Catalyst- and solvent-free approach to 2-arylated quinolines via [5+1] annulation of 2-methylquinolines with diynones

(Electronic Supplementary Information)

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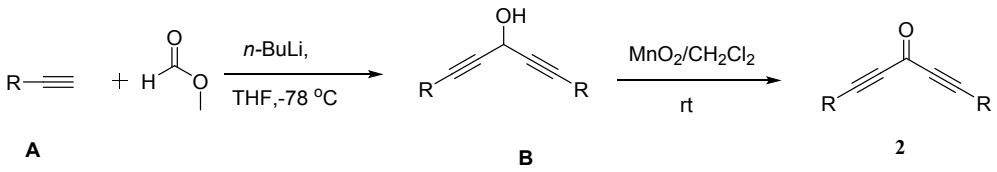
General methods and materials. Proton nuclear magnetic resonance spectra (**^{1}H NMR**) and carbon nuclear magnetic resonance spectra (**^{13}C NMR**) were recorded at 400 MHz and 100 MHz or 500 MHz and 125 MHz, respectively, using DMSO-d_6 as reference standard (δ 2.50 ppm) for **^{1}H NMR** and (δ 40.00 ppm) for **^{13}C NMR** or $CDCl_3$ as reference standard (δ 7.26 ppm) for ^{1}H NMR and (δ 77.00 ppm) for ^{13}C NMR. **HRMS** (ion trap) were recorded using ESI. Melting points were uncorrected. Precoated silica gel plates F-254 were used for analytical thin-layer chromatography. Column chromatography was performed on silica gel (300-400 mesh). Starting materials were readily prepared according to literature procedures. Unless otherwise noted, all reagents were obtained commercially and used without further purification.

Procedure of synthesis of starting materials 1[1]**:**

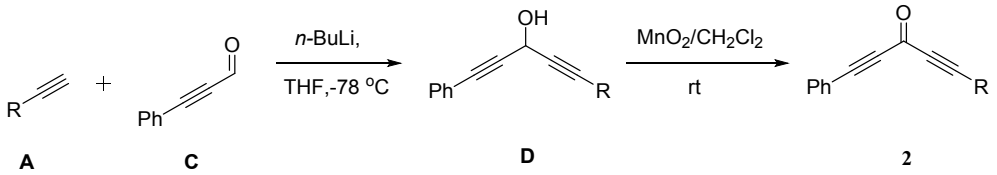
1) To a stirred solution of acetylene (**A**; 10.2 mmol)) in dry THF (30 mL) under argon was added *n*-BuLi (4.5 mL, 11.2 mmol, 2.5 M solution in hexane) via a syringe at 0 °C. The mixture was allowed to stir for 30 min at 0 °C. Then methyl formate (0.28 mL, 4.52 mmol) was added. The mixture was allowed to stir for an additional 30 min at 0 °C, and then for 2 h at room temperature. The mixture was poured into an aqueous saturated solution of NH_4Cl, and the product was extracted with ethyl acetate. The combined organic layers were washed with a saturated aqueous sodium chloride solution, dried over $MgSO_4$, and filtered, and the solvents were removed under reduced pressure. The residue was purified by flash column chromatography (silica gel, PE/EA = 10/1) to give **B**.

Procedure A: MnO_2 (15 equiv.) was added to a solution of **B** (5 mmol) in CH_2Cl_2 (15 mL) at room temperature. The resulting mixture was stirred overnight. Then the solid was filtered, and the solvents were removed under reduced pressure. The residue was purified by flash column chromatography (silica gel, PE/EA = 50/1) to give **2**.



2) To a stirred solution of acetylene (**A**, 8 mmol) in dry THF (30 mL) under argon was added *n*-BuLi (3.36 mL, 8.4 mmol, 2.5 M solution in hexane) via a syringe at 0 °C. The mixture was allowed to stir for 30 min at 0 °C. Then 3-phenylpropiolaldehyde (**C**, 8 mmol) was added. The mixture was allowed to stir for an additional 30 min at 0 °C, and then for 2 h at room temperature. It was then poured into aqueous saturated NH_4Cl solution and extracted with ethyl acetate. The combined organic layers were washed with a saturated aqueous sodium chloride solution, dried over $MgSO_4$, and filtered, and the solvents were removed under reduced pressure. The residue was purified by flash column chromatography (silica gel, PE/EA = 10/1) to give **D**.

D used the same procedure as general procedure A to give **2** (silica gel, PE/EA = 50/1).



Synthesis of 4-(quinolin-2-yl)phenol Derivatives 3a-3c, 3e-3f, 3i, 3k-3z.

The reaction mixture of **1** (1.5 mmol), **2** (0.5 mmol), were stirred at 100 °C for 6-10 h in a sealed tube, and monitored periodically by TLC. After the resulting solution cooled to room temperature, the target product **3** was purified and raw material **1** was recycled by column chromatography on silica gel using a mixture of ethyl acetate and petroleum ether.

Synthesis of 4-(quinolin-2-yl)phenol Derivatives 3d, 3g, 3h, and 3j.

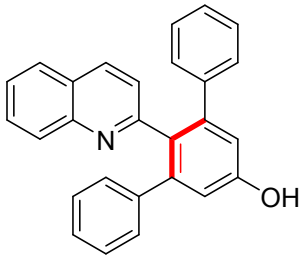
1 (0.6 mmol) and **2** (0.5 mmol) were dissolved in PhCl (1 mL), and stirred at 100 °C for 10 h in a sealed tube. The reaction monitored periodically by TLC. After the resulting solution cooled to room temperature, the target product **3** was purified by column chromatography on silica gel using a mixture of ethyl acetate and petroleum ether.

References

[1] Q.-H. Teng, Y.-L. Xu, Y. Liang, H.-S. Wang, Y.-C. Wang, Y.-M. Pan, *Adv. Synth. Catal.* **2016**, 358, 1897.

Spectral data of all compounds

2'-(quinolin-2-yl)-[1,1':3',1"-terphenyl]-5'-ol **(3a)**



3a

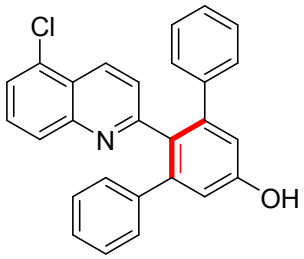
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1,5-diphenylpenta-1,4-diyn-3-one (**2a**) (115.1 mg, 0.5 mmol) at 100 °C for 10 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 158.7 mg (85%) of **3a** as light yellow solid. **m.p.** 205-207 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 10.05 (s, 1H), 7.86 (d, J = 8.4 Hz, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.66 (d, J = 8.4 Hz, 1H), 7.55–7.53 (m, 1H), 7.42–7.40 (m, 1H), 7.05 (s, 10H), 6.97 (d, J = 8.4 Hz, 1H), 6.88 (s, 2H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 159.8, 157.4, 147.4, 143.6, 141.9, 135.0, 130.7, 129.7, 129.2, 128.2, 128.1, 127.0, 126.7, 126.2, 125.7, 116.6.

HRMS (*m/z*) (ESI): calcd for $C_{27}H_{20}NO$ 374.1539 [M+H$^+$]; found 374.1535.

2'-(5-chloroquinolin-2-yl)-[1,1':3',1''-terphenyl]-5'-ol **(3b)**



3b

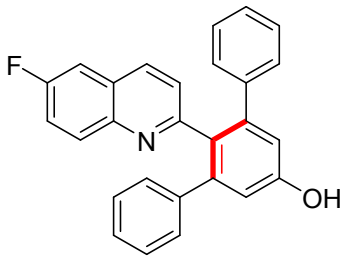
The reaction of 5-chloro-2-methylquinoline (**1b**) (266.4 mg, 1.5 mmol), and 1,5-diphenylpenta-1,4-diyn-3-one (**2a**) (115.1 mg, 0.5 mmol) at 100 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 118.3 mg (58%) of **3b** as light yellow solid. **m.p.** 221-223 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 10.01 (s, 1H), 8.09 (d, J = 8.7 Hz, 1H), 7.68–7.64 (m, 3H), 7.14 (d, J = 8.7 Hz, 1H), 7.11–7.02 (m, 10H), 6.87 (s, 2H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 160.8, 157.6, 148.0, 143.5, 141.6, 131.0, 130.3, 129.9, 129.8, 129.6, 128.8, 128.2, 127.0, 126.9, 126.8, 123.8, 116.5 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{27}H_{18}ClNO$ 408.1150 [M+H$^+$]; found 408.1146.

2'-(6-fluoroquinolin-2-yl)-[1,1':3',1''-terphenyl]-5'-ol **(3c)**



3c

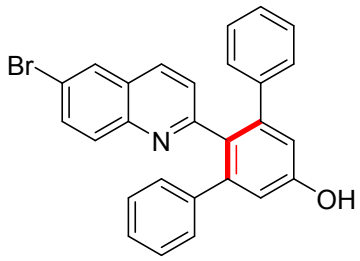
The reaction of 6-fluoro-2-methylquinoline (**1c**) (241.8 mg, 1.5 mmol), and 1,5-diphenylpenta-1,4-diyn-3-one (**2a**) (115.1 mg, 0.5 mmol) at 100 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 107.7 mg (55%) of **3c** as light yellow solid. **m.p.** 238-240 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.97 (s, 1H), 7.88 (d, J = 8.5 Hz, 1H), 7.69–7.66 (m, 1H), 7.54–7.50 (m, 1H), 7.46–7.44 (m, 1H), 7.09–7.03 (m, 10H), 7.03–6.99 (m, 1H), 6.88 (s, 2H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 161.2, 159.2, 158.7, 157.4, 144.5, 143.5, 141.7, 134.4, 131.8, 130.2, 129.6, 128.1, 126.9, 126.7, 126.3, 119.5, 116.5, 111.1 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{27}H_{19}FNO$ 392.1445 [M+H$^+$]; found 392.1440.

2'-(6-bromoquinolin-2-yl)-[1,1':3',1''-terphenyl]-5'-ol **(3d)**



3d

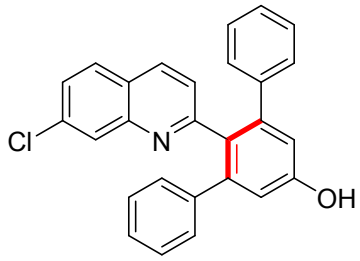
The reaction of 6-bromo-2-methylquinoline (**1d**) (133.3 mg, 0.6 mmol), and 1,5-diphenylpenta-1,4-diyn-3-one (**2a**) (115.1 mg, 0.5 mmol) in PhCl (1 mL) at 100 °C for 10 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 174.2 mg (77%) of **3d** as light yellow solid. **m.p.** 239-241 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.97 (s, 1H), 8.04 (d, J = 2.2 Hz, 1H), 7.87 (d, J = 8.5 Hz, 1H), 7.67–7.62 (m, 1H), 7.56 (d, J = 9.0 Hz, 1H), 7.07–7.00 (m, 11H), 6.86 (s, 2H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 160.4, 157.5, 145.9, 143.4, 141.6, 134.1, 132.6, 131.3, 130.2, 130.0, 129.6, 128.1, 127.4, 126.9, 126.5, 119.5, 116.5 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{27}H_{19}BrNO$ 452.0645, 454.0624 [M+H$^+$]; found 452.0643, 454.0621.

2'-(7-chloroquinolin-2-yl)-[1,1':3',1''-terphenyl]-5'-ol **(3e)**



3e

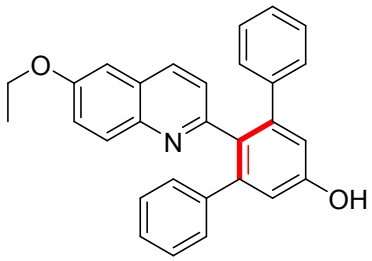
The reaction of 7-chloro-2-methylquinoline (**1e**) (266.4 mg, 1.5 mmol), and 1,5-diphenylpenta-1,4-diyn-3-one (**2a**) (115.1 mg, 0.5 mmol) at 100 °C for 7 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 122.4 mg (60%) oef **3c** as light yellow solid. **m.p.** 125-127 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.96 (s, 1H), 7.94 (d, J = 8.4 Hz, 1H), 7.92 (d, J = 8.5 Hz, 1H), 7.81 (d, J = 8.7 Hz, 1H), 7.66 (d, J = 2.1 Hz, 1H), 7.48–7.44 (m, 1H), 7.10–7.02 (m, 9H), 7.01 (d, J = 8.5 Hz, 1H), 6.85 (s, 2H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 161.1, 157.5, 147.6, 143.4, 141.6, 134.9, 134.1, 130.1, 130.1, 129.6, 128.1, 127.6, 127.2, 126.9, 126.1, 124.7, 116.5 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{27}H_{18}ClNO$ 408.1150 [M+H$^+$]; found 408.1145.

2'-(6-ethoxyquinolin-2-yl)-[1,1':3',1''-terphenyl]-5'-ol **(3f)**



3f

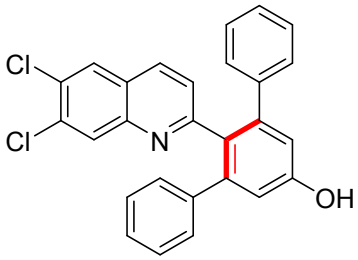
The reaction of 6-ethoxy-2-methyl-quinolin (**1f**) (280.86 mg, 1.5 mmol), and 1,5-diphenylpenta-1,4-diyn-3-one (**2a**) (115.1 mg, 0.5 mmol) at 100 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 121.1 mg (58%) of **3f** as light yellow solid. **m.p.** 155-157 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.90 (s, 1H), 7.75 (d, J = 8.5 Hz, 1H), 7.56 (d, J = 9.2 Hz, 1H), 7.20–7.12 (m, 1H), 7.11 (d, J = 2.7 Hz, 1H), 7.07 (d, J = 5.9 Hz, 10H), 6.91 (d, J = 8.4 Hz, 1H), 6.88 (s, 2H), 4.06 (q, J = 6.8 Hz, 2H), 1.34 (t, J = 6.8 Hz, 3H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 157.2, 156.9, 156.7, 143.3, 143.2, 141.9, 133.7, 130.6, 130.5, 129.6, 128.0, 127.1, 126.7, 125.7, 122.0, 116.4, 106.4, 63.8, 15.0 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{29}H_{24}NO_2$ 418.1802 [M+H$^+$]; found 418.1803.

2'-(6,7-dichloroquinolin-2-yl)-[1,1':3',1''-terphenyl]-5'-ol **(3g)**



3g

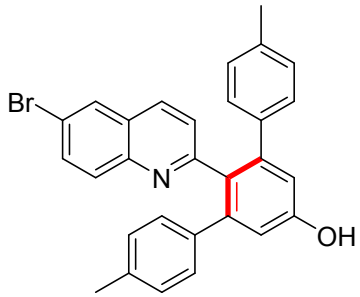
The reaction of 6,7-dichloro-2-methylquinoline (**1g**) (127.2 mg, 0.6 mmol), and 1,5-diphenylpenta-1,4-diyn-3-one (**2a**) (115.1 mg, 0.5 mmol) in PhCl (1 mL) at 100 °C for 10 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 161.4 mg (73%) of **3g** as light yellow solid. **m.p.** 186-187 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 10.02 (s, 1H), 8.15 (s, 1H), 7.92 (d, J = 8.5 Hz, 1H), 7.88 (s, 1H), 7.11–7.05 (m, 7H), 7.03–6.97 (m, 4H), 6.85 (s, 2H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 161.7, 157.6, 146.0, 143.4, 141.5, 134.2, 132.3, 130.0, 129.8, 129.6, 129.3, 129.2, 128.2, 127.0, 125.6, 116.5 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{27}H_{18}Cl_2NO$ 442.0760 [M+H$^+$]; found 442.0775.

2'-(6-bromoquinolin-2-yl)-4,4''-dimethyl-[1,1':3',1''-terphenyl]-5'-ol **(3h)**



3h

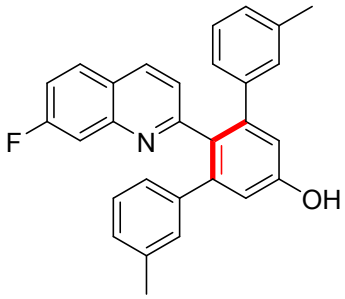
The reaction of 6-bromo-2-methylquinoline (**1d**) (133.3 mg, 0.6 mmol), and 1,5-di-p-tolylpenta-1,4-diyn-3-one (**2b**) (129.1 mg, 0.5 mmol) in PhCl (1 mL) at 100 °C for 10 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 167.7 mg (70%) of **3h** as light yellow solid. **m.p.** 136-139 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.88 (s, 1H), 8.05 (d, J = 2.1 Hz, 1H), 7.89 (d, J = 8.5 Hz, 1H), 7.69 –7.62 (m, 1H), 7.61 (d, J = 9.0 Hz, 1H), 7.03 (d, J = 8.5 Hz, 1H), 6.89–6.83 (m, 8H), 6.80 (s, 2H), 2.11 (s, 6H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 160.8, 157.4, 145.8, 143.2, 138.7, 135.9, 134.1, 132.6, 131.4, 130.1, 130.0, 129.5, 128.7, 127.5, 126.6, 119.4, 116.3, 21.0 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{29}H_{23}BrNO$ 480.0958 482.0937 [M+H$^+$]; found 480.0959 482.0934.

2'-(7-fluoroquinolin-2-yl)-3,3''-dimethyl-[1,1':3',1''-terphenyl]-5'-ol **(3i)**



3i

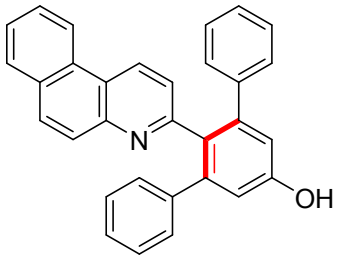
The reaction of 7-Fluoro-2-methylpyridine (**1h**) (241.8 mg, 1.5 mmol), and 1,5-di-m-tolylpenta-1,4-diyn-3-one (**2c**) (129.1 mg, 0.5 mmol) at 100 °C for 7 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 130.0 mg (62%) of **3i** as light yellow solid. **m.p.** 171-173 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.88 (s, 1H), 7.94 (d, J = 8.5 Hz, 1H), 7.86–7.80 (m, 1H), 7.40–7.32 (m, 3H), 6.97–6.93 (m, 3H), 6.91–6.86 (m, 2H), 6.88–6.82 (m, 3H), 6.78 (d, J = 7.5 Hz, 2H), 2.06 (s, 6H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 163.8, 161.4, 161.2, 157.4, 148.0, 143.3, 141.5, 137.1, 134.9, 130.6, 130.5, 130.2, 127.8, 127.5, 126.8, 125.1, 123.3, 116.7, 116.3, 112.4, 21.3 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{29}H_{23}FNO$ 420.1758 [M+H$^+$]; found 420.1748.

2'-(benzo[f]quinolin-3-yl)-[1,1':3',1"-terphenyl]-5'-ol **(3j)**



3j

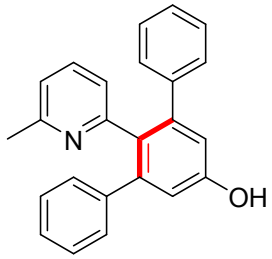
The reaction of 3-methylbenzo[f]quinoline (**1i**) (116.0 mg, 0.6 mmol), and 1,5-diphenylpenta-1,4-diyn-3-one (**2a**) (115.1 mg, 0.5 mmol) in PhCl (1 mL) at 100 °C for 10 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 173.6 mg (82%) of **3j** as light yellow solid. **m.p.** 153-155 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.93 (s, 1H), 8.78 (d, J = 8.6 Hz, 1H), 8.65 (d, J = 7.8 Hz, 1H), 7.97–7.90 (m, 2H), 7.67–7.61 (m, 2H), 7.57 (d, J = 9.1 Hz, 1H), 7.14 (d, J = 8.5 Hz, 1H), 7.10–7.01 (m, 10H), 6.89 (s, 2H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 159.2, 157.3, 146.9, 143.5, 141.8, 131.5, 130.6, 130.3, 130.3, 129.6, 129.0, 128.3, 128.0, 127.6, 127.6, 126.8, 125.8, 123.5, 122.8, 116.5 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{31}H_{22}NO$ 424.1696 [M+H$^+$]; found 424.1690.

2'-(6-methylpyridin-2-yl)-[1,1':3',1"-terphenyl]-5'-ol **(3k)**



3k

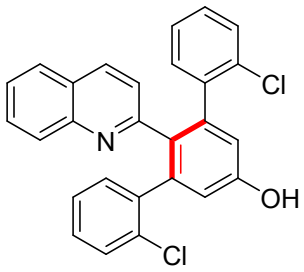
The reaction of 2,6-dimethyl-pyridin (**1j**) (160.7 mg, 1.5 mmol), and 1,5-diphenylpenta-1,4-diyn-3-one (**2a**) (115.1 mg, 0.5 mmol) at 100 °C for 9 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 114.7 mg (68%) of **3k** as light yellow solid. **m.p.** 153-155 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.91 (s, 1H), 7.20 (d, J = 7.7 Hz, 1H), 7.16–7.11 (m, 6H), 7.04–7.00 (m, 4H), 6.79 (d, J = 5.9 Hz, 3H), 6.56 (d, J = 7.6 Hz, 1H), 2.13 (s, 3H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 158.1, 157.1, 156.5, 143.2, 142.0, 135.6, 130.5, 129.6, 127.9, 126.7, 124.2, 120.3, 116.3, 24.3 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{24}H_{19}NO$ 338.1539 [M+H$^+$]; found 338.1540.

2,2''-dichloro-2'-(quinolin-2-yl)-[1,1':3',1''-terphenyl]-5'-ol **(3l)**



3l

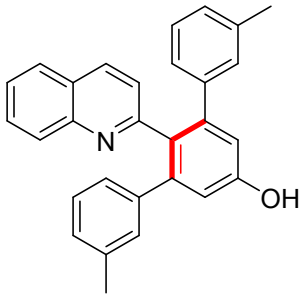
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1,5-bis(2-chlorophenyl)penta-1,4-diyn-3-one (**2d**) (149.6 mg, 0.5 mmol) at 100 °C for 8 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 181.4 mg (82%) of **3l** as light yellow solid. **m.p.** 235-237 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 10.10 (s, 1H), 7.86 (d, J = 8.5 Hz, 1H), 7.70 (d, J = 8.1 Hz, 1H), 7.55–7.49 (m, 2H), 7.40–7.32 (m, 1H), 7.17–7.10 (m, 4H), 6.98–6.91 (m, 7H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 160.5, 158.4, 158.1, 157.2, 147.2, 137.3, 134.7, 132.3, 132.0, 129.7, 129.6, 129.5, 129.2, 129.1, 129.0, 127.9, 126.5, 126.0, 124.3, 124.1, 117.7, 115.6, 115.4 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{27}H_{18}Cl_2NO$ 442.0760 [M+H$^+$]; found 442.0765.

3,3''-dimethyl-2'-(quinolin-2-yl)-[1,1':3',1''-terphenyl]-5'-ol **(3m)**



3m

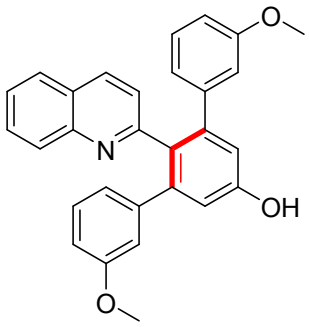
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1,5-di-m-tolylpenta-1,4-diyn-3-one (**2c**) (129.1 mg, 0.5 mmol) at 100 °C for 9 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 150.6 mg (75%) of **3m** as light yellow solid. **m.p.**187-189 °C.

^{1}H NMR (500 MHz, DMSO-d_6): δ 9.90 (s, 1H), 7.89 (d, J = 8.5 Hz, 1H), 7.73–7.68 (m, 2H), 7.59–7.54 (m, 1H), 7.44–7.39 (m, 1H), 6.97 (d, J = 8.2 Hz, 3H), 6.92–6.73 (m, 8H), 2.04 (s, 6H) ppm.

^{13}C NMR (125 MHz, DMSO-d_6): δ 159.9, 157.3, 147.2, 143.4, 141.6, 137.0, 134.8, 130.5, 130.5, 129.6, 129.1, 128.0, 127.8, 127.5, 126.8, 126.5, 126.1, 125.6, 116.3, 21.3 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{29}H_{24}NO$ 402.1852 [M+H$^+$]; found 402.1849.

3,3"-dimethoxy-2'-(quinolin-2-yl)-[1,1':3',1"-terphenyl]-5'-ol **(3n)**



3n

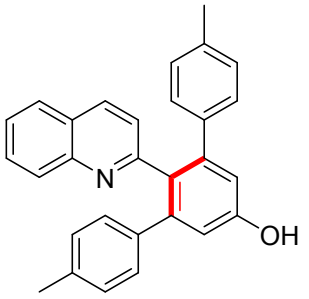
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1,5-bis(3-methoxyphenyl)penta-1,4-diyn-3-one (**2e**) (145.2 mg, 0.5 mmol) at 100 °C for 10 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 140.8 mg (65%) of **3n** as light yellow solid. **m.p.** 103-104 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.99 (s, 1H), 7.92 (d, J = 8.5 Hz, 1H), 7.75 (d, J = 8.5 Hz, 2H), 7.59–7.52 (m, 1H), 7.45–7.40 (m, 1H), 7.05 (d, J = 8.4 Hz, 1H), 7.00–6.92 (m, 2H), 6.93 (s, 2H), 6.71 (d, J = 7.6 Hz, 2H), 6.61–6.56 (m, 4H), 3.38 (s, 6H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 160.0, 158.8, 157.4, 147.3, 143.2, 143.1, 135.1, 130.6, 129.7, 129.2, 129.1, 128.0, 126.6, 126.2, 125.5, 122.1, 116.5, 115.1, 113.1, 55.0 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{29}H_{24}NO_3$ 434.1751 [M+H$^+$]; found 434.1751.

4,4"-dimethyl-2'-(quinolin-2-yl)-[1,1':3',1"-terphenyl]-5'-ol **(3o)**



3o

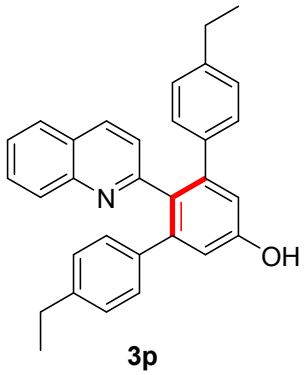
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1,5-di-p-tolylpenta-1,4-diyn-3-one (**2b**) (129.1 mg, 0.5 mmol) at 100 °C for 9 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 146.6 mg (73%) of **3o** as light yellow solid. **m.p.** 178-180 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.80 (s, 1H), 7.76 (d, J = 8.4 Hz, 1H), 7.61–7.56 (m, 2H), 7.50–7.43 (m, 1H), 7.36–7.25 (m, 1H), 6.89–6.72 (m, 5H), 6.81–6.68 (m, 6H), 1.96 (s, 6H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 160.0, 157.3, 147.3, 143.3, 138.9, 135.8, 134.9, 130.5, 129.5, 129.2, 128.7, 128.0, 126.4, 126.2, 125.6, 116.4, 20.9 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{29}H_{24}NO$ 402.1852 [M+H$^+$]; found 402.1856.

4,4''-diethyl-2'-(quinolin-2-yl)-[1,1':3',1''-terphenyl]-5'-ol **(3p)**



3p

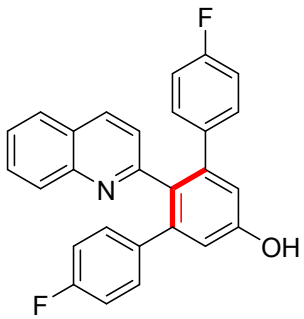
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1,5-bis(4-ethylphenyl)penta-1,4-diyn-3-one (**2f**) (143.2 mg, 0.5 mmol) at 100 °C for 9 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 150.3 mg (70%) of **3p** as light yellow solid. **m.p.** 176-178 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.87 (s, 1H), 7.87 (d, J = 8.5 Hz, 1H), 7.71–7.60 (m, 2H), 7.55–7.48 (m, 1H), 7.42–7.38 (m, 1H), 6.98–6.81 (m, 5H), 6.89–6.74 (m, 6H), 2.40 (q, J = 8.5 Hz, 4H), 1.01 (t, J = 8.4 Hz, 6H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 159.9, 157.3, 147.3, 143.3, 142.1, 139.2, 134.8, 130.5, 129.5, 129.4, 129.2, 128.0, 127.4, 126.4, 126.1, 125.6, 116.4, 28.0, 15.6 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{31}H_{28}NO$ 430.2165 [M+H$^+$]; found 430.2162.

4,4''-difluoro-2'-(quinolin-2-yl)-[1,1':3',1''-terphenyl]-5'-ol **(3q)**



3q

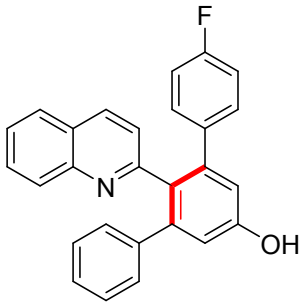
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1,5-bis(4-fluorophenyl)penta-1,4-diyn-3-one (**2g**) (133.2 mg, 0.5 mmol) at 100 °C for 7 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 161.7 mg (79%) of **3q** as light yellow solid. **m.p.** 226-228 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 10.13 (s, 1H), 7.91 (d, J = 8.5 Hz, 1H), 7.75 (d, J = 7.7 Hz, 1H), 7.67 (d, J = 8.4 Hz, 1H), 7.60–7.55 (m, 1H), 7.46–7.41 (m, 1H), 7.07 (m, 4H), 6.96 (d, J = 8.5 Hz, 1H), 6.86–6.69 (m, 6H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 162.7, 160.3, 159.6, 157.6, 147.5, 142.6, 138.2, 135.4, 131.7, 131.7, 130.8, 130.0, 129.2, 128.3, 126.9, 126.3, 125.7, 116.8, 115.2, 115.0 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{27}H_{18}F_2NO$ 410.1351 [M+H$^+$]; found 410.1349.

4-fluoro-2'-(quinolin-2-yl)-[1,1':3',1"-terphenyl]-5'-ol **(3r)**



3r

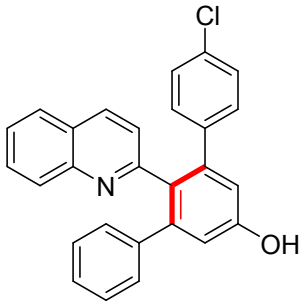
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1-(4-fluorophenyl)-5-phenylpenta-1,4-diyn-3-one (**2h**) (124.1 mg, 0.5 mmol) at 100 °C for 8 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 148.8 mg (76%) of **3r** as light yellow solid. **m.p.** 189-191 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 10.03 (s, 1H), 7.90 (d, J = 8.5 Hz, 1H), 7.74 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 8.4 Hz, 1H), 7.59–7.54 (m, 1H), 7.45–7.41 (m, 1H), 7.07–6.86 (m, 7H), 6.99 (d, J = 8.4 Hz, 1H), 6.93–6.84 (m, 4H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 162.5, 160.1, 159.6, 157.4, 147.4, 143.5, 142.5, 141.7, 138.2, 135.0, 131.5, 130.6, 129.6, 129.1, 128.1, 128.1, 126.9, 126.6, 126.1, 125.6, 116.6, 115.0, 114.8 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{27}H_{19}FNO$ 392.1445 [M+H$^+$]; found 392.1442.

4-chloro-2'-(quinolin-2-yl)-[1,1':3',1"-terphenyl]-5'-ol **(3s)**



3s

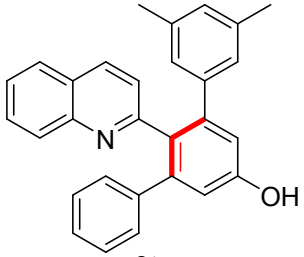
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1-(4-chlorophenyl)-5-phenylpenta-1,4-diyn-3-one (**2i**) (132.4 mg, 0.5 mmol) at 100 °C for 8 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 150.9 mg (74%) of **3s** as light yellow solid. **m.p.** 232-235 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.99 (s, 1H), 7.92 (d, J = 8.5 Hz, 1H), 7.76 (d, J = 7.9 Hz, 1H), 7.67 (d, J = 8.3 Hz, 1H), 7.60–7.56 (m, 1H), 7.45–7.39 (m, 1H), 7.12 (d, J = 8.5 Hz, 2H), 7.07 (d, J = 8.2 Hz, 7H), 6.99 (d, J = 8.4 Hz, 1H), 6.87 (s, 2H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 159.3, 157.4, 147.3, 143.5, 142.1, 141.6, 140.7, 135.0, 131.7, 131.3, 130.4, 129.6, 129.6, 129.1, 128.1, 128.0, 126.9, 126.6, 126.1, 125.5, 116.8, 116.4 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{27}H_{19}ClNO$ 408.1150 [M+H$^+$]; found 408.1147.

3,5-dimethyl-2'-(quinolin-2-yl)-[1,1':3',1''-terphenyl]-5'-ol **(3t)**



3t

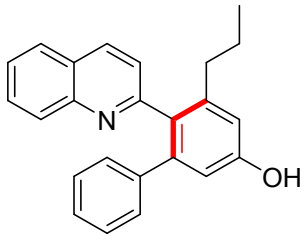
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1-(3,5-dimethylphenyl)-5-phenylpenta-1,4-diyn-3-one (**2j**) (129.2 mg, 0.5 mmol) at 100 °C for 9 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 136.5 mg (68%) of **3t** as light yellow solid. **m.p.** 132-134 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.90 (s, 1H), 7.87 (d, J = 8.5 Hz, 1H), 7.76–7.69 (m, 2H), 7.57–7.52 (m, 1H), 7.45–7.41 (m, 1H), 7.11–7.01 (m, 5H), 6.97 (d, J = 8.4 Hz, 1H), 6.88–6.82 (m, 2H), 6.70 (s, 2H), 6.64 (s, 1H), 1.95 (s, 6H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 159.9, 157.2, 147.2, 143.5, 143.2, 141.8, 141.4, 136.7, 134.7, 130.5, 129.6, 129.5, 129.1, 128.2, 128.0, 127.9, 127.7, 126.8, 126.4, 126.1, 125.5, 116.3, 116.2, 21.1 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{29}H_{23}NO$ 402.1852 [M+H$^+$]; found 402.1848.

5-propyl-6-(quinolin-2-yl)-[1,1'-biphenyl]-3-ol **(3u)**



3u

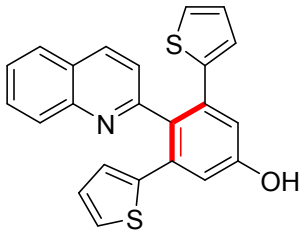
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1-phenylocta-1,4-diyn-3-one (**2k**) (98.2 mg, 0.5 mmol) at 100 °C for 10 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 118.8 mg (70%) of **3u** as light yellow solid. **m.p.** 90-93 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.68 (s, 1H), 7.98 (m, 2H), 7.84 (d, J = 8.1 Hz, 1H), 7.70 (m, 1H), 7.55–7.51 (m, 1H), 7.07–7.01 (m, 5H), 6.96 (d, J = 8.4 Hz, 1H), 6.79 (d, J = 2.3 Hz, 1H), 6.69 (d, J = 2.1 Hz, 1H), 2.38 (t, J = 7.2 Hz, 2H), 1.36–1.30 (m, 2H), 0.63 (t, J = 7.6 Hz, 3H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 160.2, 157.3, 147.5, 143.0, 142.5, 141.9, 135.4, 131.0, 129.8, 129.6, 129.3, 128.2, 128.1, 126.9, 126.7, 126.4, 125.1, 115.8, 114.8, 35.7, 24.2, 14.4 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{24}H_{22}NO$ 340.1696 [M+H$^+$]; found 340.1694.

4-(quinolin-2-yl)-3,5-di(thiophen-2-yl)phenol **(3v)**



3v

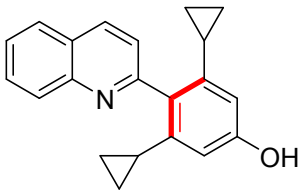
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1,5-di(thiophen-2-yl)penta-1,4-diyn-3-one (**2l**) (121.2 mg, 0.5 mmol) at 100 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 171.5 mg (89%) of **3v** as light yellow solid. **m.p.** 184-186 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 10.07 (s, 1H), 8.12 (d, J = 8.4 Hz, 1H), 7.95–7.89 (m, 2H), 7.72–7.65 (m, 1H), 7.57–7.51 (m, 1H), 7.26–7.15 (m, 2H), 7.18 (d, J = 8.4 Hz, 1H), 7.05 (s, 2H), 6.75–6.68 (m, 2H), 6.68–6.61 (m, 2H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 159.3, 157.4, 147.5, 142.5, 136.2, 135.8, 130.2, 130.0, 129.5, 128.4, 127.5, 127.4, 127.2, 127.1, 125.2, 116.6 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{23}H_{16}NOS_2$ 386.0673 [M+H$^+$]; found 386.0657.

3,5-dicyclopropyl-4-(quinolin-2-yl)phenol **(3w)**



3w

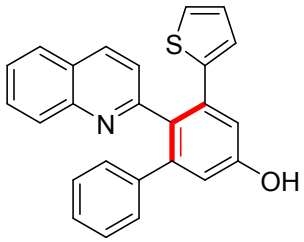
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1,5-dicyclopropylpenta-1,4-diyn-3-one (**2m**) (79.1 mg, 0.5 mmol) at 100 °C for 10 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 85.9 mg (57%) of **3w** as White solid. **m.p.** 171-173 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.34 (s, 1H), 8.37 (d, J = 8.4 Hz, 1H), 8.00–7.91 (m, 2H), 7.74–7.67 (m, 1H), 7.59–7.53 (m, 1H), 7.49 (d, J = 8.4 Hz, 1H), 6.19 (s, 2H), 1.41–1.33 (m, 2H), 0.49 (d, J = 54.5 Hz, 8H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6) δ 160.8, 158.0, 148.2, 142.6, 136.2, 133.8, 130.0, 129.4, 128.4, 126.9, 126.8, 125.0, 108.3, 13.9, 9.9, 8.6 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{21}H_{19}NO$ 302.1539 [M+H$^+$]; found 302.1531.

6-(quinolin-2-yl)-5-(thiophen-2-yl)-[1,1'-biphenyl]-3-ol **(3x)**



3x

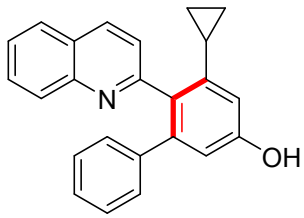
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1-phenyl-5-(thiophen-2-yl)penta-1,4-diyn-3-one (**2n**) (118.2 mg, 0.5 mmol) at 100 °C for 7 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 165.1 mg (87%) of **3x** as light yellow solid. **m.p.** 207-208 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 10.04 (s, 1H), 7.98 (d, J = 8.4 Hz, 1H), 7.82–7.76 (m, 2H), 7.66–7.61 (m, 1H), 7.48–7.42 (m, 1H), 7.24–7.16 (m, 1H), 7.12–7.08 (m, 4H), 7.06–7.02 (m, 3H), 6.88 (d, J = 2.4 Hz, 1H), 6.74–6.65 (m, 1H), 6.67–6.61 (m, 1H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 159.5, 157.4, 147.4, 143.7, 142.9, 141.4, 135.4, 130.5, 129.8, 129.6, 129.3, 128.1, 128.0, 127.3, 127.0, 126.9, 126.8, 126.6, 125.4, 117.0, 116.2 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{25}H_{18}NOS$ 380.1104 [M+H$^+$]; found 380.1086.

5-cyclopropyl-6-(quinolin-2-yl)-[1,1'-biphenyl]-3-ol **(3y)**



3y

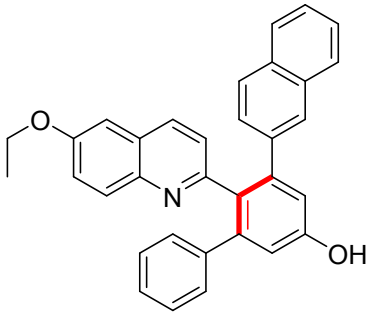
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1-cyclopropyl-5-phenylpenta-1,4-diyn-3-one (**2o**) (97.1 mg, 0.5 mmol) at 100 °C for 9 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 113.0 mg (67%) of **3y** as light yellow solid. **m.p.** 118-120 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.65 (s, 1H), 8.07 (d, J = 8.4 Hz, 1H), 7.96 (d, J = 8.4 Hz, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.70–7.62 (m, 1H), 7.54–7.48 (m, 1H), 7.12 (d, J = 8.4 Hz, 1H), 7.08–7.02 (m, 5H), 6.66 (d, J = 2.4 Hz, 1H), 6.47 (d, J = 2.3 Hz, 1H), 1.71–1.62 (m, 1H), 0.58 (s, 4H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6): δ 160.3, 157.7, 147.6, 143.8, 142.3, 141.8, 135.5, 132.0, 129.7, 129.6, 129.3, 128.1, 128.1, 126.8, 126.6, 126.4, 125.2, 114.4, 110.3, 13.8, 9.3 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{24}H_{20}NO$ 338.1539 [M+H$^+$]; found 338.1537.

6-(6-ethoxyquinolin-2-yl)-5-(naphthalen-2-yl)-[1,1'-biphenyl]-3-ol **(3z)**



3z

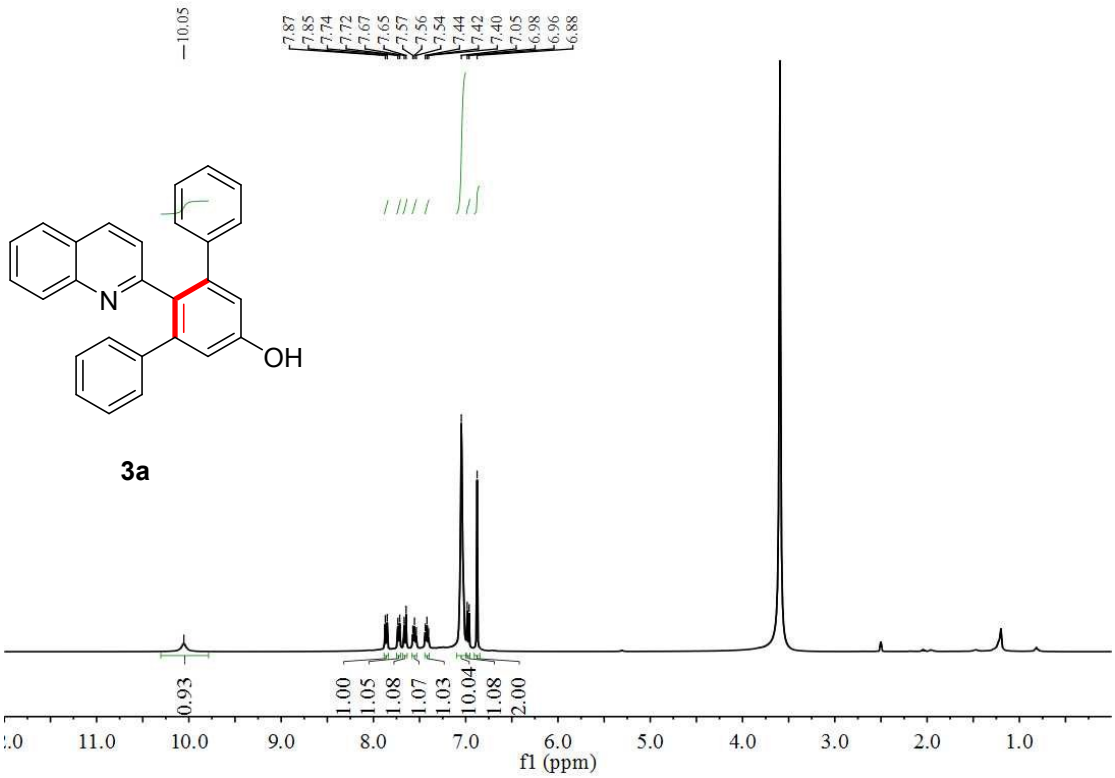
The reaction of 2-methylquinoline (**1a**) (214.8 mg, 1.5 mmol), and 1-(naphthalen-2-yl)-5-phenylpenta-1,4-diyn-3-one (**2p**) (140.2 mg, 0.5 mmol) at 100 °C for 8 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 147.3 mg (63%) of **3z** as light yellow solid. **m.p.** 136-137 °C.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.93 (s, 1H), 7.76 (d, J = 1.1 Hz, 1H), 7.71–7.63 (m, 3H), 7.52–7.46 (m, 2H), 7.42–7.36 (m, 2H), 7.16–7.11 (m, 1H), 7.10–7.04 (m, 7H), 6.95–6.88 (m, 2H), 6.88 (d, J = 2.5 Hz, 1H), 4.03 (q, J = 7.6 Hz, 2H), 1.32 (t, J = 7.2 Hz, 3H) ppm.

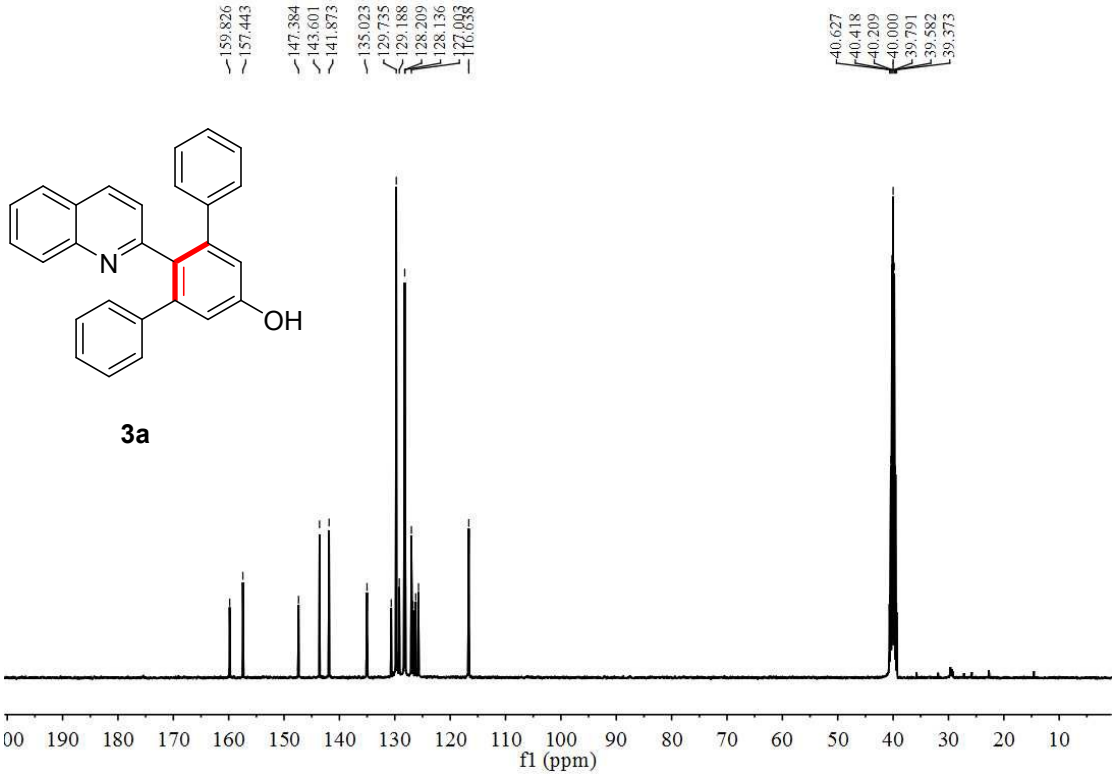
^{13}C NMR (100 MHz, DMSO-d_6): δ 157.2, 156.9, 156.7, 143.5, 143.2, 143.2, 141.8, 139.5, 133.8, 133.0, 131.8, 130.8, 130.5, 128.3, 128.2, 128.1, 127.8, 127.1, 127.0, 126.8, 126.5, 126.3, 125.7, 122.1, 116.7, 116.5, 106.5, 63.8, 15.0 ppm.

HRMS (*m/z*) (ESI): calcd for $C_{33}H_{26}NO_2$ 468.1958 [M+H$^+$]; found 468.1956.

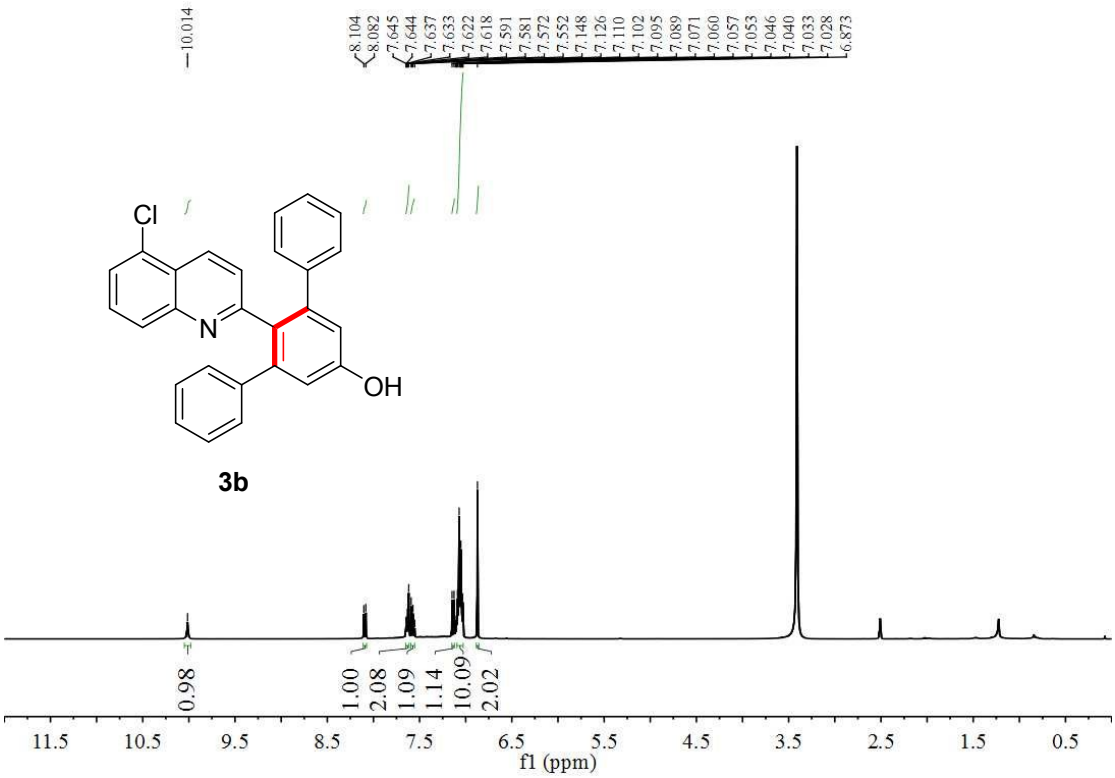
Copies of ^{1}H NMR and ^{13}C NMR spectra of all compounds



3a



3a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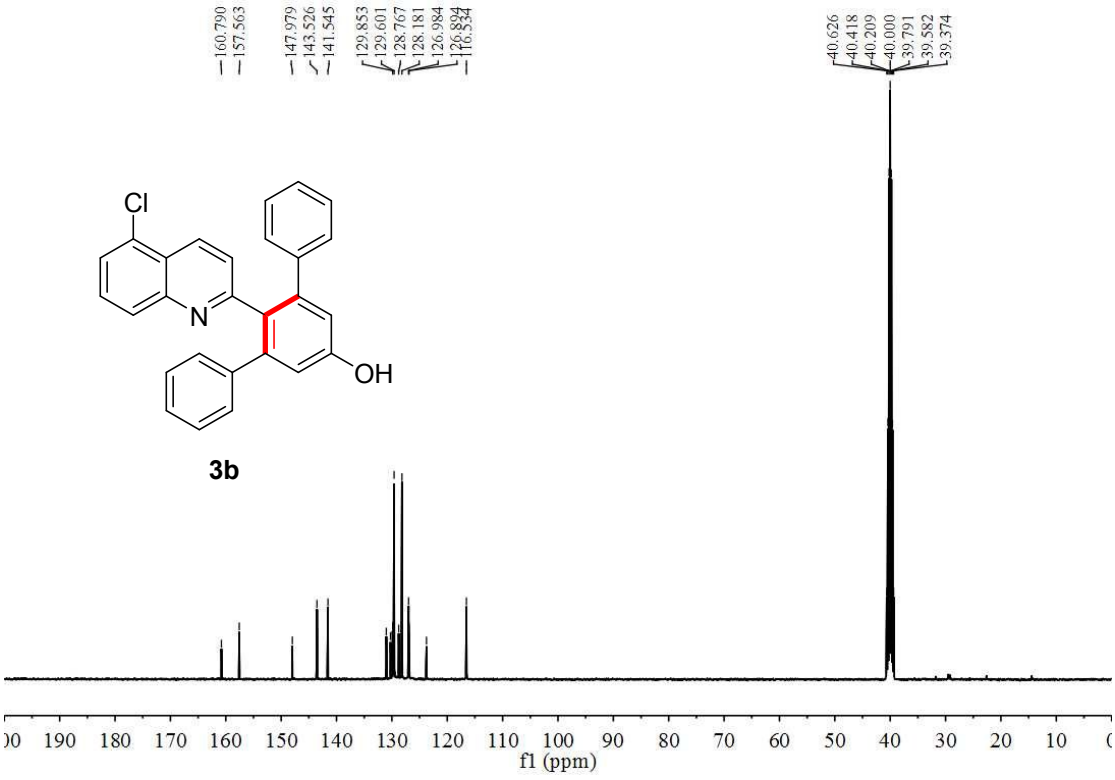
7.637
7.633
7.622
7.618
7.591
7.581
7.572
7.552
7.148
7.126
7.110
7.102
7.095
7.089
7.071
7.060
7.057
7.053
7.046
7.040
7.033
7.028
6.873
Cl
N
OH
0.98
1.00
2.08
1.09
1.14
10.09
2.02
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

3b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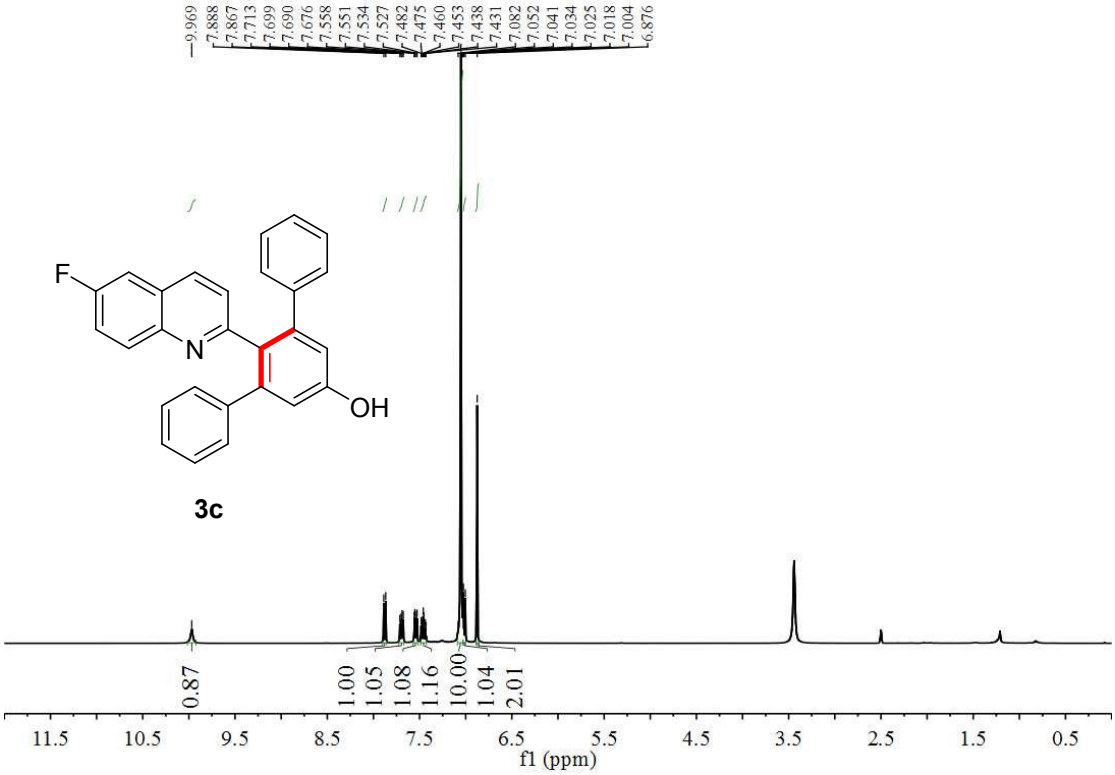
147.979
143.526
141.545
129.853
129.601
128.767
128.181
126.984
126.894
116.534
40.626
40.418
40.209
40.000
39.791
39.582
39.374
Cl
N
OH
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

3b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7.888
7.867
7.713
7.699
7.690
7.676
7.558
7.551
7.534
7.527
7.482
7.475
7.460
7.453
7.438
7.431
7.082
7.052
7.041
7.034
7.025
7.018
7.004
6.876
F
N
OH
3c
0.87
1.00
1.05
1.08
1.16
10.00
1.04
2.01
11.5
10.5
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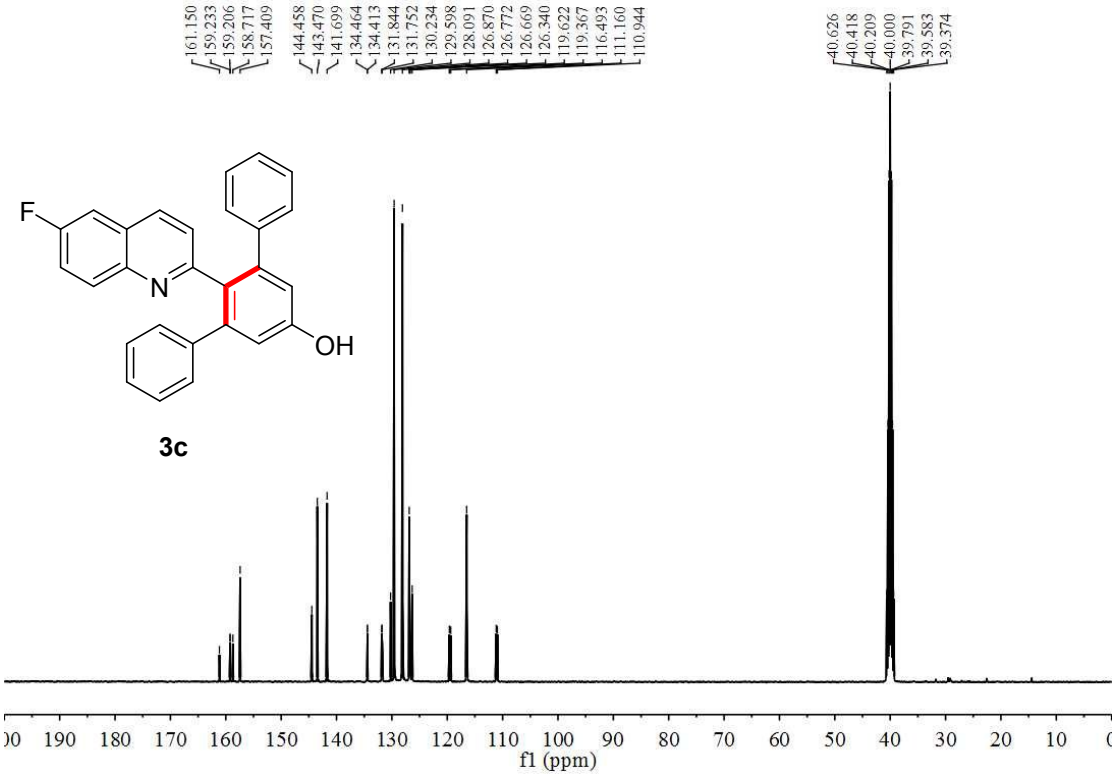
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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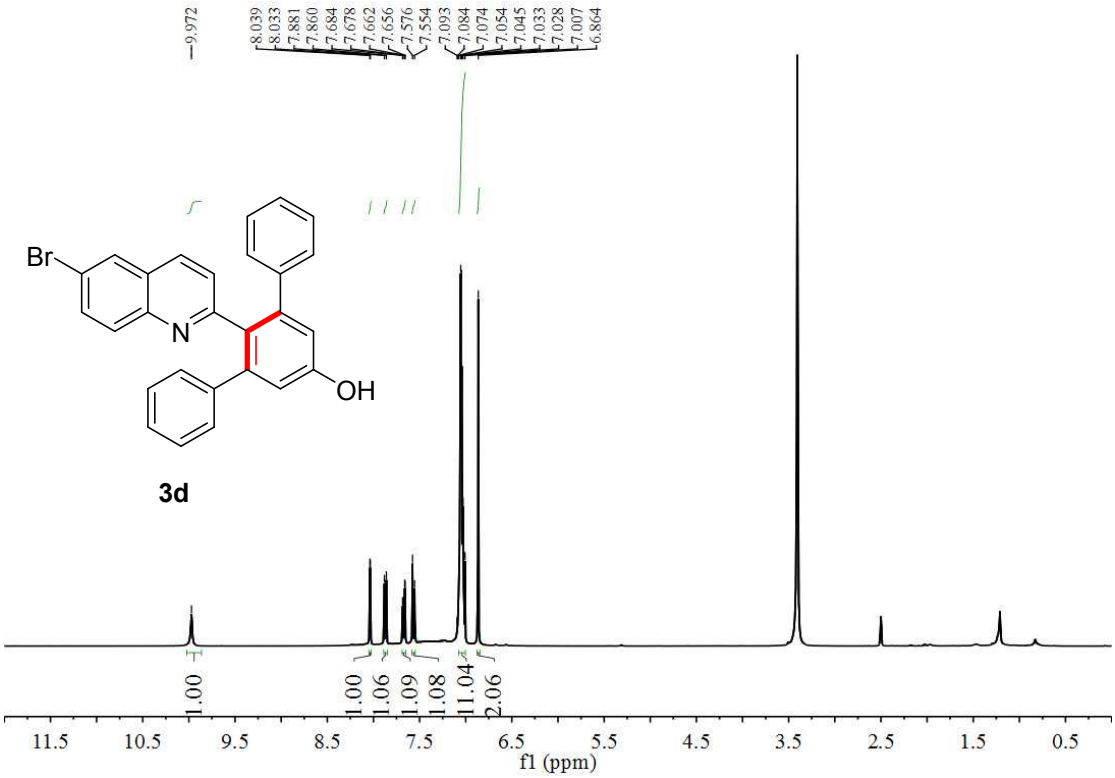
159.233
159.206
158.717
157.409
144.458
143.470
141.699
134.464
134.413
131.844
131.752
130.234
129.598
128.091
126.870
126.772
126.669
126.340
119.622
119.367
116.493
111.160
110.944
40.626
40.418
40.209
40.000
39.791
39.583
39.374
F
N
OH
3c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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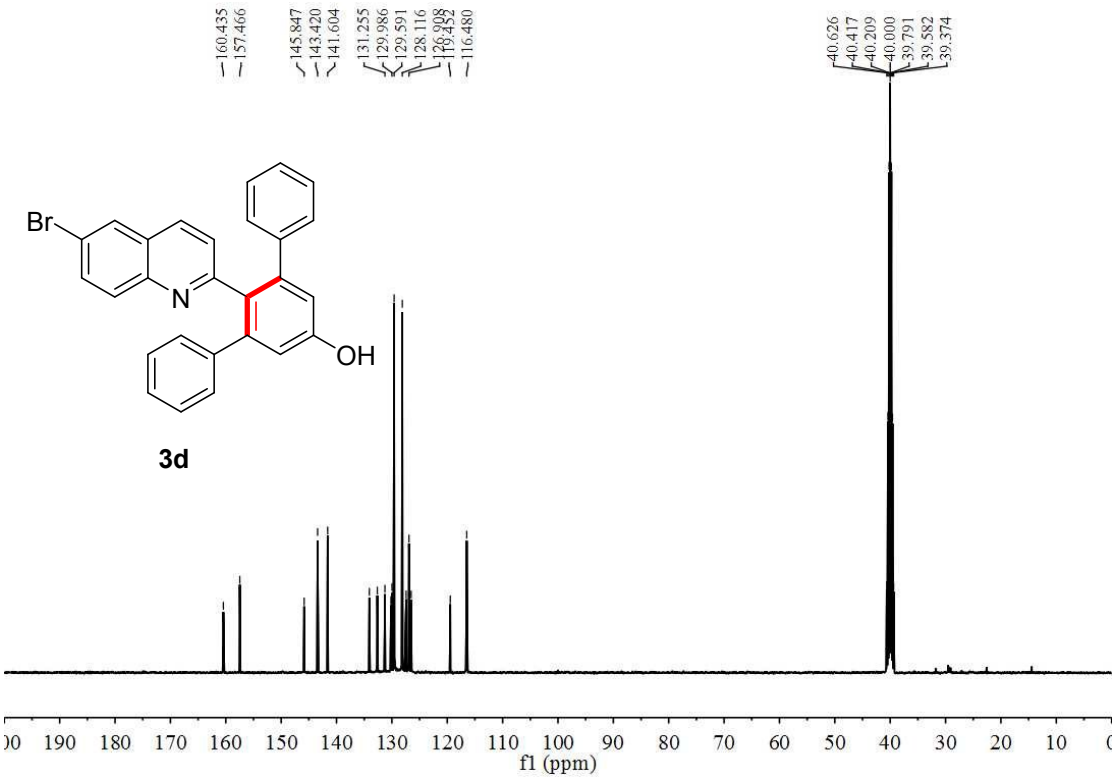
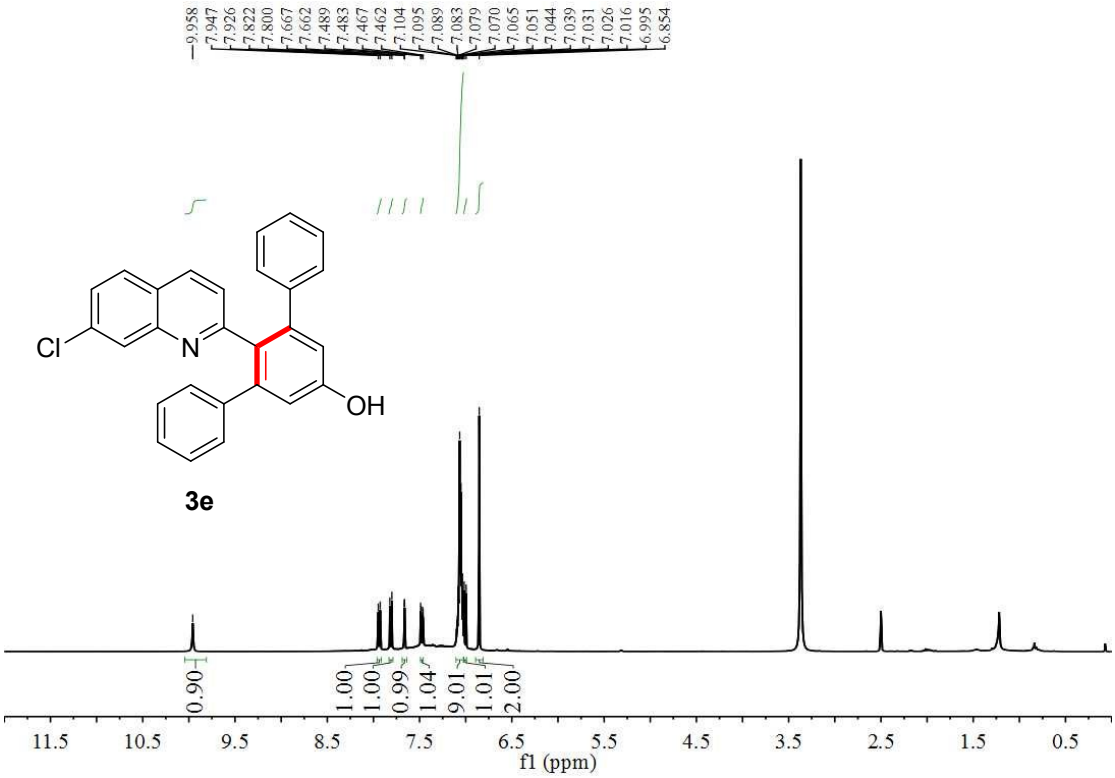
8.039
8.033
7.881
7.860
7.684
7.678
7.662
7.656
7.576
7.554
7.093
7.084
7.074
7.054
7.045
7.033
7.028
7.007
6.864
Br
N
OH
3d
1.00
1.00
1.06
1.09
1.08
11.04
2.06
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


160.435
157.466
145.847
143.420
141.604
131.255
129.986
129.591
128.116
116.480
40.626
40.417
40.209
40.000
39.791
39.582
39.374
Br
N
OH
3d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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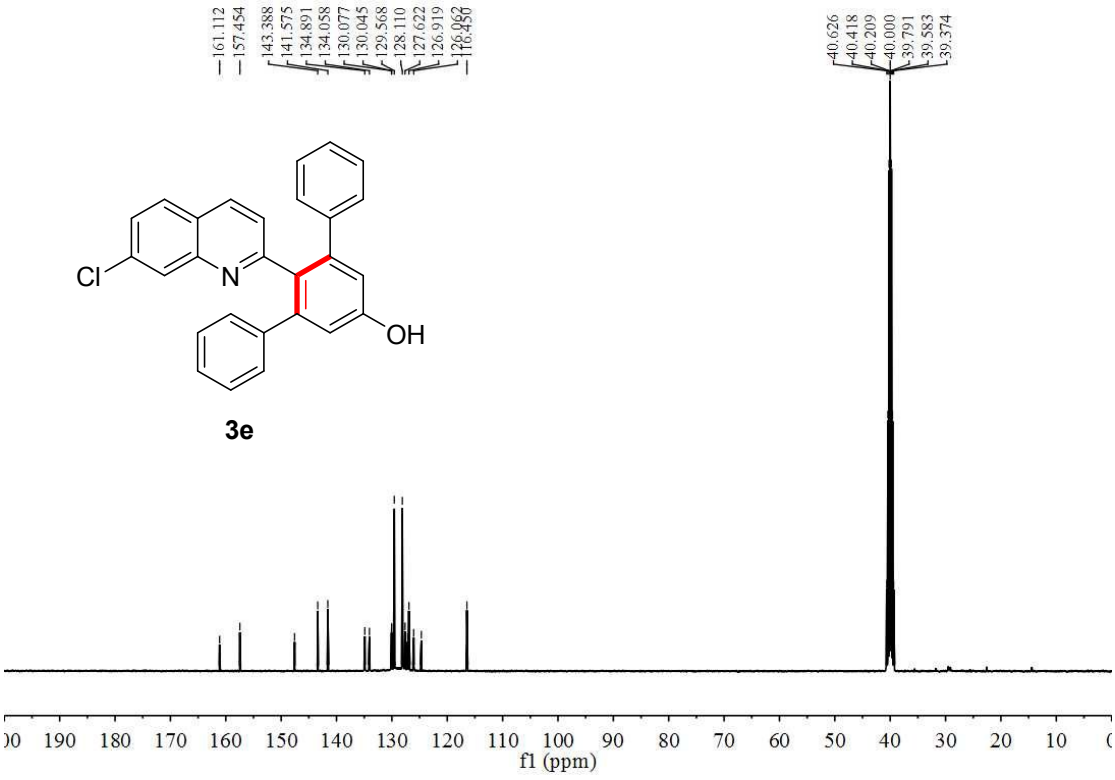
7.947
7.926
7.822
7.800
7.667
7.662
7.489
7.483
7.467
7.462
7.104
7.095
7.089
7.083
7.079
7.070
7.065
7.051
7.044
7.039
7.031
7.026
7.016
6.995
6.854
Cl
N
OH
3e
0.90
1.00
1.00
0.99
1.04
9.01
1.01
2.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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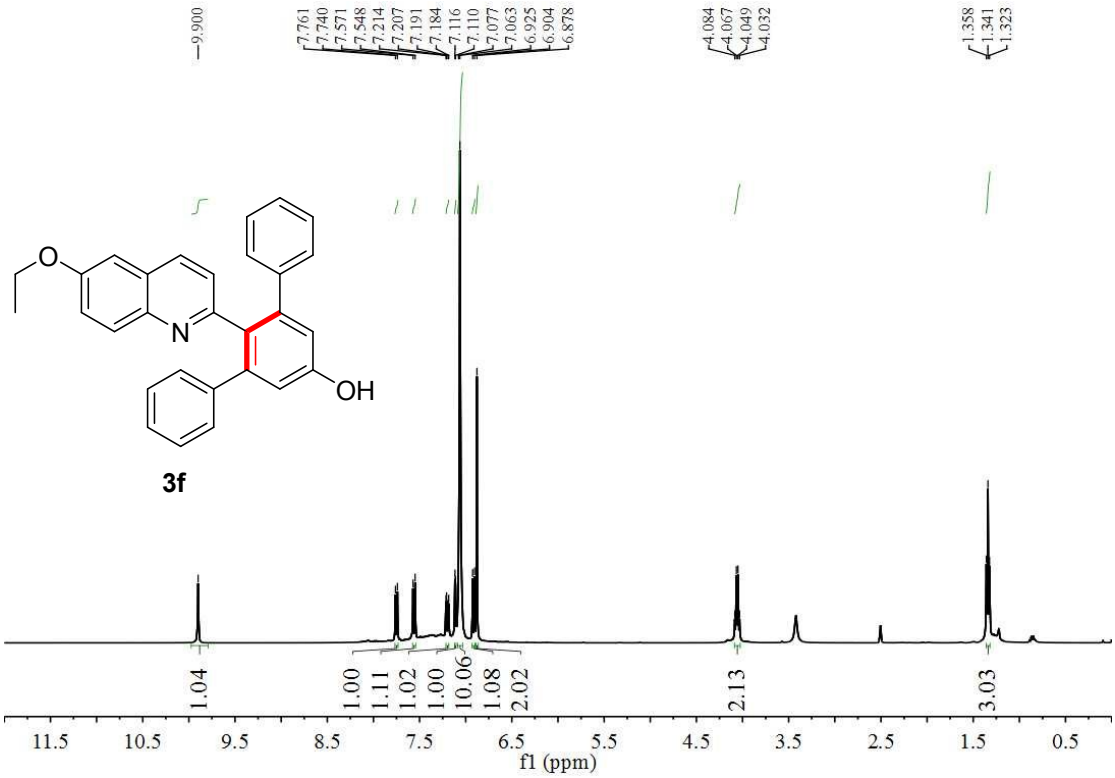
143.388
141.575
134.891
134.058
130.077
130.045
129.568
128.110
127.622
126.919
126.062
116.456
40.626
40.418
40.209
40.000
39.791
39.583
39.374
Cl
N
OH
3e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.740
7.571
7.548
7.214
7.207
7.191
7.184
7.116
7.110
7.077
7.063
6.925
6.904
6.878
4.084
4.067
4.049
4.032
1.358
1.341
1.323
O
N
OH
3f
1.04
1.00
1.11
1.02
1.00
10.06
1.08
2.02
2.13
3.03
11.5
10.5
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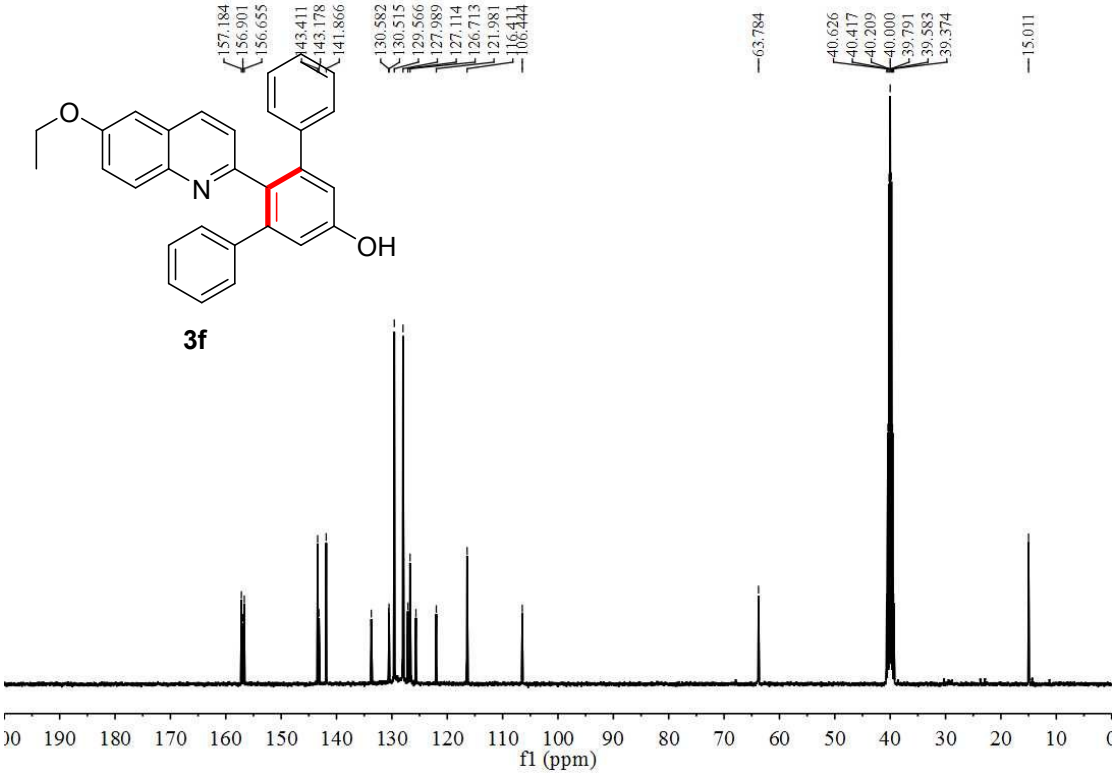
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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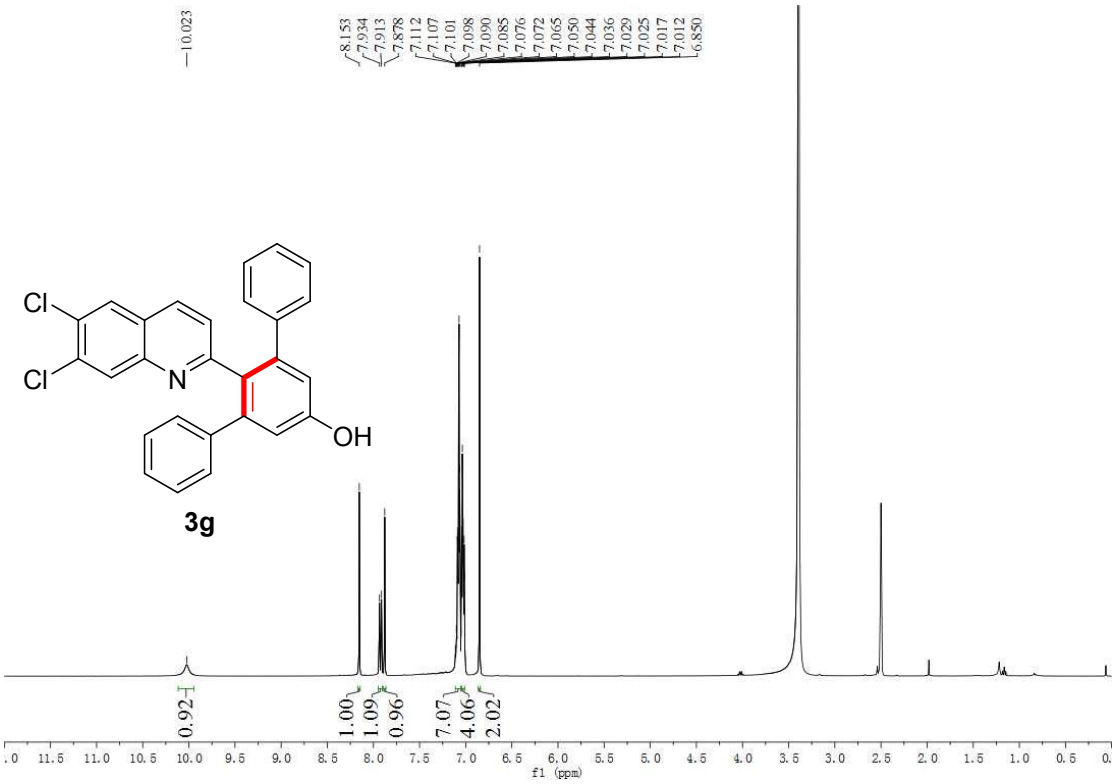
156.655
143.411
143.178
141.866
130.582
130.515
129.566
127.989
127.114
126.713
121.981
116.411
116.444
63.784
40.626
40.417
40.209
40.000
39.791
39.583
39.374
15.011
O
N
OH
3f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


10.023
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7.934
7.913
7.878
7.112
7.107
7.101
7.098
7.090
7.085
7.076
7.072
7.065
7.050
7.044
7.036
7.029
7.025
7.017
7.012
6.850
Cl
Cl
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OH
3g
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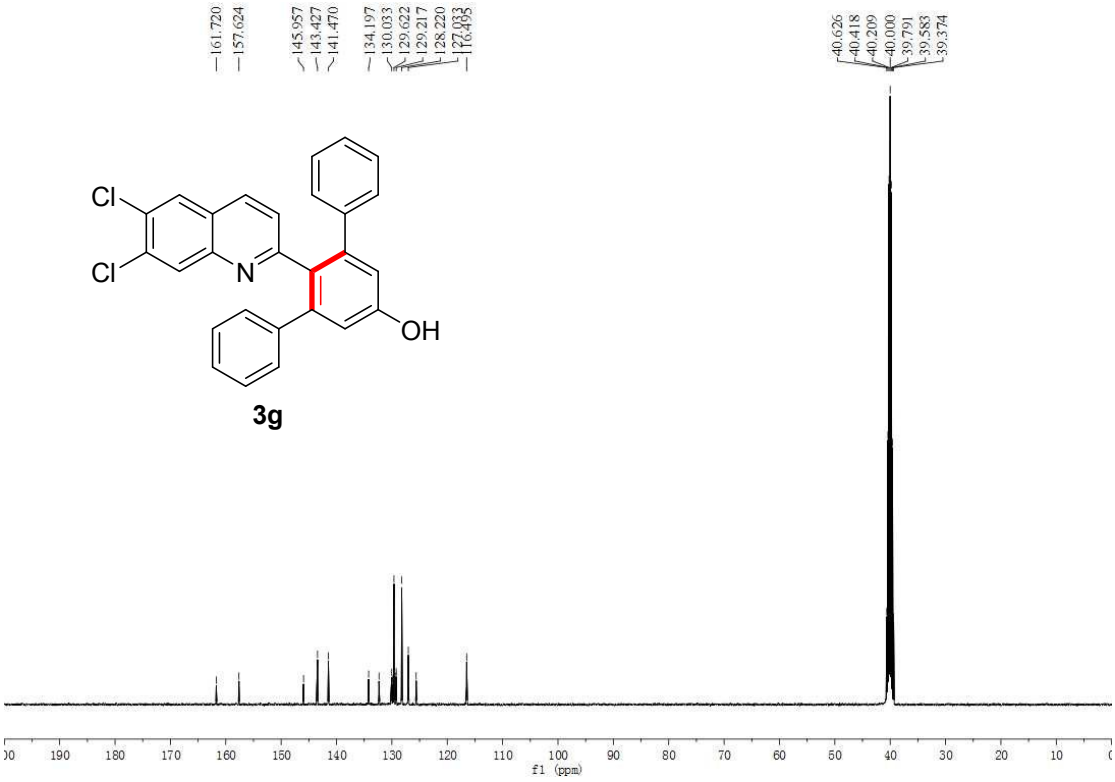
1.00
1.09
0.96
7.07
4.06
2.02
f1 (ppm)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143.427
141.470
134.197
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129.622
129.217
128.220
127.033
116.495
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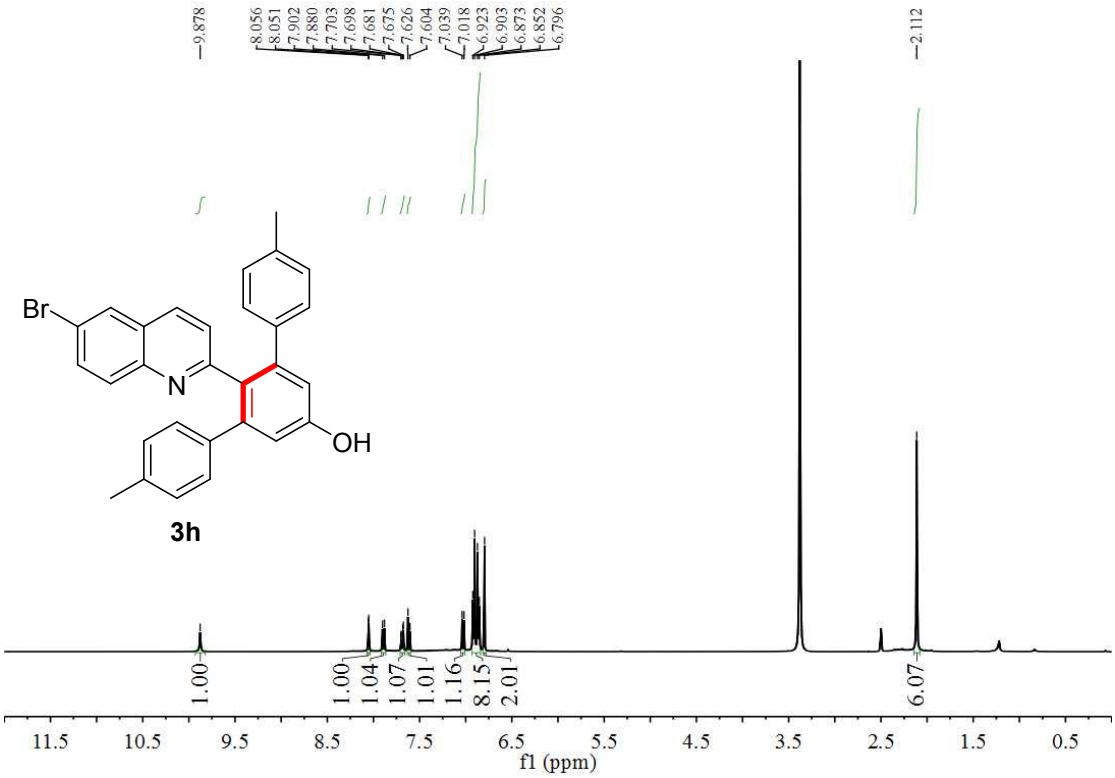
40.418
40.209
40.000
39.791
39.583
39.374
Cl
Cl
N
OH
3g
f1 (ppm)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8.051
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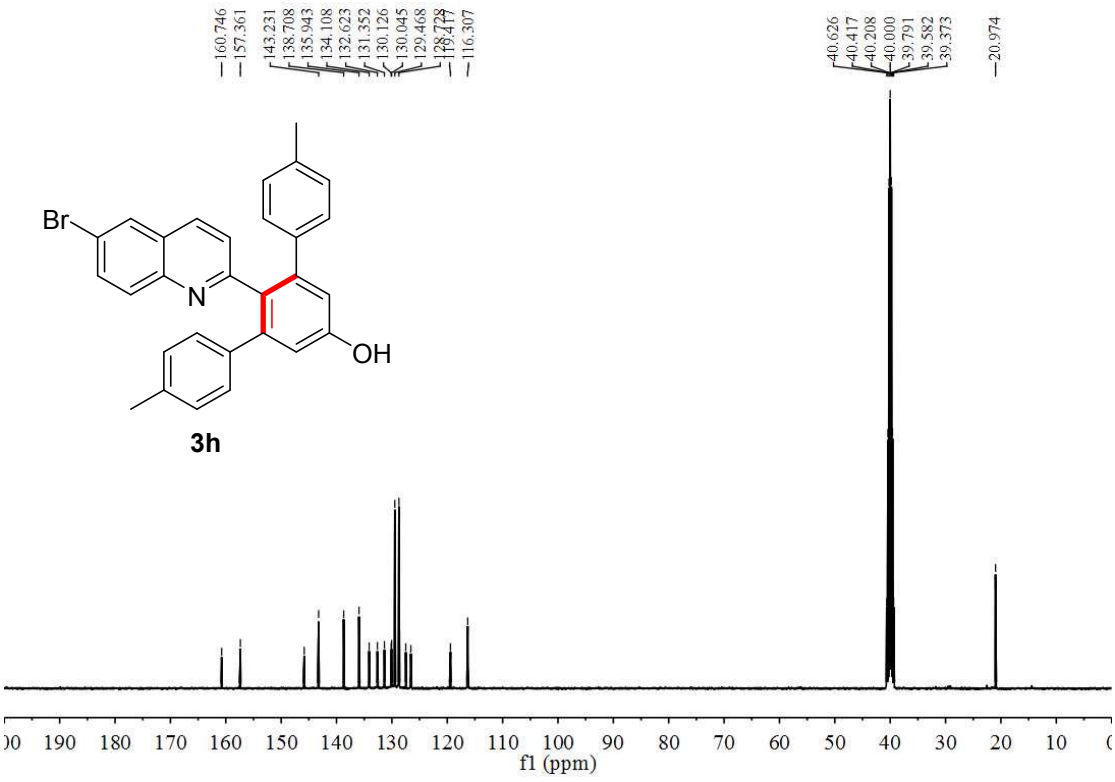
7.703
7.698
7.681
7.675
7.626
7.604
7.039
7.018
6.923
6.903
6.873
6.852
6.796
2.112
Br
N
OH
3h
1.00
1.00
1.04
1.07
1.01
1.16
8.15
2.01
6.07
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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135.943
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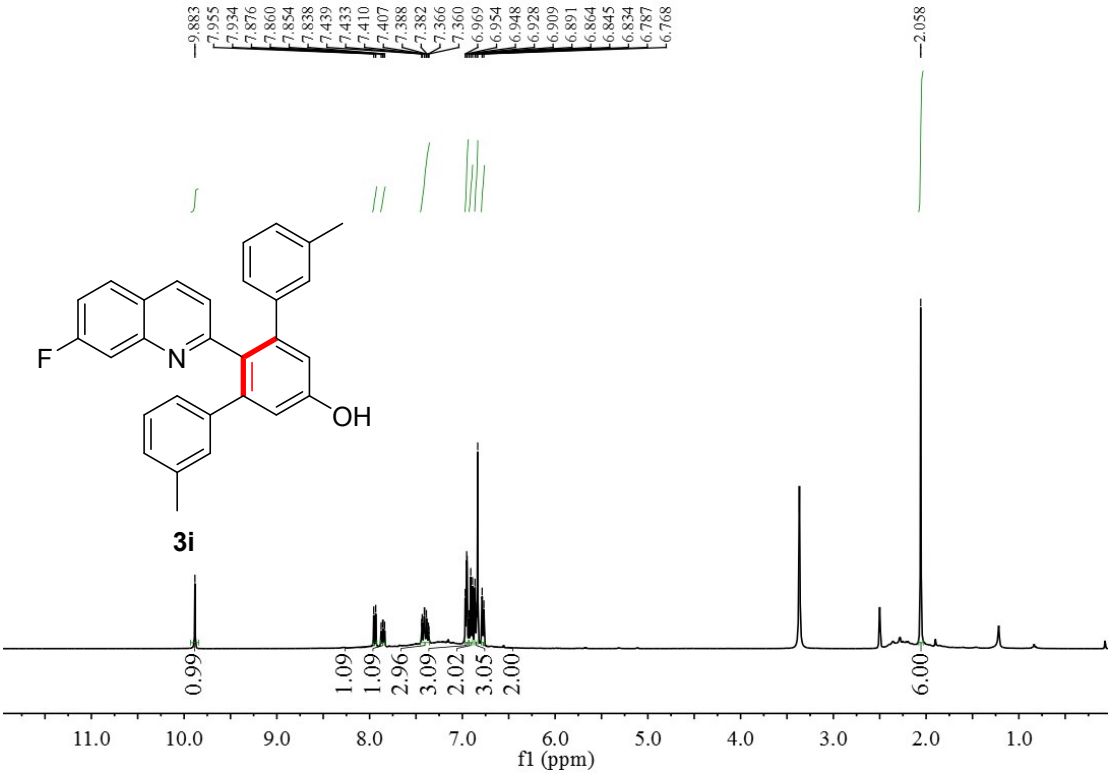
131.352
130.126
130.045
129.468
116.307
40.626
40.417
40.208
40.000
39.791
39.582
39.373
20.974
Br
N
OH
3h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.854
7.838
7.439
7.433
7.410
7.407
7.388
7.382
7.366
7.360
6.969
6.954
6.948
6.928
6.909
6.891
6.864
6.845
6.834
6.787
6.768
2.058
F
N
OH
3i
0.99
1.09
1.09
2.96
3.09
2.02
3.05
2.00
6.00
11.0
10.0
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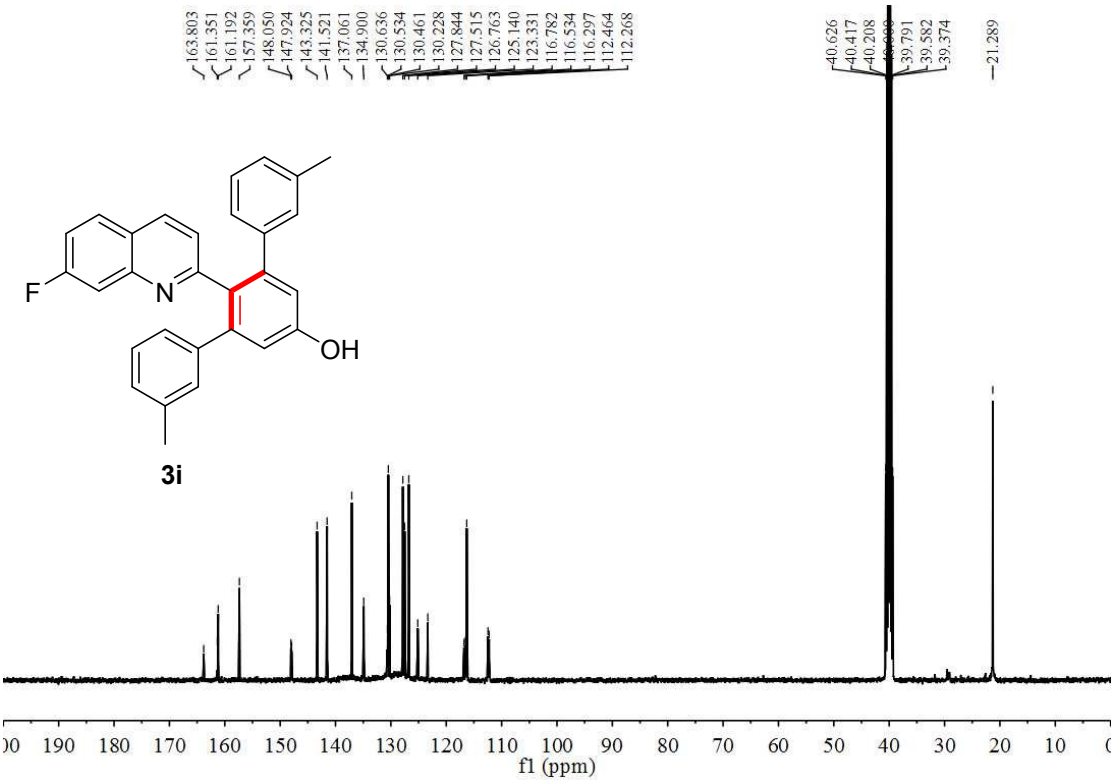
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)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147.924
143.325
141.521
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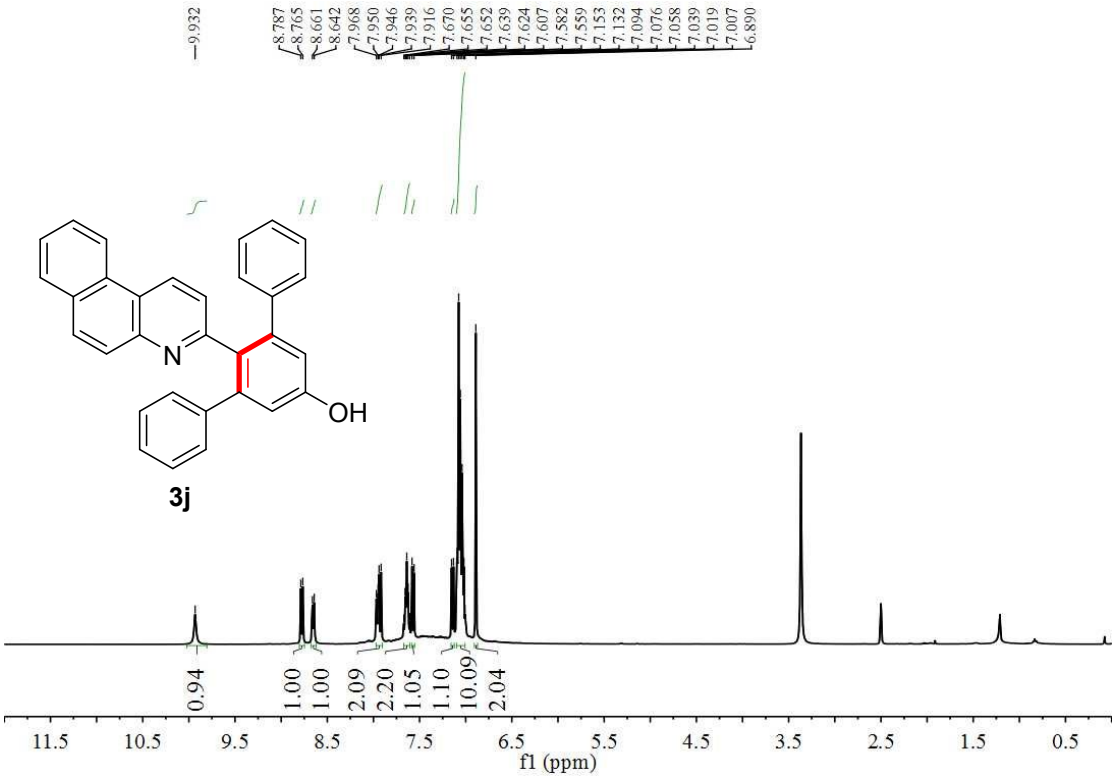
134.900
130.636
130.534
130.461
130.228
127.844
127.515
126.763
125.140
123.331
116.782
116.534
116.297
112.464
112.268
40.626
40.417
40.208
39.791
39.582
39.374
21.289
F
N
OH
3i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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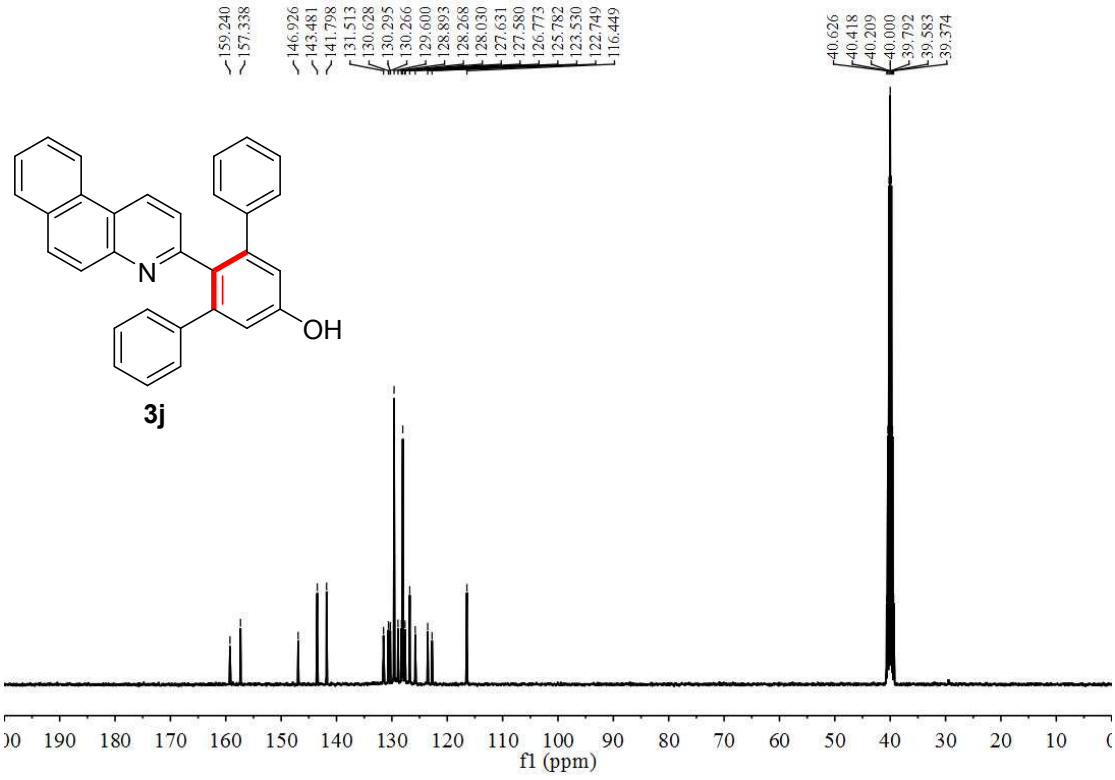
7.950
7.946
7.939
7.916
7.670
7.655
7.652
7.639
7.624
7.607
7.582
7.559
7.153
7.132
7.094
7.076
7.058
7.039
7.019
7.007
6.890
N
OH
3j
0.94
1.00
1.00
2.09
2.20
1.05
1.10
10.09
2.04
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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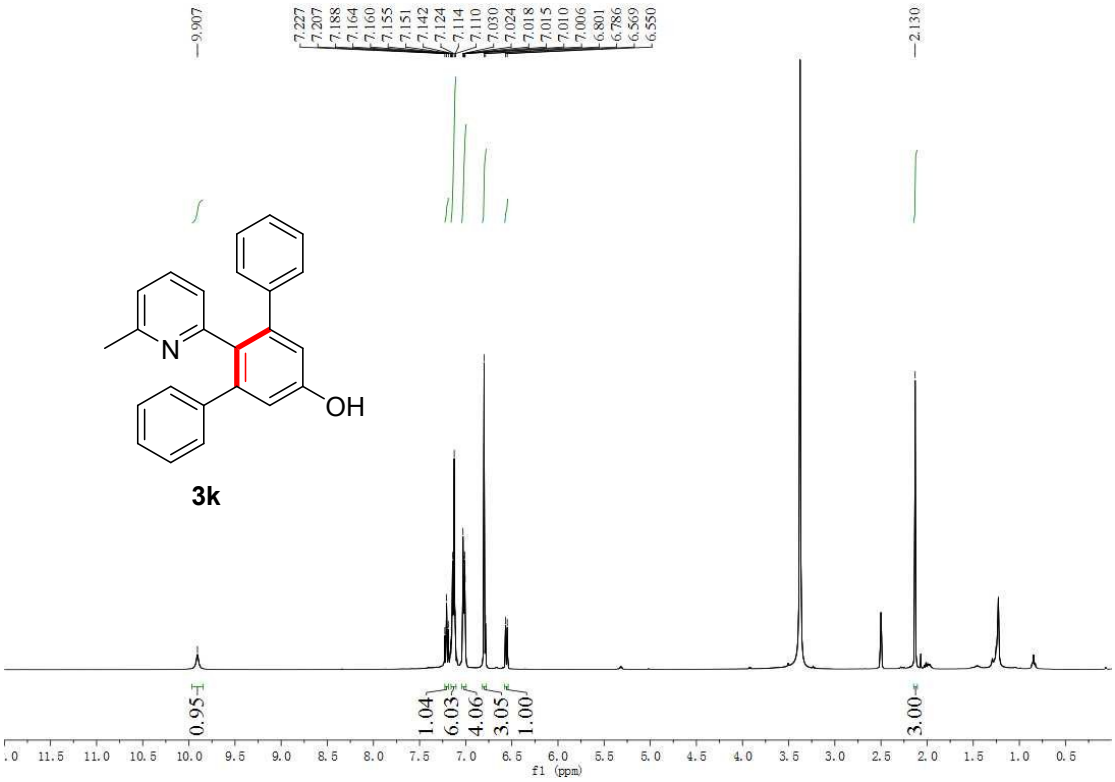
131.513
130.628
130.295
130.266
129.600
128.893
128.268
128.030
127.631
127.580
126.773
125.782
123.530
122.749
116.449
40.626
40.418
40.209
40.000
39.792
39.583
39.374
N
OH
3j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.164
7.160
7.155
7.151
7.142
7.124
7.114
7.110
7.030
7.024
7.018
7.015
7.010
7.006
6.801
6.786
6.569
6.550
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OH
0.95
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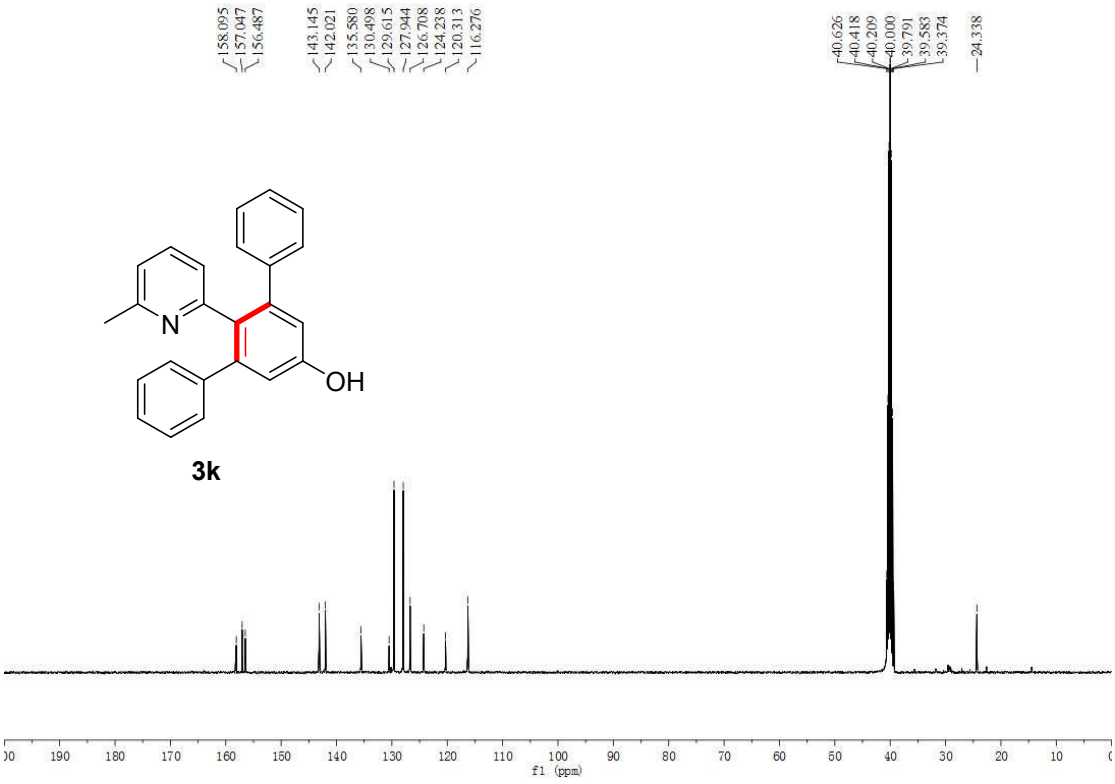
6.03
4.06
3.05
1.00
3.00
f1 (ppm)

3k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129.615
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124.238
120.313
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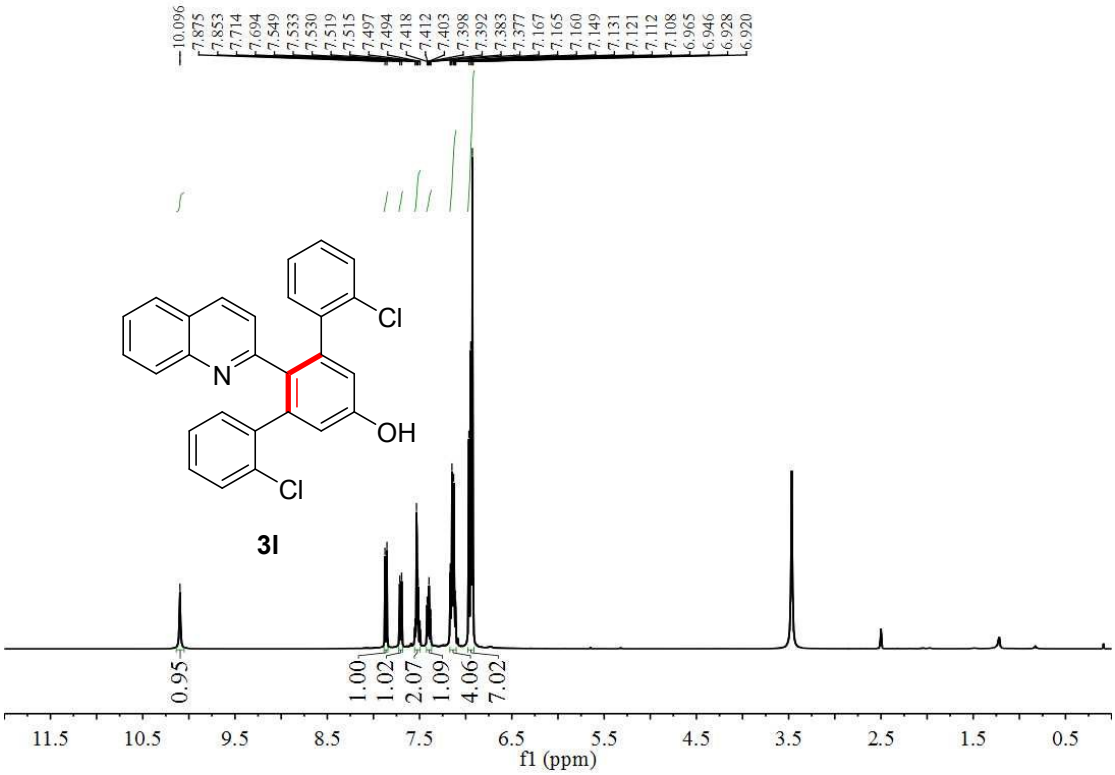
40.000
39.791
39.583
39.374
24.338
N
OH
f1 (ppm)

3k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7.530
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7.515
7.497
7.494
7.418
7.412
7.403
7.398
7.392
7.383
7.377
7.167
7.165
7.160
7.149
7.131
7.121
7.112
7.108
6.965
6.946
6.928
6.920
Cl
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OH
Cl
3l
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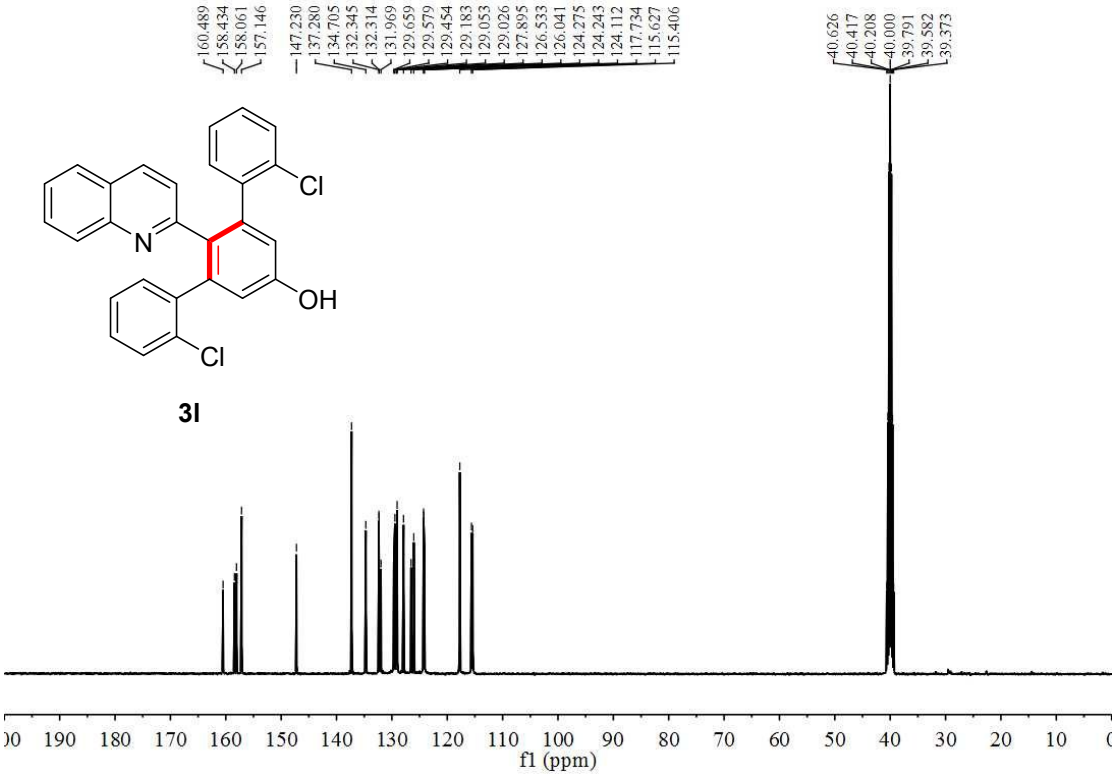
1.02
2.07
1.09
4.06
7.02
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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129.183
129.053
129.026
127.895
126.533
126.041
124.275
124.243
124.112
117.734
115.627
115.406
40.626
40.417
40.208
40.000
39.791
39.582
39.373
Cl
N
OH
Cl
3l
190
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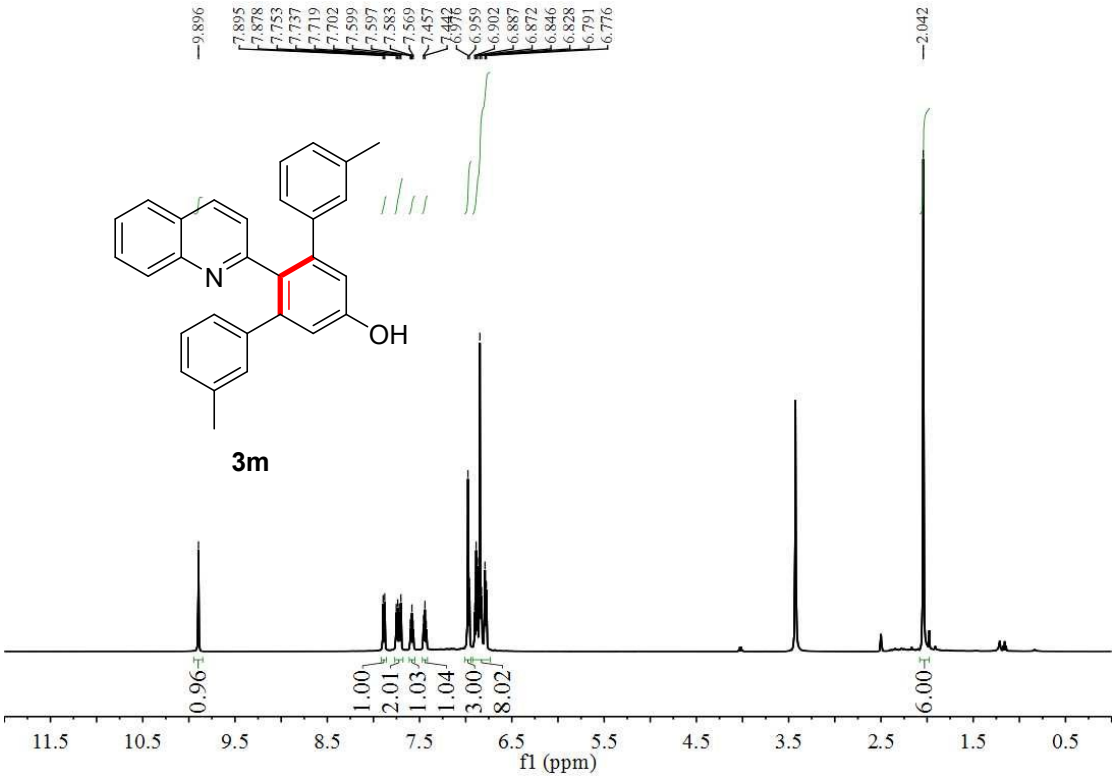
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.599
7.597
7.583
7.569
7.457
7.442
6.976
6.959
6.902
6.887
6.872
6.846
6.828
6.791
6.776
2.042
N
OH
3m
0.96
1.00
2.01
1.03
1.04
3.00
8.02
6.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
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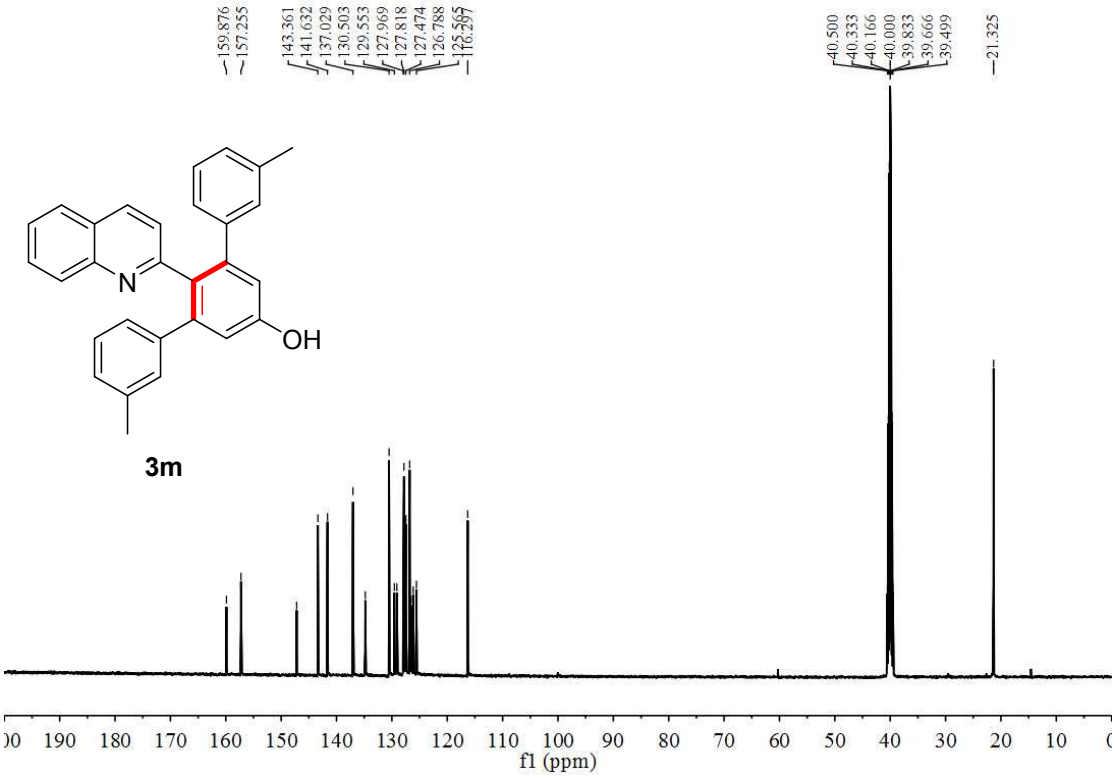
0.5
f1 (ppm)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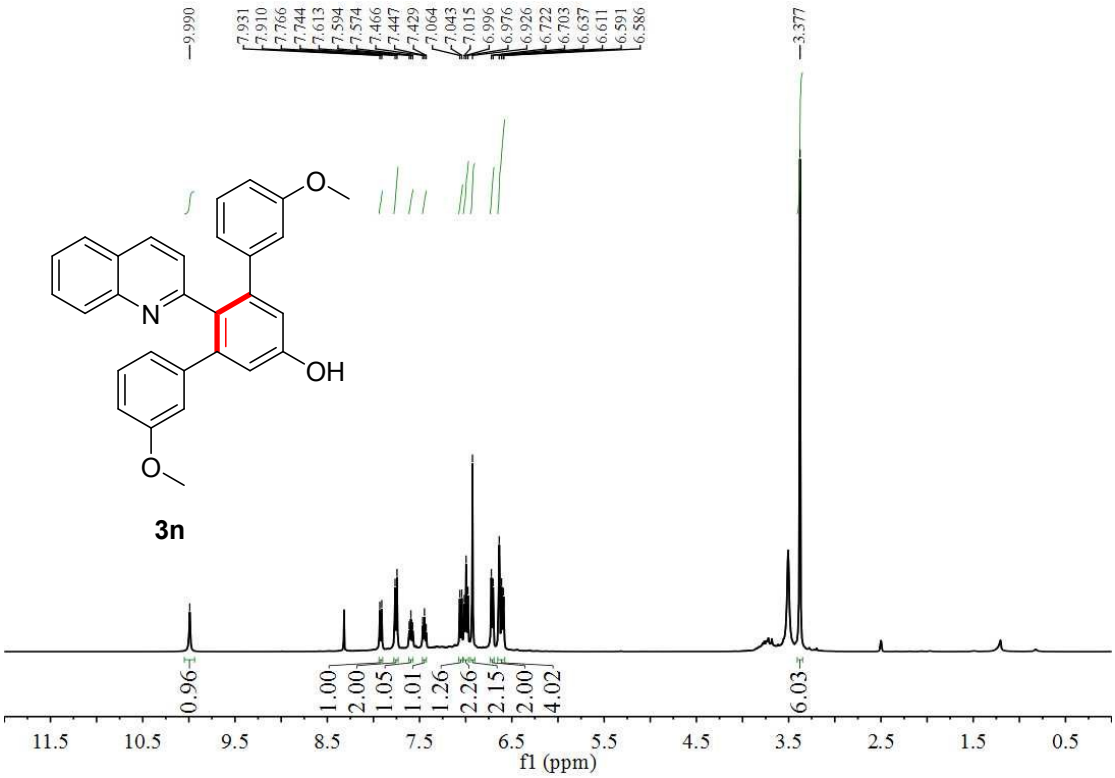
125.565
116.297
40.500
40.333
40.166
40.000
39.833
39.666
39.499
21.325
N
OH
3m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.429
7.064
7.043
7.015
6.996
6.976
6.926
6.722
6.703
6.637
6.611
6.591
6.586
3.377
O
N
OH
O
3n
0.96
1.00
2.00
1.05
1.01
1.26
2.26
2.15
2.00
4.02
6.03
11.5
10.5
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7.5
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5.5
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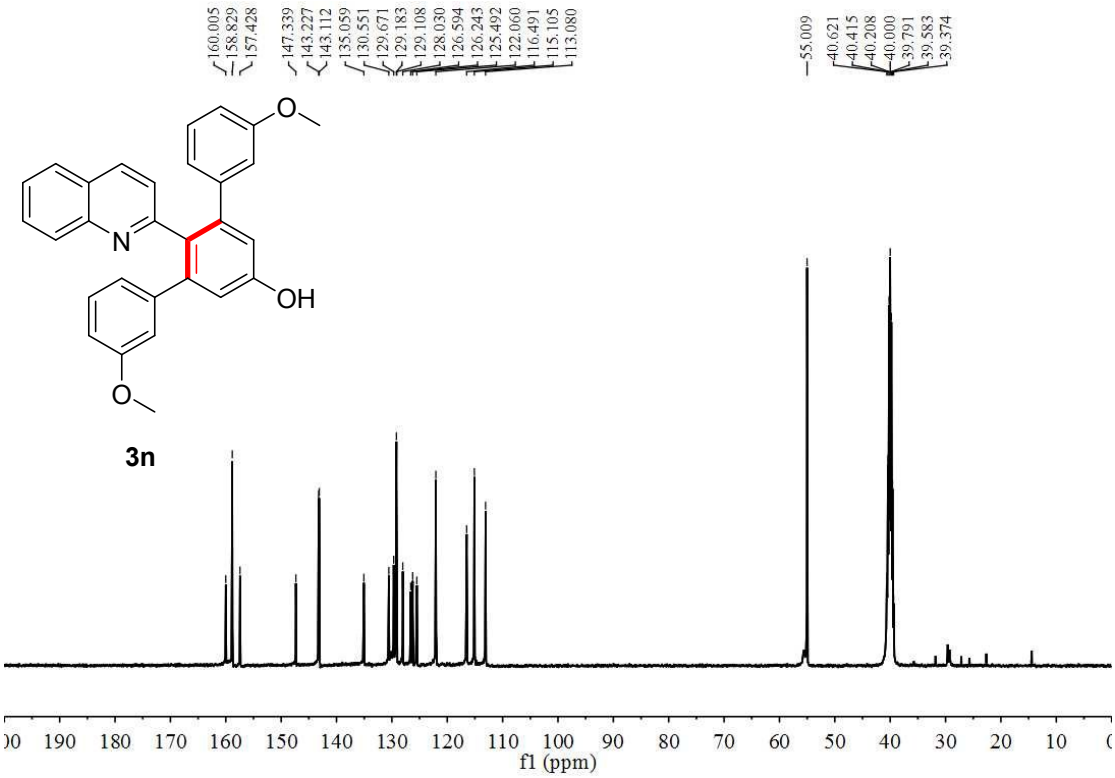
1.5
0.5
f1 (ppm)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130.551
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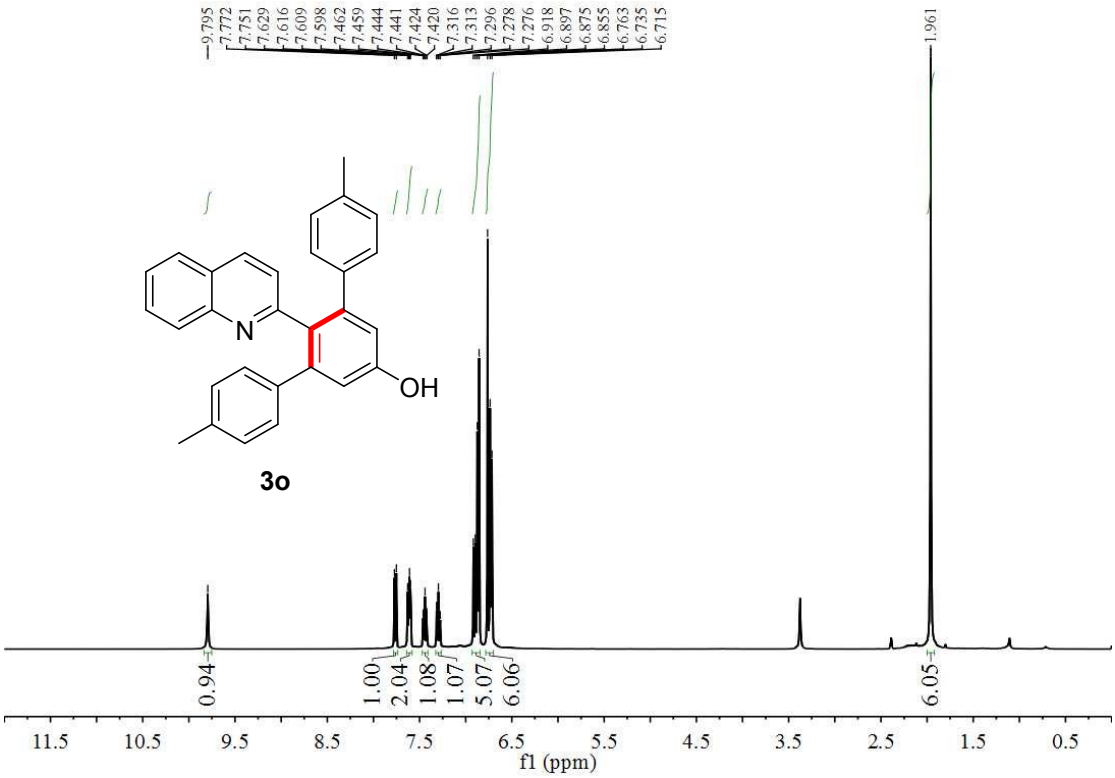
129.108
128.030
126.594
126.243
125.492
122.060
116.491
115.105
113.080
55.009
40.621
40.415
40.208
40.000
39.791
39.583
39.374
O
N
OH
O
3n
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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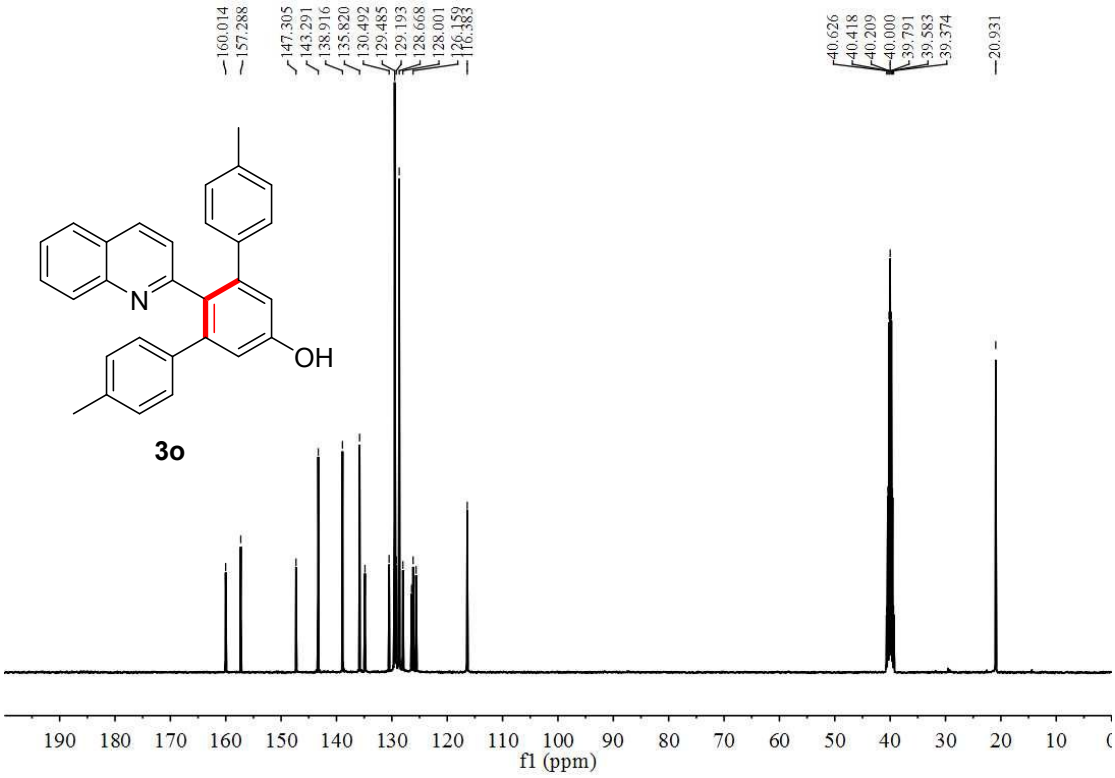
7.609
7.598
7.462
7.459
7.444
7.441
7.424
7.420
7.316
7.313
7.296
7.278
7.276
6.918
6.897
6.875
6.855
6.763
6.735
6.715
1.961
N
OH
3o
0.94
1.00
2.04
1.08
1.07
5.07
6.06
6.05
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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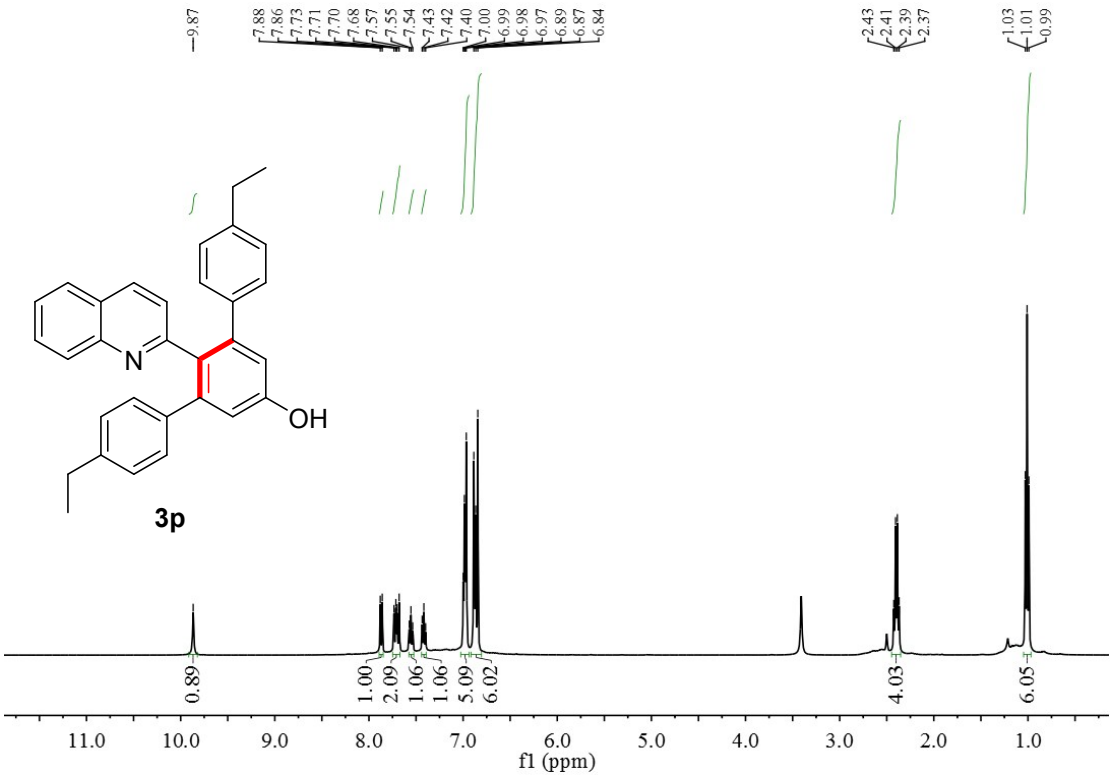
130.492
129.485
129.193
128.668
128.001
126.159
116.383
40.626
40.418
40.209
40.000
39.791
39.583
39.374
20.931
N
OH
3o
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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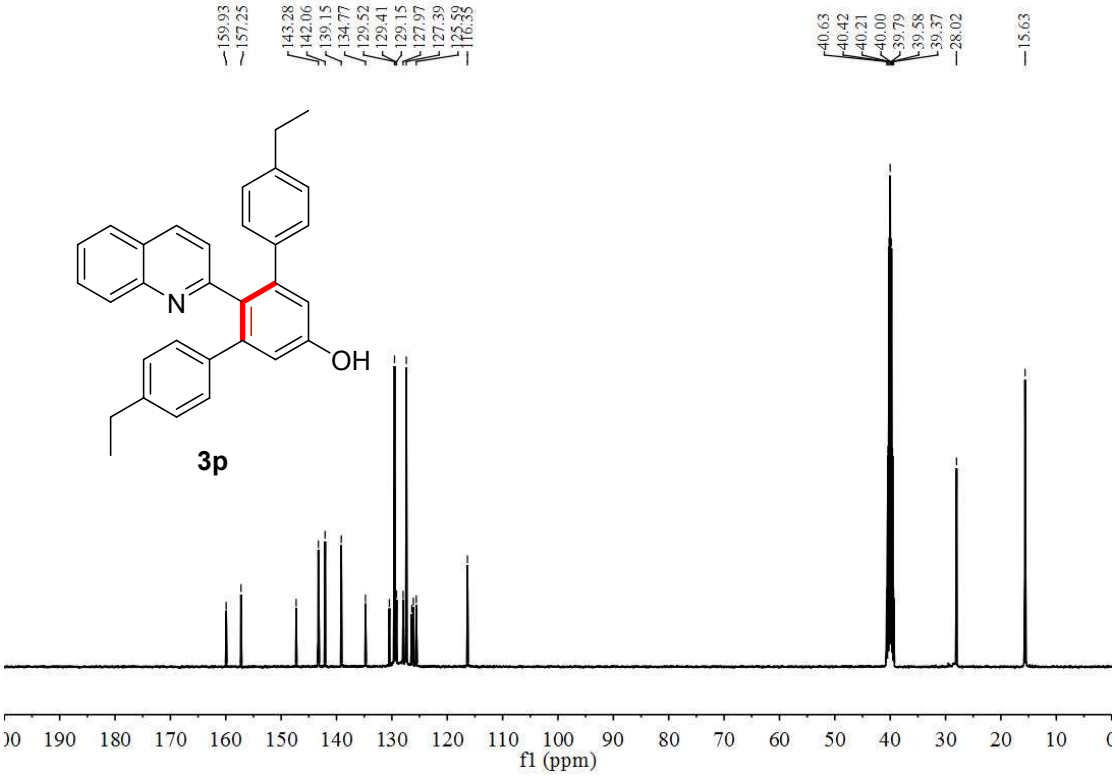
7.68
7.57
7.55
7.54
7.43
7.42
7.40
7.00
6.99
6.98
6.97
6.89
6.87
6.84
2.43
2.41
2.39
2.37
1.03
1.01
0.99
N
OH
3p
0.89
1.00
2.09
1.06
1.06
5.09
6.02
4.03
6.05
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)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139.15
134.77
129.52
129.41
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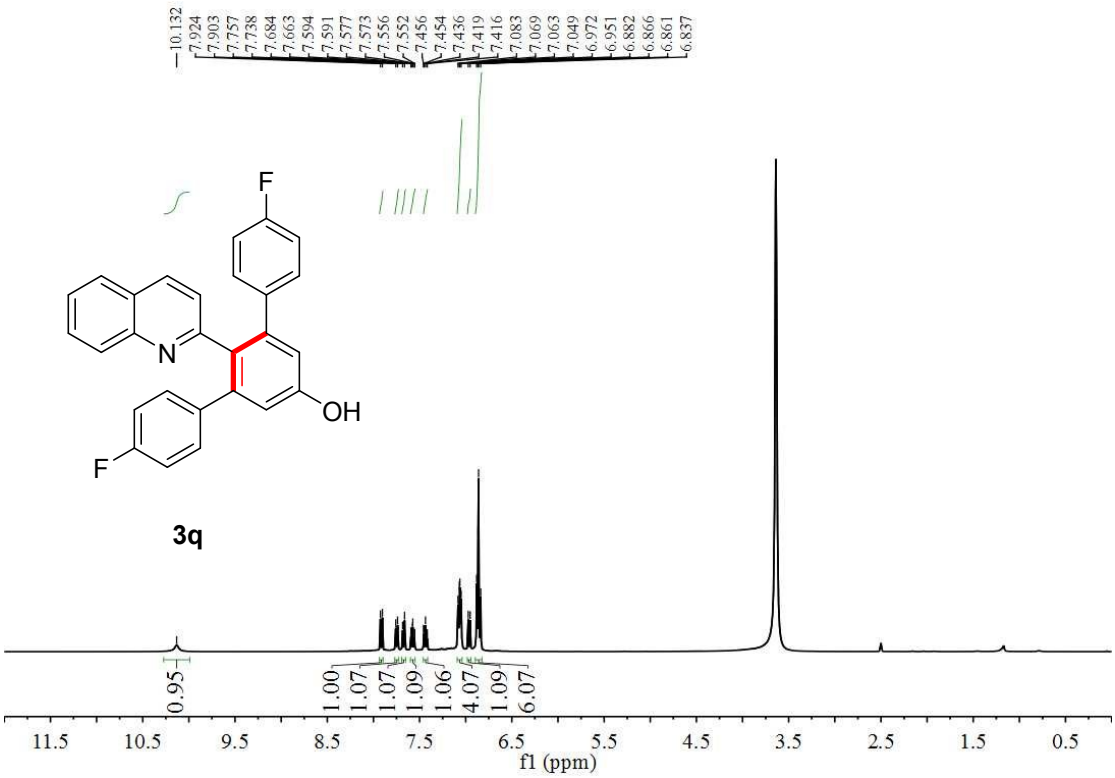
127.97
127.39
125.59
116.35
40.63
40.42
40.21
40.00
39.79
39.58
39.37
28.02
15.63
N
OH
3p
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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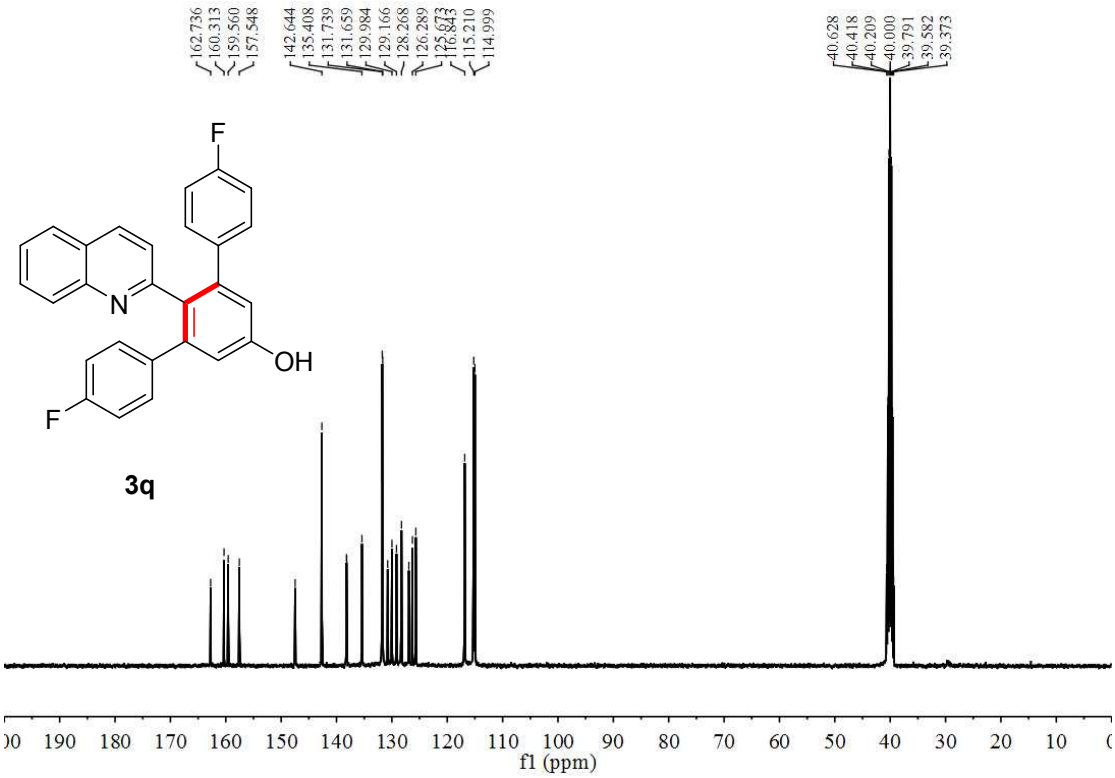
7.684
7.663
7.594
7.591
7.577
7.573
7.556
7.552
7.456
7.454
7.436
7.419
7.416
7.083
7.069
7.063
7.049
6.972
6.951
6.882
6.866
6.861
6.837
F
N
OH
F
3q
0.95
1.00
1.07
1.07
1.09
1.06
4.07
1.09
6.07
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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129.984
129.166
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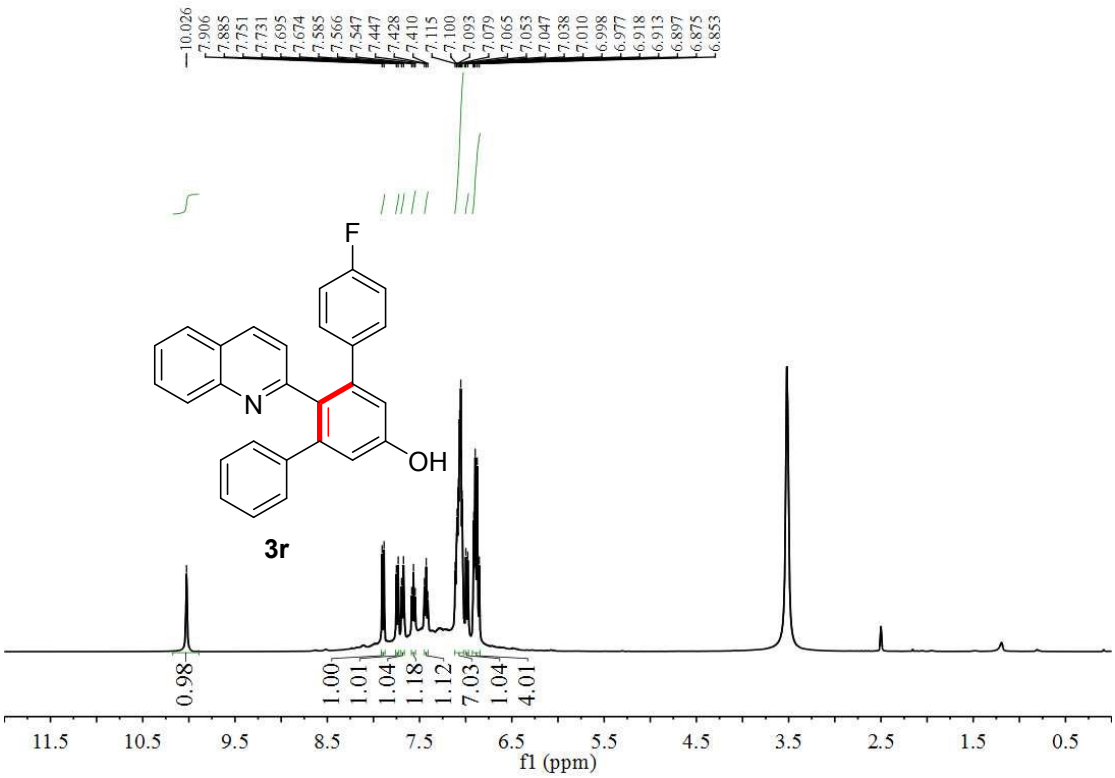
126.289
116.843
115.210
114.999
40.628
40.418
40.209
40.000
39.791
39.582
39.373
F
N
OH
F
3q
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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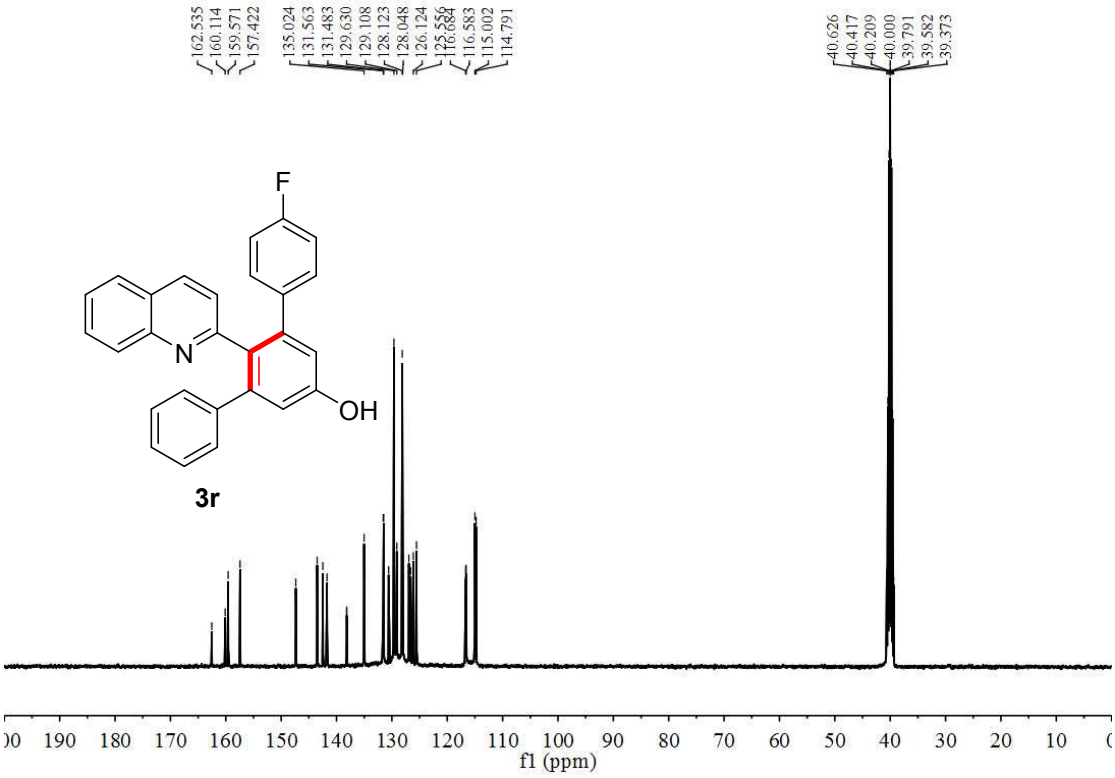
7.547
7.447
7.428
7.410
7.115
7.100
7.093
7.079
7.065
7.053
7.047
7.038
7.010
6.998
6.977
6.918
6.913
6.897
6.875
6.853
F
N
OH
3r
0.98
1.00
1.01
1.04
1.18
1.12
7.03
1.04
4.01
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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131.483
129.630
129.108
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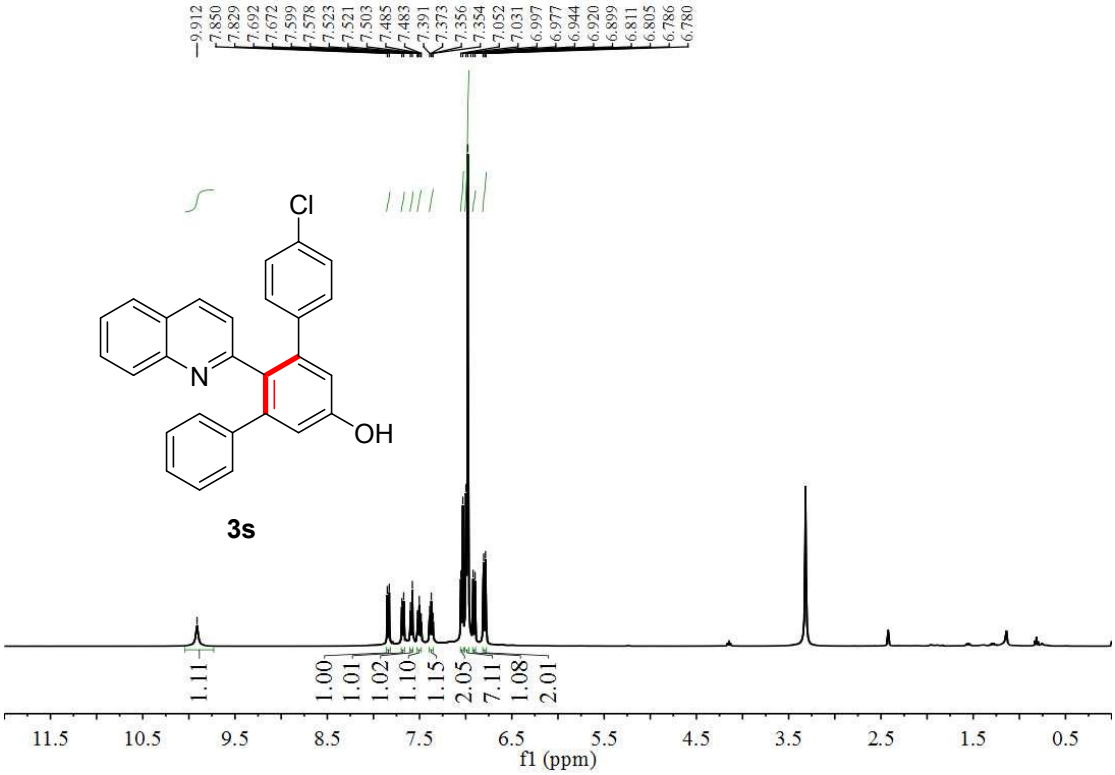
128.048
126.124
116.583
115.002
114.791
40.626
40.417
40.209
40.000
39.791
39.582
39.373
F
N
OH
3r
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.483
7.391
7.373
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7.354
7.052
7.031
6.997
6.977
6.944
6.920
6.899
6.811
6.805
6.786
6.780
Cl
N
OH
3s
1.11
1.00
1.01
1.02
1.10
1.15
2.05
7.11
1.08
2.01
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
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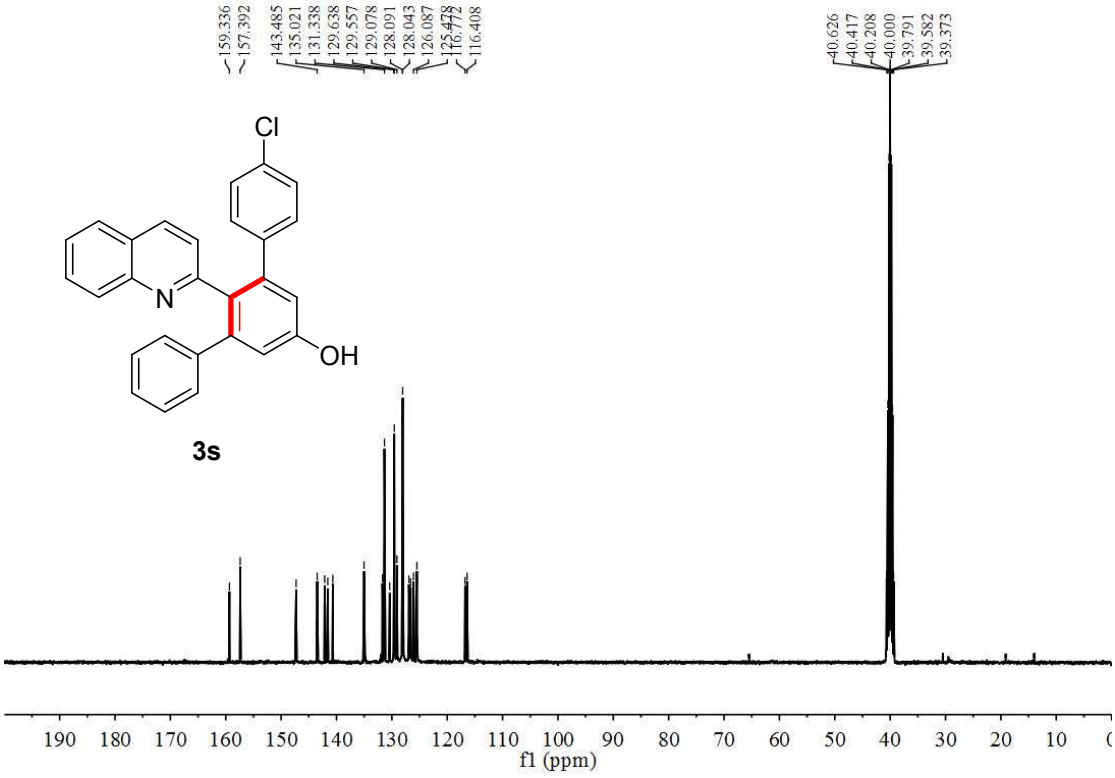
f1 (ppm)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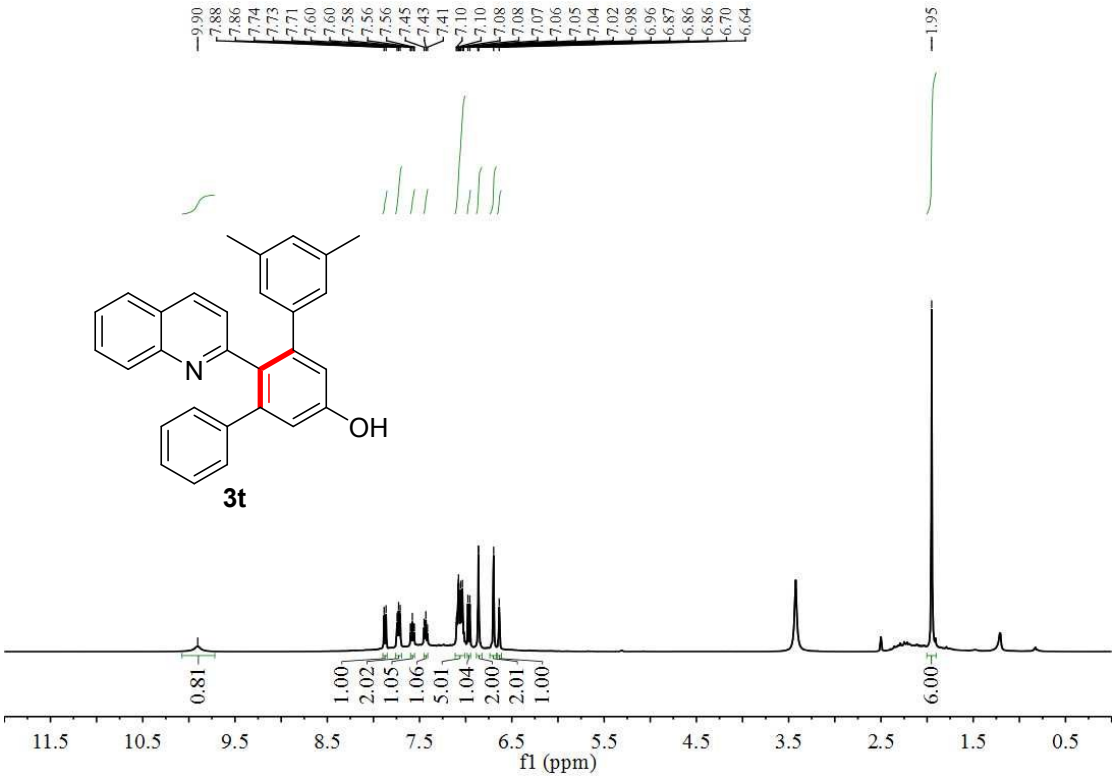
128.043
126.087
125.478
116.772
116.408
40.626
40.417
40.208
40.000
39.791
39.582
39.373
Cl
N
OH
3s
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.43
7.41
7.10
7.10
7.08
7.08
7.07
7.06
7.05
7.04
7.02
6.98
6.96
6.87
6.86
6.86
6.70
6.64
1.95
N
OH
3t
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2.02
1.05
1.06
5.01
1.04
2.00
2.01
1.00
6.00
11.5
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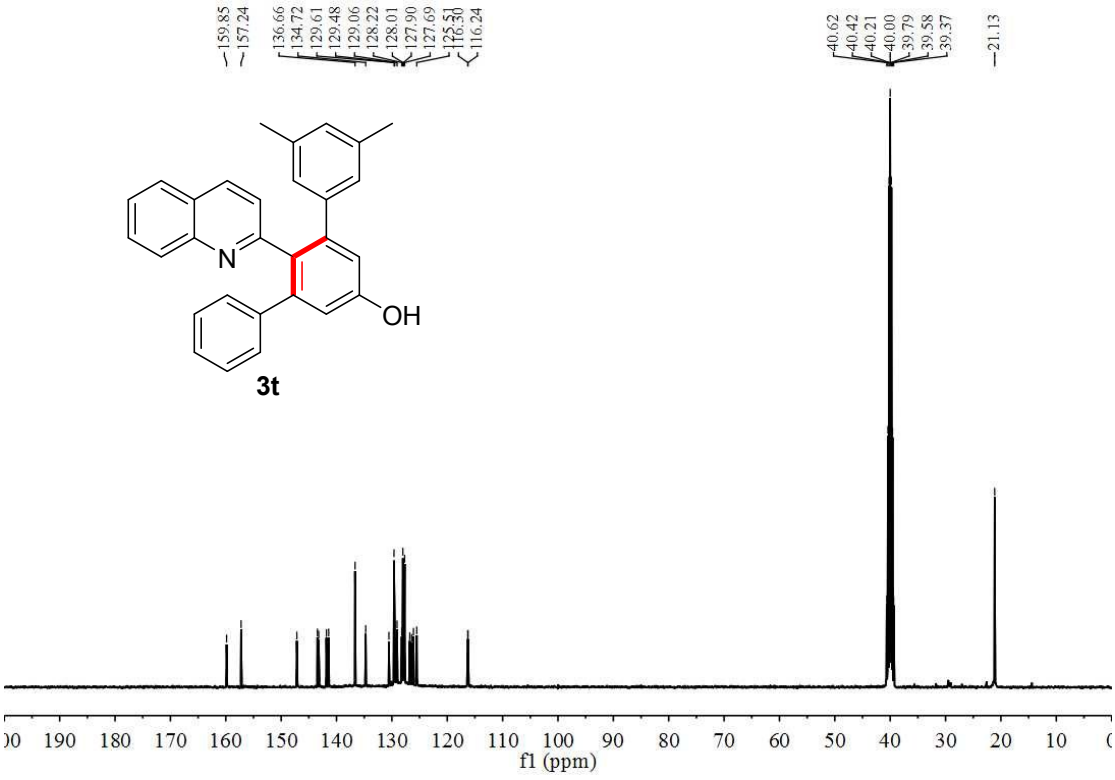
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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128.22
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127.90
127.69
125.51
116.30
116.24
40.62
40.42
40.21
40.00
39.79
39.58
39.37
21.13
N
OH
3t
190
180
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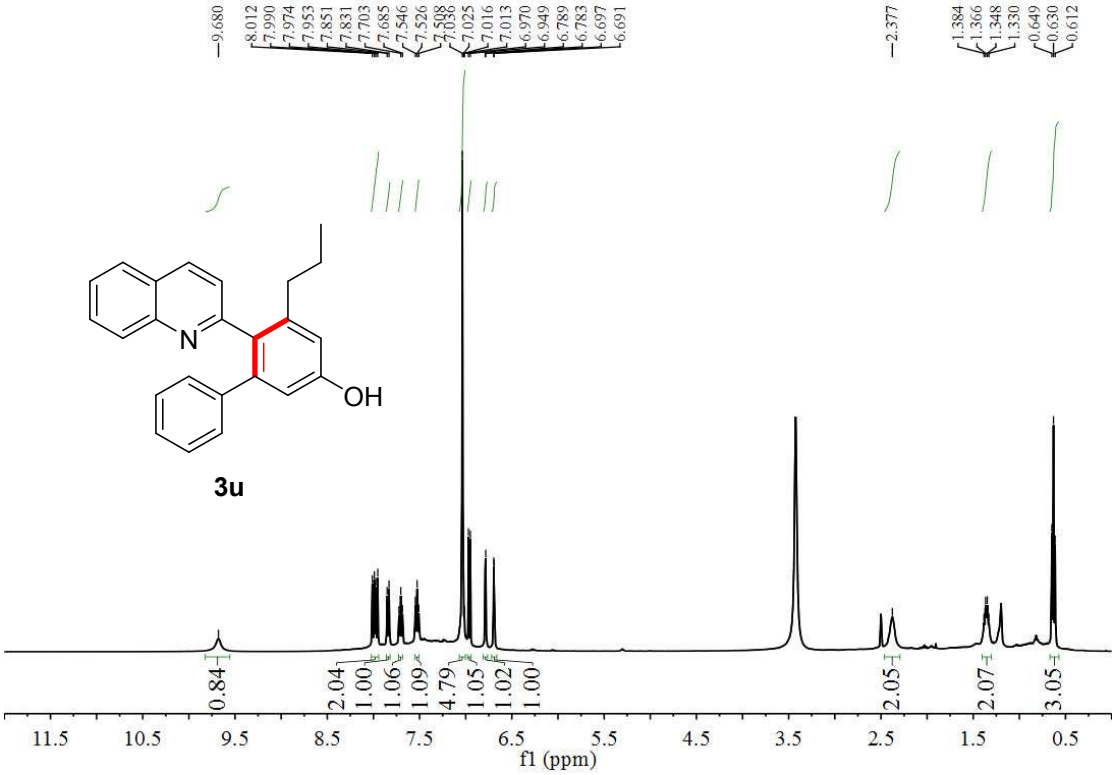
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.546
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7.038
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7.016
7.013
6.970
6.949
6.789
6.783
6.697
6.691
2.377
1.384
1.366
1.348
1.330
0.649
0.630
0.612
N
OH
3u
0.84
2.04
1.00
1.06
1.09
4.79
1.05
1.02
1.00
2.05
2.07
3.05
11.5
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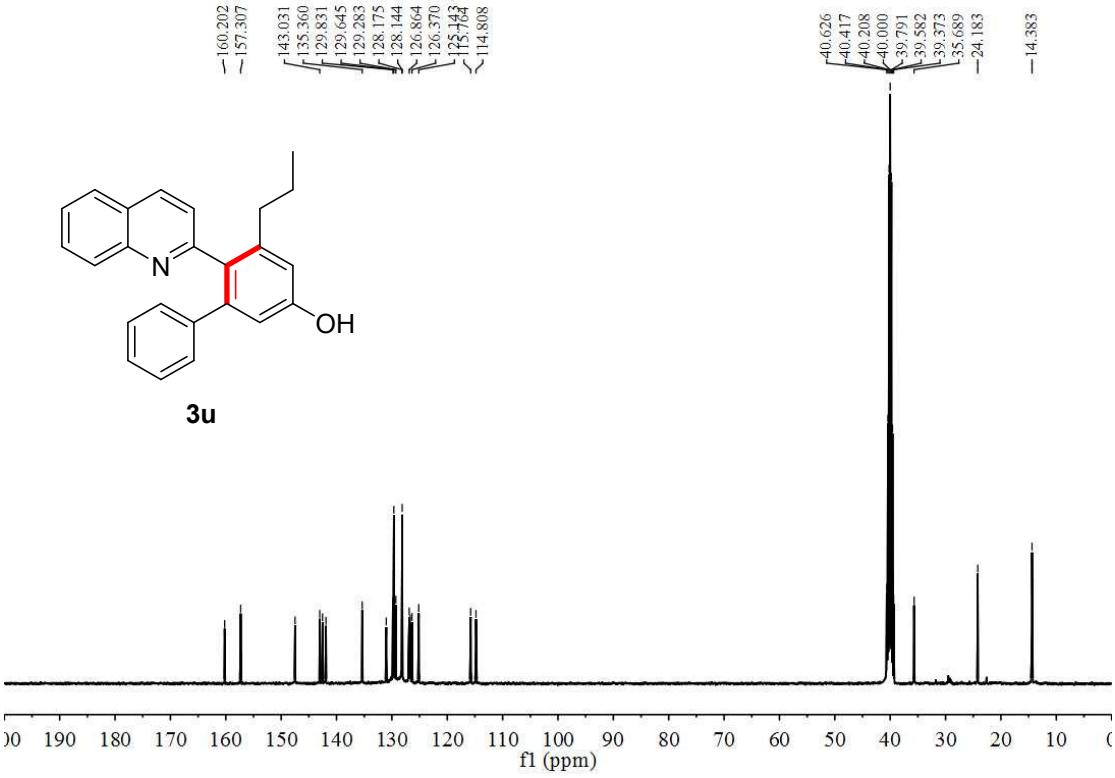
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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125.064
114.808
40.626
40.417
40.208
40.000
39.791
39.582
39.373
35.689
24.183
14.383
N
OH
3u
190
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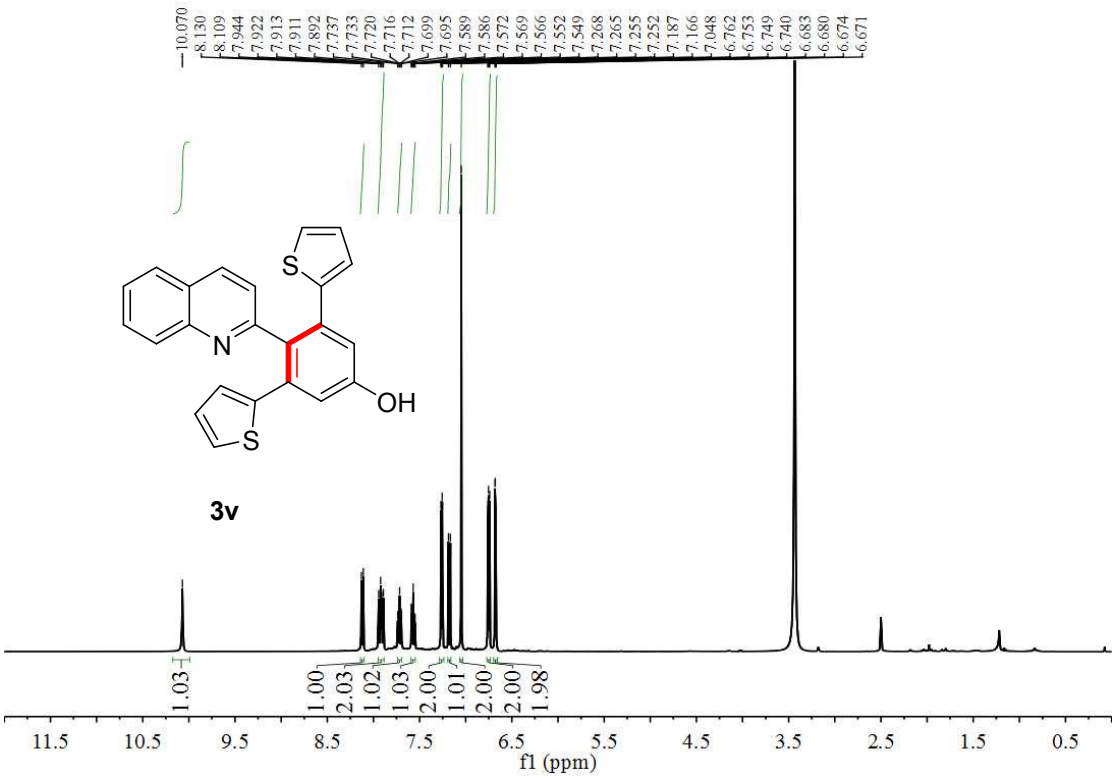
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.712
7.699
7.695
7.589
7.586
7.572
7.569
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7.265
7.255
7.252
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6.753
6.749
6.740
6.683
6.680
6.674
6.671
S
N
OH
S
3v
1.03
1.00
2.03
1.02
1.03
2.00
1.01
2.00
2.00
1.98
11.5
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6.5
5.5
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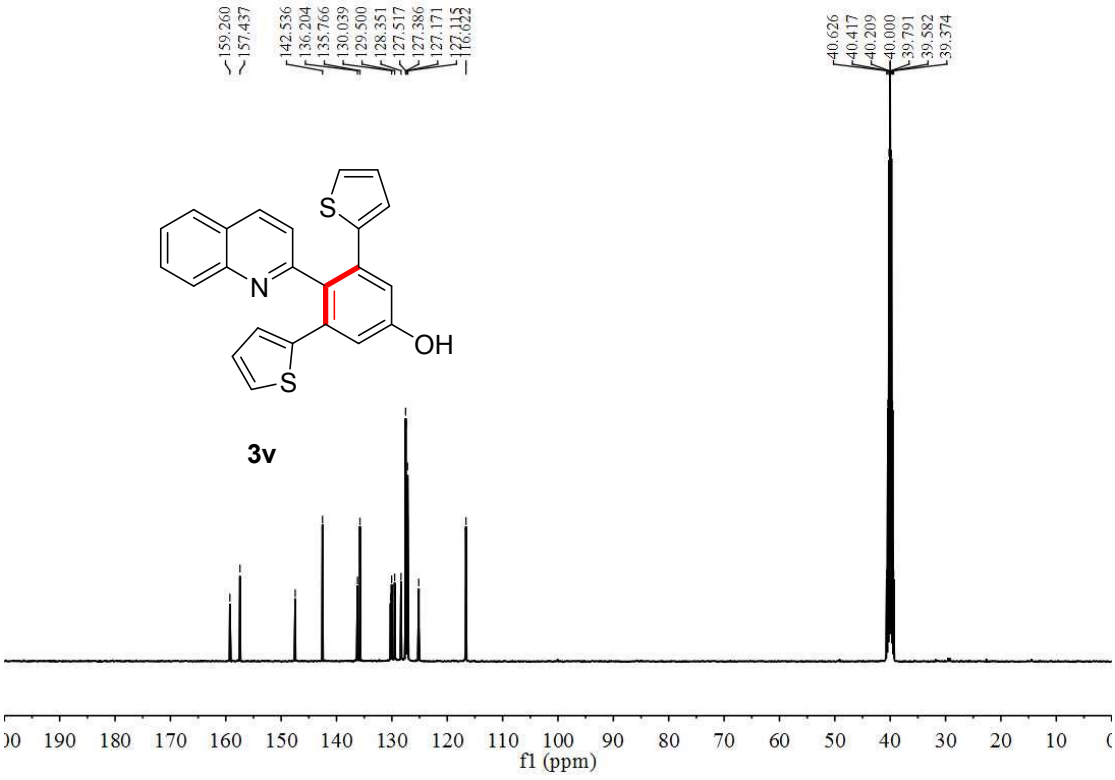
2.5
1.5
0.5
f1 (ppm)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128.351
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127.386
127.171
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40.417
40.209
40.000
39.791
39.582
39.374
S
N
OH
S
3v
190
180
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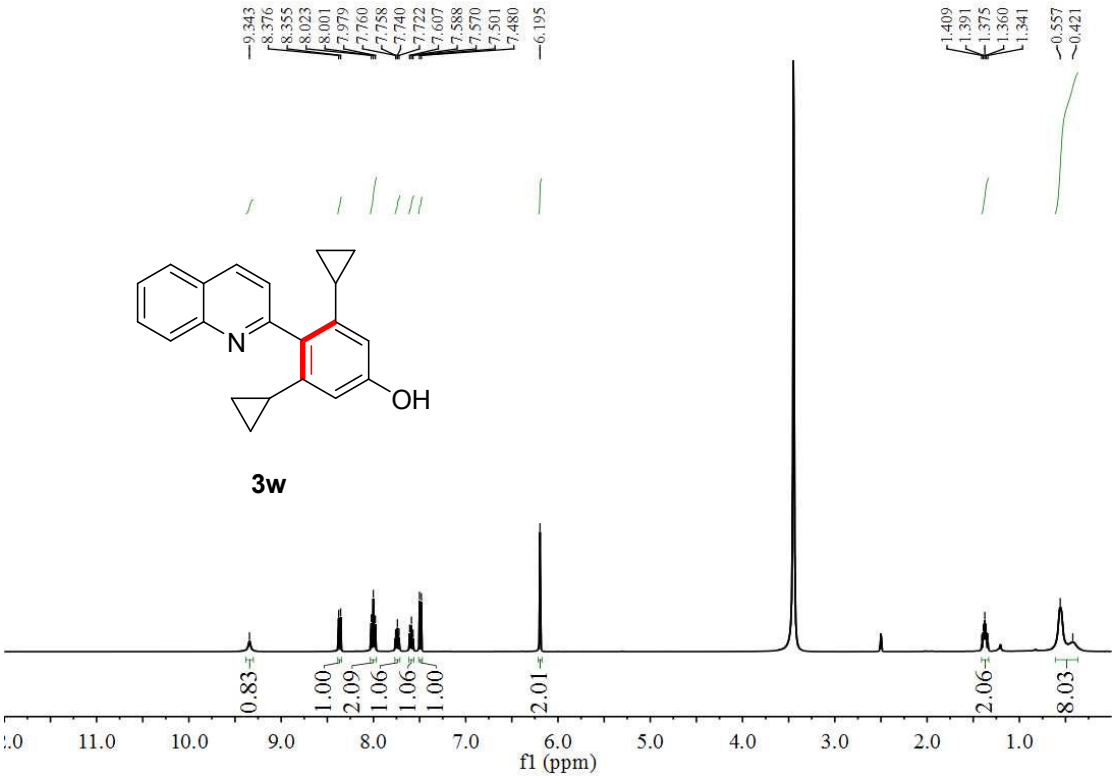
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.722
7.607
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7.570
7.501
7.480
6.195
1.409
1.391
1.375
1.360
1.341
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0.421
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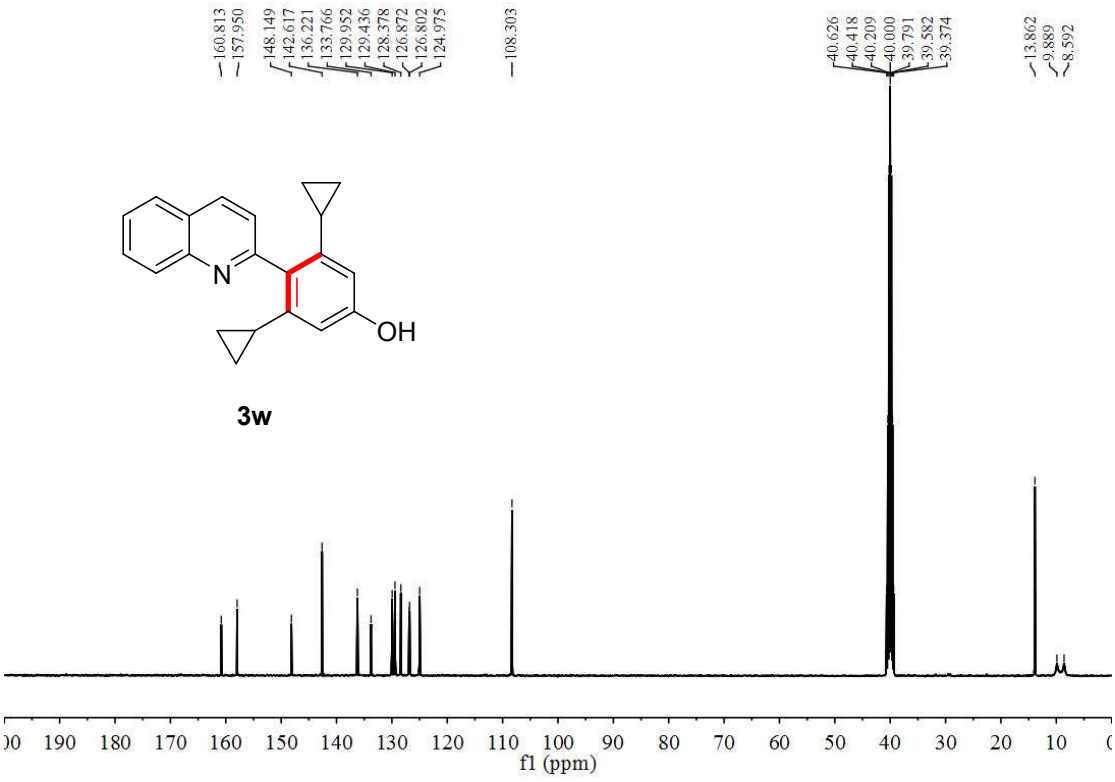
1.06
1.06
1.00
2.01
2.06
8.03
f1 (ppm)

3w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129.952
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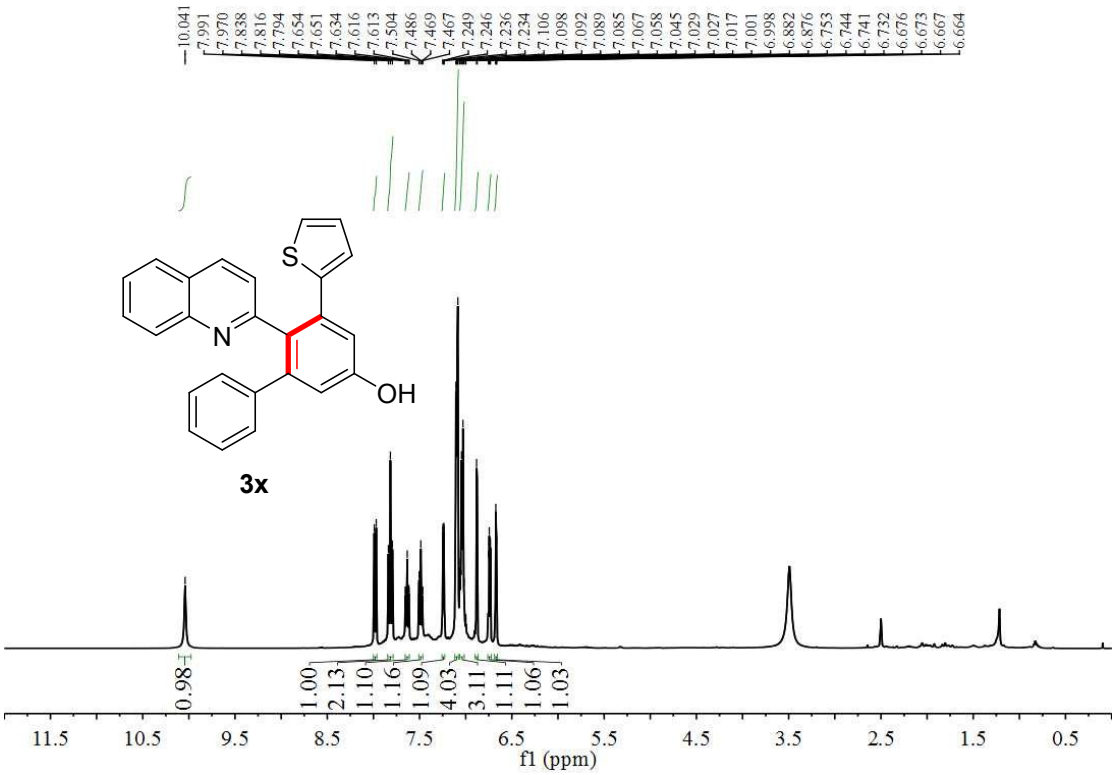
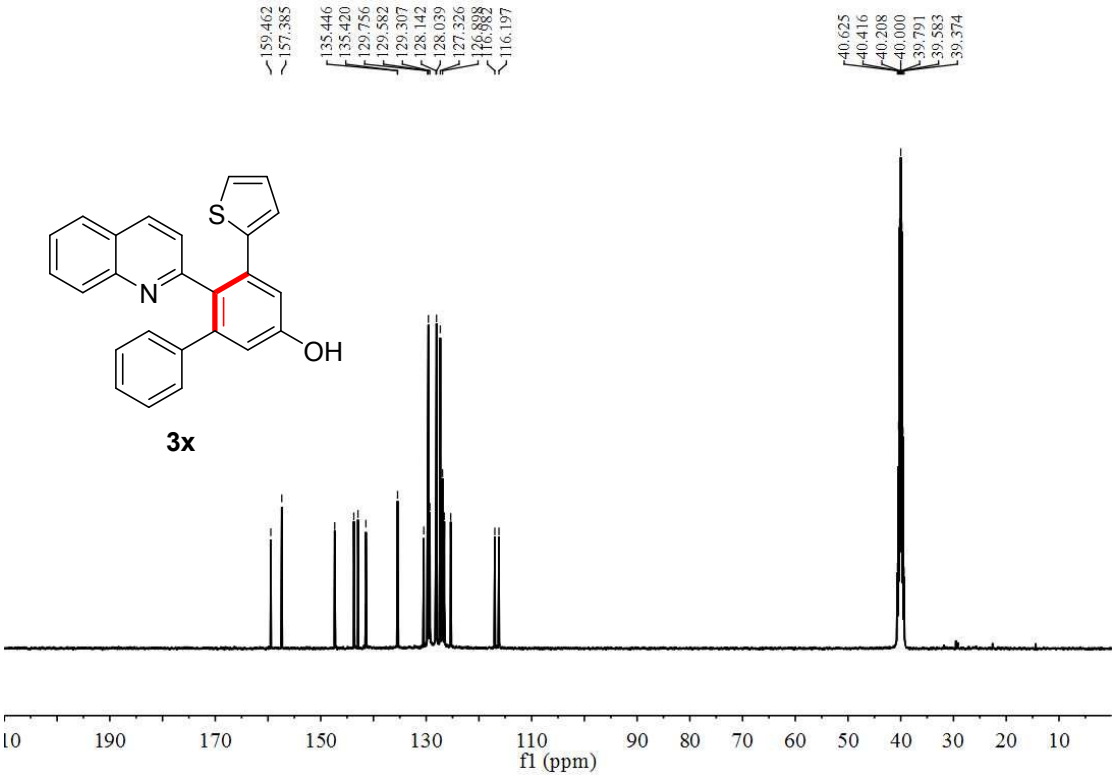
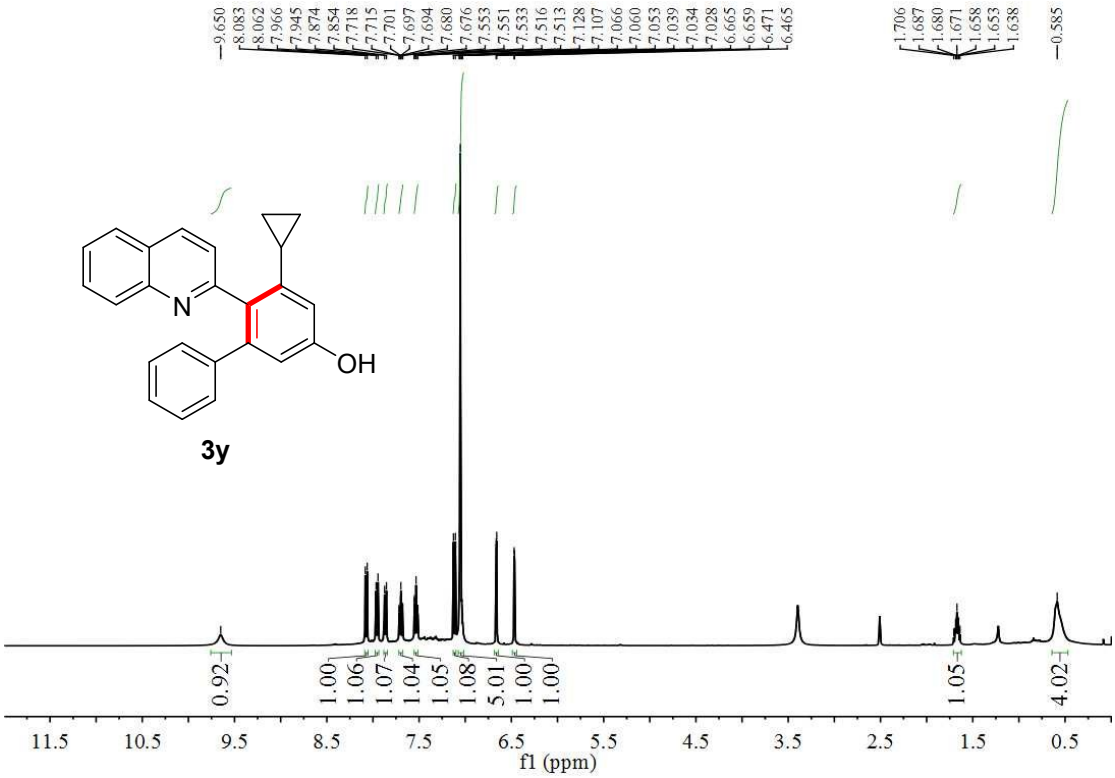
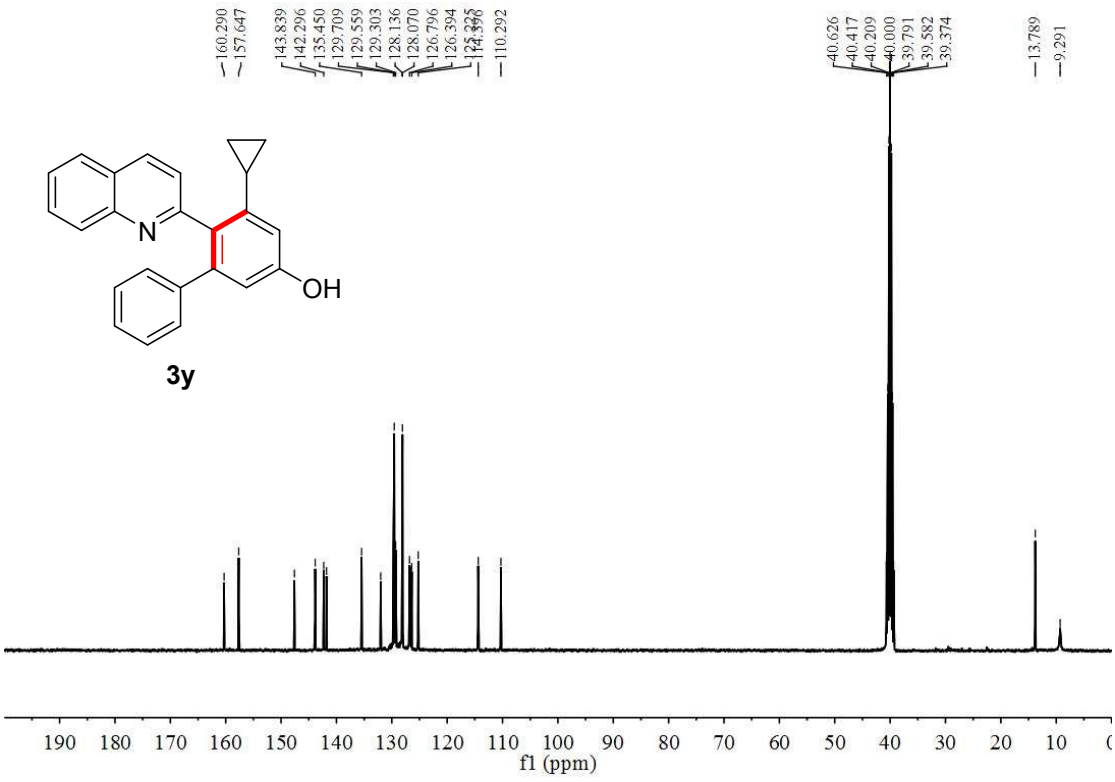
124.975
108.303
40.626
40.418
40.209
40.000
39.791
39.582
39.374
13.862
9.889
8.592
N
OH
f1 (ppm)

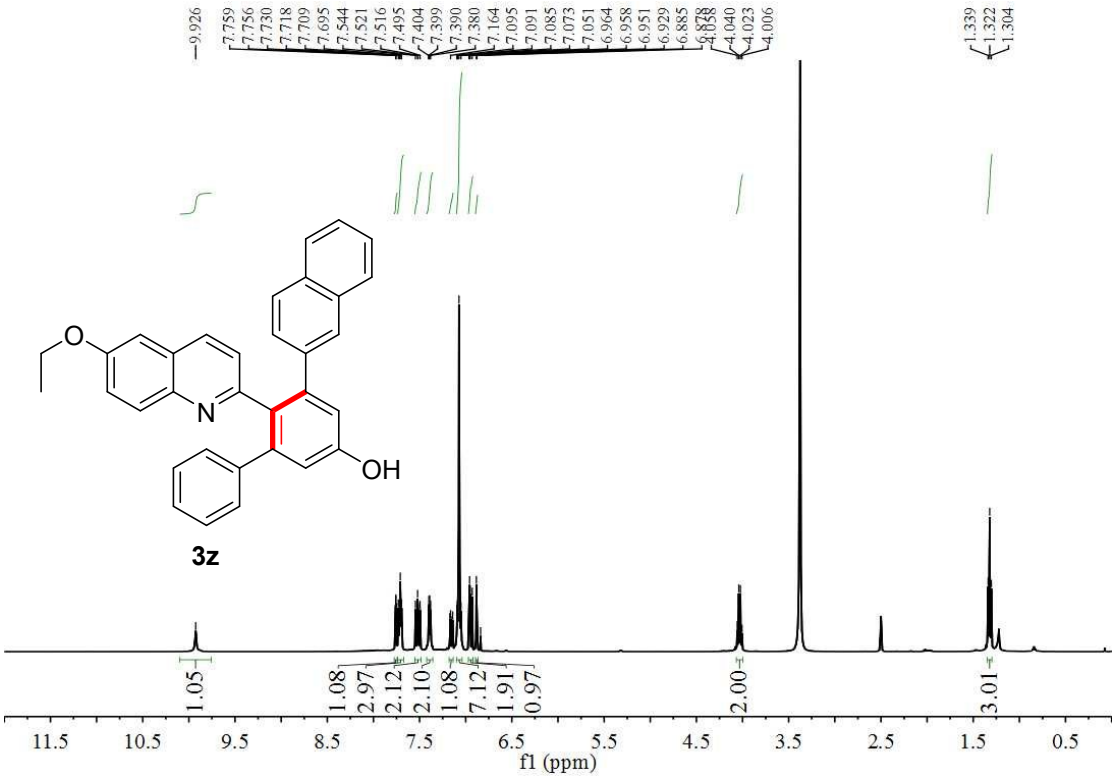
3w

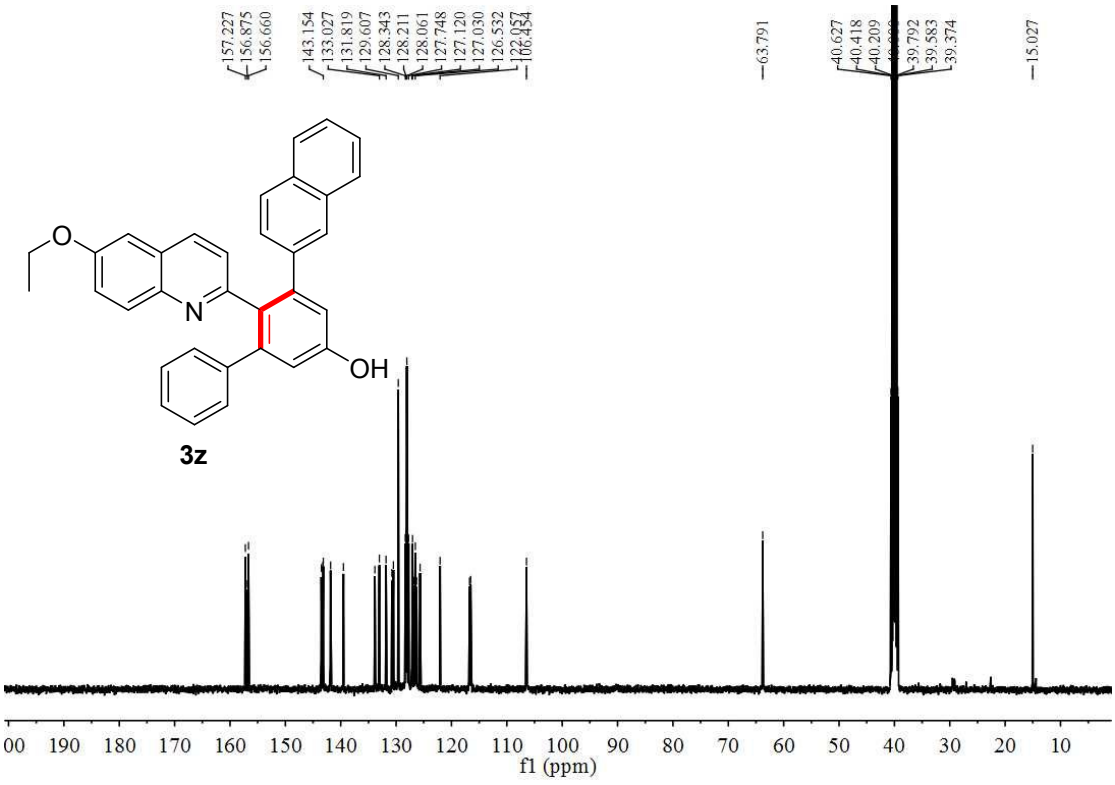

10.041
7.991
7.970
7.838
7.816
7.794
7.654
7.651
7.634
7.616
7.613
7.504
7.486
7.469
7.467
7.249
7.246
7.236
7.234
7.106
7.098
7.092
7.089
7.085
7.067
7.058
7.045
7.029
7.027
7.017
7.001
6.998
6.882
6.876
6.753
6.744
6.741
6.732
6.676
6.673
6.667
6.664
S
N
OH
3x
0.98
1.00
2.13
1.10
1.16
1.09
4.03
3.11
1.11
1.06
1.03
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


159.462
157.385
135.446
135.420
129.756
129.582
129.307
128.142
128.039
127.326
126.808
116.197
40.625
40.416
40.208
40.000
39.791
39.583
39.374
S
N
OH
3x
10
190
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)


9.650
8.083
8.062
7.966
7.945
7.874
7.854
7.718
7.715
7.701
7.697
7.694
7.680
7.676
7.553
7.551
7.533
7.516
7.513
7.128
7.107
7.066
7.060
7.053
7.039
7.034
7.028
6.665
6.659
6.471
6.465
1.706
1.687
1.680
1.671
1.658
1.653
1.638
0.585
N
OH
3y
0.92
1.00
1.06
1.07
1.04
1.05
1.08
5.01
1.00
1.00
1.05
4.02
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


160.290
157.647
143.839
142.296
135.450
129.709
129.559
129.303
128.136
128.070
126.796
126.394
110.292
40.626
40.417
40.209
40.000
39.791
39.582
39.374
13.789
9.291
N
OH
3y
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


9.926
7.759
7.756
7.730
7.718
7.709
7.695
7.544
7.521
7.516
7.495
7.404
7.399
7.390
7.380
7.164
7.095
7.091
7.085
7.073
7.051
6.964
6.958
6.951
6.929
6.885
4.040
4.023
4.006
1.339
1.322
1.304
O
N
OH
3z
1.05
1.08
2.97
2.12
2.10
1.08
7.12
1.91
0.97
2.00
3.01
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


157.227
156.875
156.660
143.154
133.027
131.819
129.607
128.343
128.211
128.061
127.748
127.120
127.030
126.532
63.791
40.627
40.418
40.209
39.792
39.583
39.374
15.027
O
N
OH
3z
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)