Supporting Information for

"Expedient Access to Unsymmetrical Triarylmethanes through *N*-Heterocyclic Carbene Catalysed 1,6-Conjugate Addition of 2-Naphthols to *para*-Quinone Methides"

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Experimental Section

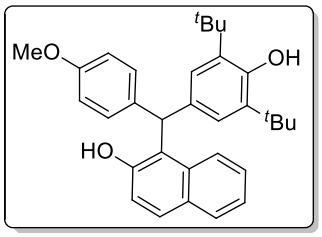
General methods

All reactions were carried out under an argon atmosphere in an oven dried vial. Solvents were dried over calcium hydride, distilled and stored with molecular sieves. Melting points were recorded on SMP20 melting point apparatus and are uncorrected. ^{1}H, ^{13}C and ^{19}F spectra were recorded in $CDCl_3$ (400, 100 and 376 MHz respectively) on Bruker FT-NMR spectrometer. Chemical shift (δ) values are reported in parts per million relative to TMS (for ^{1}H and ^{13}C) and $BF_3.Et_2O$ (for ^{19}F). High resolution mass spectra were recorded on Waters Q-TOF Premier-HAB213 spectrometer. FT-IR spectra were recorded on a Perkin–Elmer FTIR spectrometer. Single crystal X-ray data was collected using XtaLabmini X-ray difractometer. Enantiomeric excess was determined by using Waters Chiral HPLC. Most of the reagents and starting materials were purchased from commercial sources and used as such. NHC precursors were prepared according to the literature procedure.[1] All *p*-quinone methides were prepared by following a literature procedure.[2] Thin layer chromatography was performed on Merck silica gel 60 F_{254} TLC plates. Column chromatography was carried out through silica gel (100-200 mesh) using EtOAc/hexane as an eluent.

General procedure for the 1,6-conjugate addition of 2-naphthol to p-quinone methides:

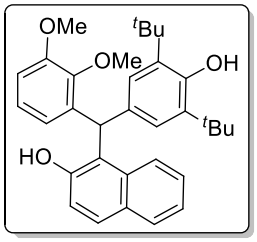
Anhydrous CH_2Cl_2 (0.3 mL) was added to the mixture of *p*-quinone methide (0.0620 mmol), 2-naphthol (0.0680 mmol), catalyst **4** (0.0062 mmol) and sodium hydride (55-60% suspension in mineral oil) (0.0124 mmol) under argon atmosphere, and the resulting suspension was stirred at room temperature until *p*-quinone methide was completely consumed. The reaction mixture was purified through silica gel column without further workup, using EtOAc/Hexane mixture as an eluent to get the pure product.

1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(4-methoxyphenyl)methyl]naphthalen-2-ol (3)



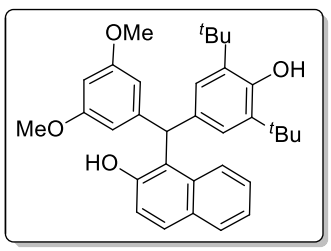
The reaction was performed at 0.062 mmol scale of *p*-quinone methide (**1**); pale yellow solid; yield 99% (28.6 mg); R_f = 0.5 (20% EtOAc in hexane); m.p. 170–172 °C; FT-IR (KBr) 3627, 3462, 2959, 1510, 1435, 1250, 743 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 8.02 (d, J = 8.6 Hz, 1H), 7.78 (dd, J = 7.9, 1.0 Hz, 1H), 7.71 (d, J = 8.8 Hz, 1H), 7.43 (ddd, J = 8.4, 6.8, 1.4 Hz, 1H), 7.34–7.30 (m, 1H), 7.16 (d, J = 8.6 Hz, 2H), 7.06 (d, J = 8.8 Hz, 1H), 7.02 (s, 2H), 6.84 (d, J = 8.8 Hz, 2H), 6.23 (s, 1H), 5.44 (s, 1H), 5.20 (s, 1H), 3.78 (s, 3H), 1.33 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 153.14, 153.13, 136.8, 134.1, 133.5, 132.2, 130.1, 129.6, 129.5, 128.8, 126.8, 125.7, 123.1, 123.0, 120.6, 120.1, 114.4, 55.4, 47.9, 34.5, 30.3; HRMS (ESI): *m/z* calcd for $C_{32}H_{37}O_3$ $[M+H]^+$: 469.2742; found: 469.2736.

1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(2,3-dimethoxyphenyl)methyl]naphthalen-2-ol (3a)



The reaction was performed at 0.28 mmol scale of *p*-quinone methide (**1a**); yellow solid; yield 89% (125 mg); R_f = 0.6 (20% EtOAc in hexane); m.p. 169–171 °C; FT-IR (KBr) 3627, 3462, 2959, 1477, 1435, 1273, 747 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 8.08 (d, J = 8.6 Hz, 1H), 7.75 (dd, J = 8.1, 1.0 Hz, 1H), 7.70 (d, J = 8.9 Hz, 1H), 7.42 (ddd, J = 8.3, 6.8, 1.3 Hz, 1H), 7.32–7.28 (m, 1H), 7.06 (d, J, = 8.9 Hz, 1H), 7.03 (s, 2H), 6.99–6.95 (m, 1H), 6.84 (dd, J = 8.2, 1.4 Hz, 1H), 6.76 (dd, J = 7.8, 1.4 Hz, 1H), 6.67 (s, 1H), 5.78 (s, 1H), 5.20 (s, 1H), 3.88 (s, 3H), 3.49 (s, 3H), 1.33 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 153.1, 152.9, 146.8, 136.8, 136.6, 133.7, 131.8, 129.6, 129.3, 128.6, 126.8, 125.6, 124.5, 123.3, 123.1, 121.7, 120.4, 120.0, 111.4, 60.6, 55.9, 42.7, 34.6, 30.4; HRMS (ESI): *m/z* calcd for $C_{33}H_{39}O_4$ $[M+H]^+$: 499.2848; found: 499.2837.

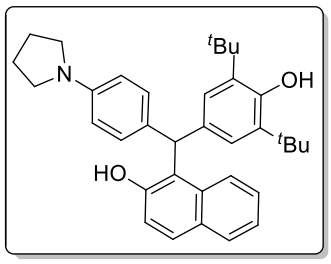
1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(3,5-dimethoxyphenyl)methyl]naphthalen-2-ol (3b)



The reaction was performed at 0.056 mmol scale of *p*-quinone methide (**1b**); pale yellow solid; yield 93% (26.2 mg); R_f = 0.5 (20% EtOAc in hexane); m.p. 72–74 °C; FT-IR (KBr) 3627, 3462, 2959, 1435, 1205, 1157, 741 cm^{-1}; ^1H NMR (400 MHz,

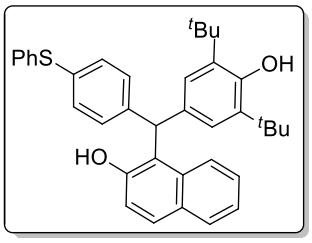
$CDCl_3$), δ 8.04 (d, J = 8.6 Hz, 1H), 7.79 (dd, J = 8.0, 1.0 Hz, 1H), 7.72 (d, J = 8.9 Hz, 1H), 7.45 (ddd, J = 8.5, 6.9, 1.5 Hz, 1H), 7.35–7.31 (m, 1H), 7.08 (d, J = 8.8 Hz, 1H), 7.07 (s, 2H), 6.41 (d, J = 2.2 Hz, 2H), 6.36 (t, J = 2.2 Hz, 1H), 6.21 (s, 1H), 5.50 (s, 1H), 5.20 (s, 1H), 3.70 (s, 6H), 1.35 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 153.3, 153.1, 145.2, 136.7, 133.6, 131.2, 129.63, 129.56, 128.8, 126.8, 125.7, 123.1, 123.0, 120.3, 120.1, 107.3, 98.9, 55.4, 48.9, 34.5, 30.4; HRMS (ESI): *m/z* calcd for $C_{33}H_{37}O_4$ $[M-H]^+$: 497.2692; found: 497.2681.

1[(3,5-di-*tert*-butyl-4-hydroxyphenyl){4-(pyrrolidin-1-yl)phenyl}methyl]naphthalen-2-ol (3c)



The reaction was performed at 0.055 mmol scale of *p*-quinone methide (**1c)**; red solid; yield 99% (27.7 mg); R_f = 0.5 (20% EtOAc in hexane); m.p. 109–111 °C; FT-IR (KBr) 3644, 3457, 2958, 1615, 1519, 1435, 1361, 817, 742 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$), δ 8.08 (d, J = 8.7 Hz, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.70 (d, J = 8.8 Hz, 1H), 7.43 (t, J = 7.6 Hz, 1H), 7.31 (t, J = 7.6 Hz, 1H), 7.10 (s, 2H), 7.08–7.04 (m, 3H), 6.52 (d, J = 8.6 Hz, 2H), 6.20 (s, 1H), 5.63 (s, 1H), 5.15 (s, 1H), 3.30–3.22 (m, 4H), 2.01–1.96 (m, 4H), 1.36 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.2, 152.8, 147.0, 136.4, 133.7, 132.3, 129.7, 129.6, 129.2, 128.7, 128.4, 126.6, 125.8, 123.1, 123.0, 121.2, 120.1, 112.3, 47.8, 47.7, 34.5, 30.4, 25.6; HRMS (ESI): *m/z* calcd for $C_{35}H_{40}NO_2$ $[M+H]^+$: 508.3215; found: 508.3200.

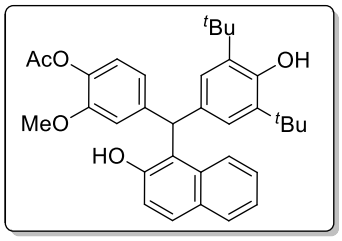
1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl){4-(phenylthio)phenyl}methyl]naphthalen-2-ol (3d)



The reaction was performed at 0.050 mmol scale of *p*-quinone methide (**1d**); pale yellow solid; yield 93% (25.4 mg); R_f = 0.4 (20% EtOAc in hexane); m.p. 171–173 °C; FT-IR (KBr) 3627, 3461, 2959, 1478, 1435, 1210, 741 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$), δ 8.00 (d, J = 8.6 Hz, 1H), 7.81 (dd, J =8.0, 1.0, Hz, 1H), 7.75 (d, J = 8.9 Hz, 1H), 7.46 (ddd, J = 8.3, 6.8, 1.3 Hz, 1H), 7.37–7.34 (m, 3H), 7.30–7.21 (m, 7H), 7.08 (d, J = 8.8 Hz, 1H), 7.01 (s, 2H), 6.29 (s, 1H), 5.41 (s, 1H), 5.26 (s, 1H), 1.35 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 153.2, 141.5, 137.0, 136.5, 133.7, 133.5, 132.3, 131.7, 130.4, 130.1, 129.78, 129.74, 129.2, 128.9, 126.87, 126.86, 125.7, 123.3, 122.9,

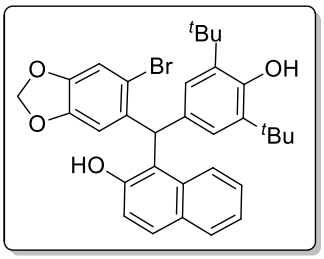
120.1, 119.9, 48.3, 34.6, 30.3; HRMS (ESI): *m/z* calcd for $C_{37}H_{37}O_2S$ $[M-H]^+$: 545.2515; found: 545.2508.

4-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(2-hydroxynaphthalen-1-yl)methyl]-2-methoxyphenyl acetate (3e)



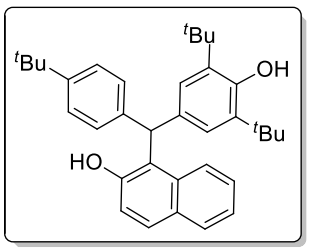
The reaction was performed at 0.052 mmol scale of *p*-quinone methide (**1e**); pale yellow solid; yield 91% (25.1 mg); R_f = 0.2 (20% EtOAc in hexane); m.p. 171–173 °C; FT-IR (KBr) 3626, 3459, 2959, 1510, 1435, 1200, 746 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 8.02 (d, J = 8.6 Hz, 1H), 7.80 (d, J = 7.7 Hz, 1H), 7.74 (d, J = 8.9 Hz, 1H), 7.47–7.42 (m, 1H), 7.34 (t, J = 7.4 Hz, 1H), 7.08 (d, J = 8.9 Hz, 1H), 7.03 (s, 2H), 6.98 (d, J = 8.1 Hz, 1H), 6.88 (d, J = 1.7 Hz, 1H), 6.80 (dd, J = 8.2, 1.8 Hz, 1H), 6.27 (s, 1H), 5.40 (s, 1H), 5.22 (s, 1H), 3.69 (s, 3H), 2.30 (s, 3H), 1.34 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 153.23, 153.16, 151.5, 141.2, 138.7, 136.9, 133.6, 131.6, 129.72, 129.69, 128.8, 126.9, 125.7, 123.3, 123.1, 123.0, 121.2, 120.2, 120.1, 113.2, 56.0, 48.5, 34.6, 30.3, 20.8; HRMS (ESI): *m/z* calcd for $C_{34}H_{37}O_5$ $[M-H]^+$: 525.2641; found: 525.2620.

1-[{6-bromobenzo(d)(1,3)dioxol-5-yl}(3,5-di-*tert*-butyl-4-hydroxyphenyl)methyl} naphthalen-2-ol (3f)



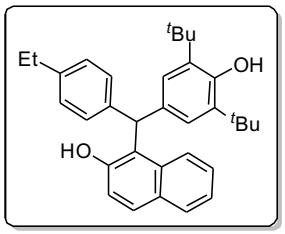
The reaction was performed at 0.24 mmol scale of *p*-quinone methide (**1f**); white solid; yield 87% (116.5 mg); R_f = 0.4 (20% EtOAc in hexane); m.p. 186–188 °C; FT-IR (KBr) 3633, 3461, 2959, 1477, 1234, 748 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 7.87 (d, J = 8.6 Hz, 1H), 7.79 (d, J = 7.3 Hz, 1H), 7.74 (d, J = 8.9 Hz, 1H), 7.47 (ddd, J = 8.4, 6.9, 1.3 Hz, 1H), 7.36–7.33 (m, 1H), 7.12 (s, 1H), 7.06 (d, J = 8.9 Hz, 1H), 6.92 (s, 2H), 6.64 (s, 1H), 6.43 (s, 1H), 5.96 (d, J = 1.3 Hz, 1H), 5.85 (d, J = 1.2 Hz, 1H), 5.46 (s, 1H), 5.25 (s, 1H), 1.34 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.6, 153.5, 147.9, 147.3, 137.2, 134.2, 133.6, 130.0, 129.9, 129.7, 128.8, 127.1, 125.2, 123.4, 123.0, 120.2, 119.8, 115.7, 113.0, 110.5, 101.8, 48.7, 34.6, 30.4; HRMS (ESI): *m/z* calcd for $C_{32}H_{34}BrO_4$ $[M+H]^+$: 561.1640; found: 561.1632.

1-{[4-(*tert*-butyl)phenyl](3,5-di-*tert*-butyl-4-hydroxyphenyl)methyl}naphthalen-2-ol (3g)



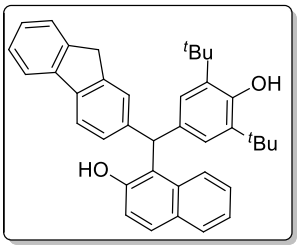
The reaction was performed at 0.057 mmol scale of *p*-quinone methide (**1g**); pale yellow solid; yield 90% (25.3 mg); R_f = 0.7 (20% EtOAc in hexane); m.p. 182–184 °C; FT-IR (KBr) 3633, 3465, 2961, 1435, 1210, 738 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 8.08 (d, J = 8.6 Hz, 1H), 7.80 (dd, J = 8.0, 1.0 Hz, 1H), 7.73 (d, J = 8.8 Hz, 1H), 7.46 (ddd, J = 8.3, 6.8, 1.4 Hz, 1H), 7.36–7.32 (m, 3H), 7.18 (d, J = 8.3 Hz, 2H), 7.09 (d, J = 8.8 Hz, 1H), 7.03 (s, 2H), 6.28 (s, 1H), 5.42 (s, 1H), 5.20 (s, 1H), 1.35 (s, 18H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.1, 153.0, 150.0, 139.1, 136.6, 133.6, 131.9, 129.7, 129.4, 128.8, 128.6, 126.8, 126.0, 125.8, 123.1, 123.0, 120.7, 120.1, 48.1, 34.6, 34.5, 31.5, 30.3; HRMS (ESI): *m/z* calcd for $C_{35}H_{41}O_2$ $[M-H]^+$: 493.3107; found: 493.3100.

1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(4-ethylphenyl)methyl]naphthalen-2-ol (3h)



The reaction was performed at 0.062 mmol scale of *p*-quinone methide (**3h**); pale yellow solid; yield 87% (25.2 mg); R_f = 0.6 (20% EtOAc in hexane); m.p. 129–131 °C; FT-IR (KBr) 3633, 3465, 2959, 1435, 1206, 738 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 8.06 (d, J = 8.6 Hz, 1H), 7.79 (dd, J = 8.0, 1.0 Hz, 1H), 7.72 (d, J = 8.8 Hz, 1H), 7.44 (ddd, J = 8.3, 6.8, 1.3 Hz, 1H), 7.35–7.31 (m, 1H), 7.16 (s, 4H), 7.08 (d, J = 8.8 Hz, 1H), 7.03 (s, 2H), 6.27 (s, 1H), 5.43 (s, 1H), 5.20 (s, 1H), 2.62 (q, J = 7.6 Hz, 2H), 1.34 (s, 18H), 1.21 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.14, 153.06, 143.0, 139.4, 136.7, 133.6, 131.9, 129.6, 129.5, 129.0, 128.8, 128.6, 126.8, 125.8, 123.1, 123.0, 120.7, 120.1, 48.3, 34.5, 30.3, 28.6, 15.7; HRMS (ESI): *m/z* calcd for $C_{33}H_{39}O_2$ $[M+H]^+$: 467.2950; found: 467.2938.

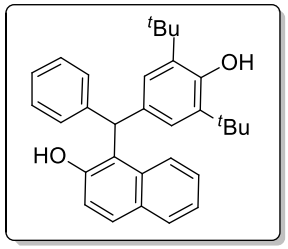
1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(9H-fluoren-2-yl)methyl]naphthalen-2-ol (3i)



The reaction was performed at 0.052 mmol scale of *p*-quinone methide (**1i**); pale yellow solid; yield 90% (24.8 mg); R_f = 0.5 (20% EtOAc in hexane); m.p. 212–214 °C; FT-IR 3629, 3465, 2958, 1435, 1210, 741 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 8.08 (d, J = 8.6 Hz, 1H), 7.81 (dd, J = 8.0, 1.0 Hz, 1H), 7.78–7.74 (m, 3H), 7.52 (d, J = 7.4 Hz, 1H), 7.47–7.43 (m, 2H), 7.39–7.27 (m, 4H), 7.11 (d, J, = 8.9 Hz, 1H), 7.08 (s, 2H), 6.39 (s, 1H), 5.53 (s, 1H), 5.24 (s, 1H), 3.88 (d, J = 22.0 Hz, 1H), 3.79 (d, J = 22.0 Hz, 1H), 3.49 (s, 3H), 1.34 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 153.2, 144.2, 143.5, 141.6, 140.9, 140.7, 136.9, 136.9, 133.6, 132.1, 129.7, 129.6, 128.8, 127.9, 126.8,

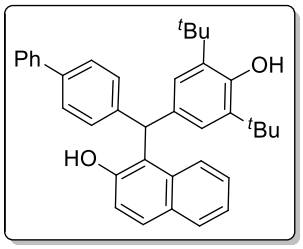
126.7, 125.8, 125.7, 125.2, 123.2, 123.0, 120.5, 120.3, 120.1, 120.0, 48.9, 37.1, 34.6, 30.4; HRMS (ESI): *m/z* calcd for $C_{38}H_{39}O_2$ $[M+H]^+$: 527.2950; found: 527.2941.

1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(phenyl)methyl]naphthalen-2-ol (3j)



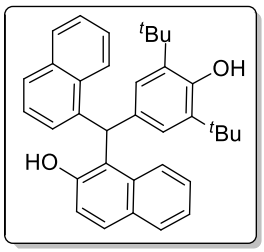
The reaction was performed at 0.068 mmol scale of *p*-quinone methide (**1j**); pale yellow solid; yield 86% (25.6 mg); R_f = 0.7 (20% EtOAc in hexane); m.p. 129–131 °C; FT-IR (KBr) 3644, 3465, 2924, 1749, 1615, 1435, 747 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 8.04 (d, J = 8.6 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 8.9 Hz, 1H), 7.45 (ddd, J = 8.5, 6.8, 1.3 Hz, 1H), 7.36–7.24 (m, 6H), 7.09 (d, J = 8.9 Hz, 1H), 7.03 (s, 2H), 6.31 (s, 1H), 5.43 (s, 1H), 5.23 (s, 1H), 1.35 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.22, 153.17, 142.2, 136.8, 133.6, 131.9, 129.7, 129.6, 129.1, 129.0, 128.8, 127.0, 126.8, 125.8, 123.2, 123.0, 120.3, 120.1, 48.7, 34.6, 30.3; HRMS (ESI): *m/z* calcd for $C_{31}H_{33}O_2$ $[M-H]^+$: 437.2481; found: 437.2469.

1-[(1,1'-biphenyl)-4-yl(3,5-di-*tert*-butyl-4-hydroxyphenyl)methyl]naphthalen-2-ol (3k)



The reaction was performed at 0.27 mmol scale of *p*-quinone methide (**1k**); pale yellow solid; yield 86% (119 mg); R_f = 0.5 (20% EtOAc in hexane); m.p. 135–137 °C; FT-IR (KBr) 3629, 3465, 2922, 1435, 1266, 746 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 8.08 (d, J = 8.6 Hz, 1H), 7.81 (d, J = 7.6 Hz, 1H), 7.76 (d, J = 8.9 Hz, 1H), 7.61–7.56 (m, 4H), 7.48–7.42 (m, 3H), 7.37–7.32 (m, 4H), 7.10 (d, J = 8.9 Hz, 1H), 7.07 (s, 2H), 6.36 (s, 1H), 5.47 (s, 1H), 5.24 (s, 1H), 1.35 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.2, 153.2, 141.3, 140.8, 139.7, 136,9, 133.6, 131.8, 129.7, 129.6, 129.5, 128.9, 128.8, 127.7, 127.4, 127.1, 126.8, 125.8, 123.2, 123.0, 120.3, 120.1, 48.4, 34.6, 30.3; HRMS (ESI): *m/z* calcd for $C_{37}H_{37}O_2$ $[M-H]^+$: 513.2794; found: 513.2789.

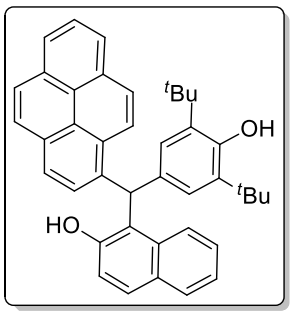
1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(naphthalen-1-yl)methyl]naphthalen-2-ol (3l)



The reaction was performed at 0.058 mmol scale of *p*-quinone methide (**1l**); pale yellow solid; yield 92% (26.1 mg); R_f = 0.6 (20% EtOAc in hexane); m.p. 170–172 °C; FT-IR (KBr) 3629, 3465, 2959, 1435, 1210, 742 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 8.5 Hz, 1H), 7.90 (dd, J = 8.2, 2.7 Hz, 2H), 7.81 (dd, J = 7.9, 1.2 Hz, 1H), 7.80 (d, J = 8.2 Hz, 1H), 7.74 (d, J = 8.9 Hz, 1H), 7.52–7.46 (m, 1H), 7.43–7.30 (m, 4H),

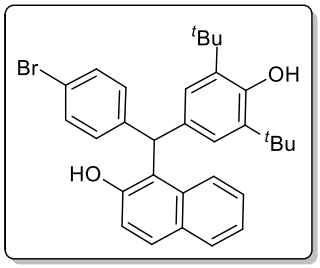
7.16 (d, J = 7.1 Hz, 1H), 7.04 (d, J = 8.9 Hz, 1H), 7.01 (brs, 2H), 6.89 (s, 1H), 5.62 (s, 1H), 5.20 (s, 1H), 1.29 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 153.2, 138.5, 136.9, 136.8, 134.2, 133.4, 132.0, 131.5, 129.7, 129.6, 129.0, 128.8, 128.3, 127.0, 126.9, 126.6, 126.0, 125.9, 125.8, 124.2, 123.2, 122.8, 120.0, 46.0, 34.5, 30.3; HRMS (ESI): *m/z* calcd for $C_{35}H_{37}O_2$ $[M+H]^+$: 489.2793; found: 489.2787.

1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(pyren-1-yl)methyl]naphthalen-2-ol (3m)



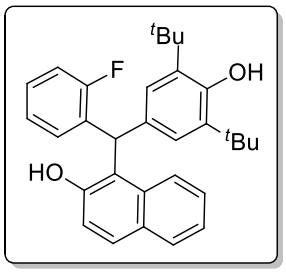
The reaction was performed at 0.048 mmol scale of *p*-quinone methide (**1m**); yellow solid; yield 75% (20.2 mg); R_f = 0.5 (20% EtOAc in hexane); m.p. 226–228 °C; FT-IR (KBr) 3629, 3465, 2959, 1435, 1210, 742 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25–8.15 (m, 3H), 8.10–7.99 (m, 5H), 7.98–7.92 (m, 1H), 7.84–7.79 (m, 1H), 7.77 (d, J = 8.9 Hz, 1H), 7.74 (d, J = 8.0 Hz, 1H), 7.36–7.27 (m, 3H), 7.23 (s, 1H), 7.09 (d, J = 8.9 Hz, 2H), 7.06 (brs, 1H), 5.57 (s, 1H), 5.23 (s, 1H), 1.27 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 153.3, 137.08, 137.06, 135.9, 133.5, 131.9, 131.6, 130.9, 130.7, 129.7, 129.2, 128.8, 128.2, 127.7, 127.4, 127.0, 126.9, 126.1, 126.0, 125.5, 125.48, 125.44, 125.3, 125.0, 123.4, 123.2, 122.9, 120.4, 120.1, 46.4, 34.5, 30.3; HRMS (ESI): *m/z* calcd for $C_{41}H_{39}O_2$ $[M+H]^+$: 563.2950; found: 563.2945.

1-[(4-bromophenyl)(3,5-di-*tert*-butyl-4-hydroxyphenyl)methyl]naphthalen-2-ol (3n)



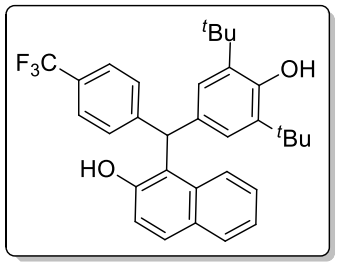
The reaction was performed at 0.054 mmol scale of *p*-quinone methide (**1n**); pale yellow solid; yield 92% (25.5 mg); R_f = 0.5 (20% EtOAc in hexane); m.p. 158–160 °C; FT-IR (KBr) 3627, 3460, 2960, 1486, 1435, 1210, 741 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.95 (d, J = 8.6 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 8.9 Hz, 1H), 7.45–7.42 (m, 3H), 7.34 (t, J = 7.4 Hz, 1H), 7.16 (d, J = 8.4 Hz, 2H), 7.07 (d, J = 8.9 Hz, 1H), 7.00 (s, 2H), 6.26 (s, 1H), 5.37 (s, 1H), 5.26 (s, 1H), 1.34 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 153.1, 141.3, 137.1, 133.4, 132.0, 131.4, 131.0, 129.8, 129.7, 128.9, 126.9, 125.7, 123.3, 122.9, 120.8, 120.0, 119.8, 48.2, 34.6, 30.3; HRMS (ESI): *m/z* calcd for $C_{31}H_{32}BrO_2$ $[M-H]^+$: 515.1586; found: 515.1579.

1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(2-fluorophenyl)methyl]naphthalen-2-ol (3o)



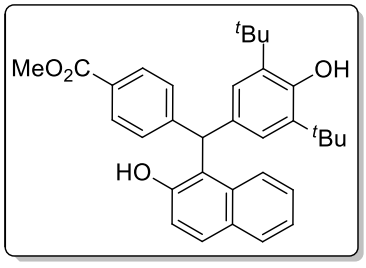
The reaction was performed at 0.064 mmol scale of *p*-quinone methide (**1o**); pale yellow solid; yield 97% (28.4 mg); R_f = 0.6 (20% EtOAc in hexane); m.p. 134–136 °C; FT-IR (KBr) 3629, 3459, 2959, 1487, 1435, 1228, 758 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.6 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 8.9 Hz, 1H), 7.45 (t, J = 7.7 Hz, 1H), 7.33 (t, J = 7.4 Hz, 1H), 7.28–7.22 (m, 1H), 7.18–7.09 (m, 2H), 7.08–7.02 (m, 2H), 6.97 (s, 2H), 6.58 (s, 1H), 5.50 (s, 1H), 5.25 (s, 1H), 1.32 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7 (d, J = 245.0 Hz), 153.7, 153.5, 137.2, 133.5, 130.7 (d, J = 3.7 Hz), 130.6, 129.8, 129.6, 128.9, 128.8 (d, J = 4.2 Hz), 128.7, 127.0, 125.1, 124.7 (d, J = 3.5 Hz), 123.3, 122.7, 120.1, 119.2, 115.5 (d, J = 22.3 Hz), 41.4 (d, J = 3.3 Hz), 34.6, 30.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.2; HRMS (ESI): *m/z* calcd for $C_{31}H_{34}FO_2$ $[M+H]^+$: 457.2543; found: 457.2533.

1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl){4-(trifluoromethyl)phenyl}methyl]naphthalen-2-ol (3p)



The reaction was performed at 0.055 mmol scale of *p*-quinone methide (**1p**); pale yellow solid; yield 86% (24.1 mg); R_f = 0.7 (20% EtOAc in hexane); m.p. 160–162 °C; FT-IR 3637, 3462, 2961, 1435, 1326, 1123, 744 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 7.95 (d, J = 8.6 Hz, 1H), 7.81 (dd, J = 8.0, 1.0 Hz, 1H), 7.76 (d, J = 8.9 Hz, 1H), 7.58 (d, J = 8.2 Hz, 2H), 7.46–7.44 (m, 1H), 7.41 (d, J = 7.9 Hz, 2H), 7.37–7.33 (m, 1H), 7.09 (d, J = 8.9 Hz, 1H), 6.99 (s, 2H), 6.37 (s, 1H), 5.37 (s, 1H), 5.28 (s, 1H), 1.34 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.4, 153.2, 146.6 (apparent d, J = 1.0 Hz), 137.1, 133.4, 131.2, 130.0, 129.8, 129.6, 129.3, 129.0, 128.6, 127.0, 125.8 (q, J = 3.7 Hz), 125.7, 124.3 (q, J = 270.3 Hz), 123.4, 122.8, 120.0, 119.6, 48.5, 34.6, 30.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.4; HRMS (ESI): *m/z* calcd for $C_{32}H_{34}F_3O_2$ $[M+H]^+$: 507.2511; found: 507.2502.

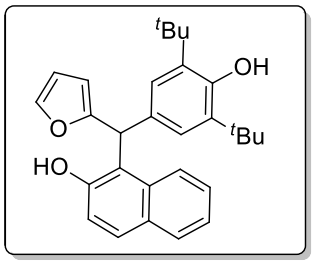
Methyl-4-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(2-hydroxynaphthalen-1-yl)methyl] benzoate (3q)



The reaction was performed at 0.057 mmol scale of *p*-quinone methide (**1q**); pale yellow solid; yield 92% (25.93 mg); R_f = 0.4 (20% EtOAc in hexane); m.p. 184–186 °C; FT-IR (KBr) 3620, 3455, 2955, 1712, 1510, 1433, 1200, 745 cm^{-1}; ^1H NMR

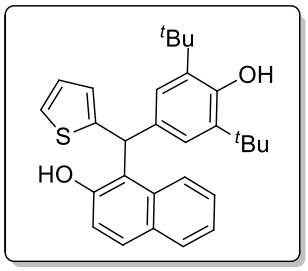
(400 MHz, $CDCl_3$) δ 7.98 (d, J = 8.3 Hz, 2H), 7.94 (d, J = 8.6 Hz, 1H), 7.79 (d, J = 7.9 Hz, 1H), 7.74 (d, J = 8.9 Hz, 1H), 7.44–7.38 (m, 1H), 7.36 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 7.3 Hz, 1H), 7.08 (d, J = 8.9 Hz, 1H), 6.98 (s, 2H), 6.34 (s, 1H), 5.38 (s, 1H), 5.25 (s, 1H), 3.89 (s, 3H), 1.32 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 153.4, 153.2, 147.8, 137.1, 133.4, 131.3, 130.2, 129.9, 129.7, 129.3, 128.9, 128.8, 126.9, 125.7, 123.3, 122.9, 120.0, 119.6, 52.2, 48.8, 34.6, 30.3; HRMS (ESI): *m/z* calcd for $C_{32}H_{35}O_4$ $[M-H]^+$: 495.2536; found: 495.2517.

1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(furan-2-yl)methyl]naphthalen-2-ol (3r)



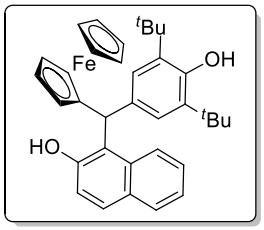
The reaction was performed at 0.070 mmol scale of *p*-quinone methide (**1r**); brown solid; yield 68% (20.5 mg); R_f = 0.5 (20% EtOAc in hexane); m.p. 71–73 °C; FT-IR (KBr) 3628, 3468, 2959, 1436, 1234, 741 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 8.6 Hz, 1H), 7.80 (d, J = 8.1 Hz, 1H), 7.74 (d, J = 8.9 Hz, 1H), 7.47 (ddd, J = 8.5, 6.8, 1.4 Hz, 1H), 7.43 (d, J = 1.1 Hz, 1H), 7.38–7.31 (m, 1H), 7.10 (d, J = 8.9 Hz, 1H), 7.04 (s, 2H), 6.34 (dd, J = 3.2, 1.9 Hz, 1H), 6.31 (s, 1H), 6.09 (d, J = 3.2 Hz, 1H), 5.77 (s, 1H), 5.21 (s, 1H), 1.35 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.9, 153.3, 142.6, 136.7, 133.3, 129.80, 129.78, 129.6, 128.9, 126.9, 124.9, 123.2, 122.5, 119.8, 117.8, 110.5, 108.8, 42.2, 34.5, 30.3; HRMS (ESI): *m/z* calcd for $C_{29}H_{33}O_3$ $[M+H]^+$: 429.2429; found: 429.2425.

1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(thiophen-2-yl)methyl]naphthalen-2-ol (3s)



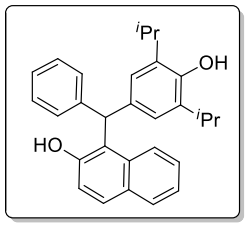
The reaction was performed at 0.067 mmol scale of *p*-quinone methide (**1s**); yellow solid; yield 75% (22.2 mg); R_f = 0.6 (20% EtOAc in hexane); m.p. 119–121 °C; FT-IR (KBr) 3627, 3464, 2959, 1435, 1210, 743 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 8.6 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 8.9 Hz, 1H), 7.47 (ddd, J = 8.5, 6.9, 1.3 Hz, 1H), 7.37–7.33 (m, 1H), 7.27–7.25 (m, 1H), 7.16 (s, 2H), 7.10 (d, J = 8.9 Hz, 1H), 6.95 (dd, J = 5.1, 3.5 Hz, 1H), 6.83 (d, J = 3.5 Hz, 1H), 6.48 (s, 1H), 5.59 (s, 1H), 5.22 (s, 1H), 1.36 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 153.1, 146.8, 136.7, 133.1, 131.5, 129.8, 129.6, 128.9, 127.0, 126.9, 126.8, 125.7, 125.2, 123.3, 122.7, 120.5, 120.0, 43.7, 34.6, 30.3; HRMS (ESI): *m/z* calcd for $C_{29}H_{33}O_2S$ $[M+H]^+$: 445.2201; found: 445.2208.

Cyclopenta-2,4-dien-1-yl[2-{(3,5-di-tert-butyl-4-hydroxyphenyl)(3-hydroxynaphthalen-2-yl)methyl}cyclopenta-2,4-dien-1-yl]iron (3t)



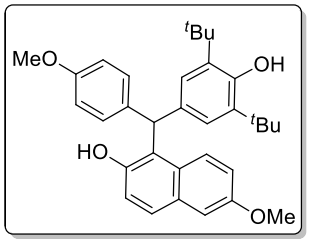
The reaction was performed at 0.050 mmol scale of *p*-quinone methide (**1t**); dark green solid; yield 74% (20.1 mg); R_f = 0.7 (20% EtOAc in hexane); m.p. 139–141 °C; FT-IR (KBr) 3637, 3467, 2958, 1435, 1232, 820, 745 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 8.17 (d, J = 8.7 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 8.8 Hz, 1H), 7.52 (t, J = 7.4 Hz, 1H), 7.34 (t, J = 7.5 Hz, 1H), 7.20 (s, 2H), 7.06 (d, J = 8.8 Hz, 1H), 6.06 (s, 1H), 5.59 (s, 1H), 5.11 (s, 1H), 4.27–4.25 (m, 2H), 4.20 (s, 1H), 4.05 (s, 5H), 3.97 (s, 1H), 1.38 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.67, 152.65, 136.0, 133.2, 132.5, 129.5, 129.1, 128.9, 126.5, 125.2, 123.1, 123.0, 121.9, 120.1, 91.9, 69.4, 69.4, 69.3, 68.6, 67.6, 43.2, 34.5, 30.5; HRMS (ESI): *m/z* calcd for $C_{35}H_{39}FeO_2$ $[M+H]^+$: 547.2299; found: 547.2288.

1-[(4-hydroxy-3,5-diisopropylphenyl)(phenyl)methyl]naphthalen-2-ol (3u)



The reaction was performed at 0.074 mmol scale of *p*-quinone methide (**1s**); pale yellow solid; yield 75% (22.93 mg); R_f = 0.5 (20% EtOAc in hexane); m.p. 119–121 °C; FT-IR (KBr) 3626, 3459, 2959, 1510, 1435, 1200, 746 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 8.6 Hz, 1H), 7.83–7.72 (m, 3H), 7.44 (ddd, J = 8.3, 7.0, 1.2 Hz, 1H), 7.36–7.26 (m, 4H), 7.15–7.09 (m, 1H), 7.09 (d, J = 8.9 Hz, 1H), 6.91 (s, 2H), 6.33 (s, 1H), 5.43 (s, 1H), 4.82 (s, 1H), 3.11 (sept, J = 6.9 Hz, 1H), 1.16 (d, J = 1.0 Hz, 6H), 1.14 (d, J = 1.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.2, 149.4, 142.0, 134.8, 133.4, 129.6, 129.13, 129.06, 128.8, 127.9, 127.1, 126.8, 126.5, 124.3, 122.9, 120.1, 117.9, 109.6, 48.6, 27.5, 22.8, 22.7; HRMS (ESI): *m/z* calcd for $C_{29}H_{29}O_2$ $[M-H]^+$: 409.2167; found: 409.2152.

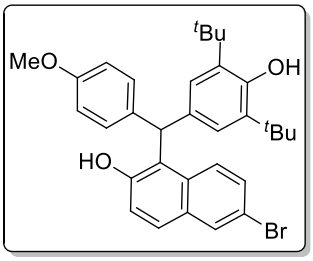
1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(4-methoxyphenyl)methyl]-6-methoxynaphthalen-2-ol (10a)



The reaction was performed at 0.062 mmol scale of *p*-quinone methide (**1**); orange solid; yield 92% (28.3 mg); R_f = 0.3 (20% EtOAc in hexane); m.p. 81–83 °C; FT-IR (KBr) 3627, 3468, 2958, 1606, 1510, 1435, 1233, 739 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 7.94 (d, J = 9.6 Hz, 1H), 7.62 (d, J = 8.8 Hz, 1H), 7.16 (d, J = 8.7 Hz, 2H), 7.13–7.10 (m, 2H), 7.05 (d, J = 8.8 Hz, 1H), 7.03 (s, 2H), 6.85 (d, J = 8.7 Hz, 2H),

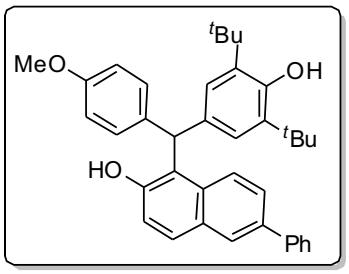
6.20 (s, 1H), 5.28 (s, 1H), 5.21 (s, 1H), 3.89 (s, 3H), 3.78 (s, 3H), 1.34 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 155.7, 153.1, 151.5, 136.7, 134.2, 132.2, 130.6, 130.1, 128.7, 128.2, 125.7, 124.6, 121.0, 120.6, 118.9, 114.4, 107.2, 55.5, 55.4, 48.0, 34.5, 30.4; HRMS (ESI): *m/z* calcd for $C_{33}H_{39}O_4$ $[M+H]^+$: 499.2848; found: 499.2838.

6-bromo-1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(4-methoxyphenyl)methyl]naphthalen-2-ol (10b)



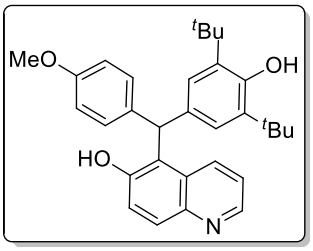
The reaction was performed at 0.062 mmol scale of *p*-quinone methide (**1**); pale yellow solid; yield 95% (32.1 mg); R_f = 0.4 (20% EtOAc in hexane); m.p. 151–153 °C; FT-IR (KBr) 3629, 3461, 2958, 1509, 1435, 1251 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.92 (d, J = 2.1 Hz, 1H), 7.87 (d, J = 9.2 Hz, 1H), 7.63 (d, J = 8.9 Hz, 1H), 7.47 (dd, J = 9.2, 2.1 Hz, 1H), 7.13 (d, J = 8.7 Hz, 2H), 7.08 (d, J = 8.9 Hz, 1H), 6.99 (s, 2H), 6.85 (d, J = 8.7 Hz, 2H), 6.16 (s, 1H), 5.47 (s, 1H), 5.22 (s, 1H), 3.78 (s, 3H), 1.33 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 153.4, 153.2, 136.9, 133.7, 132.1, 131.7, 130.9, 130.6, 130.1, 129.9, 128.6, 125.6, 124.9, 121.2, 120.9, 116.9, 114.5, 55.4, 47.9, 34.6, 30.3; HRMS (ESI): *m/z* calcd for $C_{32}H_{34}BrO_3$ $[M-H]^+$: 545.1692; found: 545.1680.

1-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(4-methoxyphenyl)methyl]-6-phenylnaphthalen-2-ol (10c)



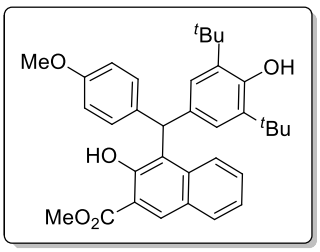
The reaction was performed at 0.062 mmol scale of *p*-quinone methide (**1**); yellow solid; yield 64% (99%); R_f = 0.4 (20% EtOAc in hexane); m.p. 89–91 °C; FT-IR (KBr) 3626, 3460, 2922, 1436, 1265, 746 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 9.0 Hz, 1H), 8.00 (d, J = 1.8 Hz, 1H), 7.79 (d, J = 8.9 Hz, 1H), 7.83–7.72 (m, 3H), 7.68 (s, 1H), 7.47 (t, J = 7.6 Hz, 2H), 7.36 (t, J = 7.4 Hz, 1H), 7.20 (d, J = 8.6 Hz, 2H), 7.11 (d, J = 8.8 Hz, 1H), 7.06 (s, 2H), 6.88 (d, J = 8.7 Hz, 2H), 6.27 (s, 1H), 5.49 (s, 1H), 5.23 (s, 1H), 3.79 (s, 3H), 1.35 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 153.3, 153.2, 141.0, 136.8, 135.9, 134.0, 132.7, 132.1, 130.1, 129.9, 129.8, 128.9, 127.3, 127.2, 126.7, 126.4, 125.7, 123.6, 120.6, 120.5, 114.4, 55.4, 48.0, 34.6, 30.4; HRMS (ESI): *m/z* calcd for $C_{38}H_{39}O_3$ $[M-H]^+$: 543.2899; found: 543.2880.

5-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(4-methoxyphenyl)methyl]quinolin-6-ol (10d)



The reaction was performed at 0.062 mmol scale of *p*-quinone methide (**1**); yellow solid; yield 86% (24.9 mg); R_f = 0.3 (50% EtOAc in hexane); m.p. 239–241 °C; FT-IR (KBr) 3636, 3450, 2958, 1509, 1248, 739 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 8.71 (d, J = 4.2 Hz, 1H), 8.32 (d, J = 8.6 Hz, 1H), 7.95 (d, J = 9.1 Hz, 1H), 7.32 (d, J = 9.0 Hz, 1H), 7.30–7.28 (m, 1H), 7.14 (d, J = 8.6 Hz, 2H), 7.02 (s, 2H), 6.85 (d, J = 8.7 Hz, 2H), 6.53 (s, 1H), 6.24 (s, 1H), 5.23 (s, 1H), 3.78 (s, 3H), 1.33 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 153.5, 153.1, 146.9, 144.6, 136.8, 134.0, 132.1, 131.7, 130.2, 130.1, 128.7, 125.7, 123.7, 121.2, 120.7, 114.4, 55.4, 47.4, 34.5, 30.3; HRMS (ESI): *m/z* calcd for $C_{31}H_{36}NO_3$ $[M+H]^+$: 470.2695; found: 470.2685.

Methyl-4-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(4-methoxyphenyl)methyl]-3-hydroxy-2-naphthoate (10e)



The reaction was performed at 0.062 mmol scale of *p*-quinone methide (**1**); yellow solid; yield 64% (20.8 mg); R_f = 0.4 (20% EtOAc in hexane); m.p. 148–150 °C; FT-IR (KBr) 3635, 2957, 1710, 1510, 1439, 750 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$), δ 10.98 (s, 1H), 8.48 (s, 1H), 7.78 (d, J = 7.9 Hz, 2H), 7.28–7.21 (m, 2H), 7.13 (d, J = 8.3 Hz, 2H), 7.12 (s, 2H), 6.77 (d, J = 8.8 Hz, 2H), 6.57 (s, 1H), 5.05 (s, 1H), 4.02 (s, 3H), 3.76 (s, 3H), 1.31 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 157.5, 154.4, 152.0, 136.8, 136.7, 135.4, 132.5, 132.2, 132.1, 130.3, 129.8, 128.2, 127.7, 126.4, 124.6, 123.2, 113.9, 113.5, 55.3, 52.8, 45.5, 34.5, 30.4; HRMS (ESI): *m/z* calcd for $C_{34}H_{37}O_5Na$ $[M+Na]^+$: 549.2617; found: 549.2605.

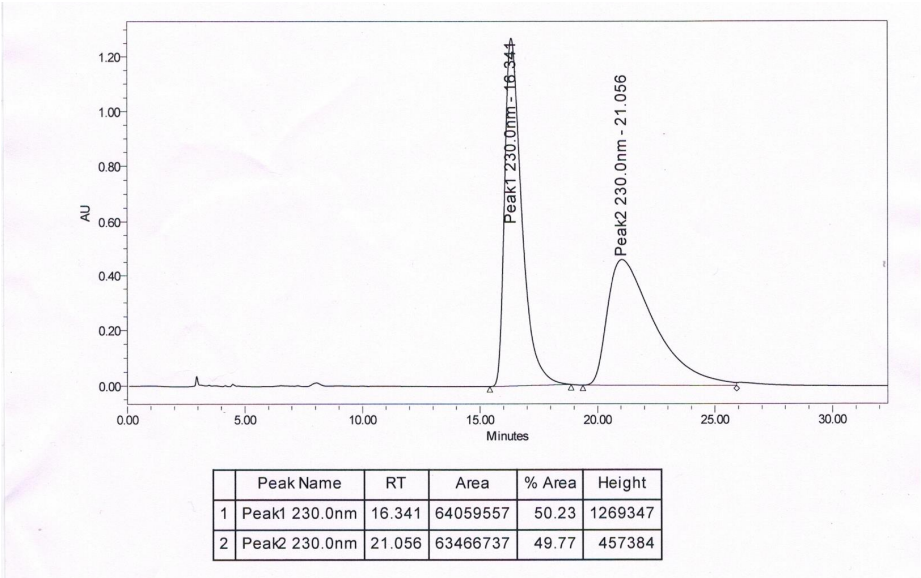
Enantioselective 1,6-conjugate addition of 2-naphthol to 1 :

Anhydrous HFIP (0.5 mL) was added to the mixture of *p*-quinone methide (**1**) (20 mg, 0.0620 mmol), 2-naphthol (8 mg, 0.0680 mmol), catalyst (3mg, 0.0062 mmol) and sodium hydride (55-60% suspension in mineral oil) (0.6 mg, 0.0124 mmol) under argon atmosphere, and the resulting suspension was stirred at room temperature. After 48 h the reaction was quenched by 2 mL of water and extracted with CH_2Cl_2 (2X3 mL). The organic layer dried over anhydrous Na_2SO_4 and solvent was removed under reduced pressure. The residue was purified through silica gel column, using EtOAc/Hexane mixture as an eluent, to gate pale

yellow solid (8 mg, 30%, 8% ee). The enantiomeric excess was determined by HPLC: CHIRALCEL AD-H, n-hexane/i-PrOH (99/1).

HPLC data for 3 (racemic)

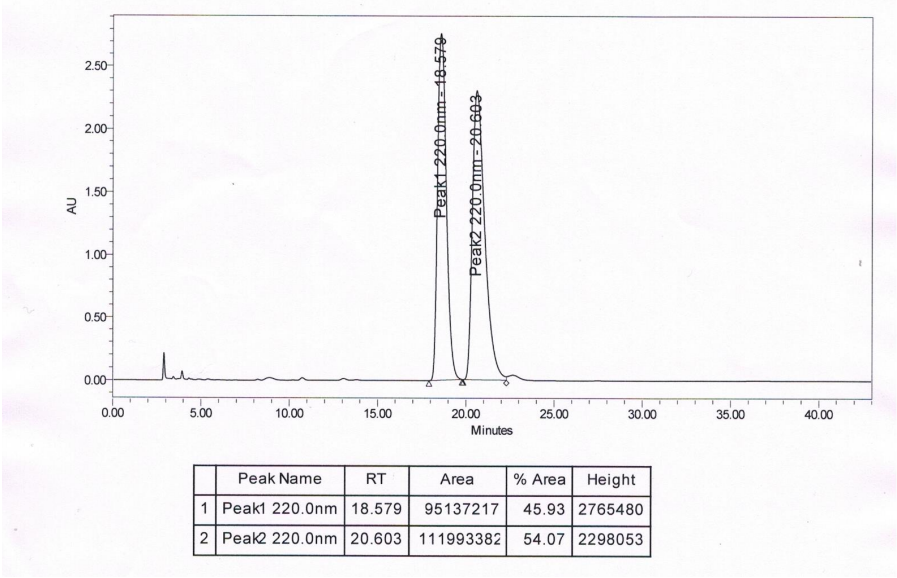
Retention time 1.0 mL min^{-1}, 220 nm.



	Peak Name	RT	Area	% Area	Height
1	Peak1 230.0nm	16.341	64059557	50.23	1269347
2	Peak2 230.0nm	21.056	63466737	49.77	457384

HPLC data for 3 (enentioenriched)

Retention time 1.0 mL min^{-1}, 220 nm, 18.58 min (minor enantiomer), 20.60 min (major enantiomer).

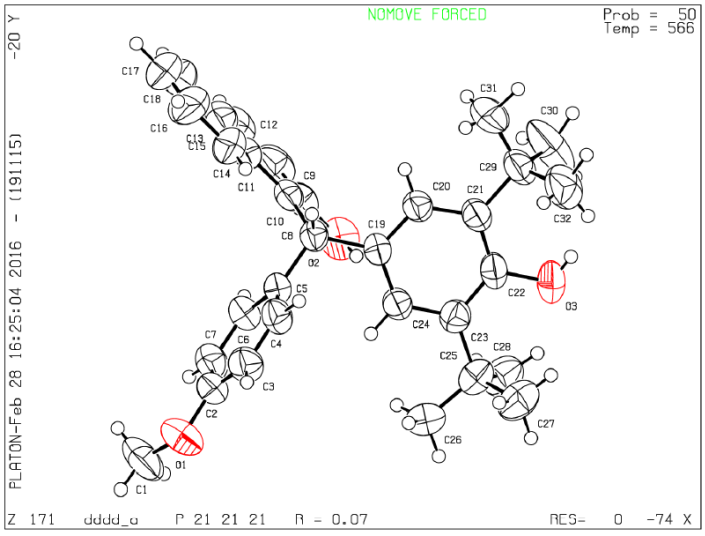


	Peak Name	RT	Area	% Area	Height
1	Peak1 220.0nm	18.579	95137217	45.93	2765480
2	Peak2 220.0nm	20.603	111993382	54.07	2298053

X-Ray crystallographic analysis for compound 3:[3]

Crystal data and structure refinement for compound 3.

Identification code	**3**
Empirical formula	$C_{32}H_{36}O_3$
Formula weight	468.61
Temperature/K	566(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	10.9865(10)
b/Å	11.6624(10)
c/Å	20.9000(17)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2677.9(4)
Z	4
ρ_{calc}g/cm^3	1.162
μ/mm^{-1}	0.073
F(000)	1008.0
Crystal size/mm^3	0.200 × 0.200 × 0.200
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.416 to 54.954
Index ranges	$-14 \le h \le 14$, $-15 \le k \le 15$, $-27 \le l \le 27$
Reflections collected	29152
Independent reflections	6127 [R_{int} = 0.2643, R_{sigma} = 0.1361]
Data/restraints/parameters	6127/0/325
Goodness-of-fit on F^2	0.957
Final R indexes [I>=2σ (I)]	R_1 = 0.0738, wR_2 = 0.2027
Final R indexes [all data]	R_1 = 0.1081, wR_2 = 0.2382
Largest diff. peak/hole / e Å^{-3}	0.22/-0.15
Flack parameter	-2.8(10)



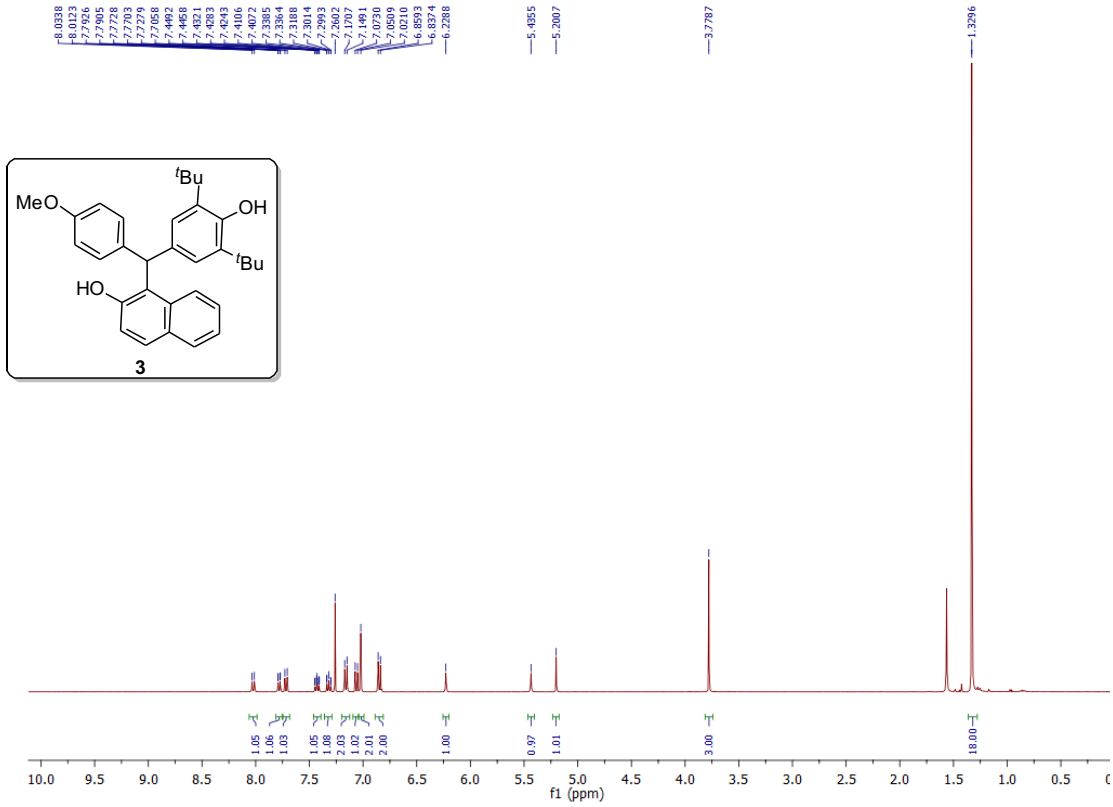
Reference:

[1] D. Enders, K. Breuer, U. Kallfass, T. Balensiefer, *Synthesis* 2003, 1292.

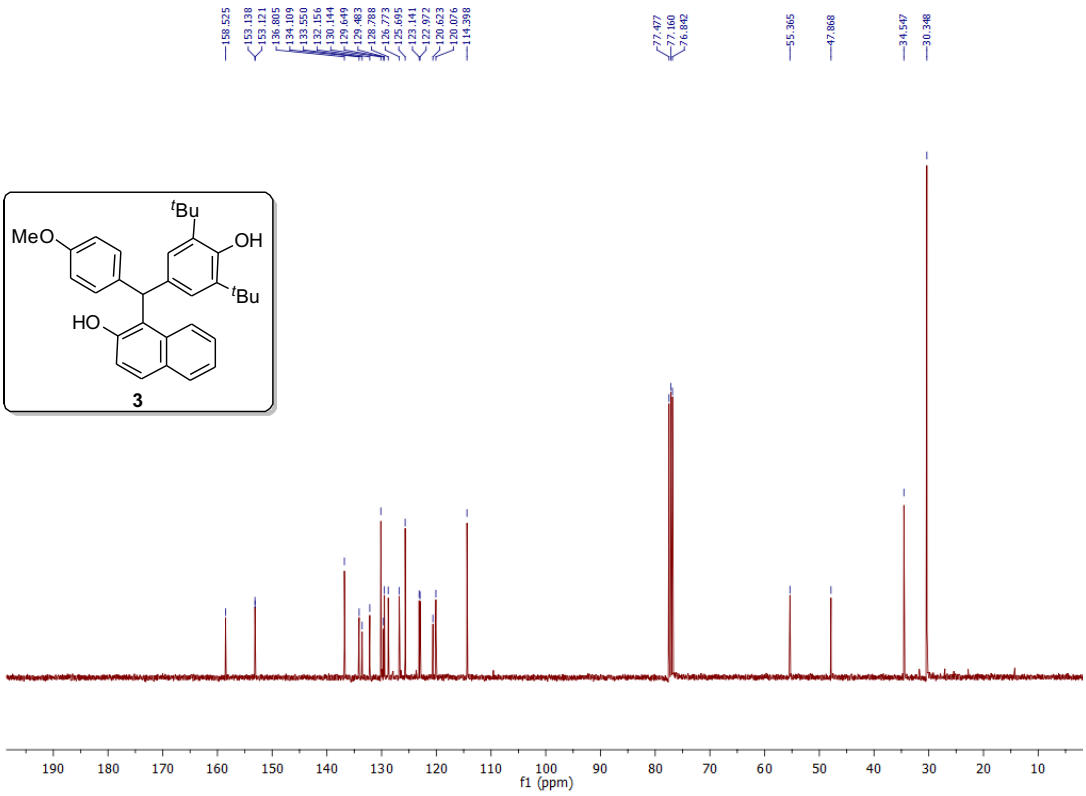
[2] (a) W. D. Chu, L. F. Zhang, X. Bao, X. H. Zhao, C. Zeng, J. Y. Du, G. B. Zhang, F. X. Wang, X. Y. C. A. Ma, Fan, *Angew. Chem. Int. Ed*. 2013, **52**, 9229; (b) V. Reddy, R. V. Anand, *Org. Lett*. 2015, **17**, 3390-3393

[3] CCDC NO: 1452070.

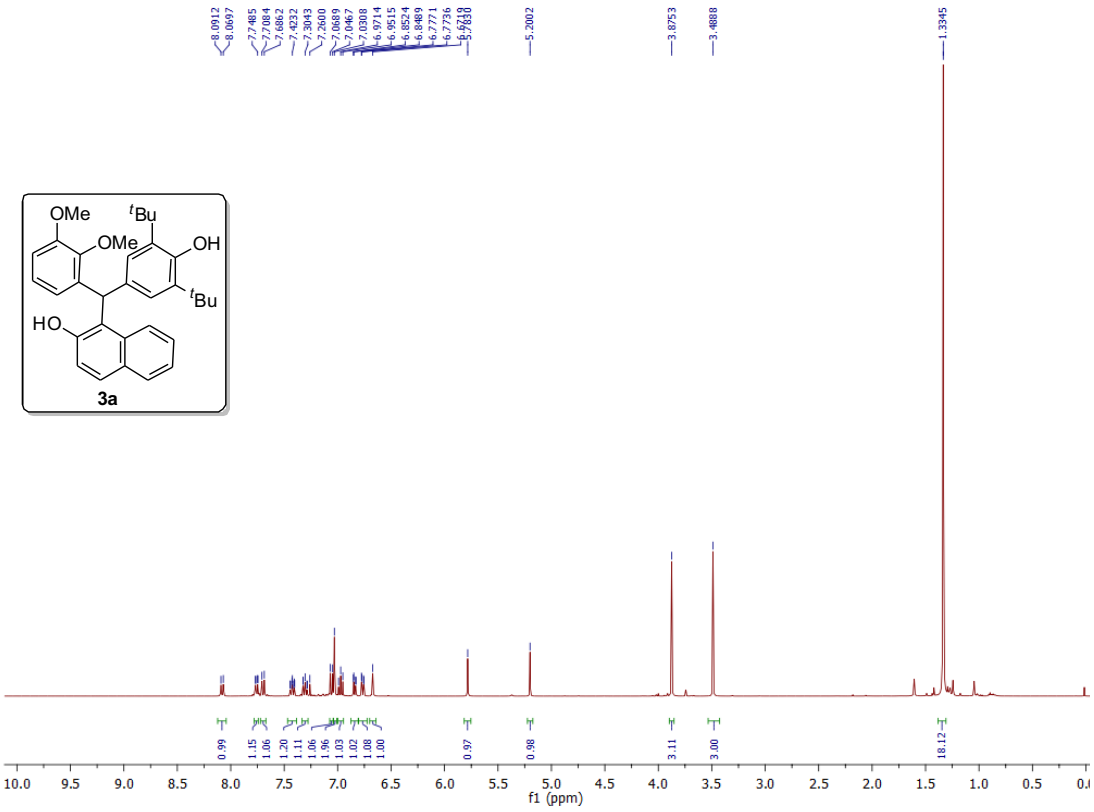
^{1}H NMR Spectrum of 3



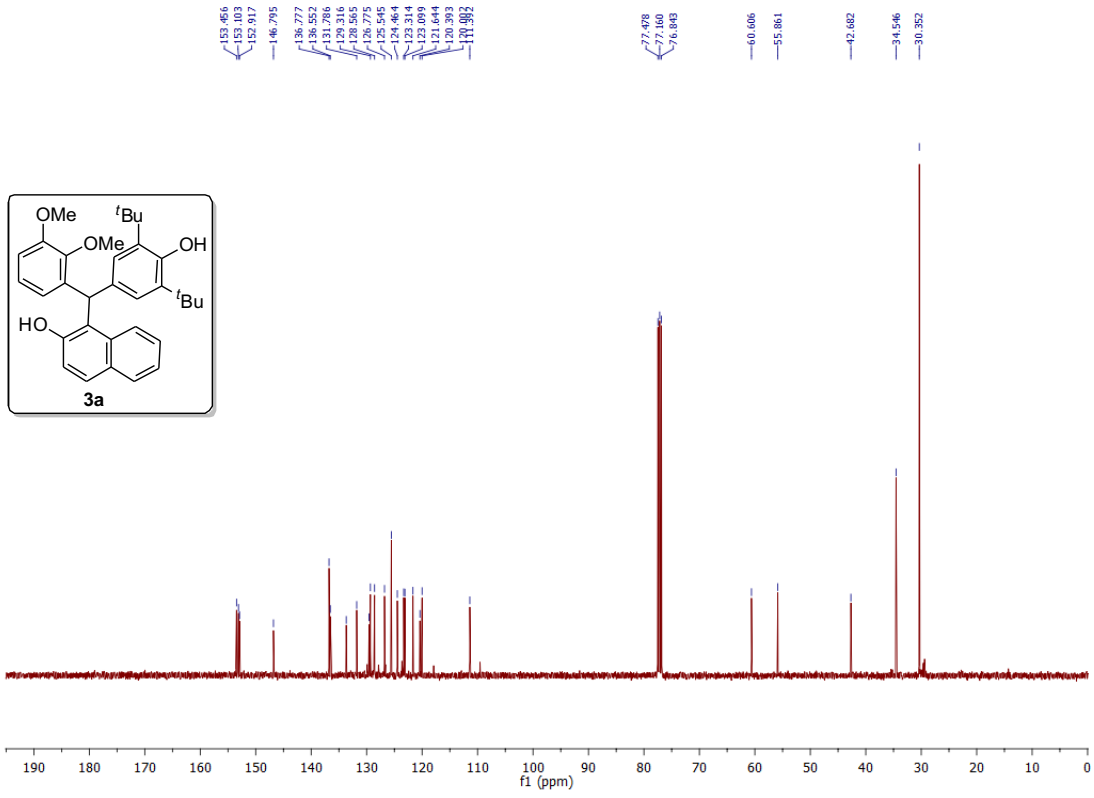
^{13}C NMR Spectrum of 3



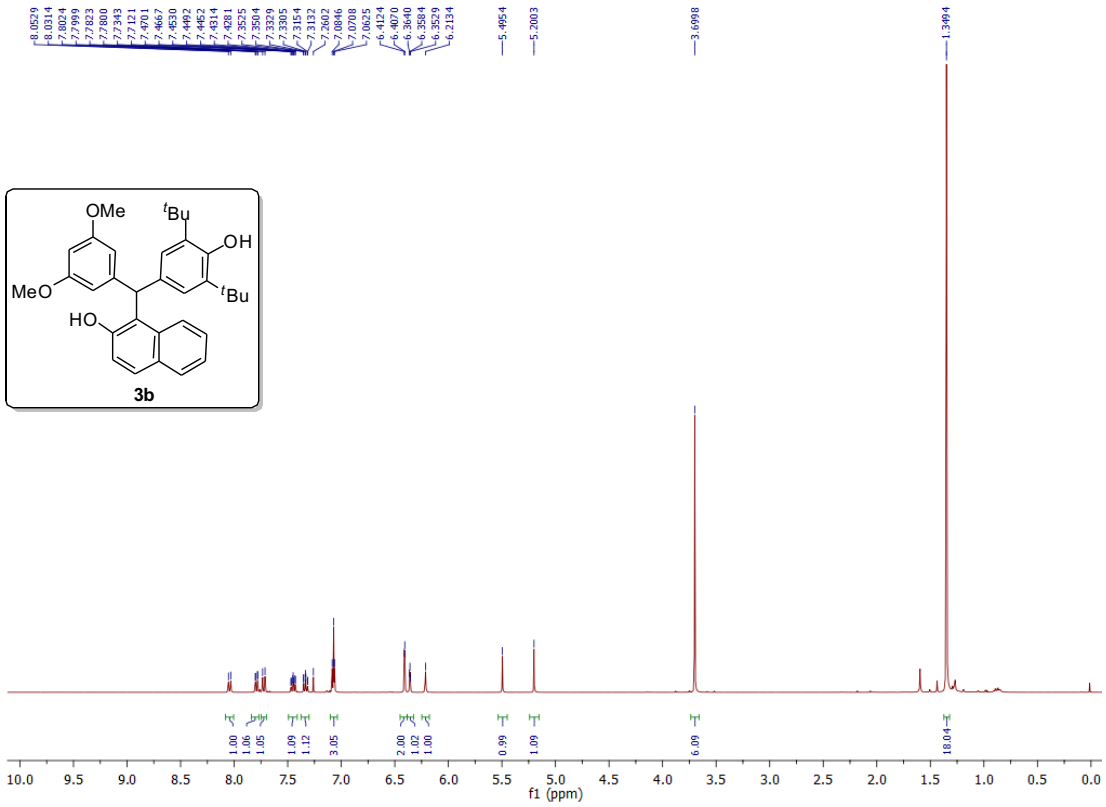
^{1}H NMR Spectrum of 3a



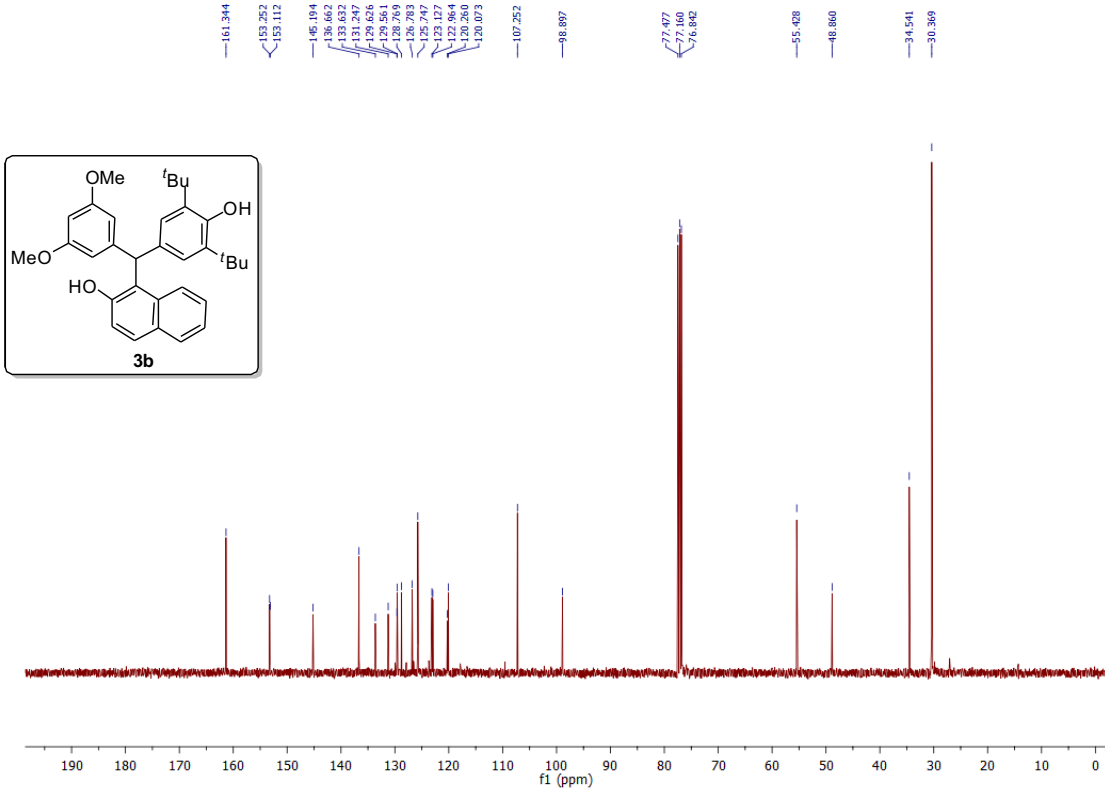
^{13}C NMR Spectrum of 3a



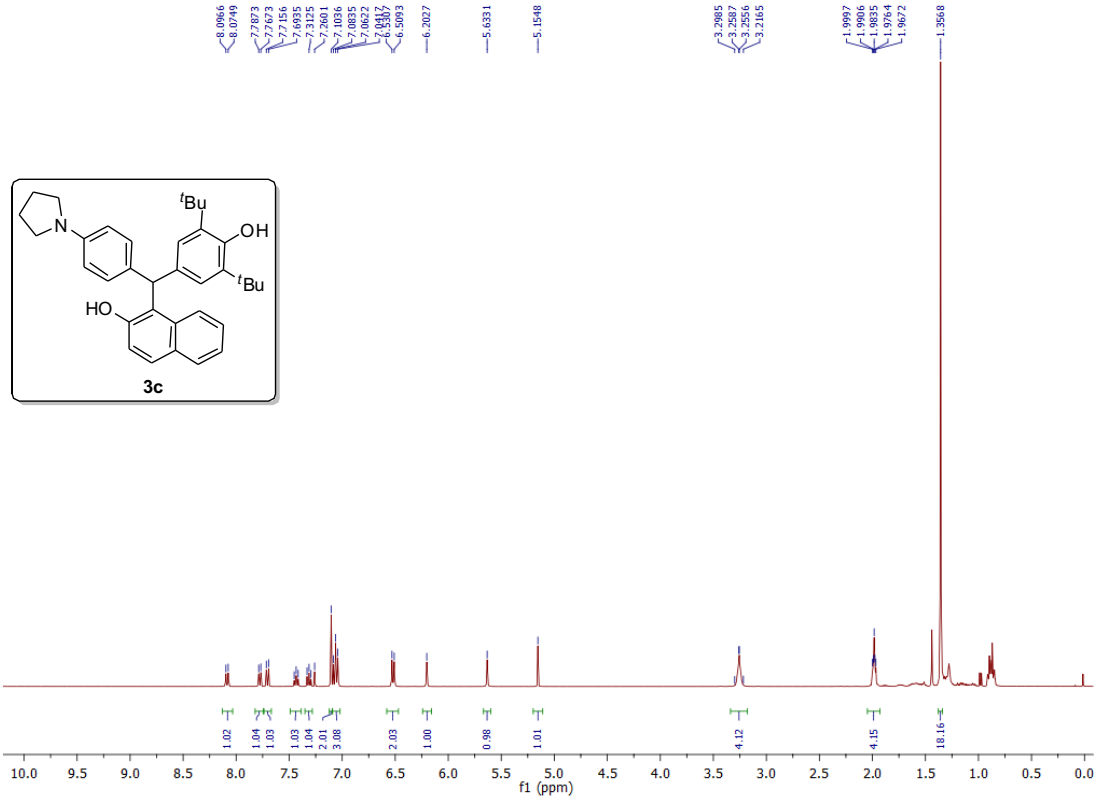
^{1}H NMR Spectrum of 3b



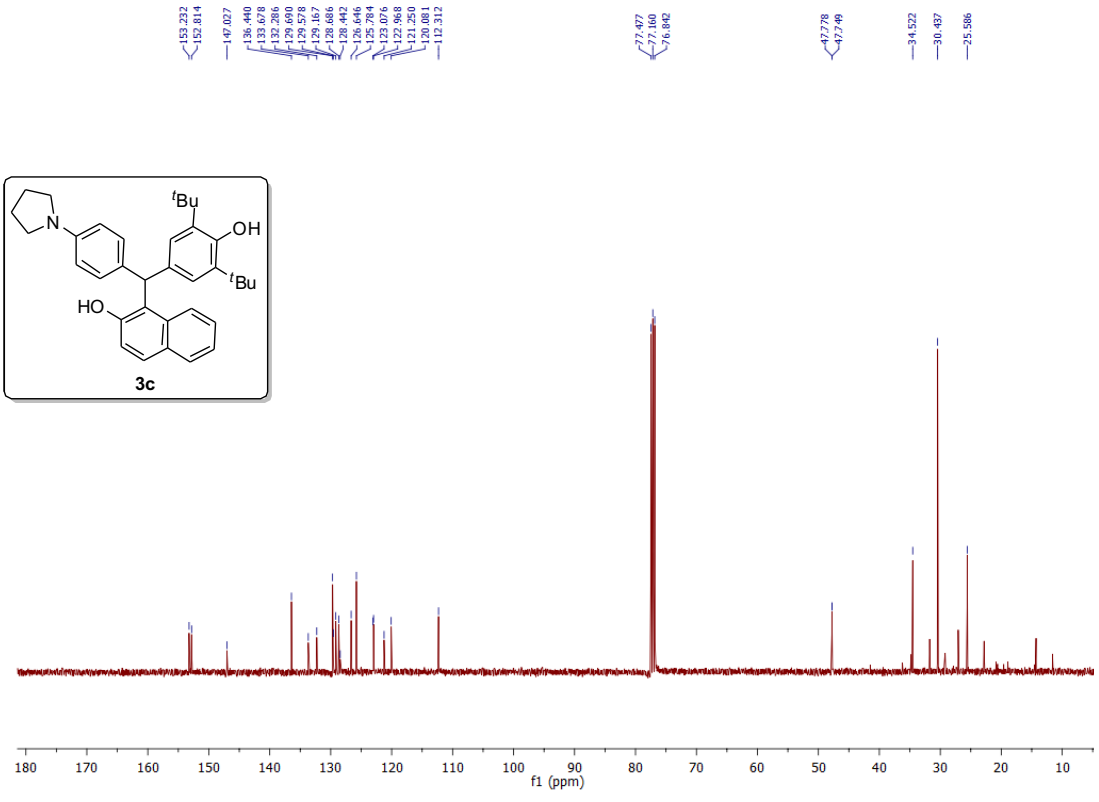
^{13}C NMR Spectrum of 3b



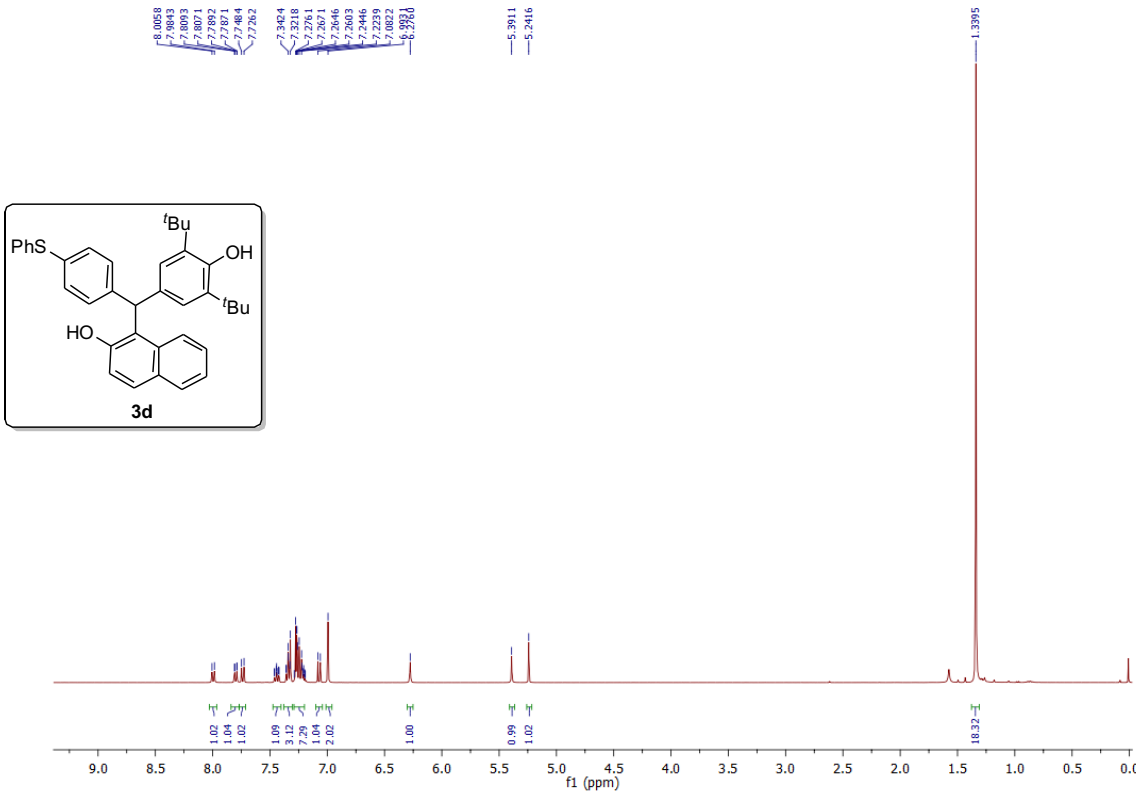
^{1}H NMR Spectrum of 3c



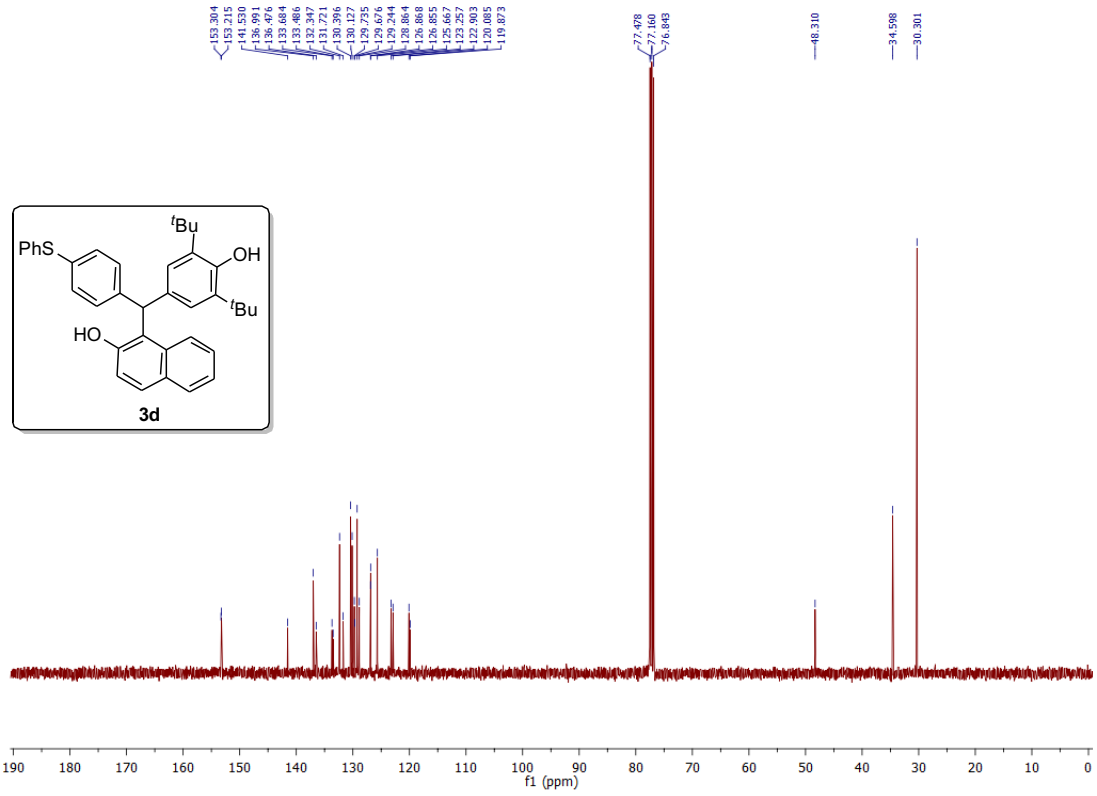
^{13}C NMR Spectrum of 3c



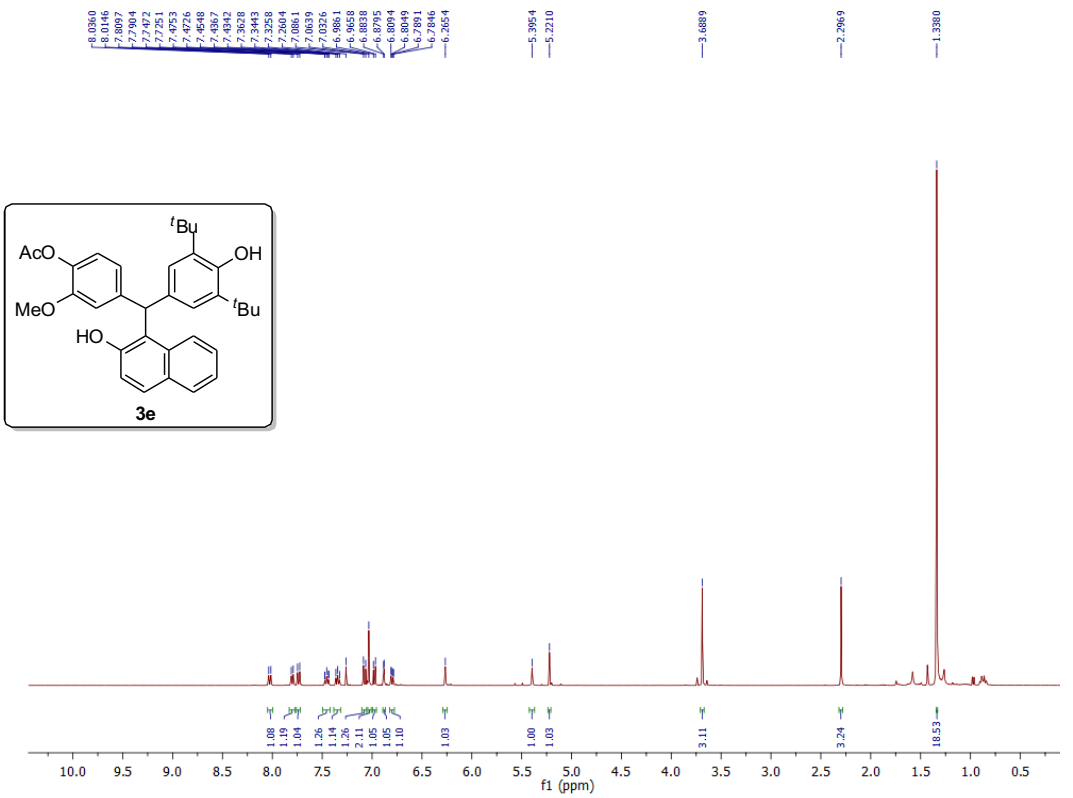
^{1}H NMR Spectrum of 3d



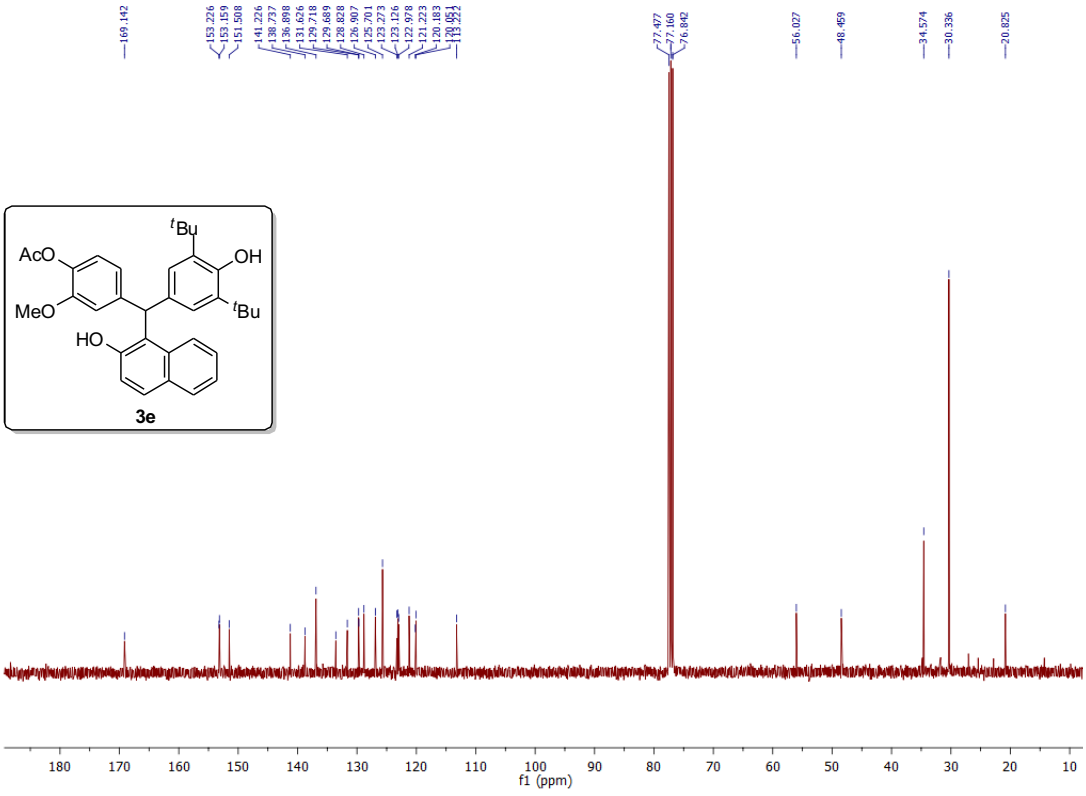
^{13}C NMR Spectrum of 3d



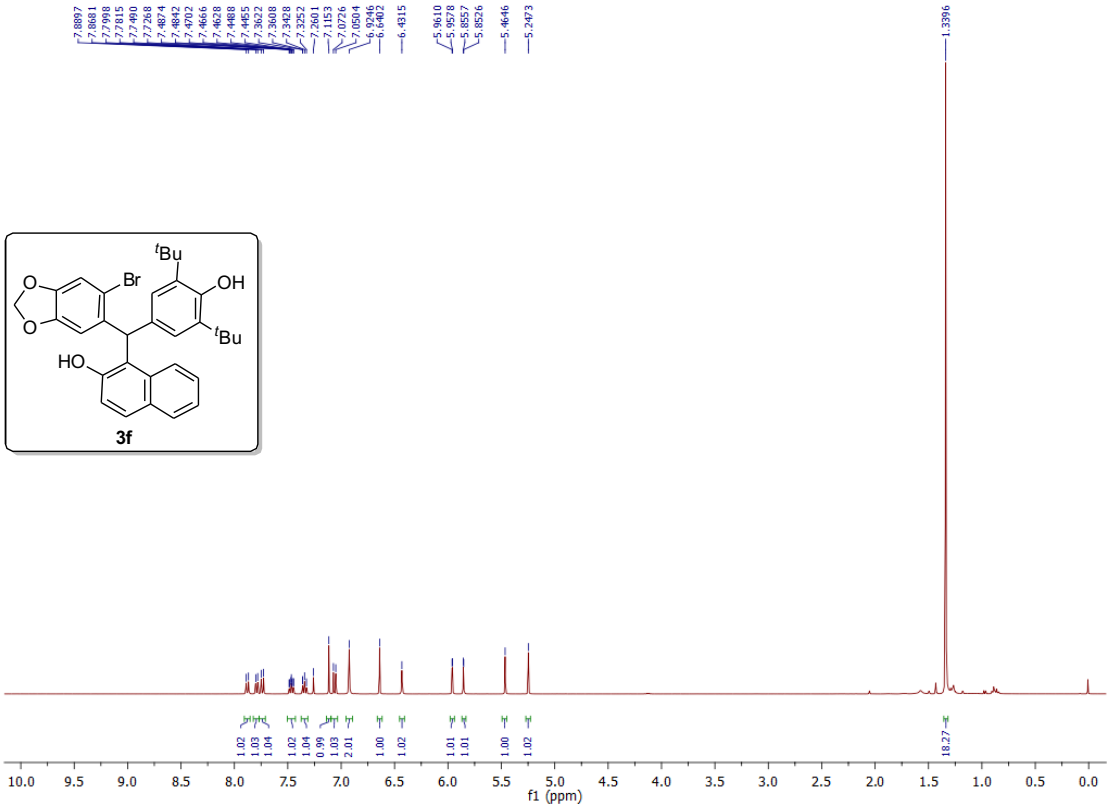
^{1}H NMR Spectrum of 3e



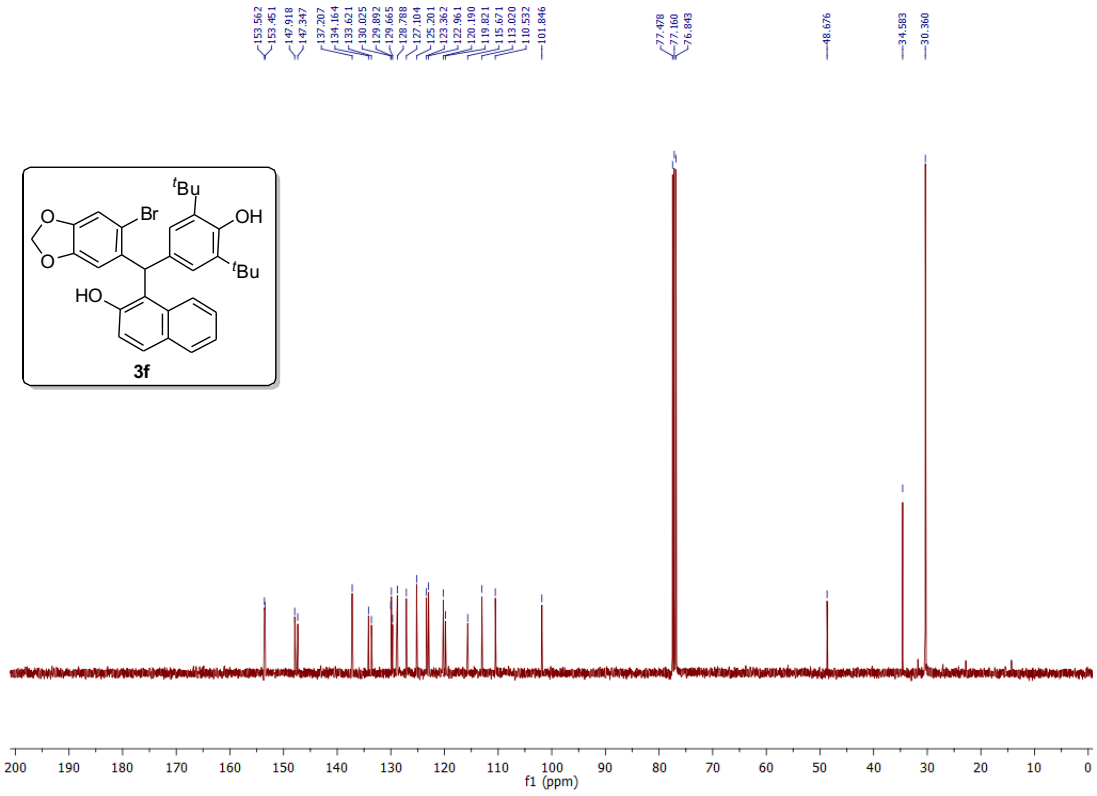
^{13}C NMR Spectrum of 3e



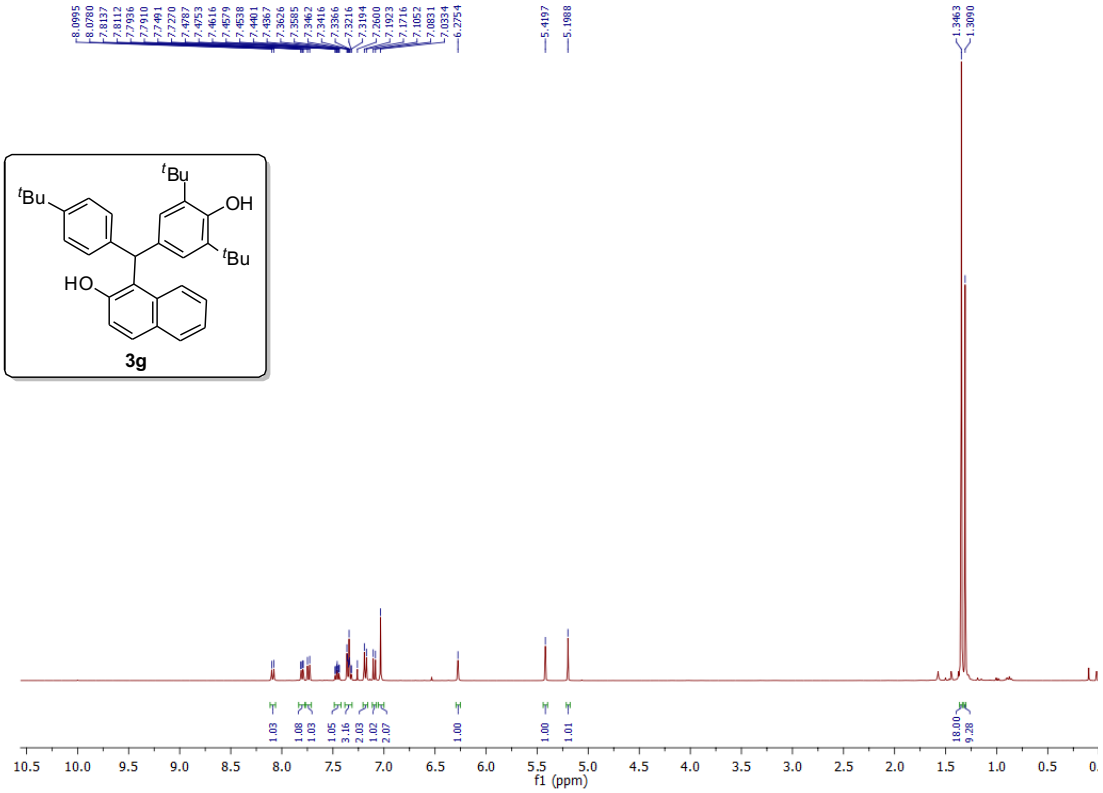
^{1}H NMR Spectrum of 3f



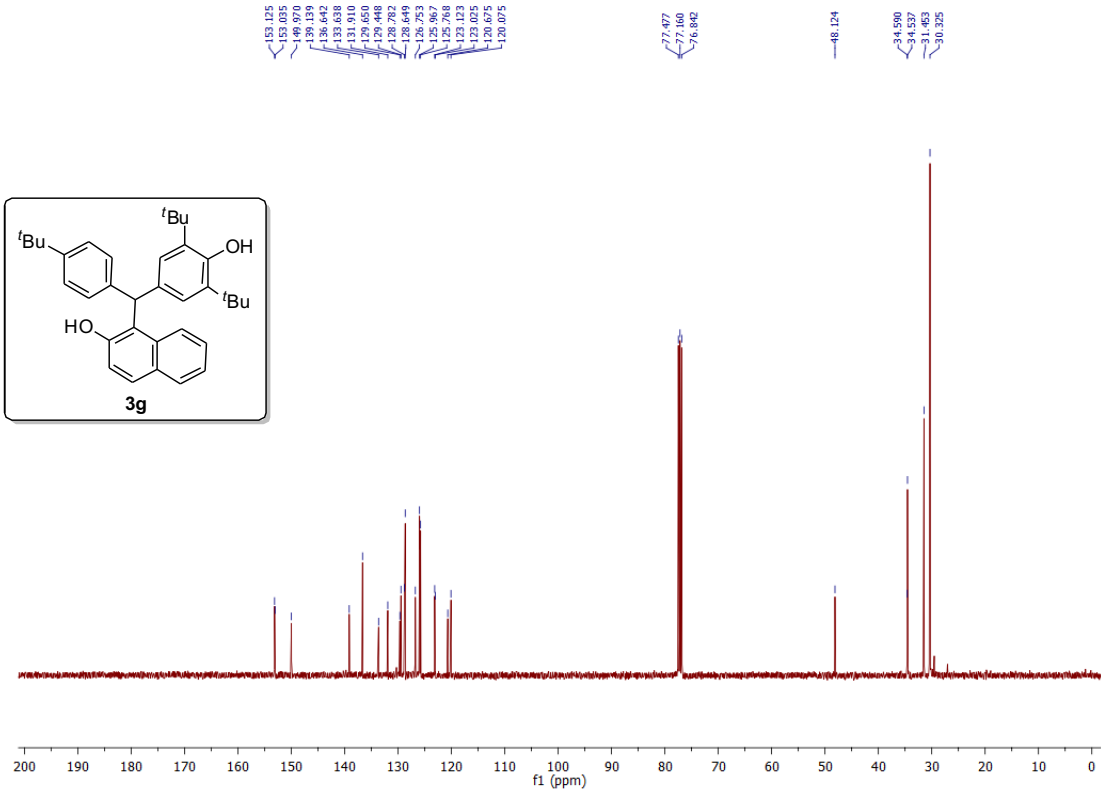
^{13}C NMR Spectrum of 3f



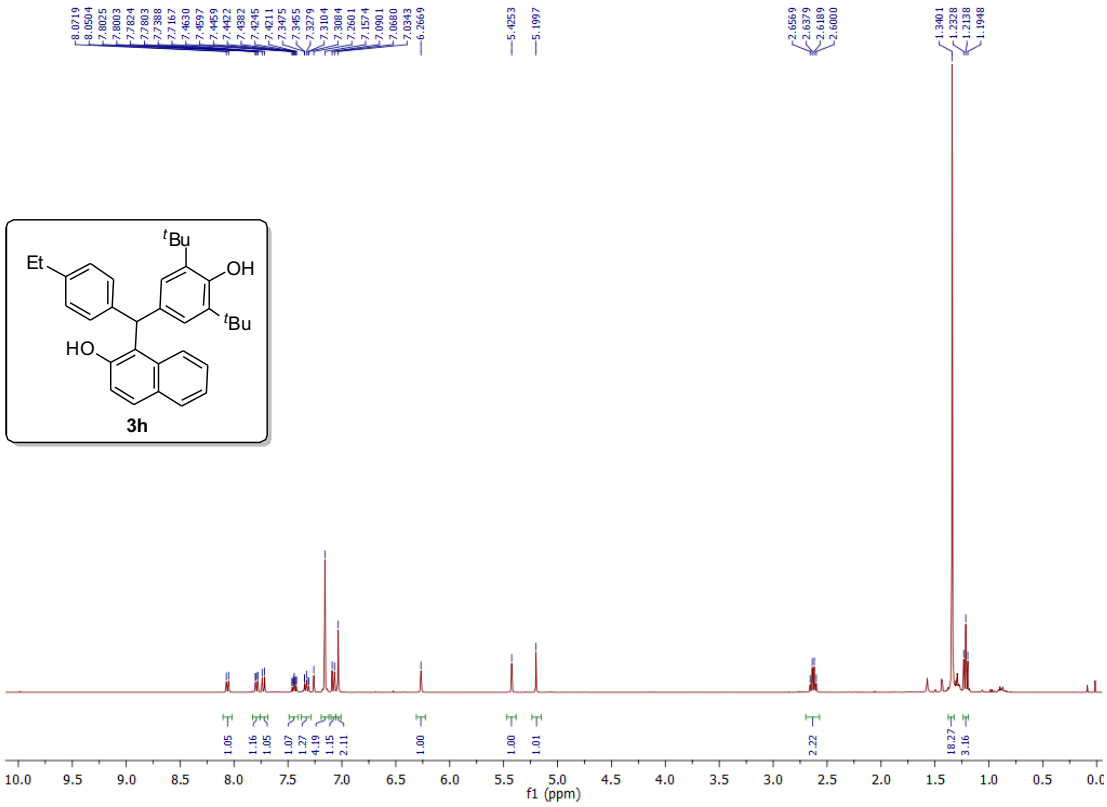
^{1}H NMR Spectrum of 3g



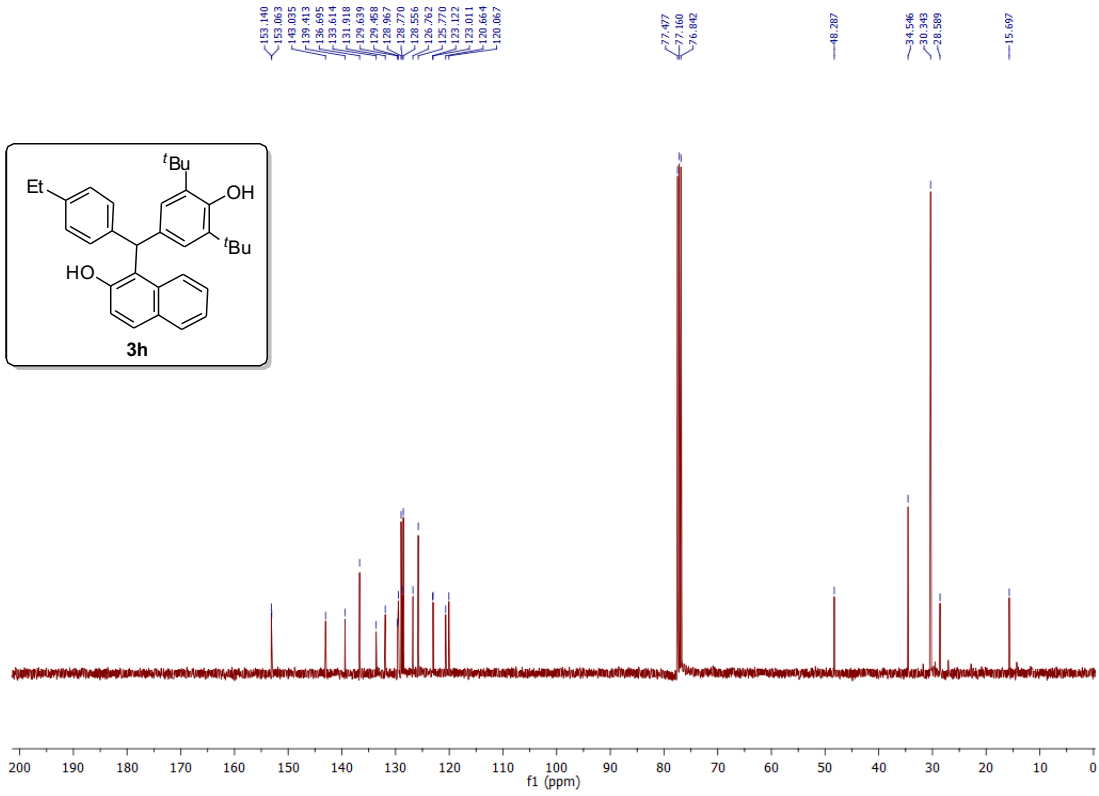
^{13}C NMR Spectrum of 3g



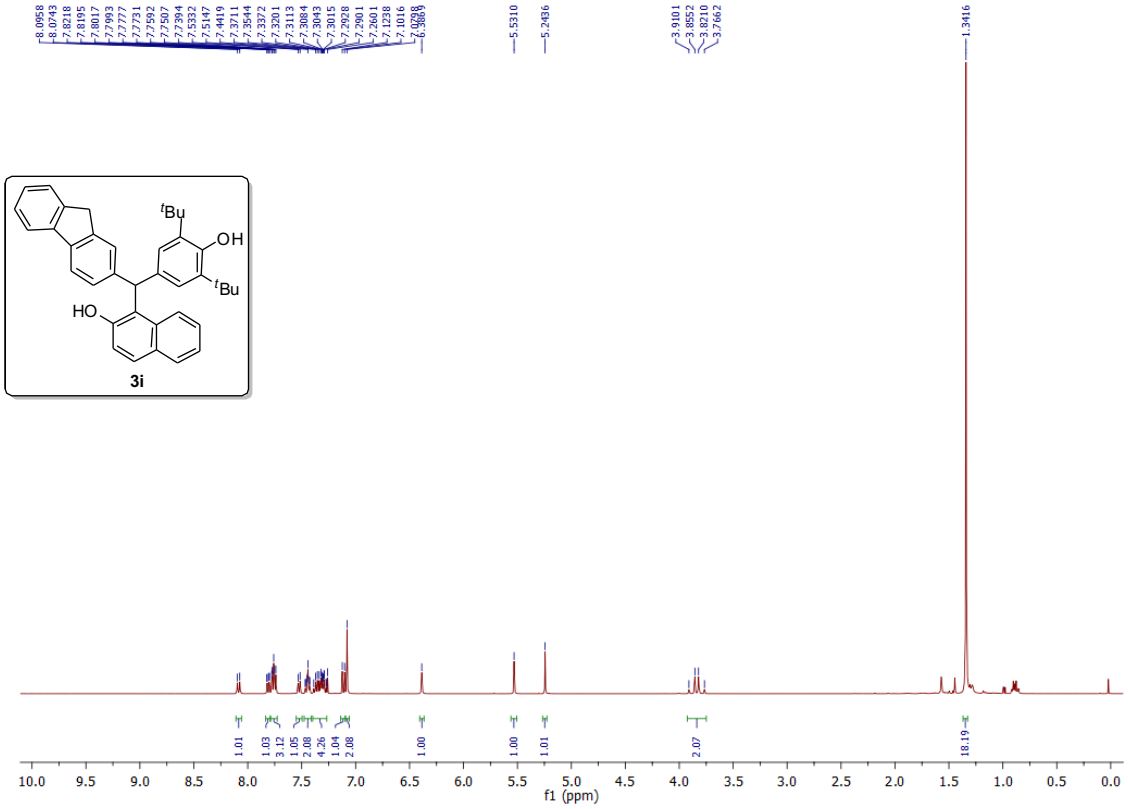
^{1}H NMR Spectrum of 3h



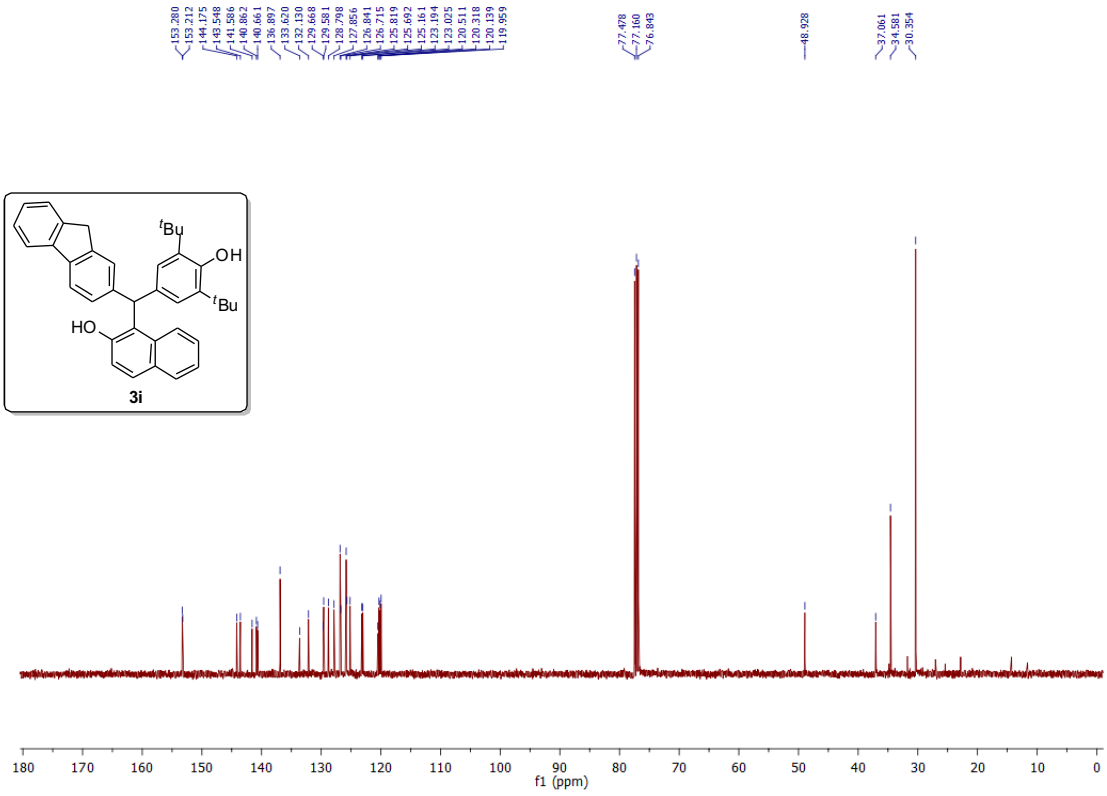
^{13}C NMR Spectrum of 3h



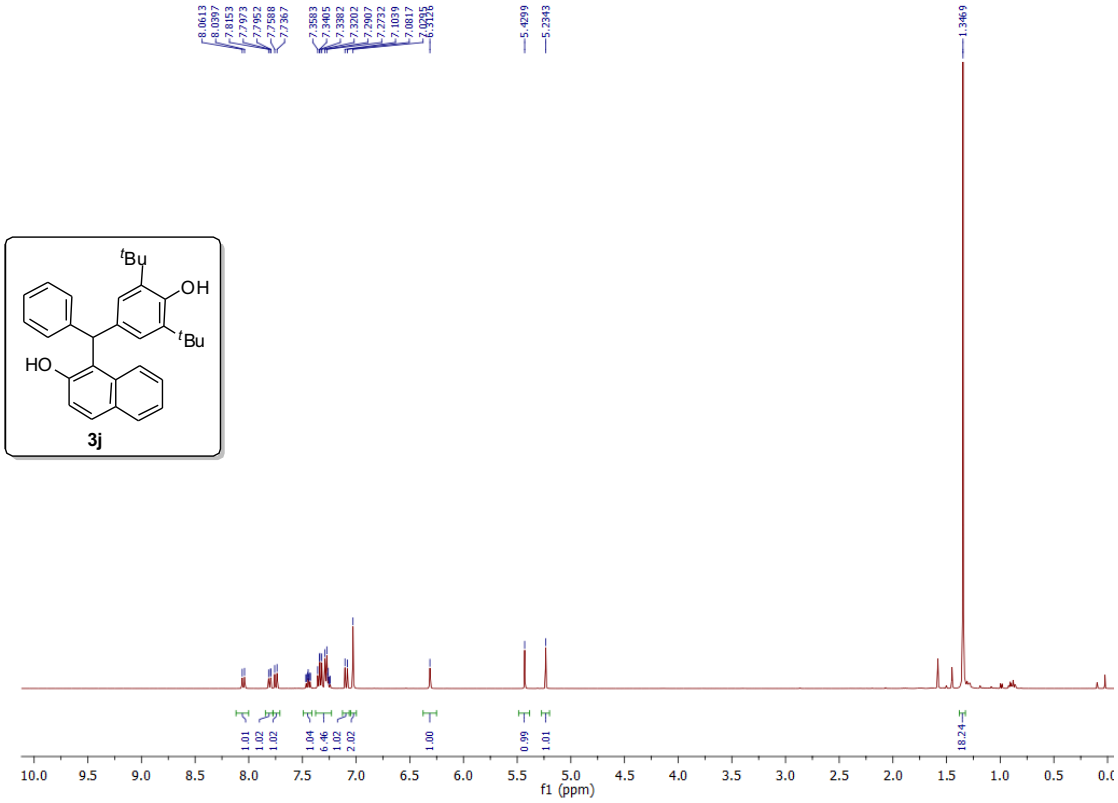
^{1}H NMR Spectrum of 3i



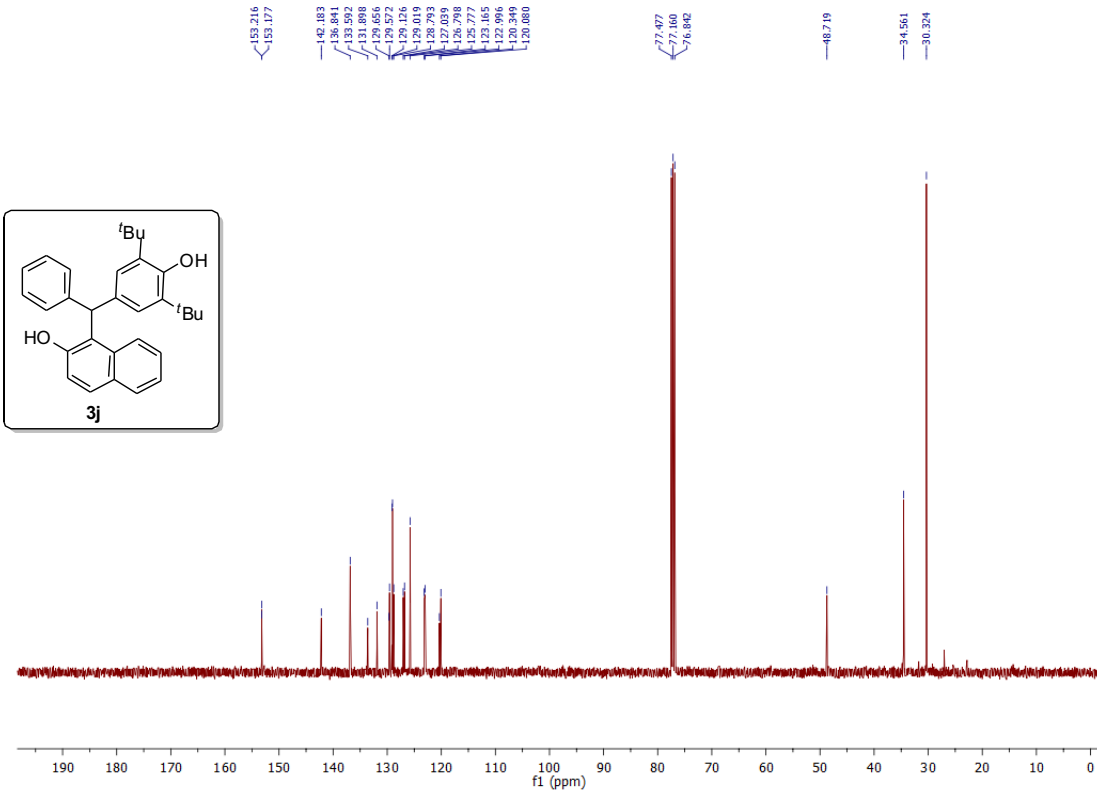
^{13}C NMR Spectrum of 3i



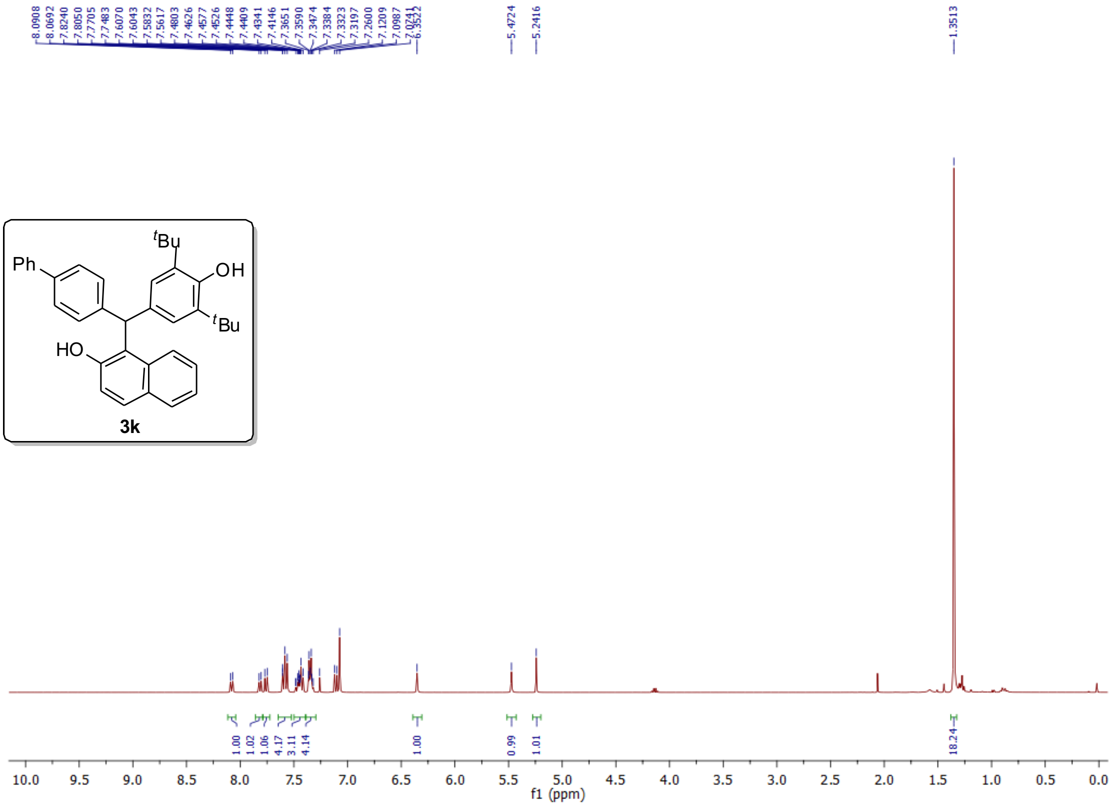
^{1}H NMR Spectrum of 3j



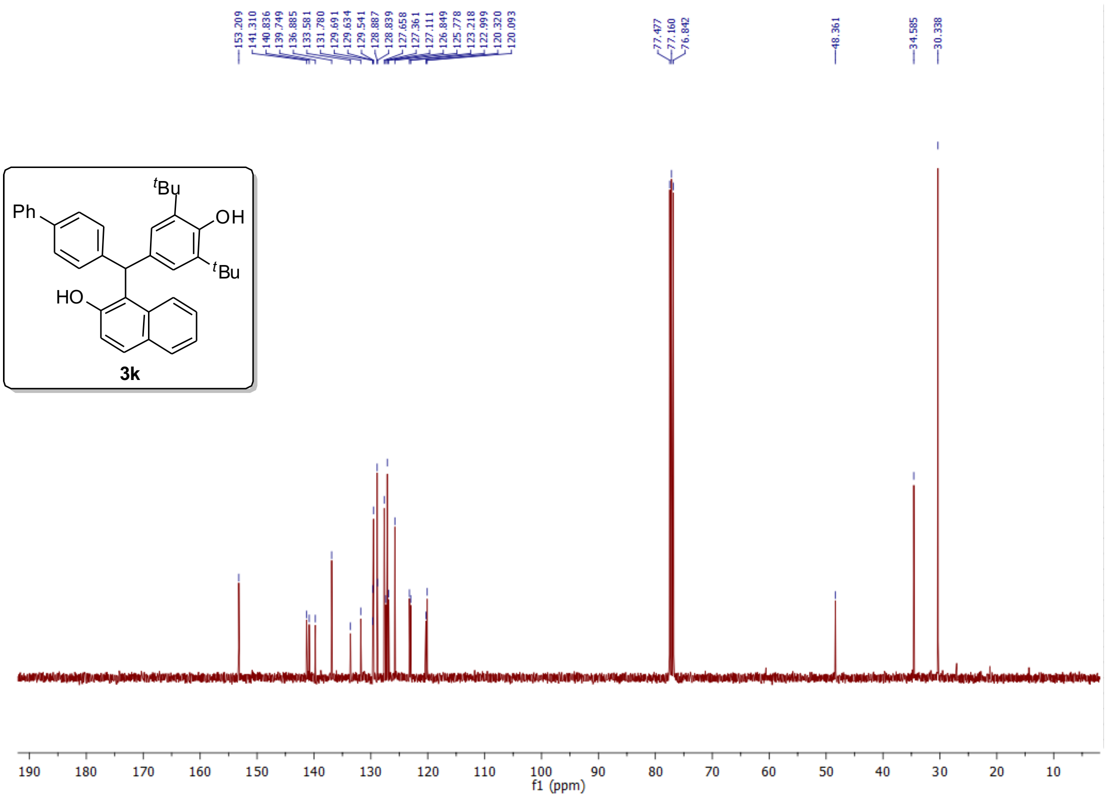
^{13}C NMR Spectrum of 3j



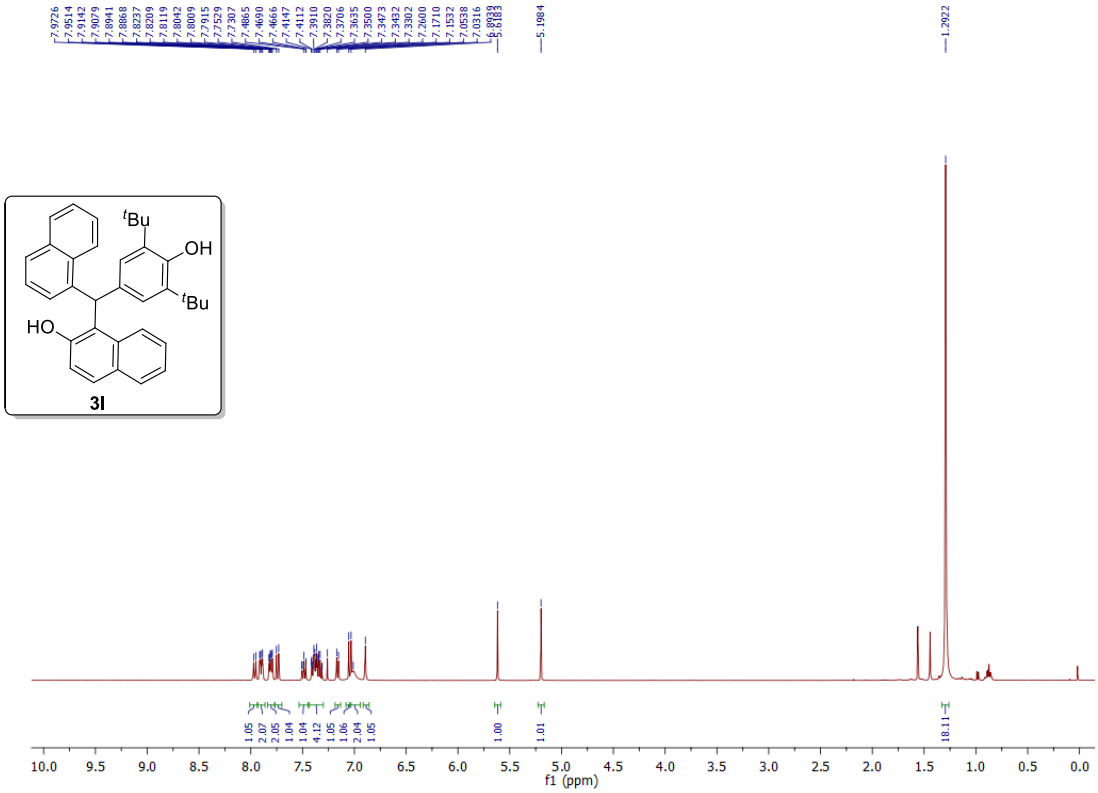
^{1}H NMR Spectrum of 3k



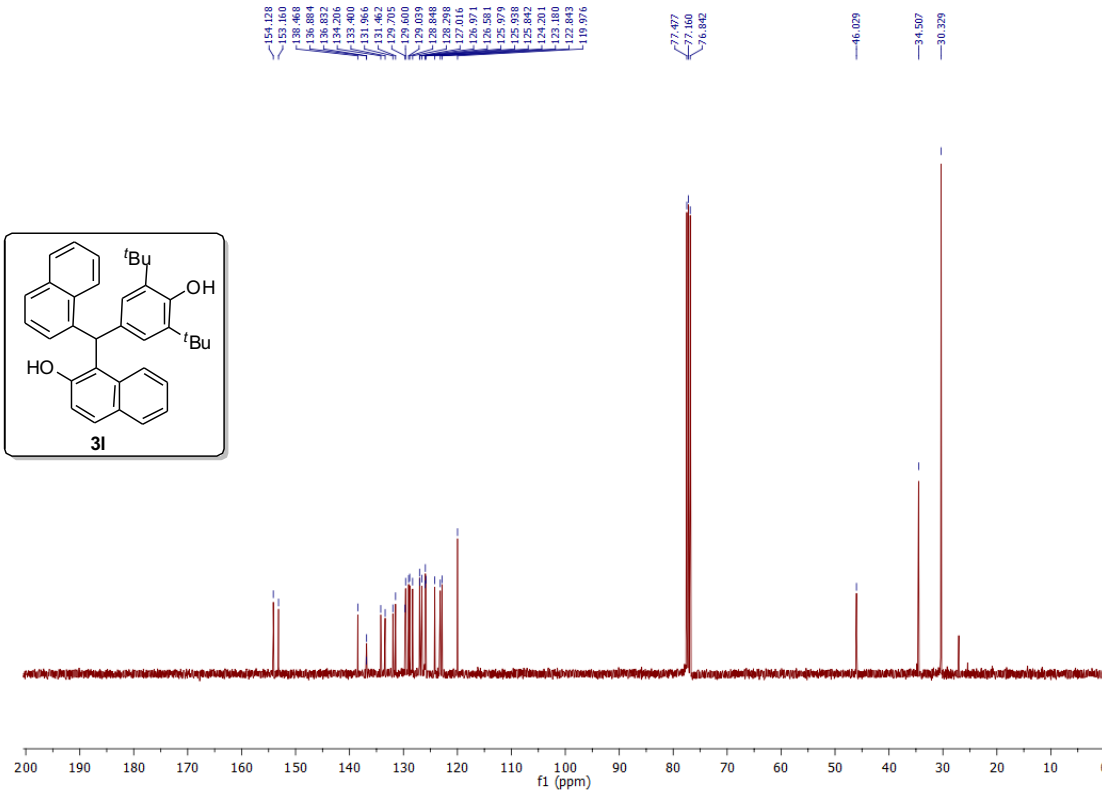
^{13}C NMR Spectrum of 3k



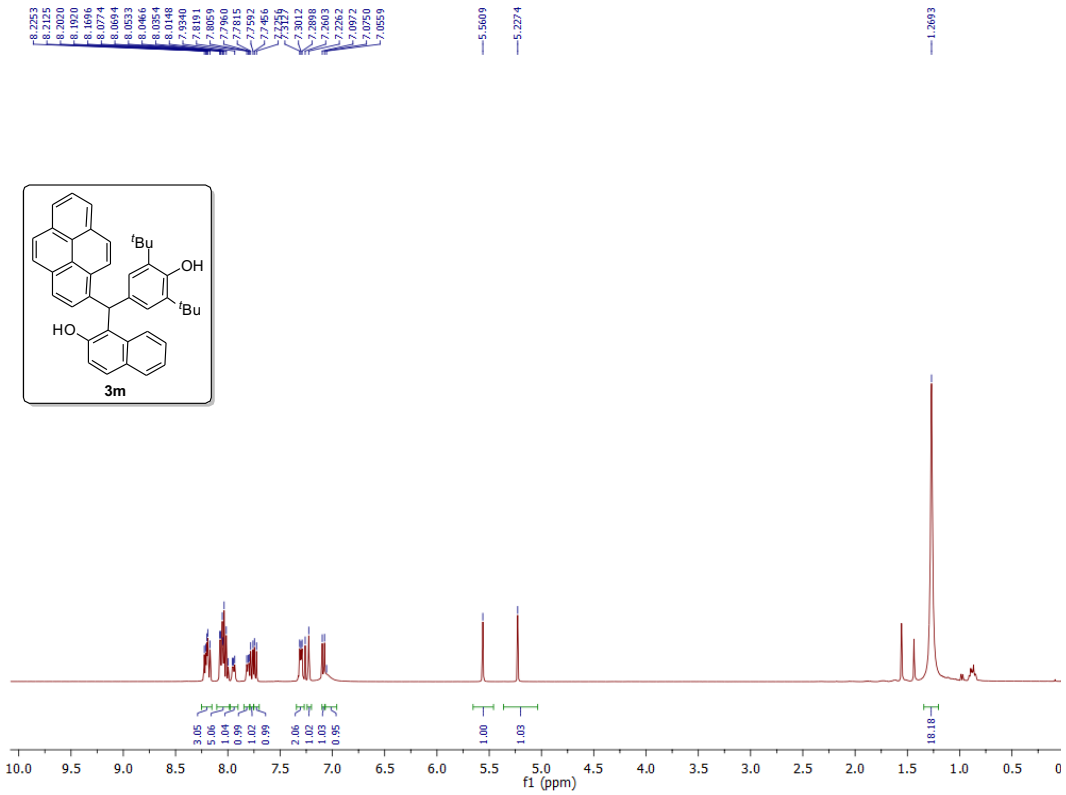
^{1}H NMR Spectrum of 3l



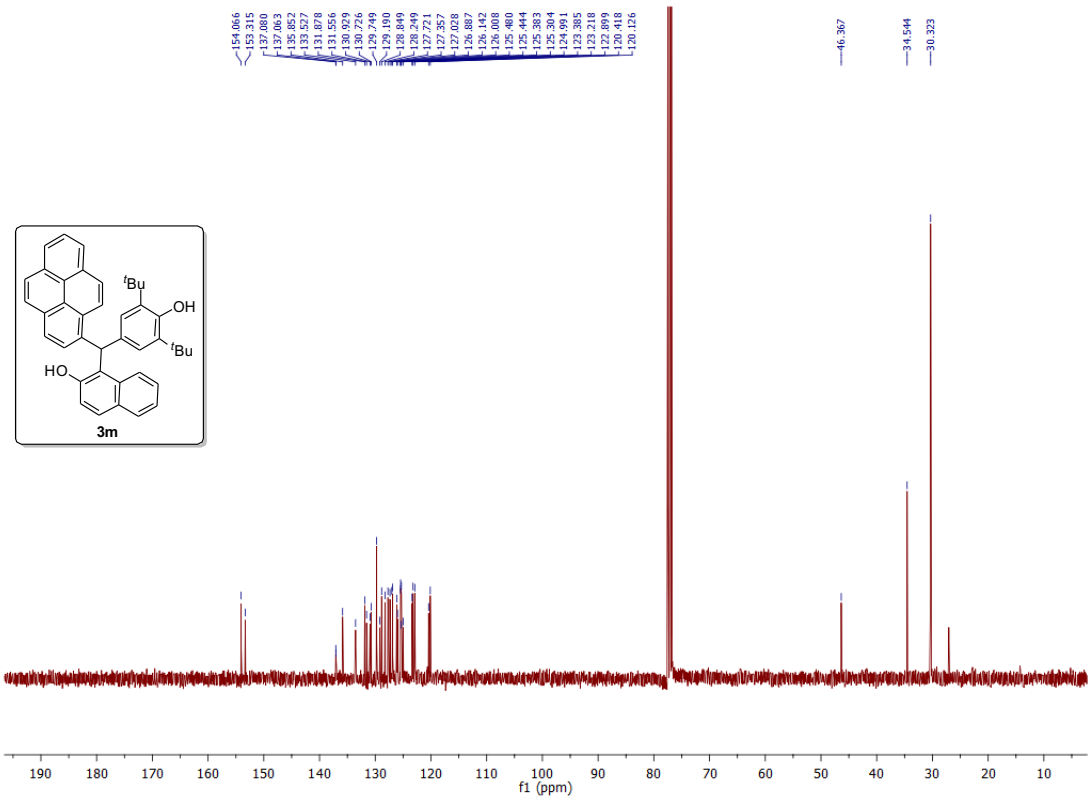
^{13}C NMR Spectrum of 3l



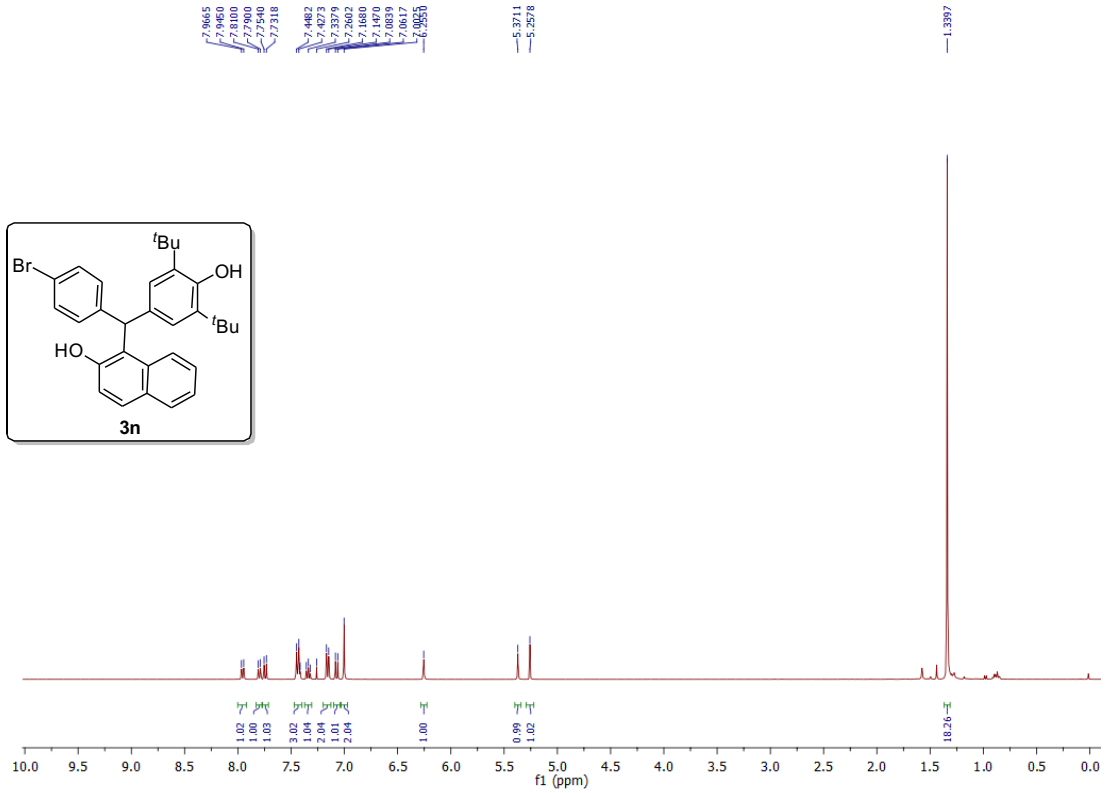
^{1}H NMR Spectrum of 3m



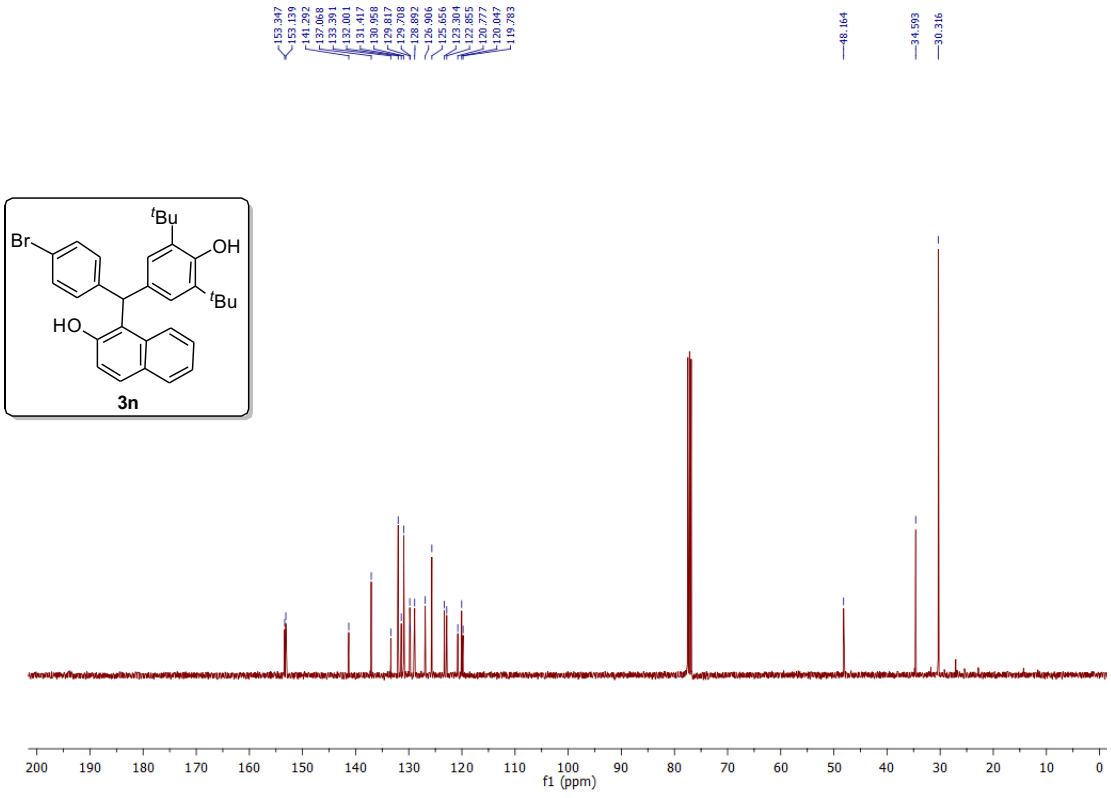
^{13}C NMR Spectrum of 3m



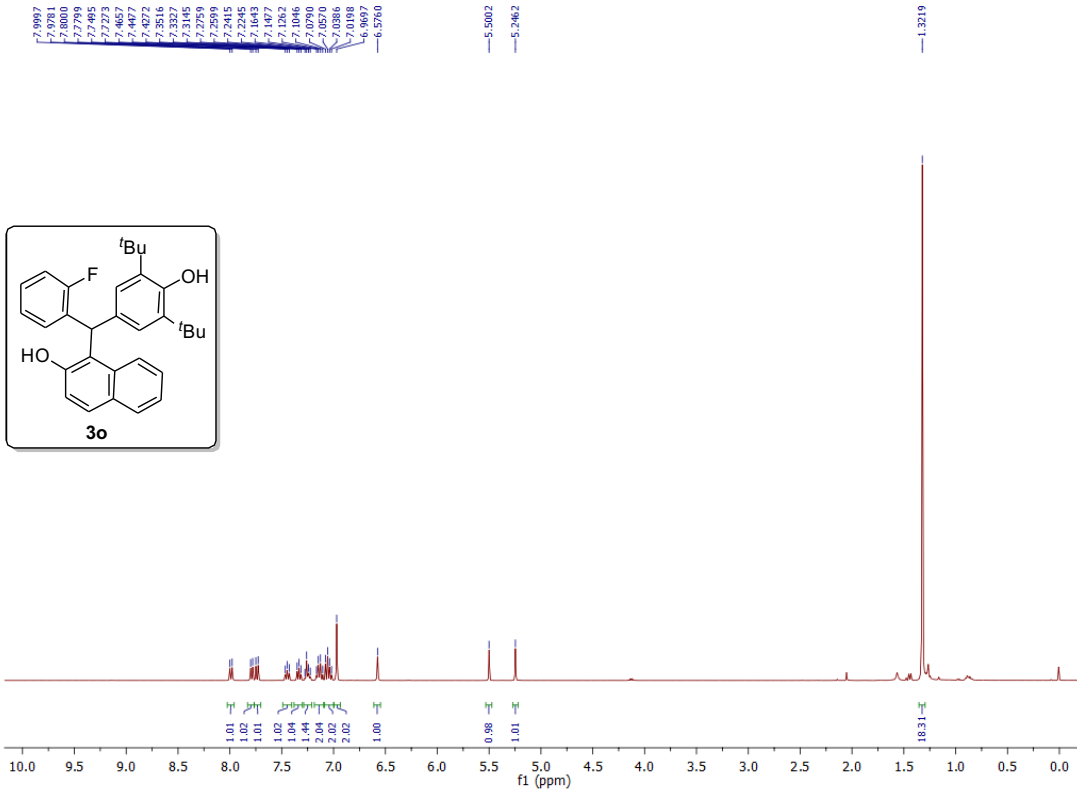
^{1}H NMR Spectrum of 3n



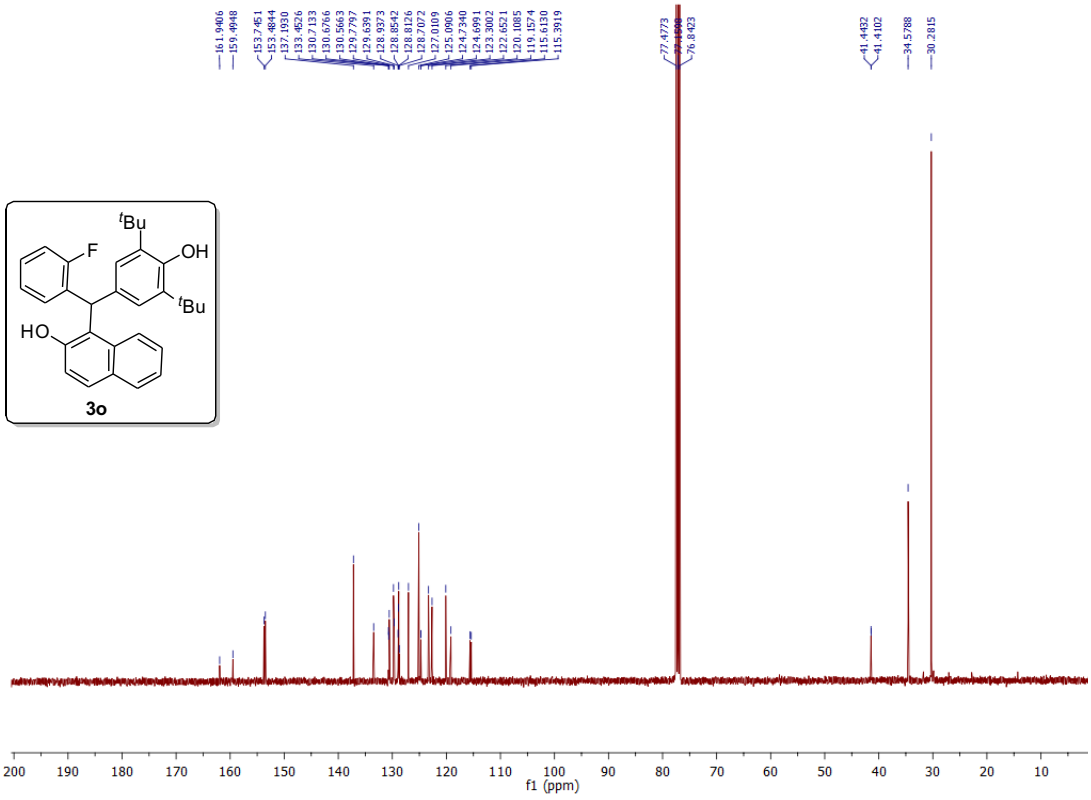
^{13}C NMR Spectrum of 3n



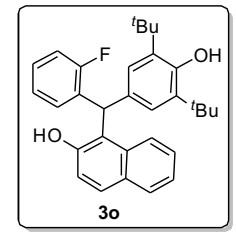
^{1}H NMR Spectrum of 3o



^{13}C NMR Spectrum of 3o

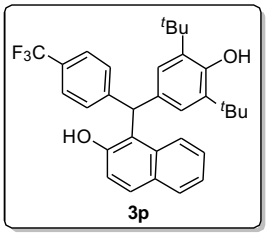


^{19}F NMR Spectrum of 3o



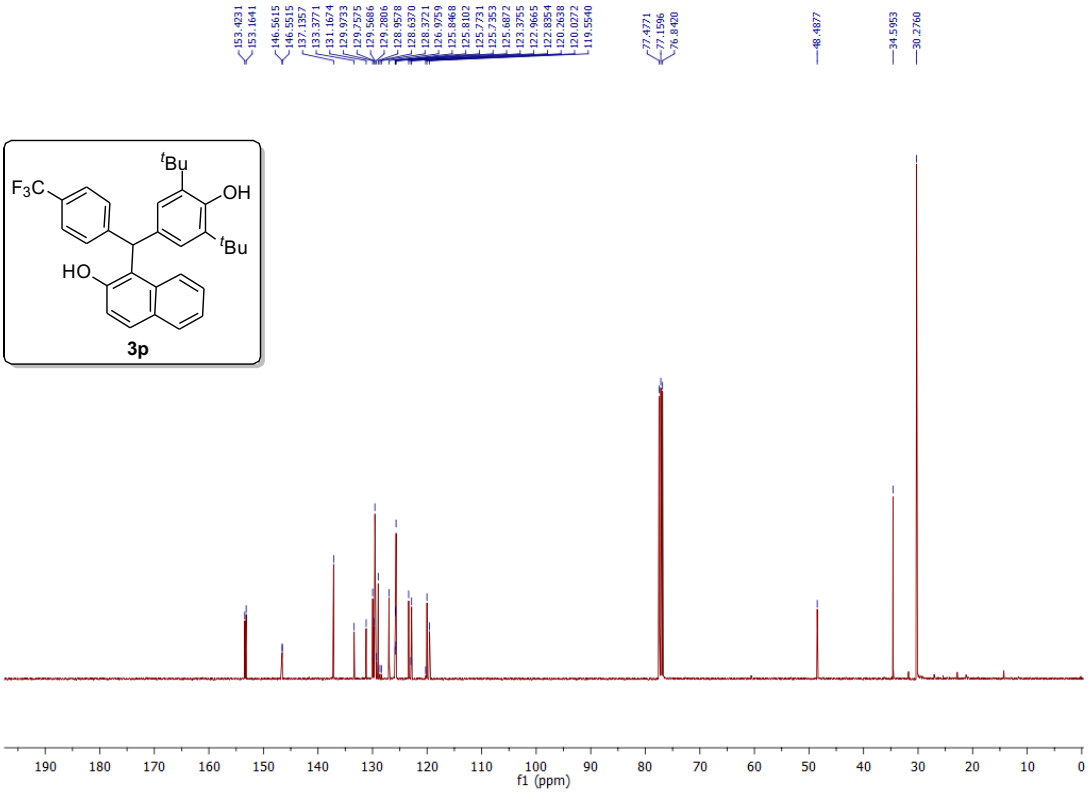
3o

^{1}H NMR Spectrum of 3p

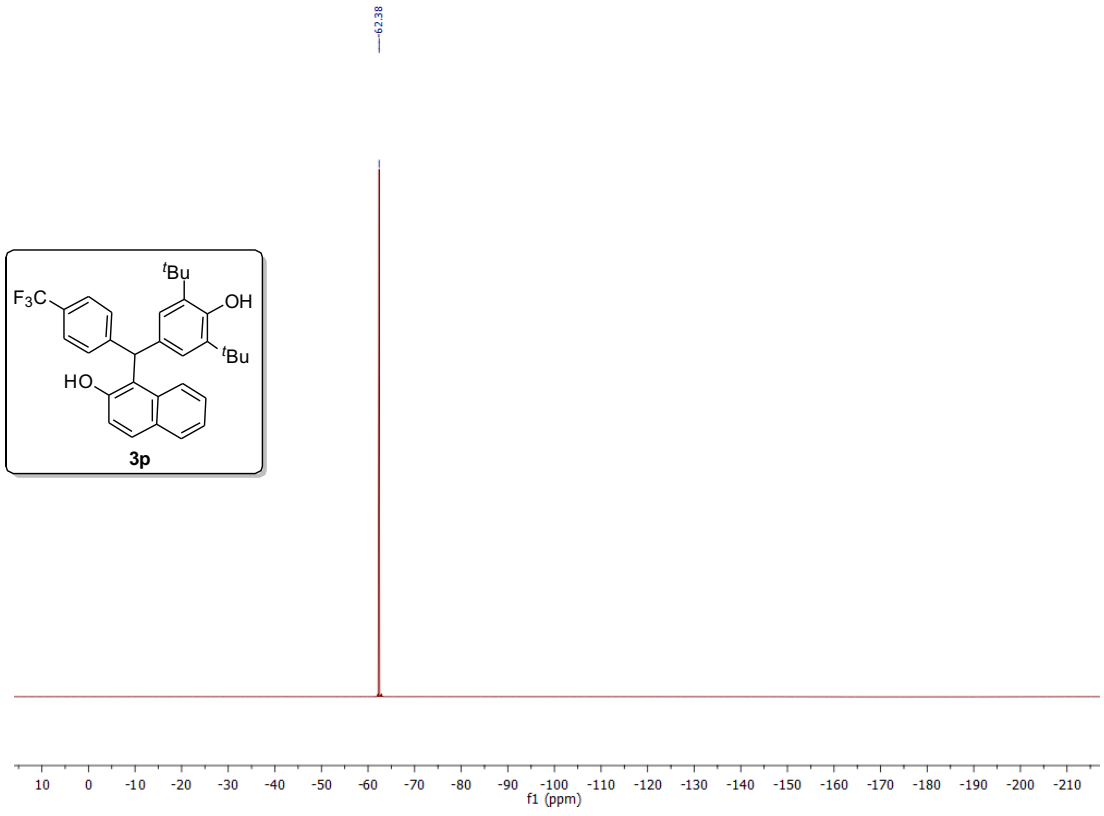


3p

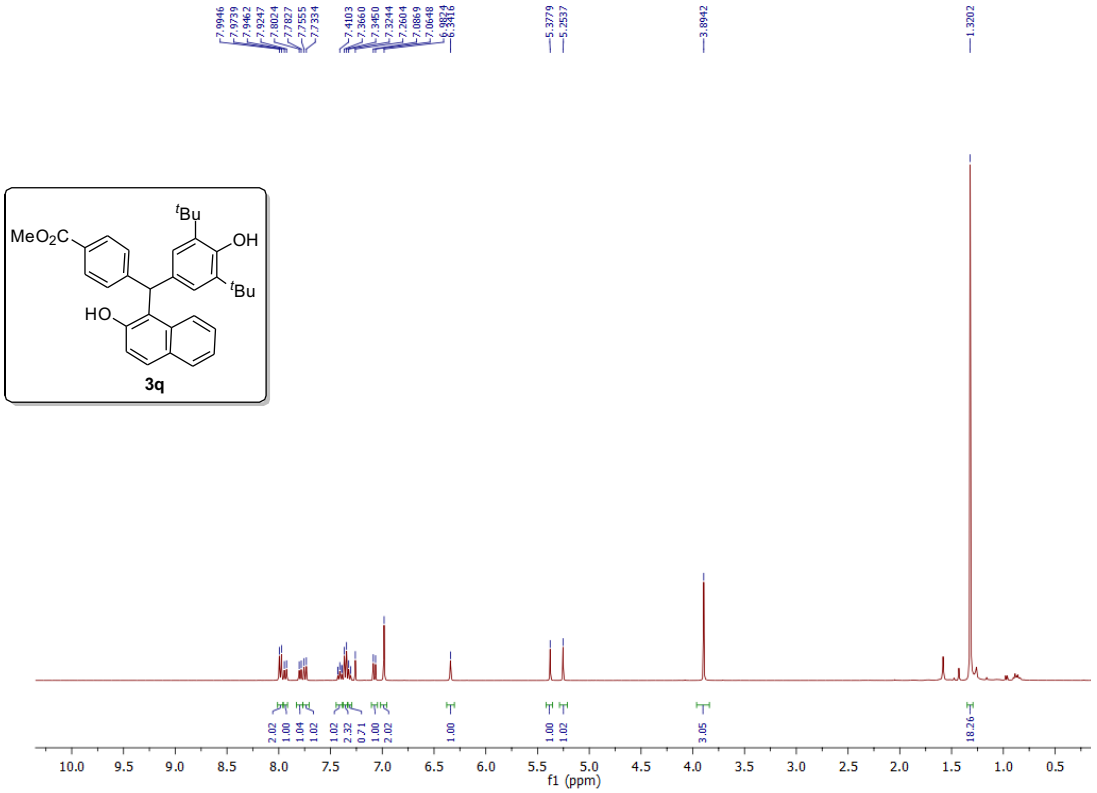
^{13}C NMR Spectrum of 3p



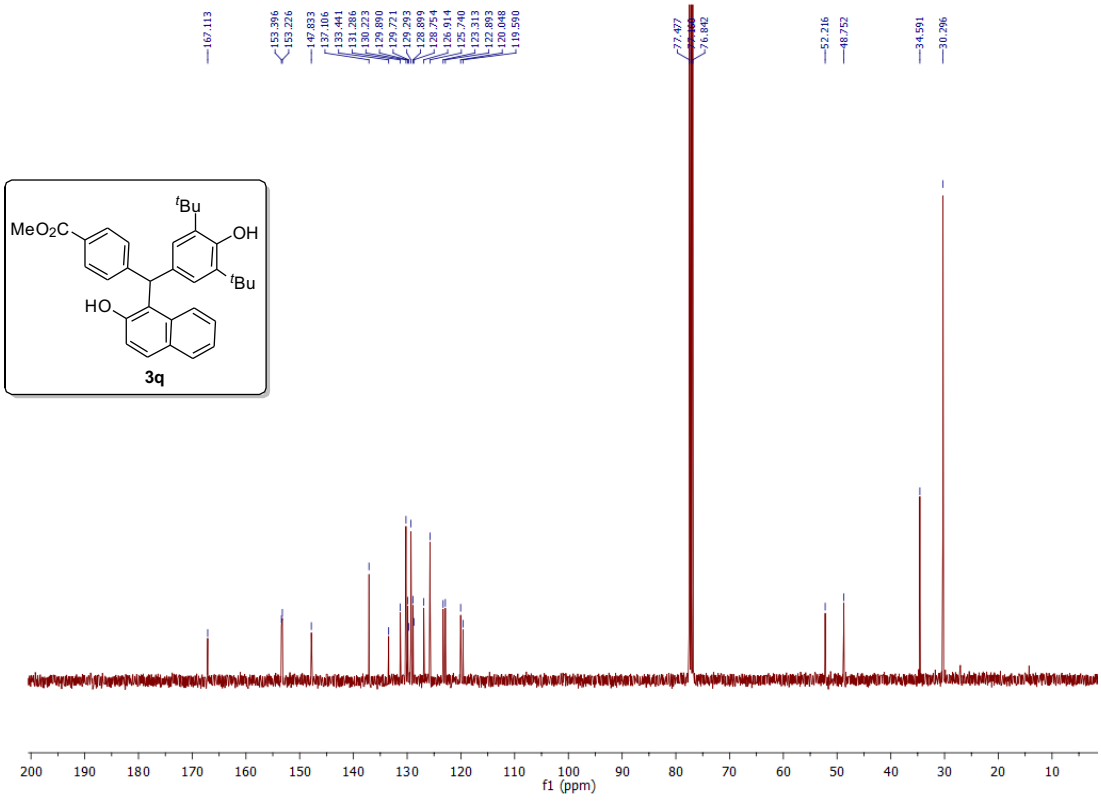
^{19}F NMR Spectrum of 3p



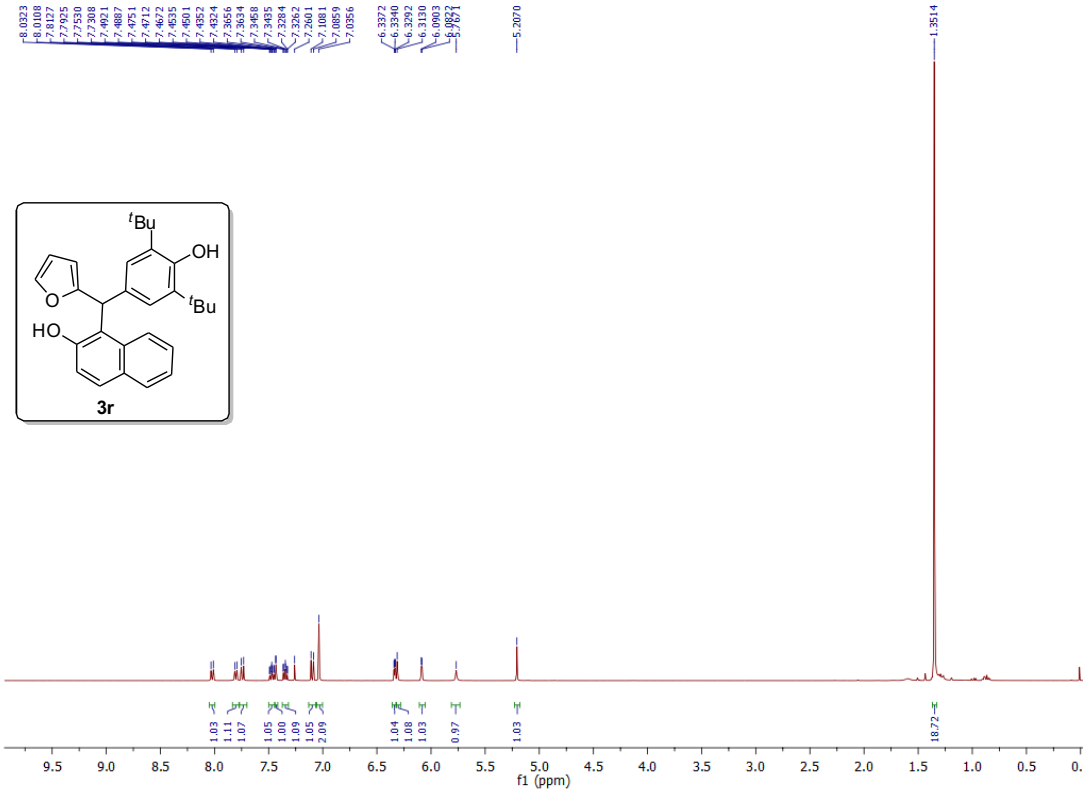
^{1}H NMR Spectrum of 3q



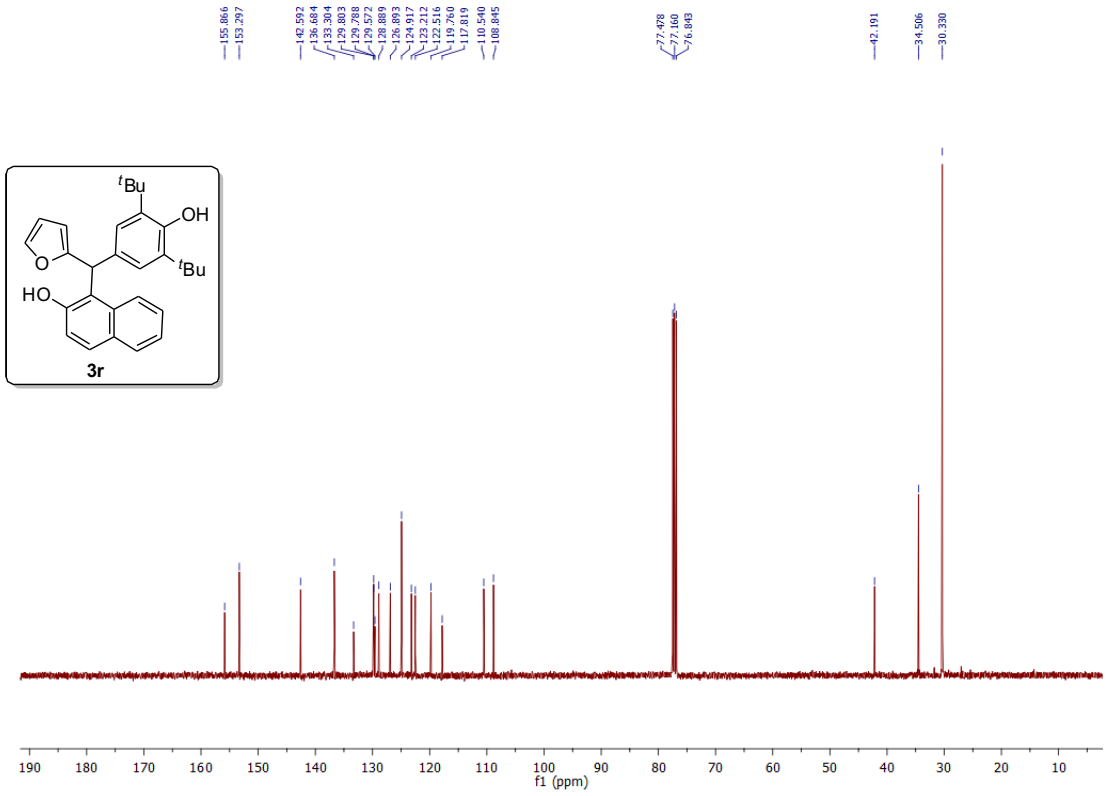
^{13}C NMR Spectrum of 3q



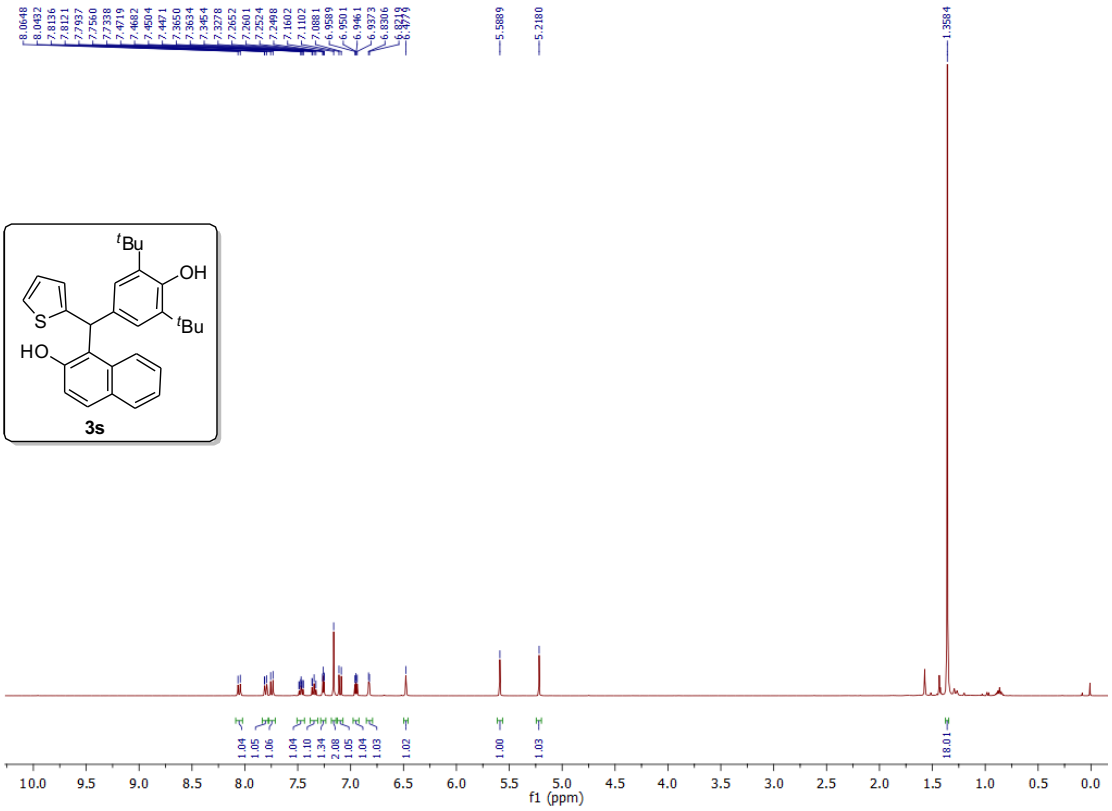
^{1}H NMR Spectrum of 3r



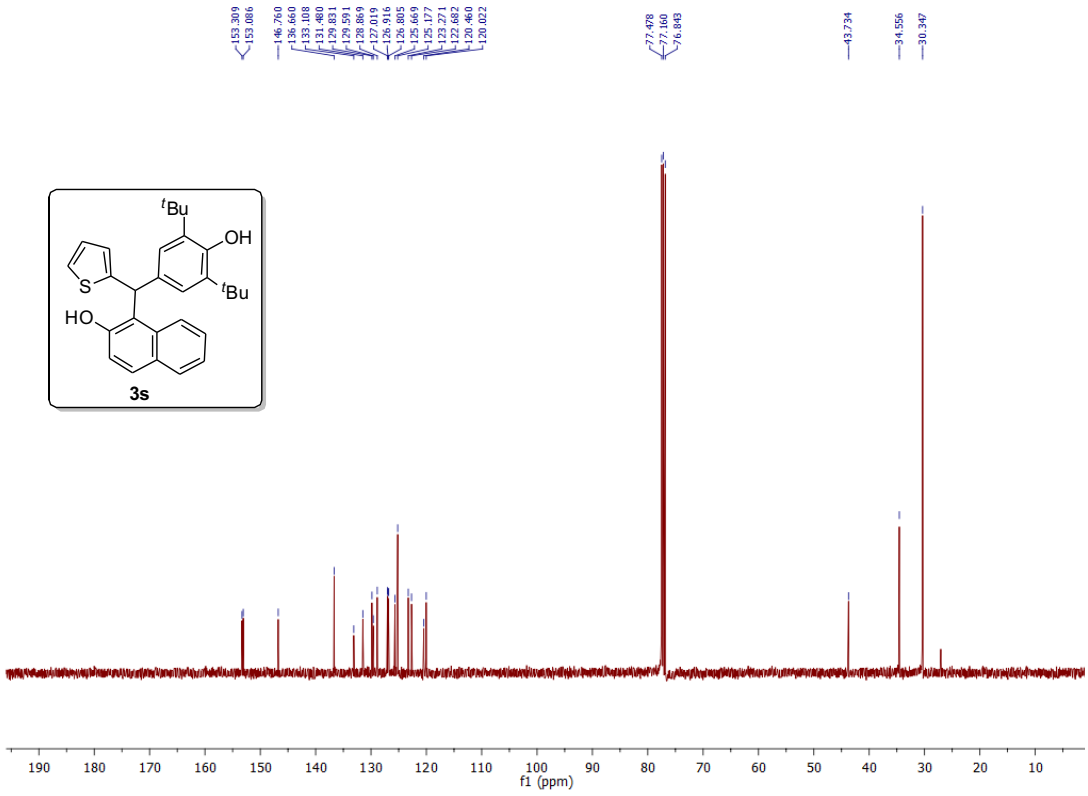
^{13}C NMR Spectrum of 3r



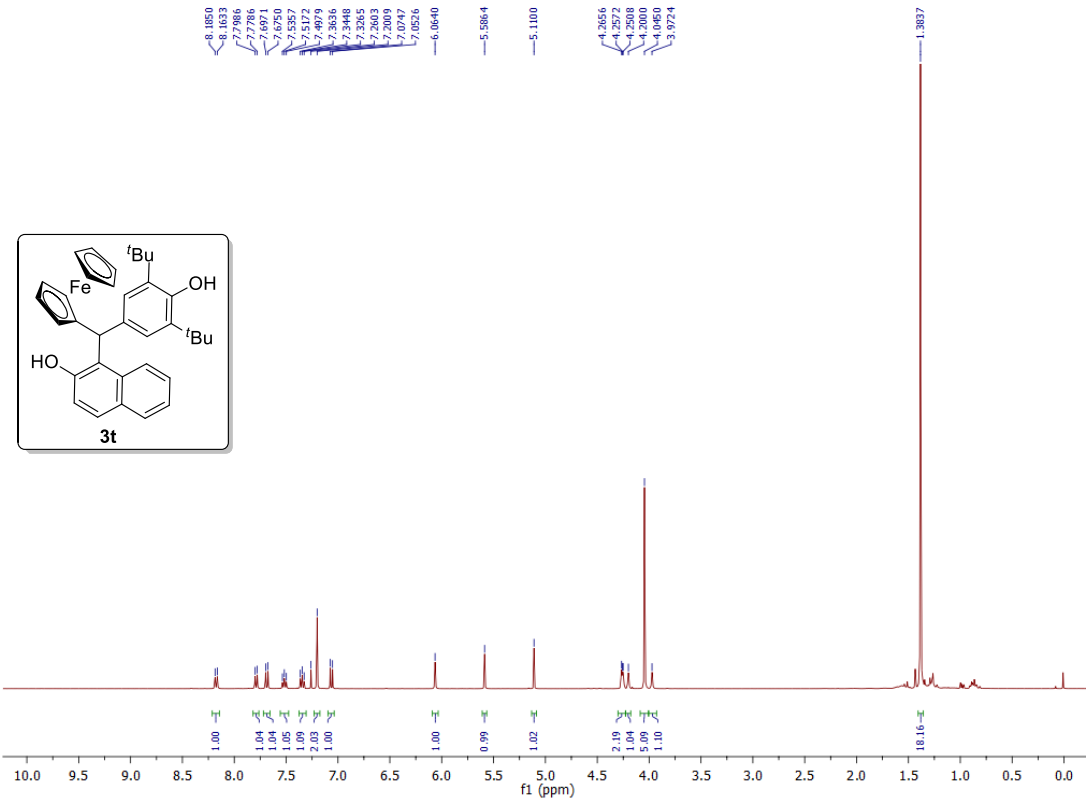
^{1}H NMR Spectrum of 3s



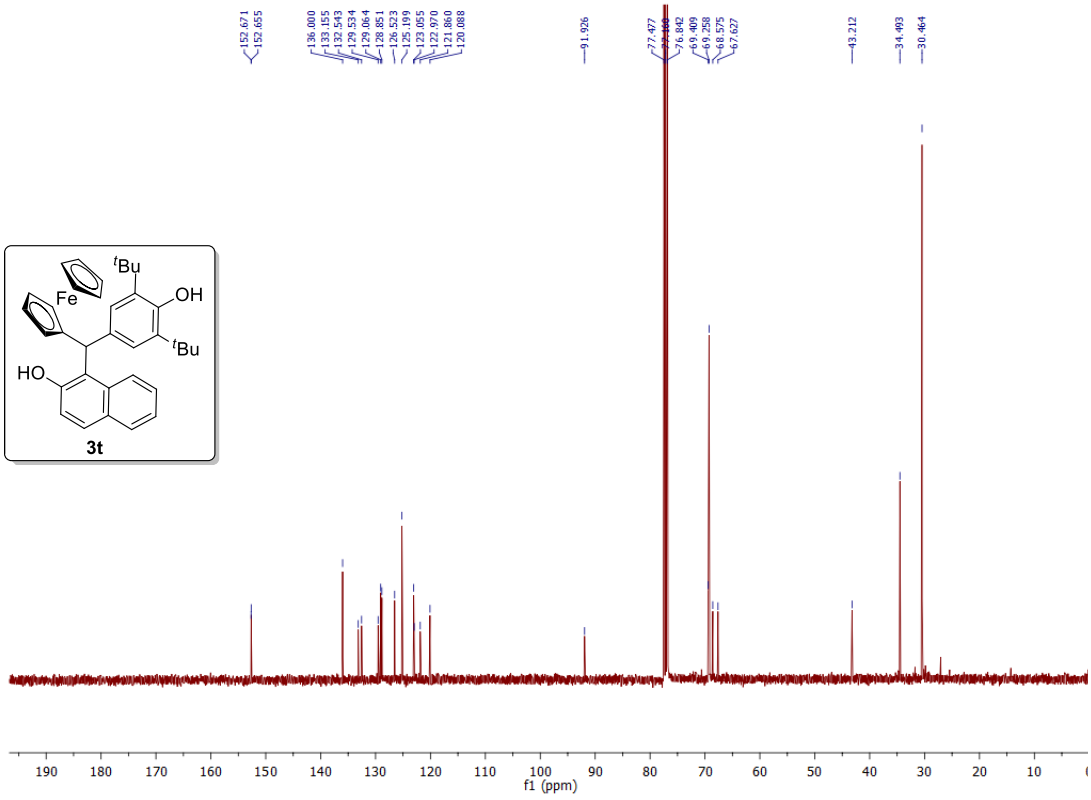
^{13}C NMR Spectrum of 3s



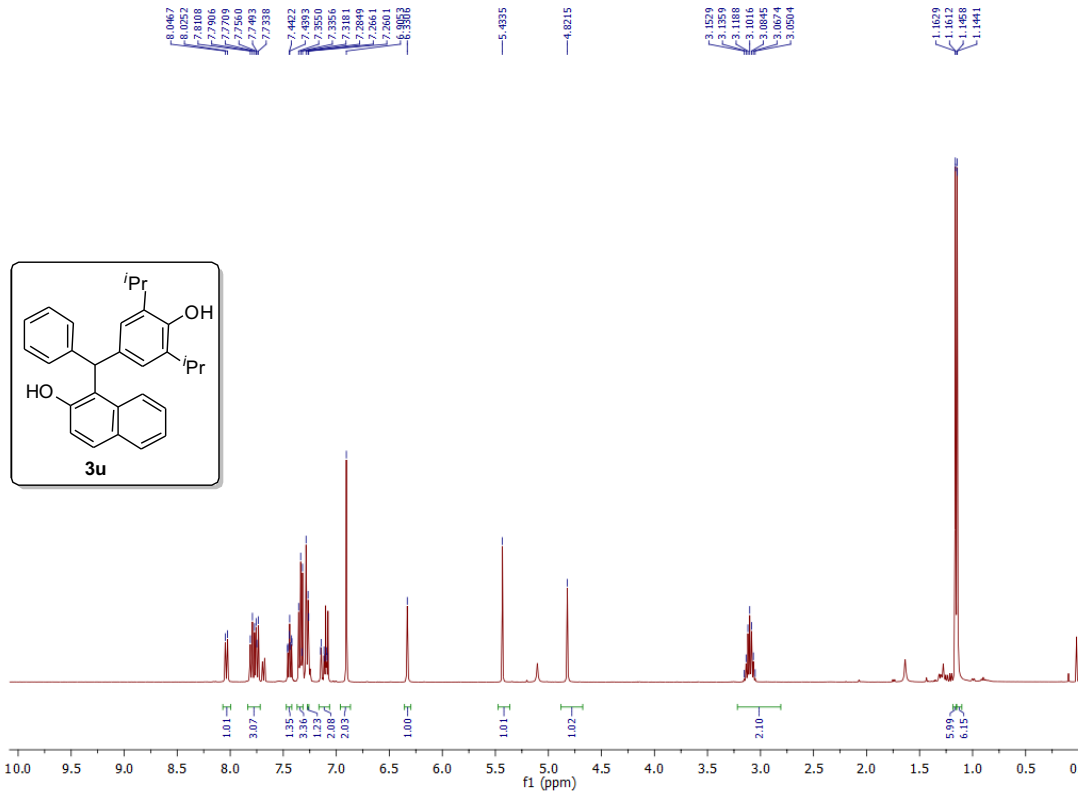
^{1}H NMR Spectrum of 3t



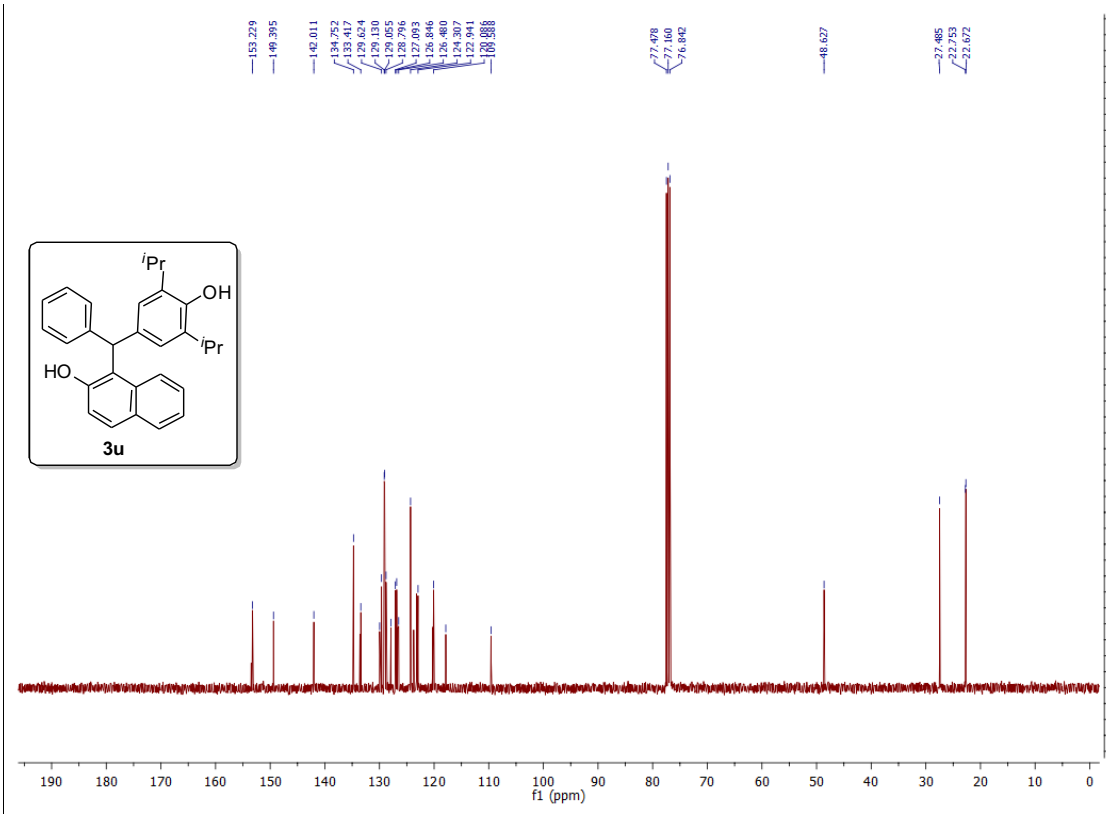
^{13}C NMR Spectrum of 3t



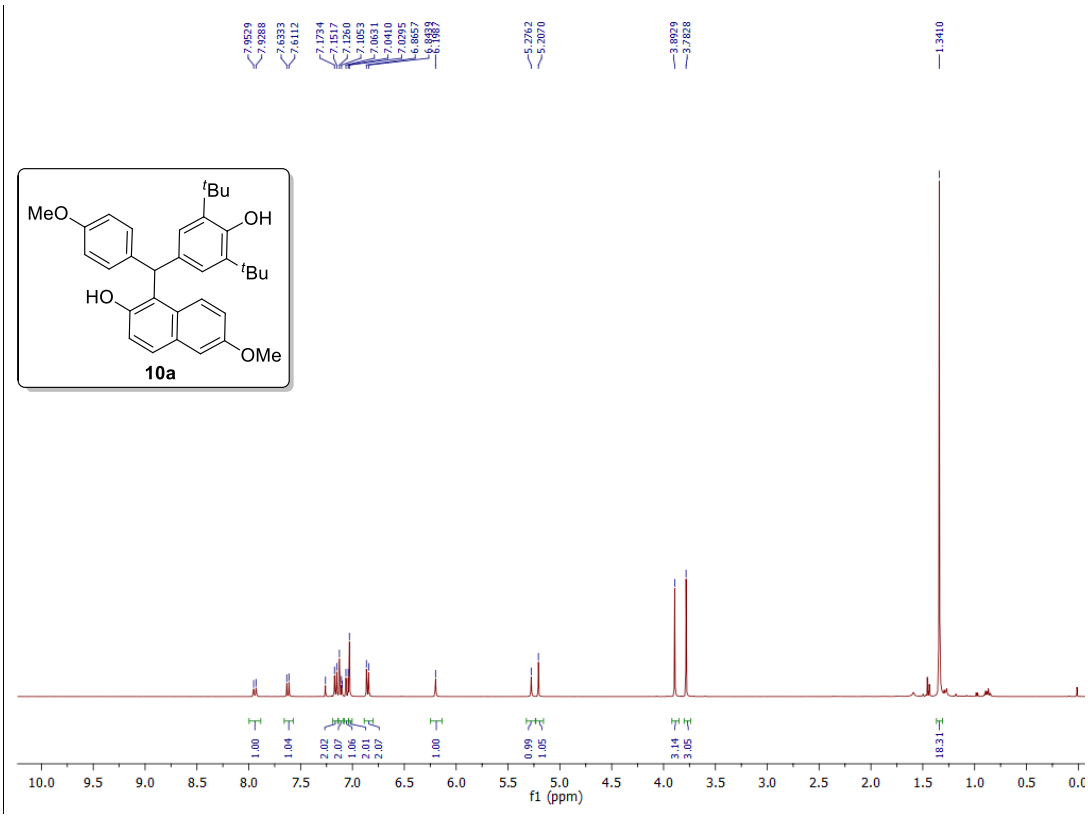
^{1}H NMR Spectrum of 3u



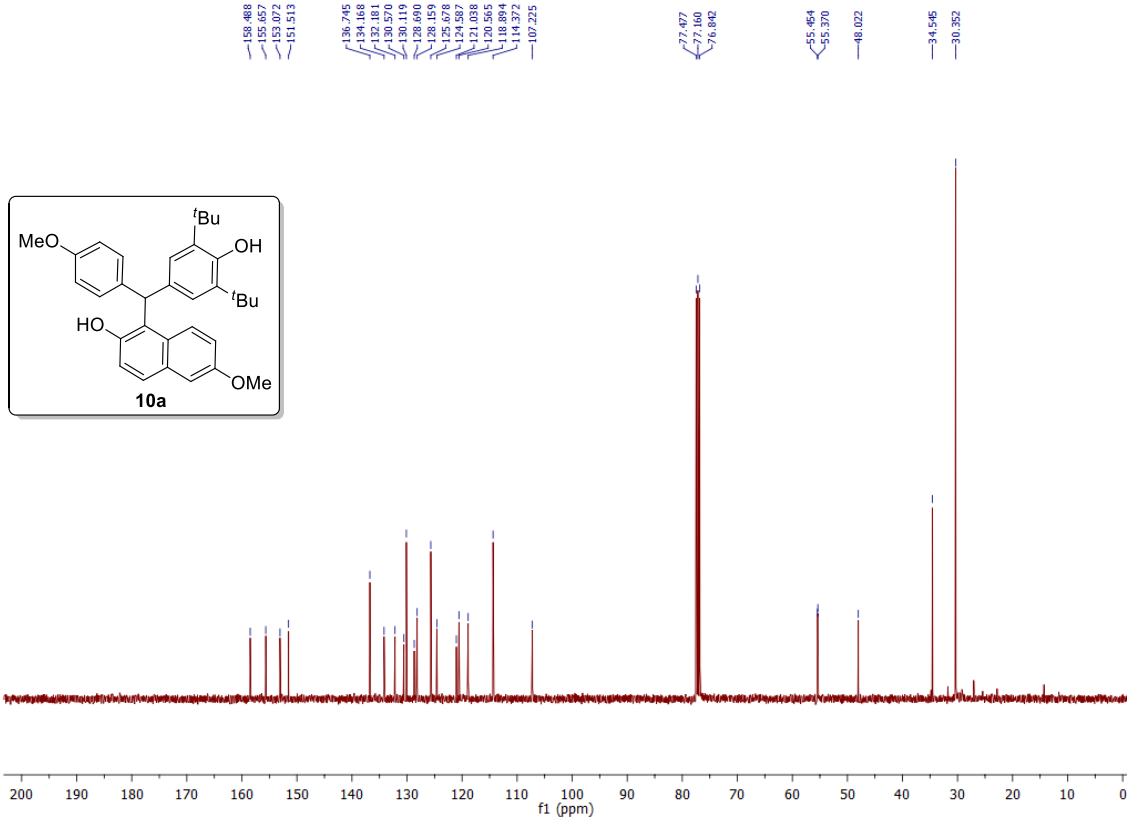
^{13}C NMR Spectrum of 3u



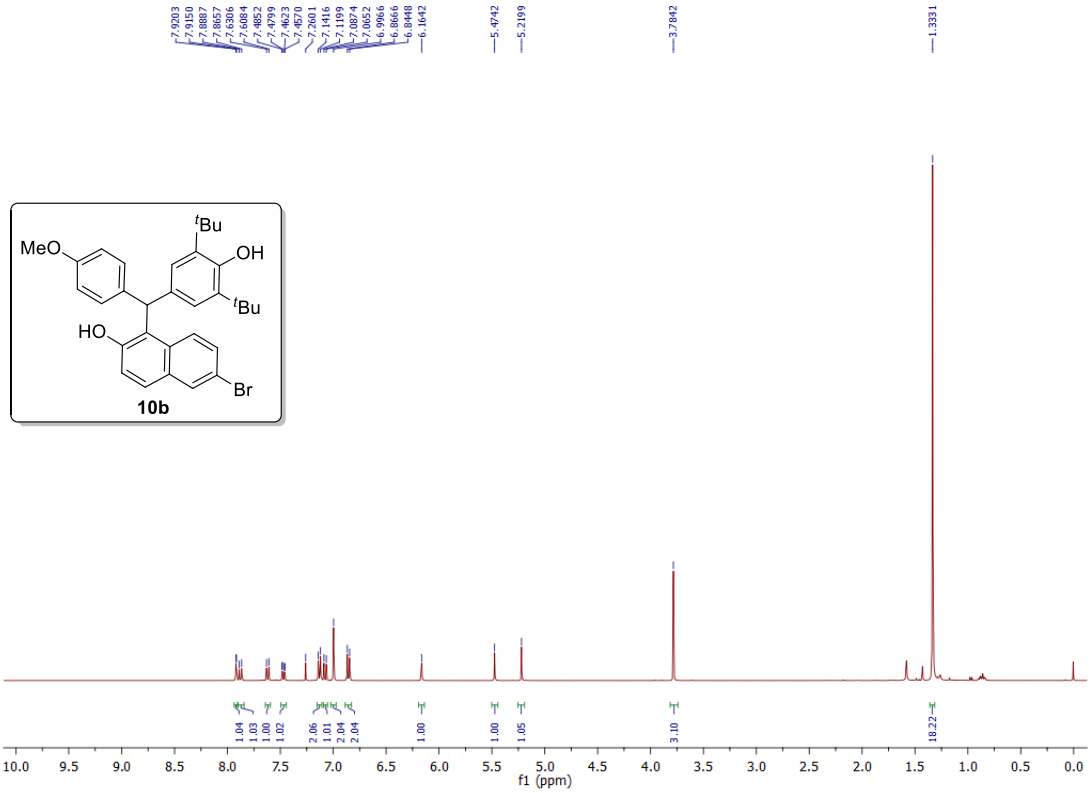
^{1}H NMR Spectrum of 10a



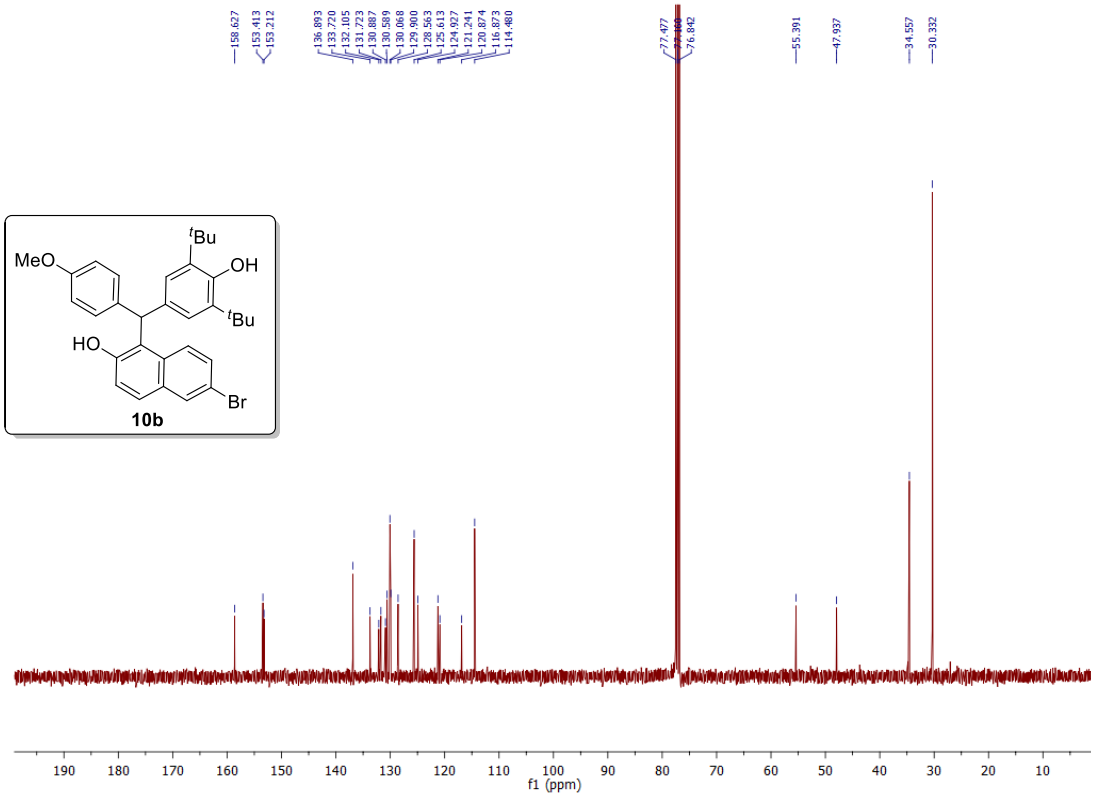
^{13}C NMR Spectrum of 10a



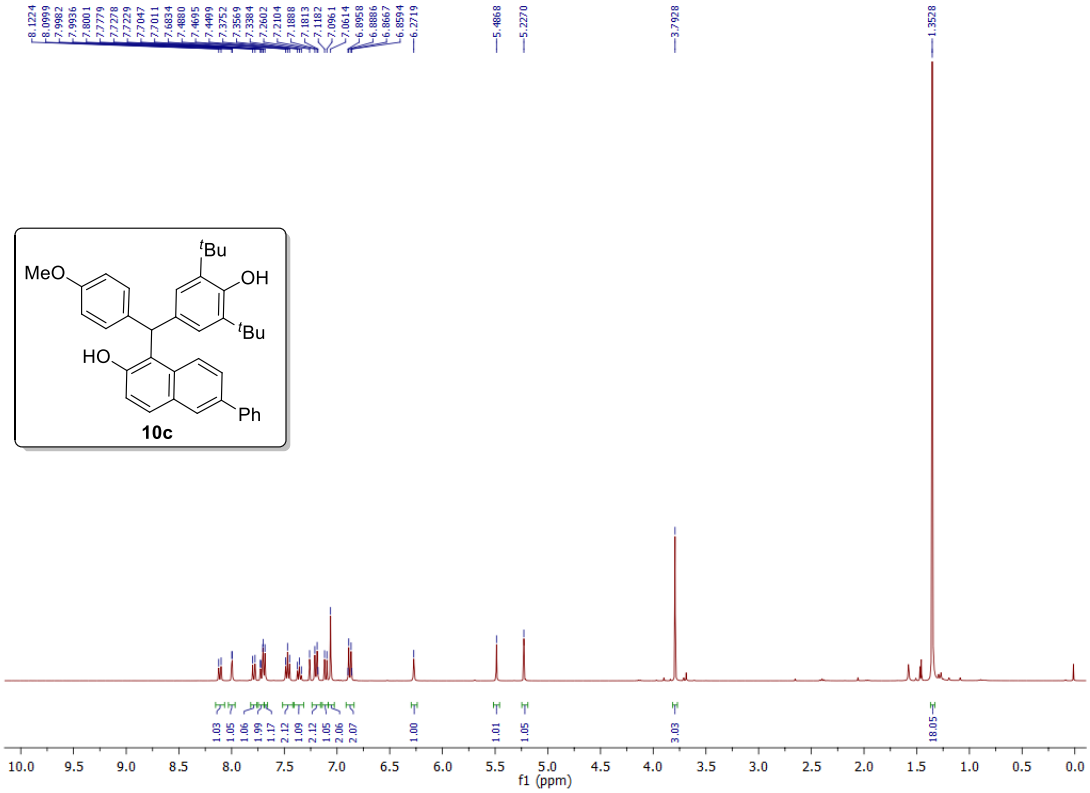
^{1}H NMR Spectrum of 10b



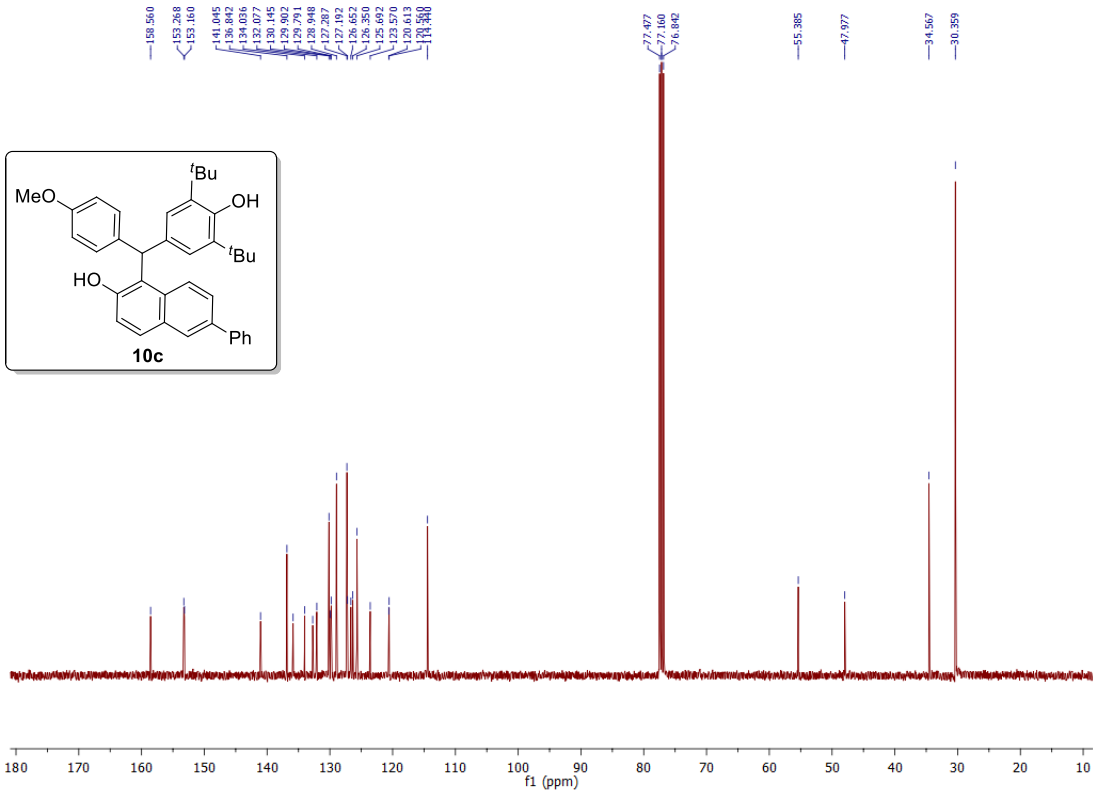
^{13}C NMR Spectrum of 10b



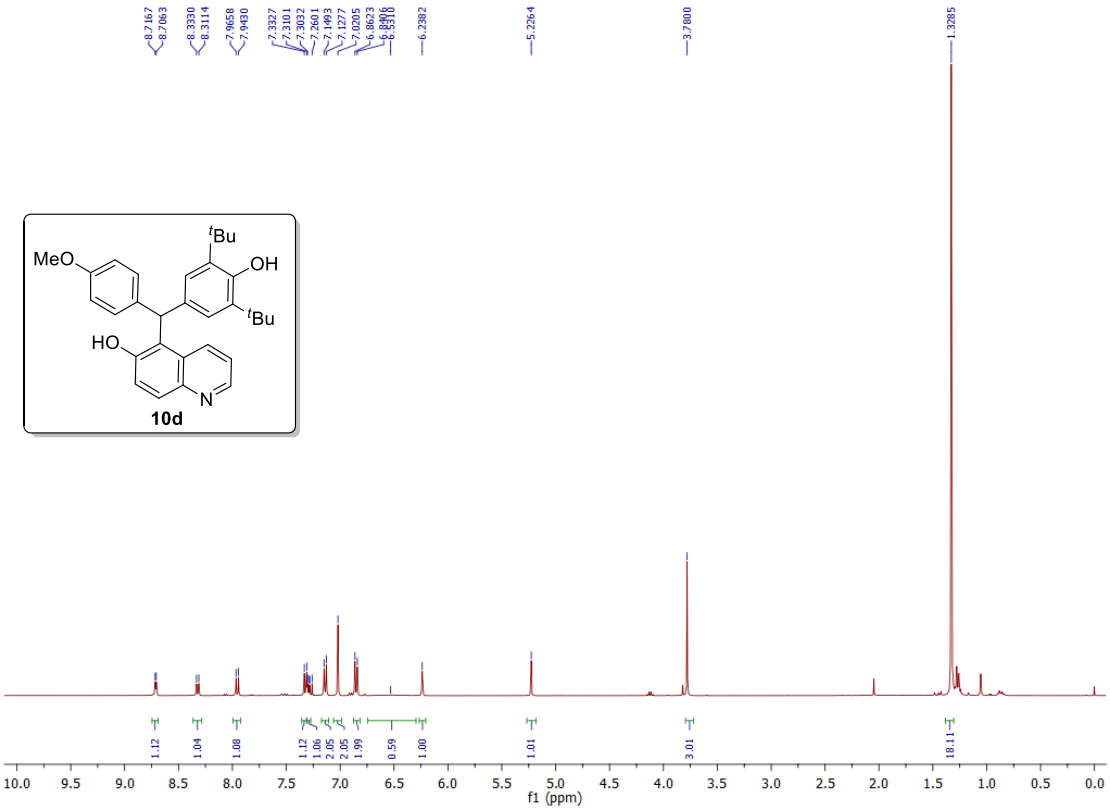
^{1}H NMR Spectrum of 10c



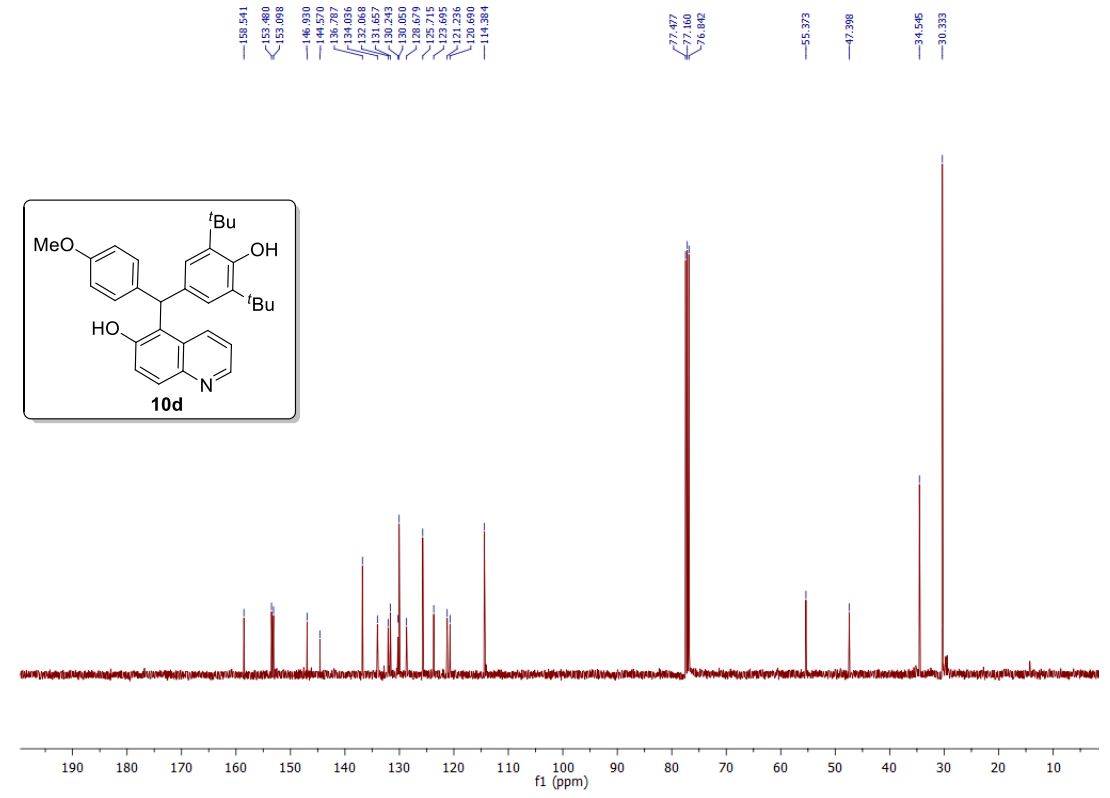
^{13}C NMR Spectrum of 10c



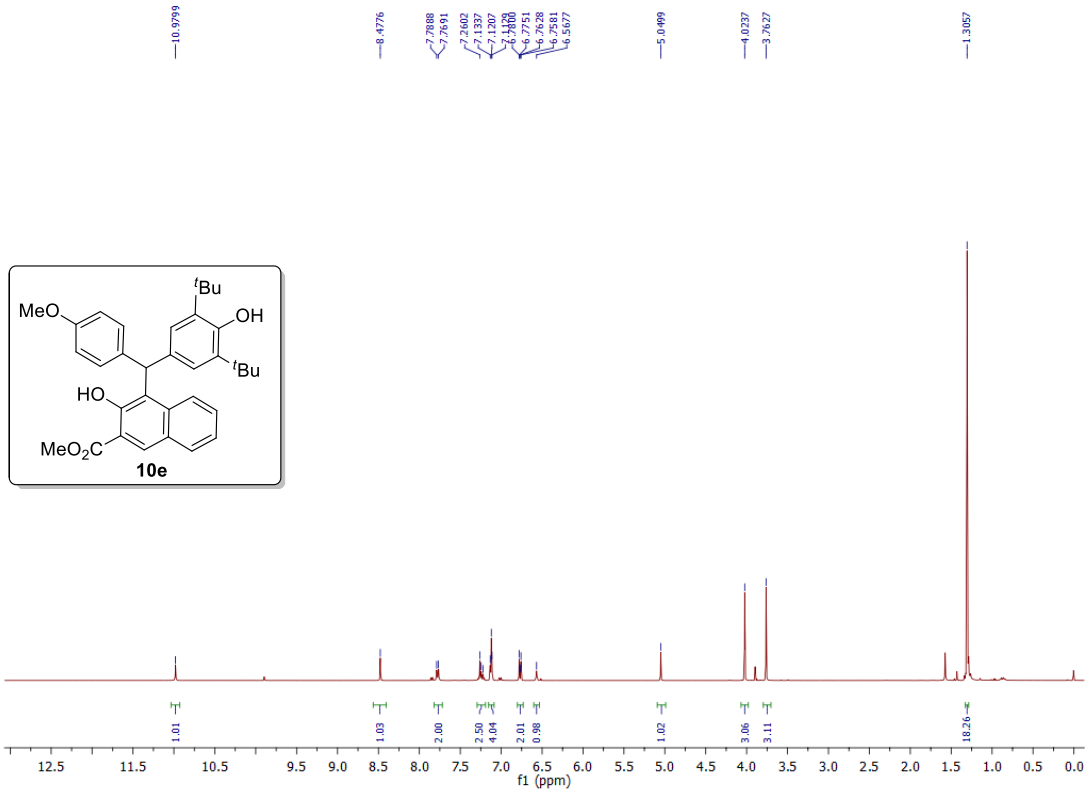
^{1}H NMR Spectrum of 10d



^{13}C NMR Spectrum of 10d



^{1}H NMR Spectrum of 10e



^{13}C NMR Spectrum of 10e