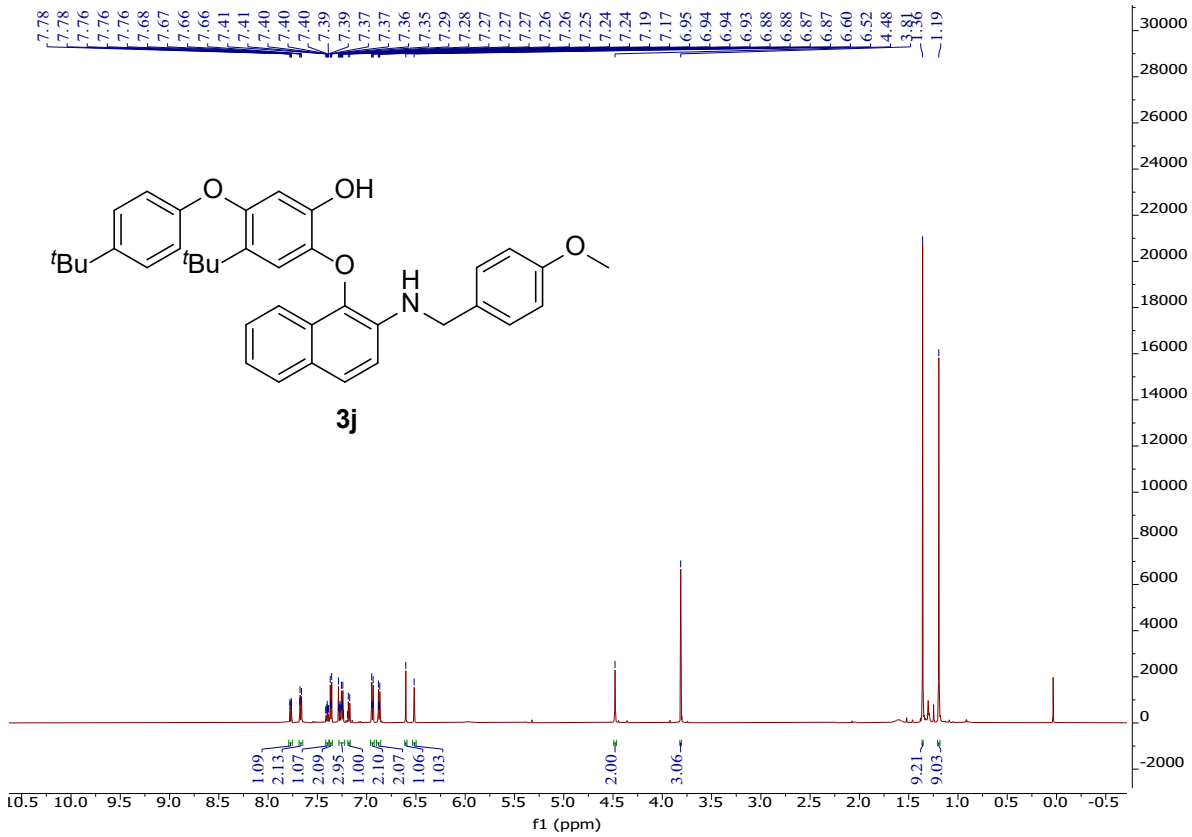
128.0
127.7
127.1
126.8
126.6
126.5
122.4
119.6
118.2
114.5
112.0
108.0
47.5
34.3
34.3
31.6
30.1
28.6
15.7
OH
O
tBu
tBu
O
H
N
Et
3i
f1 (ppm)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7.19
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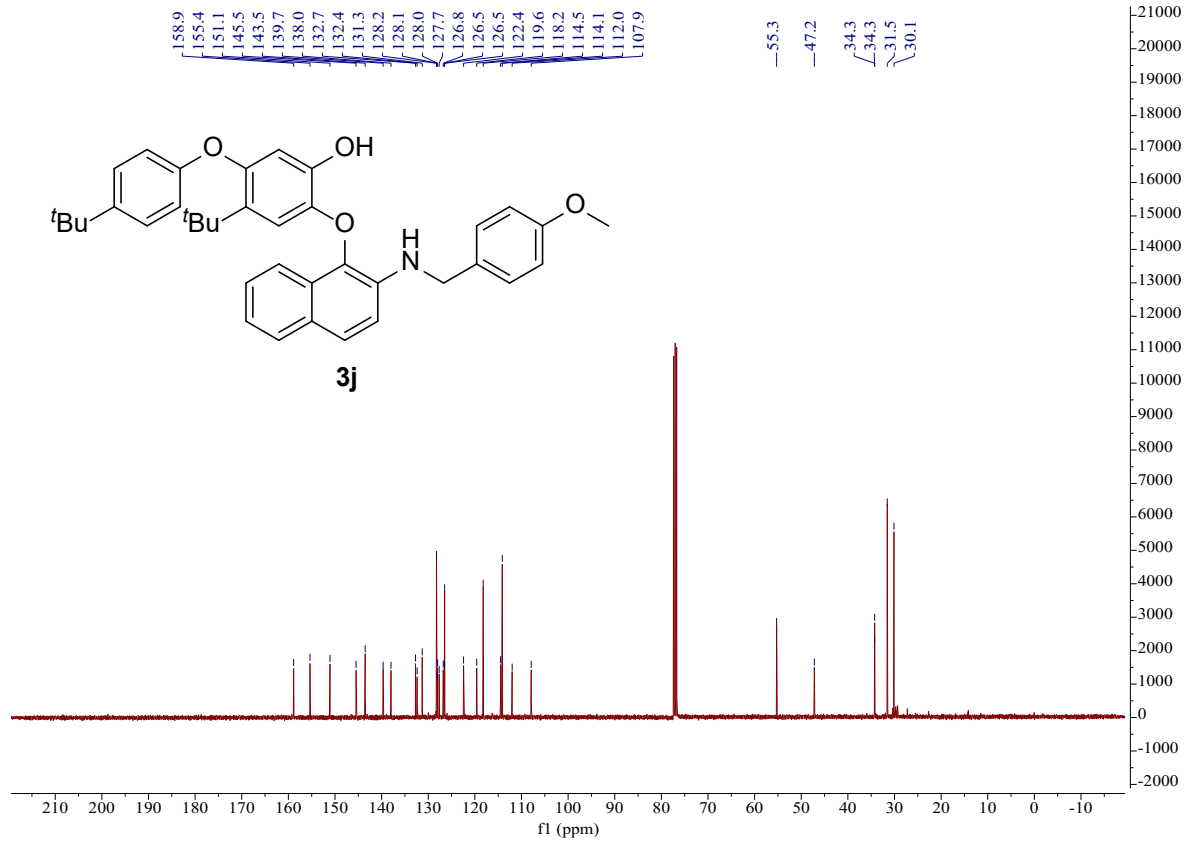
6.94
6.93
6.88
6.88
6.87
6.87
6.60
6.52
4.48
3.81
1.36
1.19
OH
O
tBu
tBu
O
H
N
O
3j
1.09
2.13
1.07
2.09
2.95
1.00
2.10
2.07
1.06
1.03
2.00
3.06
9.21
9.03
f1 (ppm)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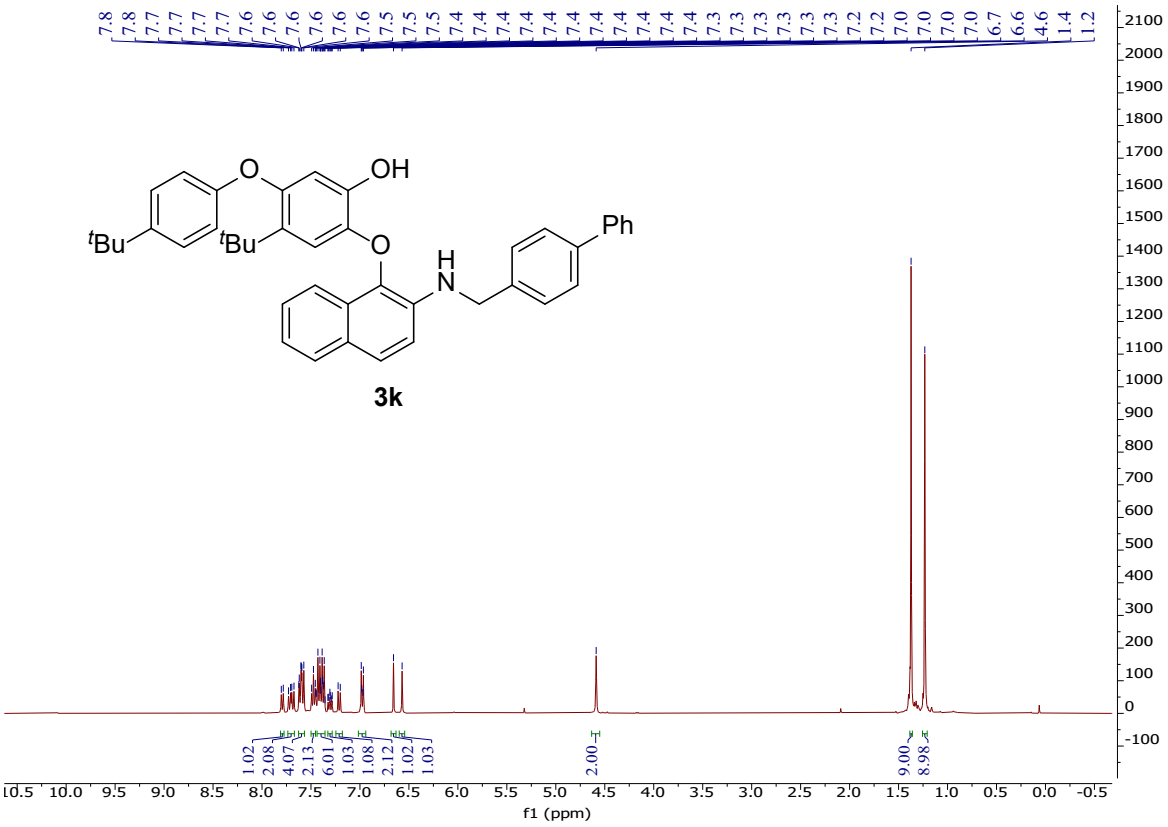
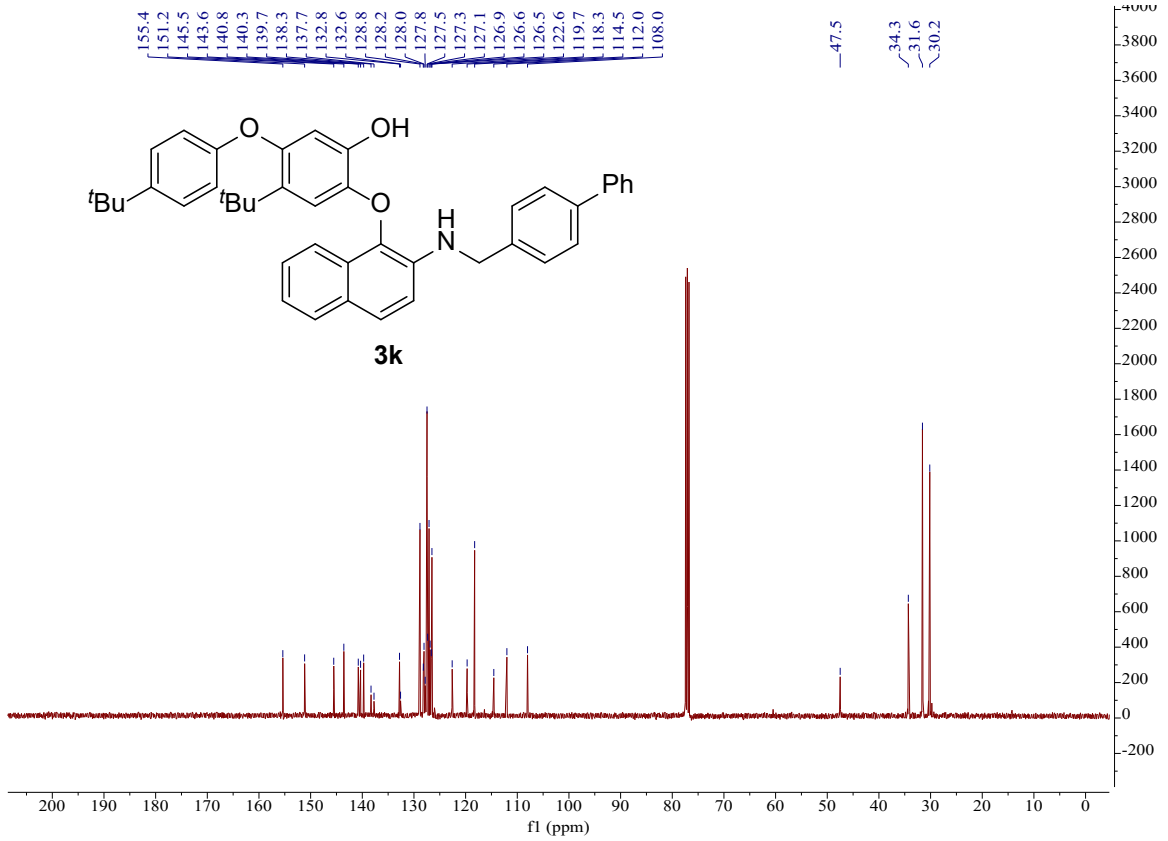
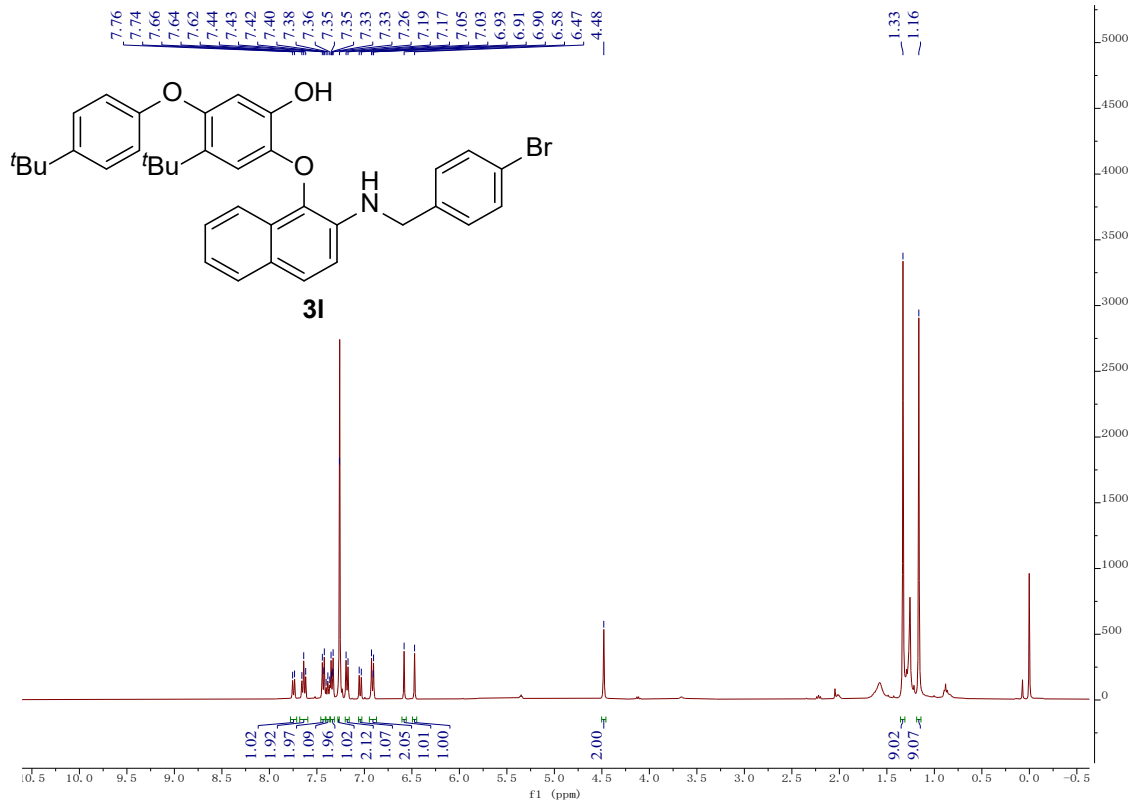
151.1
145.5
143.5
139.7
138.0
132.7
132.4
131.3
128.2
128.1
128.0
127.7
126.8
126.5
126.5
122.4
119.6
118.2
114.5
114.1
112.0
107.9
55.3
47.2
34.3
34.3
31.5
30.1
OH
O
tBu
tBu
O
H
N
O
3j
f1 (ppm)


OH
O
O
H
N
Ph
tBu
tBu
3k
f1 (ppm)


OH
O
O
H
N
Ph
tBu
tBu
3k
f1 (ppm)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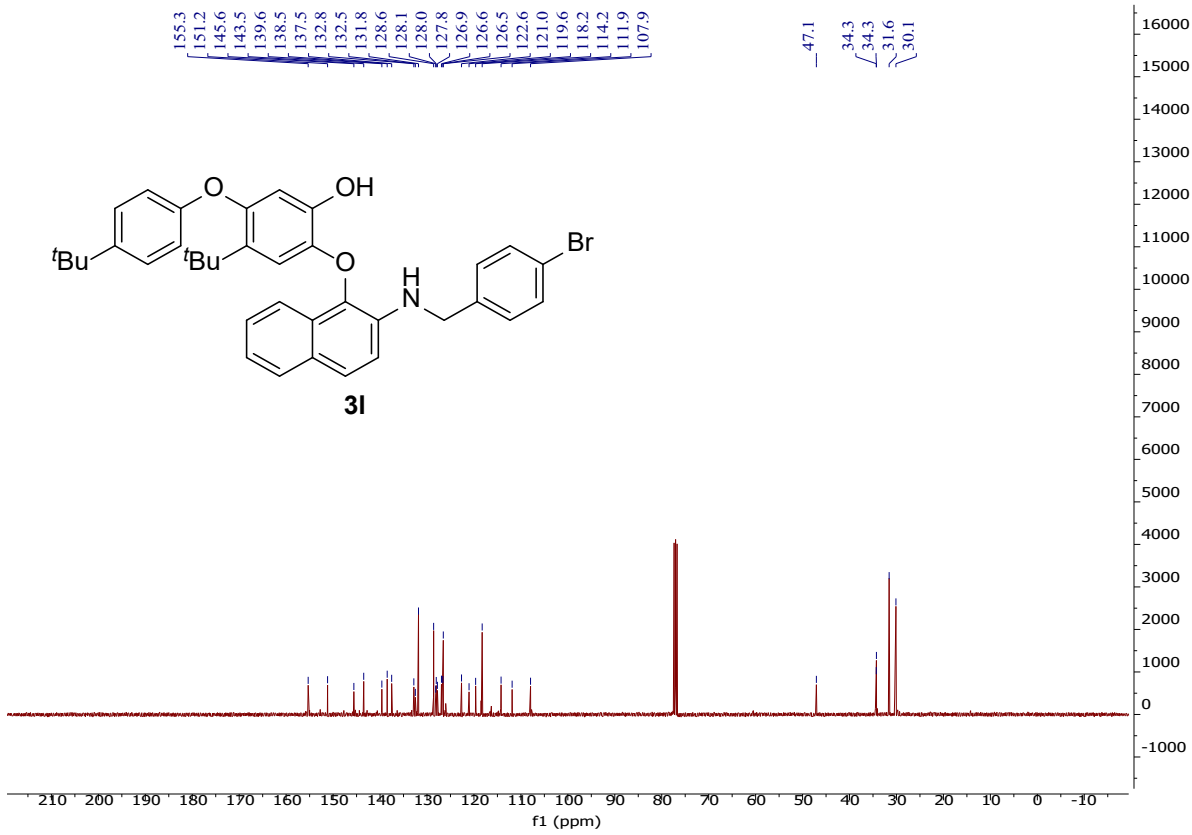
7.44
7.43
7.42
7.40
7.38
7.36
7.35
7.35
7.33
7.33
7.26
7.19
7.17
7.05
7.03
6.93
6.91
6.90
6.58
6.47
4.48
1.33
1.16
OH
O
tBu
tBu
O
H
N
Br
3l
1.02
1.92
1.97
1.09
1.96
1.02
2.12
1.07
2.05
1.01
1.00
2.00
9.02
9.07
f1 (ppm)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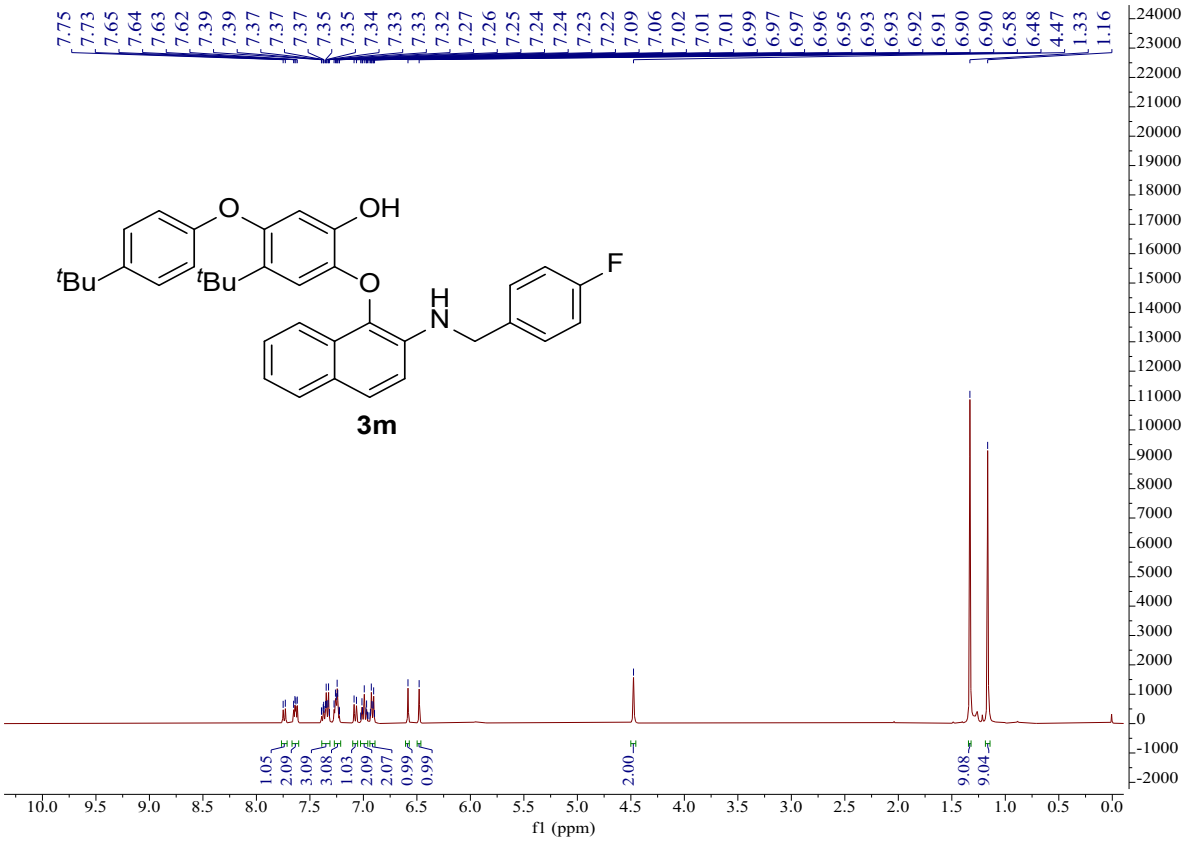
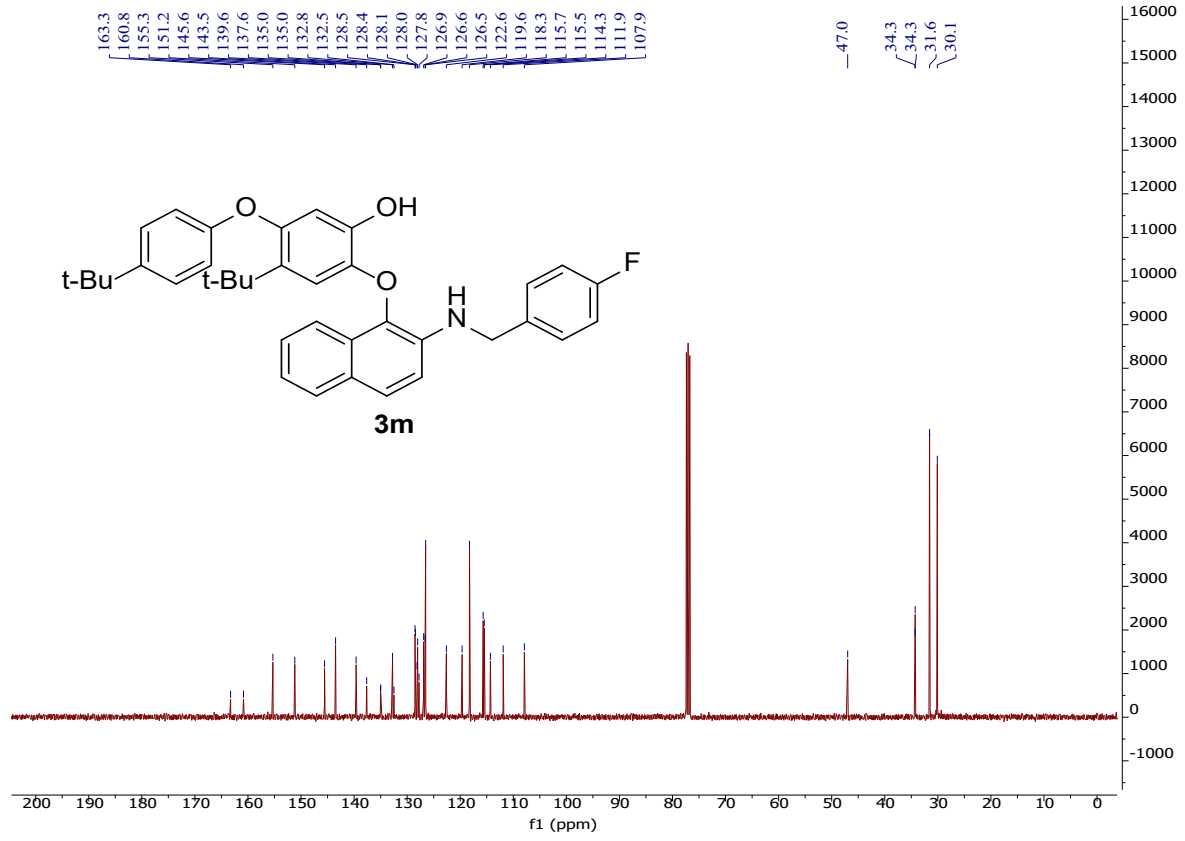
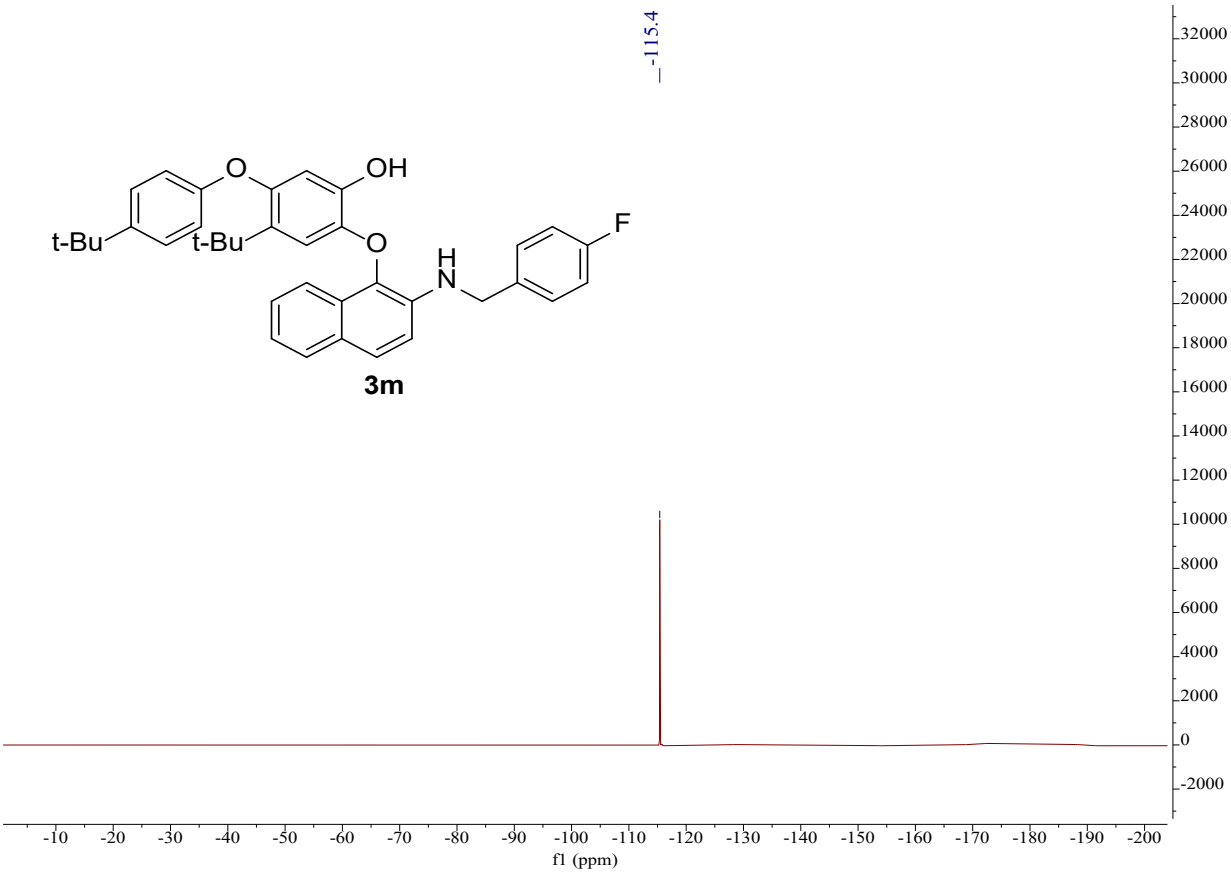
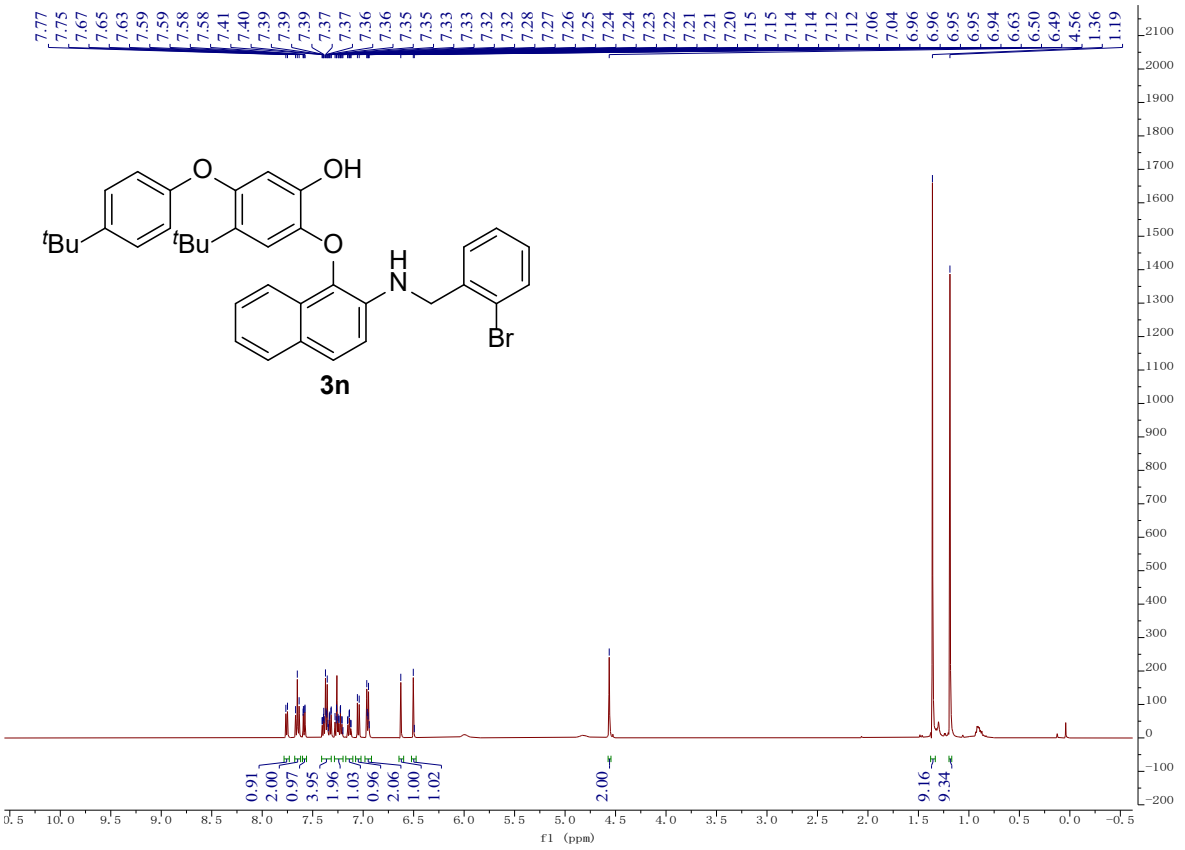
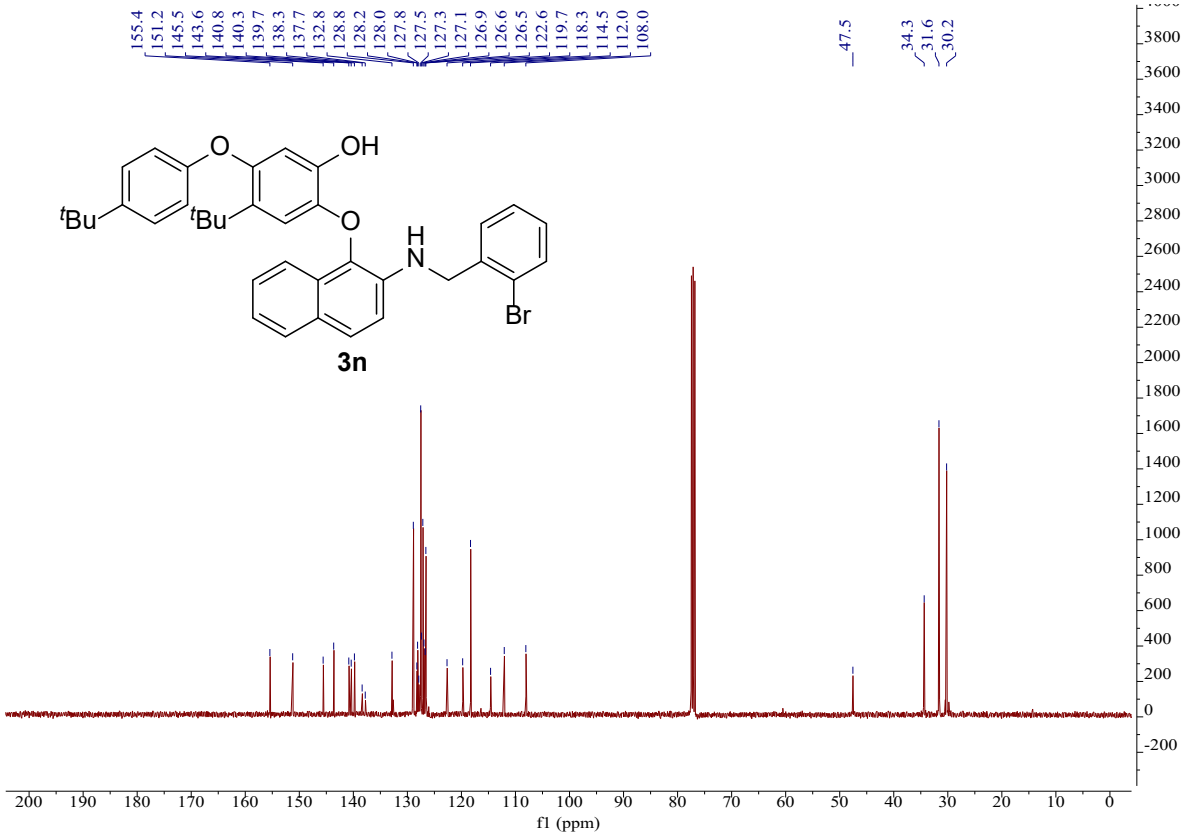
151.2
145.6
143.5
139.6
138.5
137.5
132.8
132.5
131.8
128.6
128.1
128.0
127.8
126.9
126.6
126.5
122.6
121.0
119.6
118.2
114.2
111.9
107.9
47.1
34.3
34.3
31.6
30.1
OH
O
tBu
tBu
O
H
N
Br
3l
f1 (ppm)

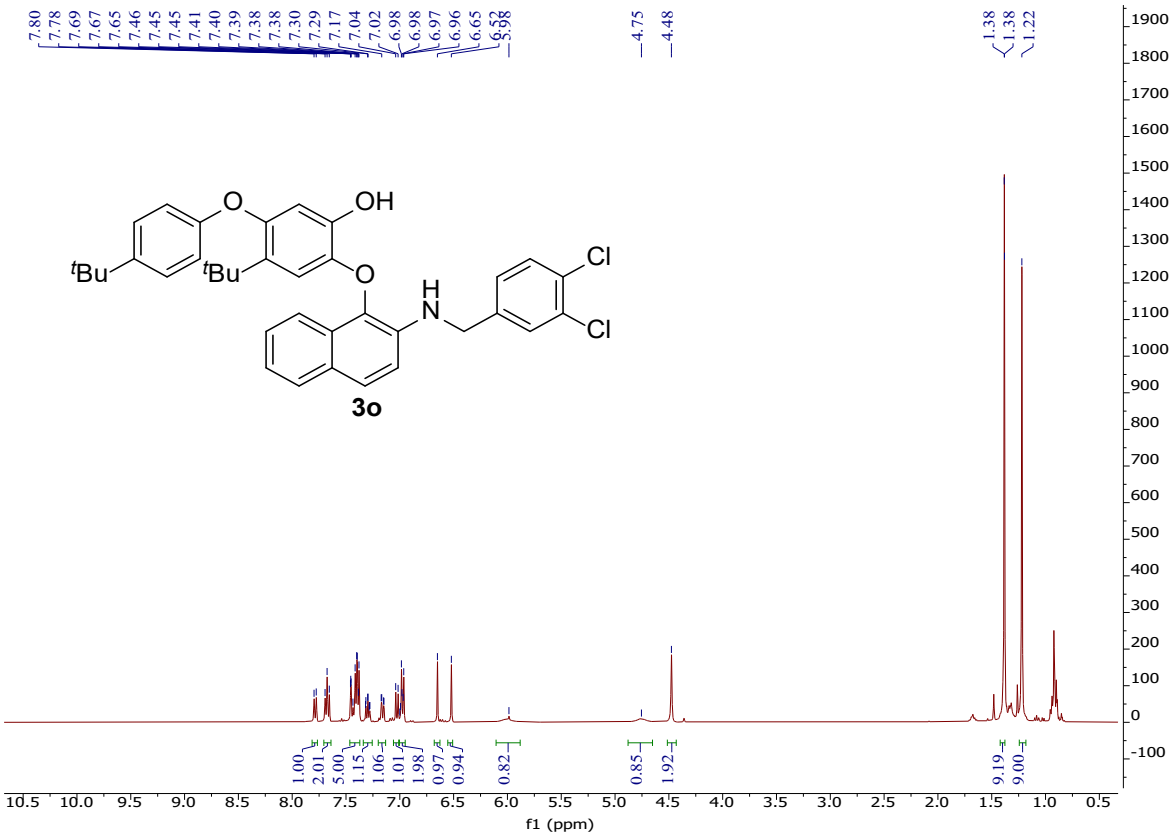

7.75 7.73 7.65 7.64 7.63 7.62 7.39 7.39 7.37 7.37 7.37 7.35 7.35 7.34 7.33 7.33 7.32 7.27 7.26 7.25 7.24 7.24 7.23 7.22 7.09 7.06 7.02 7.01 7.01 6.99 6.97 6.97 6.96 6.95 6.93 6.93 6.92 6.91 6.90 6.90 6.58 6.48 4.47 1.33 1.16
O
OH
tBu
tBu
O
H
N
F
3m
1.05 2.09 3.09 3.08 1.03 2.09 2.07 0.99 0.99 2.00 9.08 9.04
f1 (ppm)


163.3 160.8 155.3 151.2 145.6 143.5 139.6 137.6 135.0 135.0 132.8 132.5 128.5 128.4 128.1 128.0 127.8 126.9 126.6 126.5 122.6 119.6 118.3 115.7 115.5 114.3 111.9 107.9
47.0
34.3 34.3 31.6 30.1
O
OH
t-Bu
t-Bu
O
H
N
F
3m
f1 (ppm)


-115.4
O
OH
t-Bu
t-Bu
O
H
N
F
3m
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


7.77 7.75 7.67 7.65 7.63 7.59 7.59 7.58 7.58 7.41 7.40 7.39 7.39 7.39 7.37 7.37 7.36 7.36 7.35 7.35 7.33 7.33 7.32 7.32 7.28 7.27 7.26 7.25 7.24 7.24 7.23 7.22 7.21 7.21 7.20 7.15 7.15 7.14 7.14 7.12 7.12 7.06 7.04 6.96 6.96 6.95 6.95 6.94 6.63 6.50 6.49 4.56 1.36 1.19
OH
O
tBu
tBu
O
H
N
Br
3n
0.91 2.00 0.97 3.95 1.96 1.03 0.96 2.06 1.00 1.02 2.00 9.16 9.34
f1 (ppm)


155.4 151.2 145.5 143.6 140.8 140.3 139.7 138.3 137.7 132.8 128.8 128.2 128.0 127.8 127.5 127.3 127.1 126.9 126.6 126.5 122.6 119.7 118.3 114.5 112.0 108.0
47.5
34.3 31.6 30.2
OH
O
tBu
tBu
O
H
N
Br
3n
f1 (ppm)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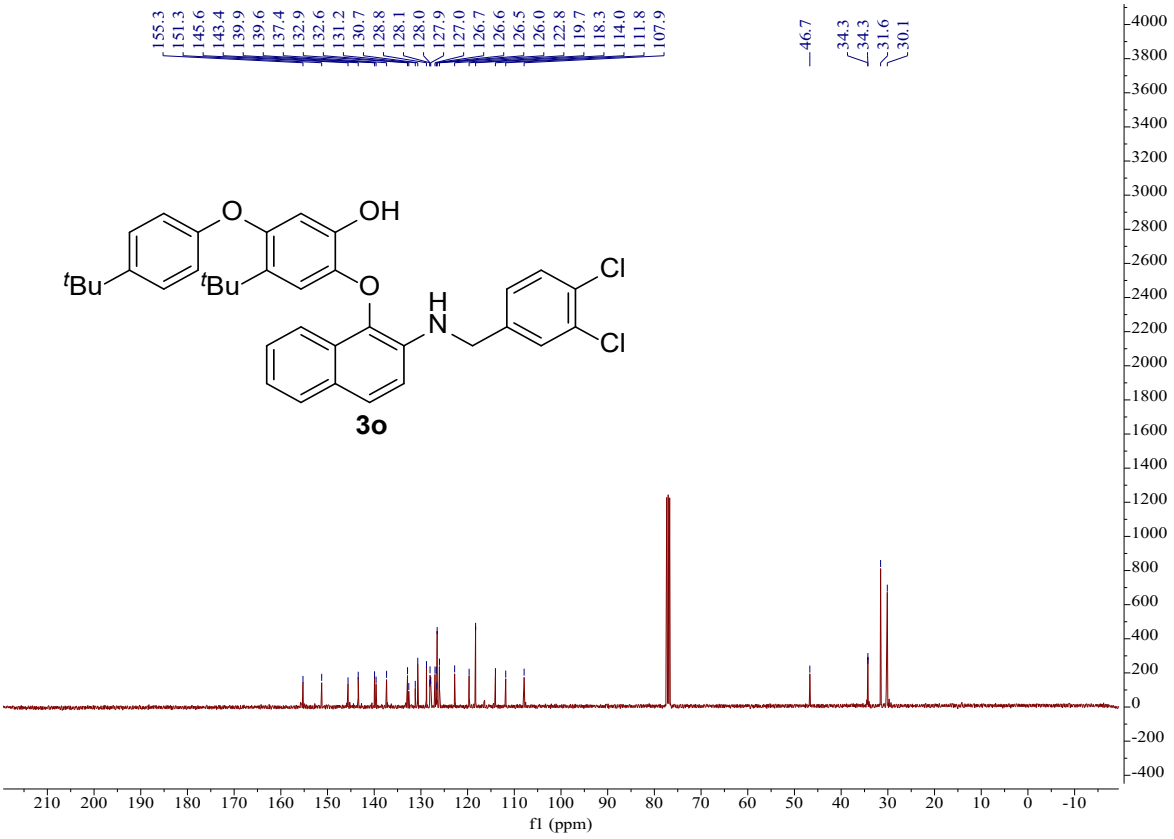
7.45
7.41
7.40
7.39
7.38
7.38
7.30
7.29
7.17
7.04
7.02
6.98
6.98
6.97
6.96
6.65
6.52
5.98
4.75
4.48
1.38
1.38
1.22
O
OH
tBu
tBu
O
H
N
Cl
Cl
3o
1.00
2.01
5.00
1.15
1.06
1.01
1.98
0.97
0.94
0.82
0.85
1.92
9.19
9.00
f1 (ppm)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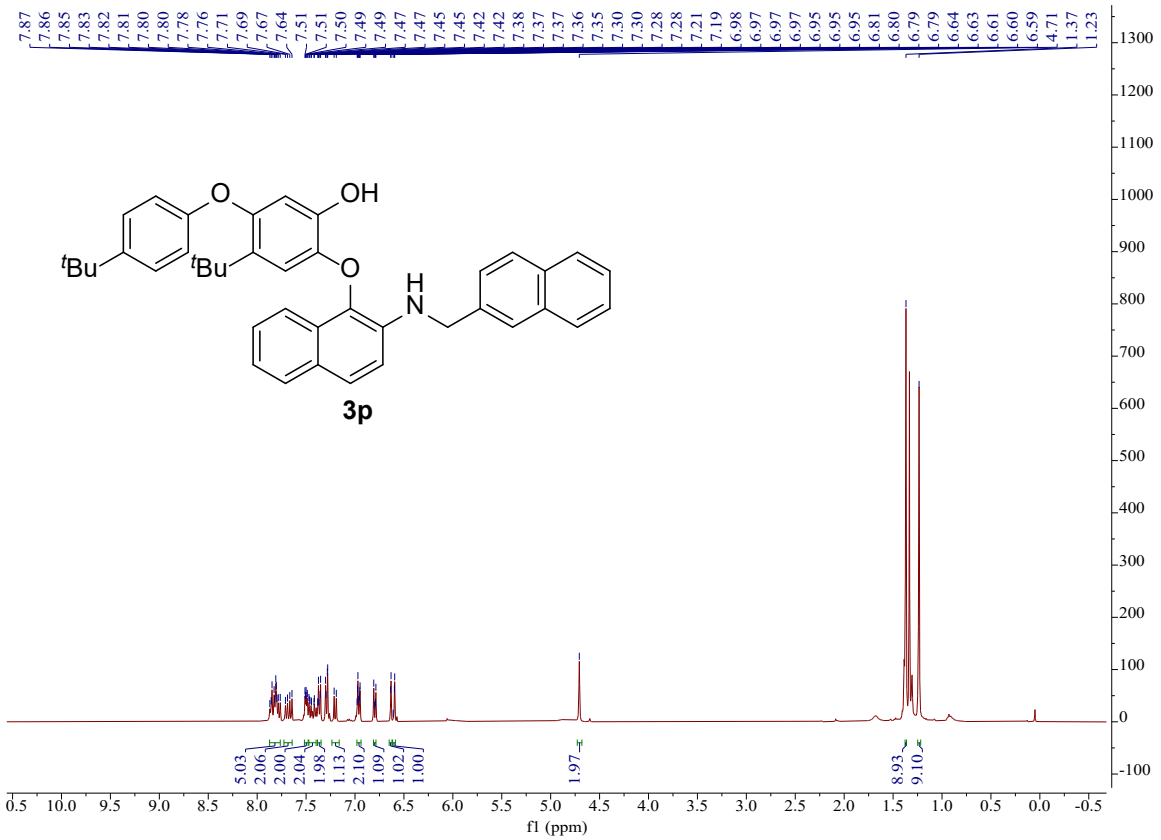
151.3
145.6
143.4
139.9
139.6
137.4
132.9
132.6
131.2
130.7
128.8
128.1
128.0
127.9
127.0
126.7
126.6
126.5
126.0
122.8
119.7
118.3
114.0
111.8
107.9
46.7
34.3
34.3
31.6
30.1
O
OH
tBu
tBu
O
H
N
Cl
Cl
3o
f1 (ppm)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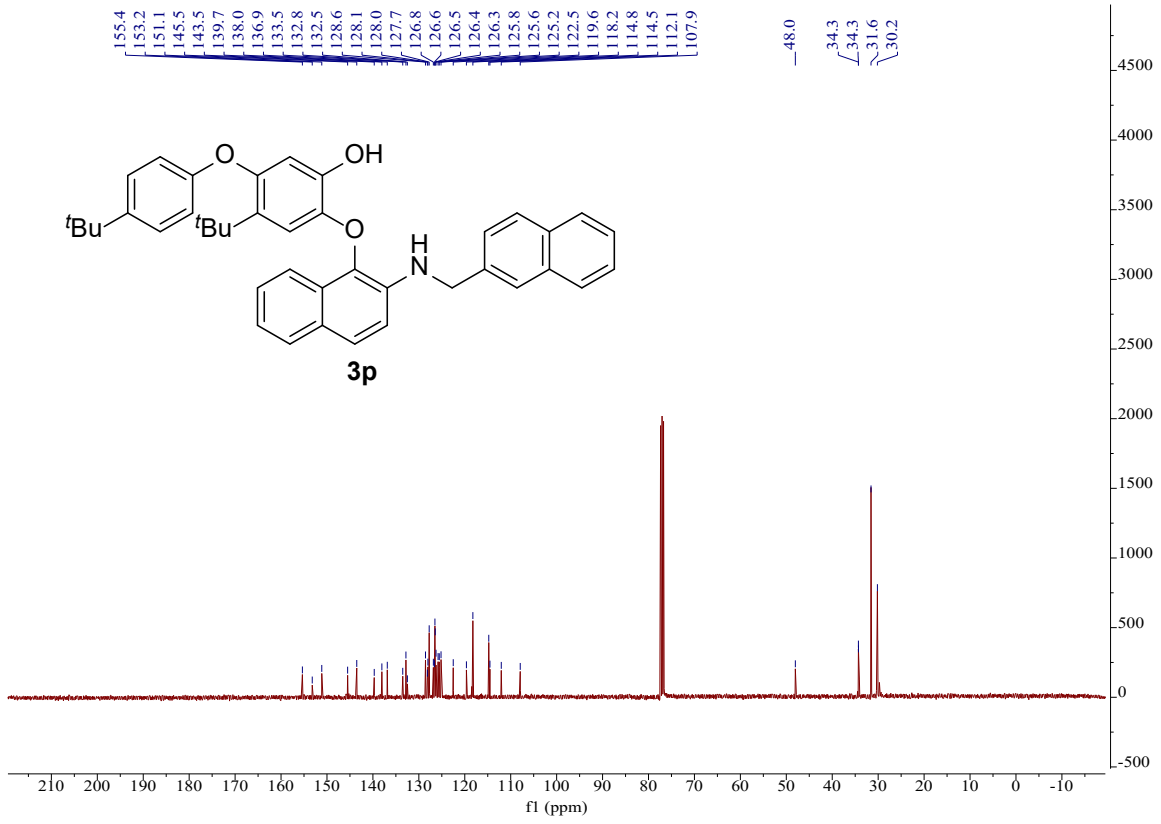
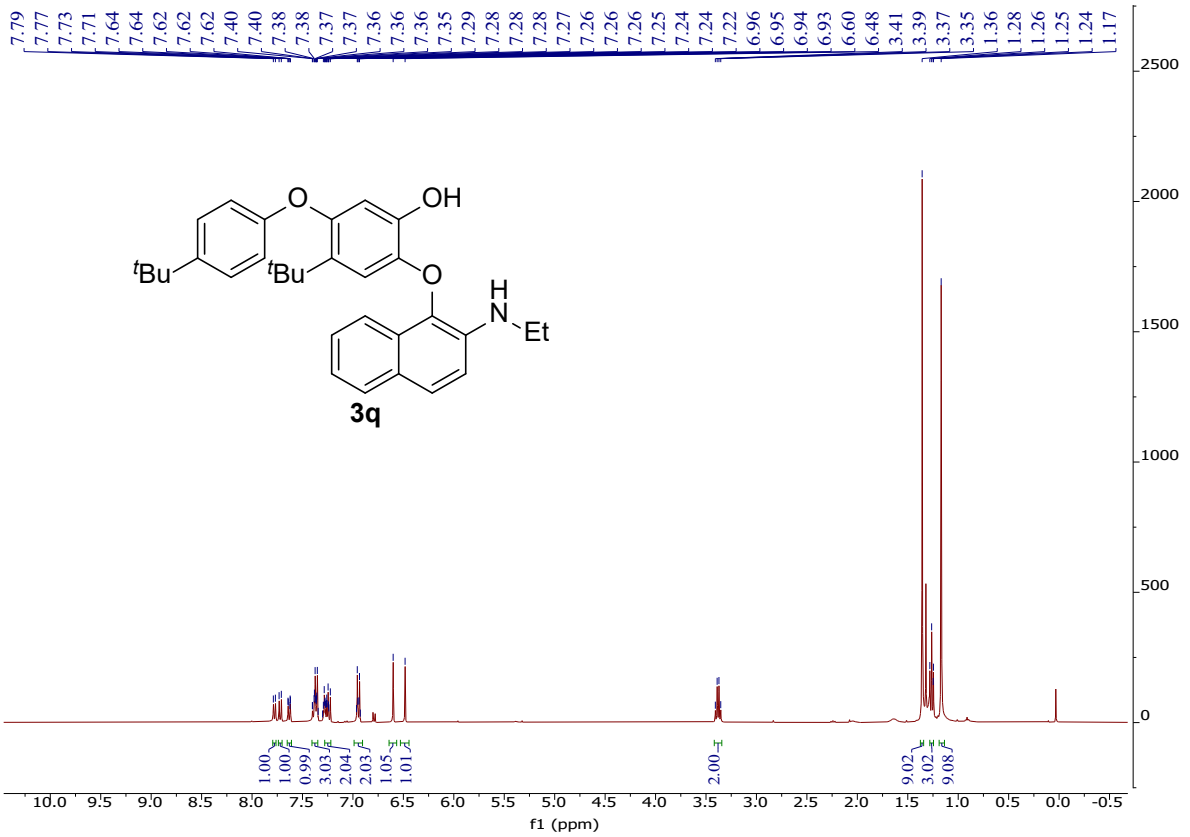
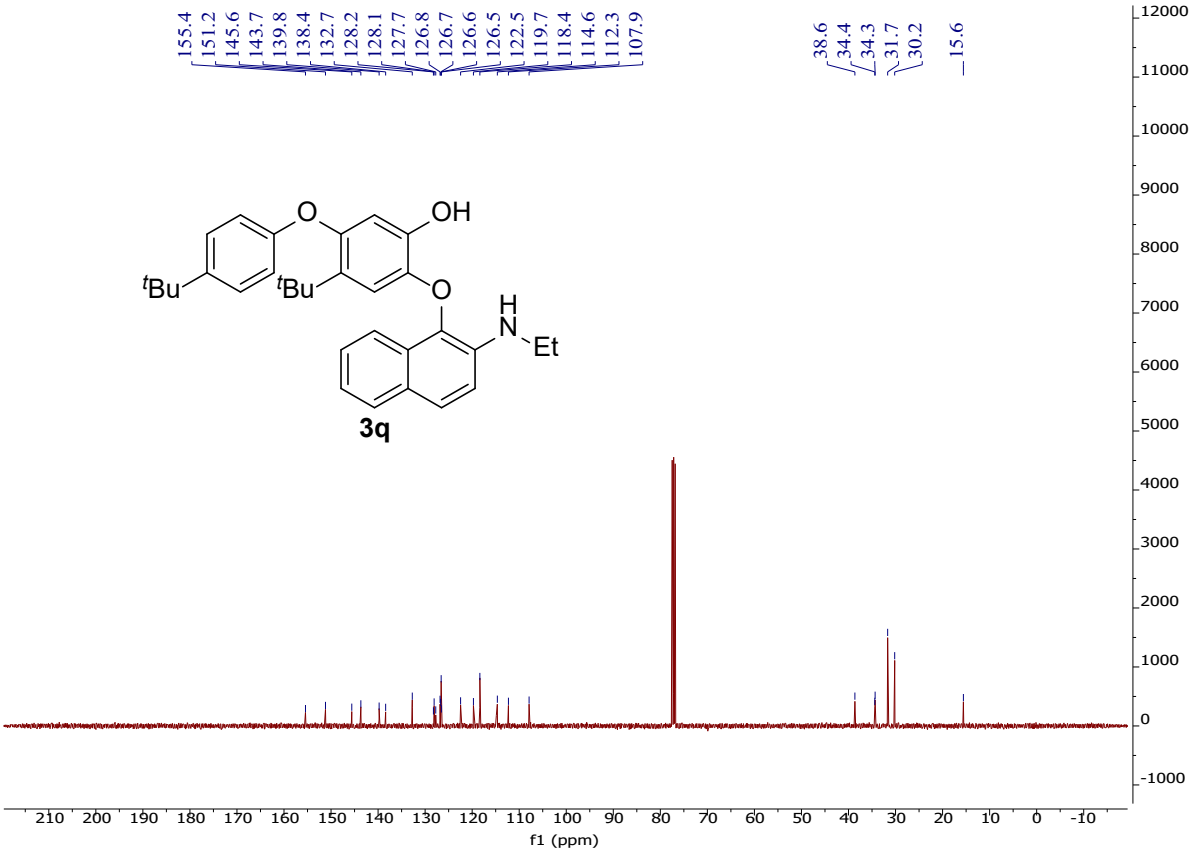
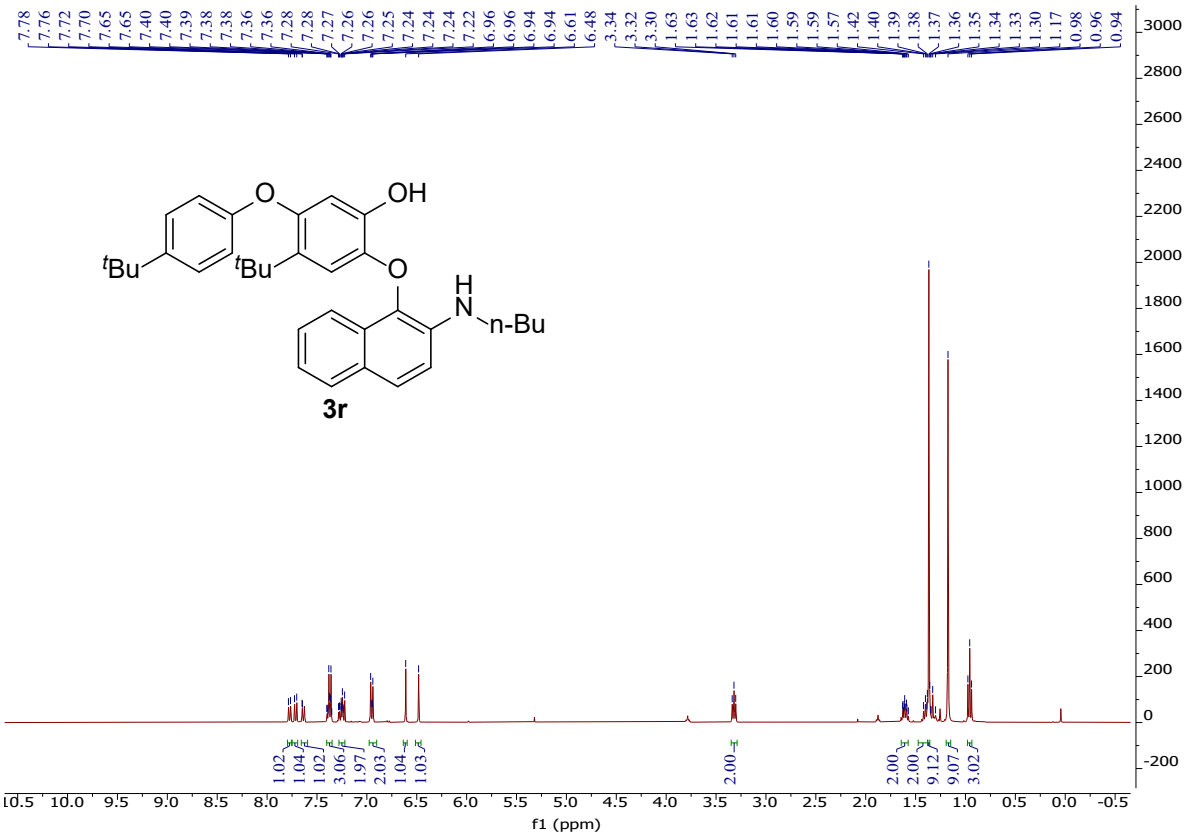
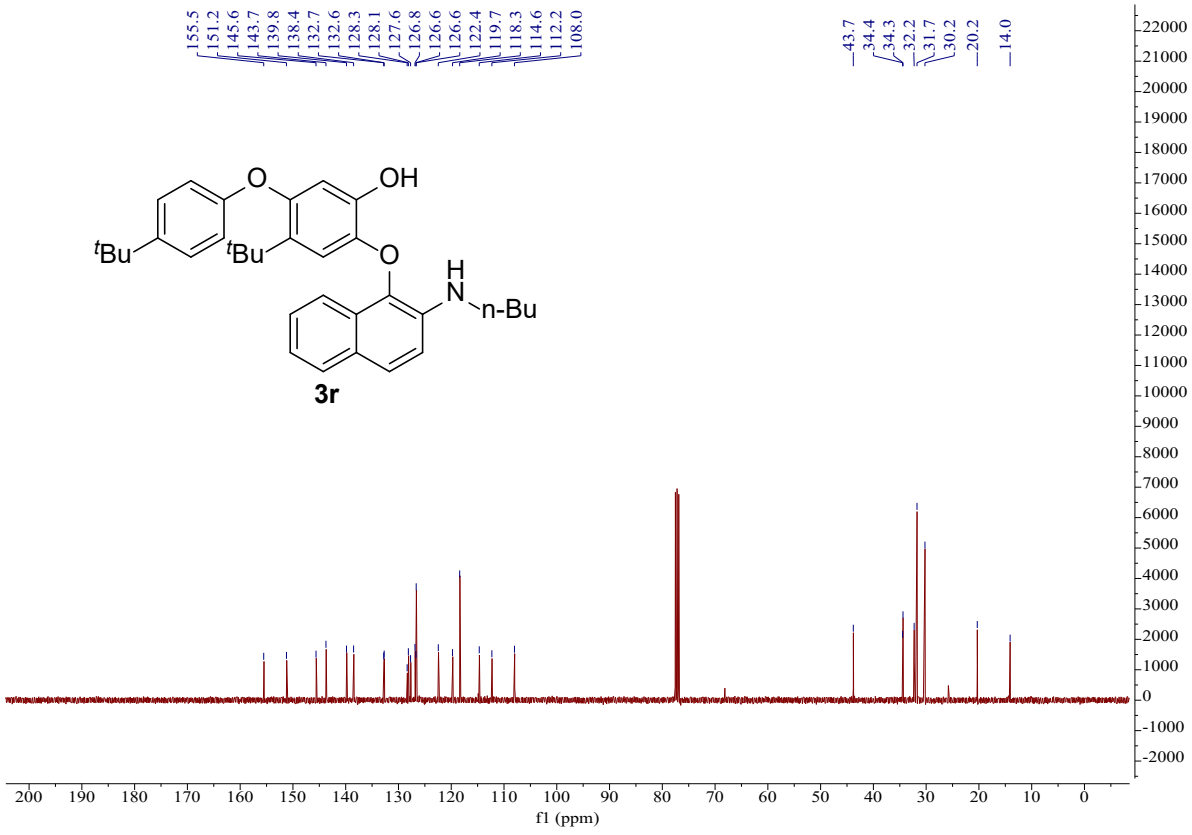
O
OH
tBu
tBu
O
H
N
3p
5.03 2.06 2.00 2.04 1.98 1.13 2.10 1.09 1.02 1.00 1.97 8.93 9.10
f1 (ppm)

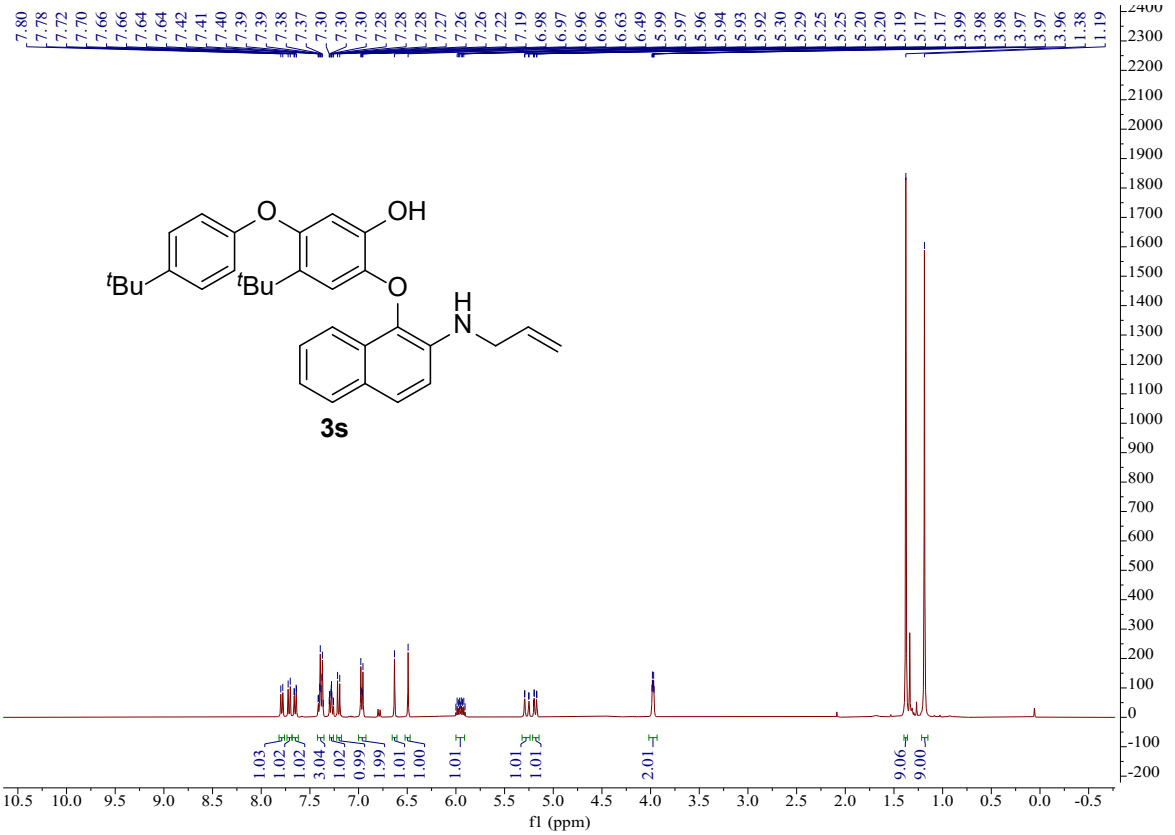

155.4 153.2 151.1 145.5 143.5 139.7 138.0 136.9 133.5 132.8 132.5 128.6 128.1 128.0 127.7 126.8 126.6 126.5 126.4 126.3 125.8 125.6 125.2 122.5 119.6 118.2 114.8 114.5 112.1 107.9
48.0
34.3
34.3
31.6
30.2
O
OH
tBu
tBu
O
H
N
3p
f1 (ppm)


7.79 7.77 7.73 7.71 7.64 7.64 7.62 7.62 7.62 7.40 7.40 7.38 7.38 7.37 7.37 7.37 7.36 7.36 7.36 7.35 7.29 7.28 7.28 7.28 7.27 7.26 7.26 7.26 7.25 7.24 7.24 7.22 6.96 6.95 6.94 6.93 6.60 6.48 3.41 3.39 3.37 3.35 1.36 1.28 1.26 1.25 1.24 1.17
O
OH
tBu
tBu
O
H
N
Et
3q
1.00 1.00 0.99 3.03 2.04 2.03 1.05 1.01 2.00 9.02 3.02 9.08
f1 (ppm)


155.4 151.2 145.6 143.7 139.8 138.4 132.7 128.2 128.1 127.7 126.8 126.7 126.6 126.5 122.5 119.7 118.4 114.6 112.3 107.9
38.6 34.4 34.3 31.7 30.2 15.6
O
OH
tBu
tBu
O
H
N
Et
3q
f1 (ppm)


OH
O
O
tBu
tBu
H
N
n-Bu
3r
f1 (ppm)


OH
O
O
tBu
tBu
H
N
n-Bu
3r
f1 (ppm)


7.80 7.78 7.72 7.70 7.66 7.64 7.64 7.42 7.41 7.40 7.39 7.38 7.37 7.30 7.30 7.30 7.28 7.28 7.28 7.27 7.26 7.26 7.22 7.19 6.98 6.97 6.96 6.96 6.63 6.49 5.99 5.97 5.96 5.94 5.93 5.92 5.30 5.29 5.25 5.25 5.20 5.20 5.19 5.17 5.17 3.99 3.98 3.98 3.97 3.97 3.96 1.38 1.19
OH
O
tBu
tBu
O
H
N
3s
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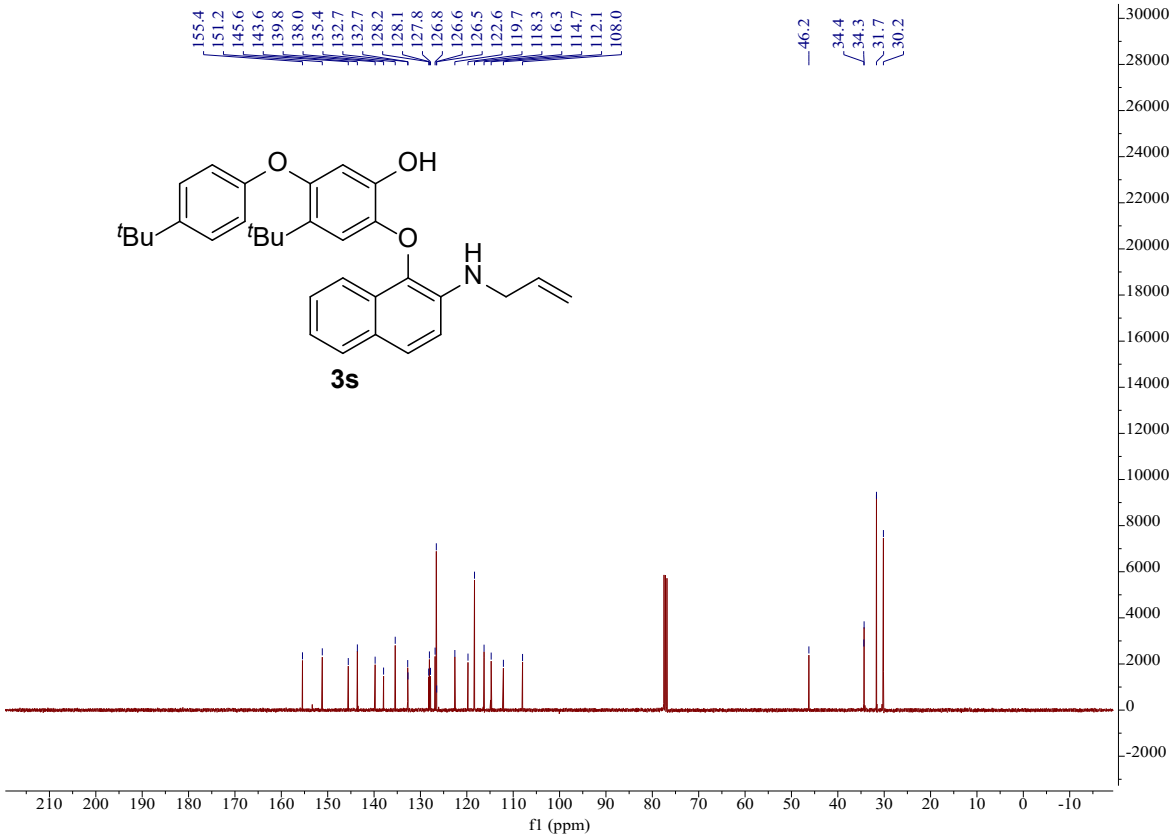
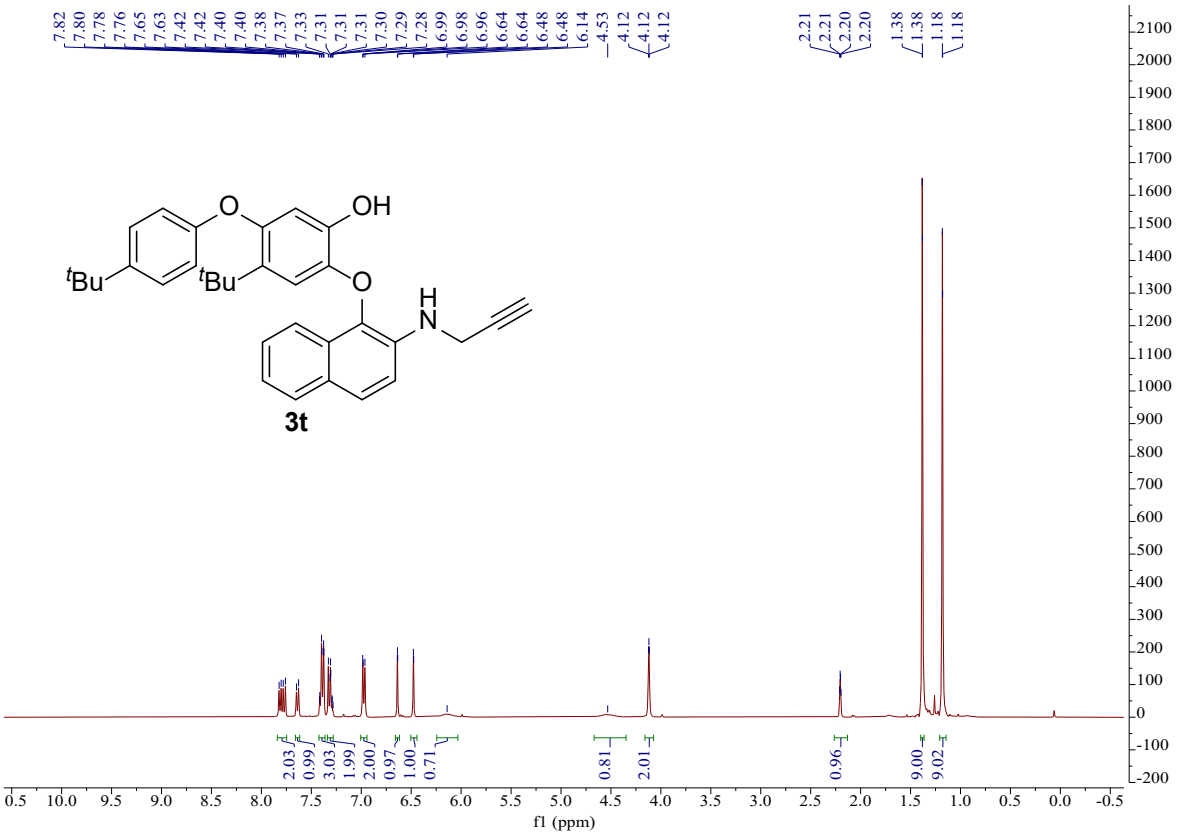
f1 (ppm)


155.4 151.2 145.6 143.6 139.8 138.0 135.4 132.7 132.7 128.2 128.1 127.8 126.8 126.6 126.5 122.6 119.7 118.3 116.3 114.7 112.1 108.0
46.2 34.4 34.3 31.7 30.2
OH
O
tBu
tBu
O
H
N
3s
f1 (ppm)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7.80
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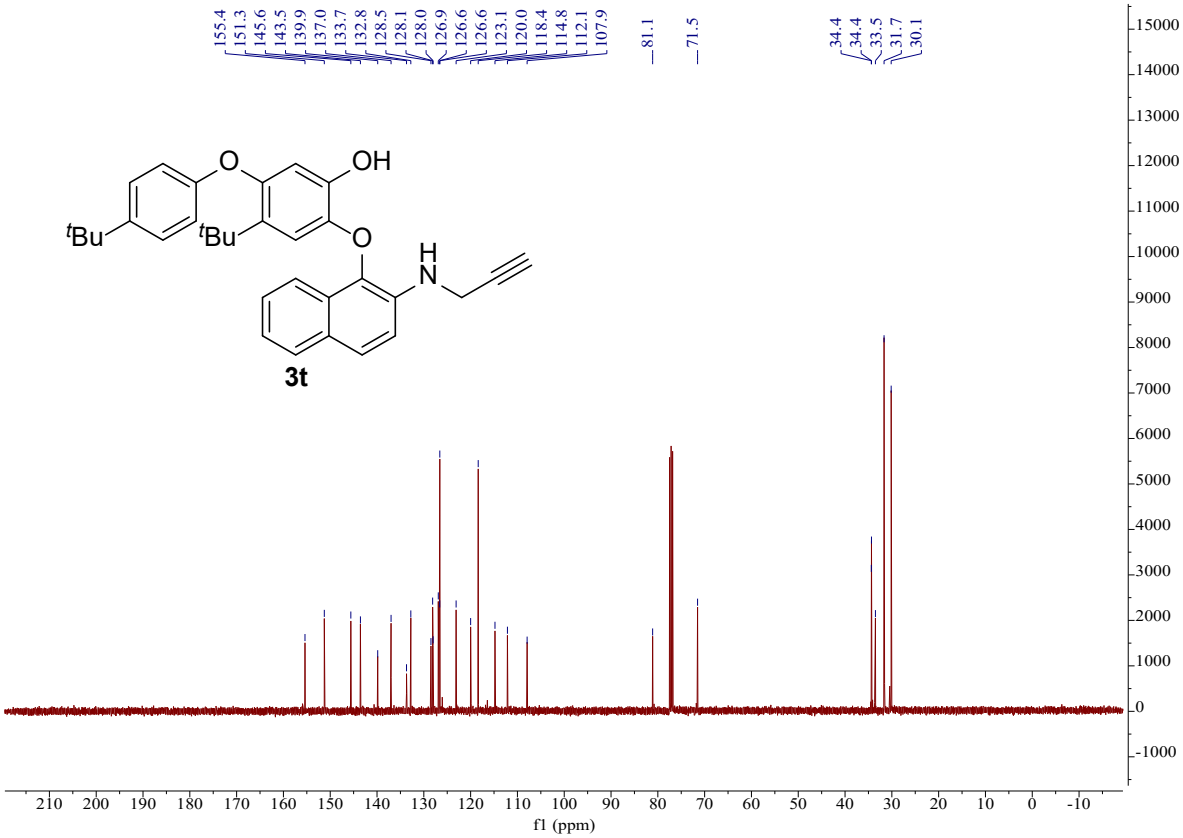
7.40
7.38
7.37
7.33
7.31
7.31
7.31
7.30
7.29
7.28
6.99
6.98
6.96
6.64
6.64
6.48
6.48
6.14
4.53
4.12
4.12
4.12
2.21
2.21
2.20
2.20
1.38
1.38
1.18
1.18
O
OH
tBu
tBu
O
H
N
3t
2.03
0.99
3.03
1.99
2.00
0.97
1.00
0.71
0.81
2.01
0.96
9.00
9.02
f1 (ppm)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143.5
139.9
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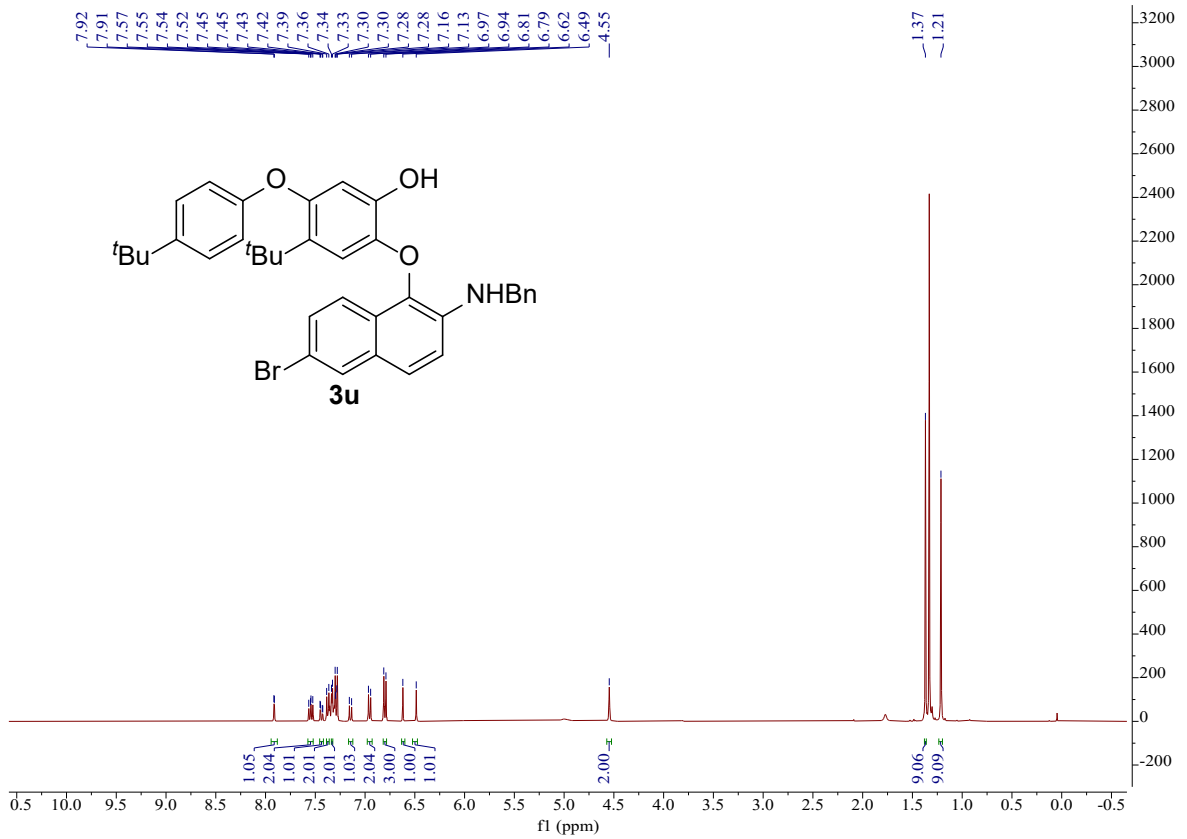
133.7
132.8
128.5
128.1
128.0
126.9
126.6
126.6
123.1
120.0
118.4
114.8
112.1
107.9
81.1
71.5
34.4
34.4
33.5
31.7
30.1
O
OH
tBu
tBu
O
H
N
3t
f1 (ppm)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7.45
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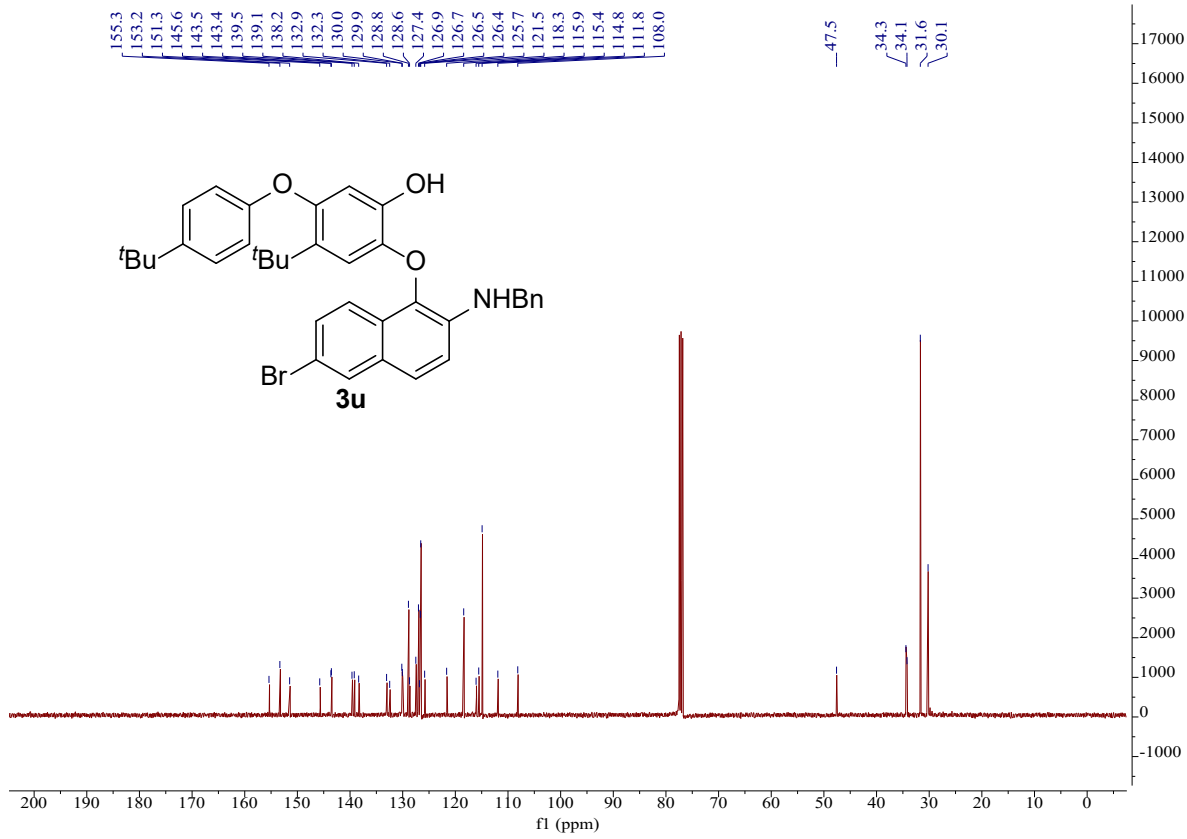
7.39
7.36
7.34
7.33
7.30
7.30
7.28
7.28
7.16
7.13
6.97
6.94
6.81
6.79
6.62
6.49
4.55
1.37
1.21
O
OH
tBu
tBu
O
NHBn
Br
3u
1.05
2.04
1.01
2.01
2.01
1.03
2.04
3.00
1.00
1.01
2.00
9.06
9.09
f1 (ppm)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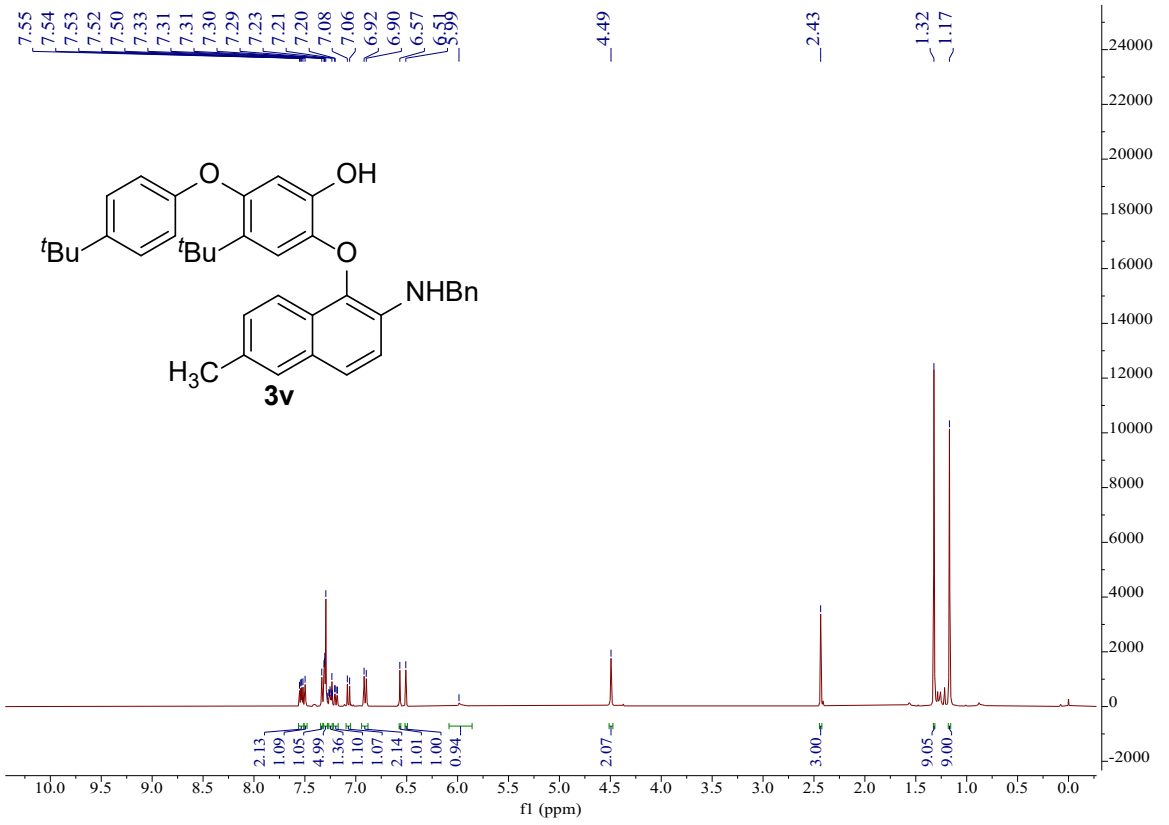
151.3
145.6
143.5
143.4
139.5
139.1
138.2
132.9
132.3
130.0
129.9
128.8
128.6
127.4
126.9
126.7
126.5
126.4
125.7
121.5
118.3
115.9
115.4
114.8
111.8
108.0
47.5
34.3
34.1
31.6
30.1
O
OH
tBu
tBu
O
NHBn
Br
3u
f1 (ppm)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7.31
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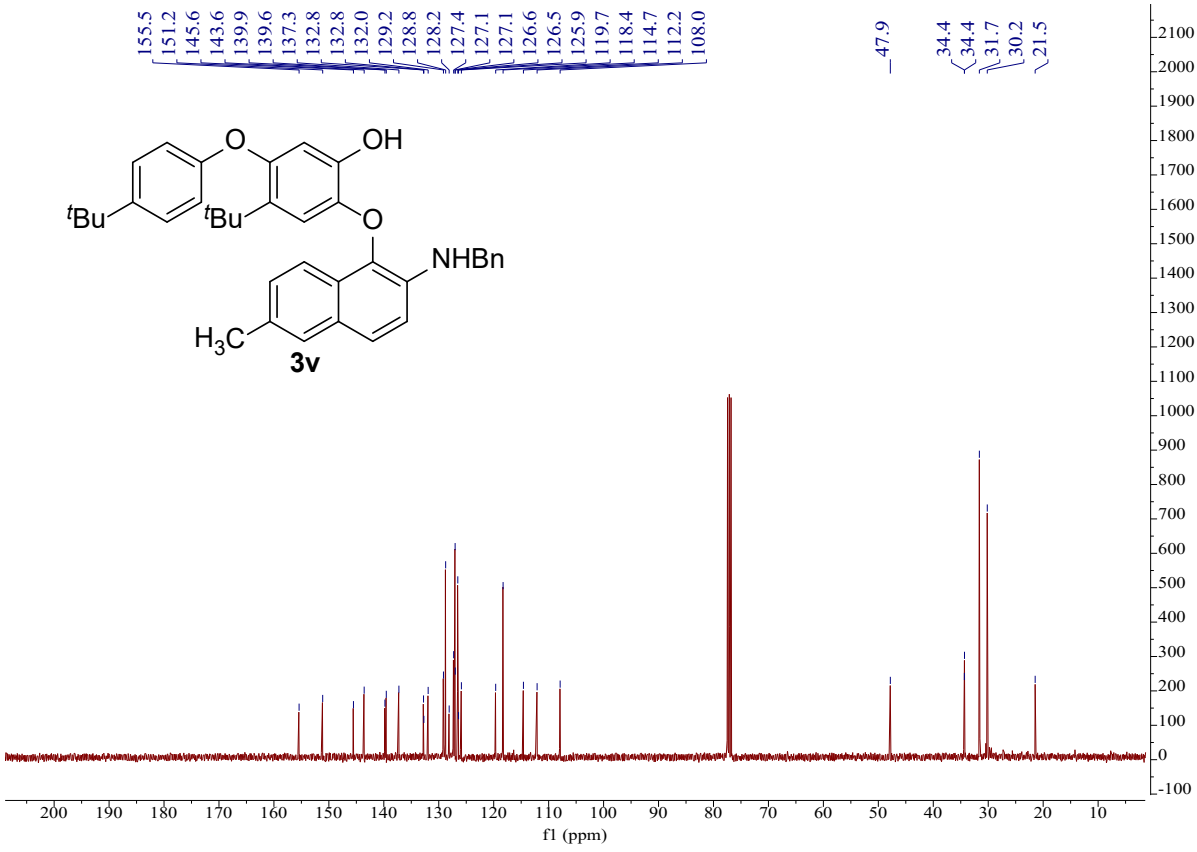
7.29
7.23
7.21
7.20
7.08
7.06
6.92
6.90
6.57
6.51
5.99
4.49
2.43
1.32
1.17
OH
O
tBu
tBu
O
NHBn
H3C
3v
2.13
1.09
1.05
4.99
1.36
1.10
1.07
2.14
1.01
1.00
0.94
2.07
3.00
9.05
9.00
f1 (ppm)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143.6
139.9
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137.3
132.8
132.8
132.0
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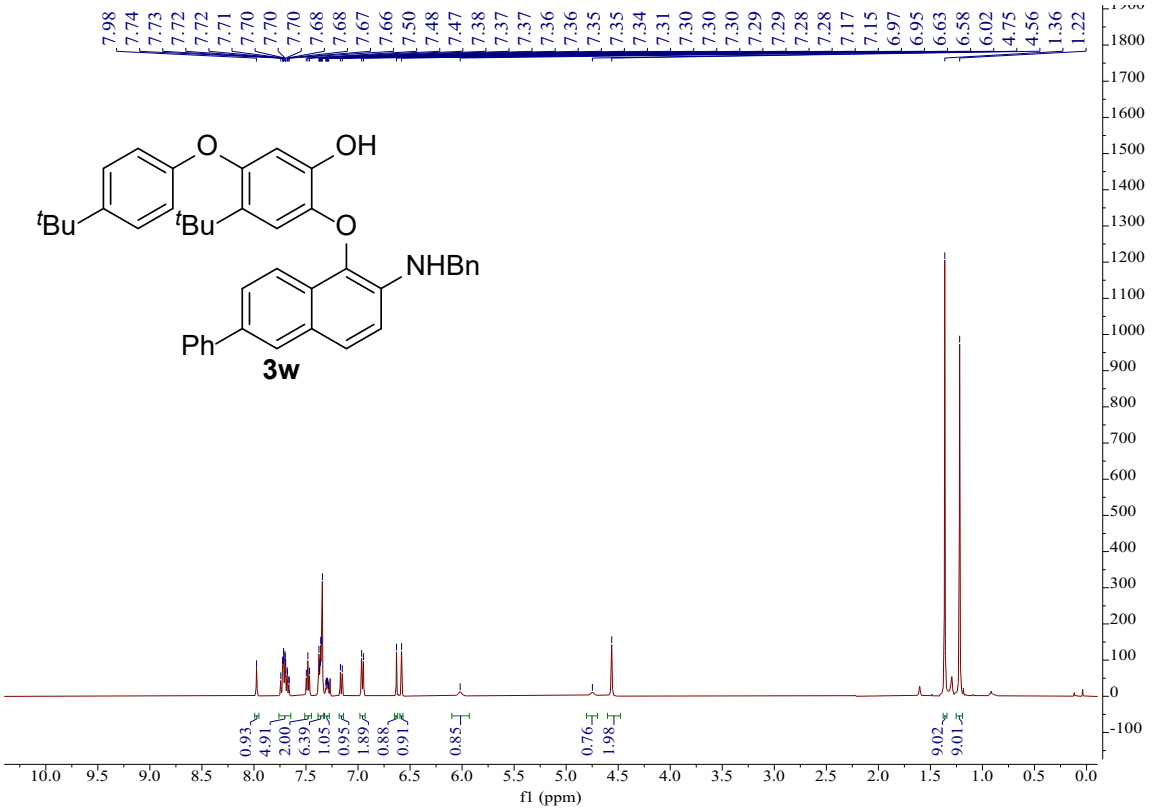
128.8
128.2
127.4
127.1
127.1
126.6
126.5
125.9
119.7
118.4
114.7
112.2
108.0
47.9
34.4
34.4
31.7
30.2
21.5
OH
O
tBu
tBu
O
NHBn
H3C
3v
f1 (ppm)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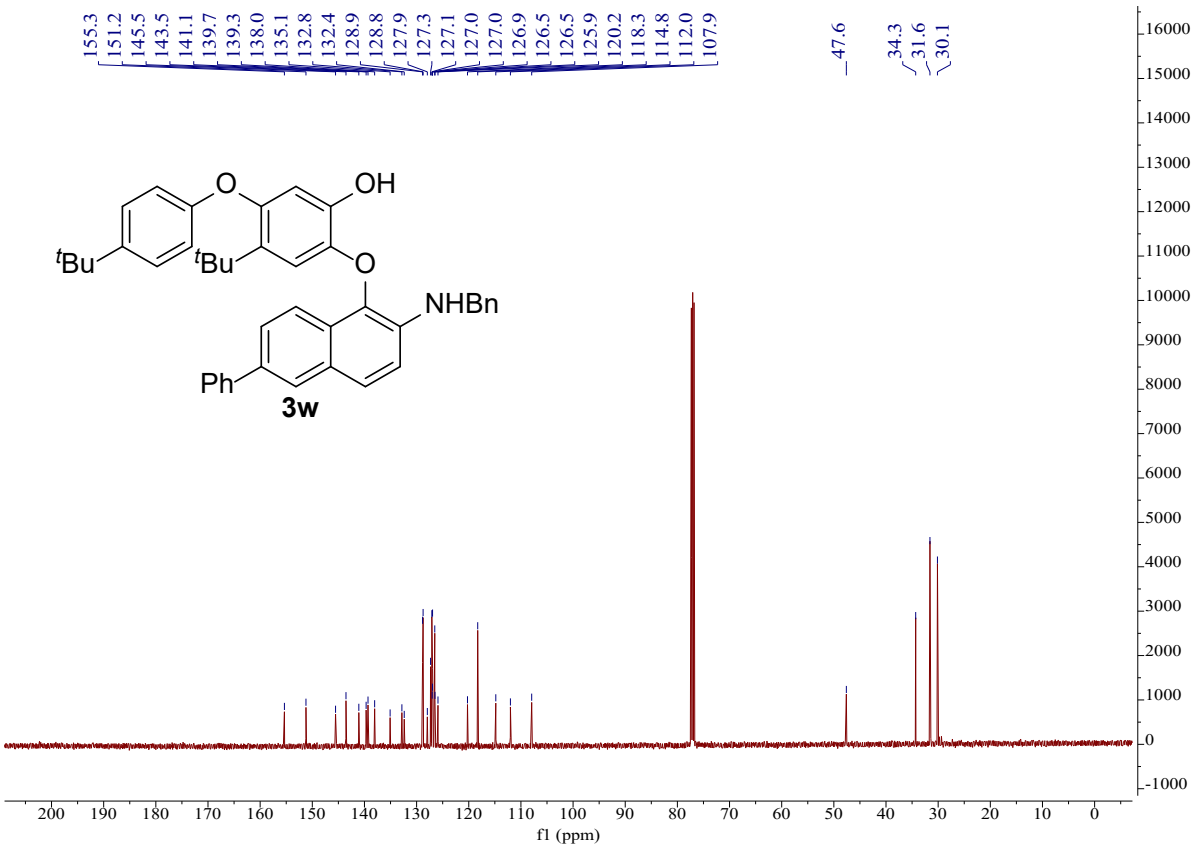
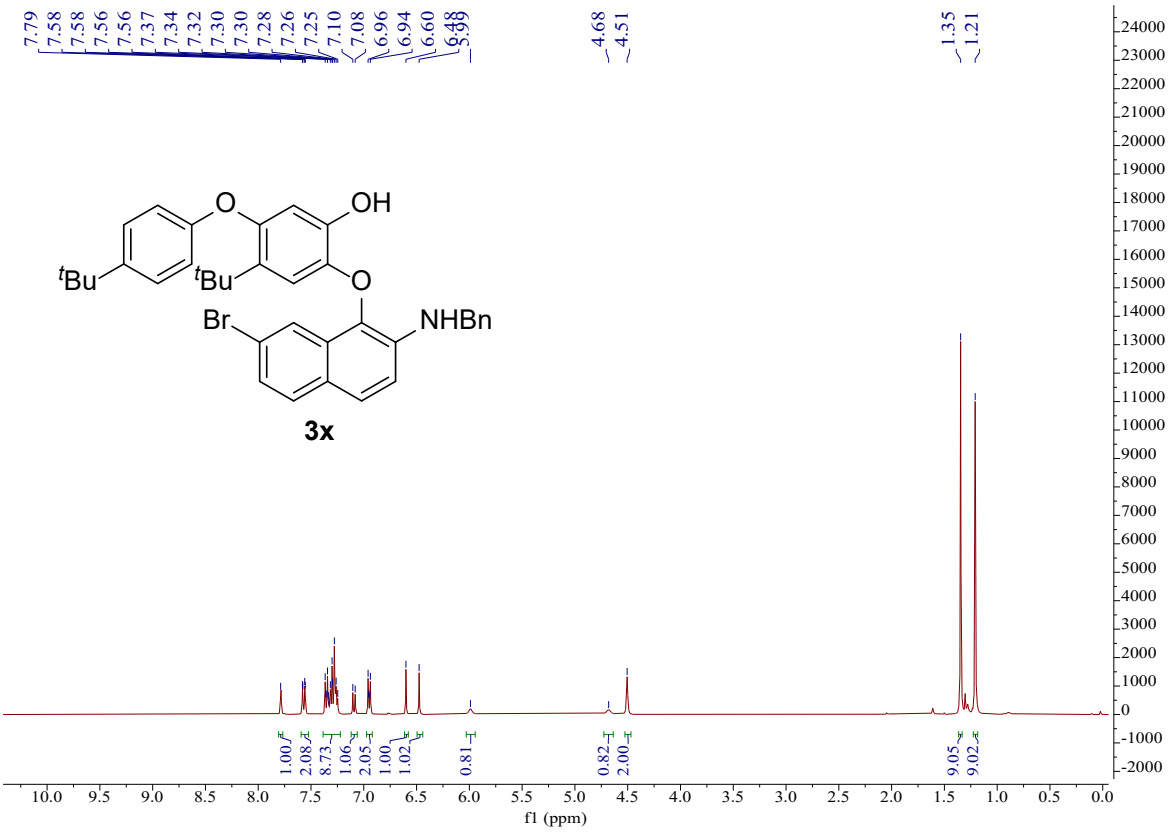
O
OH
tBu
tBu
O
NHBn
Ph
3w
0.93 4.91 2.00 6.39 1.05 0.95 1.89 0.88 0.91 0.85 0.76 1.98 9.02 9.01
f1 (ppm)


155.3 151.2 145.5 143.5 141.1 139.7 139.3 138.0 135.1 132.8 132.4 128.9 128.8 127.9 127.3 127.1 127.0 127.0 126.9 126.5 126.5 125.9 120.2 118.3 114.8 112.0 107.9
47.6
34.3 31.6 30.1
O
OH
tBu
tBu
O
NHBn
Ph
3w
f1 (ppm)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7.56
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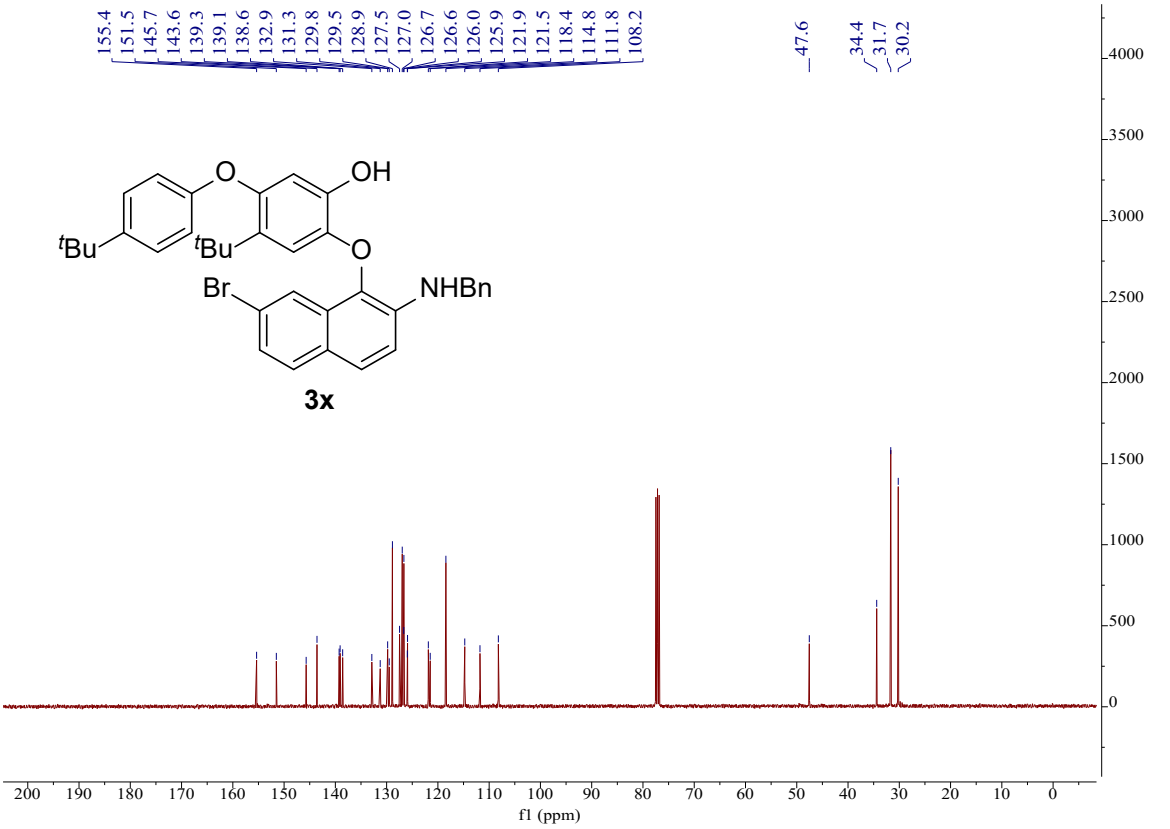
7.32
7.30
7.30
7.28
7.26
7.25
7.10
7.08
6.96
6.94
6.60
6.48
5.99
4.68
4.51
1.35
1.21
O
OH
tBu
tBu
O
Br
NHBn
3x
1.00
2.08
8.73
1.06
2.05
1.00
1.02
0.81
0.82
2.00
9.05
9.02
f1 (ppm)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145.7
143.6
139.3
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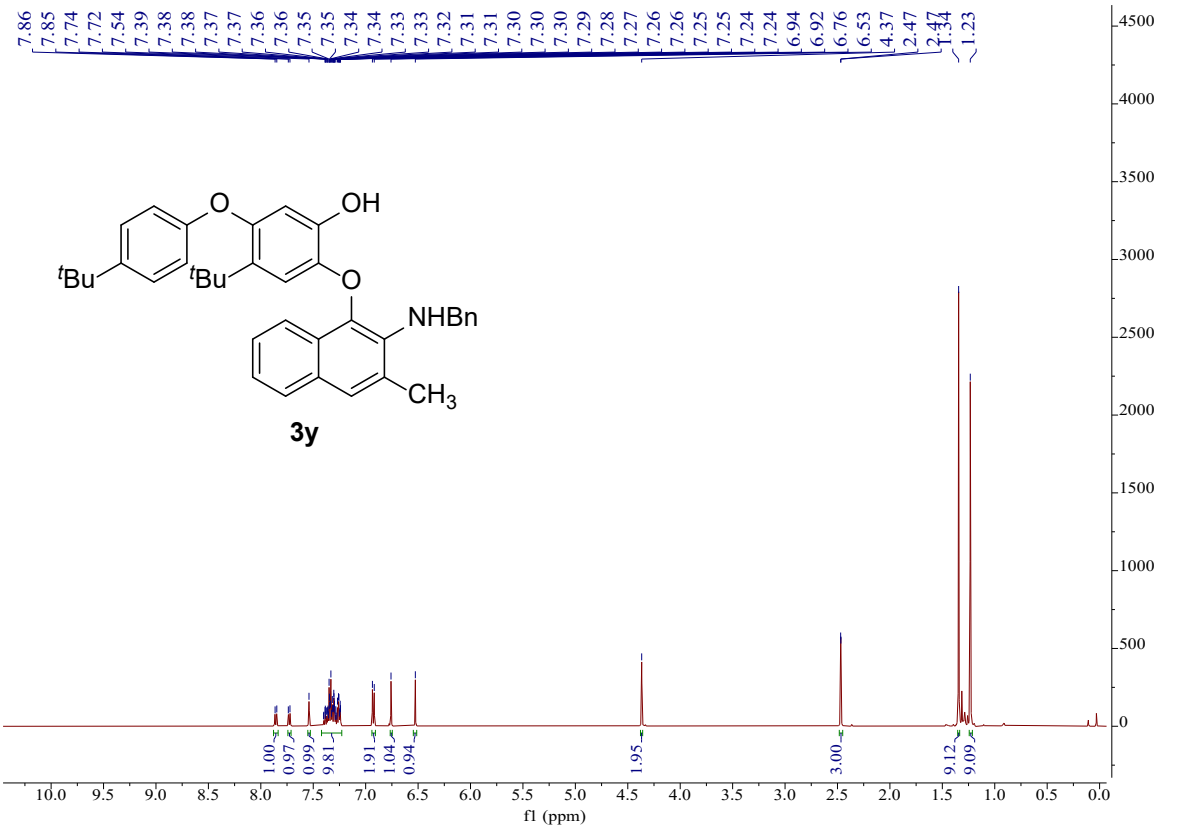
138.6
132.9
131.3
129.8
129.5
128.9
127.5
127.0
126.7
126.6
126.0
125.9
121.9
121.5
118.4
114.8
111.8
108.2
47.6
34.4
31.7
30.2
O
OH
tBu
tBu
O
Br
NHBn
3x
f1 (ppm)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7.38
7.38
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7.37
7.36
7.36
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7.34
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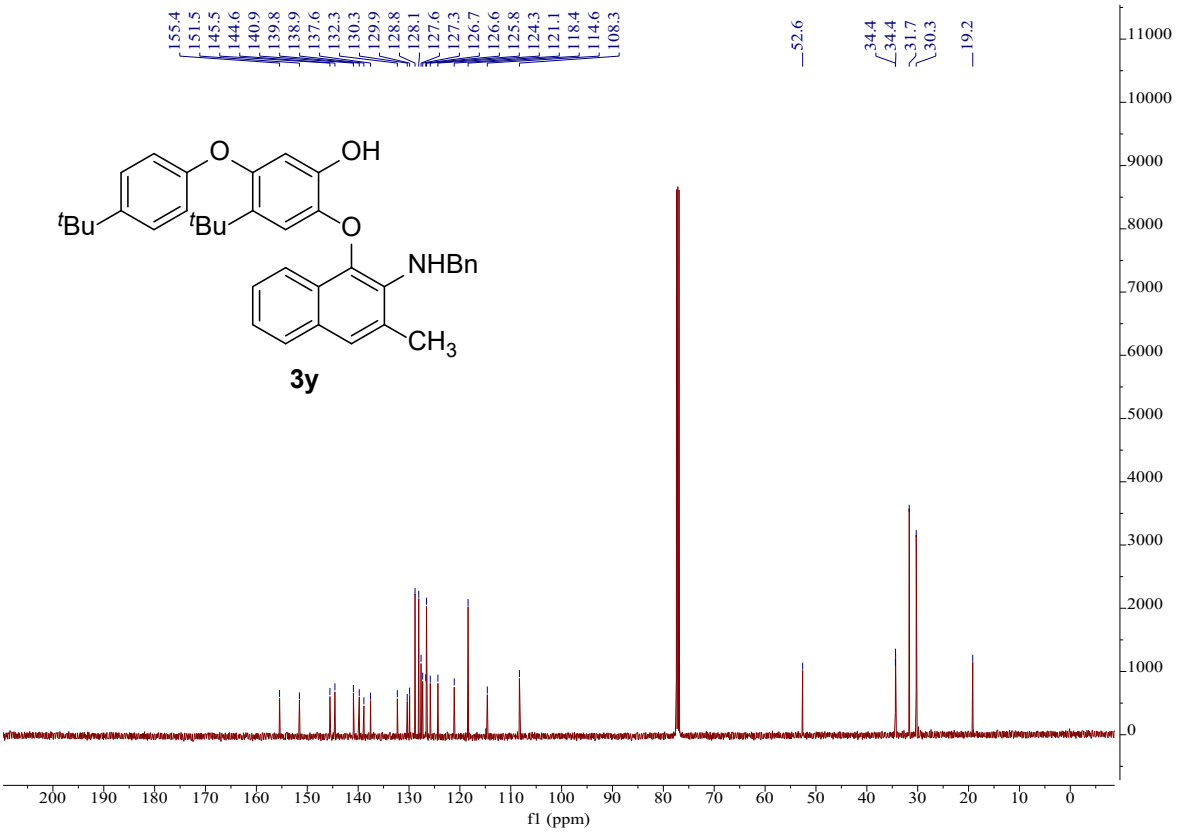
7.30
7.30
7.30
7.29
7.28
7.27
7.26
7.26
7.25
7.25
7.24
7.24
6.94
6.92
6.76
6.53
4.37
2.47
2.44
1.34
1.23
OH
O
tBu
tBu
O
NHBn
CH3
3y
1.00
0.97
0.99
9.81
1.91
1.04
0.94
1.95
3.00
9.12
9.09
f1 (ppm)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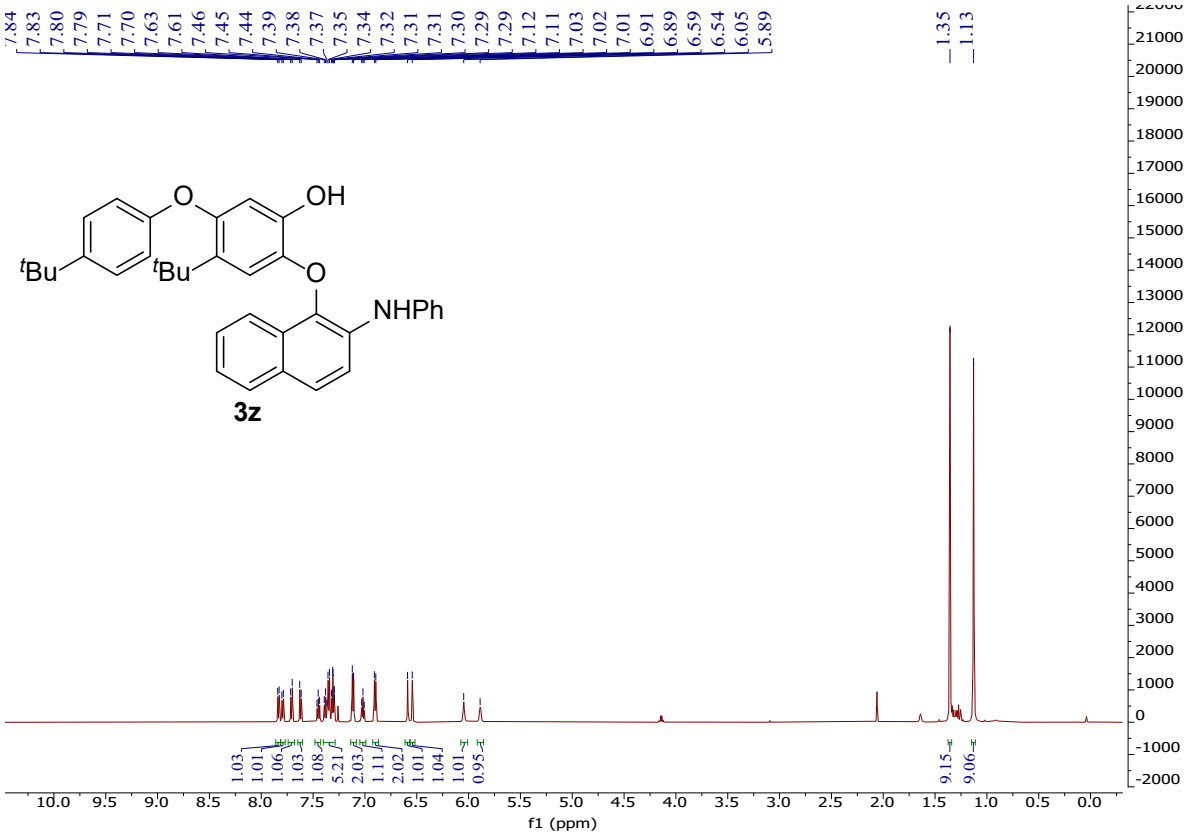
151.5
145.5
144.6
140.9
139.8
138.9
137.6
132.3
130.3
129.9
128.8
128.1
127.6
127.3
126.7
126.6
125.8
124.3
121.1
118.4
114.6
108.3
52.6
34.4
34.4
31.7
30.3
19.2
OH
O
tBu
tBu
O
NHBn
CH3
3y
f1 (ppm)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7.61
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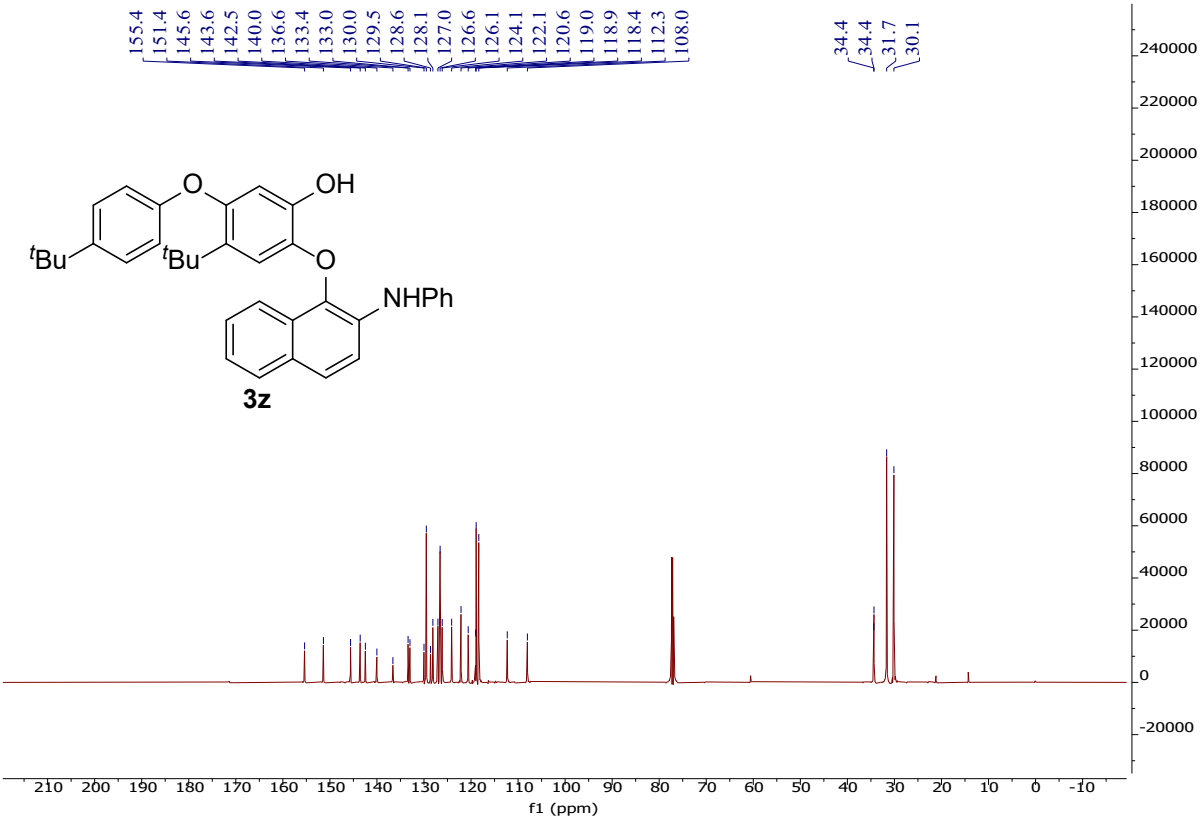
7.45
7.44
7.39
7.38
7.37
7.35
7.34
7.32
7.31
7.31
7.30
7.29
7.29
7.12
7.11
7.03
7.02
7.01
6.91
6.89
6.59
6.54
6.05
5.89
1.35
1.13
O
OH
tBu
tBu
O
NHPh
3z
1.03
1.01
1.06
1.03
1.08
5.21
2.03
1.11
2.02
1.01
1.04
1.01
0.95
9.15
9.06
f1 (ppm)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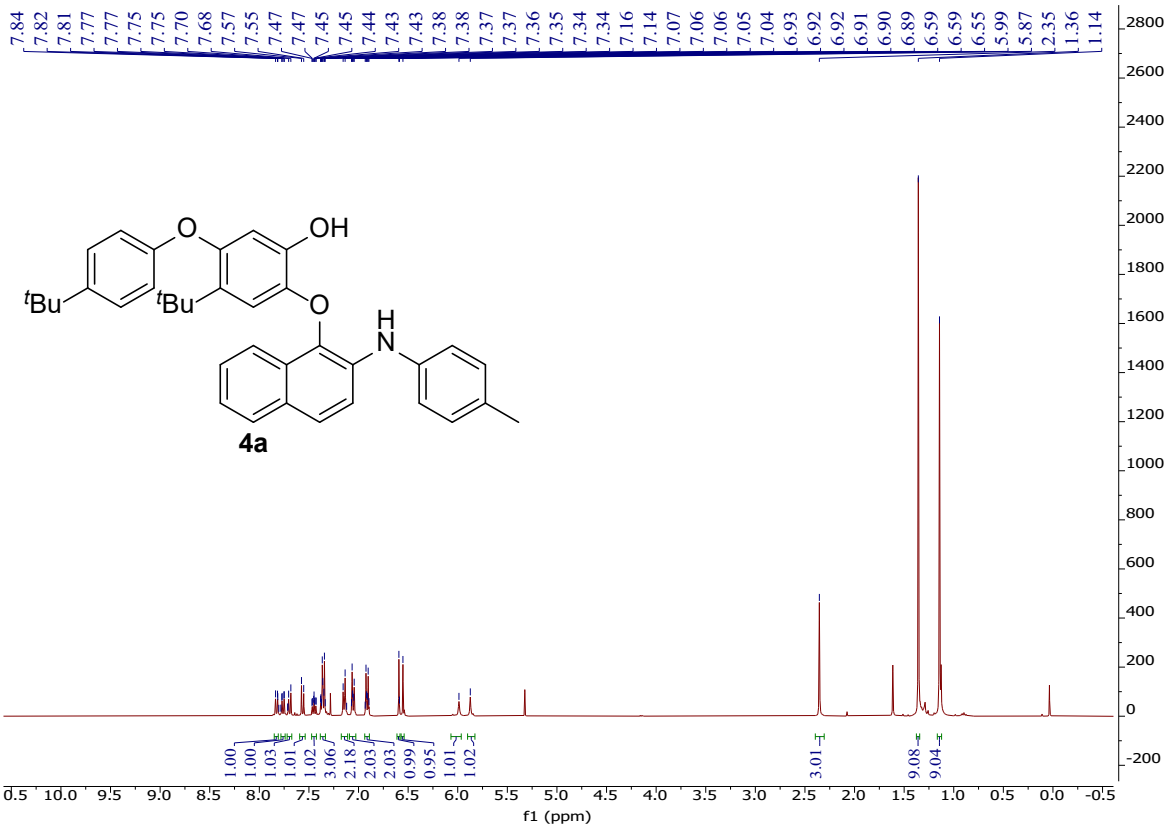
151.4
145.6
143.6
142.5
140.0
136.6
133.4
133.0
130.0
129.5
128.6
128.1
127.0
126.6
126.1
124.1
122.1
120.6
119.0
118.9
118.4
112.3
108.0
34.4
34.4
31.7
30.1
O
OH
tBu
tBu
O
NHPh
3z
f1 (ppm)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O
OH
tBu
tBu
O
H
N
4a
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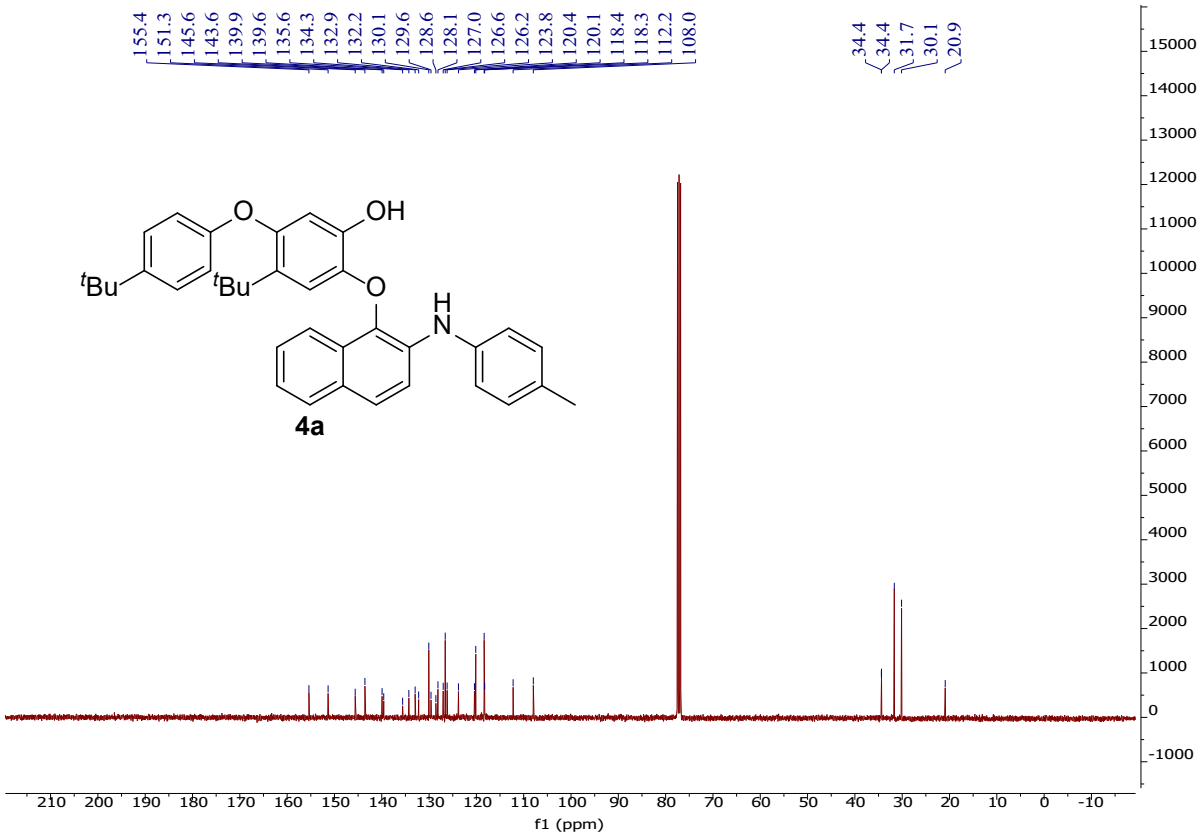
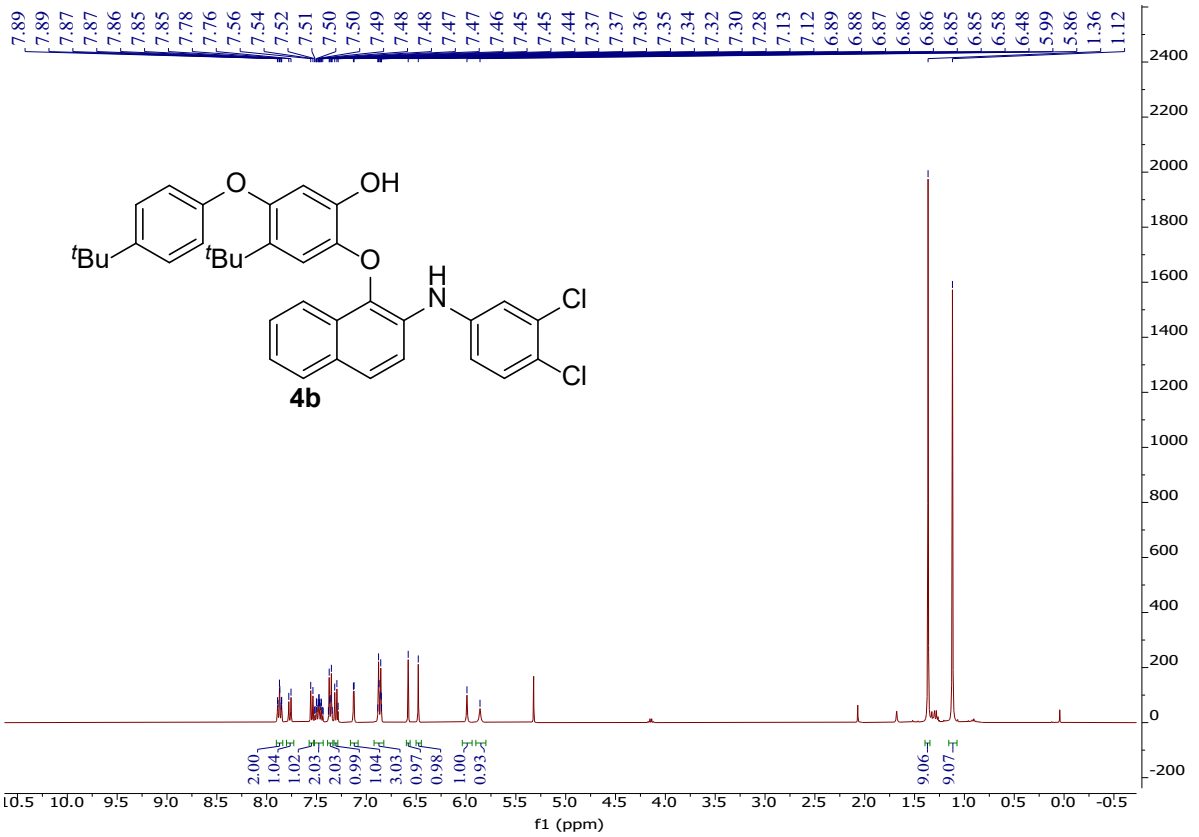
f1 (ppm)


155.4 151.3 145.6 143.6 139.9 139.6 135.6 134.3 132.9 132.2 130.1 129.6 128.6 128.1 127.0 126.6 126.2 123.8 120.4 120.1 118.4 118.3 112.2 108.0
34.4 34.4 31.7 30.1 20.9
O
OH
tBu
tBu
O
H
N
4a
f1 (ppm)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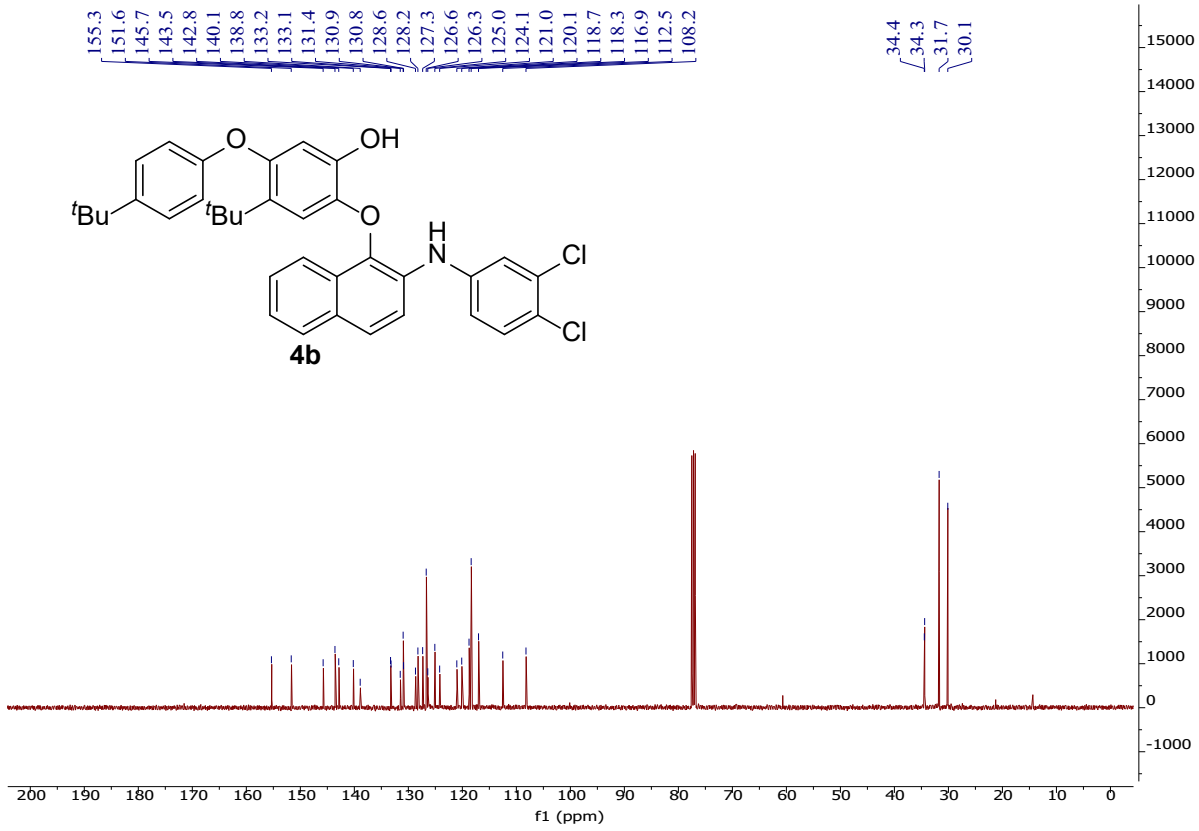
OH
O
tBu
tBu
O
H
N
Cl
Cl
4b
2.00 1.04 1.02 2.03 2.03 0.99 1.04 3.03 0.97 0.98 1.00 0.93 9.06 9.07
f1 (ppm)


155.3 151.6 145.7 143.5 142.8 140.1 138.8 133.2 133.1 131.4 130.9 130.8 128.6 128.2 127.3 126.6 126.3 125.0 124.1 121.0 120.1 118.7 118.3 116.9 112.5 108.2
34.4 34.3 31.7 30.1
OH
O
tBu
tBu
O
H
N
Cl
Cl
4b
f1 (ppm)