

Supporting Information

Cu^I-Catalyzed Ring-Opening Cross-Coupling of Oxabicyclic Olefin with Organoboron Reagent

Bowen Liu,^a Guochun Peng,^b Yu Zhang,^b Chunhui Liu,^{c,d} Jinbo Zhao*^a

^a Department of Chemistry and Biology, Changchun University of Technology, Changchun,
Jilin 130012, P. R. China

^b Key Laboratory of Functional Molecule Design of Jilin Province, Department of Chemistry,
Northeast Normal University, Changchun Jilin 130024 P. R. China

^c College of Chemical and Materials Engineering, Xuchang University, Xuchang, Henan,
461000, P. R. China;

^d College of Chemistry and Institute of Green Catalysis, Zhengzhou Univeristy, Zhengzhou,
Henan, 450001, P. R. China

Email: zhaojinbo@ccut.edu.cn

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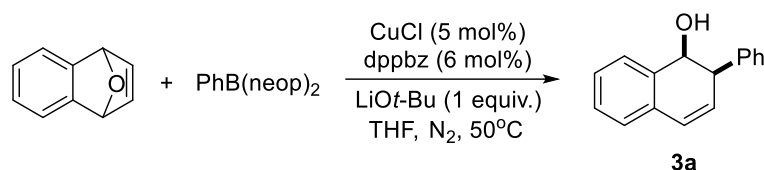
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1. General information.

Unless otherwise noted, all reactions were carried out with distilled and dried solvents under a nitrogen atmosphere. All commercial chemicals were used without further purification. Tetrahydrofuran and toluene were distilled over sodium with benzophenone as indicator. Tertiary butanol was distilled from calcium hydride. All Cu salts, ligands and NaO*t*-Bu were purchased from commercial sources. Oxabicyclic olefins¹⁻⁴ and neopentyl boronic esters^{5,6} were synthesized according to literature. ¹H NMR and ¹³C NMR spectra were recorded on Varian 400 or Bruker 400, 500 or 600 MHz spectrometer at 25°C. Chemical shifts (δ) are expressed in parts per million (ppm) relative to internal standards (0 ppm (TMS) for ¹H NMR and 77.0 ppm (CDCl₃) for ¹³C NMR). High resolution mass spectra were recorded on Bruker microTOF spectrometer. Copies of NMR were processed with MestReNova Software. Enantiomeric excesses (ee) were determined by Agilent 1260 Series HPLC on chiral stationary phases. Flash chromatography was performed on silica gel 60 (particle size 300-400 mesh ASTM, purchased from Taizhou, China).

2. Experimental procedures and Compound Characterization

2.1 General procedure for the Cu-catalyzed ring-opening cross coupling reaction of oxabicyclic olefin with organoboronic esters.

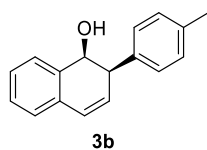


In a N₂ filled glove box, a 25 mL pressure tube was charged successfully with CuCl (5 mol%), dppbz (6 mol%), and anhydrous THF (2 mL). After stirring for 15 min, LiOt-Bu (0.2 mmol, 1 equiv.) **2a** (0.3 mmol, 1.5 equiv.) and **1a** (0.2 mmol) were sequentially added with stirring. The tube was sealed, taken out of the glove box and placed in a 50°C oil bath to react for 24 h, at which time the mixture was added saturated Na₂CO₃ and extracted with DCM (10 mL x 3). The organic phases were combined, and the solvent was removed in vacuo. The residue was subjected to flash chromatography to obtain the product **3a** (26.7 mg, 60% yield) as a yellow oil.

2-Phenyl-1,2-dihydronaphthalen-1-ol (3a): ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.28 – 7.12 (m, 9H), 6.68 (d, *J* = 8.0 Hz, 1H), 6.10 (dd, *J* = 8.0, 4.0 Hz, 1H), 5.17 (d, *J* = 4.0 Hz, 1H), 4.87 (t, *J* = 4.0 Hz, 1H), 3.72 (t, *J* = 4.0 Hz, 1H).

¹³C NMR (126 MHz, DMSO-*d*₆) δ 139.4, 138.1, 133.1, 131.3, 129.8, 128.1, 128.0, 127.7, 126.8, 126.4, 126.2, 70.2, 46.9.

HRMS (ESI-TOF) (*m/z*): Calcd for C₁₆H₁₄ONa ([M+Na]⁺), 245.0937, found 245.0943.

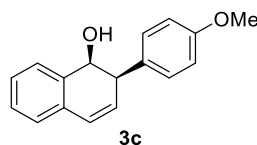


2-(*p*-Tolyl)-1,2-dihydronaphthalen-1-ol (3b): following the general procedure, the reaction of **1a** (0.2 mmol) and 5,5-dimethyl-2-(*p*-tolyl)-1,3,2-dioxaborinane (61.2 mg, 0.3 mmol) afforded the product **3b** (26.0 mg, 55% yield) as a colorless oil.

¹H NMR (600 MHz, DMSO-*d*₆) δ 7.30 – 7.13 (m, 4H), 7.00 (q, *J* = 8.1 Hz, 4H), 6.67 (d, *J* = 9.6 Hz, 1H), 6.08 (dd, *J* = 9.6, 4.7 Hz, 1H), 5.10 (d, *J* = 5.4 Hz, 1H), 4.85 (t, *J* = 5.9 Hz, 1H), 3.67 (t, *J* = 5.1 Hz, 1H), 2.22 (s, 3H).

¹³C NMR (151 MHz, DMSO-*d*₆) δ 137.66, 135.63, 135.20, 132.66, 130.95, 129.17, 128.22, 127.39, 127.34, 127.16, 125.79, 125.59, 69.71, 45.96, 20.61.

HRMS (ESI-TOF) (*m/z*): Calcd for C₁₆H₁₆ONa ([M+Na]⁺), 259.1093, found 263.1083.



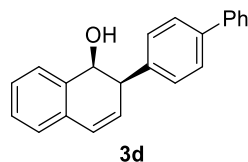
2-(4-Methoxyphenyl)-1,2-dihydronaphthalen-1-ol (3c): following the general procedure, the reaction of **1a** (0.2 mmol) and 2-(4-methoxyphenyl)-5,5-dimethyl-1,3,2-dioxaborinane (66.0 mg, 0.3 mmol) afforded the product **3c** (28.2 mg, 56% yield) as a colorless oil.

¹H NMR (500 MHz, DMSO-*d*₆) δ 7.29 – 7.25 (m, 1H), 7.21 (m, 2H), 7.15 (dd, *J* = 5.0 Hz, 1H), 7.03 (d, *J* = 10.0 Hz, 2H), 6.77 – 6.74 (m, 2H), 6.67 – 6.63 (m, 1H), 6.07 (dd, *J* = 10.0, 5.0 Hz, 1H), 5.10

(d, $J = 5.0$ Hz, 1H), 4.84 (t, $J = 10.0, 45.0$ Hz, 1H), 3.68 – 3.63 (m, 4H).

^{13}C NMR (126 MHz, DMSO- d_6) δ 158.4, 138.2, 133.2, 131.6, 130.9, 130.7, 127.9, 127.7, 127.6, 126.2, 126.1, 113.6, 70.2, 55.4, 46.0.

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{16}\text{H}_{16}\text{O}_2\text{Na}$ ($[\text{M}+\text{Na}]^+$), 275.1043, found 275.1050.

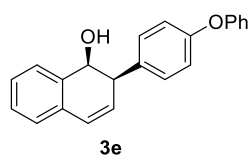


2-([1,1'-Biphenyl]-4-yl)-1,2-dihydronaphthalen-1-ol (3d): following the general procedure, the reaction of **1a** (0.2 mmol) and 2-([1,1'-biphenyl]-4-yl)-5,5-dimethyl-1,3,2-dioxaborinane (79.8 mg, 0.3 mmol) afforded the product **3d** (29.8 mg, 50% yield) as a colorless oil.

^1H NMR (400 MHz, DMSO- d_6) δ 7.63 – 7.58 (m, 2H), 7.52 – 7.46 (m, 2H), 7.43 (m, 2H), 7.36 – 7.29 (m, 2H), 7.27 – 7.17 (m, 5H), 6.72 (dd, $J = 8.0, 4.0$ Hz, 1H), 6.13 (dd, $J = 8.0, 4.0$ Hz, 1H), 5.25 (d, $J = 4.0$ Hz, 1H), 4.94 (t, $J = 4.0$ Hz, 1H), 3.78 (t, $J = 4.0$ Hz, 1H).

^{13}C NMR (126 MHz, DMSO- d_6) δ 140.6, 138.8, 138.6, 138.1, 133.1, 131.1, 130.4, 129.3, 128.0, 127.9, 127.7, 127.6, 127.0, 126.5, 126.3, 126.2, 70.2, 46.5.

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{22}\text{H}_{18}\text{ONa}$ ($[\text{M}+\text{Na}]^+$), 321.1250, found 321.1248.

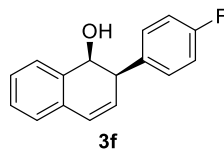


2-(4-Phenoxyphenyl)-1,2-dihydronaphthalen-1-ol (3e): following the general procedure, the reaction of **1a** (0.2 mmol) and 5,5-dimethyl-2-(4-phenoxyphenyl)-1,3,2-dioxaborinane (86.4 mg, 0.3 mmol) afforded the product **3e** (34.5 mg, 55% yield) as a colorless oil.

^1H NMR (500 MHz, DMSO- d_6) δ 7.38 – 7.29 (m, 3H), 7.22 (s, 2H), 7.15 (m, 3H), 7.10 (m, 1H), 6.95 (d, $J = 10.0$ Hz, 2H), 6.85 (d, $J = 5.0$ Hz, 2H), 6.68 (d, $J = 5.0$ Hz, 1H), 6.09 (dd, $J = 10.0, 5.0$ Hz, 1H), 5.17 (s, 1H), 4.87 (d, $J = 10.0$ Hz, 1H), 3.74 (s, 1H).

^{13}C NMR (126 MHz, DMSO- d_6) δ 157.4, 155.6, 138.0, 134.5, 133.1, 131.3, 130.4, 128.0, 127.9, 127.7, 126.4, 126.2, 123.6, 118.8, 118.5, 70.1, 46.1.

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{22}\text{H}_{18}\text{O}_2\text{Na}$ ($[\text{M}+\text{Na}]^+$), 337.1143, found 337.1139.



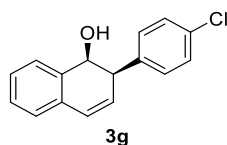
2-(4-Fluorophenyl)-1,2-dihydronaphthalen-1-ol (3f): following the general procedure, the reaction of **1a** (0.2 mmol) and 2-(4-fluorophenyl)-5,5-dimethyl-1,3,2-dioxaborinane (62.4 mg, 0.3 mmol) afforded the product **3f** (25.0 mg, 52% yield) as a white solid. mp 85 – 86 °C.

^1H NMR (400 MHz, Acetone- d_6) δ 7.35 (d, $J = 6.9$ Hz, 1H), 7.20 (dd, $J = 19.3, 8.4$ Hz, 4H), 6.97 (t, $J = 8.2$ Hz, 2H), 6.71 (d, $J = 9.4$ Hz, 1H), 6.10 (dd, $J = 9.7, 4.3$ Hz, 1H), 4.97 (t, $J = 6.2$ Hz, 1H), 4.02 (d, $J = 6.3$ Hz, 1H), 3.82 (t, $J = 5.3$ Hz, 1H).

^{13}C NMR (101 MHz, acetone- d_6) δ 162.7 (d, $^1J_{\text{C-F}} = 243.0$ Hz), 138.3, 135.8 (d, $^4J_{\text{C-F}} = 2.9$ Hz), 133.8, 132.1 (d, $^3J_{\text{C-F}} = 7.9$ Hz), 131.3, 128.7, 128.5, 128.4, 127.1, 126.8, 115.2 (d, $^2J_{\text{C-F}} = 21.2$ Hz);

^{19}F NMR (376 MHz, acetone- d_6) δ -118.51.

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{16}\text{H}_{13}\text{FONa}$ ($[\text{M}+\text{Na}]^+$), 263.0843, found 263.0849.

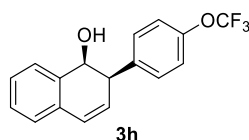


2-(4-Chlorophenyl)-1,2-dihydronaphthalen-1-ol (3g): following the general procedure, the reaction of **1a** (0,2 mmol) and 2-(4-chlorophenyl)-5,5-dimethyl-1,3,2-dioxaborinane (67.3 mg, 0.3 mmol) afforded the product **3g** (20.0 mg, 39% yield) as a white solid. mp 113 – 114 °C.

^1H NMR (600 MHz, DMSO- d_6) δ 7.29 – 7.24 (m, 3H), 7.22 (m, 2H), 7.19 – 7.13 (m, 3H), 6.70 (dd, J = 12.0, 6.0 Hz, 1H), 6.08 (dd, J = 12.0, 6.0 Hz, 1H), 5.21 (d, J = 6.0 Hz, 1H), 4.87 (t, J = 6.0 Hz, 1H), 3.77 – 3.71 (m, 1H).

^{13}C NMR (151 MHz, DMSO- d_6) δ 138.3, 137.8, 132.9, 131.5, 131.5, 130.7, 128.2, 128.0, 128.0, 127.8, 126.3, 126.2, 69.9, 46.0.

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{16}\text{H}_{13}\text{ClONa}$ ($[\text{M}+\text{Na}]^+$), 279.0843, found 279.0845.



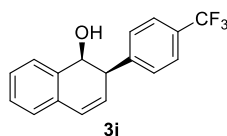
2-(4-(Trifluoromethoxy)phenyl)-1,2-dihydronaphthalen-1-ol (3h): following the general procedure, the reaction of **1a** (0,2 mmol) and 5,5-dimethyl-2-(4-(trifluoromethoxy)phenyl)-1,3,2-dioxaborinane (82.2 mg, 0.3 mmol) afforded the product **3h** (28.8 mg, 47% yield) as a yellow oil.

^1H NMR (400 MHz, Acetone- d_6) δ 7.35 (d, J = 6.9 Hz, 1H), 7.20 (dd, J = 19.3, 8.4 Hz, 4H), 6.97 (t, J = 8.2 Hz, 2H), 6.71 (d, J = 9.4 Hz, 1H), 6.10 (dd, J = 9.7, 4.3 Hz, 1H), 4.97 (t, J = 6.2 Hz, 1H), 4.02 (d, J = 6.3 Hz, 1H), 3.82 (t, J = 5.3 Hz, 1H).

^{13}C NMR (101 MHz, Acetone- d_6) δ 148.74, 139.47, 138.24, 133.75, 132.05, 130.87, 128.98, 128.63, 128.49, 127.14, 126.90, 121.50 (q, $^1J_{\text{C-F}}$ = 255.2 Hz, CF_3), 121.19, 71.33, 47.38.

^{19}F NMR (376 MHz, Acetone- d_6) δ -58.539;

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{17}\text{H}_{13}\text{F}_3\text{O}_2\text{Na}$ ($[\text{M}+\text{Na}]^+$), 329.2843, found 263.0847.



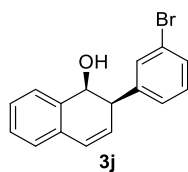
2-(4-(Trifluoromethyl)phenyl)-1,2-dihydronaphthalen-1-ol (3i): following the general procedure, the reaction of **1a** (0,2 mmol) and 5,5-dimethyl-2-(4-(trifluoromethyl)phenyl)-1,3,2-dioxaborinane (77.4 mg, 0.3 mmol) afforded the product **3i** (23.8 mg, 41% yield) as a white solid. mp 112–114 °C.

^1H NMR (400 MHz, Acetone- d_6) δ 7.35 (d, J = 6.9 Hz, 1H), 7.20 (dd, J = 19.3, 8.4 Hz, 4H), 6.97 (t, J = 8.2 Hz, 2H), 6.71 (d, J = 9.4 Hz, 1H), 6.10 (dd, J = 9.7, 4.3 Hz, 1H), 4.97 (t, J = 6.2 Hz, 1H), 4.02 (d, J = 6.3 Hz, 1H), 3.82 (t, J = 5.3 Hz, 1H).

^{13}C NMR (151 MHz, Acetone- d_6) δ 145.00, 138.13, 133.70, 131.09, 130.38, 129.20, 129.05 (q, $^2J_{\text{C-F}}$ = 32.3 Hz), 128.66, 128.53, 127.14, 126.94, 125.58 (q, $^1J_{\text{C-F}}$ = 270.7 Hz), 125.38 (q, $^3J_{\text{C-F}}$ = 3.9 Hz), 71.30, 47.87.

^{19}F NMR (376 MHz, Acetone- d_6) δ -62.78.

HRMS (ESI-TOF) (m/z): Calcd for C₁₇H₁₃F₃ONa ([M+Na]⁺), 313.2844, found 313.2849.

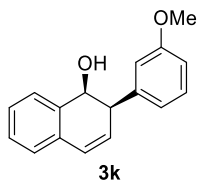


2-(3-Bromophenyl)-1,2-dihydronaphthalen-1-ol (3j): following the general procedure, the reaction of **1a** (0,2 mmol) and 2-(3-bromophenyl)-5,5-dimethyl-1,3,2-dioxaborinane (80.7 mg, 0.3 mmol) afforded the product **3j** (22.9 mg, 38% yield) as a colorless oil.

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.35 (m, 2H), 7.29 (d, 1H), 7.23 (m, 2H), 7.19 – 7.12 (m, 3H), 6.71 (dd, *J* = 8.0, 4.0 Hz, 1H), 6.08 (dd, *J* = 8.0, 4.0 Hz, 1H), 5.29 (d, *J* = 4.0 Hz, 1H), 4.87 (t, *J* = 4.0 Hz, 1H), 3.78 – 3.73 (m, 1H).

¹³C NMR (151 MHz, DMSO-*d*₆) δ 142.4, 137.7, 132.9, 132.5, 130.4, 130.2, 129.6, 128.8, 128.4, 128.1, 127.8, 126.4, 126.2, 121.5, 69.9, 46.3.

HRMS (ESI-TOF) (m/z): Calcd for C₁₆H₁₃BrONa ([M+Na]⁺), 323.0042, found 323.0036.

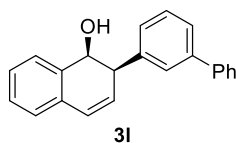


2-(3-Methoxyphenyl)-1,2-dihydronaphthalen-1-ol (3k): following the general procedure, the reaction of **1a** (0,2 mmol) and 2-(3-methoxyphenyl)-5,5-dimethyl-1,3,2-dioxaborinane (66.0 mg, 0.3 mmol) afforded the product **3k** (25.2 mg, 50% yield) as a colorless oil.

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.31 – 7.28 (m, 1H), 7.25 – 7.20 (m, 2H), 7.17 (m, 1H), 7.11 (m, 1H), 6.75 – 6.71 (m, 3H), 6.67 (dd, *J* = 8.0, 4.0 Hz, 1H), 6.09 (dd, *J* = 8.0, 4.0 Hz, 1H), 5.14 (d, *J* = 4.0 Hz, 1H), 4.88 (t, *J* = 4.0 Hz, 1H), 3.73 – 3.67 (m, 1H), 3.65 (s, 3H).

¹³C NMR (126 MHz, DMSO-*d*₆) δ 159.2, 141.0, 138.1, 133.1, 131.2, 129.0, 128.0, 127.9, 127.7, 126.3, 126.1, 122.1, 115.8, 111.9, 70.2, 55.2, 46.8.

HRMS (ESI-TOF) (m/z): Calcd for C₁₇H₁₆O₂Na ([M+Na]⁺), 275.1043, found 275.1049.

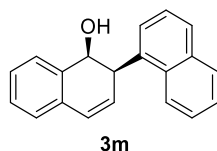


2-([1,1'-Biphenyl]-3-yl)-1,2-dihydronaphthalen-1-ol (3l): following the general procedure, the reaction of **1a** (0,2 mmol) and 2-([1,1'-biphenyl]-3-yl)-5,5-dimethyl-1,3,2-dioxaborinane (67.8 mg, 0.3 mmol) afforded the product **3l** (28.0 mg, 47% yield) as a colorless oil.

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.55 – 7.50 (m, 2H), 7.47 – 7.40 (m, 4H), 7.35 – 7.18 (m, 6H), 7.13 (s, 1H), 6.72 (dd, *J* = 8.0, 4.0 Hz, 1H), 6.17 (dd, *J* = 8.0, 4.0 Hz, 1H), 5.24 (d, *J* = 4.0 Hz, 1H), 4.93 (t, *J* = 4.0 Hz, 1H), 3.84 – 3.80 (m, 1H).

¹³C NMR (126 MHz, DMSO-*d*₆) δ 141.0, 140.1, 140.1, 138.1, 133.2, 131.2, 129.4, 128.9, 128.8, 128.5, 128.2, 128.0, 127.8, 127.8, 127.1, 126.5, 126.2, 125.3, 70.3, 46.9.

HRMS (ESI-TOF) (m/z): Calcd for C₂₂H₁₈ONa ([M+Na]⁺), 321.1250, found 321.1245.

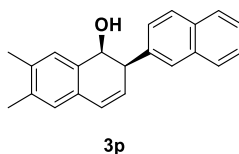


1',2'-Dihydro-[1,2'-binaphthalen]-1'-ol (3m): following the general procedure, the reaction of **1a** (0,2 mmol) and 5,5-dimethyl-2-(naphthalen-1-yl)-1,3,2-dioxaborinane (72.0 mg, 0.3 mmol) afforded the product **3m** (31.0 mg, 57% yield) as a colorless oil.

¹H NMR (600 MHz, DMSO-*d*₆) δ 8.30 (d, *J* = 12.0 Hz, 1H), 7.95 – 7.91 (m, 1H), 7.82 – 7.78 (m, 1H), 7.53 (m, 2H), 7.41 – 7.37 (m, 2H), 7.36 – 7.22 (m, 4H), 6.77 (dd, *J* = 12.0, 6.0 Hz, 1H), 6.20 (dd, *J* = 12.0, 6.0 Hz, 1H), 4.99 – 4.93 (m, 2H), 4.68 (s, 1H).

¹³C NMR (151 MHz, DMSO-*d*₆) δ 137.8, 136.2, 133.9, 133.0, 132.4, 131.8, 129.0, 128.1, 127.9, 127.8, 127.4, 127.3, 127.2, 126.4, 126.2, 125.7, 125.6, 124.5, 69.6, 42.2.

HRMS (ESI-TOF) (*m/z*): Calcd for C₂₀H₁₆ONa ([M+Na]⁺), 295.1250, found 295.1246.

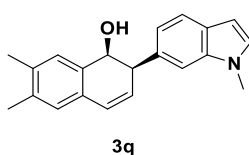


6,7-Dimethyl-1,2-dihydro-[2,2'-binaphthalen]-1-ol (3p): following the general procedure, the reaction of 6,7-dimethyl-1,4-dihydro-1,4-epoxynaphthalene (34.4 mg, 0,2 mmol) and 5,5-dimethyl-2-(naphthalen-2-yl)-1,3,2- dioxaborinane (72.0 mg, 0.3 mmol) afforded the product **3p** (38.7 mg, 64% yield) as a yellow solid.mp 110 – 112 °C.

¹H NMR (400 MHz, Acetone-*d*₆) δ 7.37 (d, *J* = 8.1 Hz, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 7.11 (s, 1H), 6.94 (s, 1H), 6.64 (d, *J* = 9.5 Hz, 1H), 5.99 (dd, *J* = 9.5, 4.3 Hz, 1H), 4.90 (t, *J* = 5.5 Hz, 1H), 3.95 (d, *J* = 6.2 Hz, 1H), 3.75 (s, 1H), 2.22 (d, *J* = 7.9 Hz, 6H).

¹³C NMR (101 MHz, Acetone-*d*₆) δ 139.71, 136.59, 136.17, 135.66, 132.50, 131.55, 131.39, 129.62, 128.85, 128.60, 128.25, 120.73, 71.20, 47.70, 19.70, 19.43.

HRMS (ESI-TOF) (*m/z*): Calcd for C₂₂H₂₀ONa ([M+Na]⁺), 323.1408, found 323.1406.

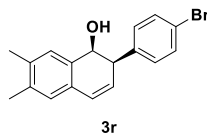


6,7-Dimethyl-2-(1-methyl-1H-indol-6-yl)-1,2-dihydronaphthalen-1-ol (3q): following the general procedure, the reaction of 6,7-dimethyl-1,4-dihydro-1,4-epoxynaphthalene (34.4 mg, 0,2 mmol) and 5-(5,5-dimethyl-1,3,2-dioxaborinan-2-yl)-1-methyl-1H-indole (72.9 mg, 0.3 mmol) afforded the product **3q** (34.0 mg, 56% yield) as a yellow solid.mp 97 – 99 °C.

¹H NMR (400 MHz, Acetone-*d*₆) δ 7.79 (ddd, *J* = 25.2, 13.7, 7.4 Hz, 4H), 7.43 (dd, *J* = 10.0, 6.2 Hz, 3H), 7.13 (s, 1H), 6.99 (s, 1H), 6.70 (d, *J* = 9.5 Hz, 1H), 6.13 (dd, *J* = 9.5, 4.1 Hz, 1H), 4.97 (d, *J* = 4.6 Hz, 1H), 3.95 (s, 1H), 3.79 (d, *J* = 6.0 Hz, 1H), 2.23 (d, *J* = 14.3 Hz, 6H).

¹³C NMR (101 MHz, Acetone-*d*₆) δ 137.33, 135.61, 135.33, 135.06, 133.53, 132.70, 130.72, 129.21, 128.20, 127.99, 127.95, 127.86, 127.64, 127.41, 127.15, 125.62, 125.24, 70.71, 47.69, 18.83, 18.60.

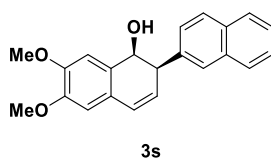
HRMS (ESI-TOF) (*m/z*): Calcd for C₂₁H₂₁NONa ([M+Na]⁺), 326.1516, found 326.1515.



2-(4-Bromophenyl)-6,7-dimethyl-1,2-dihydronaphthalen-1-ol (3r): following the general procedure, the reaction of 6,7-dimethyl-1,4-dihydro-1,4-epoxynaphthalene (34.4 mg, 0,2 mmol) and 2-(4-bromophenyl)-5,5-dimethyl-1,3,2-dioxaborinane (80.7 mg, 0.3 mmol) afforded the product **3r** (41.1 mg, 62% yield) as a white solid. mp 132 – 134 °C.

$^1\text{H NMR}$ (400 MHz, Acetone- d_6) δ 7.43 (s, 1H), 7.29 – 7.01 (m, 4H), 6.95 (s, 1H), 6.63 (d, $J = 9.5$ Hz, 1H), 6.33 (d, $J = 2.5$ Hz, 1H), 6.09 (dd, $J = 9.5, 4.2$ Hz, 1H), 4.90 (s, 1H), 3.84 (s, 1H), 3.77 (s, 3H), 2.25 (t, $J = 16.6$ Hz, 6H).

$^{13}\text{C NMR}$ (101 MHz, Acetone- d_6) δ 136.23, 135.36, 135.31, 135.08, 130.91, 130.49, 129.05, 128.95, 128.66, 127.88, 127.26, 127.21, 123.17, 121.21, 108.75, 100.36, 71.01, 47.68, 31.97, 18.84, 18.61. HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{18}\text{H}_{17}\text{BrONa}$ ($[\text{M}+\text{Na}]^+$), 351.0355, found 351.0351.

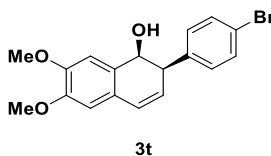


6,7-Dimethoxy-1,2-dihydro-[2,2'-binaphthalen]-1-ol (3s): following the general procedure, the reaction of 6,7-dimethoxy-1,4-dihydro-1,4-epoxynaphthalene (34.4 mg, 0,2 mmol) and 5,5-dimethyl-2-(naphthalen-2-yl)-1,3,2-dioxaborinane (72.0 mg, 0.3 mmol) afforded the product **3s** (34.3 mg, 51% yield) as a yellow oil.

$^1\text{H NMR}$ (400 MHz, Acetone- d_6) δ 7.89 – 7.71 (m, 4H), 7.43 (dd, $J = 9.6, 6.1$ Hz, 3H), 7.02 (s, 1H), 6.88 (s, 1H), 6.69 (d, $J = 9.4$ Hz, 1H), 6.09 (dd, $J = 9.5, 4.0$ Hz, 1H), 4.98 (t, $J = 5.9$ Hz, 1H), 3.94 (s, 1H), 3.84 (s, 3H), 3.80 (s, 1H), 3.77 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, Acetone- d_6) δ 149.90, 149.70, 138.26, 137.33, 134.43, 133.59, 131.74, 131.24, 129.08, 129.03, 128.88, 128.52, 128.29, 128.05, 126.80, 126.51, 126.13, 112.00, 111.51, 71.68, 56.31, 56.17, 48.45.

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{22}\text{H}_{20}\text{O}_3\text{Na}$ ($[\text{M}+\text{Na}]^+$), 355.1305, found 355.1313.

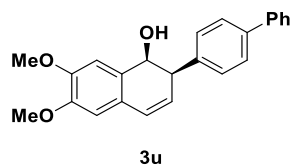


2-(4-Bromophenyl)-6,7-dimethoxy-1,2-dihydronaphthalen-1-ol (3t): following the general procedure, the reaction of 6,7-dimethoxy-1,4-dihydro-1,4-epoxynaphthalene (34.4 mg, 0,2 mmol) and 2-(4-bromophenyl)-5,5-dimethyl-1,3,2-dioxaborinane (80.7 mg, 0.3 mmol) afforded the product **3t** (40.0 mg, 55% yield) as a white solid. mp 122 – 124 °C.

$^1\text{H NMR}$ (400 MHz, Acetone- d_6) δ 7.39 (d, $J = 8.2$ Hz, 2H), 7.19 (d, $J = 8.2$ Hz, 2H), 6.99 (s, 1H), 6.83 (s, 1H), 6.63 (d, $J = 9.4$ Hz, 1H), 5.96 (dd, $J = 9.5, 4.3$ Hz, 1H), 4.90 (t, $J = 6.0$ Hz, 1H), 3.91 (d, $J = 6.4$ Hz, 1H), 3.81 (s, 3H), 3.77 (s, 3H), 3.75 (d, $J = 3.1$ Hz, 1H).

$^{13}\text{C NMR}$ (101 MHz, Acetone- d_6) δ 149.97, 149.66, 139.83, 132.53, 131.59, 130.96, 128.64, 128.58, 126.58, 120.74, 111.81, 111.49, 71.30, 56.29, 56.18, 47.60.

HRMS (ESI-TOF) (m/z): Calcd for C₂₂H₁₇BrO₃Na ([M+Na]⁺), 383.0253, found 383.0244.

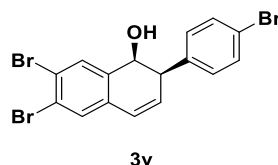


2-([1,1'-Biphenyl]-4-yl)-6,7-dimethoxy-1,2-dihydronaphthalen-1-ol (3u) following the general procedure, the reaction of 6,7-dimethoxy-1,4-dihydro-1,4-epoxynaphthalene (34.4 mg, 0,2 mmol) and 2-([1,1'-biphenyl]-4-yl)-5,5-dimethyl-1,3,2-dioxaborinane (79.8 mg, 0.3 mmol) afforded the product **3u** (35.2 mg, 49% yield) as a yellow oil.

¹H NMR (400 MHz, Acetone-*d*₆) δ 7.63 (d, *J* = 7.4 Hz, 2H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.33 (dd, *J* = 13.4, 7.6 Hz, 3H), 7.03 (s, 1H), 6.85 (s, 1H), 6.65 (d, *J* = 9.5 Hz, 1H), 6.03 (dd, *J* = 9.5, 4.3 Hz, 1H), 4.96 (t, *J* = 6.0 Hz, 1H), 3.80 (d, *J* = 18.7 Hz, 8H).

¹³C NMR (101 MHz, Acetone-*d*₆) δ 149.92, 149.64, 141.81, 140.04, 139.60, 131.25, 130.99, 129.66, 129.13, 128.40, 127.92, 127.57, 127.18, 126.76, 111.86, 111.48, 71.61, 56.31, 56.19, 47.95.

HRMS (ESI-TOF) (m/z): Calcd for C₂₄H₂₂O₃Na ([M+Na]⁺), 381.1461, found 381.1452.

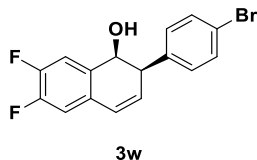


6,7-Dibromo-2-(4-bromophenyl)-1,2-dihydronaphthalen-1-ol (3v) following the general procedure, the reaction of 6,7-dibromo-1,4-dihydro-1,4-epoxynaphthalene (63.9 mg, 0,2 mmol) and 2-(4-bromophenyl)-5,5-dimethyl-1,3,2-dioxaborinane (80.7 mg, 0.3 mmol) afforded the product **3v** (9.1 mg, 10% yield) as a yellow oil.

¹H NMR (400 MHz, Acetone-*d*₆) δ 7.71 (d, *J* = 2.0 Hz, 1H), 7.52 (s, 1H), 7.41 (d, *J* = 8.1 Hz, 2H), 7.14 (d, *J* = 8.1 Hz, 2H), 6.98 (d, *J* = 9.9 Hz, 1H), 6.37 (dd, *J* = 9.9, 5.0 Hz, 1H), 5.06 (d, *J* = 6.1 Hz, 1H), 4.64 (d, *J* = 6.0 Hz, 1H), 3.86 (t, *J* = 5.9 Hz, 1H).

¹³C NMR (101 MHz, Acetone-*d*₆) δ 142.74, 137.59, 134.29, 134.17, 132.40, 132.08, 131.83, 129.53, 126.35, 122.14, 121.91, 121.28, 71.00, 46.45.

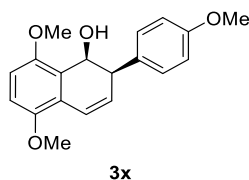
HRMS (ESI-TOF) (m/z): Calcd for C₁₆H₁₁Br₃ONa ([M+Na]⁺), 480.7361, found 480.7359.



2-(4-Bromophenyl)-6,7-difluoro-1,2-dihydronaphthalen-1-ol (3w) following the general procedure, the reaction of 6,7-difluoro-1,4-dihydro-1,4-epoxynaphthalene (36.0 mg, 0,2 mmol) and 2-(4-bromophenyl)-5,5-dimethyl-1,3,2-dioxaborinane (80.7 mg, 0.3 mmol) afforded the product **3w** (6.8 mg, 10% yield) as a yellow oil.

¹H NMR (400 MHz, Acetone-*d*₆) δ 7.42 (d, *J* = 8.1 Hz, 2H), 7.25 – 7.09 (m, 4H), 6.92 (dd, *J* = 9.8, 1.9 Hz, 1H), 6.31 (dd, *J* = 9.8, 4.4 Hz, 1H), 4.97 (t, *J* = 6.0 Hz, 1H), 4.36 (d, *J* = 6.1 Hz, 1H), 3.88 (d, *J* = 5.7 Hz, 1H).

^{13}C NMR (101 MHz, Acetone- d_6) δ 150.66 (dd, $J_{\text{C-F}} = 245.4$ Hz, 13.1 Hz), 146.55 (dd, $J_{\text{C-F}} = 248.5$ Hz, 13.6 Hz), 138.57, 135.36, 135.34, 133.75, 132.45, 131.78, 123.42-123.22 (m), 121.11, 119.80 (dd, $J_{\text{C-F}} = 4.4$ Hz, 3.3 Hz), 116.17 (d, $J_{\text{C-F}} = 17.4$ Hz), 70.38 (d, $J_{\text{C-F}} = 3.0$ Hz), 47.16.
 ^{19}F NMR (376 MHz, Acetone- d_6) δ -142.09 (d, $J = 19.9$ Hz), -149.44 (d, $J = 19.9$ Hz).
HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{16}\text{H}_{11}\text{BrF}_2\text{ONa}$ ($[\text{M}+\text{Na}]^+$), 359.3820, found 359.3826.



5,8-Dimethoxy-2-(4-methoxyphenyl)-1,2-dihydronaphthalen-1-ol (3x) following the general procedure, the reaction of 5,8-dimethoxy-1,4-dihydro-1,4-epoxynaphthalene (40.8 mg, 0.2 mmol) and 2-(4-methoxyphenyl)-5,5-dimethyl-1,3,2-dioxaborinane (66.0 mg, 0.3 mmol) afforded the product **3x** (22.9 mg, 36% yield) as a yellow oil.

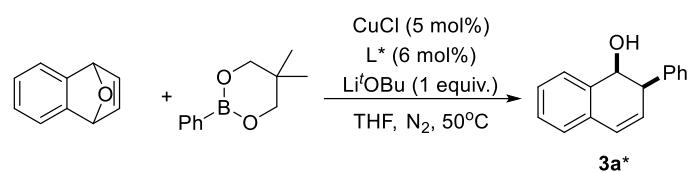
^1H NMR (400 MHz, Acetone- d_6) δ 7.41 (d, $J = 7.3$ Hz, 1H), 7.25 (t, $J = 7.7$ Hz, 1H), 7.01 (dd, $J = 9.8, 5.4$ Hz, 2H), 6.95 (t, $J = 7.5$ Hz, 1H), 6.92 – 6.84 (m, 2H), 6.02 (d, $J = 9.8$ Hz, 1H), 5.06 (t, $J = 5.0$ Hz, 1H), 4.16 (s, 1H), 3.85 (s, 3H), 3.82 (s, 3H), 3.77 (s, 3H).

^{13}C NMR (101 MHz, Acetone- d_6) δ 158.06, 151.81, 150.41, 131.90, 130.84, 130.20, 128.42, 126.72, 123.26, 122.42, 121.07, 111.82, 111.68, 111.04, 62.32, 56.44, 56.39, 55.87, 41.19.

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{19}\text{H}_{20}\text{O}_4\text{Na}$ ($[\text{M}+\text{Na}]^+$), 335.0443, found 335.0449.

2.2 Preliminary asymmetric studies with chiral ligands.

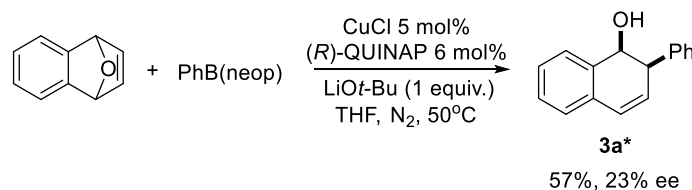
Table S1. Preliminary asymmetric studies with chiral ligands.



Entry	Ligand	Yield/% ^a	ee/% ^b
1	(<i>R</i>)-BINAP	0	0
2	(<i>R,R</i>)-Me-DuPhos	43	20
3	(<i>R</i>)-SegPhos	52	14
4	(<i>R</i>)-tol-BINAP	45	15
5	(<i>R,R</i>)- <i>i</i> -Pr-DuPhos	0	0
6	(<i>R,S</i>)-N-PINAP	0	nd
7	(<i>R,R</i>)- <i>t</i> -Bu-BOX	28	2
8	(<i>R,R</i>)-Ph-BOX	0	0
9	(<i>R</i>)-QUINAP	57	23

^a Isolated yields after column chromatography. ^b Determined by HPLC on a chiral stationary phase.

The procedure for the asymmetric catalysis.



In a N₂ filled glove box, a 25 mL pressure tube was charged successfully with CuCl (5 mol%), (*R*)-Quinap (mg, 6 mol%), and anhydrous THF (2 mL). After stirring for 15 min, LiOt-Bu (1 equiv.) **2a** (1.5 equiv.) and **1a** (1.0 equiv.) were sequentially added with stirring. The tube was sealed, taken out of the glove box and placed in a 50°C oil bath to react for 24 h, at which time the mixture was added saturated Na₂CO₃ and extracted with DCM (10 mL x 3). The organic phases were combined, and the solvent was removed in vacuo. The residue was subjected to flash chromatography to obtain the enantio-enriched product **3a*** (25.3 mg, 57% yield, 23% ee) as a yellow oil.

3. Computational Details.

The calculation was performed with Gaussian 16 software package.⁷ Geometry optimizations were performed using b3lyp hybrid functional⁸ with Grimme's DFT-D3(BJ) correction for dispersion effects.⁹ 6-31G(d) basis set was used for C, H, O, B and P atoms, and SDD pseudopotential basis set for Cu, with SMD solvation model in THF. Stationary points were checked with frequency calculation at the same level of theory to obtain thermal corrections for Gibbs free energy and to check if the structures are minima (no imaginary frequencies) or transition states (only one imaginary frequency). Intrinsic reaction coordinate (IRC) calculations were performed to check the transition structures indeed connect the starting material and product structures. Single point energy calculations were calculated with M06 functional¹⁰ with DFT-D3 dispersion correction, using 6-311+G(d,p) basis set for C, H, O, B and P atoms, and SDD pseudopotential basis set for Cu, with SMD solvation model in THF. Structures were drawn and visualized with Chemdraw and Cylview¹¹ softwares.

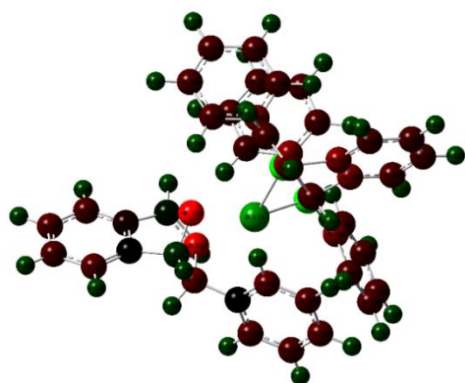
Table S2. Computed single point energies for all starting materials, products, intermediates and transition structures.

Geometry	$E_{\text{sol}}^a/\text{a.u.}$	Correction ^b /a.u.	$G_{\text{sol}}(\text{final})^c/\text{a.u.}$
NBE	-460.8268152	0.12057	-460.7062452
II	-2268.691116	0.465503	-2268.2256129
		Total (NBE+PhCuL)	-2728.9318581
III	-604.8625476	0.242423	-604.6201246
		Total (NBE+PhCuL+ III)	-3333.5519827
Ph-Bneop	-603.3639956	0.207205	-603.1567906
		Total (NBE+PhB)	-1063.863036
IV_a	-2729.538434	0.612034	-2728.9264004
TS₄	-2729.511902	0.61492	-2728.8969819
IV	-2729.584614	0.61772	-2728.9668941
TS₄₅	-2729.532201	0.612385	-2728.9198162
V	-2729.622709	0.615327	-2729.0073819
VII	-3334.452429	0.88531	-3333.567119
TS₇₈	-3334.423291	0.883012	-3333.540279
VIII	-3334.498323	0.886914	-3333.611409
IX	-3334.5165738	0.888176	-3333.6283978
VI	-1064.300798	0.350882	-1063.949916

^a Electronic energy calculated on SMD(THF)-M06-D3/6-311+G(d,p)-Cu(SDD) level of theory.

^b Thermal correction to Gibbs free energy obtained from frequency calculation on SMD(THF)-b3lyp-D3(BJ)/6-31G(d)-Cu(SDD) level of theory. ^c Final Gibbs free energy obtained by adding the first two terms.

(A)



(B)

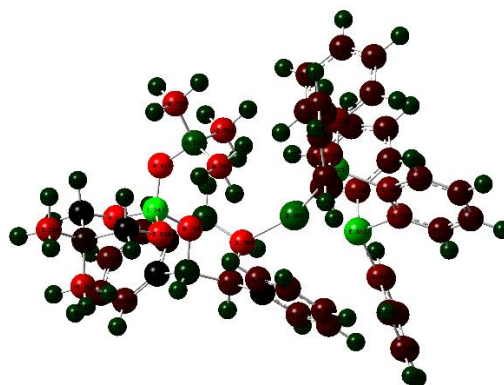
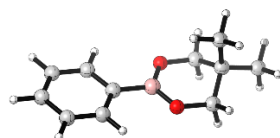


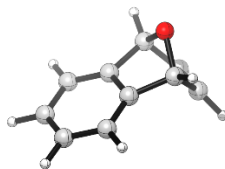
Figure S1. Natural population analysis of **TS₄₅** (A) and **TS₇₈** (B), calculated at SMD(THF)-M06-D3/6-311G(d)-Cu/SDD level of theory.

Structures and Cartesian coordinates of all stationary points and transition structures.



Ph-Bneop

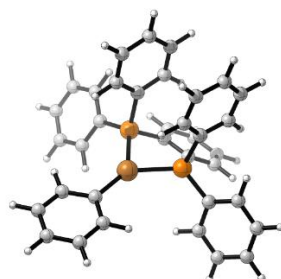
C	3.66173800	1.20932100	-0.10659600	H	-2.31481500	1.30438100	1.55710100
C	2.27463300	1.20454000	0.04085300	H	-2.43075900	-2.14932000	0.00082000
C	1.55425800	-0.00019600	0.11699500	H	-2.31605600	-1.30541100	1.55668800
C	2.27491400	-1.20474100	0.04036700	B	-0.00196200	-0.00019500	0.28074200
C	3.66202900	-1.20914500	-0.10701800	O	-0.65242300	1.20220400	0.34188500
C	4.35823600	0.00019400	-0.18076100	O	-0.65279200	-1.20219100	0.34285400
H	4.20072300	2.15155700	-0.16385600	C	-2.59865200	0.00009900	-1.65239900
H	1.73632900	2.14675100	0.09810200	H	-3.07464900	-0.88651800	-2.08701500
H	1.73689100	-2.14714800	0.09719100	H	-3.07316100	0.88768800	-2.08673400
H	4.20127000	-2.15121700	-0.16452400	H	-1.54815500	-0.00068400	-1.96077000
H	5.43911800	0.00032300	-0.29590200	C	-4.24124000	0.00029800	0.25295600
C	-2.07859300	1.23294100	0.48734600	H	-4.74415500	0.88578500	-0.15316000
C	-2.07899200	-1.23326300	0.48717300	H	-4.74447100	-0.88511400	-0.15296900
C	-2.75595200	-0.00002000	-0.12374300	H	-4.37992900	0.00042800	1.34058600
H	-2.43091300	2.14920200	0.00178600				



NBE

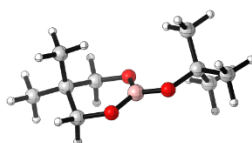
C	0.951984	-1.9863	0.667472	H	-0.772162	-1.489682	2.051494
C	-0.345696,	-1.26346	1.075603	H	-0.772162	-1.489682	-2.051494
C	-0.345696	-1.26346	-1.075603	O	-1.227701	-1.67433,	0.
C	0.951984	-1.9863	-0.667472	H	1.719626	-2.3218	1.354025
C	-0.159768	0.21572	-0.703532	H	1.719626	-2.3218	-1.354025

C	0.003429	1.383562	1.420221	H	0.283188	3.519933	-1.234341
H	0.005582	1.389966	2.507103	C	0.003429	1.383562	-1.420221
C	0.16248	2.583628	0.69633	H	0.005582	1.389966	-2.507103
H	0.283188	3.519933	1.234341	C	-0.159768	0.21572	0.703532
C	0.16248	2.583628	-0.69633				



PhCu(dppbz)

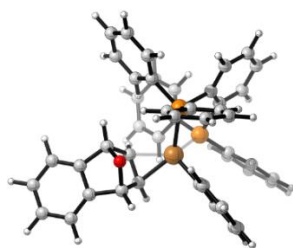
C	-1.09030200	4.04373400	1.15839800	H	6.70257100	0.76111200	-2.55878900
C	0.08571600	3.29607200	0.90745700	C	1.75858800	-1.43243100	1.00489100
C	1.29690000	3.98977700	1.14502100	C	2.22031600	-0.95639100	2.24320700
C	1.34001000	5.31384100	1.59655100	C	1.42072300	-2.78508000	0.87164000
C	0.15223300	6.01088800	1.83240500	C	2.35251100	-1.82411000	3.32598300
C	-1.06843700	5.36861300	1.60903100	H	2.46735500	0.09618700	2.35762600
H	-2.06215800	3.57683000	0.99520300	C	1.53965000	-3.64809400	1.96238400
H	2.24508600	3.48019600	0.97041600	H	1.04966700	-3.16125000	-0.07578000
H	2.29837700	5.80253800	1.76499700	C	2.00633300	-3.17117800	3.18864800
H	0.17745800	7.04006300	2.18347800	H	2.71158600	-1.44669600	4.27936100
H	-2.00182200	5.90018800	1.78748800	H	1.26127800	-4.69242300	1.85368700
C	0.62501500	-1.11282800	-1.65568800	H	2.09319800	-3.84464100	4.03665200
C	-0.78949200	-1.06196200	-1.62759300	C	-1.77469400	-1.45110300	1.04022300
C	1.26908700	-1.80175900	-2.69081400	C	-1.46228900	-1.12652900	2.36796100
C	-1.52357100	-1.69344400	-2.63869700	C	-2.15891900	-2.76268600	0.72349300
C	0.52605100	-2.43182200	-3.69005500	C	-1.53482500	-2.09924000	3.36575100
H	2.35349000	-1.83890200	-2.72037800	H	-1.14191800	-0.11718200	2.61174400
C	-0.86936400	-2.37571500	-3.66544500	C	-2.23942500	-3.73099700	1.72364200
H	-2.60808900	-1.64453400	-2.62709800	H	-2.38151600	-3.02937900	-0.30517200
H	1.03686900	-2.96018800	-4.48997100	C	-1.92528900	-3.40073800	3.04489300
H	-1.44866100	-2.85949500	-4.44675700	H	-1.27561300	-1.84295100	4.38877800
Cu	0.03606100	1.43850700	0.31419500	H	-2.53661100	-4.74505800	1.47098800
P	1.52760300	-0.20493200	-0.33324300	H	-1.97527200	-4.15974200	3.82059200
P	-1.56815100	-0.14813500	-0.22984500	C	-3.24859200	0.23646100	-0.84435700
C	3.20351400	0.05250400	-1.02064900	C	-3.36304200	1.29571500	-1.76091500
C	4.24423000	-0.87424000	-0.86390300	C	-4.40467200	-0.43235000	-0.42165800
C	3.43788900	1.24095900	-1.72918300	C	-4.61033300	1.66218700	-2.26240600
C	5.49964600	-0.61720200	-1.41712600	H	-2.47219800	1.83304200	-2.07757600
H	4.07329000	-1.79221200	-0.30992100	C	-5.65486300	-0.05464100	-0.91796900
C	4.69122800	1.49108800	-2.28788900	H	-4.33301000	-1.24512700	0.29335200
H	2.63766600	1.96956900	-1.83481800	C	-5.76018200	0.98753600	-1.84036700
C	5.72379200	0.56266000	-2.13112800	H	-4.68689000	2.47956300	-2.97399400
H	6.30227800	-1.33860200	-1.29093100	H	-6.54587300	-0.57860300	-0.58305700
H	4.86474400	2.41337400	-2.83516600	H	-6.73367300	1.27867700	-2.22470700



***t*-BuOBneop (III)**

C	-2.51148000	0.11148500	0.07499300	C	-2.09117100	-1.30412400	-0.34018000
C	-1.58202300	1.08363000	-0.65998500	H	-1.77756300	1.04866100	-1.74009900

H	-1.74835400	2.11171700	-0.32064600	C	2.77603000	0.75418600	-1.31134100
H	-2.31377100	-1.46309800	-1.40449000	H	3.68100300	1.37206900	-1.32288600
H	-2.64705800	-2.05421900	0.23338600	H	2.86474500	0.00367700	-2.10512800
B	0.19044000	-0.50782300	-0.19141600	H	1.91662600	1.39287700	-1.52913700
O	1.49540000	-0.84259400	0.01852200	O	-0.70041600	-1.55124000	-0.11982700
C	2.61959700	0.06841300	0.04929600	O	-0.19786500	0.78795800	-0.43852000
C	3.82984300	-0.82211300	0.33683400	C	-2.38397600	0.28995100	1.59581700
H	3.94524500	-1.57648100	-0.44917100	H	-2.67591200	1.30510600	1.88916300
H	4.74703300	-0.22517900	0.38198100	H	-3.03651700	-0.41660200	2.12171600
H	3.70523800	-1.34026000	1.29398300	H	-1.36067100	0.12300400	1.94698600
C	2.43183700	1.08987000	1.17522600	C	-3.95721400	0.36150800	-0.36632200
H	1.56841000	1.73130400	0.98221200	H	-4.64063900	-0.33796200	0.12927600
H	2.27896400	0.57537200	2.13086100	H	-4.27303100	1.37837500	-0.10493700
H	3.32191100	1.72255000	1.26626800	H	-4.07347400	0.23839100	-1.44969100



PhCuL-NBE complex (IV_a)

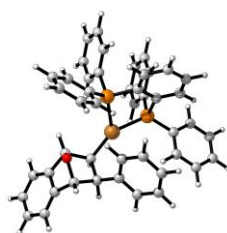
C	-0.17281100	-2.93157000	-2.12523200	C	0.43988300	4.89076300	0.19504400
C	0.28759000	-1.59817800	-2.18274900	H	0.65394800	3.43517200	-1.37422700
C	1.10746700	-1.28939300	-3.29015500	C	1.21270100	4.21163300	2.38117300
C	1.46525700	-2.23595900	-4.25763100	H	2.06300000	2.24240900	2.51820900
C	1.00000600	-3.54987400	-4.15627900	C	0.62851000	5.17033700	1.55201400
C	0.17274000	-3.89233600	-3.08344400	H	-0.01577500	5.63036900	-0.45739300
H	-0.82000200	-3.23966800	-1.30732200	H	1.35997000	4.42056500	3.43722600
H	1.49327600	-0.27675500	-3.40294000	H	0.31855400	6.12867100	1.95893800
H	2.10772600	-1.94831800	-5.08867700	C	-0.96655000	-0.37549800	2.74156200
H	1.27499000	-4.29267900	-4.90178300	C	-1.37834900	-1.13856400	3.84308400
H	-0.20351900	-4.91000200	-2.98965300	C	-1.16874800	1.01329800	2.75843500
C	2.47999300	0.08397600	1.16977700	C	-1.99037500	-0.52182700	4.93592000
C	1.67006800	-0.84969900	1.84551000	H	-1.22539300	-2.21265400	3.84941600
C	3.79978900	0.28901600	1.60207900	C	-1.76687400	1.62939600	3.85728800
C	2.18483000	-1.53980800	2.95298300	H	-0.85185400	1.61068500	1.91097500
C	4.30666500	-0.41472100	2.69198700	C	-2.18433400	0.86156500	4.94718800
H	4.42861000	1.00585300	1.08348800	H	-2.31041000	-1.12367100	5.78214000
C	3.49599900	-1.32903600	3.37204700	H	-1.90931600	2.70655500	3.85770100
H	1.55689800	-2.24920900	3.48333600	H	-2.65858500	1.33807500	5.80058900
H	5.32988700	-0.24640100	3.01561900	C	-0.37084300	-2.87241600	1.36037700
H	3.88549300	-1.87451200	4.22689000	C	0.66462500	-3.79432800	1.15033500
Cu	-0.22865700	-0.22317300	-0.84733400	C	-1.69658100	-3.33576100	1.40874300
P	1.76574600	1.04236200	-0.23397700	C	0.38227600	-5.15464000	1.01633200
P	-0.07342400	-1.07209900	1.29199300	H	1.69135700	-3.45205200	1.07810300
C	3.24658200	1.30452500	-1.28954000	C	-1.97460900	-4.69565600	1.27818800
C	3.79565300	2.56360700	-1.56546900	H	-2.51264300	-2.63165300	1.53854900
C	3.82327400	0.16397700	-1.87593800	C	-0.93553200	-5.60982700	1.08183900
C	4.89845100	2.68060000	-2.41563700	H	1.19509000	-5.85689900	0.85356200
H	3.37067600	3.45437600	-1.11510600	H	-3.00408900	-5.04000800	1.32223800
C	4.92781200	0.28383300	-2.71664400	H	-1.15379600	-6.66860100	0.97463900
H	3.40289700	-0.81673500	-1.67549000	C	-1.77782700	1.25717100	-0.68264100
C	5.46730000	1.54407300	-2.99217400	C	-3.07257700	0.65616800	-0.10515400
H	5.31580700	3.66300900	-2.61963500	C	-2.93373300	-0.17015600	-2.09969200
H	5.36360000	-0.60665300	-3.16123300	C	-1.69439700	0.73166300	-1.96332600
H	6.32534900	1.63757000	-3.65195700	C	-4.13492600	0.77870500	-2.16758400
C	1.42402400	2.68633800	0.50299100	H	-3.16047000	0.56989200	0.97489000
C	0.82276600	3.65413700	-0.32266700	H	-2.88521700	-0.99726500	-2.80424700
C	1.61334300	2.97852900	1.86098900	O	-3.07744500	-0.64837200	-0.73731200

H	-1.36477100	2.19893700	-0.34481700	C	-5.99010100	2.12653600	-2.84628300
H	-1.20165800	1.17826800	-2.81945500	H	-6.69327800	2.44577100	-3.61071700
C	-5.18164500	2.26100100	-0.54950800	C	-5.00135000	1.17416700	-3.16791800
H	-5.25356600	2.68288600	0.44976100	H	-4.93471300	0.76513400	-4.17274300
C	-6.07850300	2.65987600	-1.56173600	C	-4.22392500	1.31840100	-0.86899700
H	-6.85035500	3.39033500	-1.33487100				



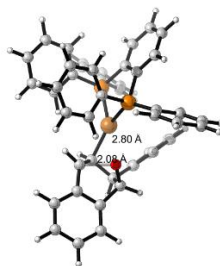
TS₄

C	1.66386400	-0.63686600	-2.78990100	H	-4.18251600	1.58660300	3.80996100
C	1.24071200	-1.49674200	-1.76301100	H	-2.91560200	0.54740200	5.67999900
C	0.72960700	-2.75134600	-2.13139600	C	-0.51367700	2.58415800	1.02621100
C	0.59583000	-3.11890000	-3.47309100	C	-1.21893900	3.79741300	1.01215200
C	0.99492200	-2.23722100	-4.48309900	C	-0.05861300	2.06736200	2.24603500
C	1.53533600	-0.99556300	-4.13551900	C	-1.46449000	4.48004100	2.20239200
H	2.08498200	0.33284000	-2.54033500	H	-1.57971600	4.20583900	0.07290400
H	0.41879900	-3.45196100	-1.35772700	C	-0.30746300	2.75147500	3.43784900
H	0.18027400	-4.09109400	-3.73023100	H	0.46407200	1.11588400	2.25107200
H	0.89651100	-2.51984800	-5.52805200	C	-1.01071900	3.95636300	3.41764800
H	1.85429800	-0.30227500	-4.91115200	H	-2.01380300	5.41739000	2.18414800
C	-2.65704100	0.19535500	-0.74469400	H	0.03884700	2.33579900	4.37963400
C	-1.97714100	1.37788900	-1.11310300	H	-1.21024500	4.48666400	4.34485300
C	-3.97951700	-0.00178600	-1.16361600	C	0.51487100	2.74383900	-1.68662700
C	-2.63877600	2.33519100	-1.89313000	C	0.41467000	2.48639100	-3.06486700
C	-4.62333100	0.95479100	-1.94836300	C	1.32941800	3.79835100	-1.24857700
H	-4.50527000	-0.90726900	-0.87805300	C	1.09868200	3.28160300	-3.98311400
C	-3.95194800	2.12400200	-2.31320400	H	-0.19794800	1.66363400	-3.41911500
H	-2.12167300	3.24324600	-2.18530400	C	2.01752800	4.58865300	-2.17097300
H	-5.64669100	0.78800700	-2.27234800	H	1.42535900	4.00426000	-0.18717000
H	-4.44959100	2.87187100	-2.92414700	C	1.90266200	4.33520000	-3.53919600
Cu	0.45689400	-0.54562300	-0.05603100	H	1.00562100	3.07553700	-5.04593100
P	-1.75738100	-1.02276900	0.30158200	H	2.64196400	5.40464800	-1.81770800
P	-0.25026500	1.58703300	-0.49664100	H	2.43731100	4.95258100	-4.25557000
C	-2.63758900	-2.59594900	-0.02467800	C	1.94808000	-0.93716500	1.26855500
C	-3.30098600	-3.32192800	0.97334400	C	3.04447300	0.13059100	1.44605000
C	-2.57887300	-3.11775000	-1.32897500	C	3.61723800	-0.84391400	-0.40106000
C	-3.89546700	-4.54978200	0.67210200	C	2.32870400	-1.58659800	0.00714100
H	-3.35808600	-2.93060200	1.98377800	C	4.68417100	-1.26975400	0.59829700
C	-3.18112000	-4.33840000	-1.62706200	H	2.80719500	1.02274400	2.02615700
H	-2.06286600	-2.56623400	-2.10855400	H	3.89036200	-0.84103300	-1.45329000
C	-3.83872000	-5.05998400	-0.62583200	O	3.32668000	0.49459500	0.06542100
H	-4.40886800	-5.10290500	1.45388100	H	1.74510800	-1.58721000	2.11777500
H	-3.13324600	-4.72838900	-2.64008400	H	2.33540100	-2.67099200	-0.05082700
H	-4.30387600	-6.01401200	-0.85761300	C	5.06252100	-0.80861000	-2.95261200
C	-2.23344100	-0.54928400	2.00906000	H	4.79507700	-0.31412900	3.88340100
C	-1.51346500	-1.12424300	3.06909800	C	6.17955900	-1.66401700	2.89547900
C	-3.20208300	0.42310700	2.28921300	H	6.78164600	-1.81728200	3.78745800
C	-1.76951800	-0.74369600	4.38538700	C	6.52768800	-2.31316100	1.71036600
H	-0.74052000	-1.85755300	2.85748800	H	7.39617000	-2.96596700	1.68855500
C	-3.44180900	0.81837000	3.60649200	C	5.76724500	-2.12704500	0.53939200
H	-3.75502600	0.88915300	1.48094100	H	6.03570600	-2.64010600	-0.38090600
C	-2.72972000	0.23577500	4.65595700	C	4.32848000	-0.61534100	1.79426600
H	-1.20871800	-1.19813800	5.19747500				



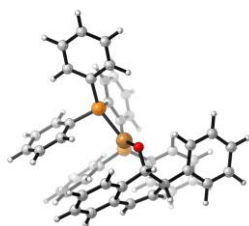
IV

C	1.71081100	-1.30507000	-1.92672100	H	-5.41309100	1.64312100	2.25453000
C	2.37780900	-2.13173000	-1.00513200	H	-4.71025300	1.29123200	4.61288600
C	2.32386300	-3.51676500	-1.20450800	C	-1.40505000	2.66131400	0.47848800
C	1.60799300	-4.06721200	-2.27342700	C	-2.44324900	3.49422500	0.03578100
C	0.92625700	-3.23571300	-3.16294800	C	-1.07943800	2.63212800	1.84119700
C	0.98656900	-1.84881900	-2.98693000	C	-3.14406000	4.28490000	0.94518800
H	1.78031600	-0.23037100	-1.80307900	H	-2.70902900	3.51667700	-1.01689000
H	2.84077500	-4.17329400	-0.50794800	C	-1.78342600	3.42250000	2.75126100
H	1.57626800	-5.14622000	-2.40232500	H	-0.28792800	1.97286500	2.18723100
H	0.35728800	-3.66049100	-3.98543400	C	-2.81609500	4.24814600	2.30404400
H	0.46735700	-1.19053700	-3.67929800	H	-3.94966300	4.92513600	0.59632900
C	-2.36893100	-0.45088100	-1.16258600	H	-1.53319600	3.38302700	3.80735700
C	-1.83032700	0.76454000	-1.64821100	H	-3.36970200	4.85798700	3.01254000
C	-3.38022900	-1.09666200	-1.88422800	C	0.35686800	2.66209700	-1.82365000
C	-2.32569000	1.30613500	-2.84132600	C	0.83853700	2.14994600	-3.04119300
C	-3.85792100	-0.55067700	-3.07588200	C	0.65728000	3.98787000	-1.47806500
H	-3.79104700	-2.03143600	-1.51636600	C	1.58782100	2.95296200	-3.89907100
C	-3.33192200	0.65197100	-3.55295900	H	0.61745500	1.12555400	-3.32392200
H	-1.91485800	2.23481100	-3.22352400	C	1.41403700	4.78698400	-2.33722500
H	-4.63867200	-1.06374700	-3.63016100	H	0.29888100	4.39856400	-0.53960600
H	-3.70265800	1.08067500	-4.47973700	C	1.87944500	4.27435700	-3.54934400
Cu	0.44644500	-0.29043100	0.51576500	H	1.94655900	2.54494500	-4.83999200
P	-1.67524800	-1.11616500	0.40716700	H	1.63613100	5.81329800	-2.05791600
P	-0.48996500	1.54191200	-0.64960200	H	2.46694200	4.89839500	-4.21677500
C	-2.14118000	-2.88417100	0.39420500	C	2.31826500	-0.59763800	1.11494600
C	-3.36580400	-3.35983800	0.88499000	C	3.17963000	0.70305200	1.03154600
C	-1.21334000	-3.78655900	-0.14476100	C	4.28320400	-0.57856200	-0.31429100
C	-3.65853400	-4.72339000	0.82713500	C	3.14341700	-1.54687600	0.16139700
H	-4.08612600	-2.66789800	1.31072200	C	5.21846800	-0.38293200	0.86027800
C	-1.51315400	-5.14698700	-0.20980000	H	2.67463100	1.64304000	1.25627900
H	-0.25799300	-3.42247300	-0.50683400	H	4.72788000	-0.80655600	-1.28333000
C	-2.73531400	-5.61732300	0.27739400	O	3.60846200	0.69898200	-0.35723000
H	-4.60780700	-5.08769500	1.21029300	H	2.37327500	-0.99710700	2.13715700
H	-0.78867200	-5.83771200	-0.63216800	H	3.59260900	-2.38101100	0.71246900
H	-2.96629100	-6.67815800	0.23516100	C	5.02522600	0.79874600	2.97332200
C	-2.72767600	-0.37965800	1.71343700	H	4.47821500	1.44019000	3.66064400
C	-2.33089900	-0.57010500	3.04732400	C	6.29425400	0.30358700	3.32044600
C	-3.84666600	0.41609300	1.43770400	H	6.73400800	0.57837700	4.27592900
C	-3.04858800	0.01938400	4.08679900	C	7.00152600	-0.53058300	2.45099700
H	-1.45442100	-1.17454500	3.26740600	H	7.98350100	-0.89802500	2.73728400
C	-4.55512500	1.01614000	2.47997600	C	6.45742600	-0.89594600	1.20678300
H	-4.15636200	0.58082800	0.41129100	H	7.00500700	-1.55603400	0.53814100
C	-4.15968200	0.81894500	3.80416500	C	4.50333200	0.45707000	1.73404500
H	-2.73417300	-0.13492200	5.11530600				



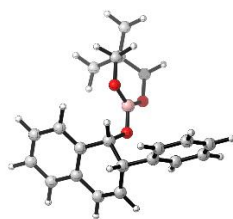
TS45

C	-1.15641500	-2.23529600	1.95361900	H	4.30132900	3.14465400	-3.20402300
C	-1.50160700	-2.96629700	0.80284800	H	2.44781200	3.32251400	-4.85075400
C	-0.85780600	-4.19209000	0.57655200	C	-0.25495200	2.61132500	-0.10755700
C	0.11596100	-4.67001700	1.45538700	C	0.76219000	3.50870200	-0.45693700
C	0.45805100	-3.93104200	2.59132000	C	-1.48584500	2.65720600	-0.78741300
C	-0.18775300	-2.71720100	2.83934300	C	0.55724200	4.43568000	-1.48047400
H	-1.65035600	-1.28946800	2.14911100	H	1.71914700	3.47122500	0.05277300
H	-1.12244900	-4.77277600	-0.30435800	C	-1.69063300	3.60043100	-1.79414000
H	0.60547900	-5.61967700	1.25500100	H	-2.26372500	1.94338700	-0.52930100
H	1.21184700	-4.30194900	3.28062900	C	-0.66753300	4.48489100	-2.14896300
H	0.05924900	-2.14542500	3.72985400	H	1.35783400	5.11567300	-1.75741500
C	2.67739500	0.51333400	0.85742500	H	-2.64515800	3.63383000	-2.31270500
C	1.76401300	1.33151200	1.56620200	H	-0.82292900	5.20591600	-2.94682200
C	4.02259600	0.47912300	1.24762000	C	-0.89357300	1.75689000	2.61074300
C	2.23183200	2.11633100	2.62934700	C	-0.73581900	0.95888200	3.75679200
C	4.46997500	1.25623700	2.31613600	C	-1.77374100	2.84565000	2.65443800
H	4.72057300	-0.15992700	0.71548000	C	-1.43754200	1.25133400	4.92451500
C	3.57542800	2.08155500	3.00214100	H	-0.05309400	0.11486700	3.73555200
H	1.53805400	2.74833100	3.17456600	C	-2.48236800	3.13099400	3.82358600
H	5.51501700	1.21921100	2.61052200	H	-1.90960600	3.47033400	1.77795000
H	3.92187600	2.69330300	3.83030500	C	-2.31707100	2.33755900	4.95996700
Cu	-0.22088700	-0.65227600	-0.21134900	H	-1.30201400	0.62888400	5.80473800
P	2.03065400	-0.45042900	-0.57224700	H	-3.16166800	3.97883300	3.84459400
P	-0.01150100	1.25018500	1.09058200	H	-2.86969500	2.56236600	5.8676400
C	3.25888800	-1.78281700	-0.80374200	C	-1.71346100	-1.62440900	-1.28992600
C	4.19825700	-1.80996800	-1.84286000	C	-2.52534900	-0.54582400	-1.75829600
C	3.19575000	-2.85914600	0.09844000	C	-3.50938000	-1.34689000	0.29119400
C	5.07089900	-2.89385800	-1.96908000	C	-2.47433300	-2.42776900	-0.22838200
H	4.25062000	-0.98962000	-2.55129300	C	-4.59257000	-1.30542200	-0.77463700
C	4.07503500	-3.93258300	-0.02505000	H	-2.06753300	0.20928900	-2.40033000
H	2.45323800	-2.85552500	0.89223400	H	-3.88831700	-1.59981000	1.29232000
C	5.01429500	-3.95283000	-1.06110100	O	-2.92417100	-0.07931500	0.23039800
H	5.79640600	-2.90763300	-2.77785700	H	-1.05930800	-2.13582200	-1.99881100
H	4.01945500	-4.75813900	0.67918300	H	-3.03798500	-3.27710300	-0.64500500
H	5.69445200	-4.79382500	-1.16274400	C	-4.74219700	-0.46854400	-3.05132900
C	2.24996900	0.71953400	-1.96760700	H	-4.28145500	-0.02633700	-3.93209400
C	1.21131600	0.82115600	-2.90502200	C	-6.10937000	-0.79796200	-3.05374000
C	3.36345400	1.56511000	-2.08353700	H	-6.71090300	-0.58872300	-3.93462200
C	1.28256500	1.75374100	-3.94028400	C	-6.69780600	-1.38308700	-1.93401600
H	0.33811800	0.18230900	-2.80530800	H	-7.75826400	-1.62174900	-1.94265300
C	3.43669700	2.49171100	-3.12345500	C	-5.93200200	-1.64886300	-0.78129200
H	4.16532000	1.51098700	-1.35372000	H	-6.39743400	-2.09163100	0.09652600
C	2.39505600	2.59006800	-4.05013900	C	-3.99226100	-0.72399200	-1.90826000
H	0.46500700	1.83510300	-4.65071100				



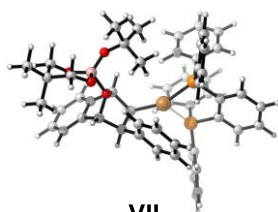
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C	3.30259800	-1.75600400	-2.15837700	H	-1.44262300	2.06107900	5.38774600
C	3.96387400	-0.59720500	-1.72900900	H	-1.73426700	4.23112900	4.21066000
C	5.25881800	-0.73161800	-1.20195300	C	-2.91380000	0.62137600	-0.07989400
C	5.87405000	-1.97838200	-1.09700500	C	-3.63054000	0.74872800	1.11733800
C	5.20133800	-3.12820400	-1.52098100	C	-2.77328400	1.73678000	-0.92181500
C	3.91711900	-3.00810000	-2.05385400	C	-4.20271200	1.97332900	1.46466200
H	2.30229200	-1.65309700	-2.56206900	H	-3.72641700	-0.10228900	1.78440100
H	5.79166500	0.15660000	-0.86925300	C	-3.35378600	2.95655600	-0.57672400
H	6.87799100	-2.05265500	-0.68668300	H	-2.19188000	1.65371400	-1.83651200
H	5.67618700	-4.10271100	-1.44161700	C	-4.06771700	3.07653700	0.61843100
H	3.38517400	-3.89390400	-2.39332100	H	-4.74614400	2.06797600	2.40053500
C	-0.79766600	-1.63787100	1.82061900	H	-3.22998800	3.81507600	-1.23069800
C	-1.90778400	-1.89390400	0.97924800	H	-4.50721100	4.03053100	0.89602300
C	-0.60040800	-2.41746900	2.96636300	C	-3.29297900	-1.84471000	-1.55566200
C	-2.80524500	-2.91310000	1.32380800	C	-2.82443300	-2.87215100	-2.38952900
C	-1.49966600	-3.43252600	3.29464800	C	-4.66690900	-1.56748200	-1.51146100
H	0.26392400	-2.23449100	3.59766200	C	-3.71821400	-3.62350600	-3.15223600
C	-2.60467100	-3.67523400	2.47571000	H	-1.75795300	-3.07867700	-2.44062300
H	-3.65914100	-3.11771100	0.68610700	C	-5.55815600	-2.31464400	-2.28353300
H	-1.33665100	-4.03247500	4.18540800	H	-5.03896200	-0.77108200	-0.87461500
H	-3.30806400	-4.46355100	2.72845300	C	-5.08660300	-3.34447000	-3.10117900
Cu	0.14394100	-0.15688600	-0.89228900	H	-3.34674700	-4.41841400	-3.79288600
P	0.32382100	-0.26388100	1.33865500	H	-6.62122800	-2.09318600	-2.24456200
P	-2.05106000	-0.91764300	-0.57717900	H	-5.78239200	-3.92377300	-3.70166400
C	1.93734000	-0.70705100	2.06821900	C	3.16551400	1.36865200	-0.39281100
C	2.57184500	0.05685100	3.05530800	C	2.40479000	2.45369100	-0.18408300
C	2.61277000	-1.80138900	1.50193700	C	2.09476800	0.98373000	-2.68754600
C	3.86399900	-0.27298200	3.47296500	C	3.35367400	0.79774000	-1.78154600
H	2.06635500	0.91215100	3.49120200	C	1.53753700	2.39860300	-2.50995800
C	3.89558400	-2.13414000	1.92905500	H	2.32211200	2.89181300	0.80789300
H	2.14082000	-2.37959600	0.71260000	H	2.46605400	0.89958500	-3.72647900
C	4.52676700	-1.36635400	2.91302000	O	1.05790200	0.07444600	-2.52021500
H	4.35095500	0.32766800	4.23635500	H	3.70486000	0.90810200	0.42938100
H	4.40962300	-2.97644100	1.47754900	H	4.11439000	1.44453100	-2.25528900
H	5.53337200	-1.61704800	3.23568600	C	0.95074300	4.27708300	-1.07673800
C	-0.30981400	1.15743800	2.30317900	H	1.02383700	4.77835000	-0.11401600
C	-0.48462000	2.38089900	1.64348200	C	0.18999300	4.83743600	-2.10092600
C	-0.66244900	1.04847700	3.65691600	H	-0.32993600	5.77828300	-1.94048300
C	-0.99130100	3.48538100	2.32876800	C	0.10661800	4.18692100	-3.33676300
H	-0.24332800	2.46327000	0.59095400	H	-0.47602200	4.62131500	-4.14498900
C	-1.17017600	2.15332500	4.34002900	C	0.77562400	2.97583700	-3.52870600
H	-0.54809300	0.10146400	4.17517500	H	0.69755700	2.45837900	-4.48251900
C	-1.33308900	3.37362700	3.67757500	C	1.63445800	3.06319100	-1.26601100
H	-1.13185100	4.42491400	1.80258300				



VI

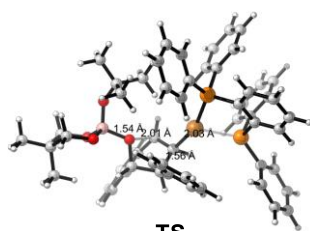
C	-2.95218300	1.23424100	0.96722600	H	1.86007500	-5.43681600	-0.01099700
C	-2.91094000	0.51294100	-0.23368100	C	1.81345100	-3.52926400	-1.01790600
C	-3.45573600	1.09459100	-1.38439900	H	2.72034400	-3.71292700	-1.58727100
C	-4.03055500	2.36627200	-1.34146200	C	1.12853700	-2.31954400	-1.16531600
C	-4.06855600	3.07529800	-0.13965600	H	1.50816900	-1.55258500	-1.83409000
C	-3.52733400	2.50419000	1.01489000	C	-0.53779000	-3.05175300	0.44307200
H	-2.52329800	0.79846400	1.86394200	C	2.57685900	1.81134300	-1.16709900
H	-3.43085700	0.54361300	-2.32191300	C	2.59178200	2.33087200	1.24230000
H	-4.45197900	2.79936500	-2.24480700	C	3.47569500	1.87637000	0.07320800
H	-4.51800000	4.06393800	-0.10166600	H	2.24532900	2.81950500	-1.44829800
H	-3.55069900	3.04983200	1.95456100	H	3.11807700	1.38337100	-2.01755700
C	-2.57719100	-1.76014500	0.85407500	H	2.26185700	3.36639900	1.08318700
C	-1.77802600	-2.78814600	1.17556700	H	3.15094000	2.29688400	2.18361400
C	-0.72934800	-0.72661800	-0.50875300	B	0.90397500	0.87873500	0.31448100
C	-2.25319200	-0.84947300	-0.30792100	O	1.43666800	1.50214100	1.41039100
C	-0.04123800	-2.07541500	-0.44700900	O	1.41875300	0.99492800	-0.95275200
H	-2.04947800	-3.47710600	1.97235000	C	4.09213900	0.49829600	0.36201200
H	-0.53936200	-0.25006700	-1.47351100	H	4.72585500	0.18029300	-0.47414600
O	-0.19166700	0.09324300	0.54046400	H	4.71389500	0.53677200	1.26389500
H	-3.51082600	-1.59476700	1.38534900	H	3.33171100	-0.27446600	0.51388300
H	-2.61961900	-1.34644900	-1.22062100	C	4.58098300	2.91222400	-0.15652400
C	0.16327400	-4.25696700	0.59197400	H	5.22768700	2.99109400	0.72515500
H	-0.21649700	-5.00994500	1.27841500	H	5.21020300	2.62664200	-1.00764600
C	1.32982000	-4.49640900	-0.13423100	H	4.16386900	3.90536600	-0.36126900



VII

C	1.68813500	-0.08524400	-2.81406800	P	-2.97290100	-1.23835500	-0.23627600
C	1.01132300	-1.21031600	-2.32356100	P	-1.79971300	1.64258500	-0.02873900
C	-0.19540200	-1.58018400	-2.94082000	C	-3.74942500	-2.73950400	-0.94666400
C	-0.72433100	-0.83689700	-3.99624900	C	-4.38709300	-3.71314300	-0.16566000
C	-0.04633100	0.29154700	-4.46808400	C	-3.62771200	-2.94701600	-2.33230800
C	1.16340700	0.65756900	-3.87488200	C	-4.89493000	-4.87096600	-0.75979500
H	2.62028500	0.22869700	-2.35847900	H	-4.48984600	-3.56866900	0.90480800
H	-0.72668100	-2.45693000	-2.57982500	C	-4.14636500	-4.09734200	-2.92332100
H	-1.66069400	-1.14291900	-4.45652200	H	-3.13574100	-2.19929200	-2.94747400
H	-0.45310300	0.87182400	-5.29201900	C	-4.77828500	-5.06574900	-2.13697900
H	1.70264300	1.53134200	-4.23179900	H	-5.38772900	-5.61799500	-0.14346700
C	-3.98732200	0.13943700	-0.90911900	H	-4.05186500	-4.24162900	-3.99607300
C	-3.43691800	1.44054500	-0.85115300	H	-5.17555300	-5.96642200	-2.59639000
C	-5.24480200	-0.04845800	-1.49830400	C	-3.40888900	-1.28560300	1.54390300
C	-4.14820900	2.51754200	-1.39528500	C	-2.57111800	-2.02598900	2.39538300
C	-5.94404700	1.03216100	-2.03637400	C	-4.46398900	-0.54676200	2.09488800
H	-5.67520600	-1.04356600	-1.54270900	C	-2.79605400	-2.03651800	3.77166000
C	-5.39458800	2.31538100	-1.98848800	H	-1.73957600	-2.58718600	1.97815800
H	-3.72128000	3.51494400	-1.36435900	C	-4.67479300	-0.54373600	3.47440200
H	-6.91598100	0.87119300	-2.49424500	H	-5.10909100	0.04098100	1.45032000
H	-5.93383700	3.15743800	-2.41290200	C	-3.84432100	-1.28876300	4.31420100
Cu	-0.72296200	-0.34601000	-0.08697400	H	-2.14470600	-2.61560100	4.42046400

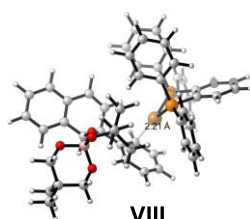
H	-5.48514200	0.04620800	3.89297300	C	4.24995500	-4.77946600	1.33178300
H	-4.00863200	-1.28091200	5.38803000	H	4.83205100	-5.69665500	1.30868800
C	-2.23897800	2.06182200	1.70030700	C	4.11855100	-4.01075400	0.16215200
C	-3.30871600	2.90924900	2.02355600	H	4.58573100	-4.33059500	-0.76551300
C	-1.49366900	1.47130500	2.73071200	C	2.78187200	-2.42516500	1.43321900
C	-3.62234900	3.16531000	3.35796300	C	6.43286600	-0.15292600	1.13492100
H	-3.90285800	3.36030600	1.23486900	C	6.04756200	0.95637700	-1.03635900
C	-1.81080700	1.72614500	4.06526000	C	6.94449700	-0.06506600	-0.31397600
H	-0.67903400	0.79811400	2.48029700	H	6.99155300	-0.92140100	1.68664100
C	-2.87485600	2.57326700	4.37998900	H	6.61798700	0.81189700	1.64074400
H	-4.45413900	3.82083000	3.60050200	H	6.26639200	0.95634200	-2.11271600
H	-1.23433600	1.25466300	4.85576700	H	6.29011100	1.96290100	-0.65681400
H	-3.12653200	2.76703100	5.41892100	B	4.20237000	0.37255800	0.44029200
C	-1.15798000	3.18615700	-0.76586700	O	3.63498200	1.37784900	1.26318700
C	-0.81837800	3.15472000	-2.12816100	C	3.02113700	2.60332400	0.85124300
C	-0.92068900	4.34839700	-0.02298200	O	4.66217500	0.70266900	-0.88265400
C	-0.26020500	4.27490500	-2.73882200	O	5.06415700	-0.48835400	1.19050300
H	-0.97899300	2.24854300	-2.70457200	C	8.39137600	0.43766500	-0.32640600
C	-0.35255800	5.46781100	-0.63736200	H	9.05368200	-0.26386500	0.19609400
H	-1.17099700	4.38172500	1.03185100	H	8.76363200	0.54293300	-1.35347000
C	-0.02258500	5.43442600	-1.99324400	H	8.48192100	1.41448900	0.16500500
H	0.00030500	4.23984800	-3.79301400	C	6.85722900	-1.44058700	-0.98662500
H	-0.16857100	6.36519800	-0.05312800	H	7.16207500	-1.38312700	-2.03937600
H	0.42159200	6.30507300	-2.46740500	H	7.51538100	-2.16073700	-0.48392300
C	0.78250300	-1.60016300	0.21947500	H	5.84045200	-1.83511900	-0.94202900
C	2.00084200	-1.17817000	1.08357500	C	4.11373400	3.67051200	0.69656100
C	2.99114200	-1.80819500	-0.79246600	H	4.71630200	3.73267200	1.61033700
C	1.49686500	-2.01752800	-1.13386100	H	4.77723500	3.42098000	-0.13709100
C	3.39223500	-2.83523900	0.23579900	H	3.67767000	4.65804500	0.50123000
H	1.85384700	-0.43593600	1.86255900	C	2.07314500	2.98766100	1.99407300
H	3.67409100	-1.61078200	-1.61286800	H	1.59967500	3.95790200	1.80655600
O	2.87953500	-0.59372000	0.04413800	H	1.28135100	2.23779900	2.09904700
H	0.36478000	-2.50629800	0.67839500	H	2.61987500	3.04348400	2.94271100
H	1.32906300	-3.07797900	-1.35134200	C	2.22467900	2.47755900	-0.45037600
C	2.89284800	-3.18783200	2.58482700	H	1.45951300	1.70076900	-0.36485300
H	2.42348400	-2.87817800	3.51525300	H	1.72815300	3.42606600	-0.67362700
C	3.64548100	-4.37288800	2.52363200	H	2.88273000	2.22204800	-1.28152400
H	3.76487100	-4.97774100	3.41874300				



TS₇₈

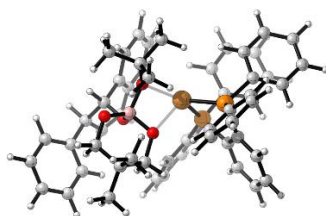
C	1.50004700	-0.33753700	-2.63396800	C	-5.09532000	2.30345300	-2.37859600
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C	-0.17190000	-2.07054100	-2.76481100	H	-6.64527500	0.88587700	-2.87343700
C	-0.71738100	-1.46389100	-3.89834800	H	-5.56824500	3.13152100	-2.89868800
C	-0.15649000	-0.28920700	-4.40549800	Cu	-0.66807300	-0.34721500	-0.01521100
C	0.95692100	0.26576000	-3.77023300	P	-2.95621800	-1.20752600	-0.21546100
H	2.36392200	0.10902400	-2.15349900	P	-1.68471000	1.66677700	-0.10918400
H	-0.61462000	-2.98538500	-2.37821300	C	-3.74362400	-2.72925400	-0.87211500
H	-1.56997200	-1.91763100	-4.39614800	C	-4.33633600	-3.69168600	-0.04260100
H	-0.57551300	0.18028200	-5.29147200	C	-3.65819500	-2.98008000	-2.25315200
H	1.40985100	1.17445300	-4.15818700	C	-4.83373300	-4.87936800	-0.58425200
C	-3.85606200	0.16207300	-1.04879900	H	-4.41374400	-3.51620700	1.02521600
C	-3.25575800	1.44339700	-1.04724400	C	-4.16553800	-4.16083000	-2.79139500
C	-5.08131300	-0.01850100	-1.70522600	H	-3.20565600	-2.24124600	-2.90610700
C	-3.88291900	2.50128000	-1.71802600	C	-4.75156400	-5.11761300	-1.95693800
C	-5.69738100	1.04367400	-2.36682100	H	-5.29257000	-5.61532900	0.07037400
H	-5.55241100	-0.99567200	-1.70522500	H	-4.09980100	-4.33622300	-3.86169900

H	-5.14130200	-6.04116300	-2.37545700	C	3.07510200	-3.24503400	2.81229300
C	-3.52481100	-1.12684900	1.52571600	H	2.55085900	-3.03718800	3.74161400
C	-2.77333700	-1.82266900	2.48730600	C	4.04973100	-4.25024300	2.74914500
C	-4.62119100	-0.35846900	1.93811600	H	4.29772400	-4.81551500	3.64321500
C	-3.12507400	-1.76413000	3.83576700	C	4.71113300	-4.52391400	1.54898200
H	-1.91273500	-2.41034800	2.17838200	H	5.47260200	-5.29860400	1.51968900
C	-4.95940100	-0.28617300	3.28974000	C	4.42236200	-3.79176100	0.38573800
H	-5.20034300	0.19571300	1.20691800	H	4.96240200	-3.98486400	-0.53709700
C	-4.21582200	-0.99018400	4.23953600	C	2.78114300	-2.53455900	1.65088600
H	-2.54113100	-2.31114300	4.57082600	C	6.42769800	-0.06431400	0.92147000
H	-5.80180300	0.32483800	3.60102600	C	5.80486600	1.11859600	-1.15937300
H	-4.48036300	-0.92966400	5.29140800	C	6.86874200	0.19356300	-0.53409600
C	-2.27259600	2.16552100	1.55471300	H	7.10429000	-0.79579500	1.39030200
C	-3.33129400	3.06884900	1.72937600	H	6.52300400	0.87830900	1.49081900
C	-1.66848000	1.58941800	2.68060200	H	6.01667200	1.26260900	-2.23006500
C	-3.77069100	3.39623200	3.01164400	H	5.87905500	2.11154200	-0.67901800
H	-3.81810300	3.50955900	0.86494500	B	4.12135400	0.27685800	0.35039700
C	-2.11105800	1.91555700	3.96269800	O	3.85927500	1.40255900	1.21091400
H	-0.86279700	0.87488500	2.54839200	C	2.95083900	2.47509600	1.02207800
C	-3.16134400	2.81983300	4.12958900	O	4.50269900	0.60301800	-1.03295200
H	-4.59205700	4.09601100	3.13803600	O	5.11745600	-0.56197100	1.00061200
H	-1.64302100	1.45496500	4.82765900	C	8.23347100	0.88623000	-0.55195200
H	-3.51015500	3.06974500	5.12763700	H	9.00294100	0.25561200	-0.08779100
C	-0.96657300	3.17504600	-0.85077000	H	8.55644100	1.09991500	-1.57932800
C	-0.52806800	3.09443500	-2.18224000	H	8.20701100	1.83760600	-0.00526800
C	-0.79854700	4.37094800	-0.14190500	C	6.93205600	-1.13138000	-1.30339900
C	0.05682600	4.19876600	-2.79762000	H	7.20586100	-0.96577100	-2.35383200
H	-0.64128600	2.16551900	-2.73266100	H	7.67895000	-1.80542600	-0.86355600
C	-0.20471600	5.47411100	-0.76045600	H	5.96358200	-1.63629100	-1.27677100
H	-1.12870400	4.44559300	0.88837700	C	3.60289400	3.69708100	1.68616000
C	0.22135400	5.39182100	-2.08706300	H	3.83437100	3.47853200	2.73531900
H	0.39212300	4.12639700	-3.82842100	H	4.54188100	3.94837500	1.17860500
H	-0.07665200	6.39733200	-0.20232300	H	2.94493800	4.57412300	1.65078800
H	0.68436300	6.25050600	-2.56480500	C	1.63852600	2.13441000	1.74525400
C	0.72385700	-1.75587900	0.40909500	H	0.94076800	2.97924200	1.73706500
C	1.69579600	-1.55312900	1.47691700	H	1.15273400	1.28652600	1.25350100
C	2.96473400	-1.80300400	-0.56179500	H	1.84167000	1.86369500	2.78861200
C	1.49905000	-2.19545200	-0.87291900	C	2.64765400	2.79903100	-0.44755100
C	3.46993500	-2.79184000	0.45561500	H	2.14503000	1.96343800	-0.93773900
H	1.40305700	-0.98191600	2.35855000	H	1.99265900	3.67441300	-0.50142900
H	3.59976500	-1.67643800	-1.43711600	H	3.56495600	3.01570700	-1.00150100
O	2.84324400	-0.55408100	0.15681300				
H	-0.02311000	-2.48394500	0.76096100				
H	1.45549500	-3.28089800	-1.03234600				



C	1.69213200	0.25901000	-2.41900900	C	-4.26465200	0.88578400	-0.24697400
C	1.00210200	-0.91748500	-2.08714600	C	-3.42576400	1.97605400	0.09306000
C	-0.25568400	-1.14951900	-2.69984300	C	-5.64314500	1.09395700	-0.38281300
C	-0.81860000	-0.20177900	-3.58226500	C	-3.98733400	3.24561500	0.27331500
C	-0.12805100	0.98093800	-3.86651300	C	-6.19063900	2.36297600	-0.19191300
C	1.13122500	1.18888300	-3.29856300	H	-6.28867600	0.26195800	-0.64598200
H	2.67844000	0.44506600	-2.00610600	C	-5.36214200	3.43920800	0.13115000
H	-0.74094300	-2.11565300	-2.57896900	H	-3.34723500	4.08572600	0.52334200
H	-1.76727800	-0.41940000	-4.06413900	H	-7.26104800	2.51077100	-0.30128600
H	-0.55663600	1.71217800	-4.54594700	H	-5.78386300	4.43017100	0.27216200
H	1.68561200	2.09422000	-3.53074500	Cu	-1.36769100	-0.06380600	-1.13536300

P	-3.49616400	-0.75496700	-0.56259700	C	1.56916700	-2.00098900	-1.18228500
P	-1.62231900	1.65744900	0.31685600	C	3.39776400	-3.02562500	0.15584100
C	-4.69800700	-1.62232900	-1.62919700	H	0.38544900	-3.40807600	1.78024700
C	-5.60268400	-2.57393400	-1.13940300	H	3.67833300	-1.71582400	-1.52926000
C	-4.69495200	-1.31028400	-2.99847800	O	3.10026300	-0.62754300	0.12581800
C	-6.49451600	-3.20272100	-2.01051600	H	-0.39813400	-2.02765600	-0.07299700
H	-5.61114500	-2.82252400	-0.08309900	H	1.63453800	-2.90787200	-1.81132600
C	-5.59362100	-1.93317200	-3.86285000	C	2.80949100	-4.67749600	1.84840800
H	-3.99234500	-0.57522700	-3.38311400	H	2.06681300	-5.11337100	2.51331500
C	-6.49306900	-2.88299500	-3.36979400	C	4.10515700	-5.18973300	1.81068400
H	-7.19307500	-3.93975400	-1.62459800	H	4.38063700	-6.02201800	2.45324300
H	-5.58759100	-1.68423700	-4.92018500	C	5.04421200	-4.63055900	0.93928700
H	-7.18839100	-3.37395200	-4.04457800	H	6.05503200	-5.02850000	0.89953400
C	-3.53327600	-1.63464200	1.03775100	C	4.68959200	-3.54983200	0.12771400
C	-2.83186000	-2.84809200	1.13182700	H	5.42799100	-3.08402600	-0.51399500
C	-4.16247200	-1.11196900	2.17431400	C	2.44003800	-3.60963900	1.01562300
C	-2.76420300	-3.52813100	2.34664100	C	6.75608400	-0.16559600	0.18190200
H	-2.33498700	-3.25713000	0.25657100	C	5.75011200	1.27588800	-1.55638000
C	-4.08143200	-1.78965600	3.39188800	C	6.93266900	0.32748900	-1.27052800
H	-4.69826000	-0.17087000	2.11514800	H	7.52935300	-0.91890800	0.40932100
C	-3.38322900	-2.99511200	3.48096100	H	6.92867900	0.68889200	0.86190600
H	-2.22111800	-4.46672100	2.40942100	H	5.77085400	1.58841500	-2.61387700
H	-4.55882400	-1.36964000	4.27220700	H	5.88374700	2.18917600	-0.94791800
H	-3.31666400	-3.51613800	4.43166800	B	4.35890800	0.14437200	0.10015500
C	-1.54429100	1.14928000	2.07212300	O	4.36224700	1.20230500	1.10653500
C	-2.29130000	1.79950700	3.06659700	C	3.37937200	2.19299400	1.31455400
C	-0.76274100	0.03786400	2.41301400	O	4.51296100	0.67696900	-1.28945700
C	-2.23430300	1.35494300	4.38699100	O	5.49854300	-0.73622900	0.40842200
H	-2.92574600	2.64187700	2.80885800	C	8.25653300	1.08262900	-1.40875100
C	-0.71330800	-0.40936300	3.73287800	H	9.11131800	0.42868000	-1.19036600
H	-0.19667300	-0.48249000	1.64958900	H	8.38942900	1.47000200	-2.42780700
C	-1.44507300	0.25078700	4.72129900	H	8.30472200	1.93515900	-0.71892000
H	-2.81211900	1.86451600	5.15290200	C	6.89272600	-0.85958700	-2.23958900
H	-0.10560600	-1.27356900	3.98342100	H	7.02524100	-0.52666200	-3.27808600
H	-1.40894000	-0.09885900	5.74913900	H	7.69000400	-1.58127200	-2.01562800
C	-0.84955300	3.30474000	0.17729000	H	5.93249200	-1.37664300	-2.16885900
C	-0.55517900	3.75727000	-1.11850500	C	4.05063300	3.26915000	2.18257100
C	-0.54267200	4.11538800	1.27814500	H	4.43384000	2.82175800	3.10738000
C	0.01794000	5.01301500	-1.31135800	H	4.89852300	3.71493100	1.64799900
H	-0.76615800	3.11934800	-1.97203100	H	3.34921500	4.07017500	2.44828800
C	0.03996200	5.36894800	1.08118100	C	2.18626100	1.58931300	2.07354300
H	-0.74905900	3.77067000	2.28528400	H	1.43150100	2.34666700	2.31539000
C	0.31651300	5.82099200	-0.21089000	H	1.73003400	0.80927800	1.46322600
H	0.24459200	5.35417600	-2.31739400	H	2.52553800	1.12701000	3.00881500
H	0.28048500	5.98955300	1.93959400	C	2.87424800	2.84457700	0.01585500
H	0.77369900	6.79498000	-0.35968700	H	2.32362500	2.12690200	-0.59395200
C	0.63775200	-2.35694100	-0.03858800	H	2.20842000	3.68219400	0.24903600
C	1.06419800	-3.11515700	0.98172400	H	3.71139900	3.22267700	-0.57989500
C	3.01097100	-1.78700400	-0.66030000				



IX

C	-5.17189200	-0.22070900	1.30564700	H	-4.44399100	-0.76344100	1.89974900
C	-5.26868900	-0.47915300	-0.06770100	H	-6.28708200	0.06028500	-1.88528300
C	-6.20039800	0.24979400	-0.81776000	H	-7.73065400	1.76469400	-0.81816400
C	-7.01586900	1.20956800	-0.21632000	H	-7.56140800	2.18664600	1.63070100
C	-6.92177200	1.44699500	1.15696100	H	-5.91474800	0.90253000	2.98497900
C	-5.99793200	0.72495000	1.91590800	C	1.86330800	-0.41177100	2.25498700

C	2.55351500	0.76447500	1.87665900	H	5.15296000	5.43328000	-0.69661100
C	1.84334300	-0.78920700	3.60432600	H	3.28115100	6.87345300	0.07645900
C	3.18732400	1.53999300	2.85562900	C	-4.04337800	-2.67378000	0.15852400
C	2.48627900	-0.01336700	4.56925600	C	-3.01373600	-3.48401300	-0.11951400
H	1.31588900	-1.68927400	3.90274600	C	-3.12991400	-0.89383500	-1.40536400
C	3.15438100	1.15482700	4.19590400	C	-4.39576400	-1.51379000	-0.74236700
H	3.70125400	2.45217600	2.56890600	C	-2.27405200	-2.02567100	-1.98499400
H	2.45989100	-0.31842100	5.61150500	H	-2.79741300	-4.35041900	0.49971500
H	3.64797100	1.76608200	4.94615400	H	-3.47500700	-0.25649800	-2.23074500
Cu	0.59991600	0.30311000	-0.54633800	O	-2.40262700	-0.12667600	-0.47889400
P	0.97896900	-1.36443300	0.94519900	H	-4.68432300	-2.87588400	1.01234900
P	2.58087000	1.20588500	0.08832800	H	-4.97462800	-1.92925000	-1.58487000
C	-0.22766900	-2.33683000	1.91411200	C	-1.35139700	-4.27353900	-1.79830800
C	-0.10305600	-3.71185600	2.14577100	H	-1.28350600	-5.21363500	-1.25572500
C	-1.31767700	-1.63812500	2.45708100	C	-0.64025900	-4.09542400	-2.98400800
C	-1.05077300	-4.37802300	2.92753300	H	-0.01107300	-4.89467700	-3.36684900
H	0.73352400	-4.26035400	1.72448700	C	-0.74490400	-2.88526300	-3.67420300
C	-2.24669700	-2.30141300	3.25552600	H	-0.20471600	-2.73689600	-4.60573900
H	-1.43577200	-0.58159900	2.24302400	C	-1.55174100	-1.86258400	-3.16636500
C	-2.11677900	-3.67375100	3.49111100	H	-1.62316500	-0.92224700	-3.69503000
H	-0.94812700	-5.44534600	3.10389600	C	-2.18341200	-3.25863000	-1.30002100
H	-3.08095400	-1.75107300	3.68173500	C	-3.55398500	2.71371800	-0.25868900
H	-2.84746400	-4.19208300	4.10578100	C	-1.77195100	2.10022000	1.35682200
C	2.22625600	-2.56230300	0.34755100	C	-2.70995600	3.24186800	0.92410800
C	1.98440700	-3.16124100	-0.89785600	H	-4.25413800	1.96576300	0.12708900
C	3.42269200	-2.83683800	1.02303100	H	-4.14907400	3.53726800	-0.67810900
C	2.91528900	-4.03933900	-1.45025200	H	-2.37186700	1.28195700	1.78292600
H	1.07140400	-2.92931700	-1.43520100	H	-1.07542500	2.44562800	2.13386300
C	4.36382500	-3.69836300	0.45652400	B	-1.82283200	1.16216100	-0.89985700
H	3.62882700	-2.36541900	1.97848500	O	-0.80749500	0.87687300	-1.96549700
C	4.11036300	-4.30443400	-0.77620100	C	-0.43456000	1.74747900	-3.05787000
H	2.71444800	-4.50148800	-2.41291500	O	-1.01519900	1.63588000	0.25729300
H	5.29689500	-3.89318600	0.97775300	O	-2.78453700	2.16069600	-1.31299700
H	4.84628900	-4.97303400	-1.21416300	C	-1.88821100	4.47261900	0.52193600
C	4.11139600	0.38776100	-0.49613600	H	-2.53766700	5.26780100	0.13326600
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C	4.04181000	-0.38962000	-1.66012100	H	-1.15434900	4.22478700	-0.24516200
C	6.43447100	-0.25562100	-0.22650700	C	-3.64443100	3.60543600	2.08318100
H	5.37577900	1.02963100	1.13501300	H	-3.07375100	3.98219600	2.94198800
C	5.16061300	-1.09545000	-2.10440700	H	-4.35266600	4.38965100	1.78601500
H	3.10395500	-0.46212300	-2.20131900	H	-4.22718000	2.74023600	2.41565000
C	6.35706000	-1.02860200	-1.38878600	C	0.78809200	1.09473300	-3.70911300
H	7.36303600	-0.20756100	0.33547600	H	1.63701800	1.09984400	-3.01607600
H	5.09215800	-1.70703100	-2.99913000	H	0.57222300	0.05606100	-3.98029300
H	7.22613000	-1.58436700	-1.72959400	H	1.08303900	1.63814600	-4.61424900
C	2.90507000	3.00295800	0.10075200	C	-0.07040500	3.14996000	-2.56458500
C	1.84219200	3.82260700	0.52139100	H	0.33768900	3.74730200	-3.38936900
C	4.09531400	3.59195600	-0.34282900	H	-0.95491100	3.65243400	-2.17233400
C	1.98138500	5.20822700	0.52091200	H	0.68268000	3.09648700	-1.77476500
H	0.90252700	3.36816900	0.82137600	C	-1.58610200	1.83630100	-4.06903000
C	4.22623200	4.98358900	-0.35080700	H	-2.48944600	2.19465200	-3.57248700
H	4.91879600	2.97132300	-0.68057000	H	-1.32395800	2.52984500	-4.87737900
C	3.17527500	5.79228700	0.08453500	H	-1.79548600	0.86255000	-4.52362900
H	1.15357100	5.83235700	0.84558600				

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4. Copies of NMR spectra for all new compounds.

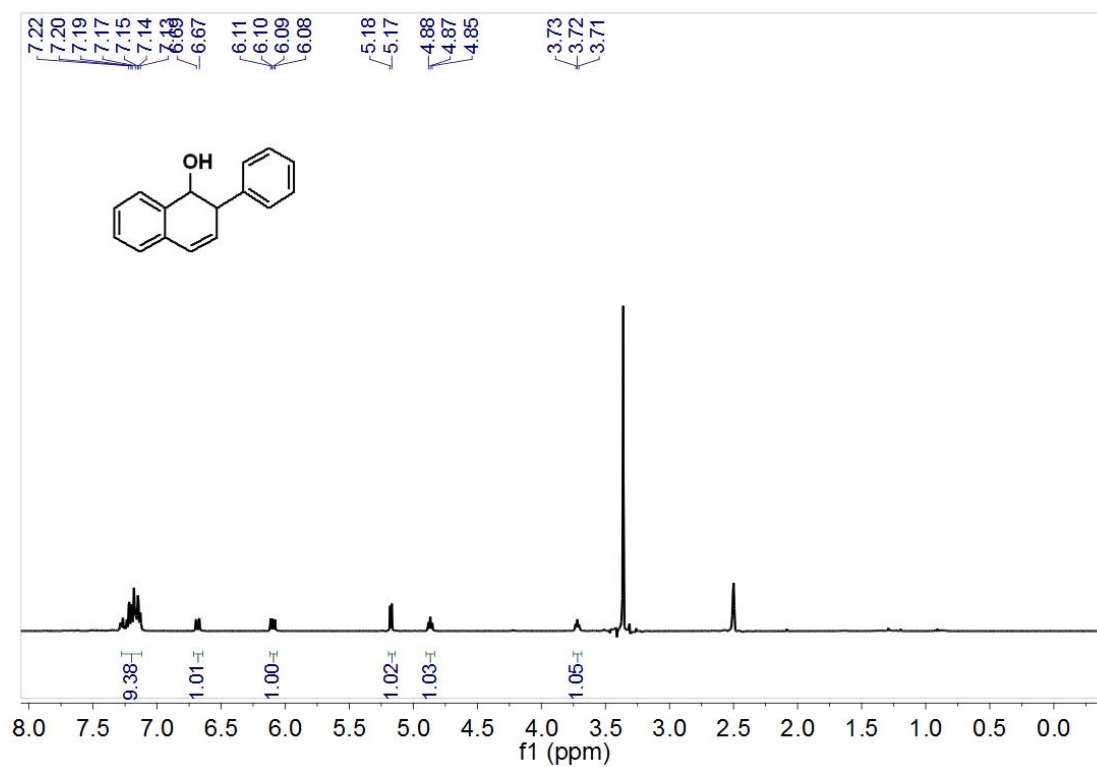


Figure S2. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) for product 3a.

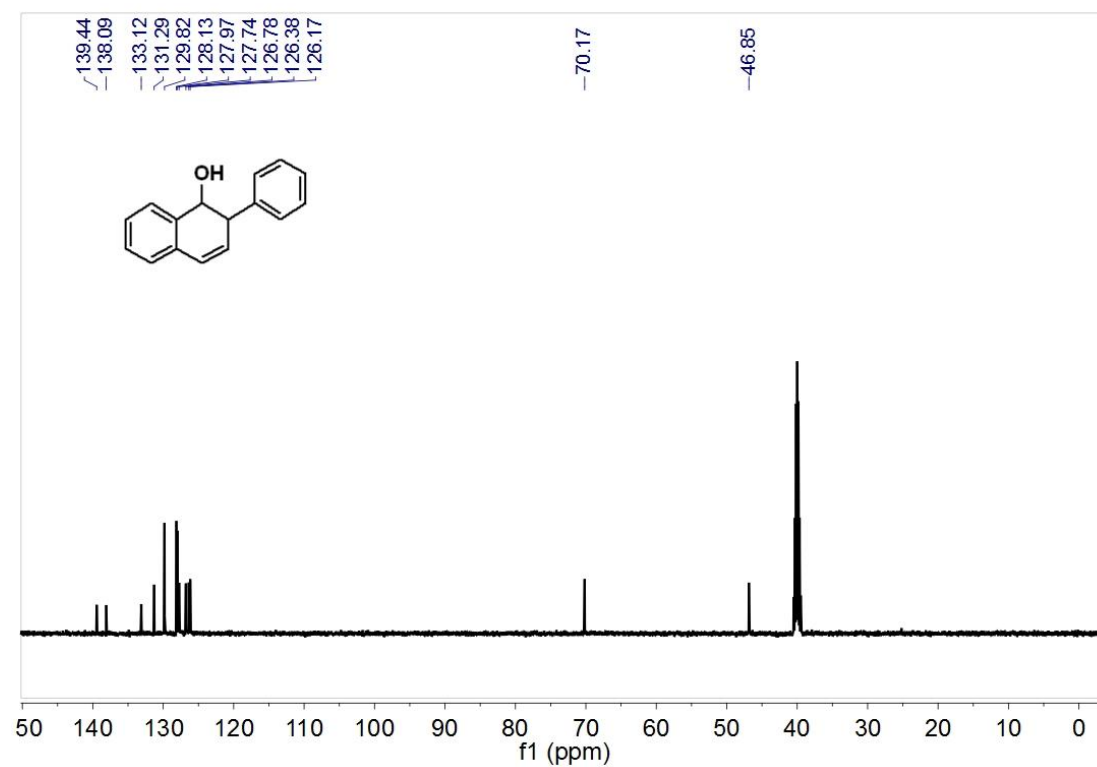


Figure S3. ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) for product 3a.

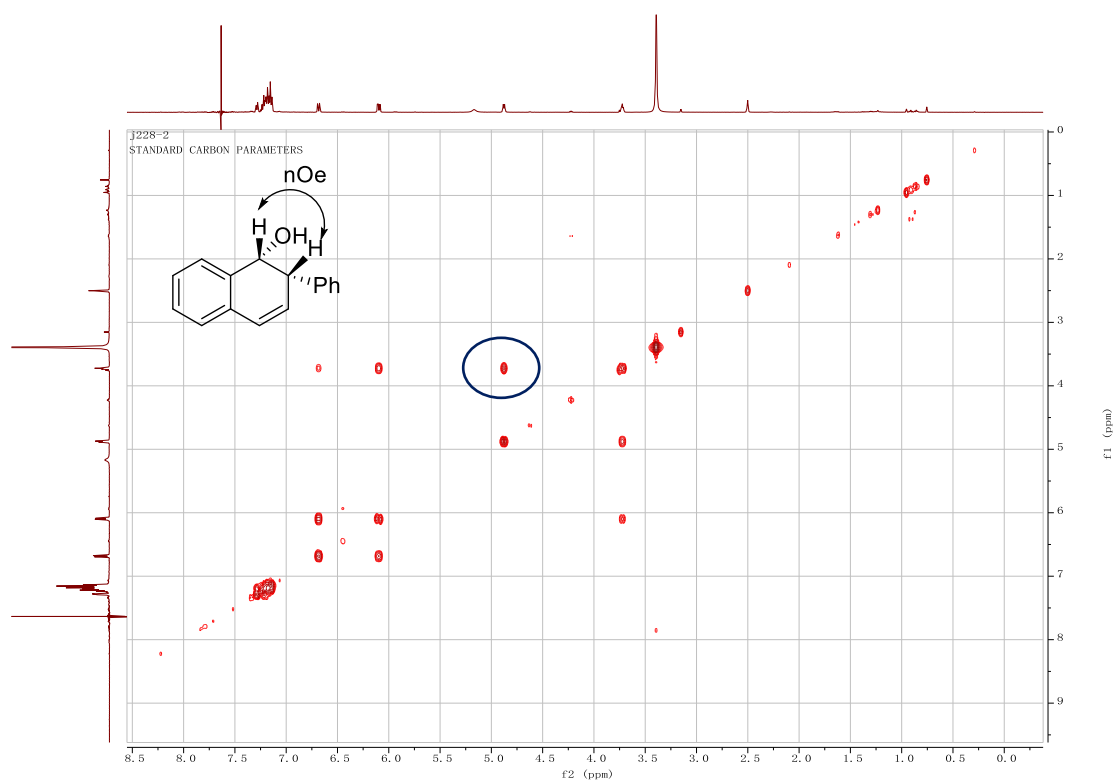


Figure S4. 2D NOESY spectrum of product **3a**

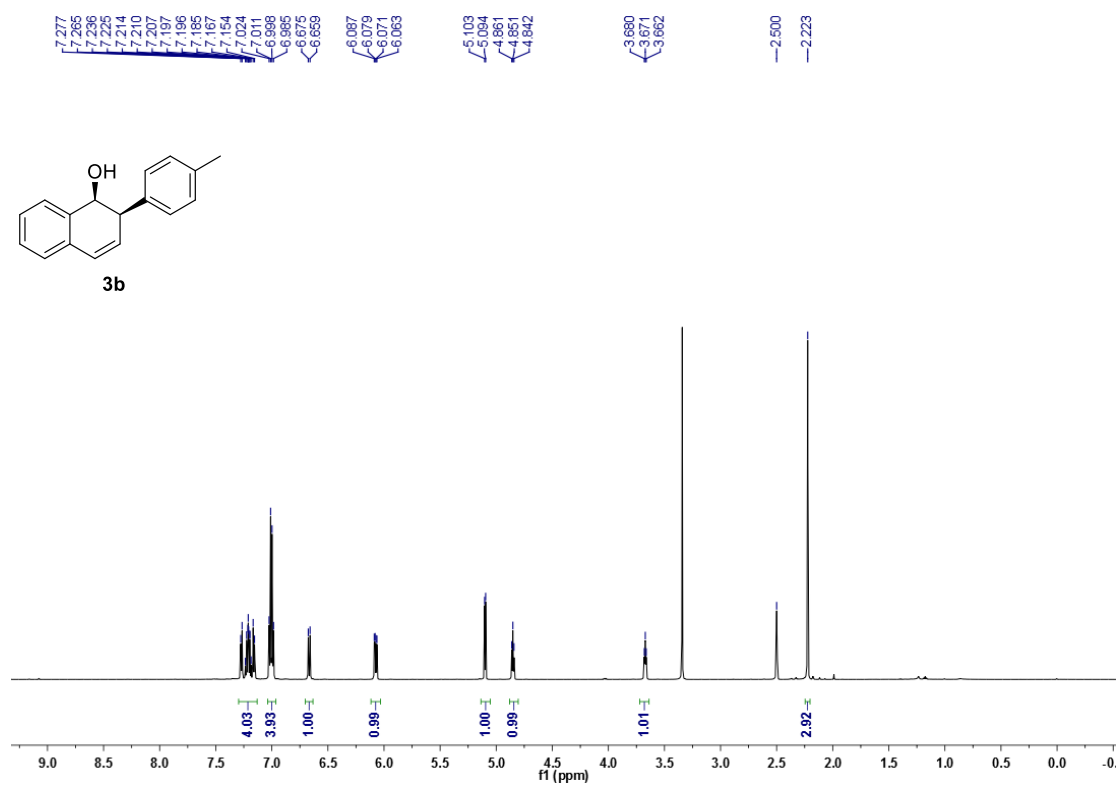


Figure S5. ^1H NMR (600 MHz, $\text{DMSO-}d_6$) for product **3b**.

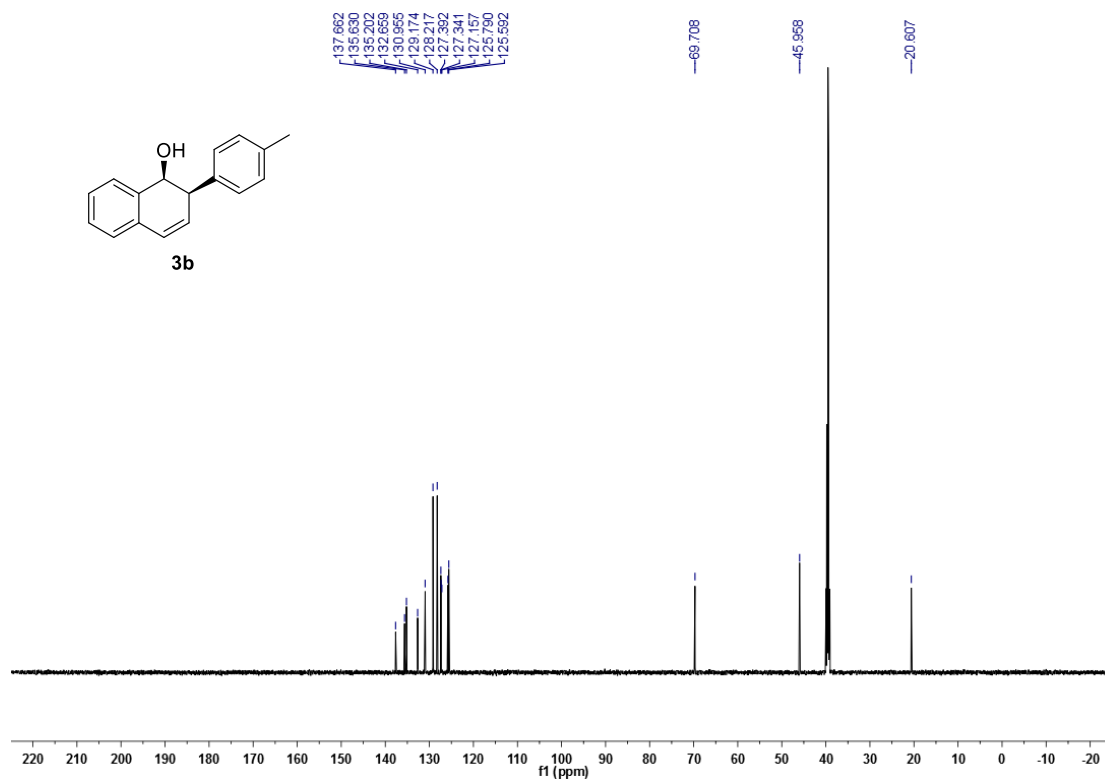


Figure S6. ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) for product **3b**.

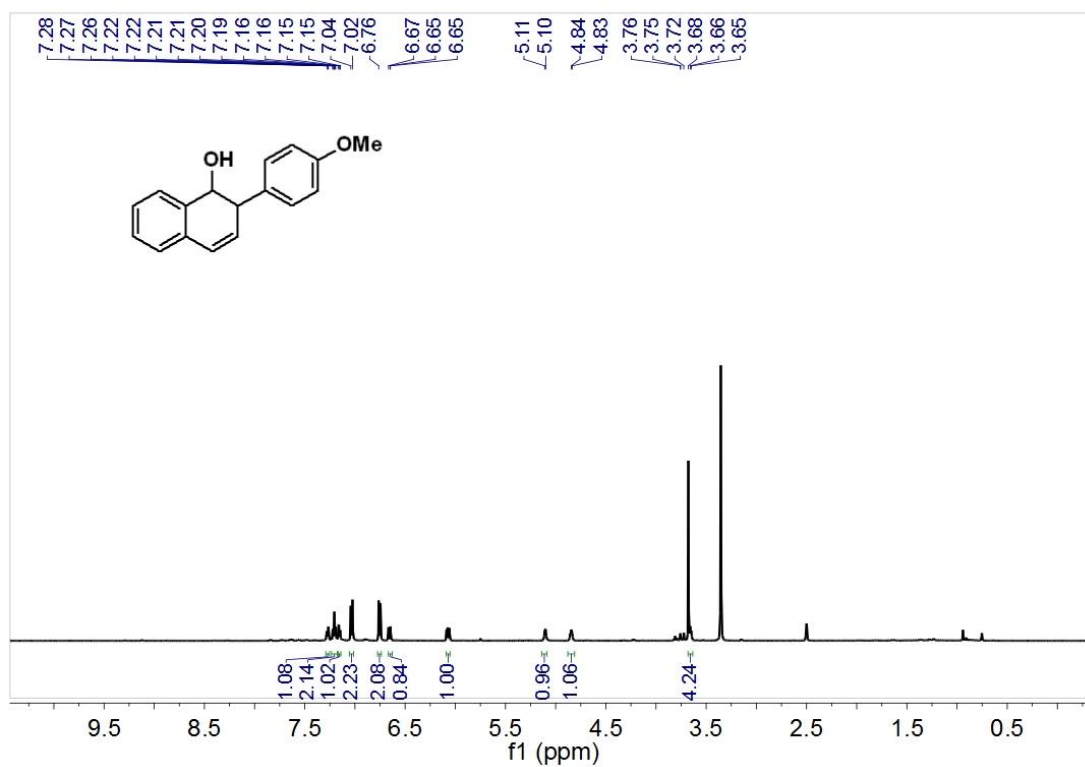


Figure S7. ^1H NMR (500 MHz, $\text{DMSO-}d_6$) for product **3c**.

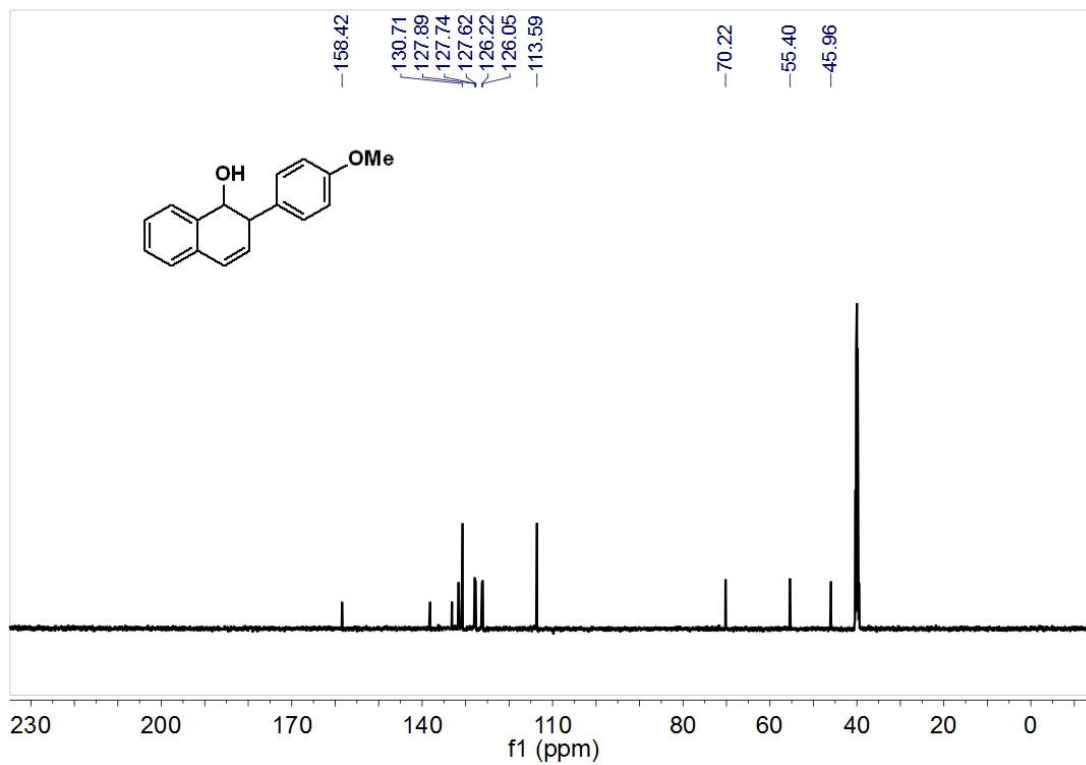


Figure S8. ¹³C NMR (126 MHz, DMSO-*d*₆) for product **3c**.

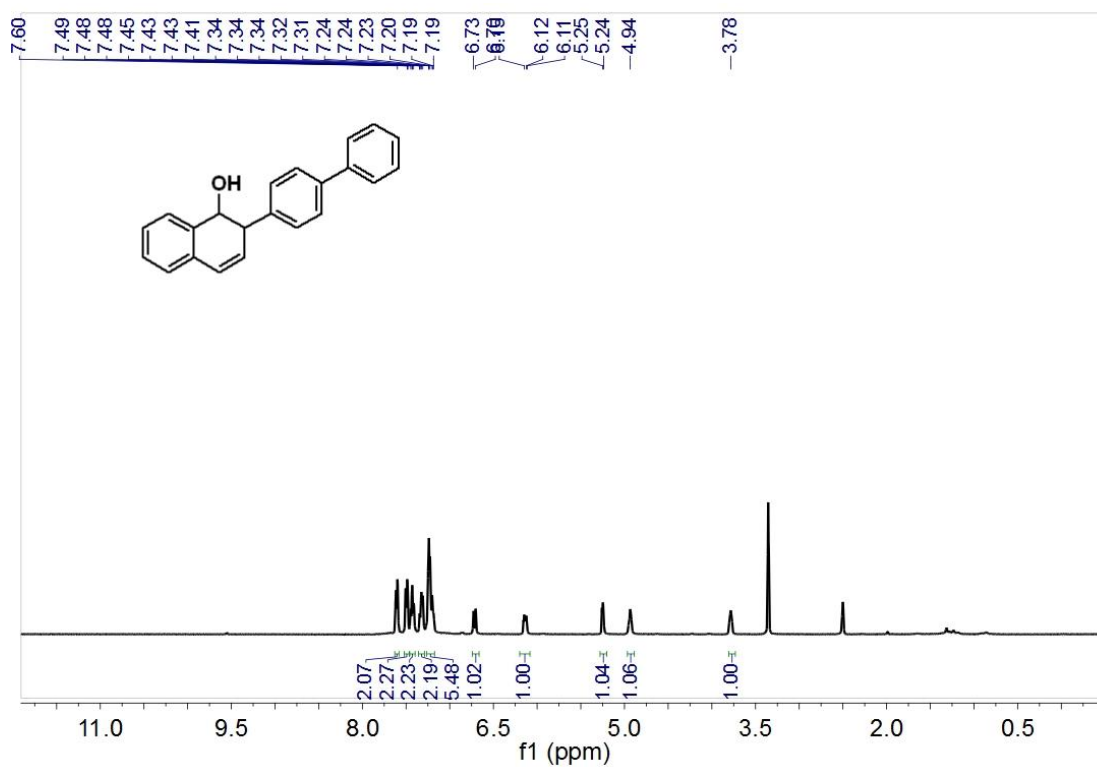


Figure S9. ¹H NMR (400 MHz, DMSO-*d*₆) for product **3d**.

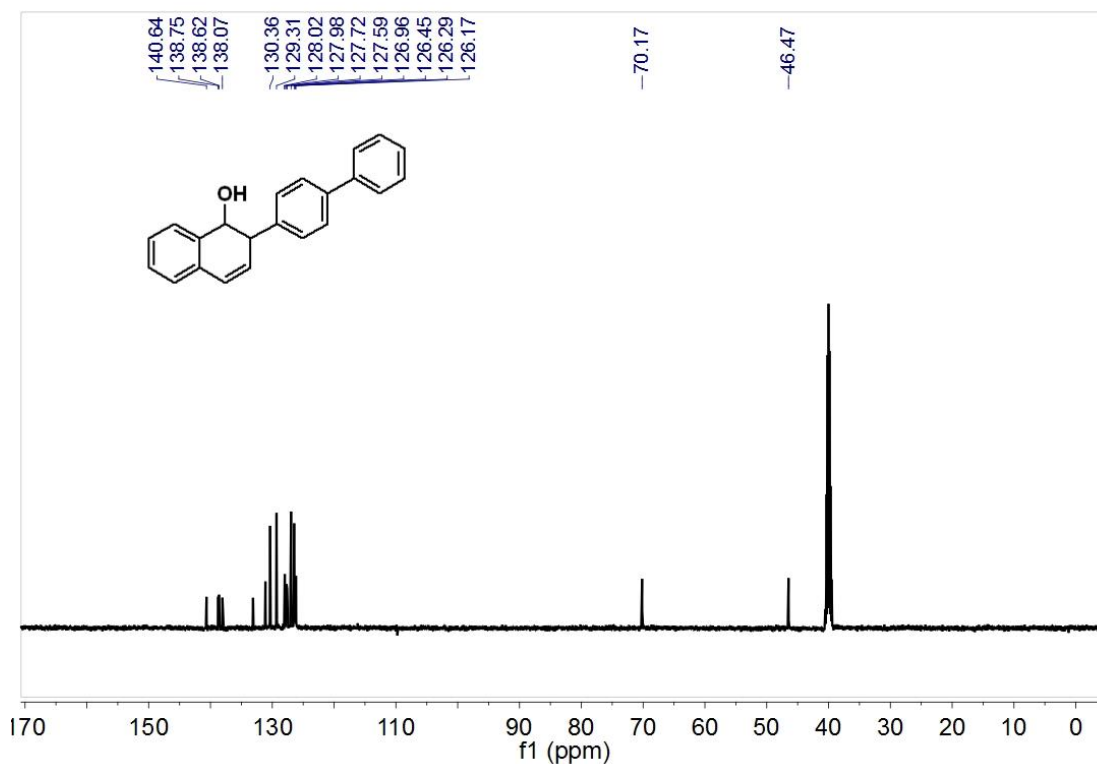


Figure S10. ¹³C NMR (126 MHz, DMSO-*d*₆) for product **3d**.

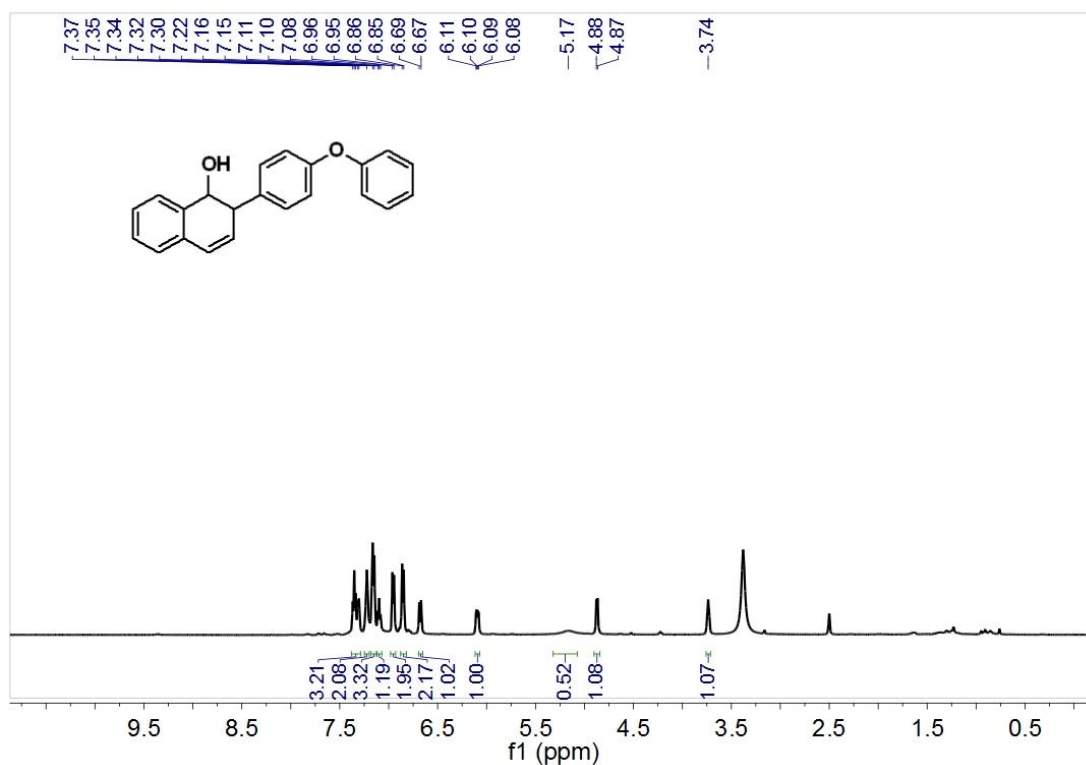


Figure S11. ¹H NMR (500 MHz, DMSO-*d*₆) for product **3e**.

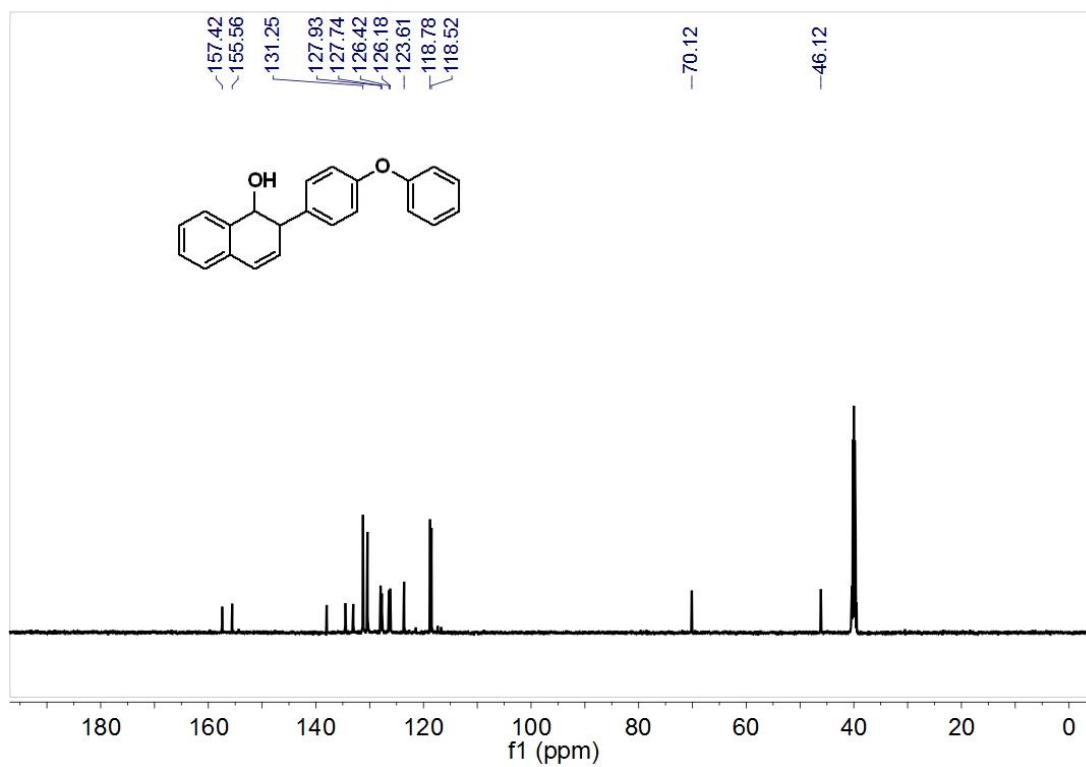


Figure S12. ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) for product **3e**.

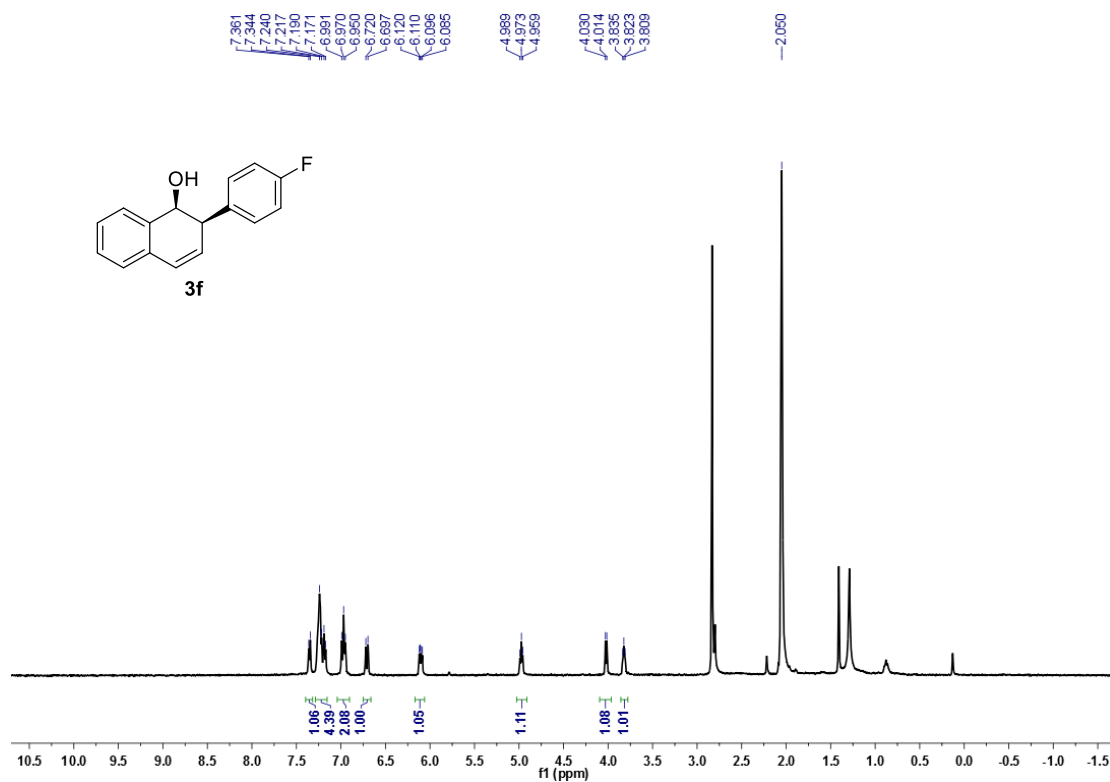


Figure S13. ^1H NMR (400 MHz, $\text{Acetone-}d_6$) for product **3f**.

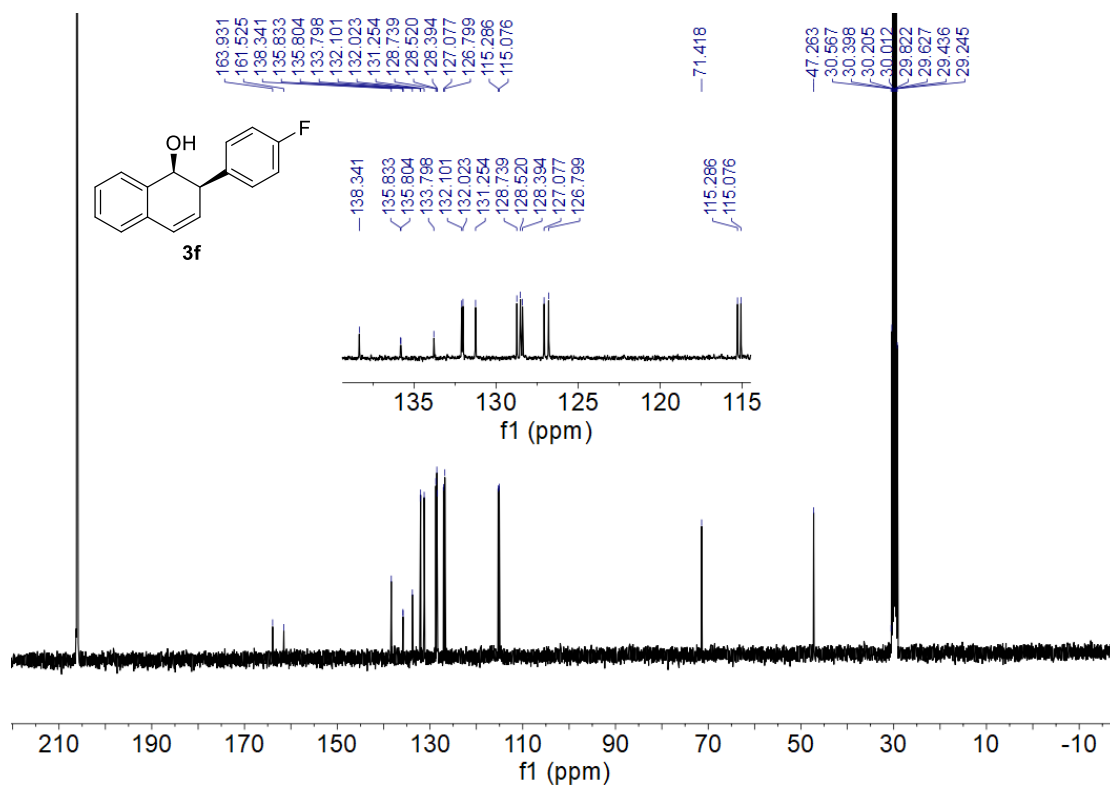


Figure S14. ^{13}C NMR (101 MHz, acetone- d_6) for product **3f**.

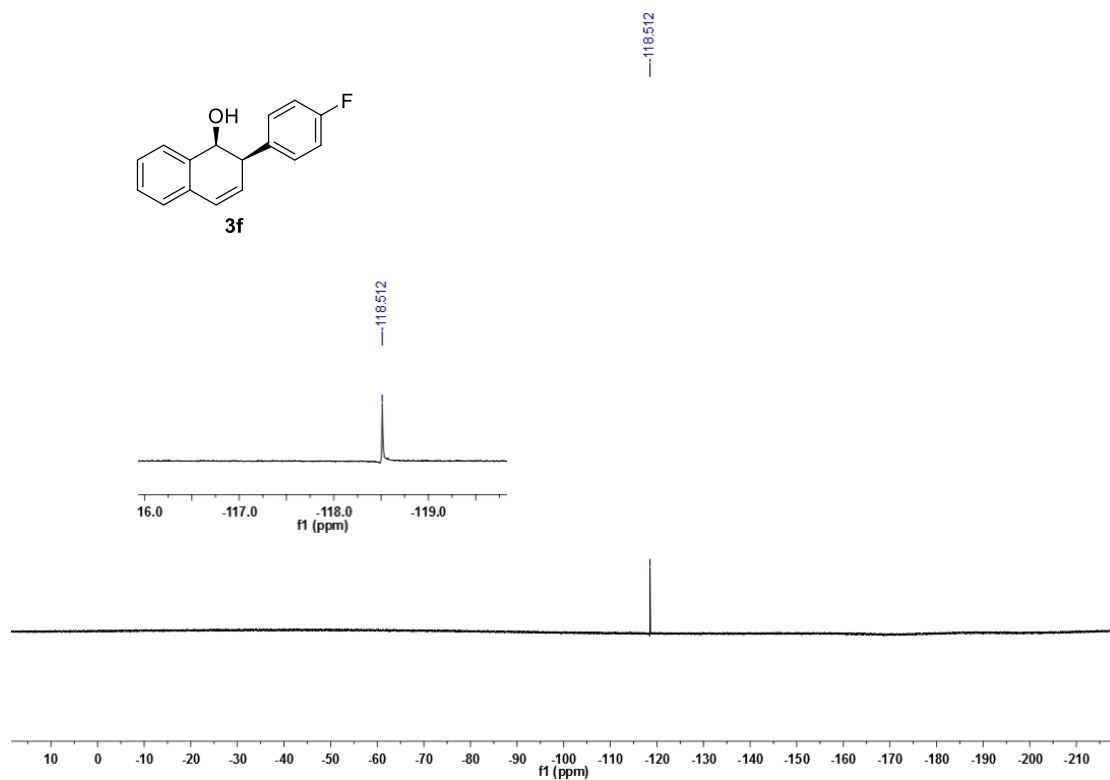


Figure S15. ^{19}F NMR (376 MHz, Acetone- d_6) for product **3f**.

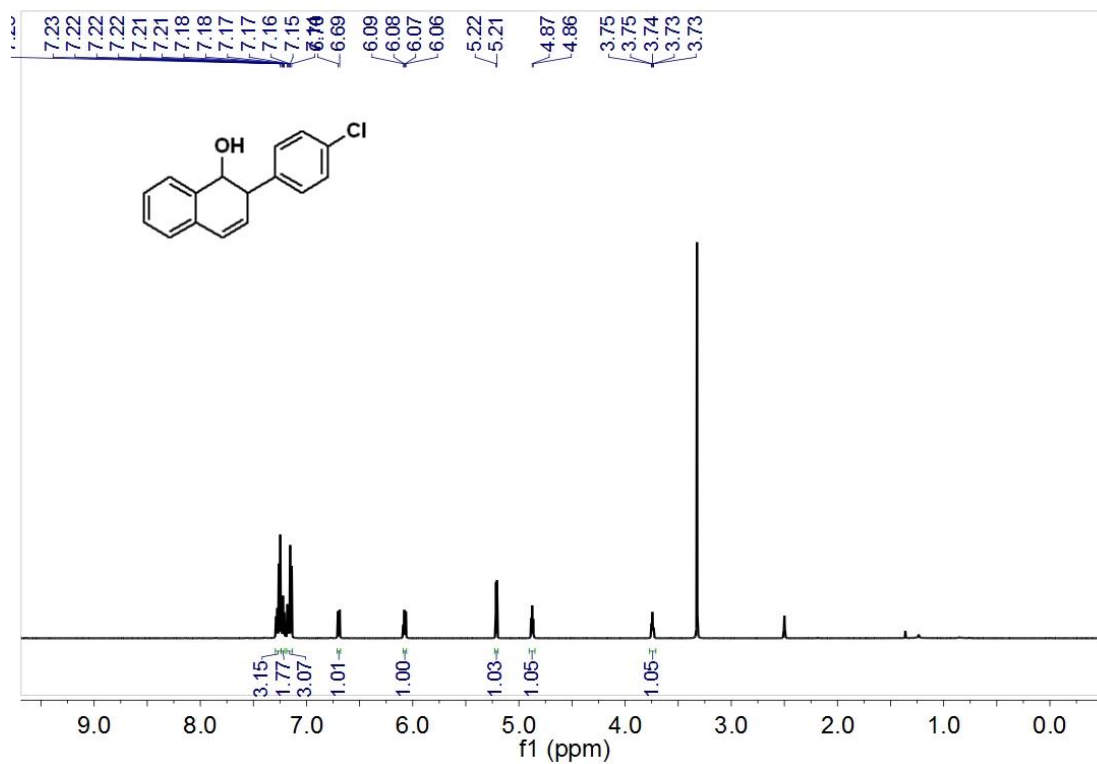


Figure S16. ^1H NMR (600 MHz, $\text{DMSO-}d_6$) for product **3g**.

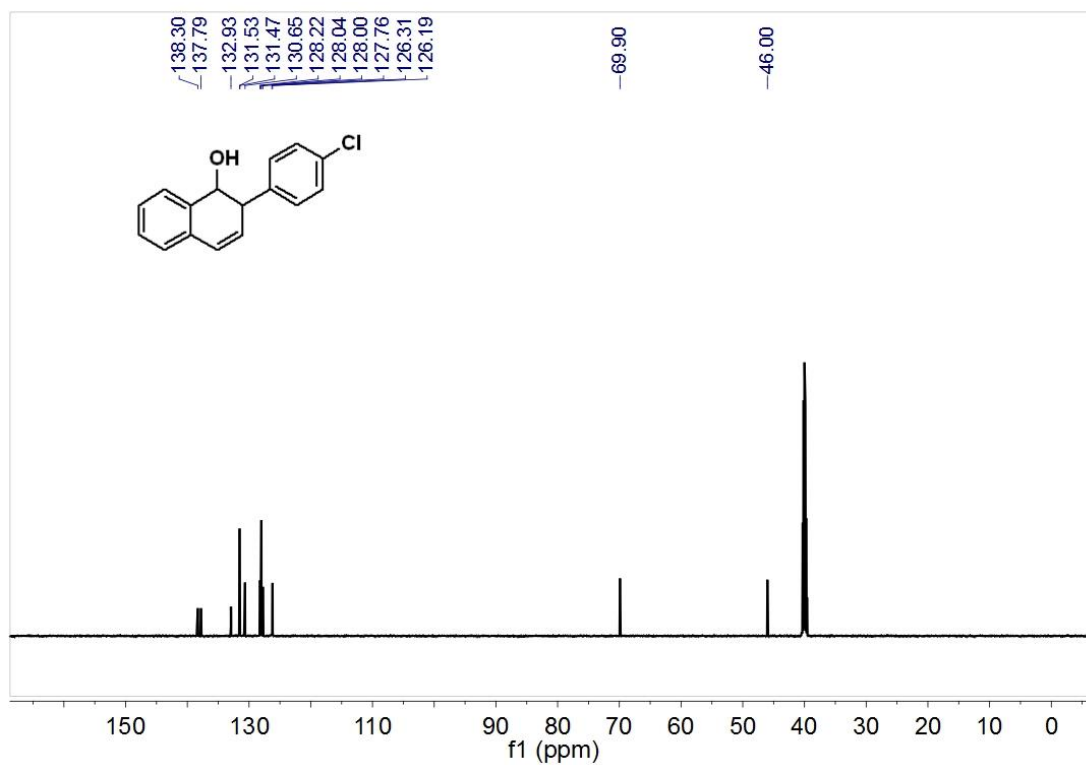


Figure S17. ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) for product **3g**.

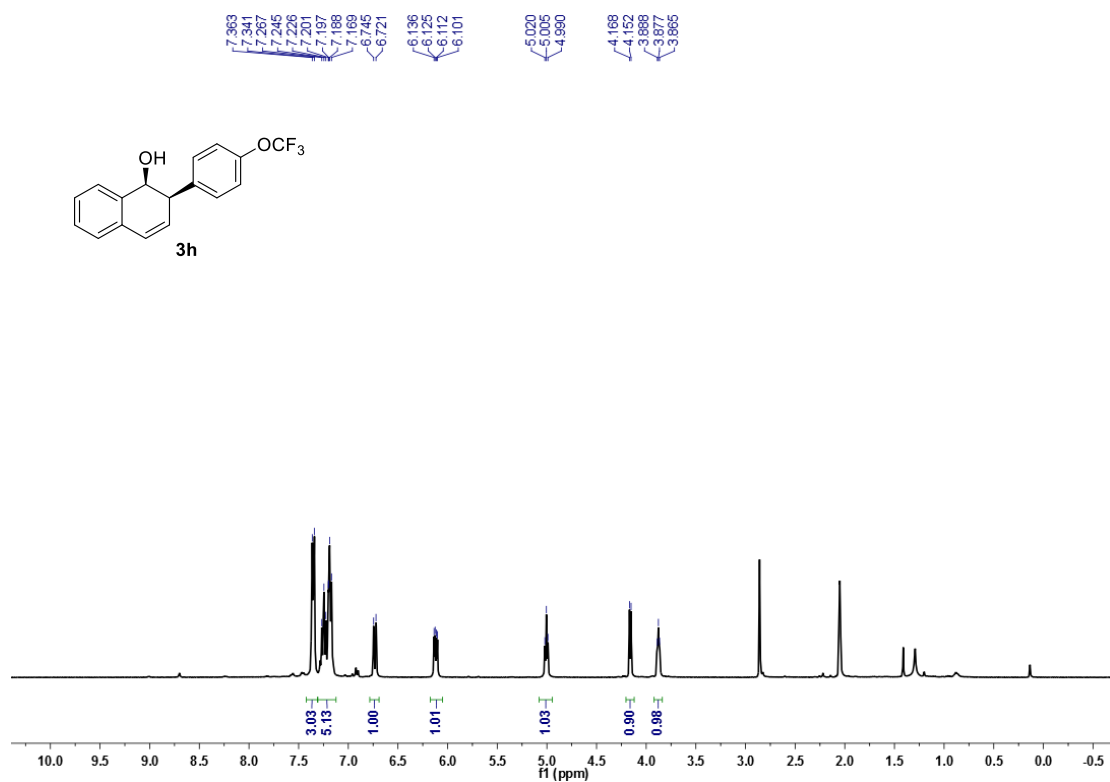


Figure S18. ¹H NMR (400 MHz, Acetone-*d*₆) for product **3h**.

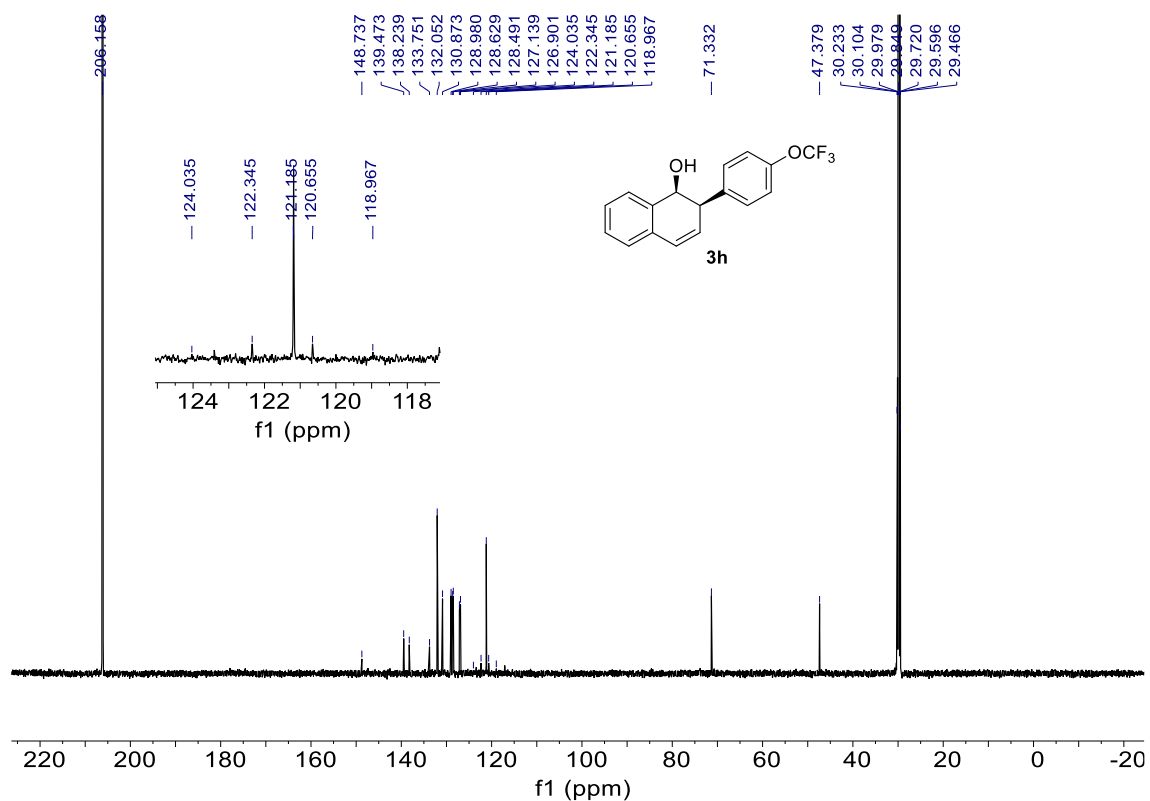


Figure S19. ¹³C NMR (101 MHz, Acetone-*d*₆) for product **3h**.

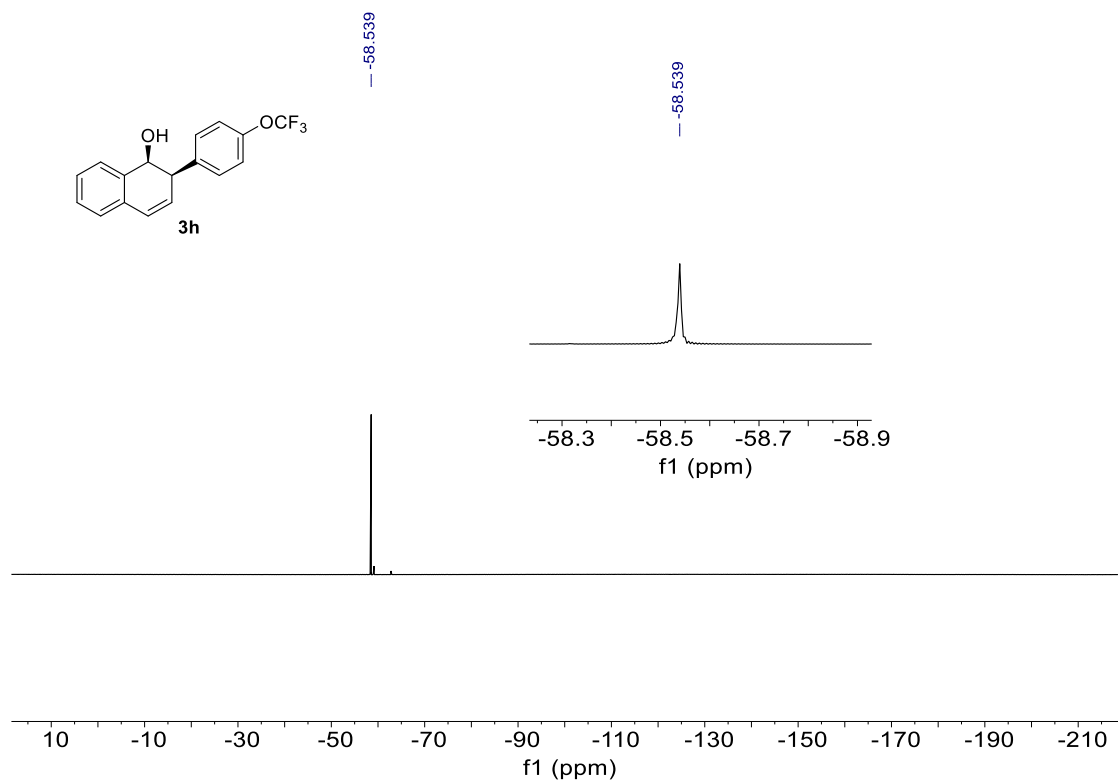


Figure S20. ^{19}F NMR (376 MHz, Acetone- d_6) for product **3h**.

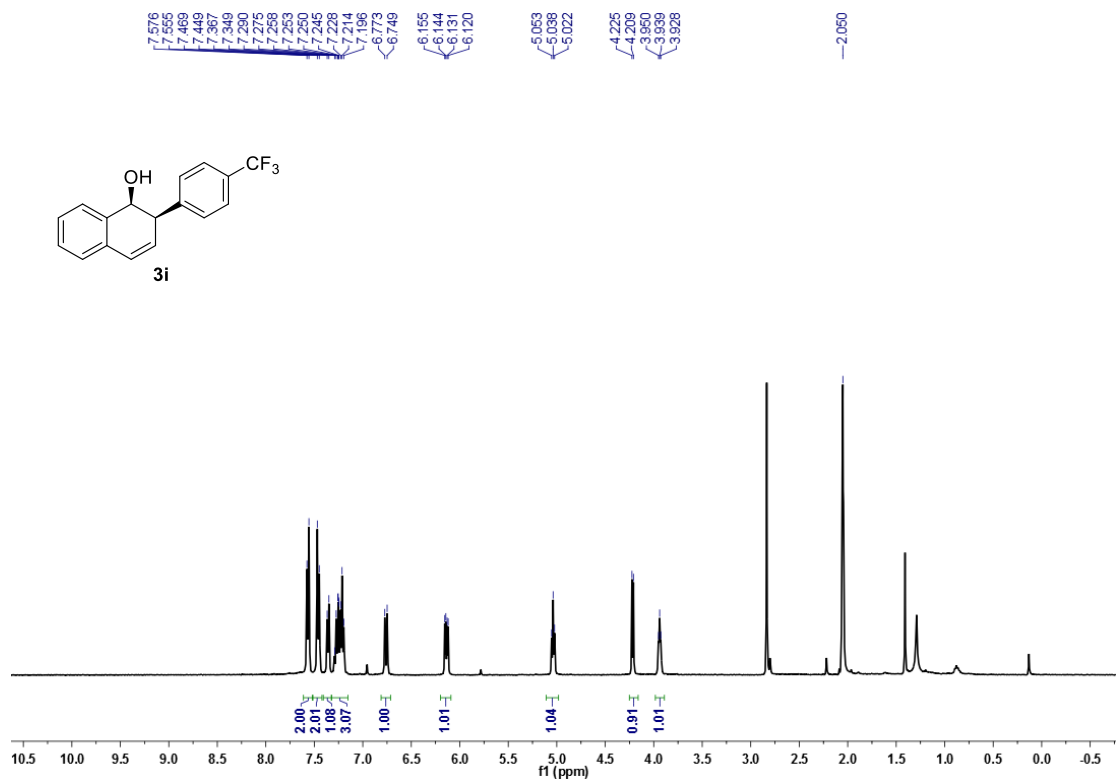


Figure S21. ^1H NMR (400 MHz, Acetone- d_6) for product **3i**.

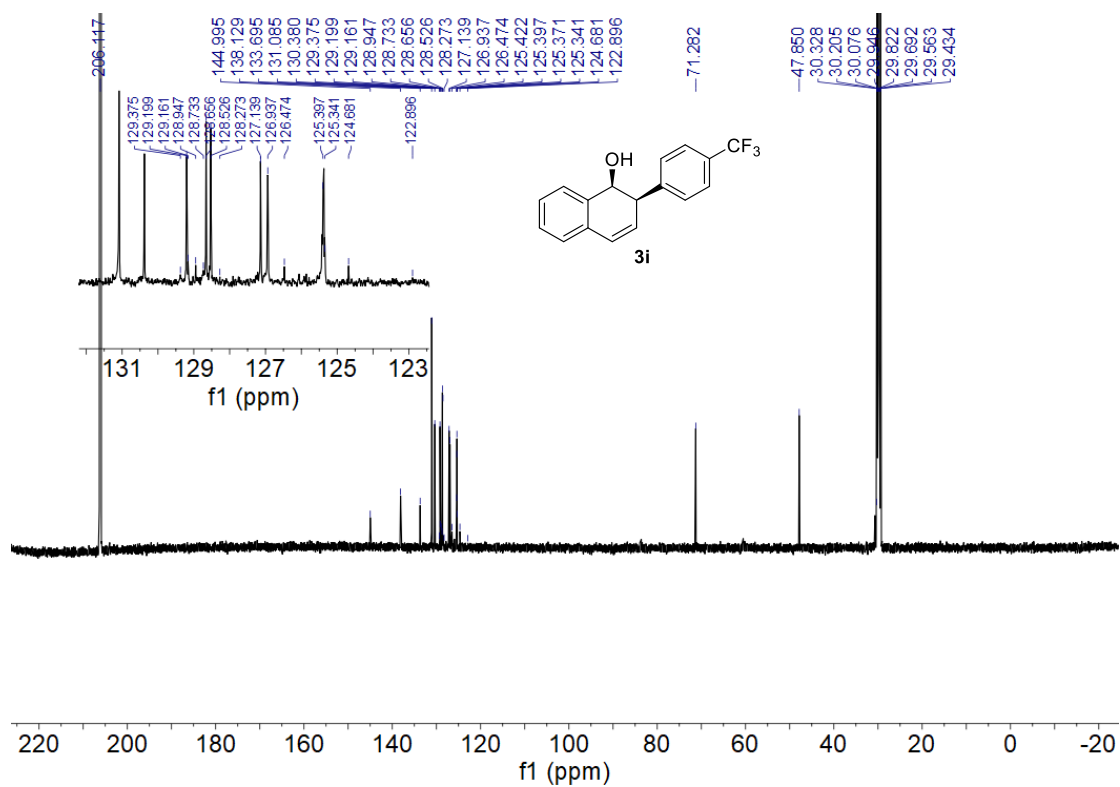


Figure S22. ^{13}C NMR (151 MHz, Acetone- d_6) for product **3i**.

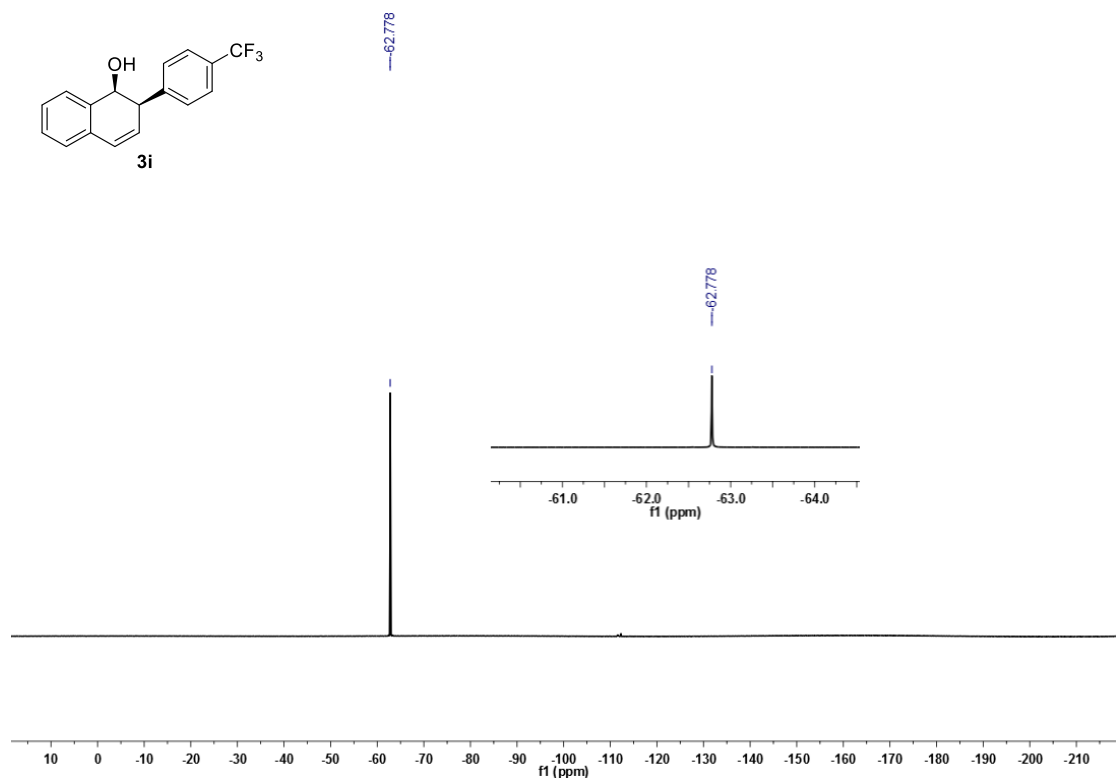


Figure S23. ^{19}F NMR (376 MHz, Acetone- d_6) for product **3i**.

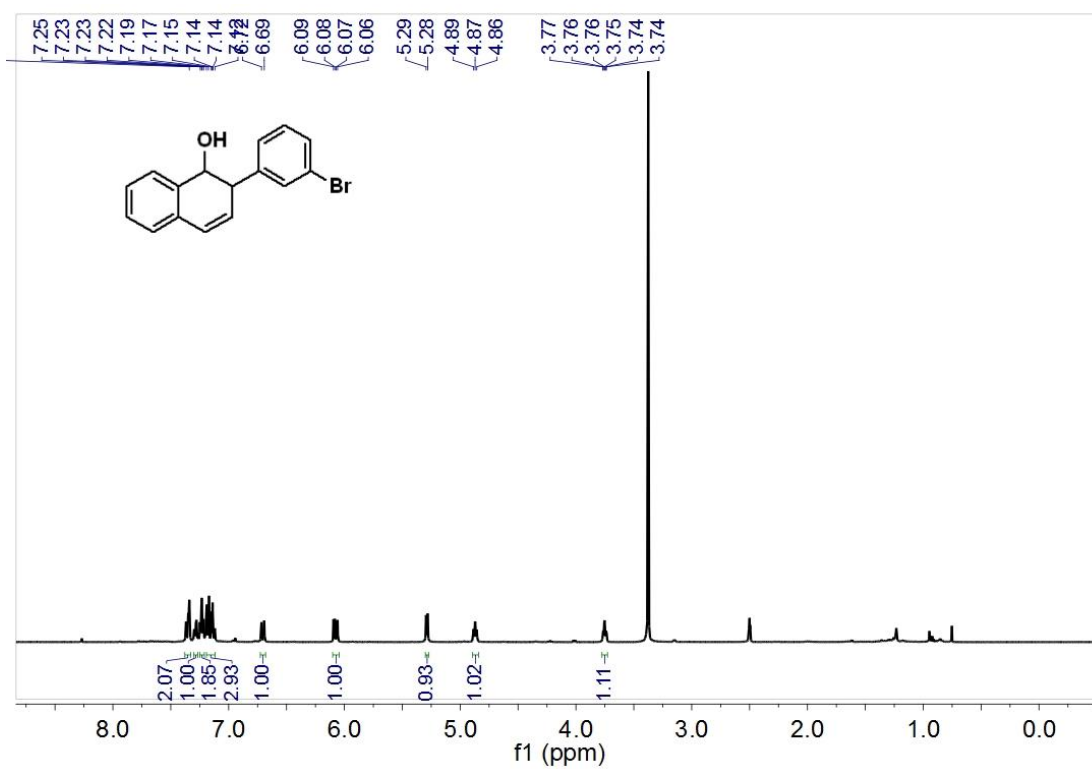


Figure S24. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) for product 3j.

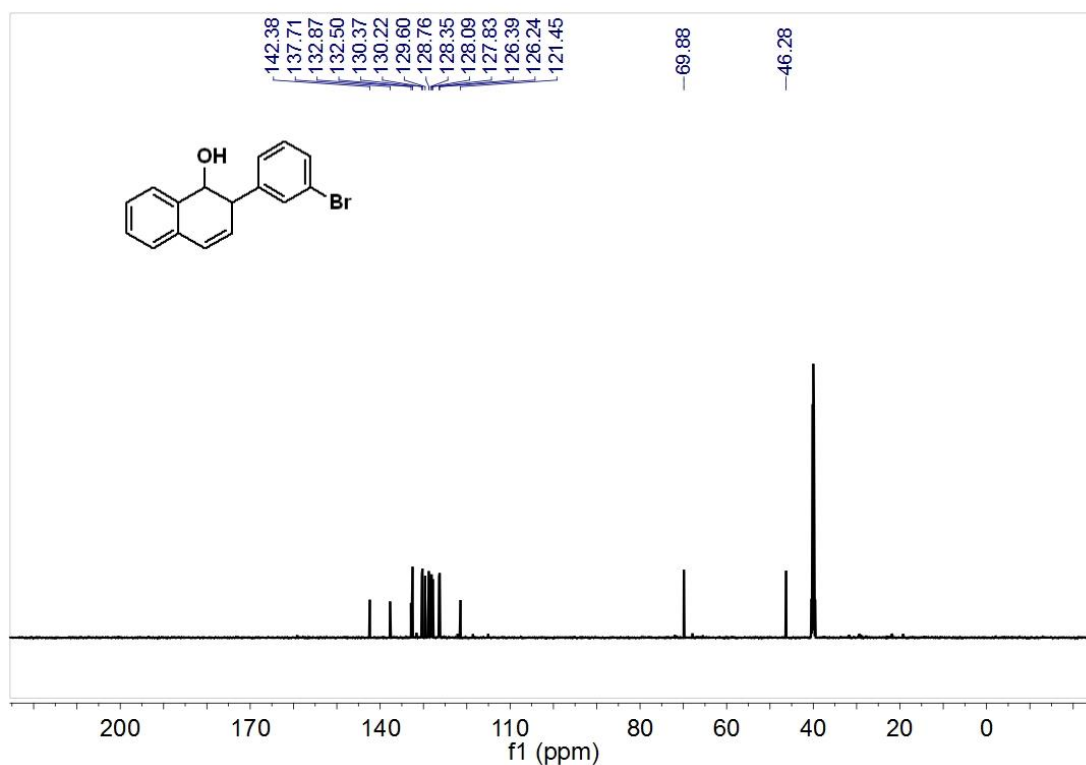


Figure S25. ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) for product 3j.

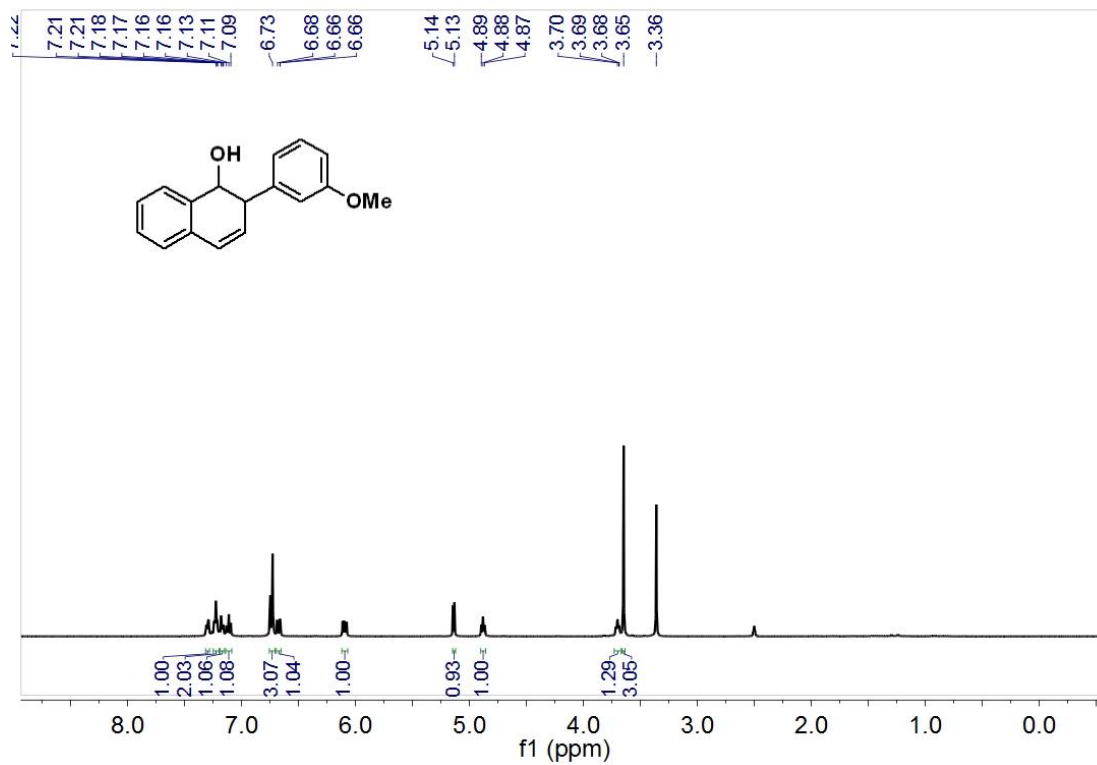


Figure S26. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) for product **3k**.

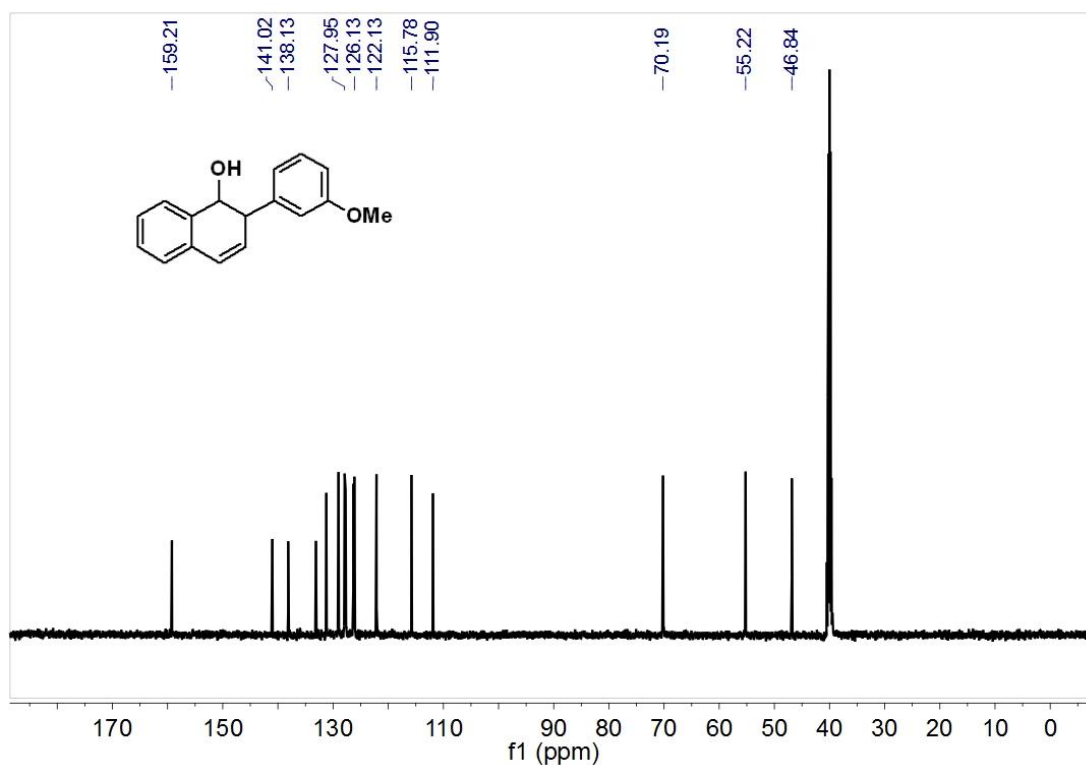


Figure S27. ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) for product **3k**.

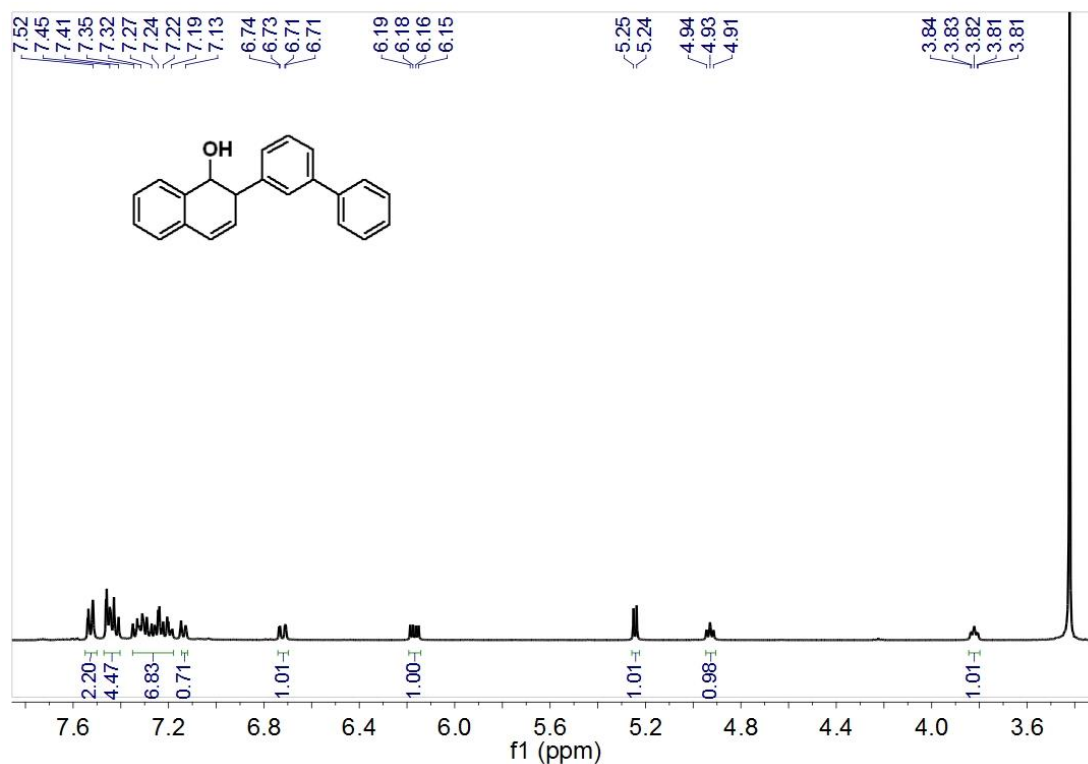


Figure S28. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) for product **31**.

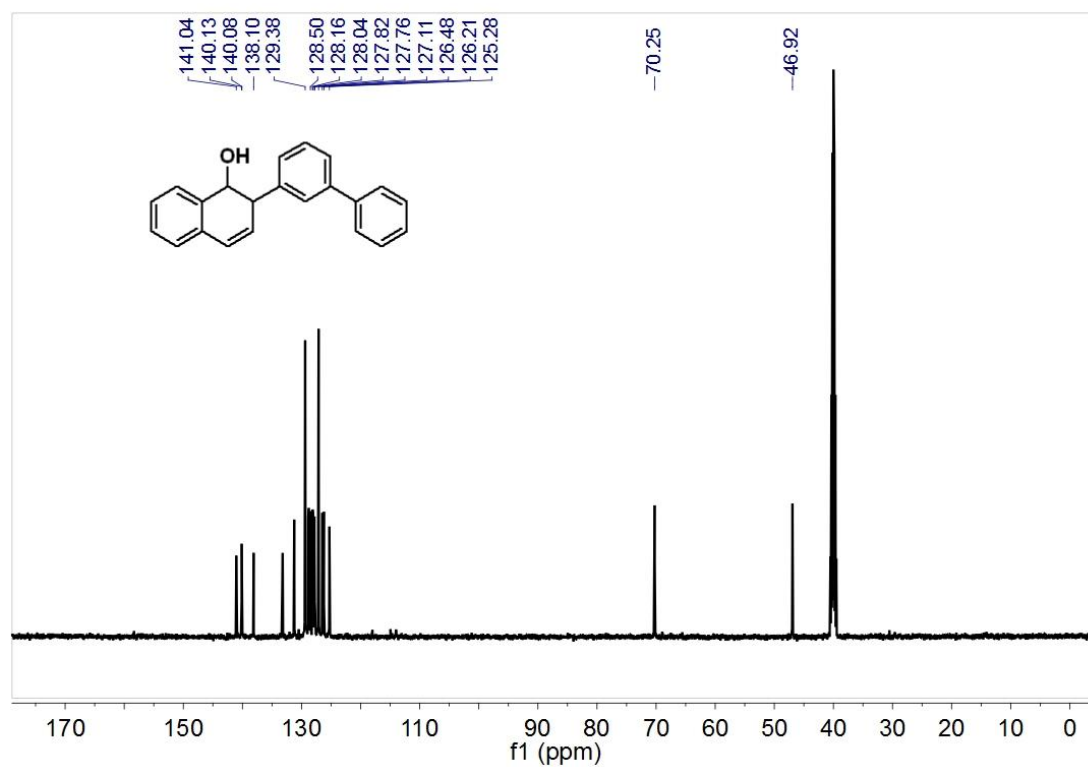


Figure S29. ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) for product **31**.

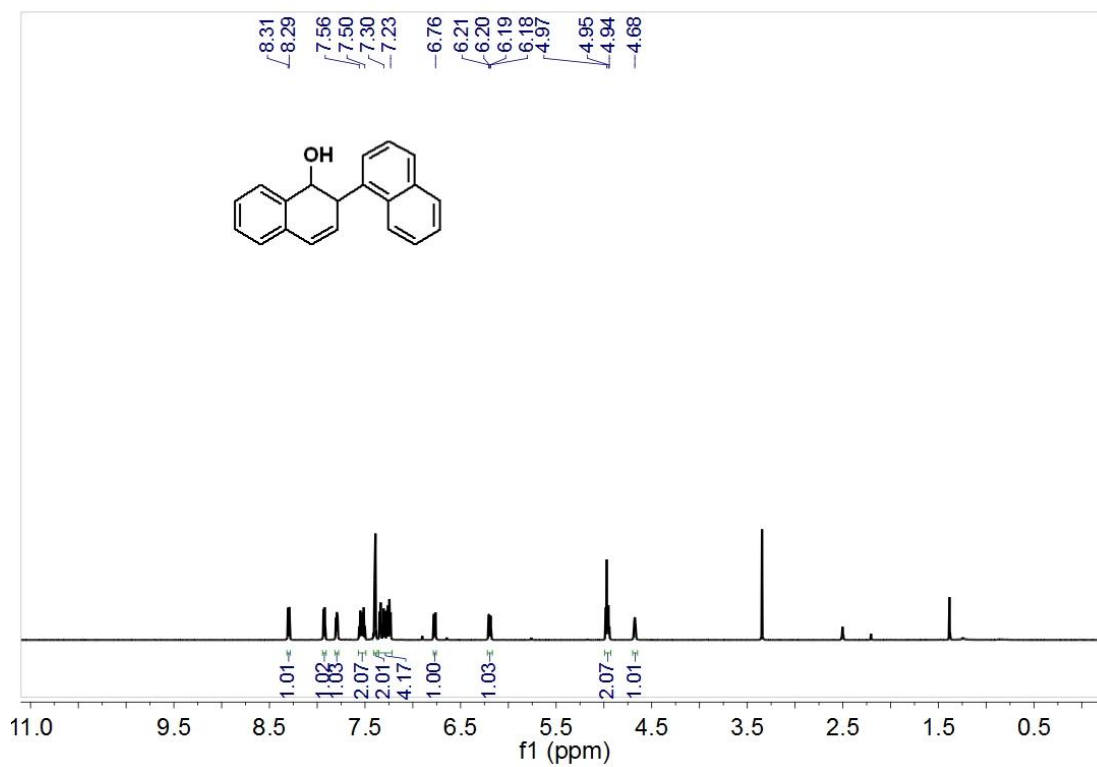


Figure S30. ^1H NMR (600 MHz, $\text{DMSO-}d_6$) for product **3m**.

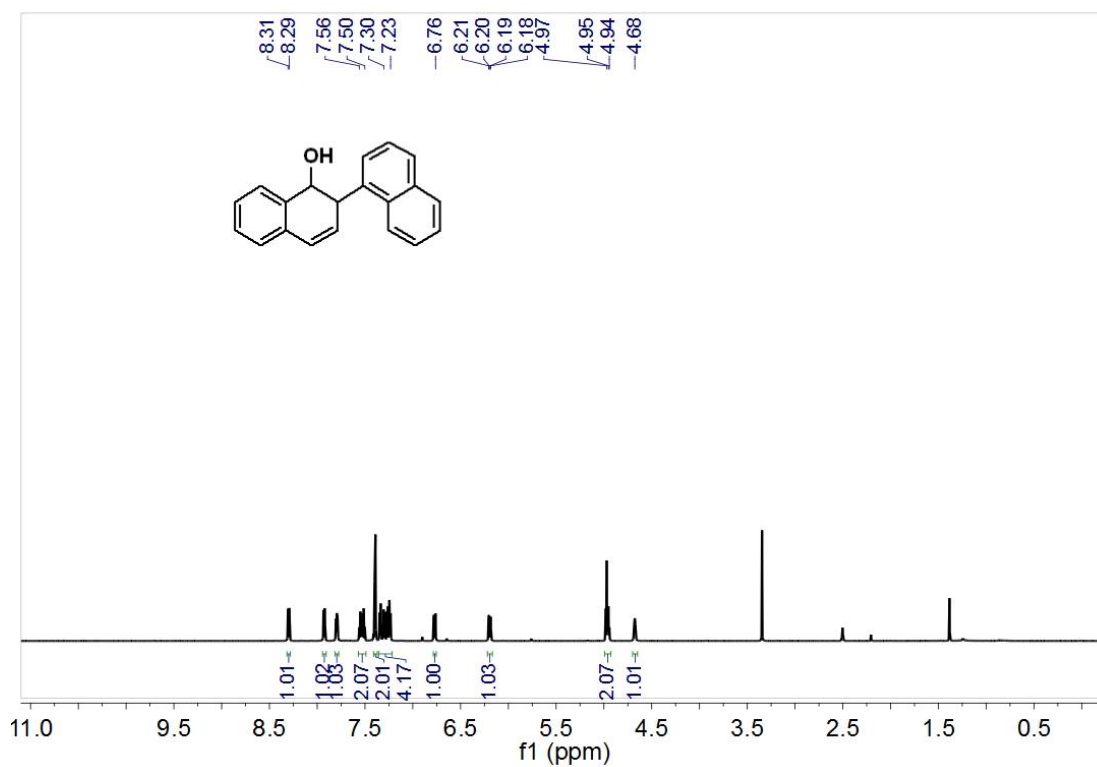


Figure S31. ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) for product **3m**.

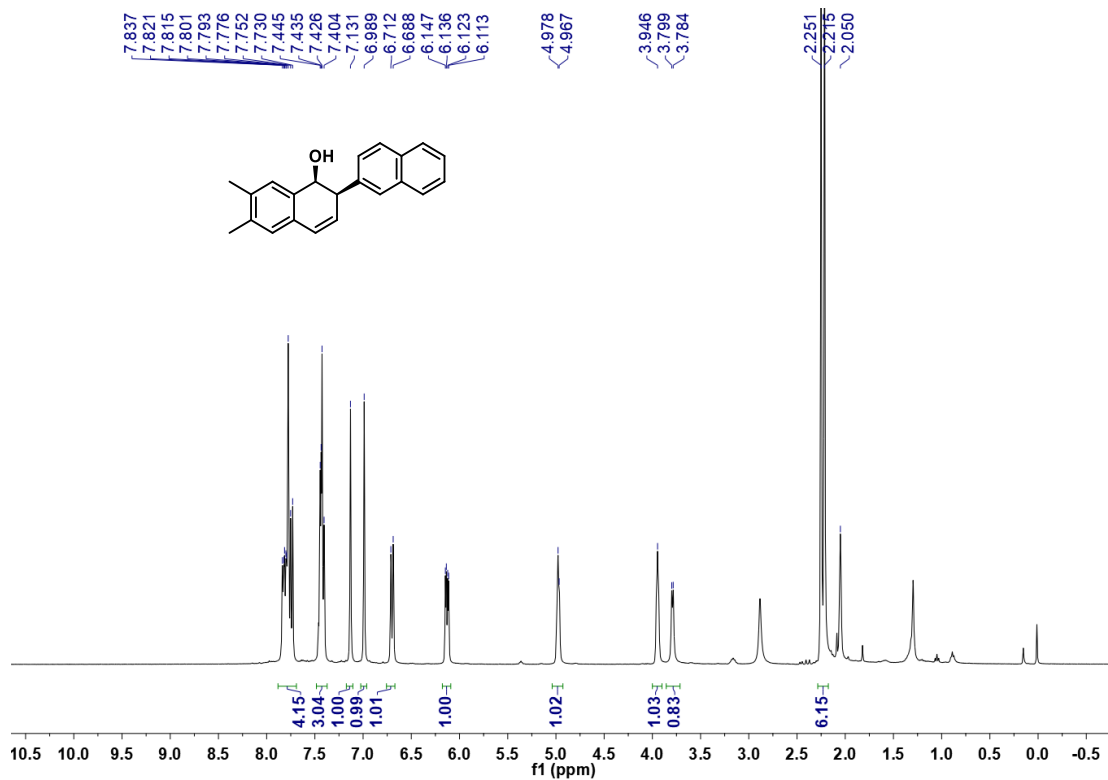


Figure S32. ^1H NMR (400 MHz, acetone- d_6) for product **3p**.

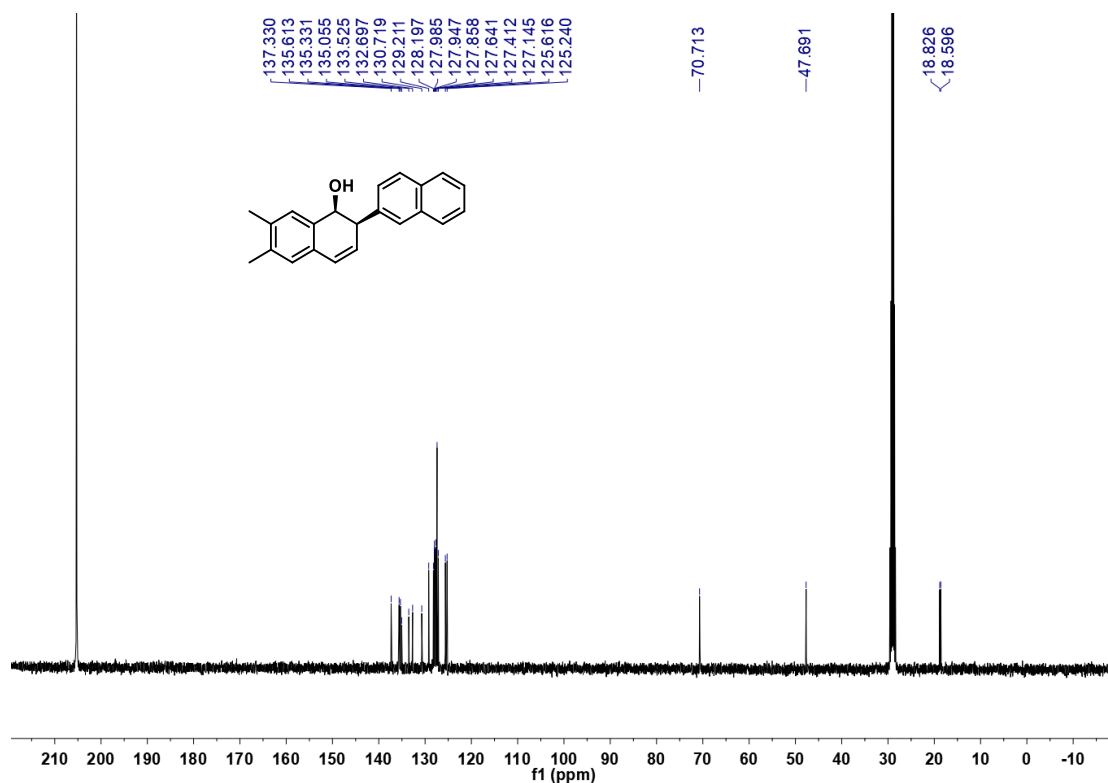


Figure S33. ^{13}C NMR (101 MHz, acetone- d_6) for product **3p**.

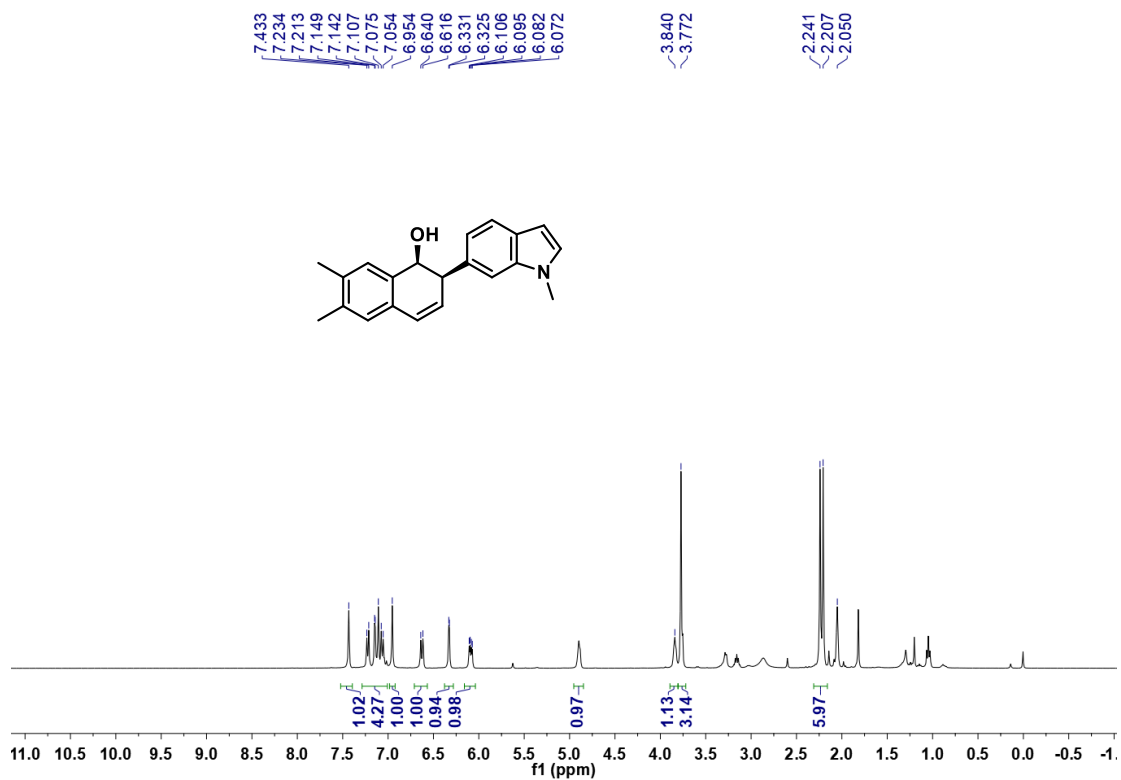


Figure S34. ¹H NMR (400 MHz, acetone-*d*₆) for product **3q**.

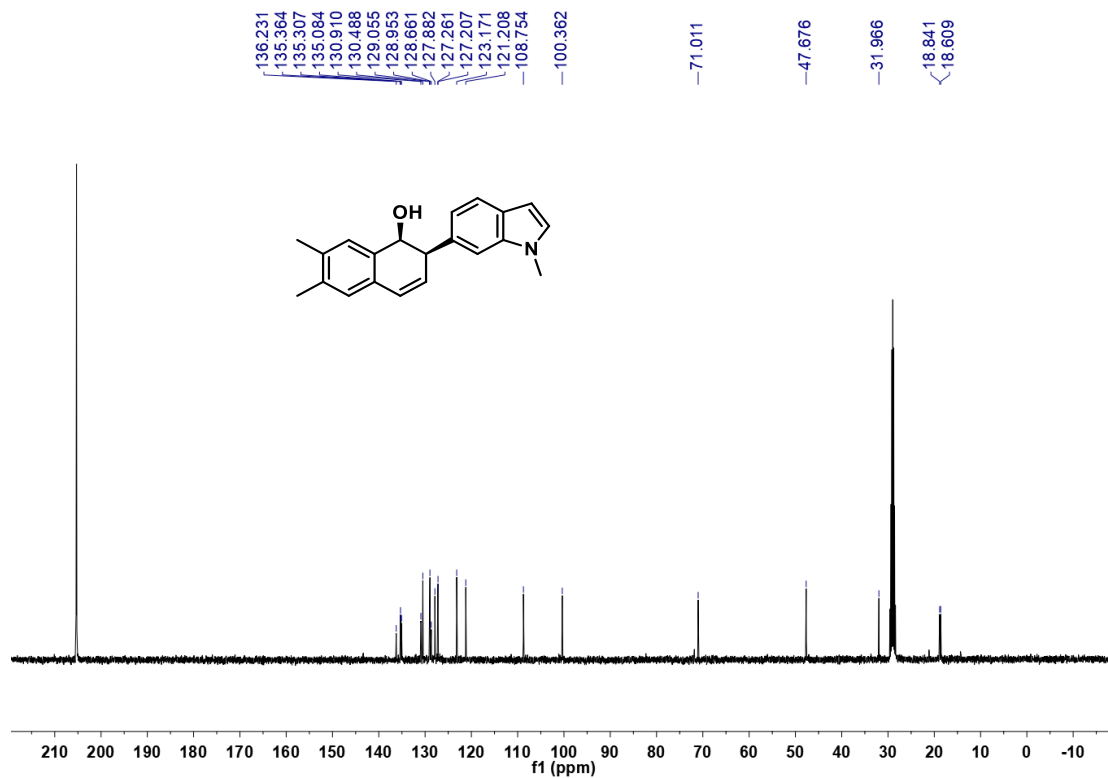


Figure S35. ¹³C NMR (101 MHz, acetone-*d*₆) for product **3q**.

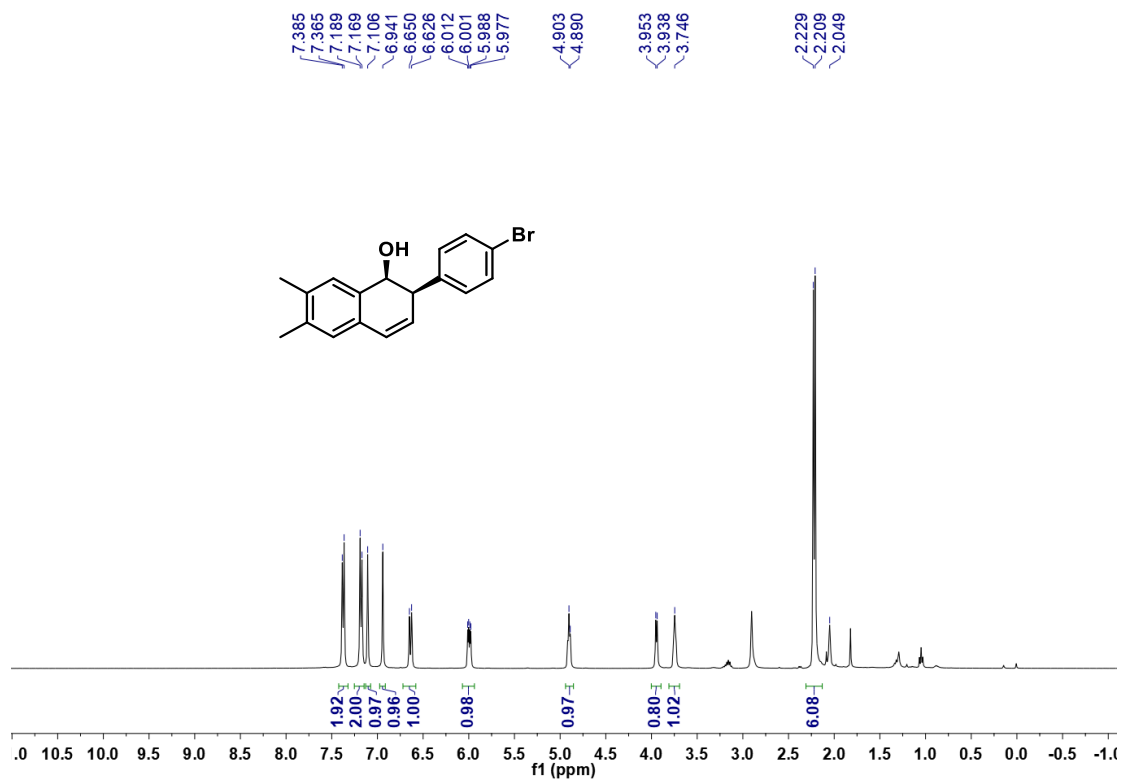


Figure S36. ¹H NMR (400 MHz, acetone-*d*₆) for product **3r**.

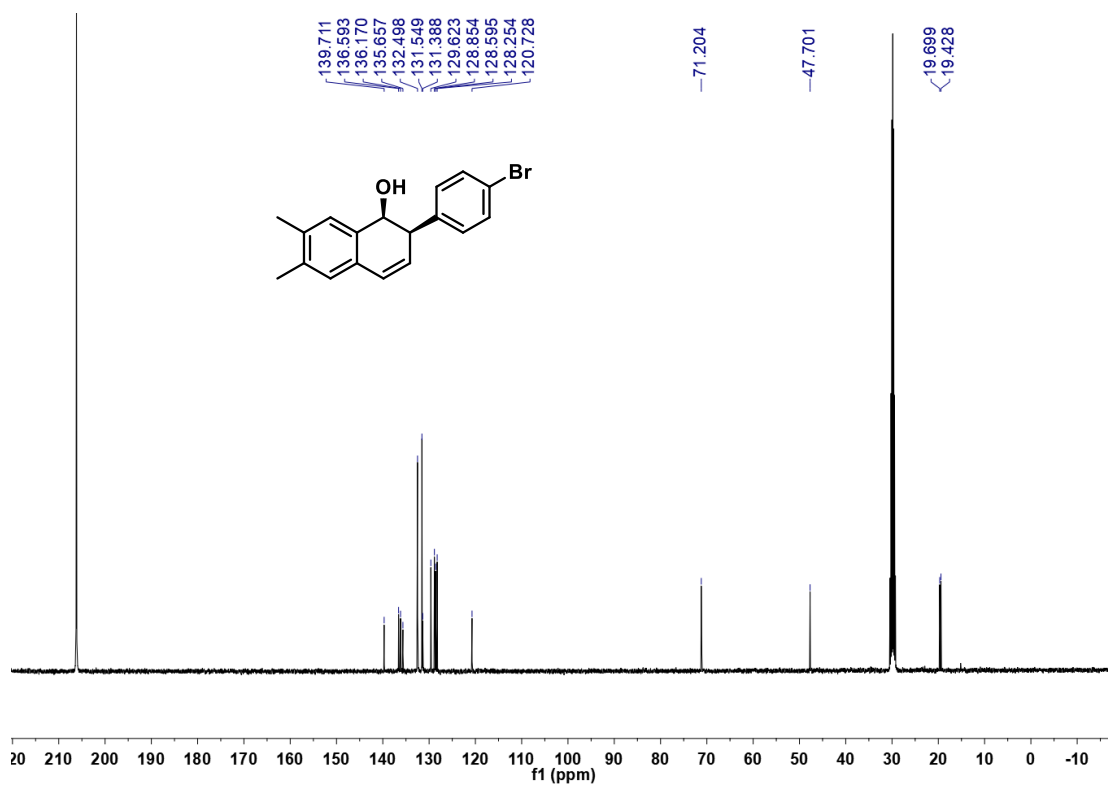


Figure S37. ¹³C NMR (101 MHz, acetone-*d*₆) for product **3r**.

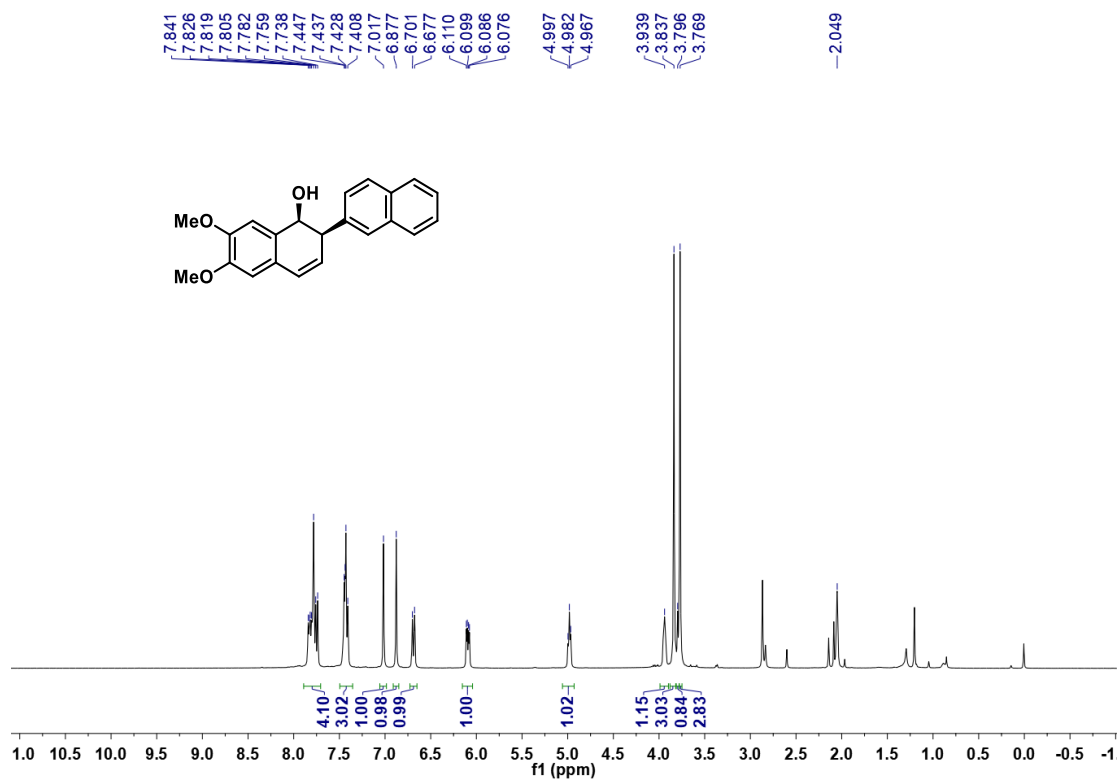


Figure S38. ¹H NMR (400 MHz, acetone-*d*₆) for product **3e**.

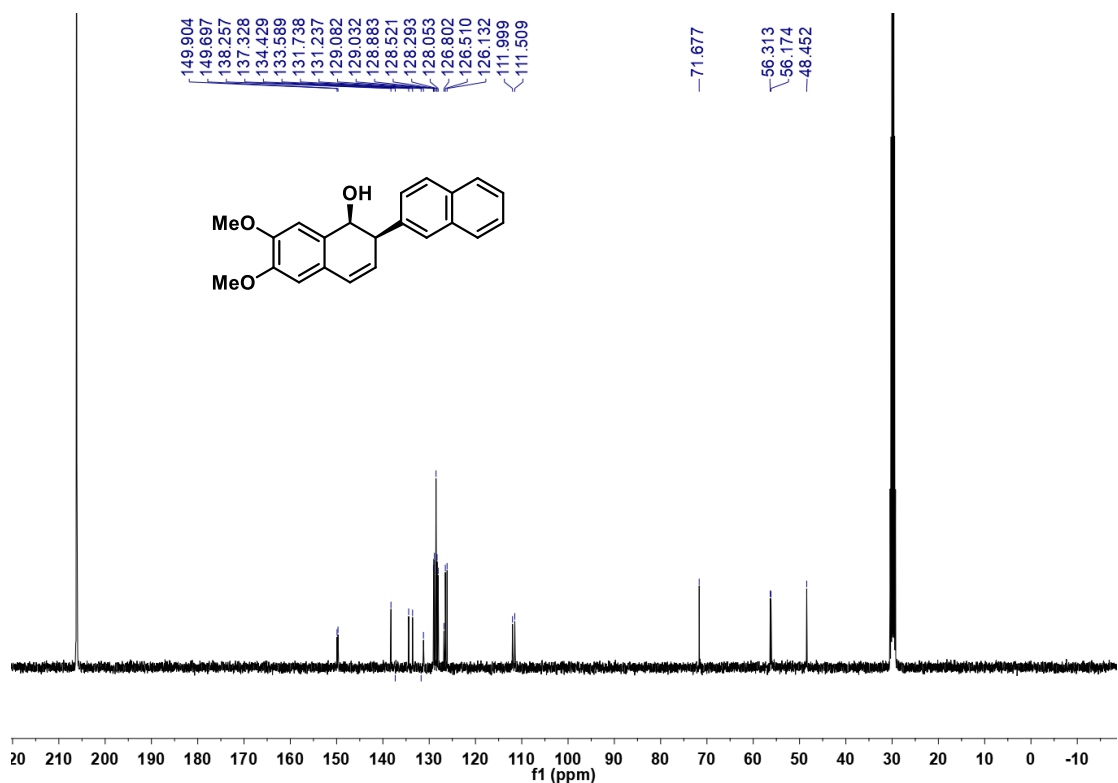


Figure S39. ¹³C NMR (101 MHz, acetone-*d*₆) for product **3e**.

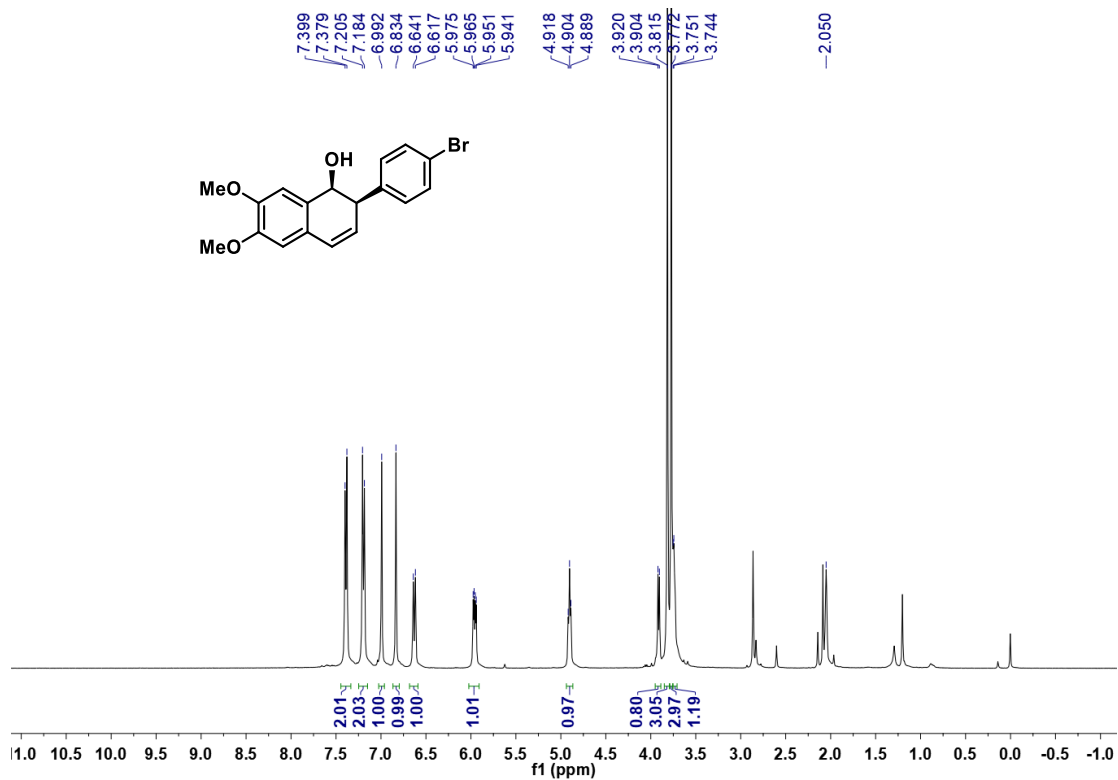


Figure S40. ^1H NMR (400 MHz, acetone- d_6) for product **3t**.

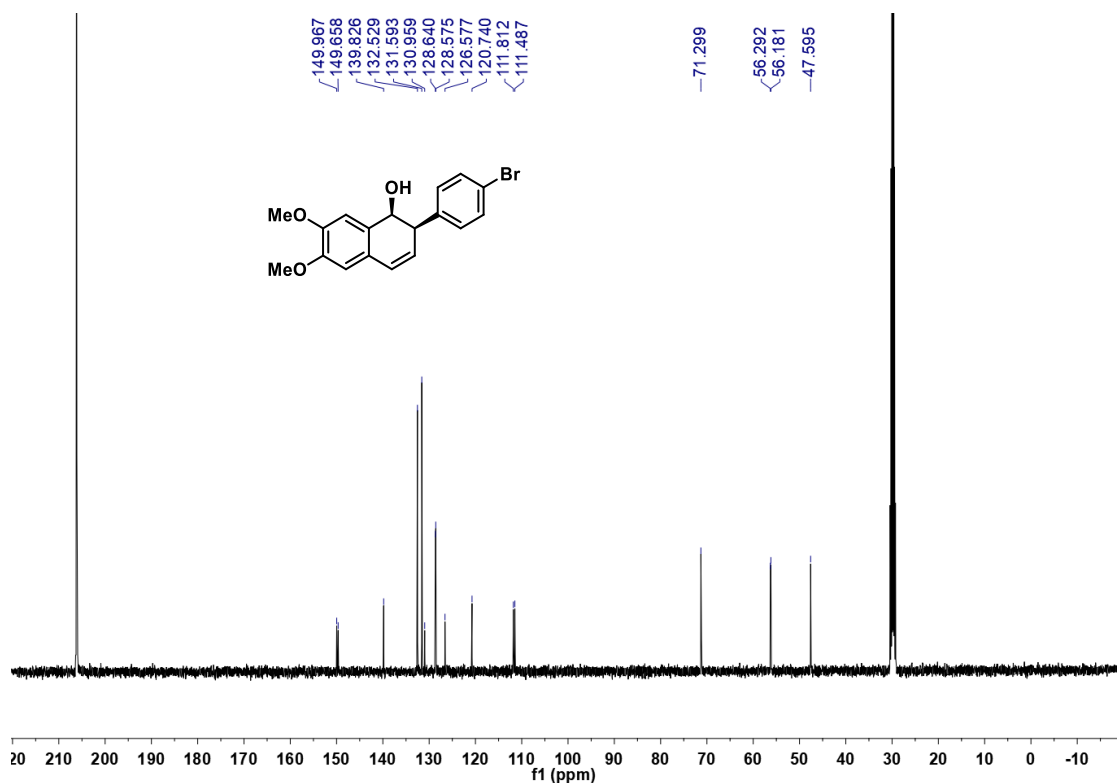


Figure S41. ^{13}C NMR (101 MHz, acetone- d_6) for product **3t**.

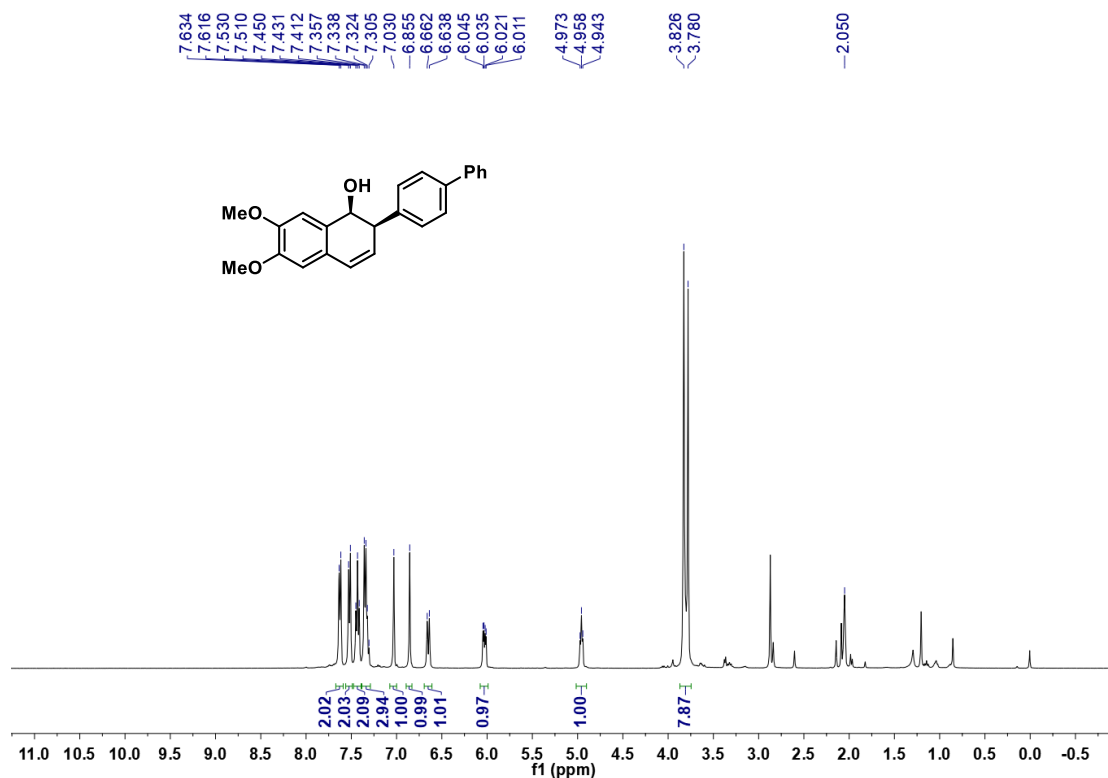


Figure S42. ¹H NMR (400 MHz, acetone-*d*₆) for product **3u**.

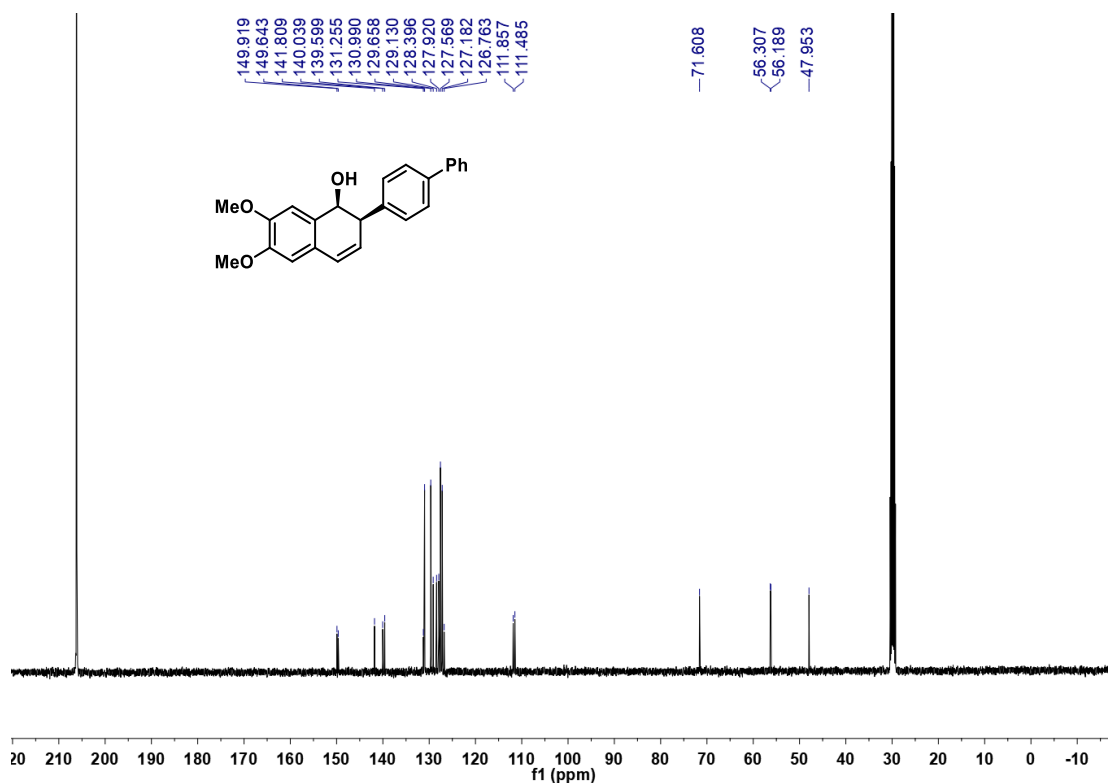


Figure S43. ¹³C NMR (101 MHz, acetone-*d*₆) for product **3u**.

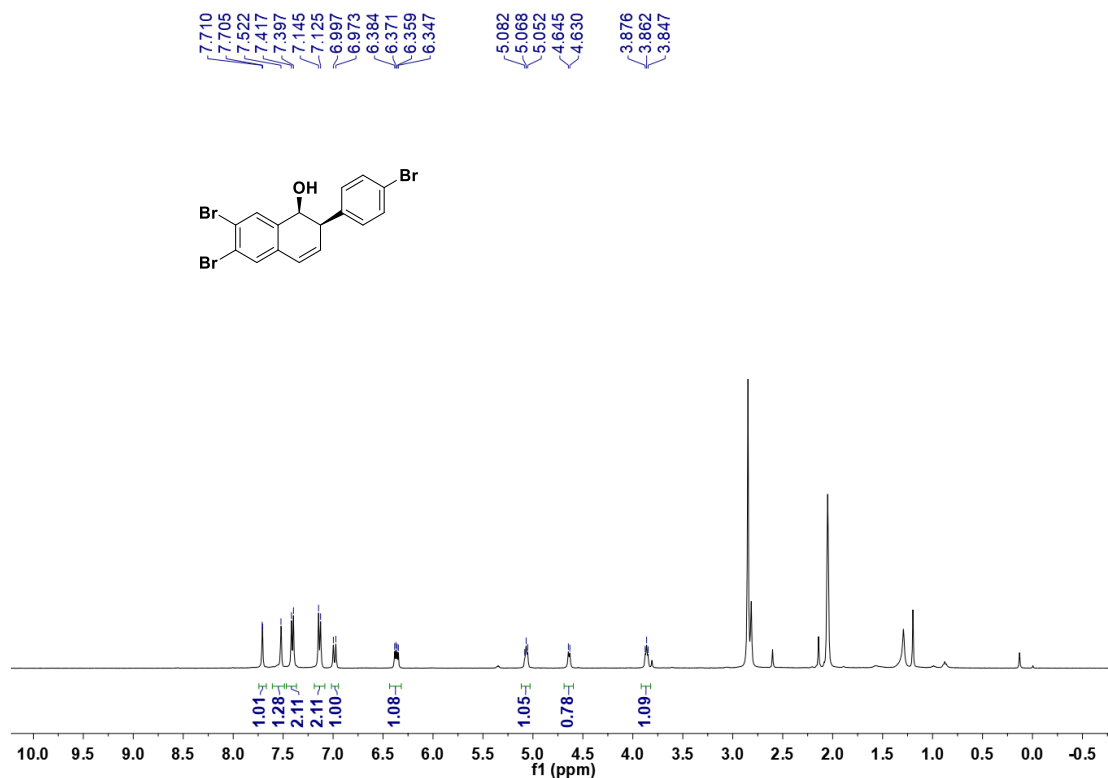


Figure S44. ¹H NMR (400 MHz, acetone-*d*₆) for product **3v**.

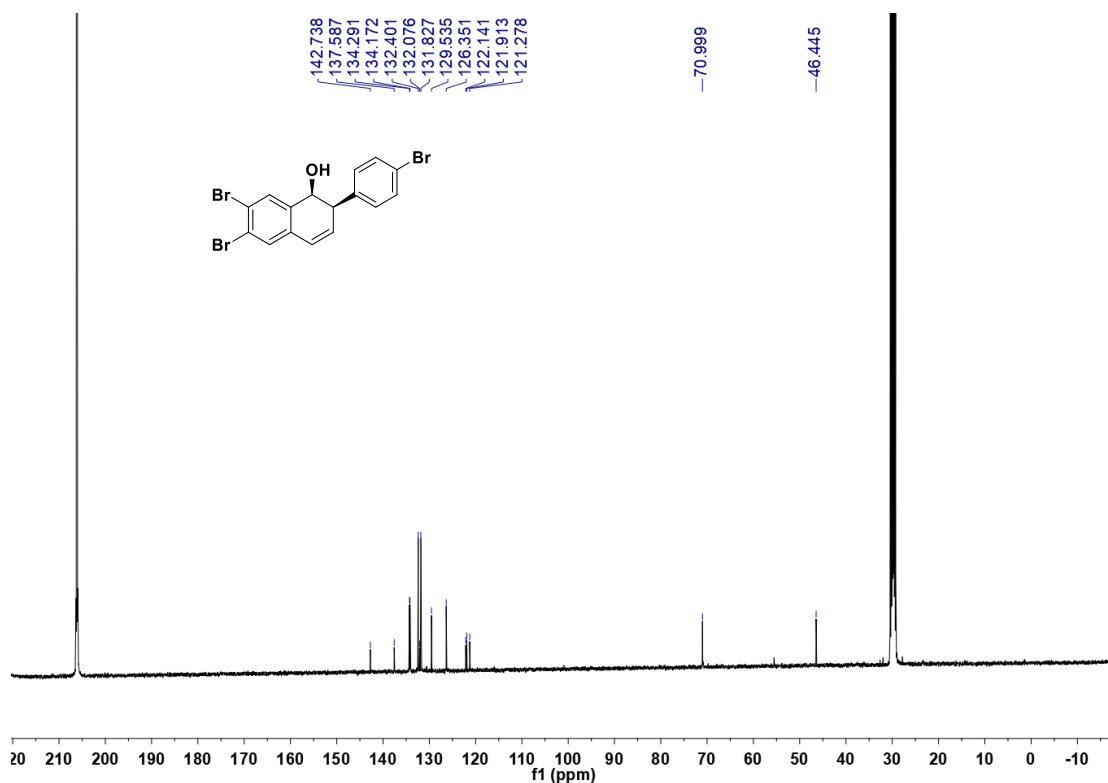


Figure S45. ¹³C NMR (101 MHz, acetone-*d*₆) for product **3v**.

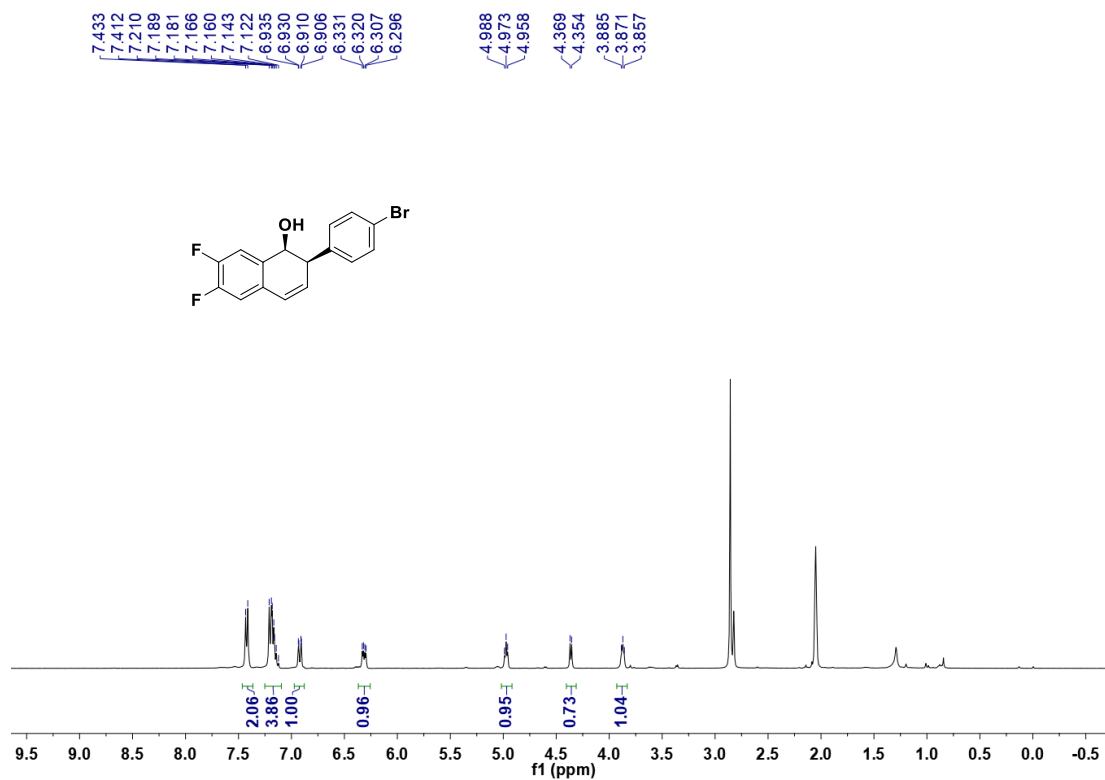


Figure S46. ¹H NMR (400 MHz, acetone-*d*₆) for product **3w**.

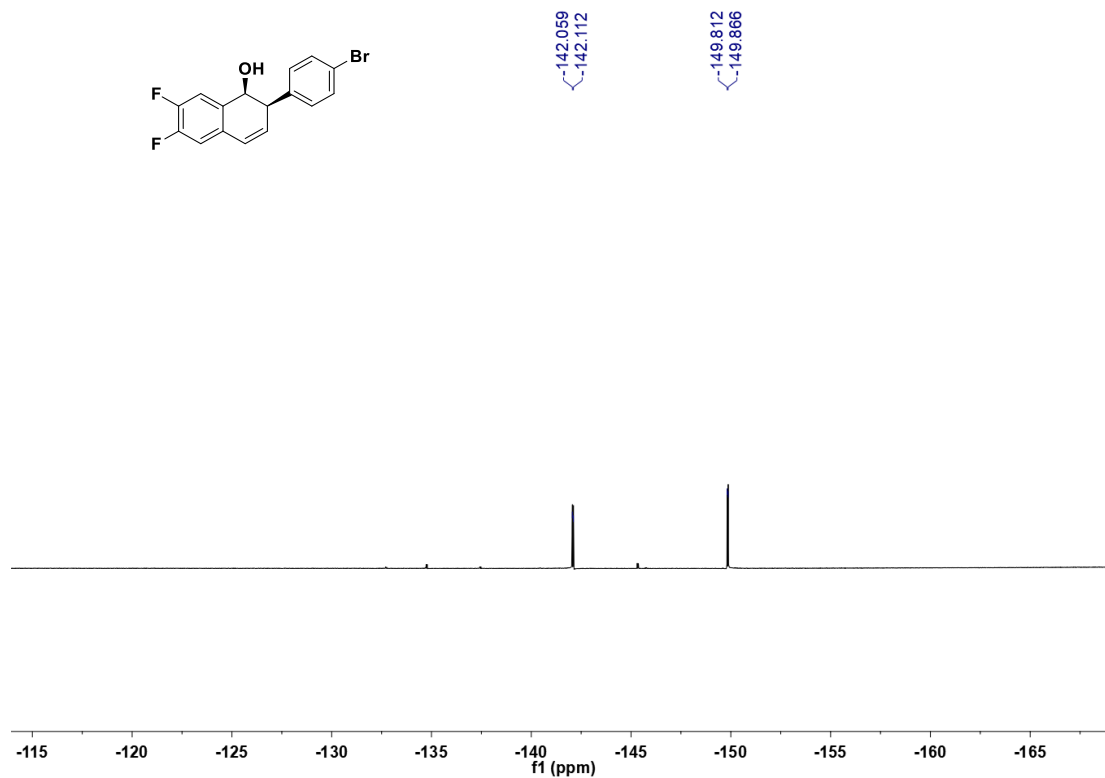


Figure S47. ¹⁹F NMR (376 MHz, acetone-*d*₆) for product **3w**.

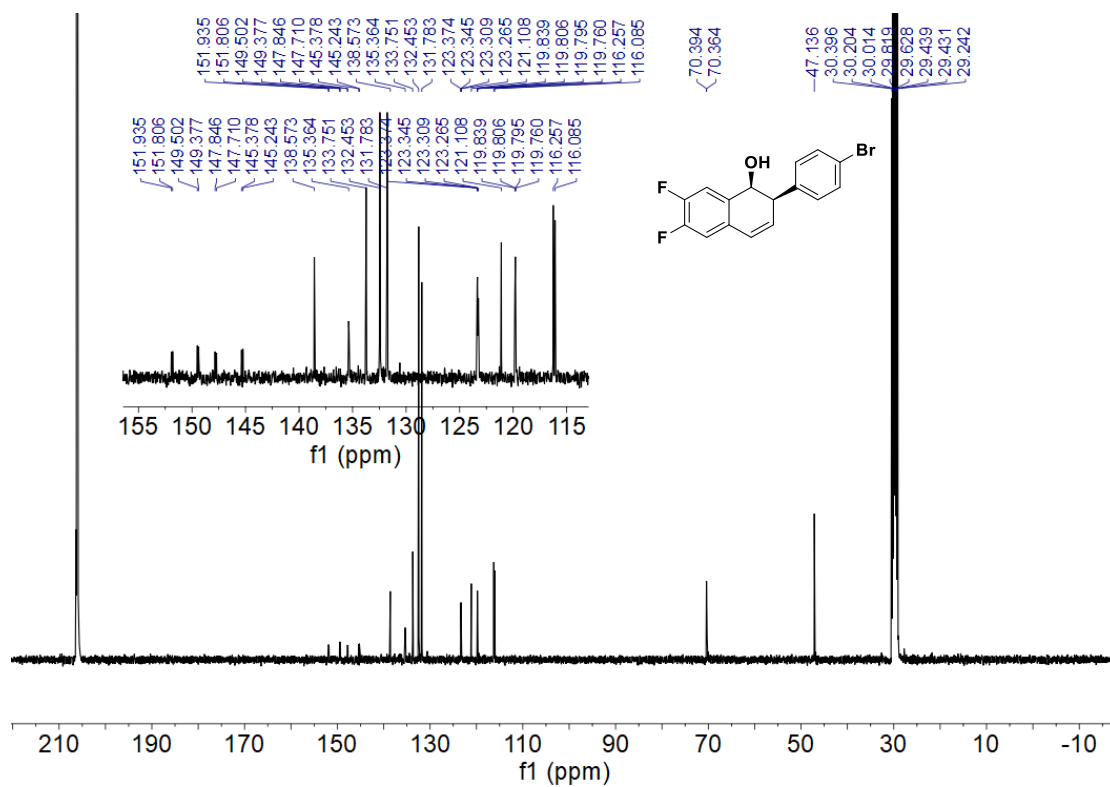


Figure S48. ^{13}C NMR (101 MHz, acetone- d_6) for product 3w.

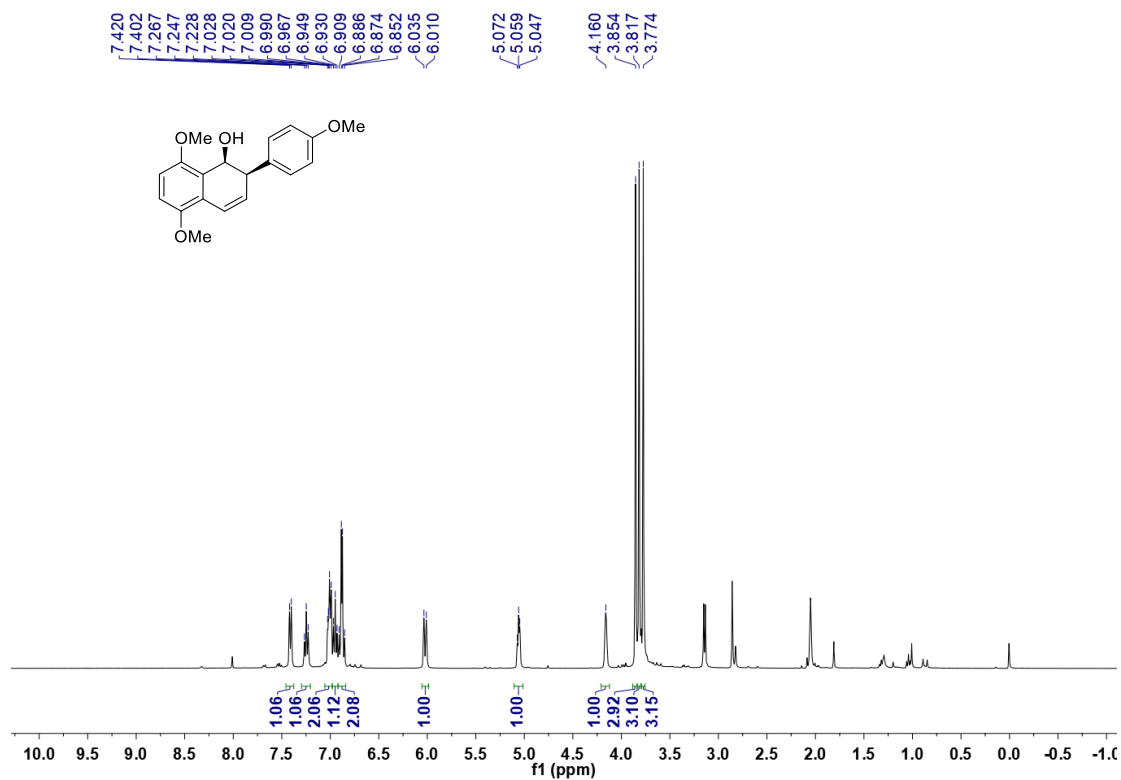


Figure S49. ^1H NMR (400 MHz, acetone- d_6) for product 3x.

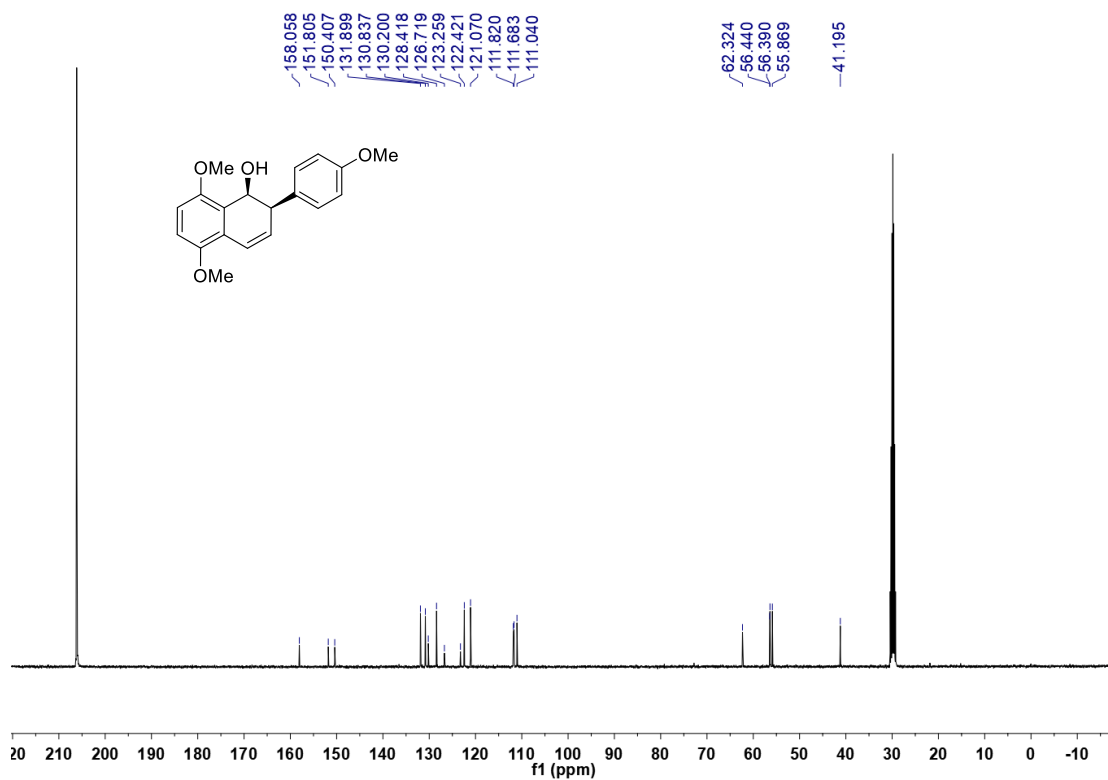
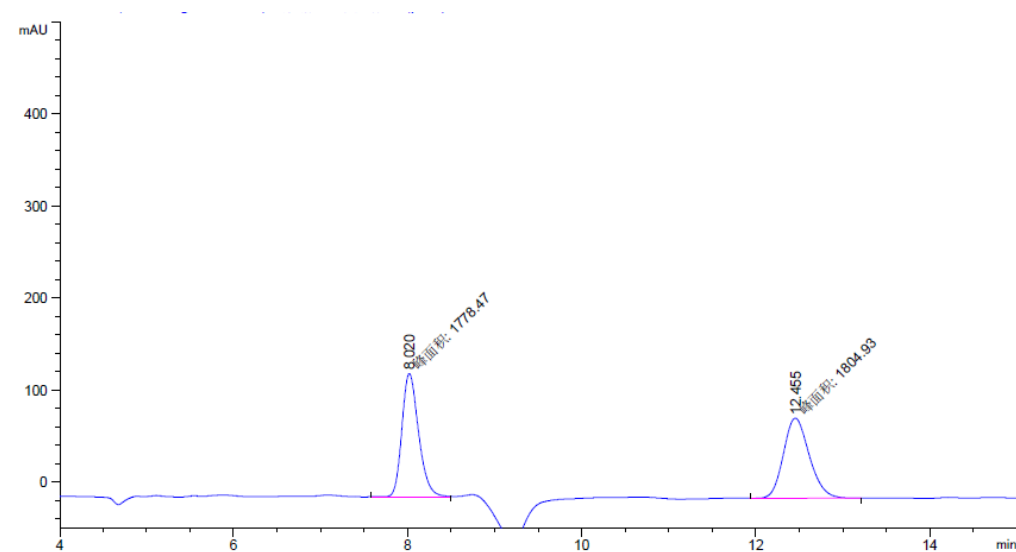


Figure S50. ^{13}C NMR (101 MHz, acetone- d_6) for product **3x**.

HPLC analysis of 3a*

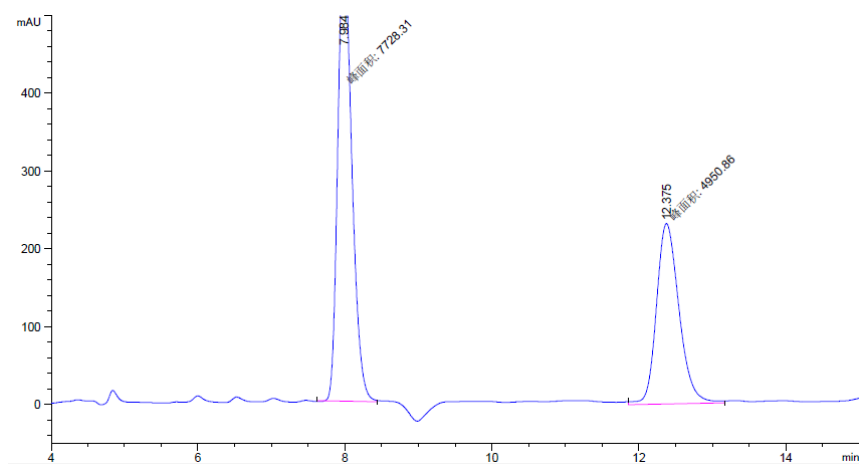
HPLC conditions: chiralpak OD-H column, hexane/*i*-PrOH = 90/10, 1.0ml/min, $\lambda=254$ nm

Racemic sample:



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.020	MM	0.2212	1778.46765	133.97203	49.6307
2	12.455	MM	0.3454	1804.93408	87.10378	50.3693

Chiral sample:



信号 1: VWD1 A, Wavelength=250 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.984	MM	0.2200	7728.30762	585.58112	60.9528
2	12.375	MM	0.3560	4950.86328	231.75279	39.0472