Electronic Supplementary Material (ESI) for Dalton Transactions.

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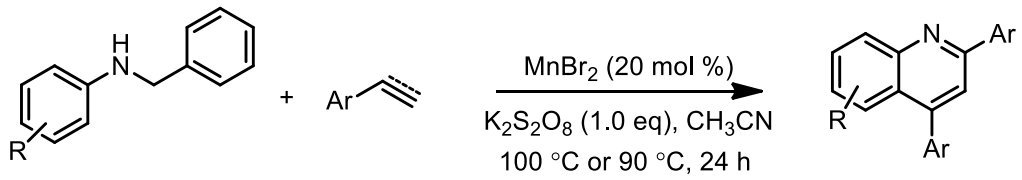
1. General Information

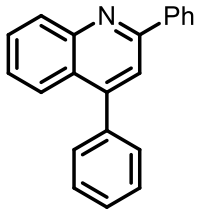
All reactions were conducted in pressure tubes under air. All solvents were received from commercial sources without further purification. Commercially available reagents were used as received. Non-commercially available substrates were synthesized following reported protocols. Thin-layer chromatography (TLC) was visualized using a combination of UV and potassium permanganate staining techniques. Silica gel (particle size 40 – 63 μm) was used for flash column chromatography. NMR spectra were recorded on Bruker AV 400 spectrometer at 400 MHz (^{1}H NMR), 100 MHz (^{13}C NMR). Proton and carbon chemical shifts are reported relative to the solvent used as an internal reference. High resolution mass spectra (HRMS) were recorded on Varian 7.0T FTICR LC/MS with Electron Spray Ionization (ESI) resource.

2. Typical Procedure for Synthesis of 2,4-Diarylquinoline

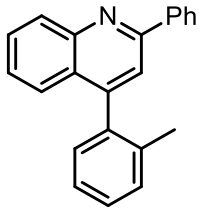


1 **2** **3**

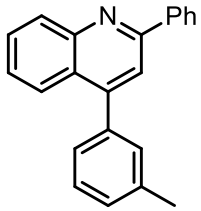
To a 15 mL pressure tube were added N-alkyl anilines **1** (0.2 mmol), $MnBr_2$ (8.6 mg, 40.0 μmol), $K_2S_2O_8$ (54 mg, 0.2 mmol), under air, and then alkenes or alkynes (0.4 mmol) and CH_3CN (1 mL) were added. The resulting dark green solution was stirred at 100 ^{o}C or 90 ^{o}C for 24 h. After the reaction was completed, the solution was cooled to room temperature, and diluted with dichloromethane and water (2 mL). The organic phase was separated and the aqueous phase was extracted with dichloromethane. The combined organic phases were washed with brine, dried over anhydrous Na_2SO_4, filtered and concentrated in *vacuo*. The crude product was purified by column chromatography (*n*-Hex/EtOAc = 100:1 to 20:1) to afford the desired product.



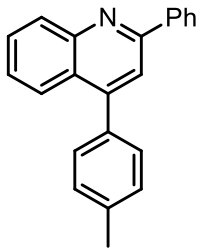
3a: 2,4-diphenylquinoline.[1] White solid (45 mg, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.4 Hz, 1H), 8.21 – 8.18 (m, 2H), 7.92 – 7.90 (m, 1H), 7.82 (s, 1H), 7.75 – 7.71 (m, 1H), 7.56 – 7.44 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 149.2, 148.9, 139.7, 138.5, 130.2, 129.7, 129.6, 129.4, 128.9, 128.7, 128.5, 127.7, 126.4, 125.8, 125.7, 119.4.



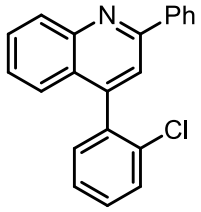
3b: 2-phenyl-4-(*o*-tolyl) quinoline.[1] White solid (39 mg, 65%yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J = 8.4 Hz, 1H), 8.20 – 8.18 (m, 2H), 7.76 (s, 1H), 7.73 – 7.69 (m, 1H), 7.54 – 7.27 (m, 9H), 2.08 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 149.3, 148.6, 139.7, 138.0, 136.3, 130.3, 130.2, 129.7, 129.7, 129.5, 128.9, 128.5, 127.7, 126.4, 126.4, 125.9, 125.9, 119.5, 20.1.



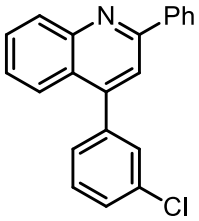
3c: 2-phenyl-4-(*m*-tolyl) quinoline.[2] White solid (41 mg, 69% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, J = 8.0 Hz, 1H), 8.21 – 8.19 (m, 2H), 7.94 (d, J = 8.0 Hz, 1H), 7.82 (s, 1H), 7.76 – 7.72 (m, 1H), 7.56 – 7.45 (m, 5H), 7.38 – 7.36 (m, 3H), 2.49 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 149.4, 148.9, 139.8, 138.5, 138.4, 130.3, 130.2, 129.6, 129.4, 129.2, 128.9, 128.5, 127.7, 126.8, 126.3, 125.9, 125.8, 119.4, 21.6.



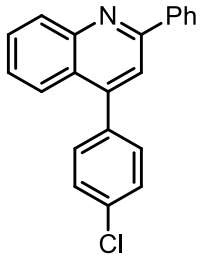
3d: 2-phenyl-4-(*p*-tolyl) quinoline.[1] White solid (45 mg, 72% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.4 Hz, 1H), 8.22 – 8.19 (m, 2H), 7.94 – 7.92 (m, 1H), 7.82 (s, 1H), 7.76 – 7.72 (m, 1H), 7.56 – 7.32 (m, 8H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.1, 149.4, 149.0, 139.9, 138.5, 135.6, 130.2, 129.6, 129.6, 129.4, 129.0, 127.7, 126.4, 126.0, 125.9, 119.5, 112.9, 21.5.



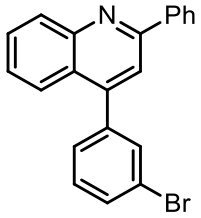
3e: 4-(2-chlorophenyl)-2-phenylquinoline.[1] White solid (52 mg, 83% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.4 Hz, 1H), 8.21 – 8.19 (m, 2H), 7.81 (s, 1H), 7.76 – 7.72 (m, 1H), 7.61 – 7.58 (m, 1H), 7.55 – 7.39 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 148.6, 146.6, 139.6, 137.1, 133.5, 131.5, 130.2, 130.0, 139.9, 129.8, 129.5, 128.9, 127.7, 126.9, 126.6, 125.9, 125.7, 119.9.



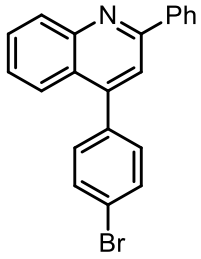
3f: 4-(3-chlorophenyl)-2-phenylquinoline.[3] White solid (54 mg, 86% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.4 Hz, 1H), 8.21 – 8.19 (m, 2H), 7.86 (d, J = 8.4 Hz, 1H), 7.80 (s, 1H), 7.78 – 7.74 (m, 1H), 7.57 – 7.44 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 148.9, 147.7, 140.2, 139.5, 134.7, 130.3, 130.0, 129.8, 129.6, 129.6, 129.0, 128.6, 127.9, 127.7, 126.7, 125.5, 125.3, 119.4.



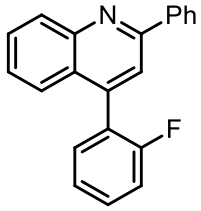
3g: 4-(4-chlorophenyl)-2-phenylquinoline.[2] White solid (56 mg, 89% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.4 Hz, 1H), 8.20 – 8.18 (m, 2H), 7.86 – 7.84 (m, 1H), 7.79 (s, 1H), 7.77 – 7.73 (m, 1H), 7.55 – 7.48 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 149.0, 148.0, 139.6, 136.9, 134.7, 131.0, 130.3, 129.8, 129.5, 129.0, 127.7, 126.6, 125.6, 125.4, 119.4.



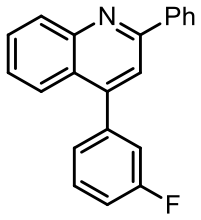
3h: 4-(3-bromophenyl)-2-phenylquinoline.[3] White solid (53 mg, 73% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.4 Hz, 1H), 8.20 – 8.18 (m, 2H), 7.85 (d, J = 8.4 Hz, 1H), 7.79 (s, 1H), 7.77 – 7.73 (m, 1H), 7.71 – 7.68 (m, 2H), 7.56 – 7.43 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 148.9, 148.0, 139.6, 137.4, 131.9, 131.3, 130.3, 129.8, 129.5, 129.0, 127.7, 126.7, 125.5, 125.3, 122.9, 119.3.



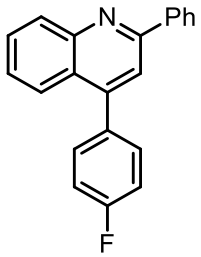
3i: 4-(4-bromophenyl)-2-phenylquinoline.[1] White solid (56 mg, 78% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.4 Hz, 1H), 8.20 – 8.18 (m, 2H), 7.85 (d, J = 8.0 Hz, 1H), 7.79 (s, 1H), 7.78 – 7.73 (m, 1H), 7.71 – 7.69 (m, 2H), 7.56 – 7.44 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 148.8, 147.9, 139.5, 137.4, 131.9, 131.2, 130.3, 129.7, 129.5, 128.9, 127.6, 126.6, 125.5, 125.3, 122.8, 119.2.



3j: 4-(2-fluorophenyl)-2-phenylquinoline.[3] White solid (43 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.4 Hz, 1H), 8.20 – 8.18 (m, 2H), 7.85 (s, 1H), 7.77 – 7.68 (m, 2H), 7.55 – 7.45 (m, 6H), 7.36 – 7.28 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8 (d, $J_{C\text{-}F}$ = 246.7 Hz), 157.0, 148.6, 143.4, 139.6, 131.8 (d, $J_{C\text{-}F}$ = 3.2 Hz), 130.6 (d, $J_{C\text{-}F}$ = 7.9 Hz), 130.2, 129.8, 129.5, 129.0, 127.7, 126.6, 125.9, 125.8, 125.6, 124.5 (d, $J_{C\text{-}F}$ = 3.6 Hz), 120.3, 116.1 (d, $J_{C\text{-}F}$ = 21.7 Hz).

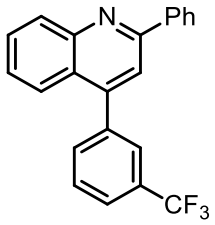


3k: 4-(3-fluorophenyl)-2-phenylquinoline.[3] White solid (45 mg, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.4 Hz, 1H), 8.20 – 8.18 (m, 2H), 7.87 (d, J = 8.4 Hz, 1H), 7.81 (s, 1H), 7.77 – 7.73 (m, 1H), 7.55 – 7.46 (m, 5H), 7.36 – 7.34 (m, 1H), 7.30 – 7.27 (m, 1H), 7.24 – 7.19 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, $J_{C\text{-}F}$ = 245.8 Hz), 157.0, 148.9, 147.8, 140.6, 139.6, 130.4, 130.3 (d, $J_{C\text{-}F}$ = 8.3 Hz), 130.3, 129.8, 129.6, 129.0, 127.7, 126.7, 125.4 (d, $J_{C\text{-}F}$ = 3.1 Hz), 125.4, 119.3, 116.7 (d, $J_{C\text{-}F}$ = 22.0 Hz), 115.5 (d, $J_{C\text{-}F}$ = 22.0 Hz).

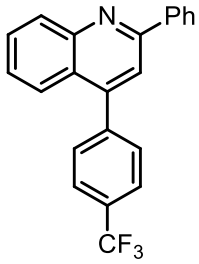


3l: 4-(4-fluorophenyl)-2-phenylquinoline.[1] White solid (48 mg, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.4 Hz, 1H), 8.20 – 8.18 (m, 2H), 7.87 – 7.85 (m, 1H), 7.79 (s, 1H), 7.76-7.72 (m, 1H), 7.56 – 7.45 (m, 6H), 7.27 – 7.23 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0 (d, $J_{C\text{-}F}$ = 245.8 Hz), 156.9, 148.8, 148.1, 139.6,

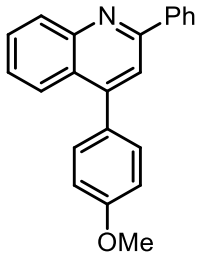
134.4 (d, $J_{C\text{-}F}$ = 3.4 Hz), 131.3 (d, $J_{C\text{-}F}$ = 8.1 Hz), 130.2, 129.7, 129.5, 128.9, 127.6, 126.5, 125.7, 125.4, 119.4, 115.7 (d, $J_{C\text{-}F}$ = 21.5 Hz).



3m: 2-phenyl-4-(3-(trifluoromethyl)phenyl)quinoline. White solid (52 mg, 74% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, J = 8.4 Hz, 1H), 8.21 – 8.18 (m, 2H), 7.84 – 7.74 (m, 5H), 7.70 – 7.68 (m, 2H), 7.56 – 7.46 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 148.8, 147.7, 142.1, 139.4, 130.3, 130.0, 129.8, 129.6, 128.9, 127.6, 126.8, 125.6 (q, $J_{C\text{-}F}$ = 3.7 Hz) , 125.3, 125.1, 119.3; HRMS (ESI-TOF) m/z Calcd for C22H15F3N $[M+H]^+$ 350.1157, Found 350.1165.

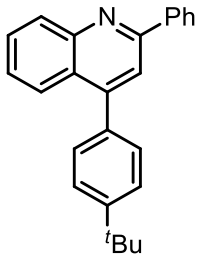


3n: 2-phenyl-4-(4-(trifluoromethyl)phenyl)quinoline.[4] White solid (53 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, J = 8.4 Hz, 1H), 8.21 – 8.19 (m, 2H), 7.83 – 7.75 (m, 6H), 7.71-7.67 (m, 1H), 7.56-7.46 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 148.8, 147.5, 139.4, 139.2, 132.8, 130.3, 129.9, 129.8, 129.5, 129.2, 128.9, 127.6, 126.8, 126.3 (q, $J_{C\text{-}F}$ = 3.9 Hz), 125.4, 125.0, 119.4.

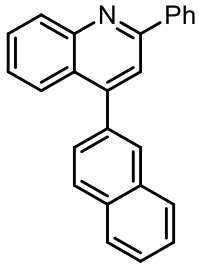


3o: 4-(4-methoxyphenyl)-2-phenylquinoline.[5] White solid (29 mg, 46% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J = 8.4 Hz, 1H), 8.20 – 8.18 (m, 2H), 7.95 (d, J = 8.4 Hz, 1H), 7.80 (s, 1H), 7.75-7.70 (m, 1H), 7.55 – 7.44 (m, 6H), 7.09 – 7.07 (m, 2H),

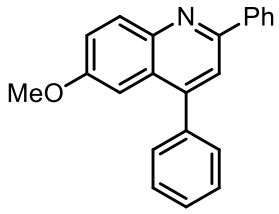
3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 157.0, 148.9, 139.8, 130.8, 130.7, 130.2, 129.6, 129.5, 129.3, 128.8, 127.6, 126.2, 126.0, 125.7, .119.4, 114.1, 55.5.



3p: 4-(4-(tert-butyl)phenyl)-2-phenylquinoline.[4] White solid (47 mg, 70% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, J = 8.4 Hz, 1H), 8.20 – 8.18 (m, 2H), 7.97 (d, J = 8.4 Hz, 1H), 7.83 (s, 1H), 7.75-7.71 (m, 1H), 7.59 – 7.44 (m, 8H), 1.43 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 151.6, 149.2, 148.9, 139.8, 135.5, 130.1, 129.5, 129.3, 129.3, 128.8, 127.6, 126.2, 125.9, 125.8, 125.6, 119.4, 31.4.

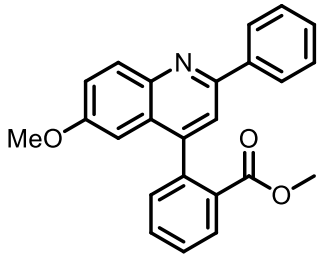


3q: 4-(naphthalen-2-yl)-2-phenylquinoline.[3] White solid (46 mg, 69% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, J = 8.0 Hz, 1H), 8.24 – 8.21 (m, 2H), 8.05 (s, 1H), 8.04 – 8.02 (m, 1H), 7.99 – 7.93 (m, 4H), 7.78 – 7.74 (m, 1H), 7.71 – 7.68 (m, 1H), 7.61 – 7.46 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 149.3, 148.9, 139.7, 136.0, 133.4, 133.1, 130.3, 129.7, 129.5, 129.0, 128.8, 128.3, 128.2, 127.9, 127.7, 127.5, 126.8, 126.8, 126.5, 126.0, 125.8, 119.8.

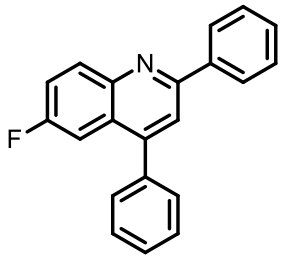


3r: 6-methoxy-2,4-diphenylquinoline.[1] White solid (51 mg, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 – 8.14 (m, 3H), 7.77 (s, 1H), 7.60 – 7.49 (m, 7H), 7.46 – 7.38 (m, 2H), 7.20 (d, J = 2.8 Hz, 1H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ

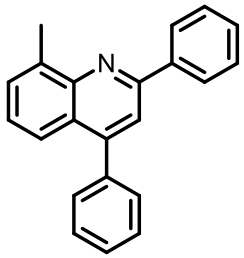
157.9, 154.7, 147.9, 144.9, 139.8, 138.8, 131.7, 129.5, 129.1, 128.9, 128.8, 128.4, 127.4, 126.8, 121.9, 119.8, 103.8, 55.6.



3s: methyl 2-(6-methoxy-2-phenylquinolin-4-yl)benzoate.[3] White solid (30 mg, 41% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 – 8.14 (m, 2H), 8.11 – 8.08 (m, 1H), 7.68 – 7.63 (m, 1H), 7.60 (s, 1H), 7.58 – 7.40 (m, 6H), 7.37 – 7.35 (m, 1H), 7.08 – 7.05 (m, 1H), 3.98 (s, 3H), 3.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 160.7, 157.1, 150.1, 149.1, 139.9, 139.3, 132.1, 131.2, 131.0, 130.6, 129.3, 128.9, 128.5, 127.6, 126.3, 121.5, 119.5, 116.8, 108.0, 55.6, 52.2.

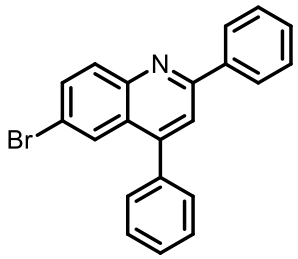


3t: 6-fluoro-2,4-diphenylquinoline.[1] White solid (45 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 – 8.22 (m, 1H), 8.19 – 8.17 (m, 2H), 7.84 (s, 1H), 7.59 – 7.45 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.8, 159.3, 156.3, 148.7 (d, $J_{C\text{-}F}$ = 5.5 Hz), 146.0, 139.4, 138.0, 132.5 (d, $J_{C\text{-}F}$ = 9.0 Hz), 129.4, 129.1 (d, $J_{C\text{-}F}$ = 76.4 Hz), 128.9, 128.8, 127.5, 126.5 (d, $J_{C\text{-}F}$ = 9.5 Hz), 119.9, 119.7 (d, $J_{C\text{-}F}$ = 20.7 Hz), 119.1 (d, $J_{C\text{-}F}$ = 23.0 Hz).

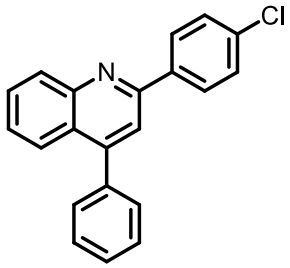


3u: 8-methyl-2,4-diphenylquinoline.[6] White solid (47 mg, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 – 8.28 (m, 2H), 7.85 (s, 1H), 7.73 (d, J = 8.4 Hz, 1H), 7.60 –

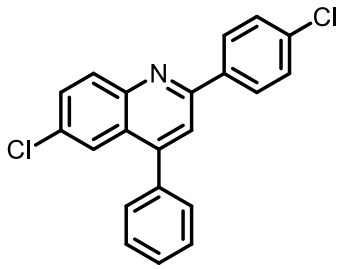
7.44 (m, 9H), 7.38 – 7.34 (m, 1H), 2.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 149.3, 147.7, 139.8, 139.0, 138.0, 129.6, 129.6, 129.3, 128.8, 128.5, 128.3, 127.5, 126.0, 123.6, 118.7, 18.5.



3v: 6-bromo-2,4-diphenylquinoline.[6] White solid (54 mg, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 – 8.17 (m, 2H), 8.10 (d, J = 8.8 Hz, 1H), 8.04 – 8.03 (m, 1H), 7.84 (s, 1H), 7.80 (dd, J = 8.8, 2.0 Hz, 1H), 7.58 – 7.46 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 148.4, 147.5, 139.2, 137.6, 133.0, 131.9, 129.7, 129.5, 128.9, 128.9, 128.8, 127.8, 127.6, 127.0, 120.5, 120.1.



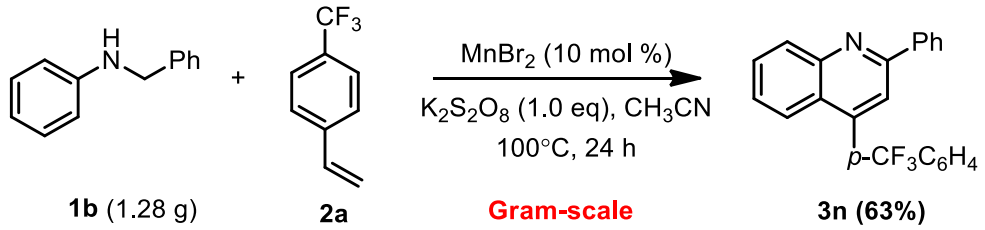
3w: 2-(4-chlorophenyl)-4-phenylquinoline.[4] White solid (49 mg, 77% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, J = 8.4 Hz, 1H), 8.15 – 8.13 (m, 2H), 7.89 (d, J = 8.4 Hz, 1H), 7.77 (s, 1H), 7.75 – 7.71 (m, 1H), 7.56 – 7.45 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.5, 149.4, 148.8, 138.3, 138.0, 135.6, 130.1, 129.7, 129.6, 129.0, 128.9, 128.7, 128.5, 126.6, 125.8, 125.7, 118.9.



3x: 6-chloro-2-(4-chlorophenyl)-4-phenylquinoline.[7] White solid (48 mg, 69% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 – 8.13 (m, 3H), 7..86 (d, J = 2.0 Hz, 1H), 7.80 (s, 1H), 7.67 (dd, J = 8.8, 2.0 Hz, 1H), 7.60 – 7.48 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$)

δ 155.7, 148.7, 147.2, 137.6, 135.9, 132.5, 131.7, 130.7, 129.4, 129.1, 128.9, 128.8, 128.8, 126.6, 124.5, 119.6.

3. Gram-scale Synthesis



According to the typical procedure: To a 250 mL pressure tube were added *N*-benzyl-4-methoxyaniline (1.28 g, 6 mmol), $MnBr_2$ (257.7 mg, 1.2 mmol), and $K_2S_2O_8$ (1.62 g, 6 mmol) under air. Then 1-(trifluoromethyl)-4-vinylbenzene (2.07 g, 12 mmol) and CH_3CN (50 mL) were added under air and this resulting dark green solution was stirred at 100 ^oC for 24 h. After column purification (*n*-Hex/EtOAc = 100:1 to 20:1), coupling product was obtained (1.32 g, 63% yield).

4. Zebrafish Experiments

At 6 hpf, embryos were screened under anatomical microscope to remove the morphologically abnormal individuals. Around 10 healthy embryos were loaded into each well of 96-well plate in E3 solution. At the setting time, E3 solutions were replaced with different **3n** treatment solutions. The control and treated groups were analyzed at different intervals. At 55 hpf, the *Tg(fli1a:nEGFP)* zebrafish embryos were collected for imaging. At 55 hpf, for confocal imaging embryos were anesthetized with E3/0.16 mg/mL tricaine/1% 1-phenyl-2-thiourea (Sigma) and embedded in 0.8% low melt agarose. Confocal imaging was performed with a Leica TCS-SP8 LSM. Analysis was performed using Imaris software.

References

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Adv. **2018**, *8*, 31603.

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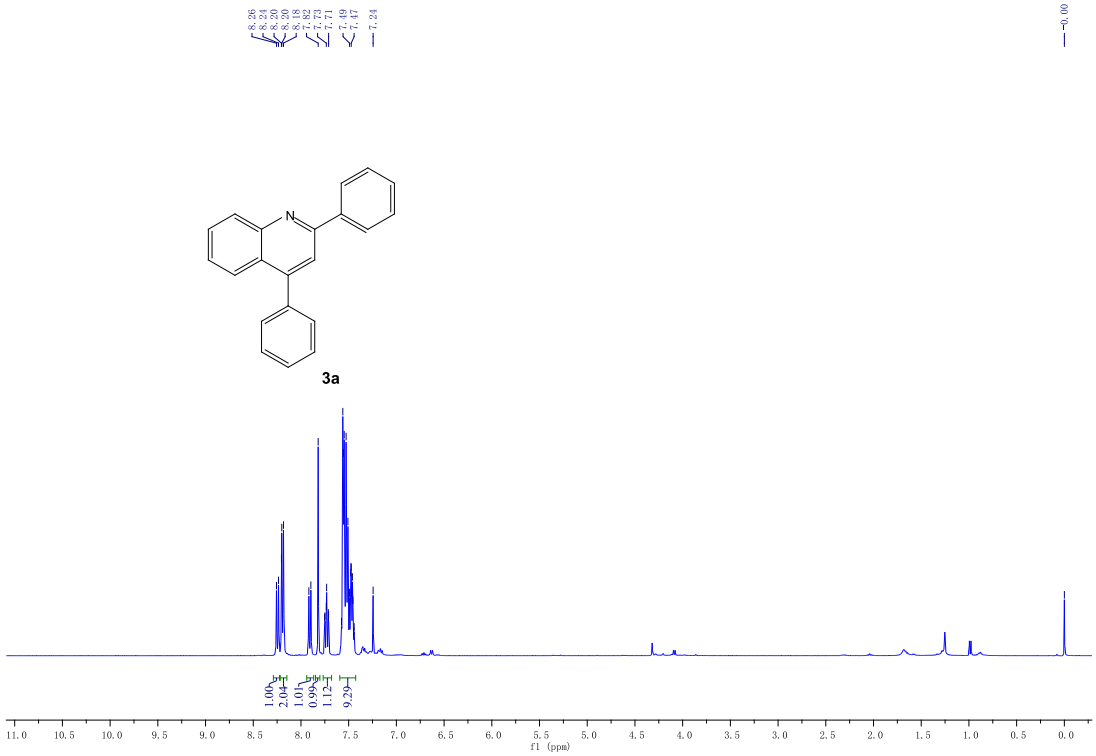
NMR Spectra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7.24
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3a
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2.04
1.01
0.99
1.12
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8.0
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7.0
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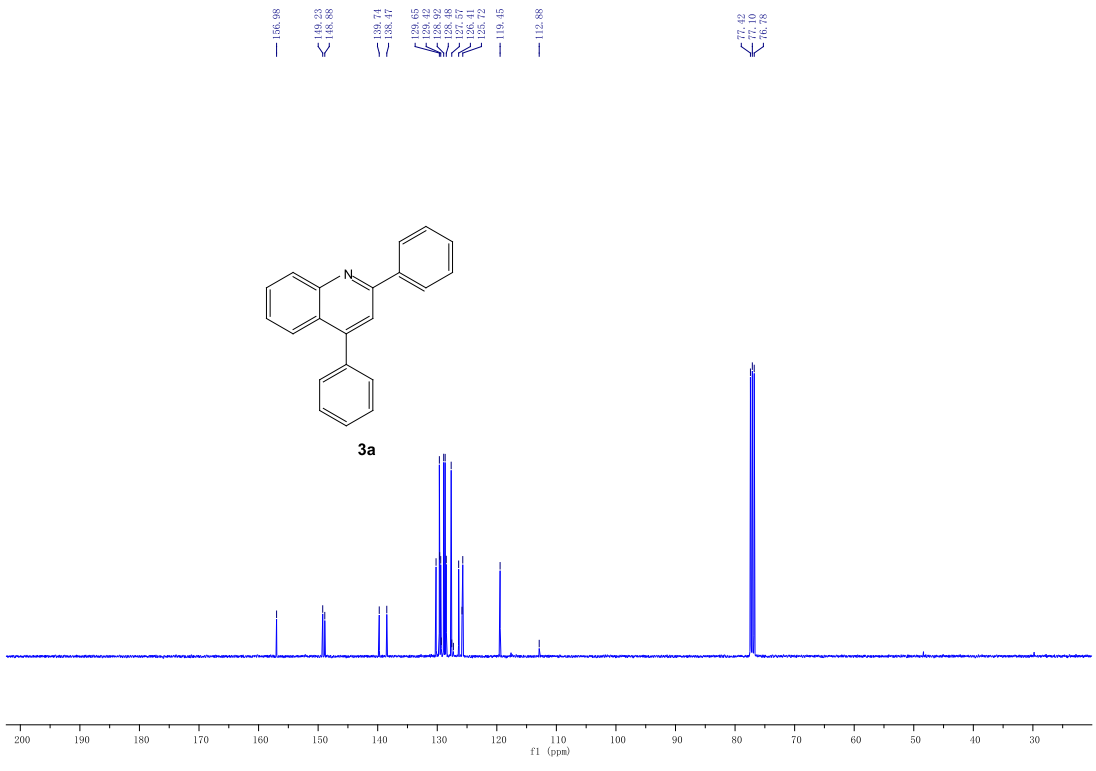
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3a
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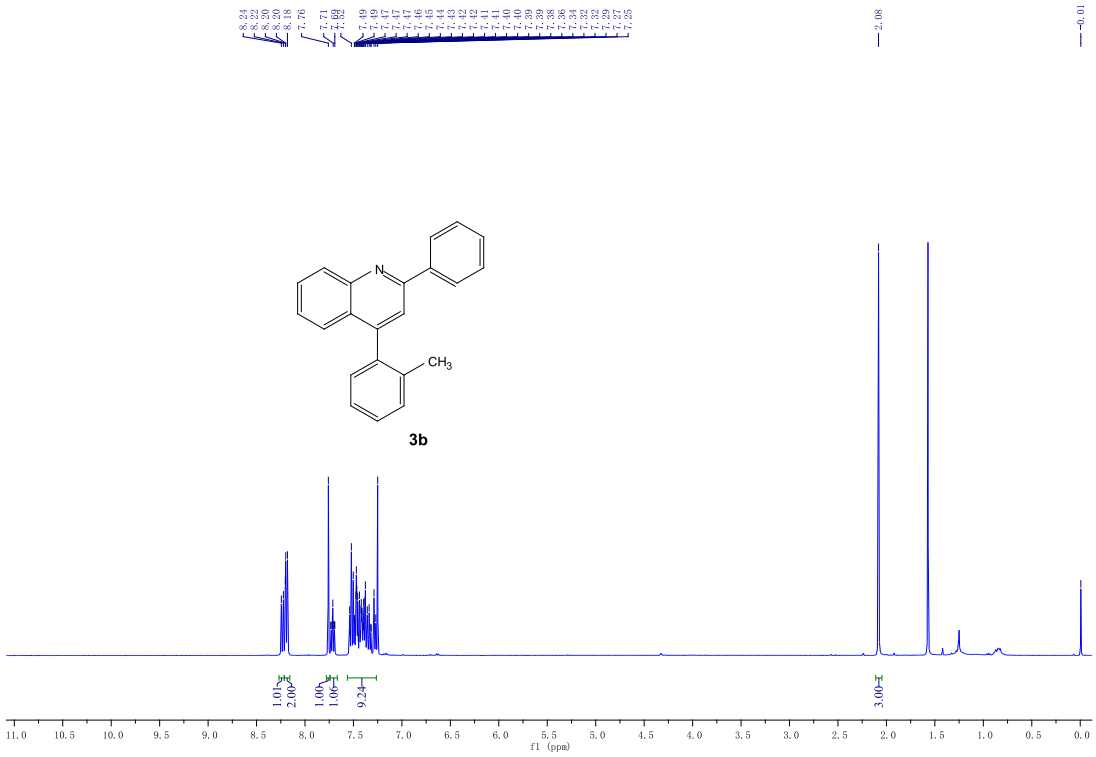
30
f1 (ppm)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2.00
1.00
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3.00
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6.0
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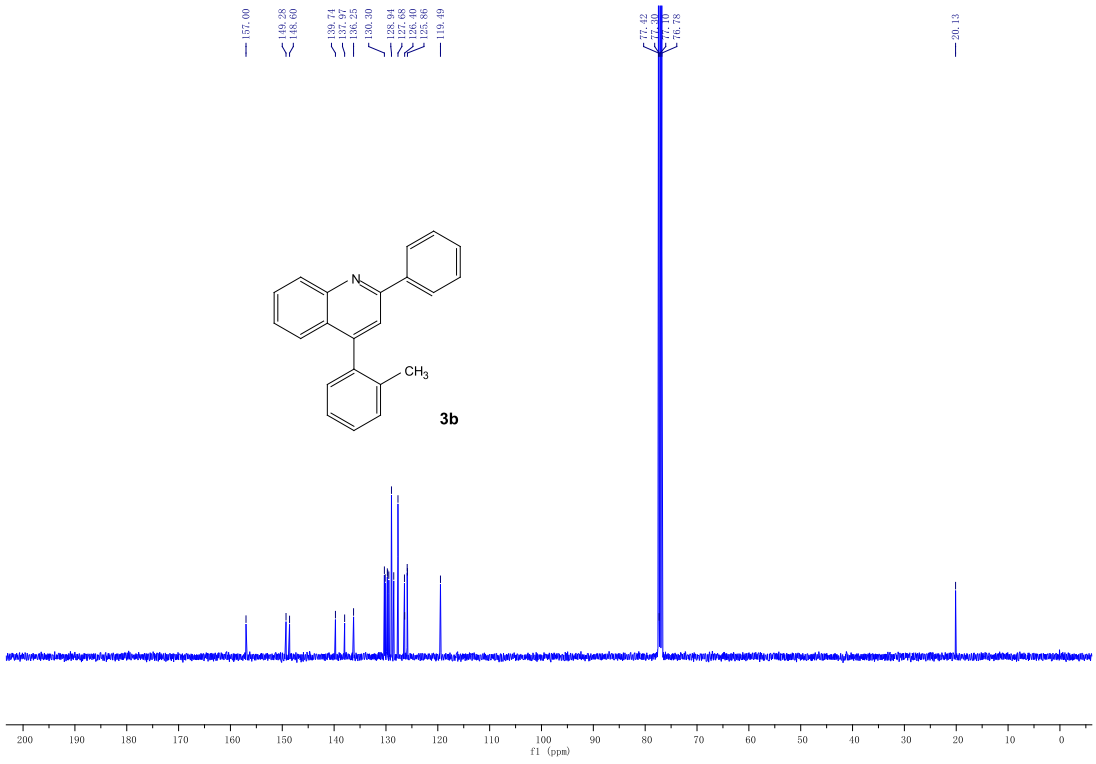
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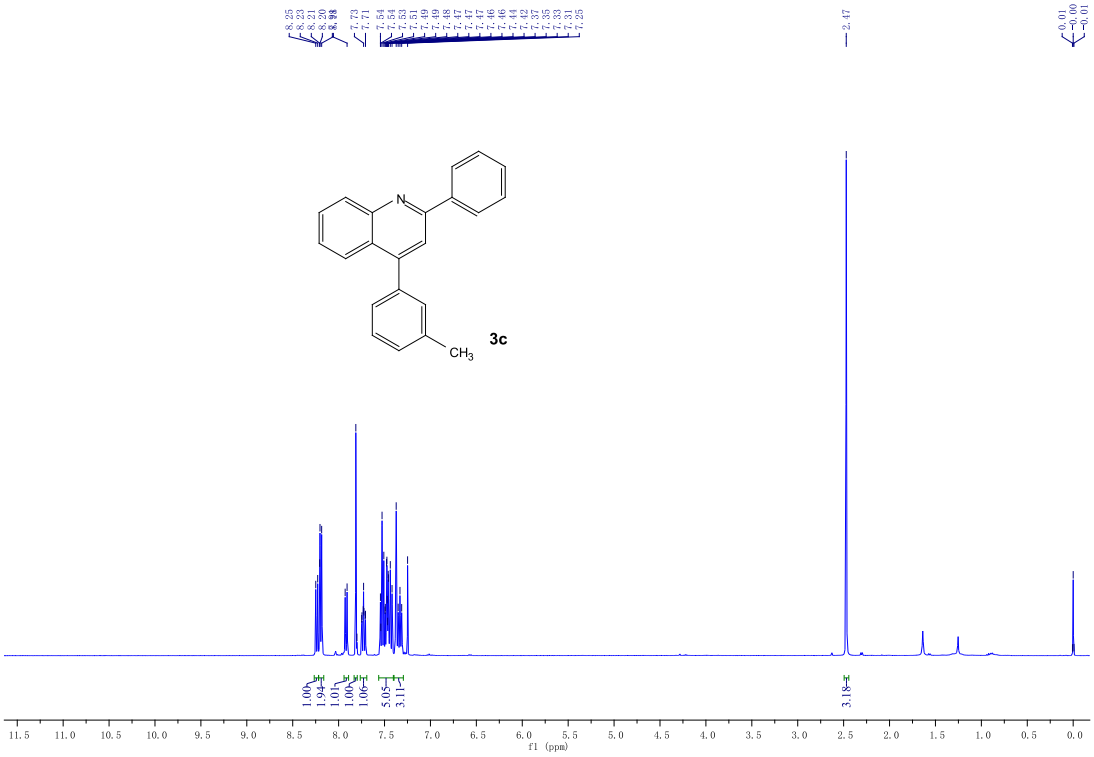
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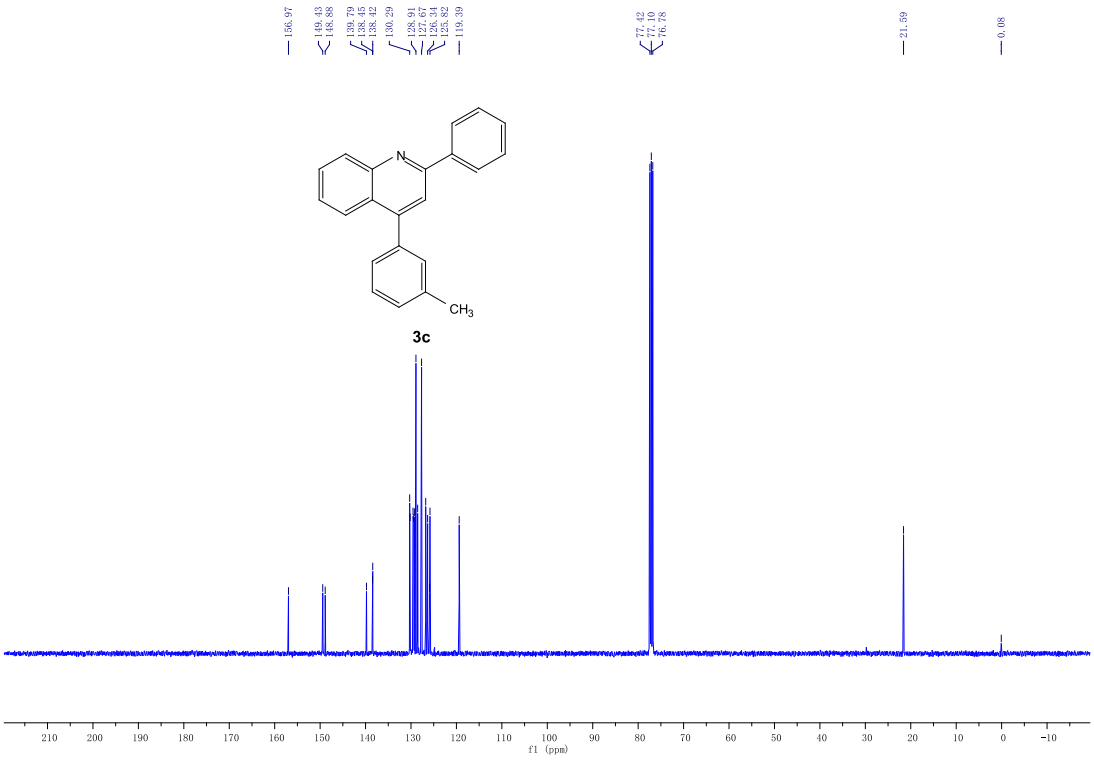
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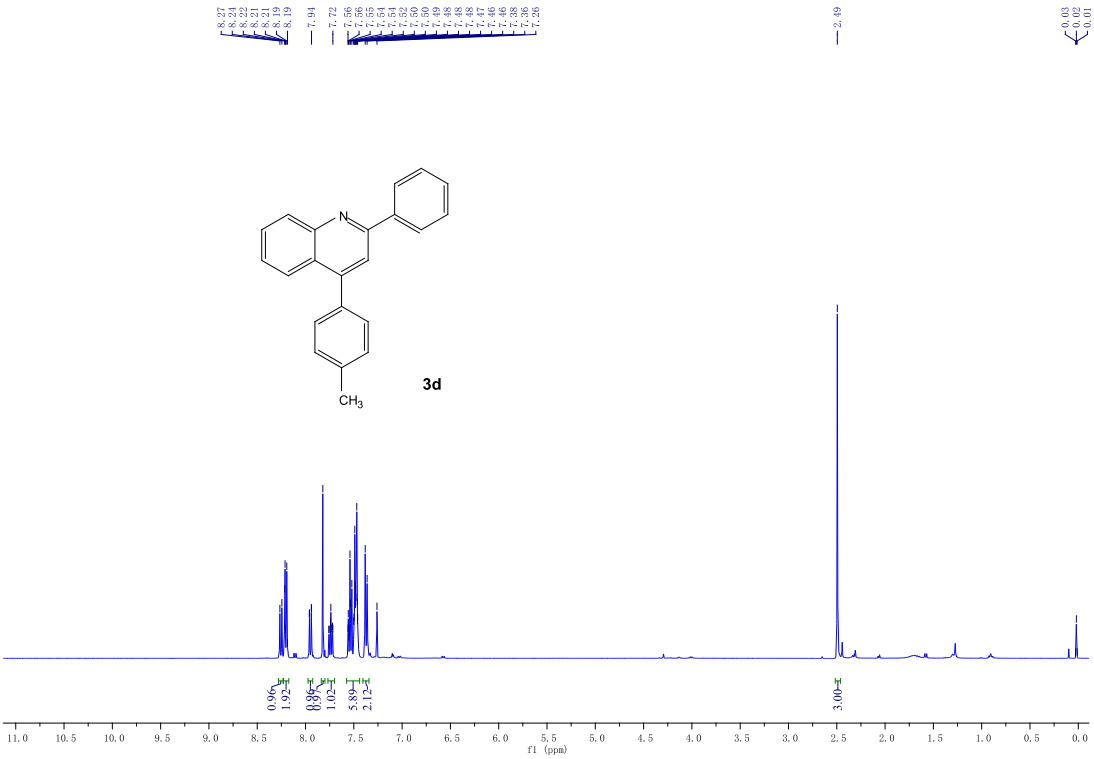
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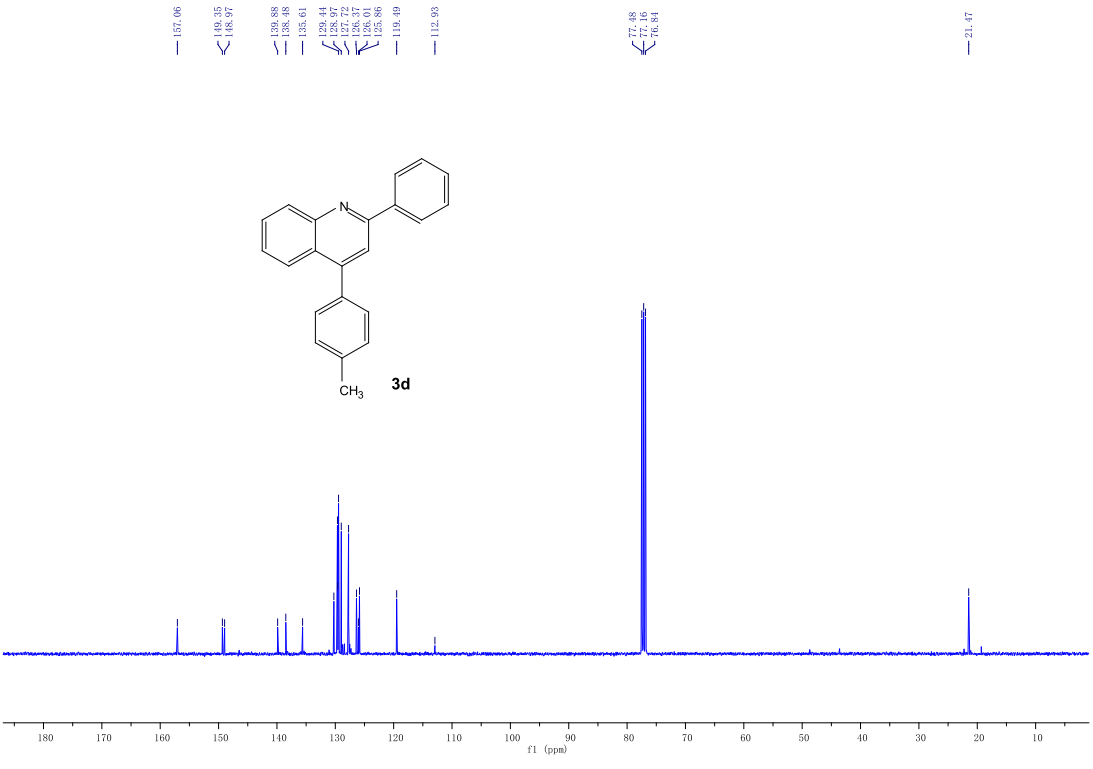
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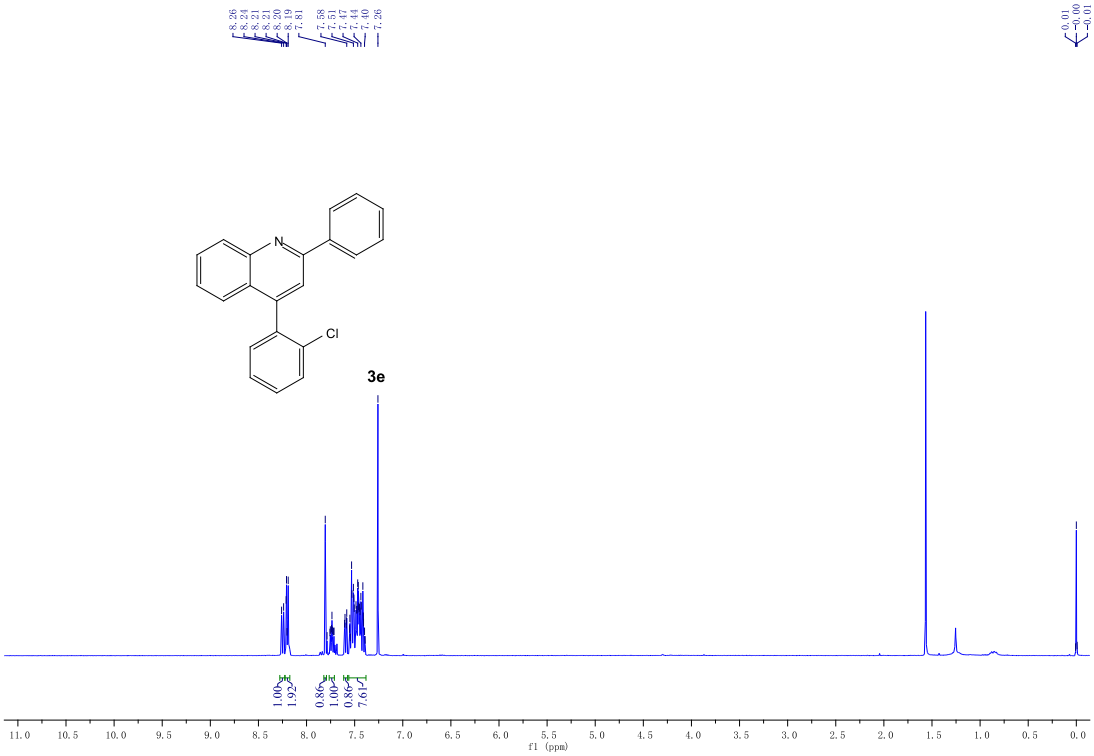
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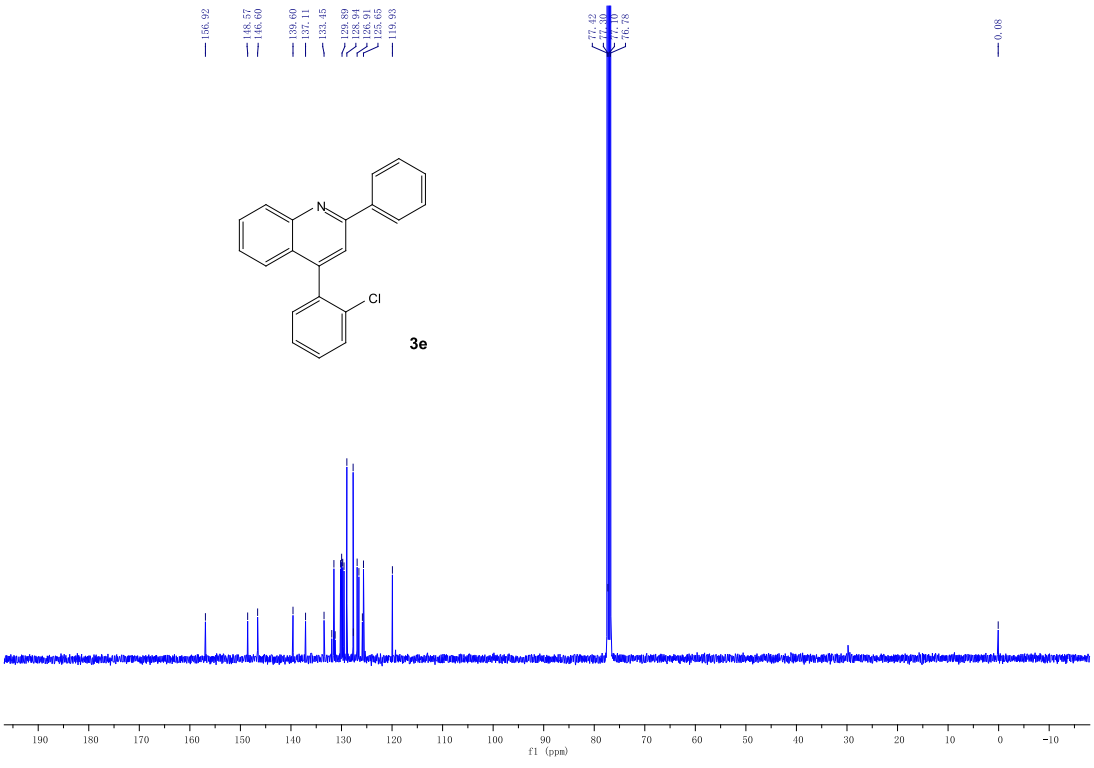
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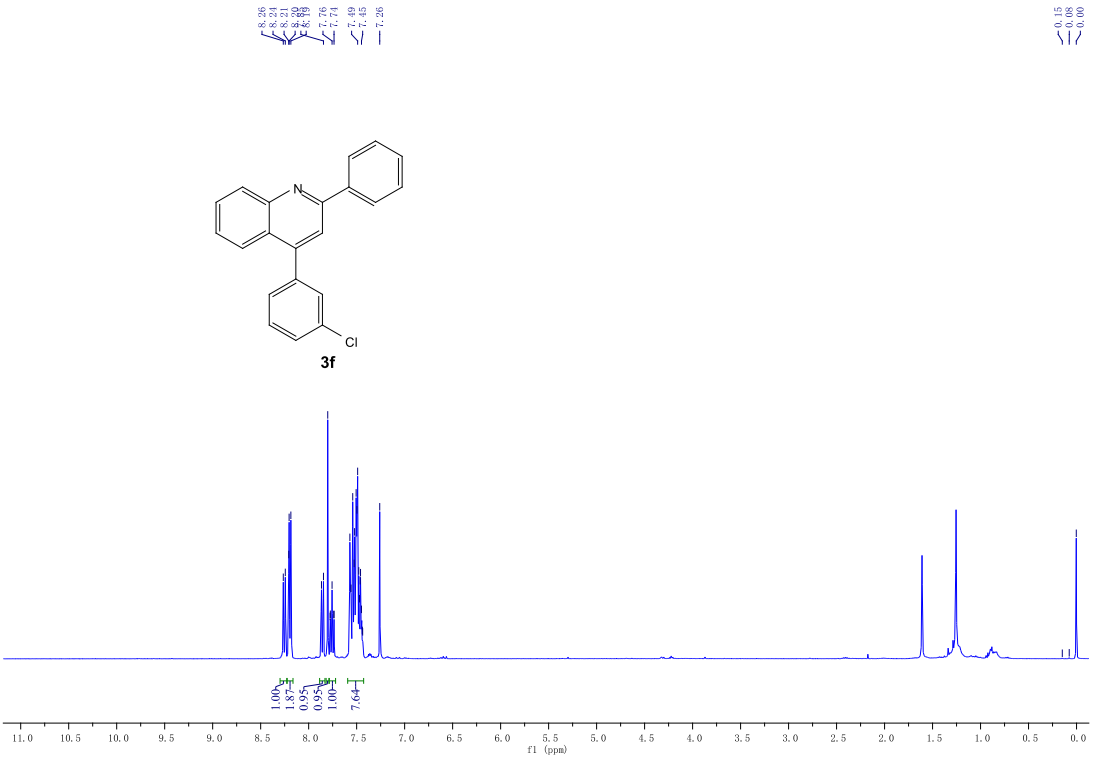
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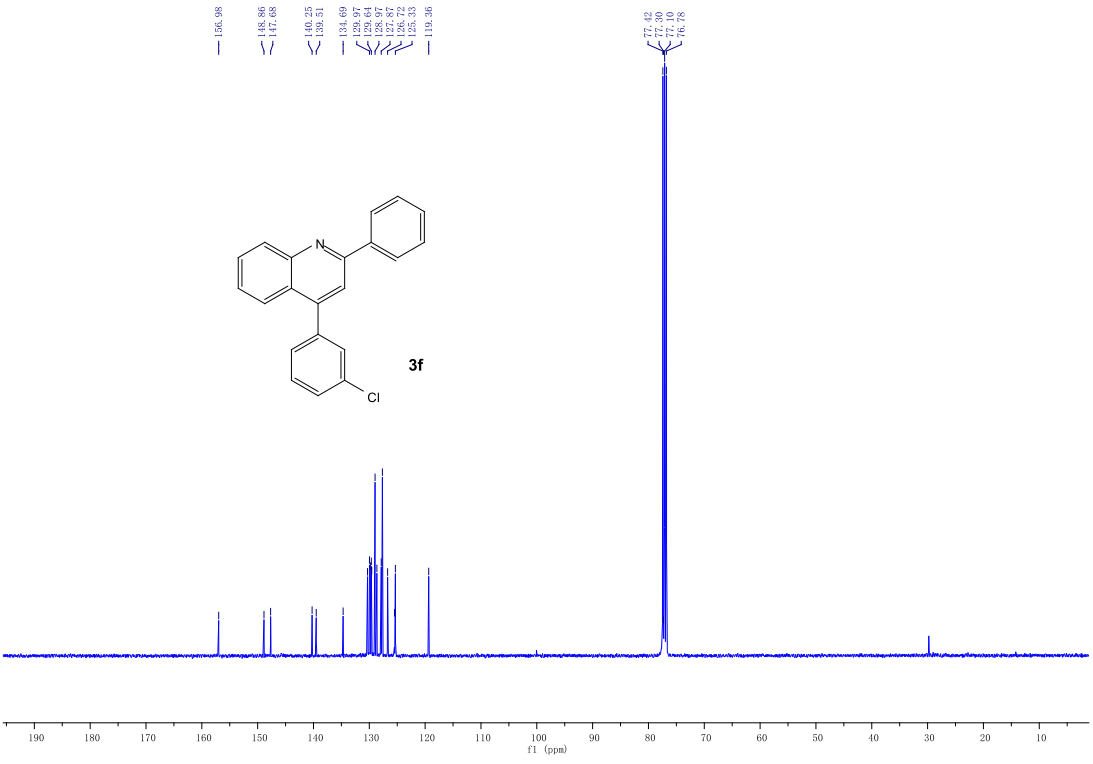
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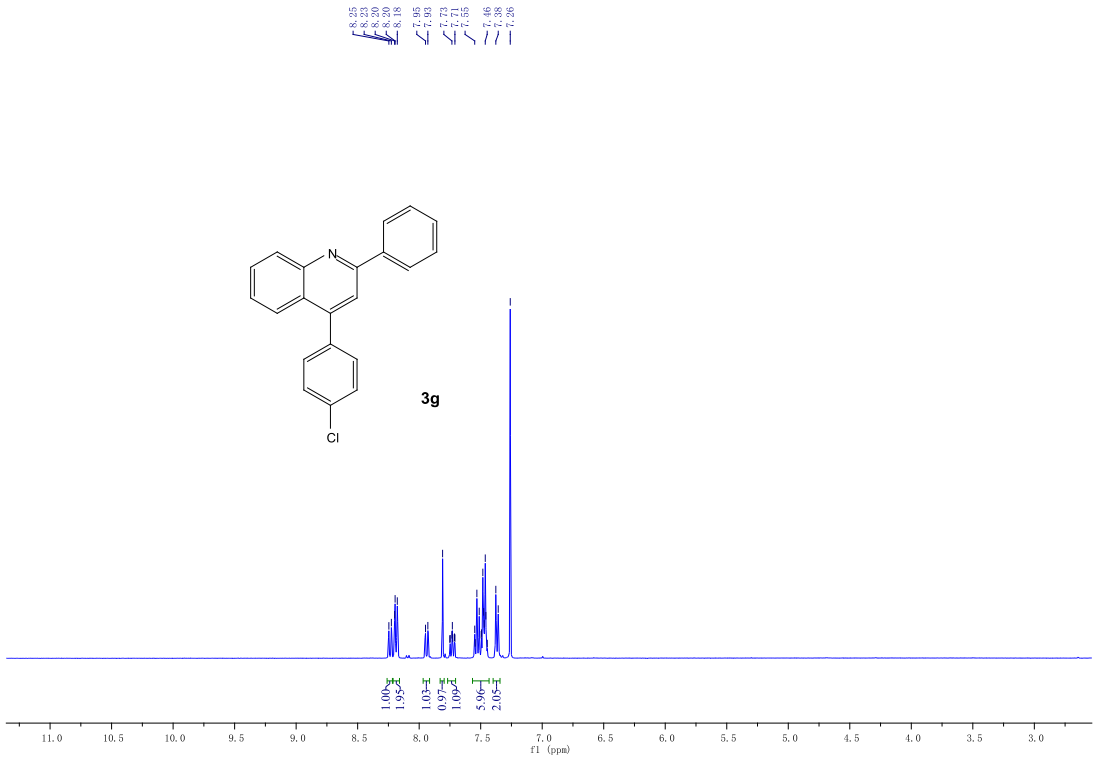
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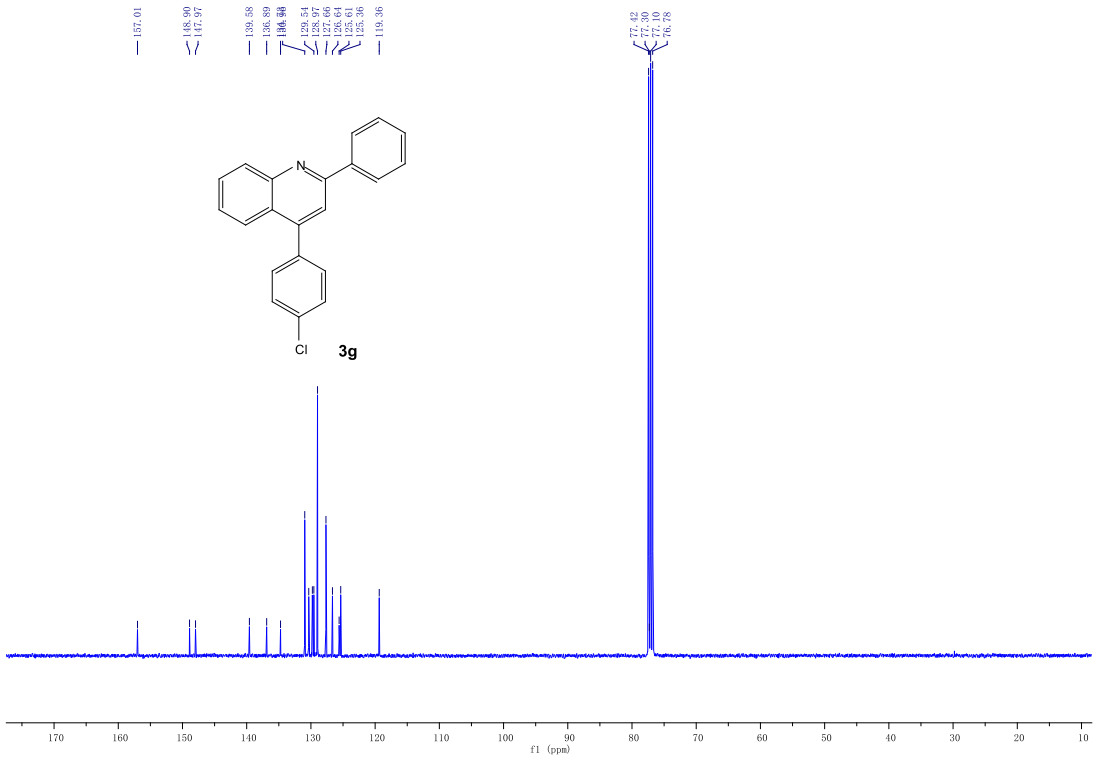
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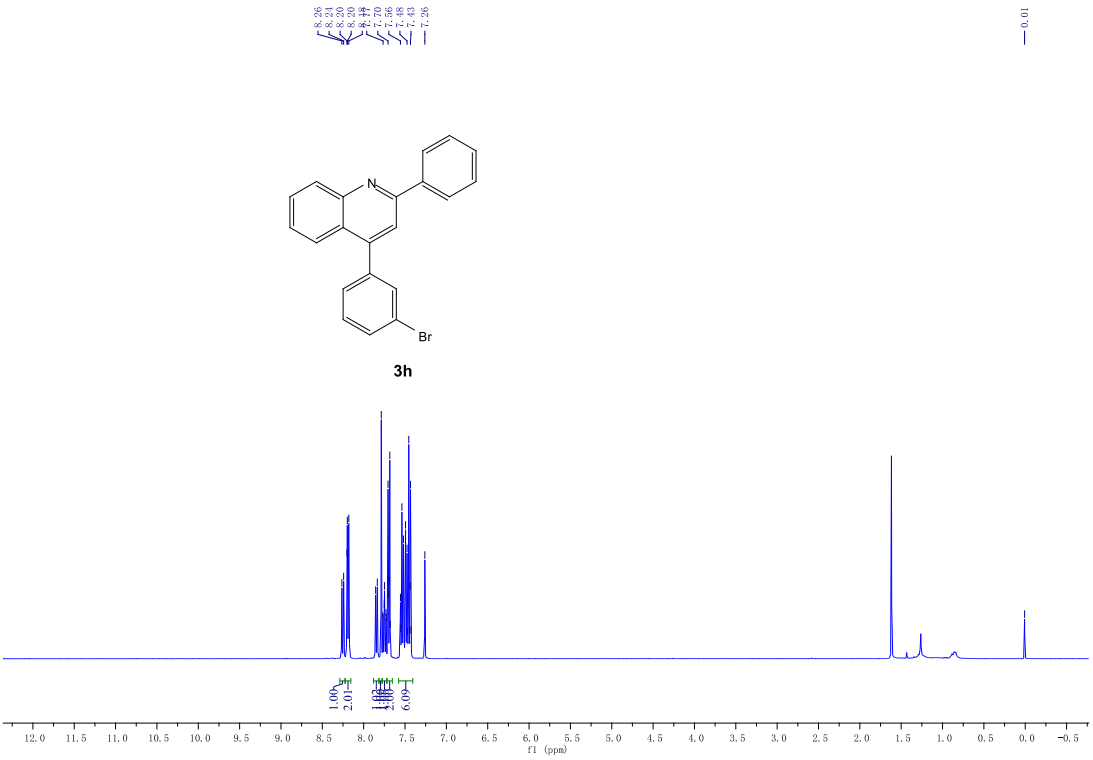
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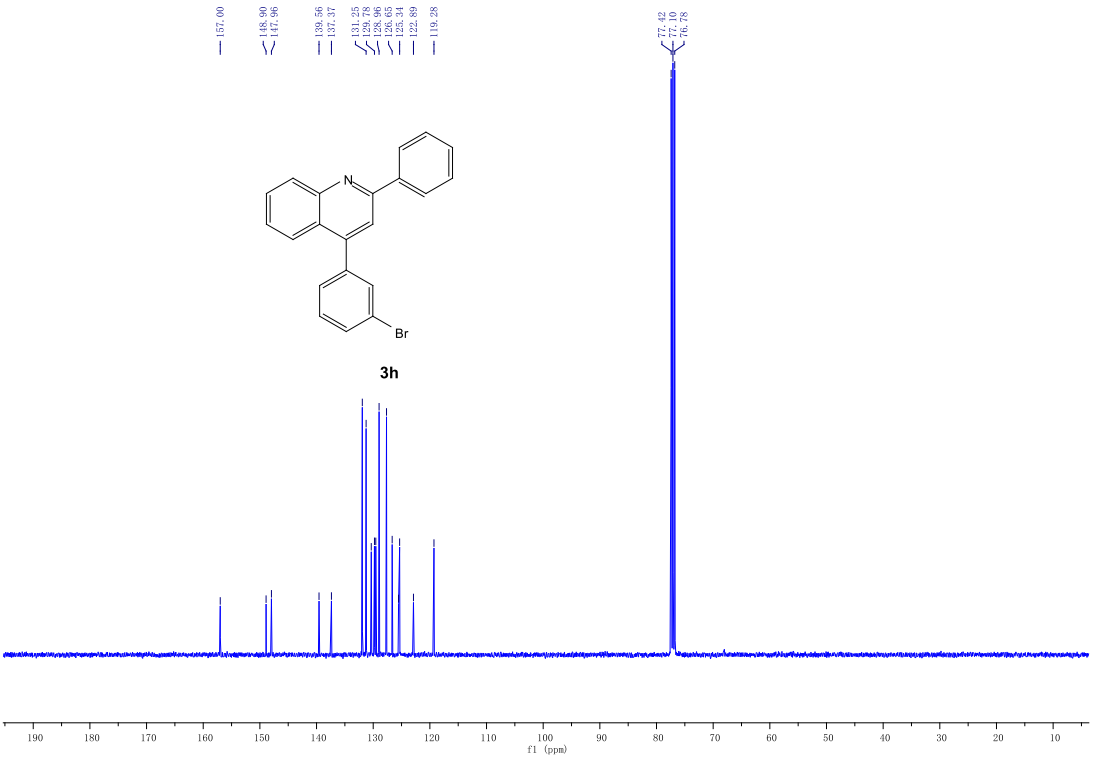
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Br
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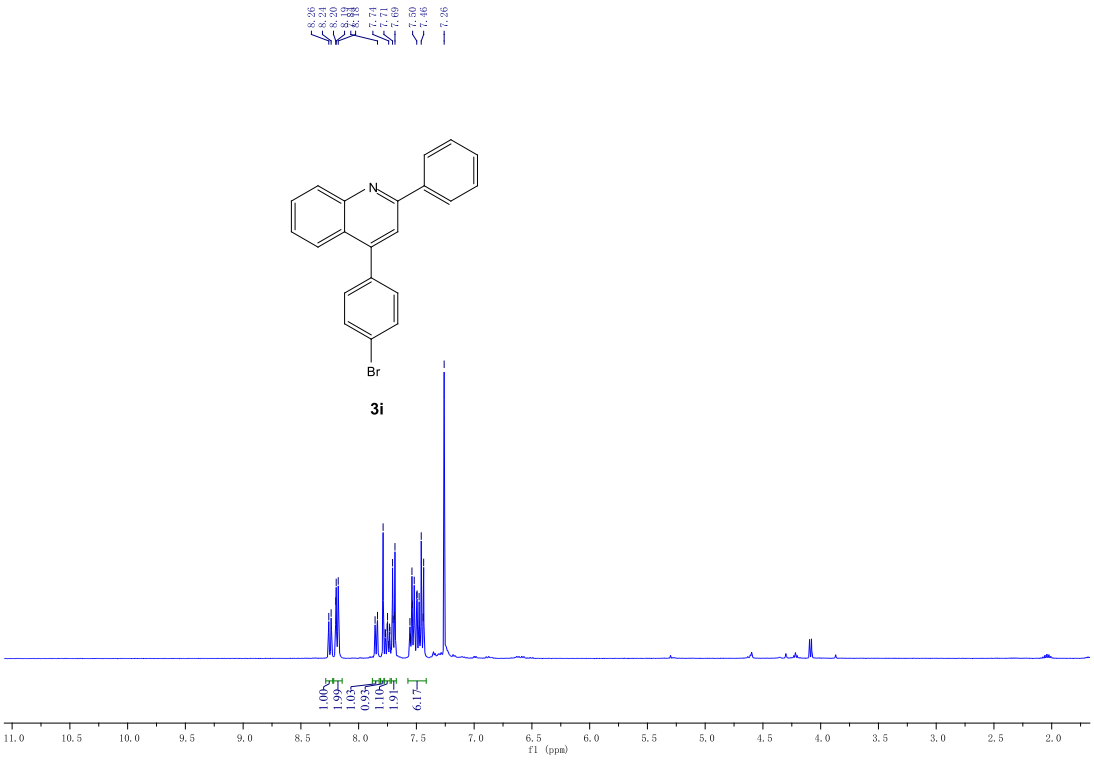
3h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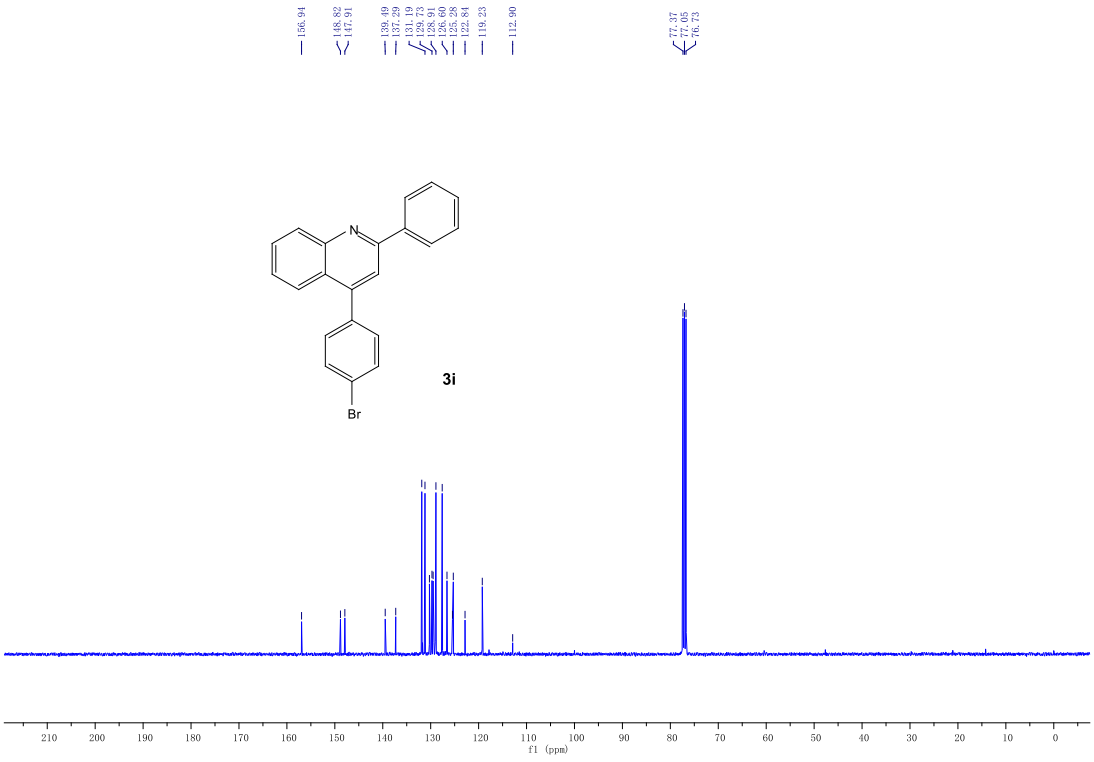
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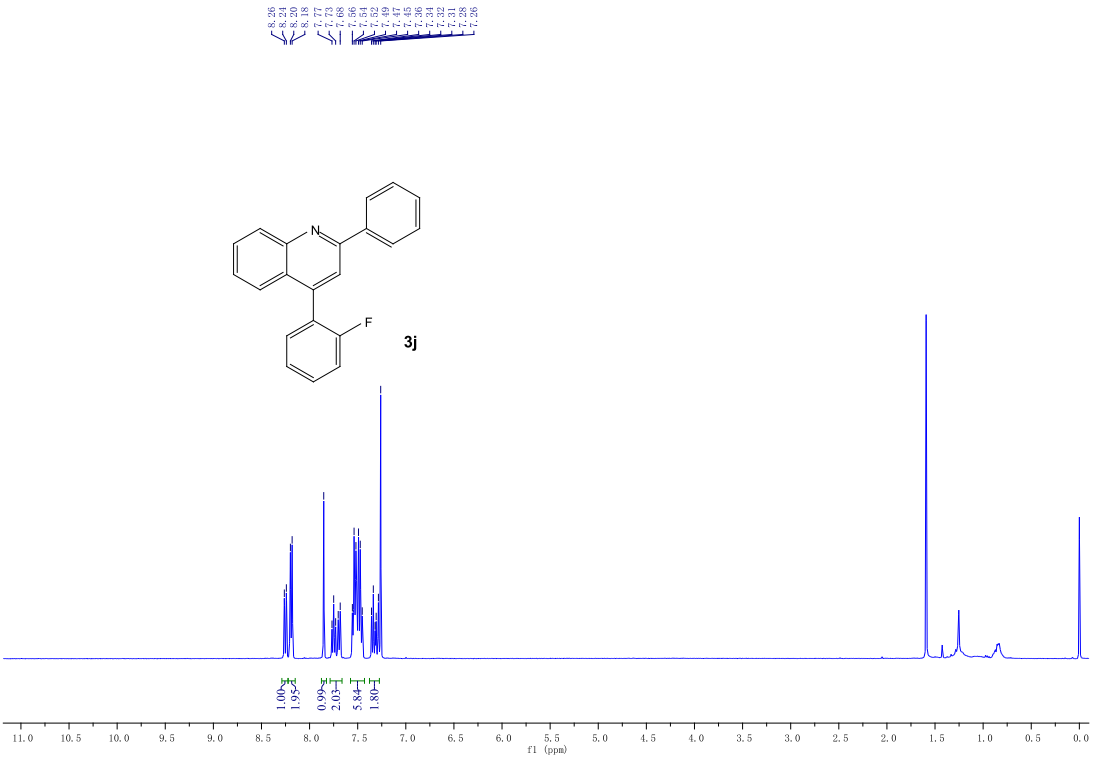
0
f1 (ppm)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8.24
8.20
8.18
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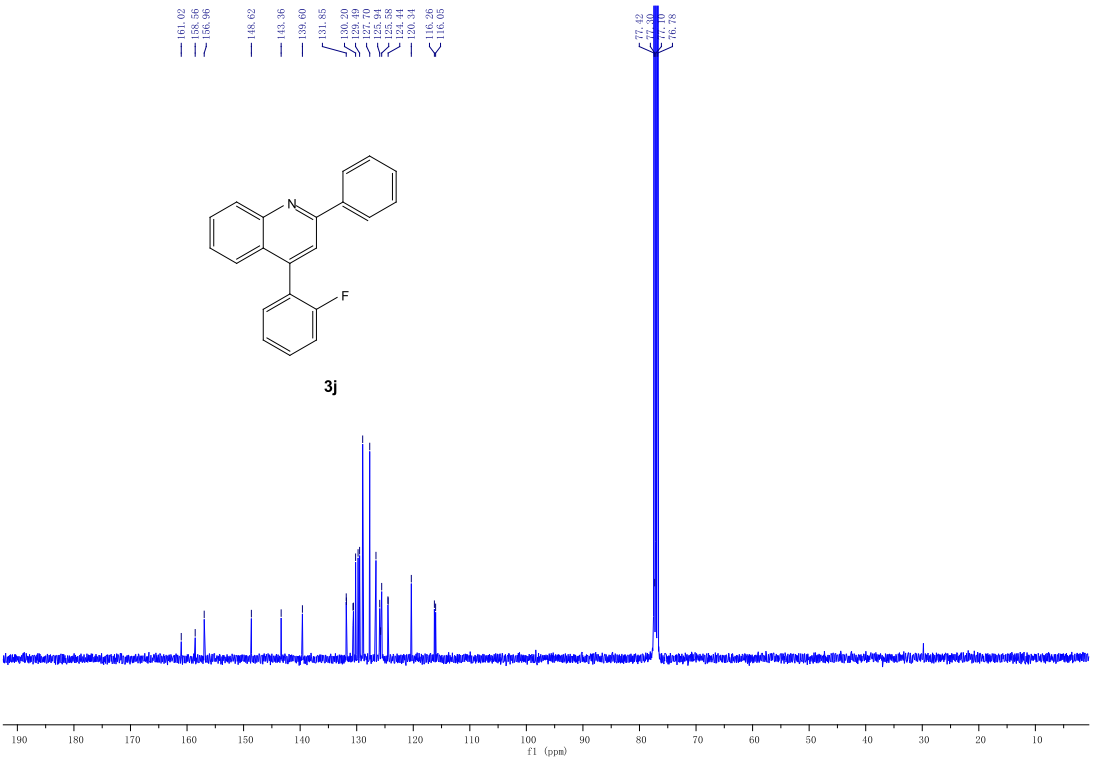
7.68
7.66
7.54
7.52
7.49
7.47
7.45
7.36
7.34
7.32
7.31
7.28
7.26
N
F
3j
1.00
1.95
0.99
2.03
5.84
1.80
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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143.36
139.60
131.85
130.20
130.09
127.70
125.94
125.58
124.44
120.34
116.26
116.05
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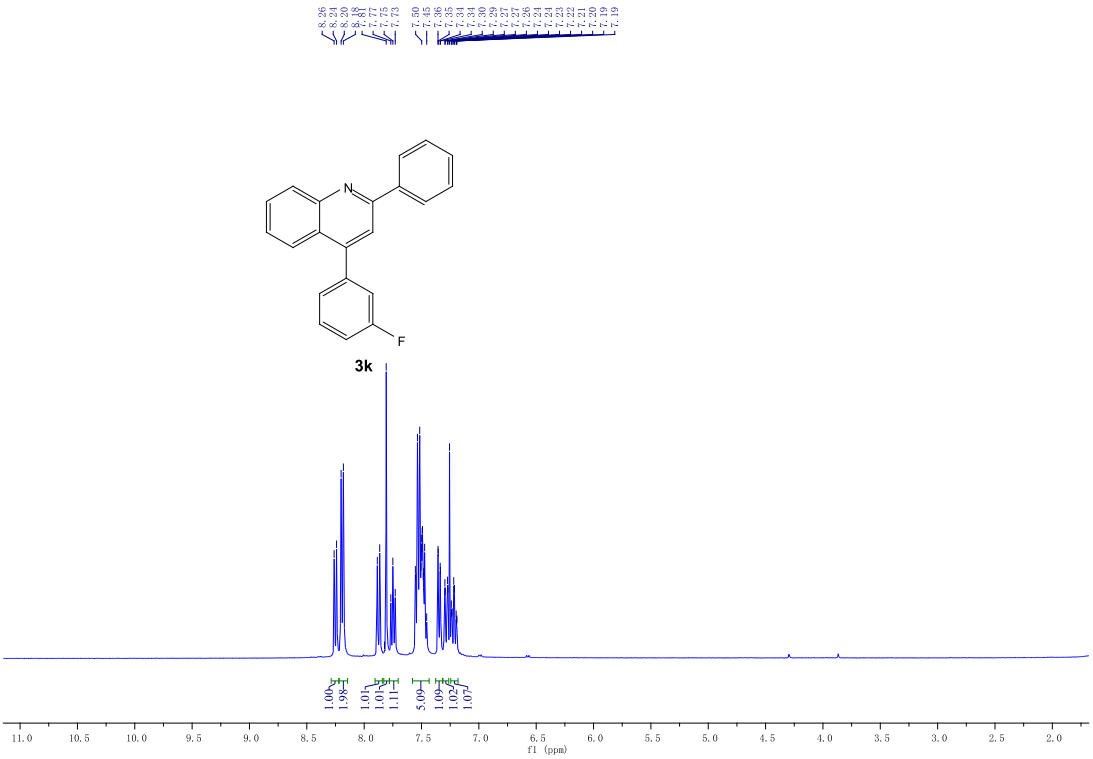
77.00
76.78
N
F
3j
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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7.73
7.50
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7.36
7.35
7.34
7.34
7.30
7.29
7.27
7.27
7.26
7.24
7.24
7.23
7.22
7.21
7.20
7.19
7.19
N
F
3k
1.00
1.98
1.01
1.01
1.11
5.09
1.09
1.02
1.07
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
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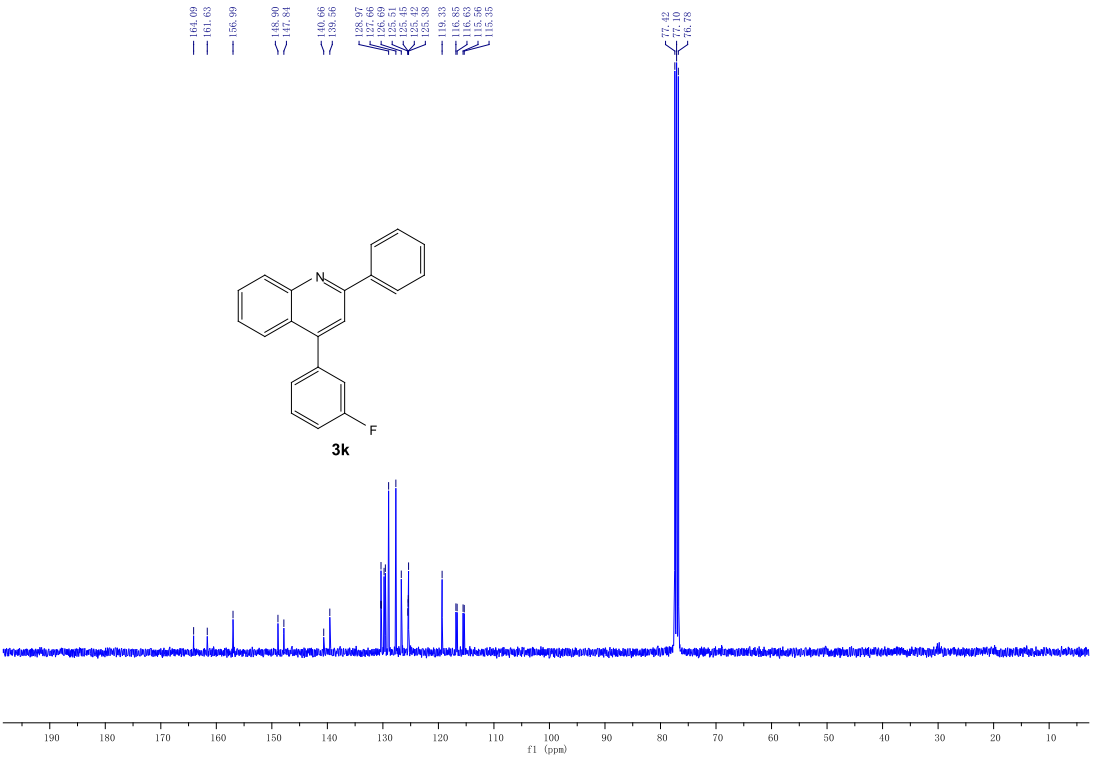
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)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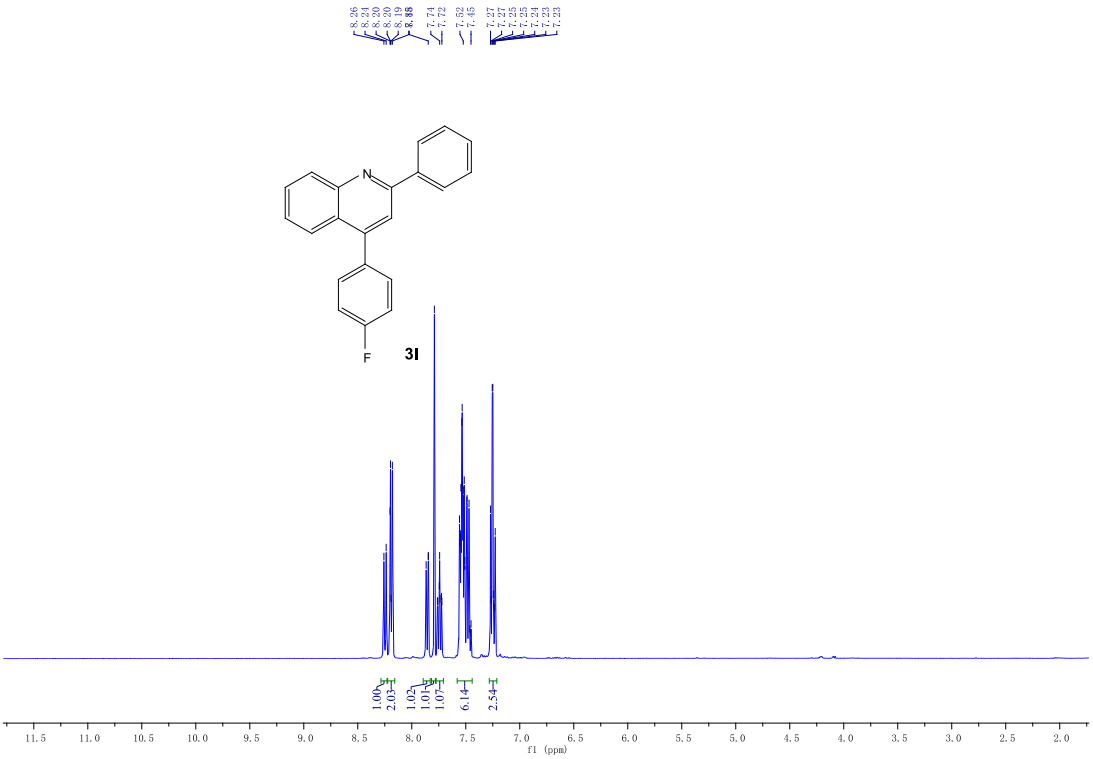
140.66
139.56
128.97
127.66
126.69
125.51
125.45
125.42
124.38
119.33
116.85
116.63
115.56
115.35
77.42
77.10
76.78
N
F
3k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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8.24
8.20
8.20
8.19
8.18
7.74
7.72
7.52
7.45
7.27
7.27
7.25
7.25
7.24
7.24
7.23
7.23
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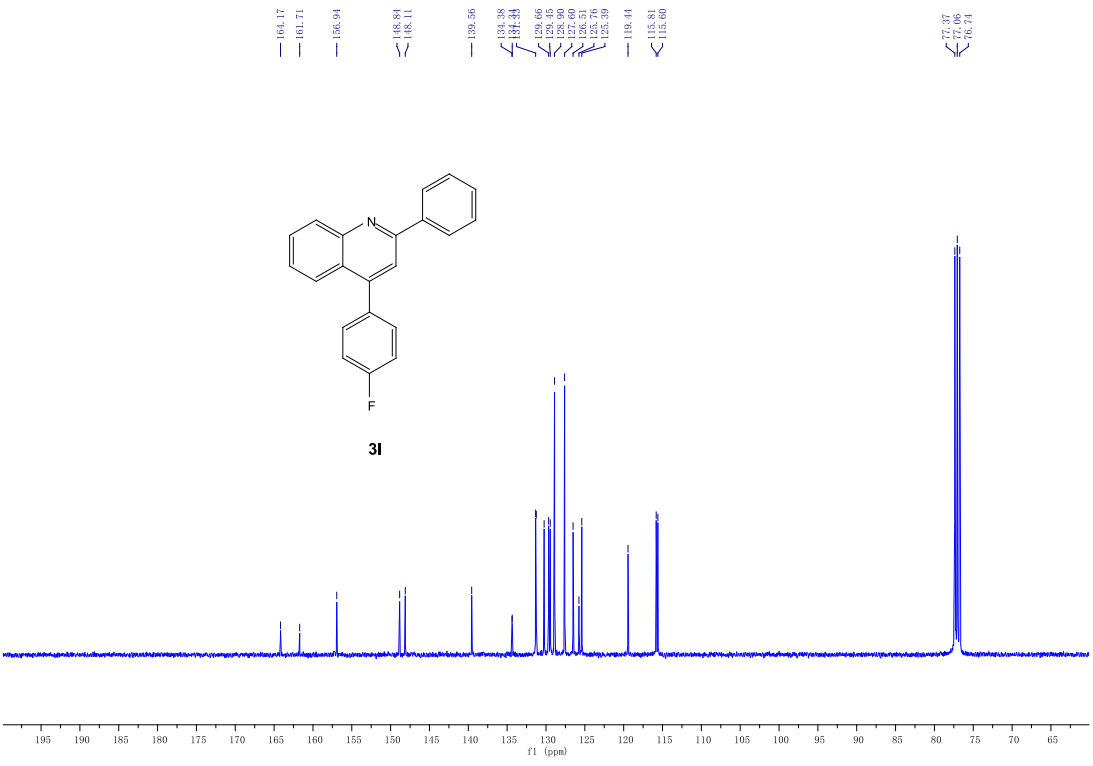
F
3l
1.00
2.03
1.02
1.01
1.07
6.14
2.54
f1 (ppm)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139.56
134.38
131.33
129.66
129.55
128.90
127.60
126.51
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125.30
119.44
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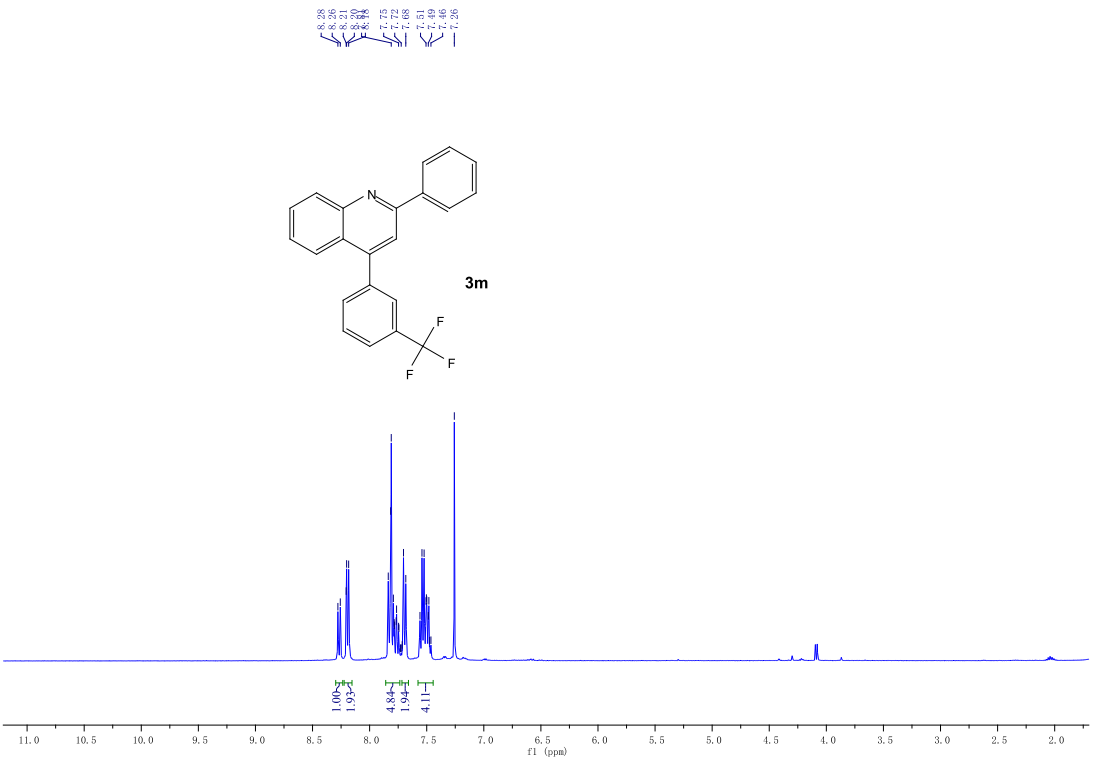
115.60
77.37
77.06
76.74
N
F
3l
f1 (ppm)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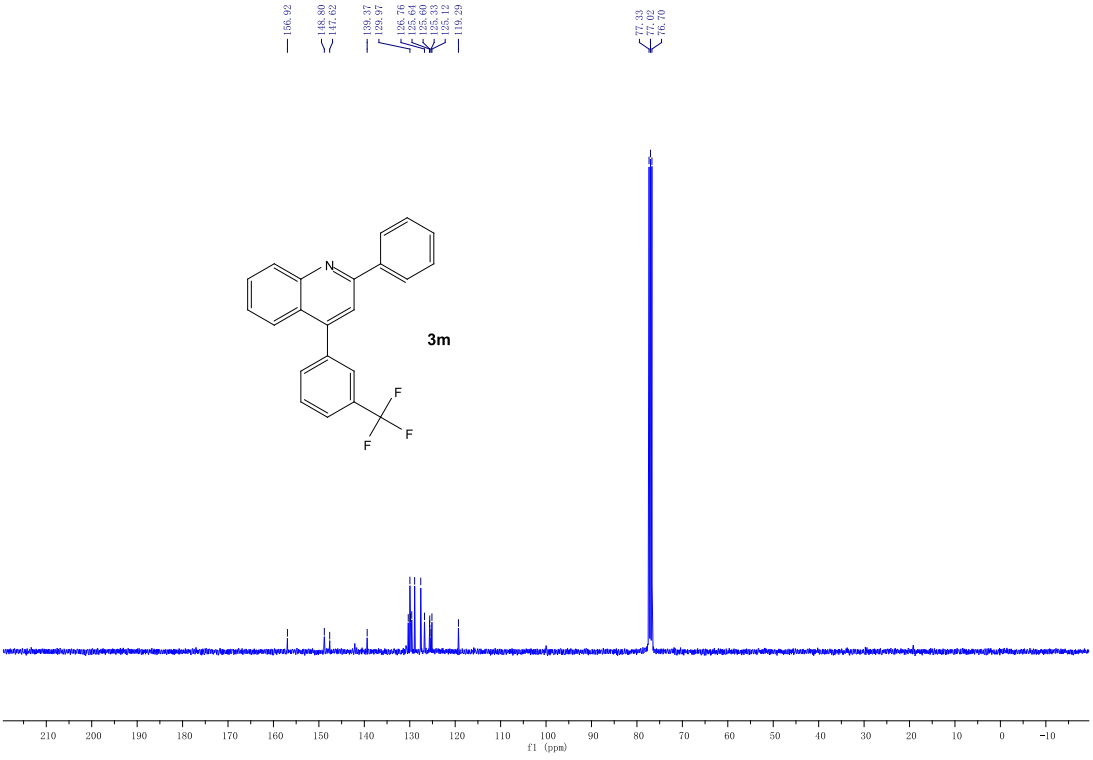
8.26
8.21
8.20
7.75
7.72
7.68
7.51
7.49
7.46
7.26
N
3m
F
F
F
1.00
1.93
4.84
1.94
4.11
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)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148.80
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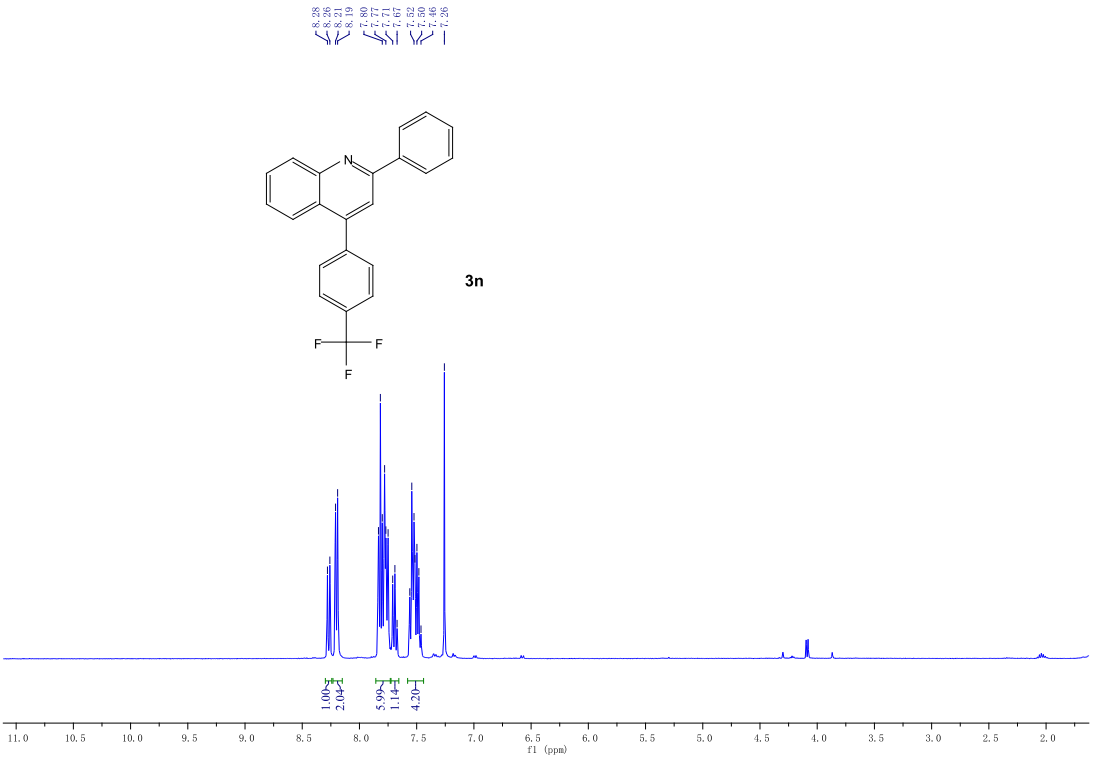
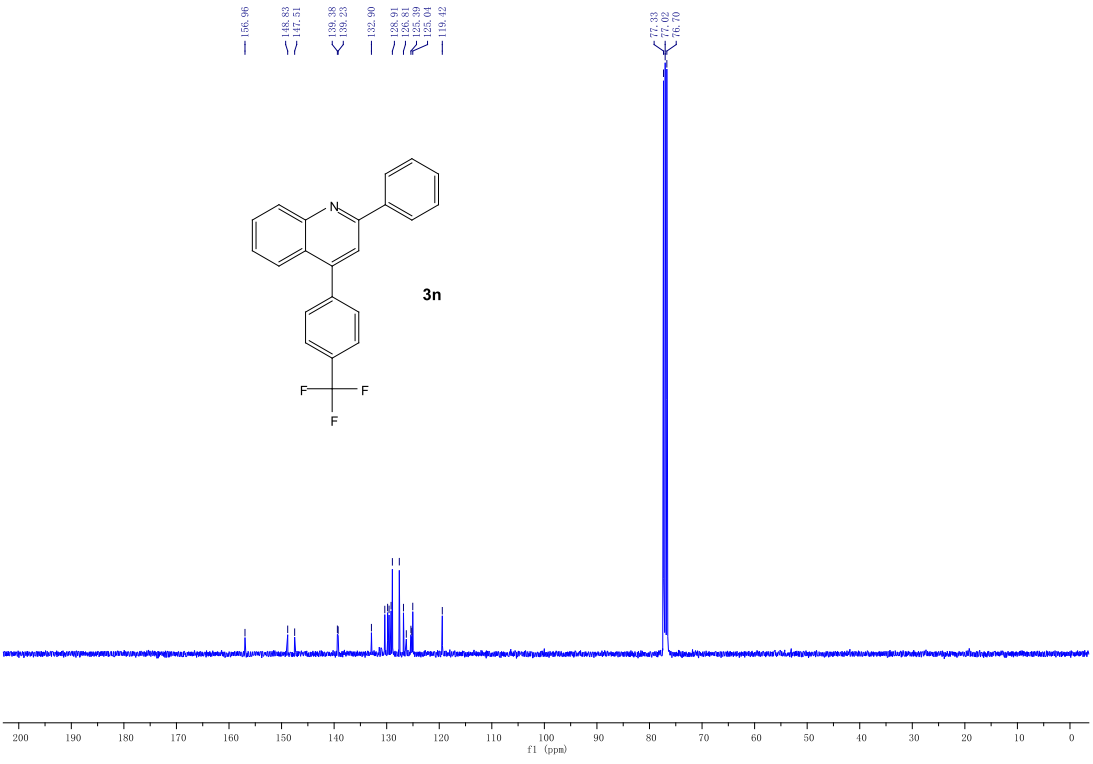
139.37
129.97
126.76
125.64
125.60
125.33
125.12
119.29
77.33
77.02
76.70
N
3m
F
F
F
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.28
8.25
8.21
8.19
7.80
7.77
7.71
7.67
7.52
7.50
7.46
7.26
N
F
F
F
3n
1.00
2.04
5.99
1.14
4.20
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)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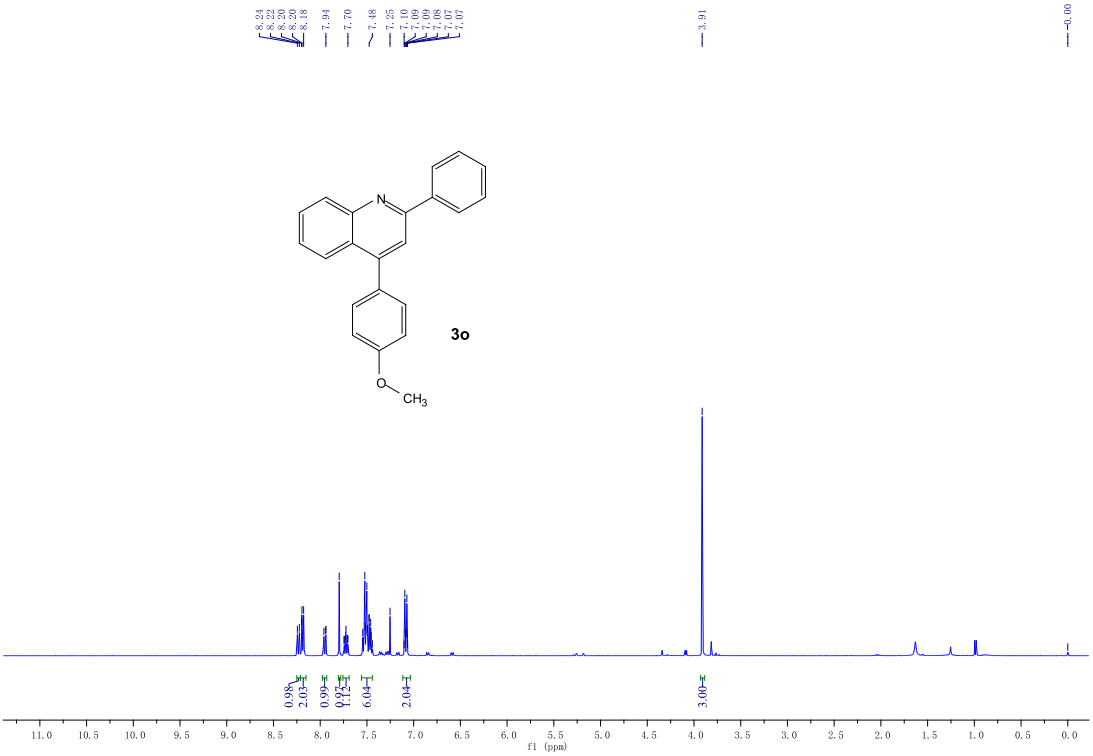
139.38
139.23
132.90
128.91
126.81
125.39
125.04
119.42
77.33
77.02
76.70
N
F
F
F
3n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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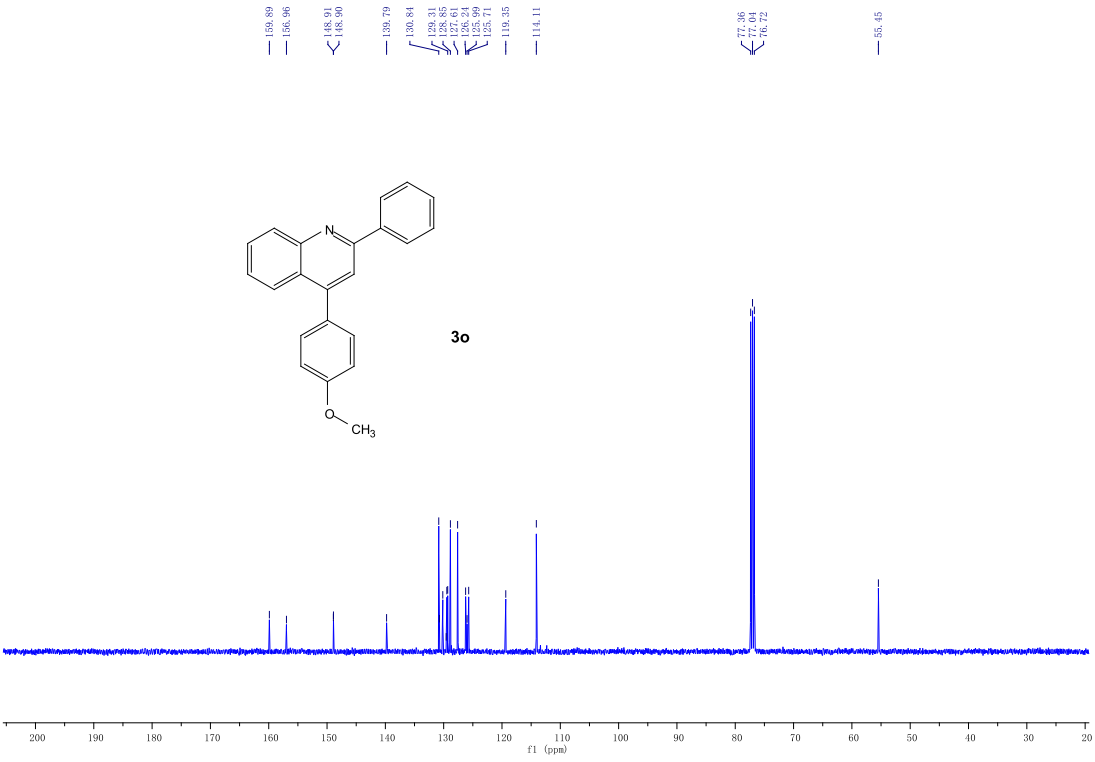
8.22
8.20
8.18
7.94
7.70
7.48
7.25
7.10
7.09
7.09
7.08
7.07
7.07
3.91
0.00
N
O
CH3
3o
0.98
2.03
0.99
0.97
1.12
6.04
2.04
3.00
f1 (ppm)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129.31
128.85
127.61
126.24
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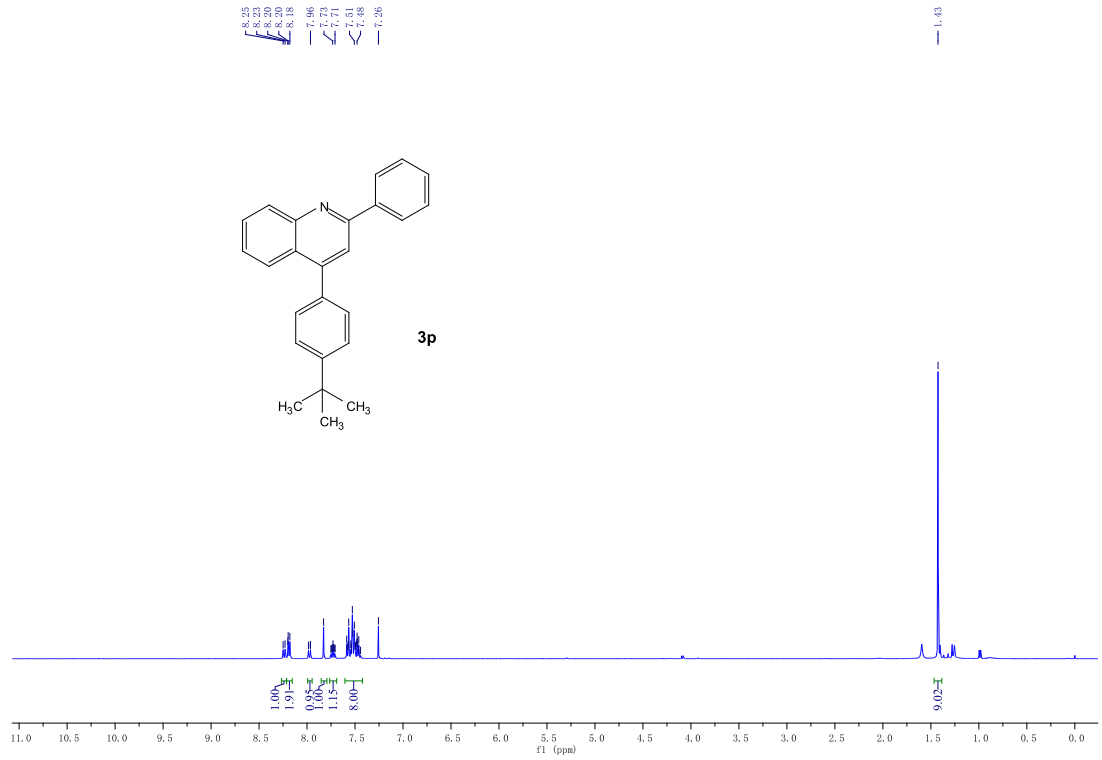
114.11
77.36
77.04
76.72
55.45
N
O
CH3
3o
f1 (ppm)


8.25
8.23
8.20
8.20
8.18
7.96
7.73
7.71
7.51
7.48
7.26
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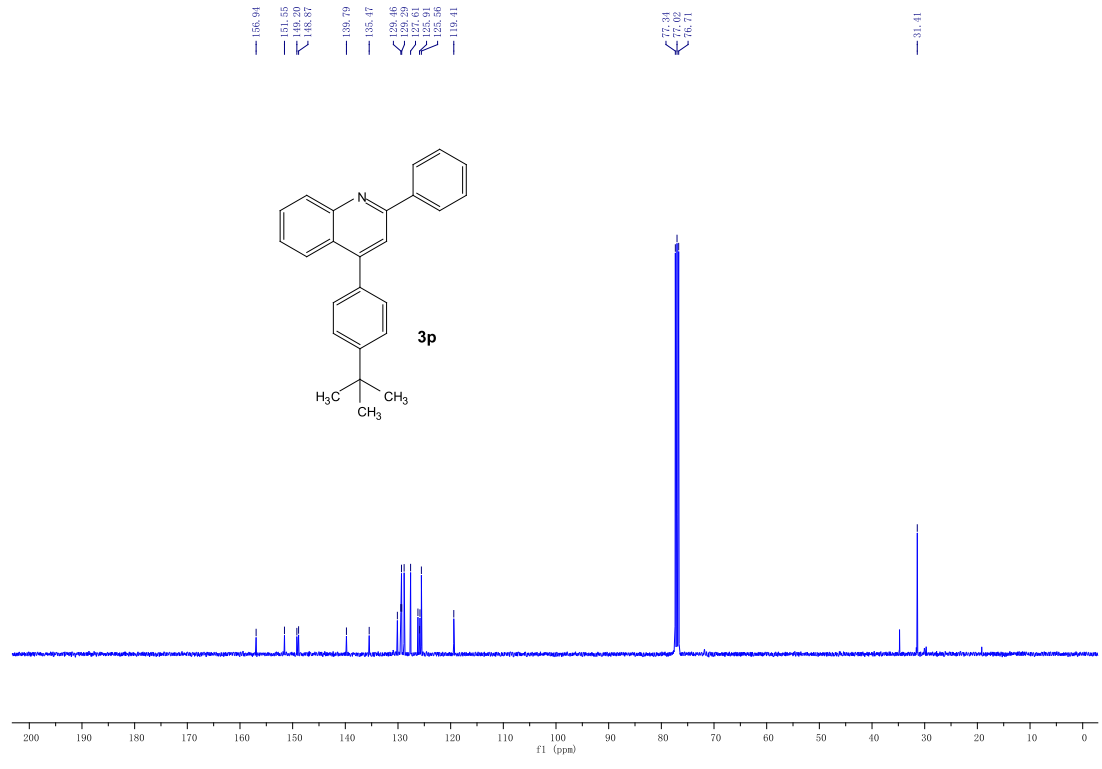
3p
1.00
1.91
0.85
1.00
1.15
8.00
9.02
f1 (ppm)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135.47
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125.56
119.41
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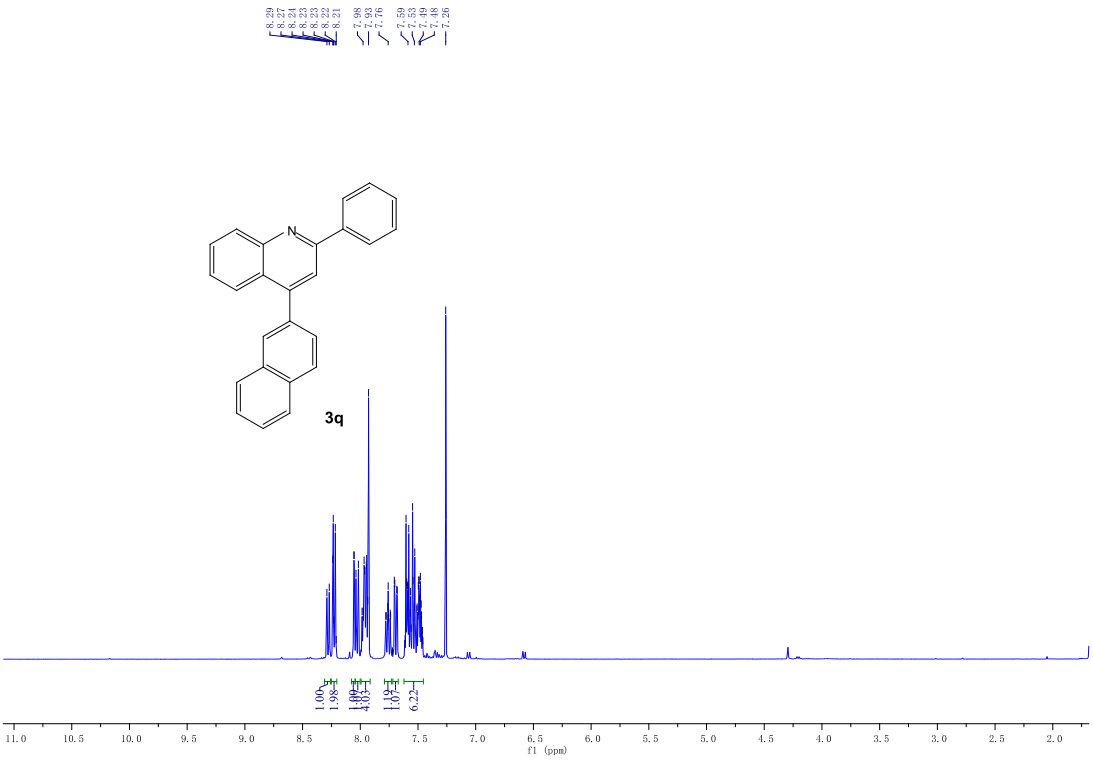
77.02
76.71
31.41
3p
f1 (ppm)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8.27
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8.23
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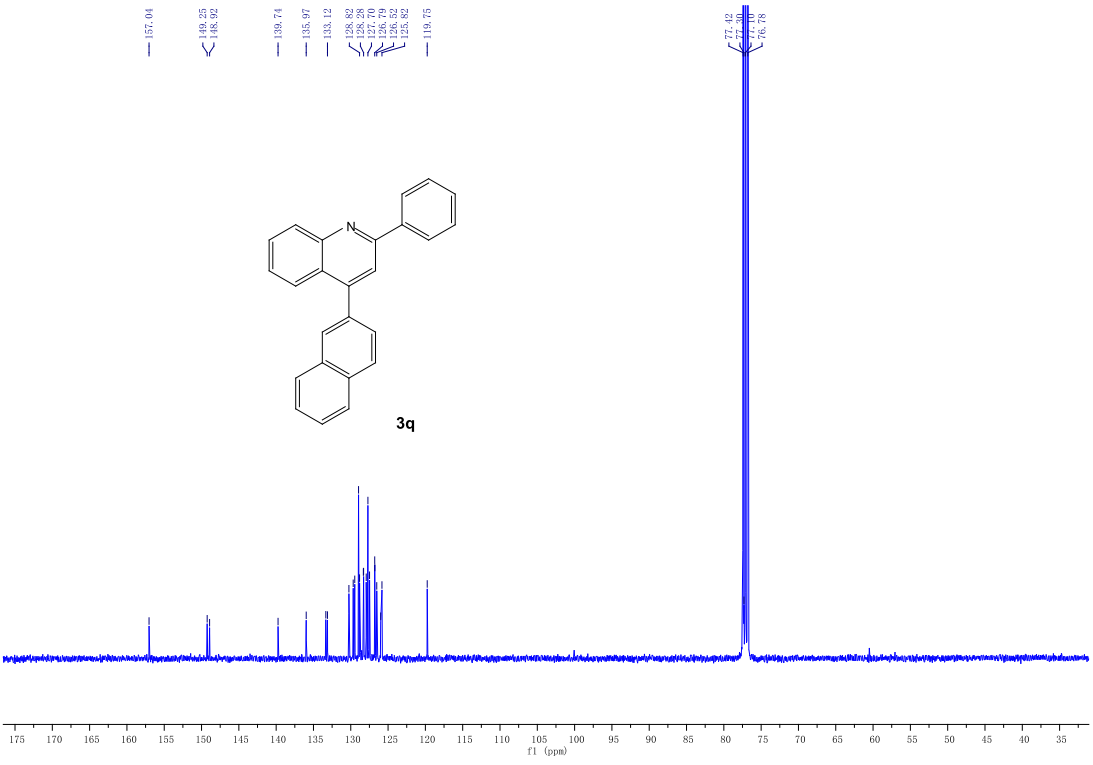
8.22
8.21
7.98
7.83
7.76
7.59
7.53
7.49
7.48
7.26
N
3q
1.00
1.98
1.00
4.03
1.07
6.22
f1 (ppm)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149.25
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133.12
128.82
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126.79
126.52
125.82
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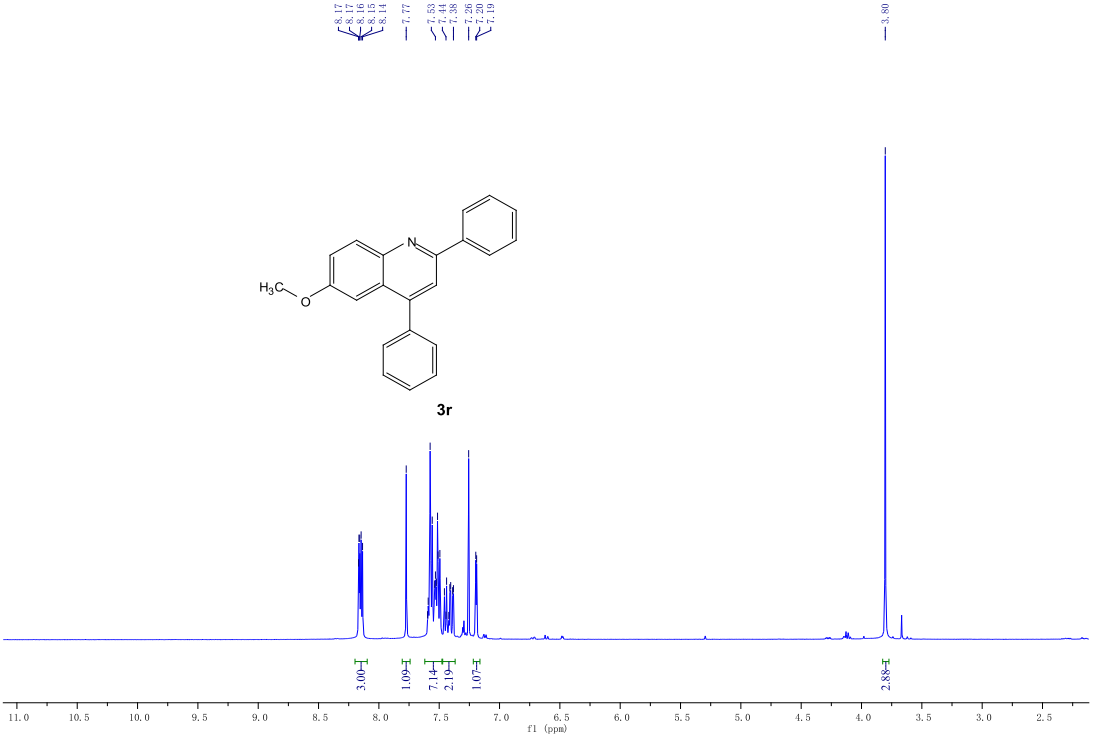
77.42
77.00
76.78
N
3q
f1 (ppm)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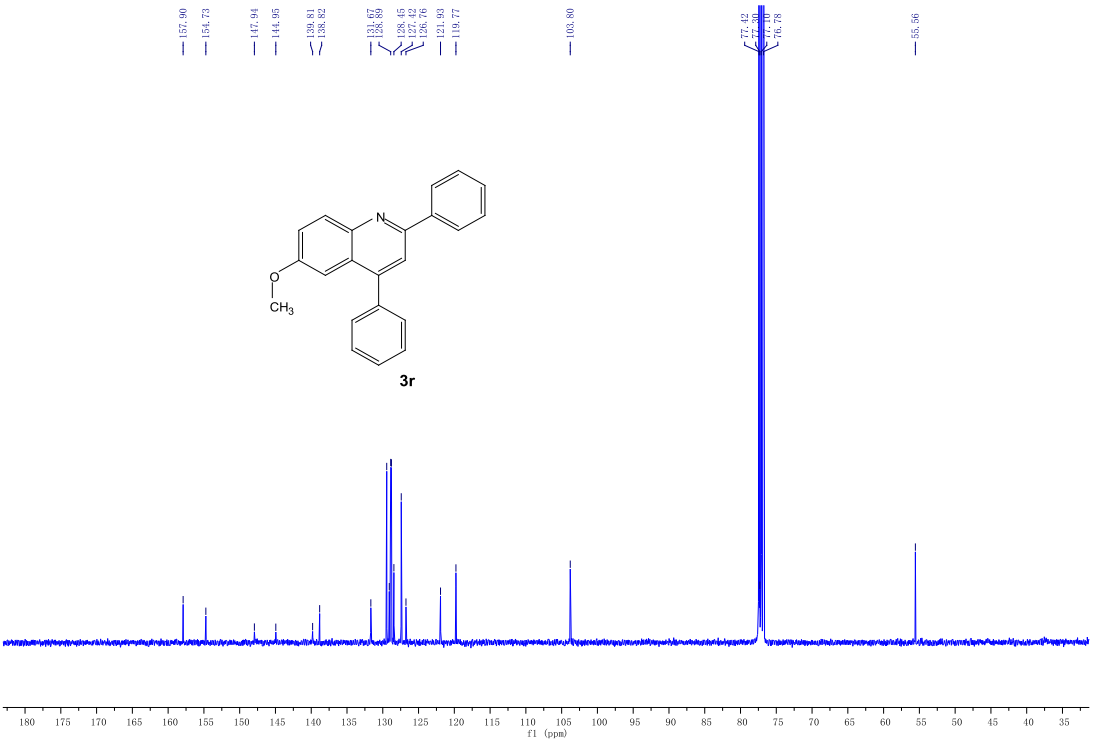
8.17
8.16
8.15
8.14
7.77
7.53
7.44
7.38
7.26
7.20
7.19
3.80
N
H3C
O
3r
3.00
1.09
7.14
2.19
1.07
2.88
f1 (ppm)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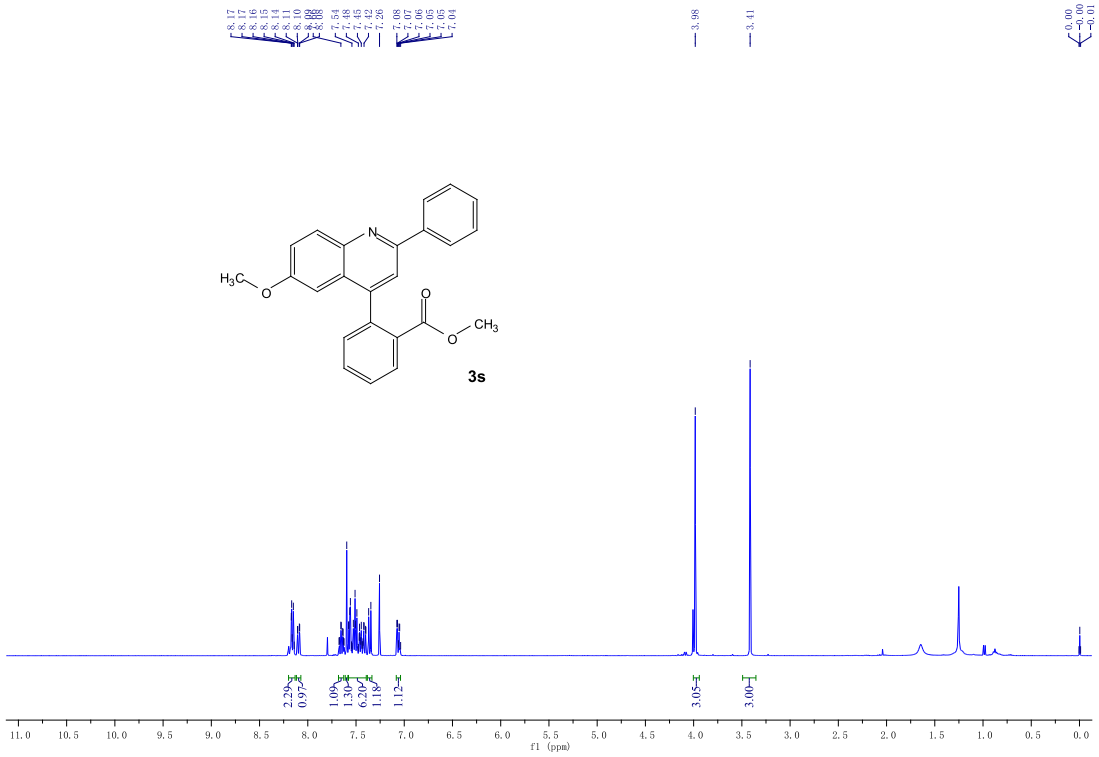
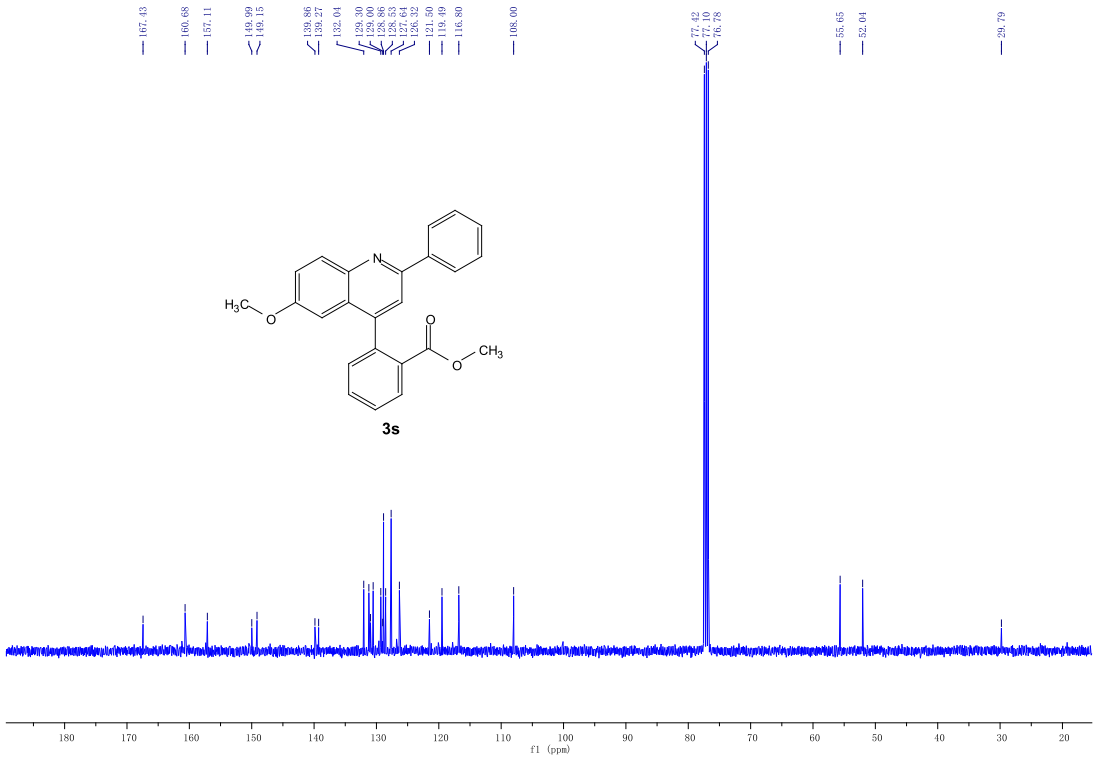
128.69
128.45
127.42
126.76
121.93
119.77
103.80
77.42
77.30
77.10
76.78
55.56
N
O
CH3
3r
f1 (ppm)


8.17
8.16
8.15
8.14
8.11
8.10
7.54
7.48
7.45
7.42
7.26
7.08
7.07
7.06
7.05
7.05
7.04
3.98
3.41
0.00
-0.00
-0.01
N
H3C
O
O
O
CH3
3s
2.29
0.97
1.09
1.30
6.20
1.18
1.12
3.05
3.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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139.86
139.27
132.04
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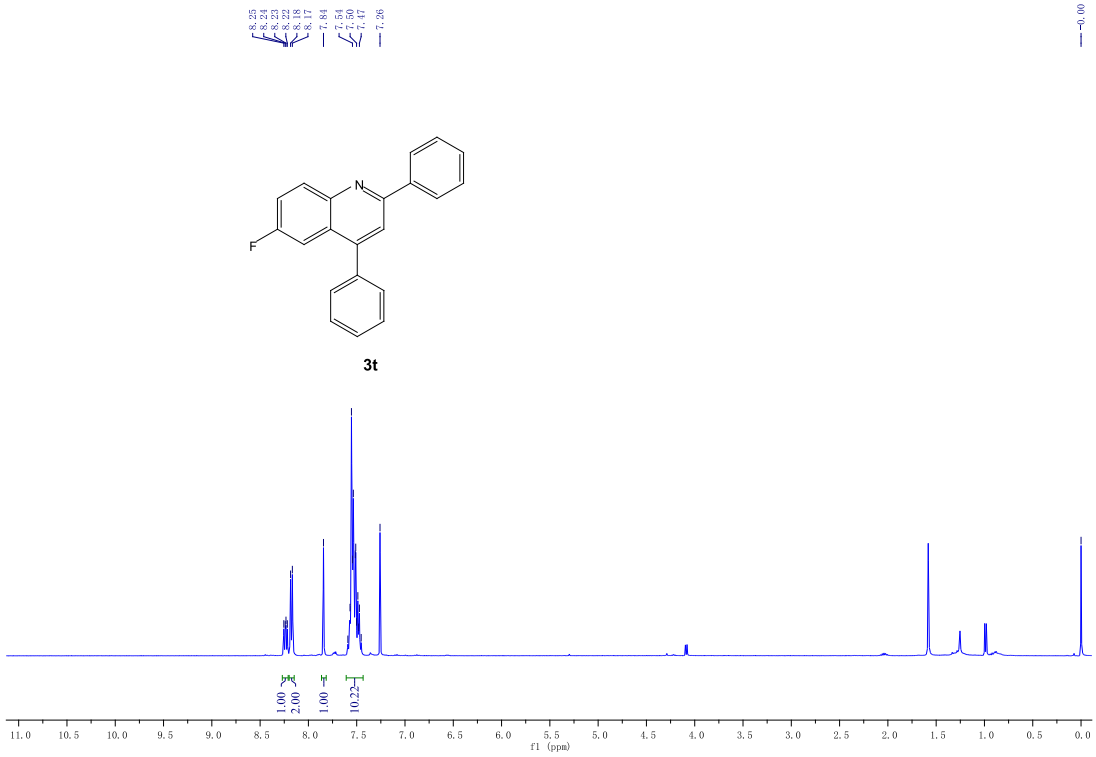
129.00
128.86
128.53
127.64
126.32
121.50
119.49
116.80
108.00
77.42
77.10
76.78
55.65
52.04
29.79
N
H3C
O
O
O
CH3
3s
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)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8.24
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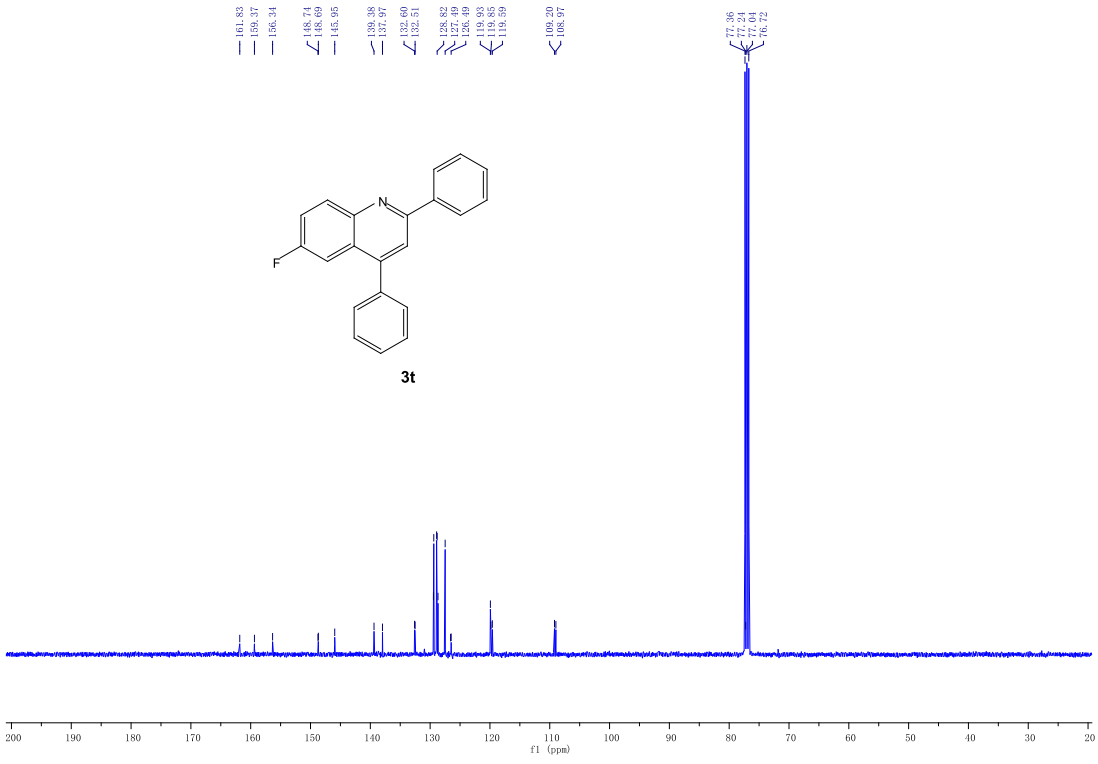
8.22
8.18
8.17
7.84
7.54
7.50
7.47
7.26
0.00
N
F
3t
1.00
2.00
1.00
10.22
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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137.97
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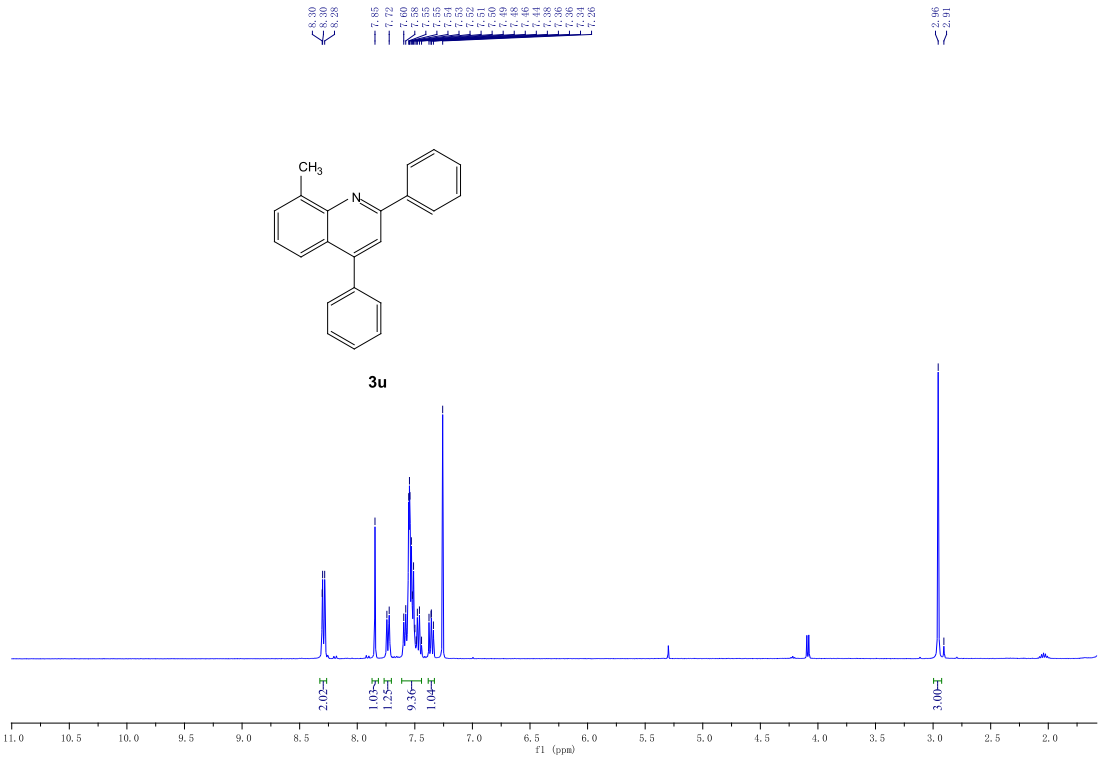
132.51
128.82
127.69
126.49
119.93
119.85
119.59
109.20
108.97
77.36
77.24
77.04
76.72
N
F
3t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)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7.55
7.55
7.54
7.53
7.52
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7.50
7.49
7.48
7.46
7.44
7.38
7.36
7.36
7.34
7.26
2.96
2.91
CH3
N
3u
2.02
1.03
1.25
9.36
1.04
3.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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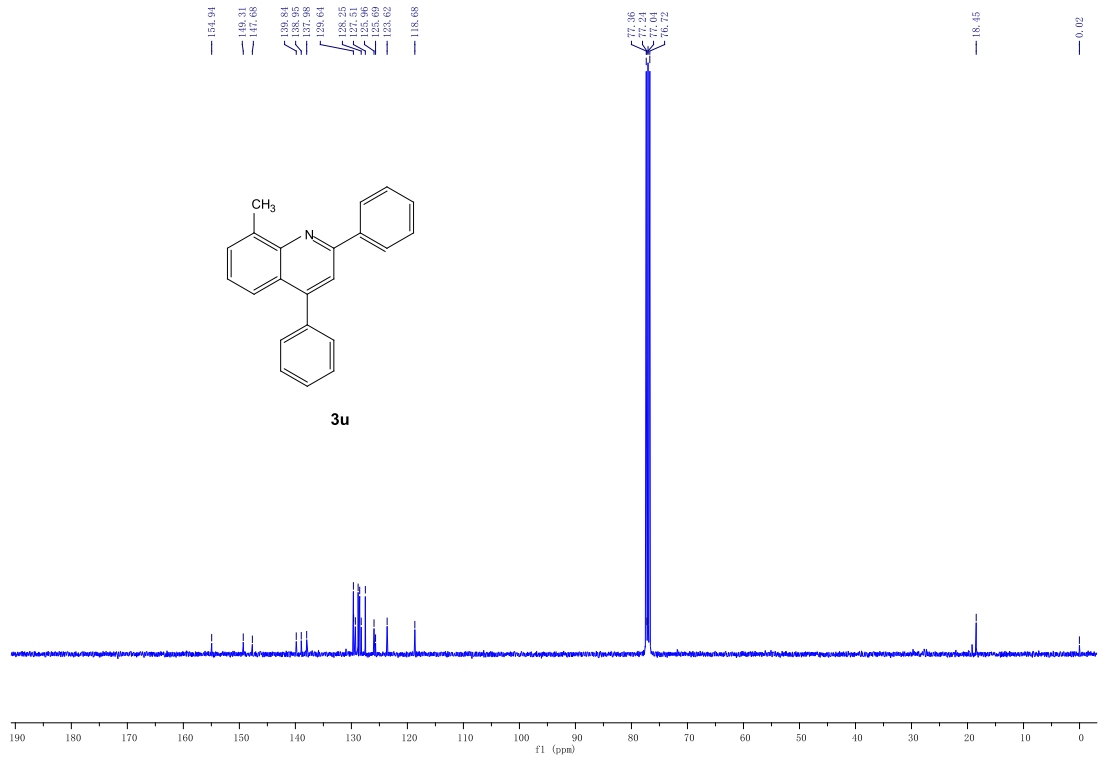
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)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149.31
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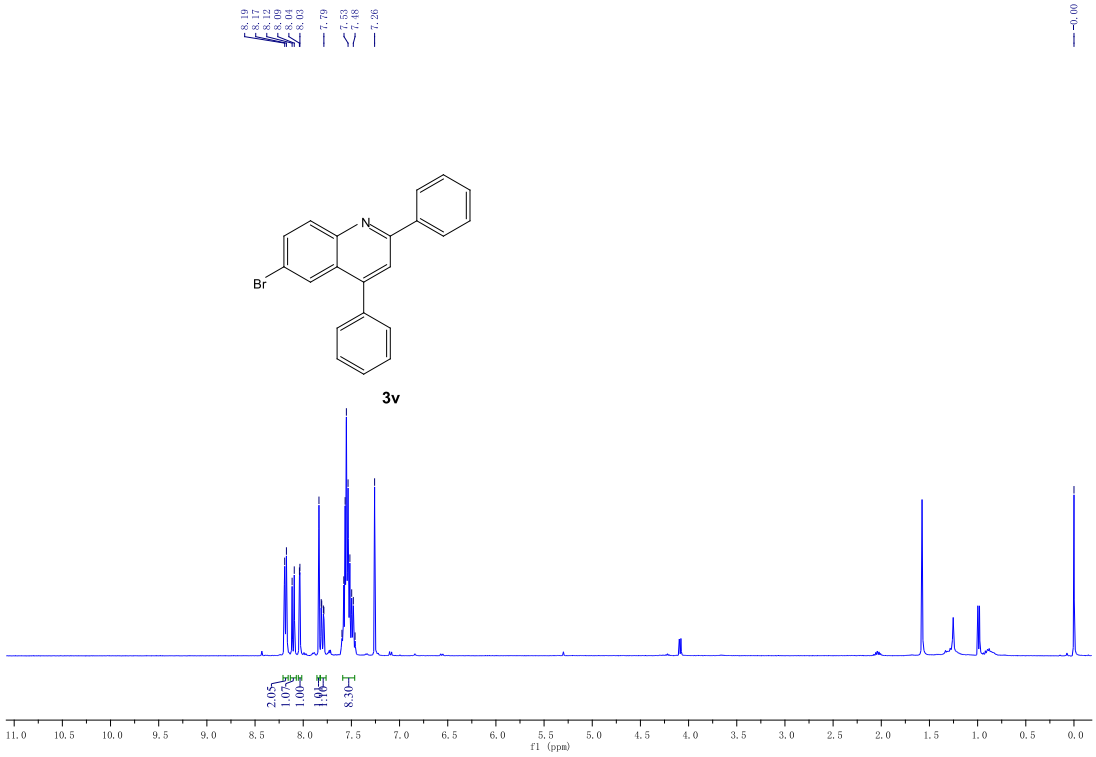
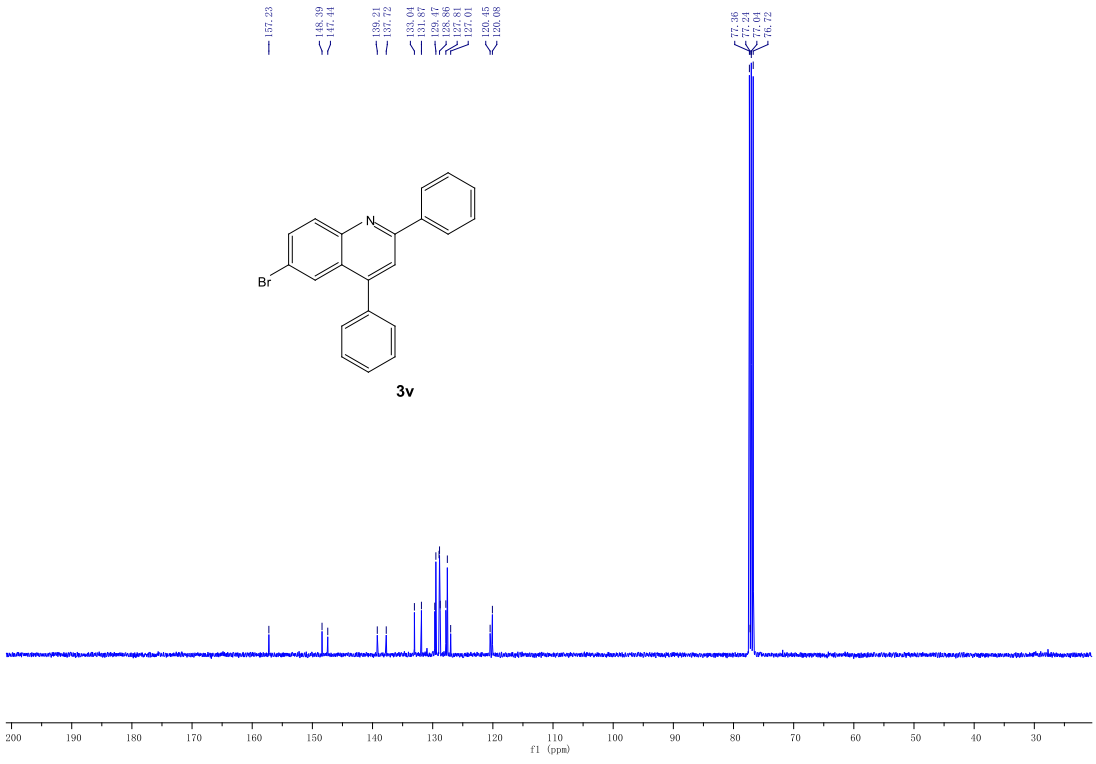
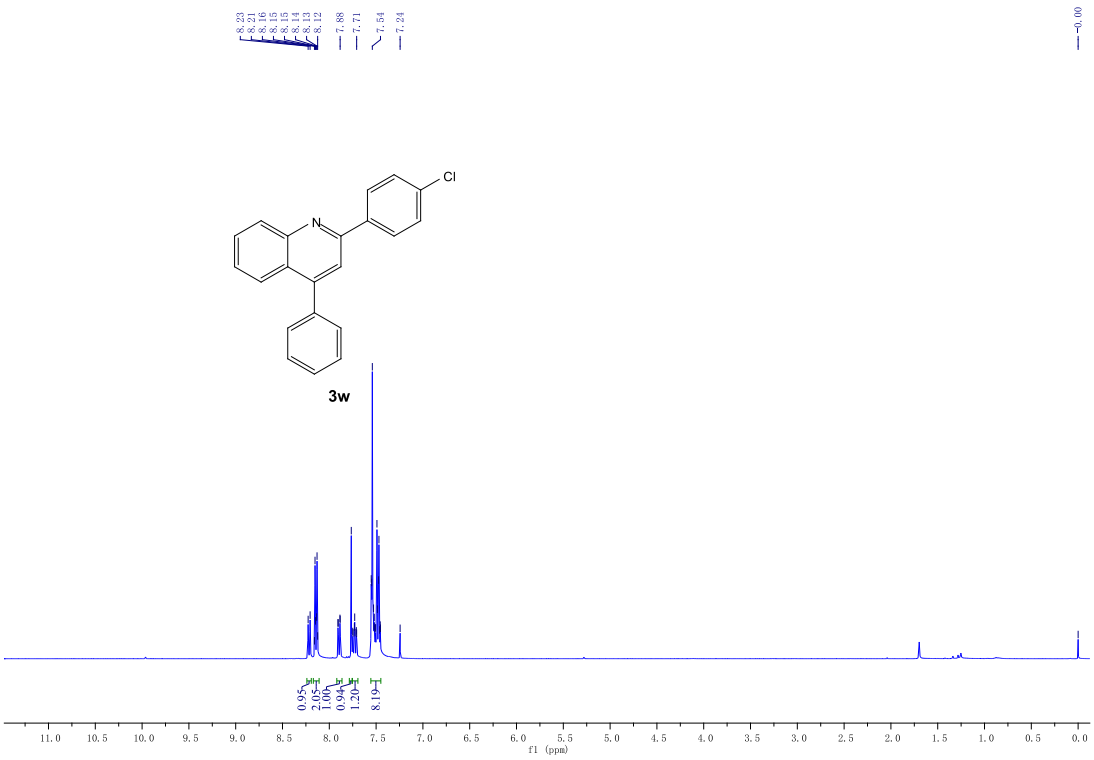
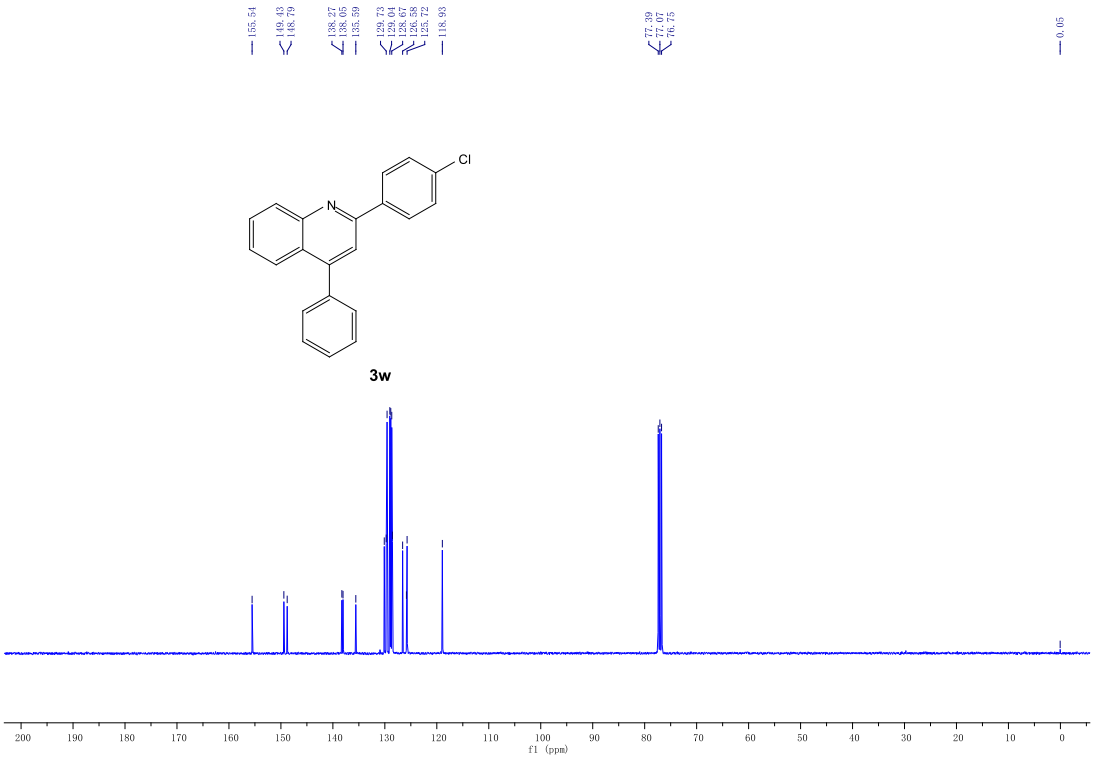
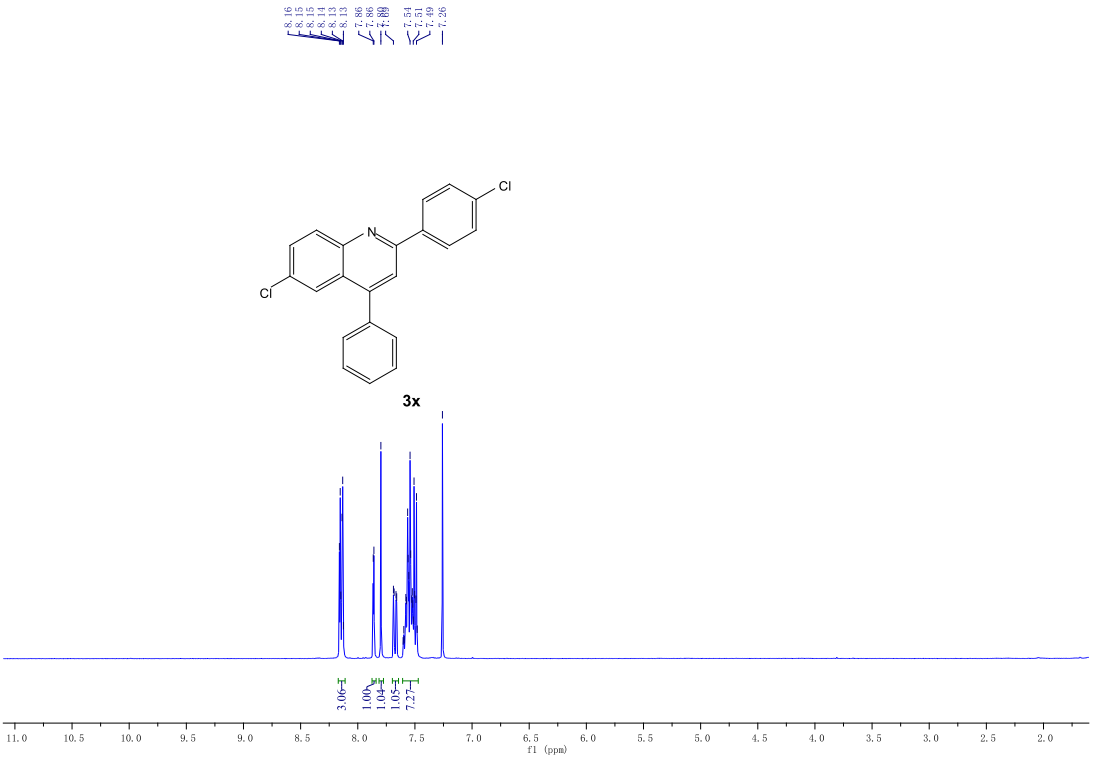
139.84
138.95
137.98
136.64
128.25
127.51
125.96
125.60
123.62
118.68
77.36
77.04
76.72
18.45
0.02
CH3
N
3u
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

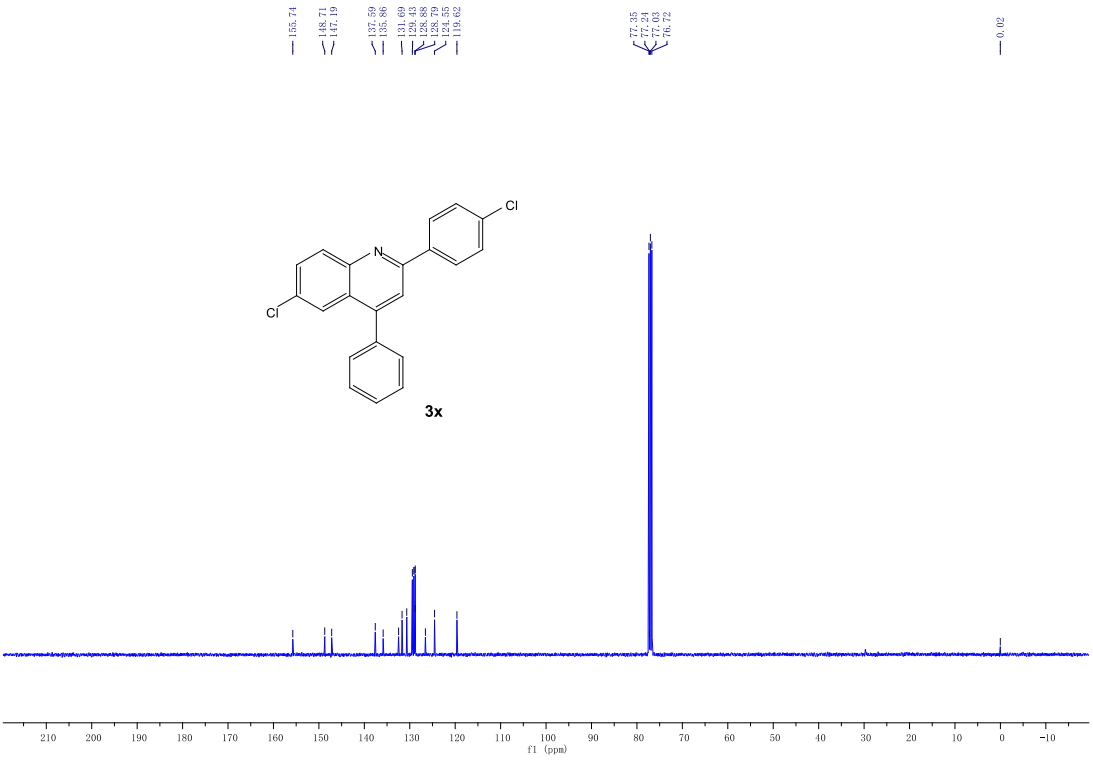

8.19
8.17
8.12
8.09
8.04
8.03
7.79
7.53
7.48
7.26
0.00
N
Br
3v
2.05
1.07
1.00
1.90
8.30
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


157.23
148.39
147.44
139.21
137.72
133.04
131.87
129.47
128.86
127.81
127.01
120.45
120.08
77.36
77.24
77.04
76.72
N
Br
3v
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30
f1 (ppm)


8.23
8.21
8.16
8.15
8.15
8.14
8.13
8.12
7.88
7.71
7.54
7.24
0.00
Cl
N
3w
0.95
2.05
1.06
0.94
1.20
8.19
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


155.54
149.43
148.79
138.27
138.05
135.89
129.73
129.04
128.67
126.58
125.72
118.93
77.39
77.07
76.75
0.05
Cl
N
3w
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.16
8.15
8.15
8.14
8.13
8.13
7.86
7.86
7.89
7.89
7.54
7.51
7.49
7.26
Cl
N
Cl
3x
3.06
1.00
1.04
1.05
7.27
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)


155.74
148.71
147.19
137.59
135.86
131.69
128.43
128.38
128.79
124.55
119.62
77.35
77.24
77.03
76.72
0.02
Cl
N
Cl
3x
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)