SUPPORTING INFORMATION

Gold-catalyzed dual annulation of azide-tethered alkynes with nitriles: expeditious synthesis of oxazolo[4,5-c]quinolines

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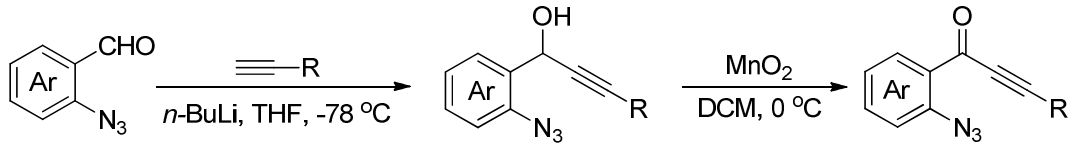
General Information

All reactions were carried out in oven-dried glassware under an atmosphere of dry argon. Metal catalysts used in this reaction were purchased from commercial sources and used without further purification. Flash column chromatography was performed using silica gel (300-400 mesh). Analytical thin-layer chromatography was performed using glass plates pre-coated with 200-300 mesh silica gel impregnated with a fluorescent indicator (254 nm). ^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 MHz spectrometer in $CDCl_3$; chemical shifts are reported in ppm with the solvent signals as reference, and coupling constants (J) are given in Hertz. The peak information is described as: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, comp = composite. High-resolution mass spectra (HRMS) were recorded on a commercial apparatus (CI Source).

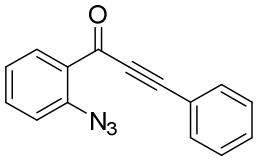
General Procedure for the Synthesis of Azide Alkynes 1.



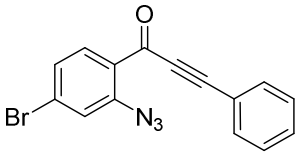
S-1 **S-2** **1**

Synthesis of S-2: To a 50-mL oven-dried flask containing a magnetic stirring bar, alkyne (11.0 mmol) in 20 mL of THF, *n*-BuLi (4.4 mL, 2.5 M, 11.0 mmol, 1.1 equiv) was added slowly at -78 ^{o}C under argon atmosphere. The reaction mixture was stirred for additional 30 mins, then **S-1** (10.0 mmol) was added to the above reaction mixture, and the reaction mixture was stirred for 8 h under these conditions. The reaction was quenched with saturated NH_4Cl (20 mL). The organic phase was separated, and the aqueous layer was extracted with DCM (3 × 20 mL). The combined organic layer was washed with brine (30 mL), dried over anhydrous $MgSO_4$ and concentrated in *vacuo* after filtration. The residue was purified by column chromatography on silica gel (eluted with petroleum ether/ethyl acetate = 5:1) to afford pure products **S-2** in >85% yields.

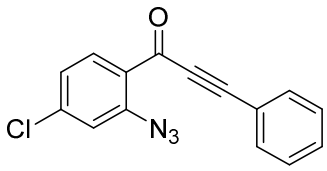
Synthesis of 1:[1] To a 50-mL oven-dried flask containing a magnetic stirring bar, and **S-2** (5.0 mmol) in DCM (10 mL), MnO_2 (6.521 g, 75.0 mmol) was added at room temperature. The resulting reaction mixture was stirred for 5 - 15 mins. After **S-2** was completely consumed (monitored by TLC), the reaction mixture was filtered through a short pad of Celite and concentrated *in vacuo* after filtration. The residue was purified by column chromatography on silica gel (eluted with petroleum ether/ethyl acetate = 30:1) to give **1** in >80% yields.



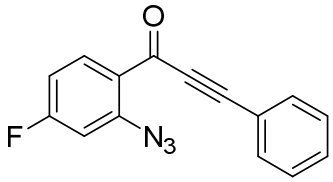
1-(2-Azidophenyl)-3-phenylprop-2-yn-1-one (1a). Yellow solid; mp: 62-65 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.19 – 8.13 (m, 1H), 7.67 – 7.62 (m, 2H), 7.61 – 7.56 (m, 1H), 7.49 – 7.45 (m, 1H), 7.44 – 7.37 (m, 2H), 7.30 – 7.23 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.2, 140.3, 134.4, 133.22, 133.18, 131.0, 129.2, 129.0, 128.8, 124.7, 120.3, 93.5, 88.4. HRMS (TOF MS CI$^+$) calculated for $C_{15}H_9N_3NaO^+$ $[M+Na]^+$: 270.0638, found 270.0642.



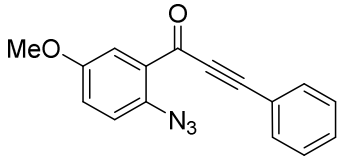
1-(2-Azido-4-bromophenyl)-3-phenylprop-2-yn-1-one (1b). Yellow solid; mp: 91-93 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.00 (d, J = 8.2 Hz, 1H), 7.65 – 7.60 (m, 2H), 7.50 – 7.44 (m, 1H), 7.43 – 7.35 (comp, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.1, 141.6, 134.3, 133.3, 131.2, 129.0, 128.9, 128.1, 127.8, 123.4, 120.1, 94.0, 88.3. HRMS (TOF MS CI$^+$) calculated for $C_{15}H_8BrN_3NaO^+$ $[M+Na]^+$: 347.9743, found 347.9745.



1-(2-Azido-4-chlorophenyl)-3-phenylprop-2-yn-1-one (1c). Yellow solid; mp: 73-75 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.09 (d, *J* = 8.3 Hz, 1H), 7.65 – 7.60 (m, 2H), 7.50 – 7.45 (m, 1H), 7.41 (t, *J* = 7.4 Hz, 2H), 7.25 – 7.20 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 141.6, 140.5, 134.3, 133.2, 131.1, 128.8, 127.3, 125.0, 120.4, 120.0, 93.9, 88.2. HRMS (TOF MS CI$^+$) calculated for $C_{15}H_8ClN_3NaO^+$ $[M+Na]^+$: 304.0248, found 304.0249.

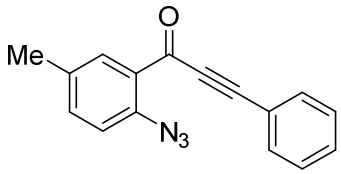


1-(2-Azido-4-fluorophenyl)-3-phenylprop-2-yn-1-one (1d). Yellow solid; mp: 58-60 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.21 (m, *J* = 9.2, 6.3 Hz, 1H), 7.66 – 7.60 (m, 2H), 7.51 – 7.45 (m, 1H), 7.41 – 7.39 (m, 2H), 7.00 – 6.90 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.7, 166.0 (d, *J* = 258.0 Hz), 143.0 (d, *J* = 9.5 Hz), 135.8 (d, *J* = 10.5 Hz), 133.2, 131.0, 128.8, 125.5, 120.1, 112.2 (d, *J* = 21.7 Hz), 107.7 (d, *J* = 25.1 Hz), 93.6, 88.2. ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.0. HRMS (TOF MS CI$^+$) calculated for $C_{15}H_8FN_3NaO^+$ $[M+Na]^+$: 288.0544, found 288.0540.

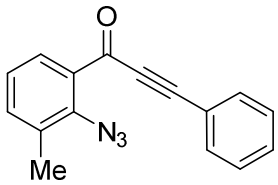


1-(2-Azido-5-methoxyphenyl)-3-phenylprop-2-yn-1-one (1e). Yellow solid; mp: 68-70 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.65 – 7.59 (comp, 3H), 7.48 – 7.42 (m, 1H), 7.41 – 7.36 (m, 2H), 7.18 – 7.09 (m, 2H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.7, 156.5, 133.1, 132.7, 131.0, 129.6, 128.7, 121.5, 120.9, 120.2, 116.6, 93.7, 88.5, 55.8. HRMS (TOF MS CI$^+$) calculated for $C_{16}H_{11}N_3NaO_2^+$ $[M+Na]^+$:

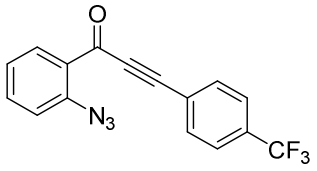
300.0743, found 300.0750.



1-(2-Azido-5-methylphenyl)-3-phenylprop-2-yn-1-one (1f). Yellow solid; mp: 69-71 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.92 (d, *J* = 1.4 Hz, 1H), 7.67 – 7.60 (m, 2H), 7.51 – 7.44 (m, 1H), 7.43 – 7.35 (comp, 3H), 7.15 (d, *J* = 8.2 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.2, 137.5, 135.1, 134.6, 133.3, 133.1, 130.9, 128.74, 128.71, 120.3, 120.2, 93.3, 88.5, 20.8. HRMS (TOF MS CI^{+}) calculated for $C_{16}H_{11}N_3NaO^{+}$ $[M+Na]^{+}$: 284.0794, found 284.0797.

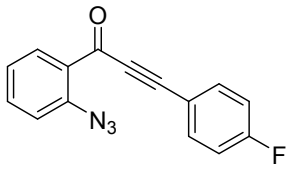


1-(2-Azido-3-methylphenyl)-3-phenylprop-2-yn-1-one (1g). Yellow solid; mp: 70-72 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.10 (d, *J* = 7.8, 1.0 Hz, 1H), 7.66 – 7.61 (m, 2H), 7.45 (d, *J* = 6.4, 3.7, 1.3 Hz, 1H), 7.41 – 7.35 (m, 3H), 7.22 (t, *J* = 7.7 Hz, 1H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.8, 138.6, 135.9, 133.7, 133.1, 131.3, 130.9, 130.7, 128.7, 125.1, 120.0, 93.0, 88.0, 18.1. HRMS (TOF MS CI^{+}) calculated for $C_{16}H_{12}N_3O^{+}$ $[M+H]^{+}$: 262.0975, found 262.0981.

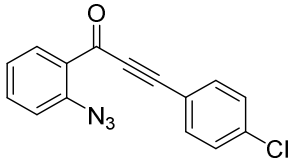


1-(2-Azidophenyl)-3-(4-(trifluoromethyl)phenyl)prop-2-yn-1-one (1h). Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.16 – 8.10 (m, 1H), 7.74 (d, *J* = 8.1 Hz, 2H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.63 – 7.57 (m, 1H), 7.30 – 7.23 (m, 2H). ^{13}C NMR (100

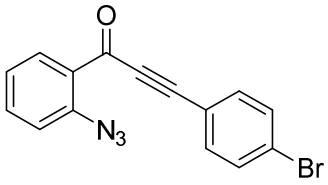
MHz, $CDCl_3$) δ 175.6, 140.5, 136.0, 134.7, 133.21, 133.15, 132.3 (q, *J* = 33.0 Hz), 128.5, 125.8 (q, *J* = 3.7 Hz), 124.8 (q, *J* = 237.1 Hz), 124.7, 120.3, 90.8, 89.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1. HRMS (TOF MS CI^+) calculated for $C_{16}H_8F_3N_3NaO^+$ $[M+Na]^+$: 338.0512, found 338.0500.



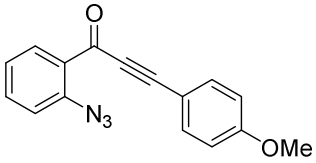
1-(2-Azidophenyl)-3-(4-fluorophenyl)prop-2-yn-1-one (1i). Yellow solid; mp: 82-84 °C. ^1H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.16 – 8.10 (m, 1H), 7.66 – 7.55 (comp, 3H), 7.30 – 7.23 (m, 2H), 7.13 – 7.06 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.0, 164.1 (d, *J* = 254.0 Hz), 140.3, 135.4 (d, *J* = 8.9 Hz), 134.4, 133.1, 128.9, 124.7, 120.3, 116.4 (d, *J* = 3.6 Hz), 116.3 (d, *J* = 22.4 Hz), 92.3, 88.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.9. HRMS (TOF MS CI^+) calculated for $C_{15}H_8FN_3NaO^+$ $[M+Na]^+$: 288.0544, found 288.0552.



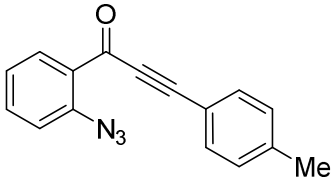
1-(2-Azidophenyl)-3-(4-chlorophenyl)prop-2-yn-1-one (1j). Yellow solid; mp: 86-88 °C. ^1H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.16 – 8.09 (m, 1H), 7.61 – 7.53 (comp, 3H), 7.38 (d, *J* = 8.5 Hz, 2H), 7.26 (t, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.9, 140.3, 137.3, 134.5, 134.3, 133.1, 129.2, 128.8, 124.7, 120.3, 118.7, 92.0, 89.1. HRMS (TOF MS CI^+) calculated for $C_{15}H_8ClN_3NaO^+$ $[M+Na]^+$: 304.0248, found 304.0254.



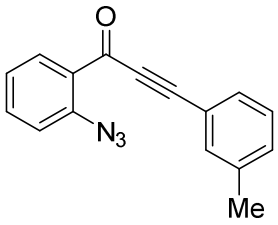
1-(2-Azidophenyl)-3-(4-bromophenyl)prop-2-yn-1-one (1k). Yellow solid; mp: 85-88 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.17 – 8.09 (m, 1H), 7.63 – 7.56 (m, 1H), 7.56 – 7.52 (m, 2H), 7.51 – 7.46 (m, 2H), 7.30 – 7.23 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.7, 140.2, 134.4, 134.3, 133.1, 132.1, 128.6, 125.7, 124.6, 120.2, 119.1, 91.9, 89.1. HRMS (TOF MS CI$^+$) calculated for $C_{15}H_8BrN_3NaO^+$ $[M+Na]^+$: 347.9743, found 347.9744.



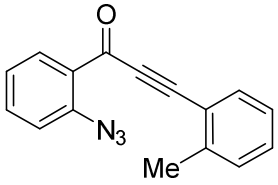
1-(2-Azidophenyl)-3-(4-methoxyphenyl)prop-2-yn-1-one (1l). Yellow solid; mp: 78-81 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.16 (d, J = 7.7 Hz, 1H), 7.63 – 7.58 (comp, 3H), 7.28 (t, J = 7.9 Hz, 2H), 6.94 (d, J = 8.5 Hz, 2H), 3.87 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.2, 161.9, 140.1, 135.3, 134.1, 133.0, 129.3, 124.7, 120.2, 114.5, 112.0, 94.8, 88.5, 55.6. HRMS (TOF MS CI$^+$) calculated for $C_{16}H_{11}N_3NaO_2^+$ $[M+Na]^+$: 300.0743, found 300.0730.



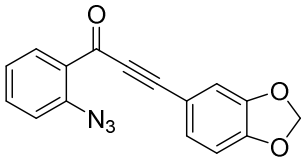
1-(2-Azidophenyl)-3-(*p*-tolyl)prop-2-yn-1-one (1m). Yellow solid; mp: 76-78 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.92 (d, J = 1.4 Hz, 1H), 7.67 – 7.60 (m, 2H), 7.51 – 7.44 (m, 1H), 7.43 – 7.35 (comp, 3H), 7.15 (d, J = 8.2 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.2, 141.7, 140.1, 134.2, 133.2, 133.1, 129.6, 129.1, 124.6, 120.2, 117.1, 94.1, 88.3, 21.8. HRMS (TOF MS CI$^+$) calculated for $C_{16}H_{11}N_3NaO^+$ $[M+Na]^+$: 284.0794, found 284.0797.



1-(2-Azidophenyl)-3-(*m*-tolyl)prop-2-yn-1-one (1n). Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.16 – 8.11 (m, 1H), 7.58 – 7.51 (m, 1H), 7.43 – 7.38 (m, 2H), 7.27 – 7.19 (comp, 4H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.8, 139.9, 138.4, 134.2, 133.4, 133.0, 131.7, 130.1, 128.6, 128.5, 124.5, 120.1, 119.7, 93.6, 88.0, 21.0. HRMS (TOF MS CI$^+$) calculated for $C_{16}H_{11}N_3NaO^+$ $[M+Na]^+$:284.0794, found 284.0784.

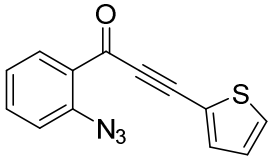


1-(2-Azidophenyl)-3-(*o*-tolyl)prop-2-yn-1-one (1o). Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.21 – 8.10 (m, 1H), 7.64 – 7.53 (m, 2H), 7.39 – 7.33 (m, 1H), 7.30 – 7.18 (comp, 4H), 2.55 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.2, 142.3, 140.2, 134.2, 133.8, 133.0, 131.0, 130.0, 129.2, 126.0, 124.7, 120.2, 120.1, 92.6, 92.3, 20.8. HRMS (TOF MS CI$^+$) calculated for $C_{16}H_{11}N_3NaO^+$ $[M+Na]^+$: 284.0794, found 284.0804.

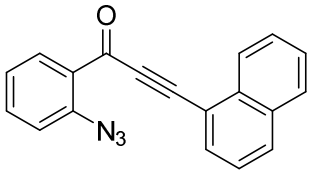


1-(2-Azidophenyl)-3-(benzo[*d*][1,3]dioxol-5-yl)prop-2-yn-1-one (1p). Yellow solid; mp: 124-126 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.36 – 8.31 (m, 1H), 7.79 – 7.77 (m, 1H), 7.49 – 7.46 (m, 2H), 7.45 – 7.41 (m, 1H), 7.26 (d, J = 1.6 Hz, 1H), 7.04 (d, J = 8.0 Hz, 1H), 6.24 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ176.1, 150.4, 147.9, 140.2, 134.2, 133.0, 129.3, 129.1, 124.7, 120.2, 113.2, 112.7, 109.0, 102.0, 94.3, 87.9.

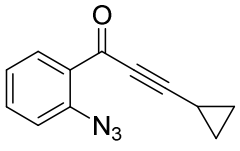
HRMS (TOF MS CI$^+$) calculated for $C_{16}H_9N_3NaO_3^+$ [M+Na]$^+$: 314.0536, found 314.0540.



1-(2-Azidophenyl)-3-(thiophen-2-yl)prop-2-yn-1-one (1q). Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.10 – 8.03 (m, 1H), 7.59 – 7.47 (comp, 3H), 7.27 – 7.20 (m, 2H), 7.09 – 7.02 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.4, 140.2, 136.8, 134.3, 132.7, 132.0, 128.6, 127.9, 124.6, 120.1, 120.0, 93.3, 87.6. HRMS (TOF MS CI$^+$) calculated for $C_{13}H_7N_3OS$ [M+Na]$^+$: 276.0202, found 276.0208.

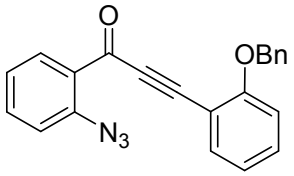


1-(2-Azidophenyl)-3-(naphthalen-1-yl)prop-2-yn-1-one (1r). Yellow solid; mp: 59-61 ^{o}C. ^{1} H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.42 (d, *J* = 8.3 Hz, 1H), 8.24 – 8.21 (m, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.92 – 7.88 (m, 2H), 7.64 – 7.54 (comp, 3H), 7.49 (t, *J* = 7.7 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.0, 140.2, 134.3, 133.8, 133.4, 133.1, 132.9, 131.7, 129.2, 128.7, 127.8, 127.0, 125.8, 125.3, 124.7, 120.2, 117.9, 93.3, 92.0. HRMS (TOF MS CI$^+$) calculated for $C_{19}H_{11}N_3NaO^+$ [M+Na]$^+$: 320.0794, found 320.0783.



1-(2-Azidophenyl)-3-cyclopropylprop-2-yn-1-one (1s). Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.99 – 7.91 (m, 1H), 7.51 – 7.41 (m, 1H), 7.19 – 7.10 (m, 2H), 1.49 – 1.40 (m, 1H), 1.01 – 0.89 (comp, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.9,

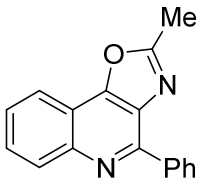
139.6, 133.8, 132.9, 128.9, 124.4, 120.0, 101.5, 76.9, 9.9. HRMS (TOF MS CI^+) calculated for $C_{12}H_9N_3NaO^+$ $[M+Na]^+$: 234.0638, found 234.0654.



1-(2-Azidophenyl)-3-(2-(benzyloxy)phenyl)prop-2-yn-1-one (1t). Yellow solid; mp: 100-102 ^oC. ^1H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.29 – 8.16 (m, 1H), 7.65 – 7.58 (m, 1H), 7.54 – 7.32 (comp, 7H), 7.18 (d, J = 7.9 Hz, 1H), 7.04 – 6.93 (m, 2H), 6.89 – 6.77 (m, 1H), 5.16 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.2, 161.0, 140.0, 136.2, 135.3, 134.2, 134.0, 132.7, 128.72, 128.68, 128.2, 127.6, 124.5, 121.1, 120.1, 112.3, 109.9, 92.5, 90.3, 70.6. HRMS (TOF MS CI^+) calculated for $C_{22}H_{15}N_3NaO_2^+$ $[M+Na]^+$: 376.1056, found 376.1041.

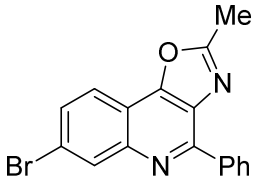
Reactions of Nitriles with Azide Alkynes

To a 10-mL oven-dried vial containing a magnetic stirring bar, azide alkynes **1** (0.2 mmol), $AuCl_3$ (2.3 mg, 5.0 mol %), and nitriles **2** (1.0 mL) were added in sequence at room temperature under argon atmosphere. The resulting reaction mixture was stirred for 12 h under these conditions. When the reaction was completed (monitored by TLC). Then the solvent was evaporated *in vacuo* and the residue was purified by flash column chromatography on silica gel without additional treatment (hexanes/ethyl acetate = 80:1 to 5:1) to afford the pure products **3** in good to high yields.

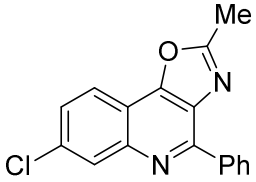


2-Methyl-4-phenyloxazolo[4,5-*c*]quinoline (3a). 49.4 mg, 95% yield. Yellow solid;

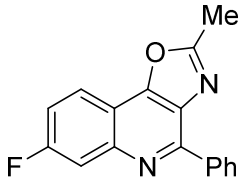
mp: 150-152 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.70 – 8.64 (m, 2H), 8.27 (d, *J* = 8.5 Hz, 1H), 8.10 – 8.08 (m, 1H), 7.73 – 7.69 (m, 1H), 7.62 – 7.55 (comp, 3H), 7.54 – 7.47 (m, 1H), 2.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 153.1, 150.4, 145.5, 137.2, 133.3, 130.1, 129.9, 129.4, 128.9, 128.7, 126.8, 119.9, 115.6, 14.7. HRMS (TOF MS CI^+) calculated for $C_{17}H_{13}N_2O^+$ $[M+H]^+$: 261.1028, found 261.1028.



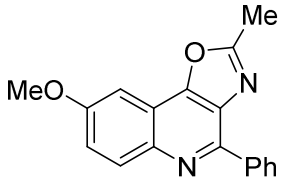
7-Bromo-2-methyl-4-phenyloxazolo[4,5-*c*]quinoline (3b). 59.7 mg, 88% yield. Yellow solid; mp: 202-204 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.67 – 8.61 (m, 2H), 8.39 (d, *J* = 1.9 Hz, 1H), 7.89 (d, *J* = 8.7 Hz, 1H), 7.64 – 7.61 (m, 1H), 7.59 – 7.55 (m, 2H), 7.54 – 7.47 (m, 1H), 2.74 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4, 152.9, 151.2, 145.9, 136.8, 133.5, 132.4, 130.2, 130.1, 129.5, 128.7, 122.8, 121.2, 114.2, 14.7. HRMS (TOF MS CI^+) calculated for $C_{17}H_{12}BrN_2O^+$ $[M+H]^+$: 339.0133, found 339.0124.



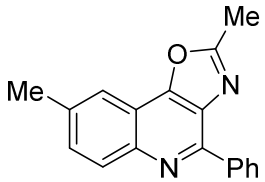
7-Chloro-2-methyl-4-phenyloxazolo[4,5-*c*]quinoline (3c). 47.7 mg, 81% yield. Yellow solid; mp: 197-199 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.67 – 8.62 (m, 2H), 8.21 (d, *J* = 2.0 Hz, 1H), 7.96 (d, *J* = 8.7 Hz, 1H), 7.60 – 7.54 (m, 2H), 7.54 – 7.47 (m, 2H), 2.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4, 152.9, 151.3, 145.74, 136.8, 134.7, 133.4, 130.2, 129.5, 129.1, 128.7, 127.7, 121.2, 113.9, 14.6. HRMS (TOF MS CI^+) calculated for $C_{17}H_{12}ClN_2O^+$ $[M+H]^+$: 295.0638, found 295.0634.



7-Fluoro-2-methyl-4-phenyloxazolo[4,5-*c*]quinoline (3d). 47.3 mg, 85% yield. White solid; mp: 189-191 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.68 – 8.61 (m, 2H), 8.07 – 8.03 (m, 1H), 7.89 – 7.85 (m, 1H), 7.61 – 7.54 (m, 2H), 7.54 – 7.48 (m, 1H), 7.40 – 7.32 (m, 1H), 2.76 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8 (d, *J* = 248.6 Hz), 163.0, 153.2, 151.5, 146.5 (d, *J* = 12.7 Hz), 136.9, 132.8, 130.2, 129.5, 128.7, 121.9 (d, *J* = 9.9 Hz), 117.1 (d, *J* = 25.7 Hz), 114.1 (d, *J* = 20.9 Hz), 112.6, 14.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -110.3. HRMS (TOF MS CI$^+$) calculated for $C_{18}H_{11}ClN_2O^+$ $[M+H]^+$: 279.0928, found 279.0932.

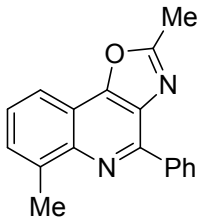


8-Methoxy-2-methyl-4-phenyloxazolo[4,5-*c*]quinoline (3e). 25.5 mg, 44% yield. Yellow solid; mp: 201-203 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.64 – 8.59 (m, 2H), 8.17 (d, *J* = 10.1 Hz, 1H), 7.60 – 7.53 (m, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.36 (d, *J* = 7.8 Hz, 2H), 3.99 (s, 3H), 2.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 158.4, 152.6, 147.9, 141.5, 137.4, 133.6, 131.8, 129.6, 129.2, 128.7, 121.4, 116.4, 98.2, 55.9, 14.8. HRMS (TOF MS CI$^+$) calculated for $C_{18}H_{15}N_2O_2^+$ $[M+H]^+$: 291.1134, found 291.1134.

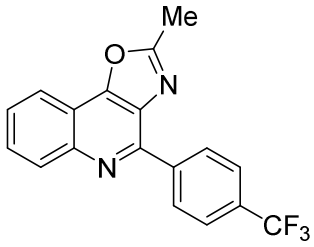


2,8-Dimethyl-4-phenyloxazolo[4,5-*c*]quinoline (3f). 42.2 mg, 77% yield. Yellow

solid; mp: 165-167 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.64 (d, *J* = 7.2 Hz, 2H), 8.13 (d, *J* = 8.7 Hz, 1H), 7.81 (s, 1H), 7.58 (t, *J* = 7.6 Hz, 2H), 7.54 – 7.46 (m, 2H), 2.73 (s, 3H), 2.55 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9, 152.6, 149.4, 144.0, 137.3, 137.0, 133.3, 131.0, 129.8, 129.7, 129.3, 128.6, 118.9, 115.5, 21.8, 14.6. HRMS (TOF MS CI$^+$) calculated for $C_{18}H_{15}N_2O^+$ [M+H]$^+$: 275.1184, found 275.1181.

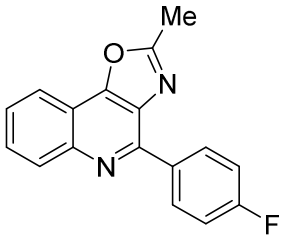


2,6-Dimethyl-4-phenyloxazolo[4,5-*c*]quinoline (3g). 25.8 mg, 47% yield. White solid; mp: 155-157 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.83 – 8.77 (m, 2H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.61 – 7.55 (comp, 3H), 7.53 – 7.46 (m, 2H), 2.95 (s, 3H), 2.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0, 153.5, 148.4, 144.3, 138.4, 137.8, 133.2, 129.8, 129.5, 129.2, 128.7, 126.7, 117.8, 115.6, 18.9, 14.8. HRMS (TOF MS CI$^+$) calculated for $C_{18}H_{15}N_2O^+$ [M+H]$^+$: 275.1184, found 275.1186.

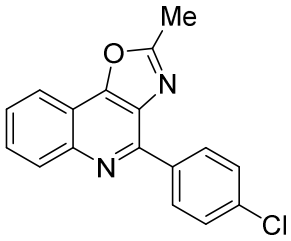


2-Methyl-4-(4-(trifluoromethyl)phenyl)oxazolo[4,5-*c*]quinoline (3h). 58.0 mg, 89% yield. White solid; mp: 150-153 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.85 – 8.74 (m, 2H), 8.27 – 8.18 (m, 1H), 8.08 – 8.05 (m, 1H), 7.80 (d, *J* = 8.1 Hz, 2H), 7.71 (m, 1H), 7.60 (m, 1H), 2.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4, 153.2, 148.4, 145.3, 140.4, 133.3, 131.4 (q, *J* = 32.3 Hz), 130.2, 129.7, 129.1, 127.4, 125.5 (q, *J* = 3.9 Hz), 124.4 (q, *J* = 272.2 Hz), 120.0, 115.8, 14.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.7. HRMS (TOF MS CI$^+$) calculated for $C_{18}H_{12}F_3N_2O^+$ [M+H]$^+$:

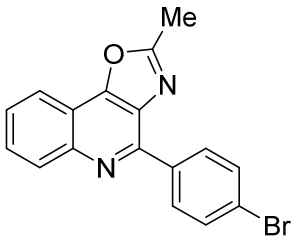
329.0902, found 329.0902.



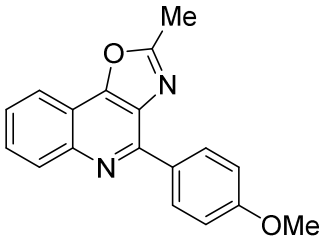
4-(4-Fluorophenyl)-2-methyloxazolo[4,5-*c*]quinoline (3i). 42.3 mg, 76% yield. Yellow solid; mp: 152-154 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.76 – 8.66 (m, 2H), 8.23 – 8.20 (m, 1H), 8.08 – 8.05 (m, 1H), 7.72 – 7.67 (m, 1H), 7.63 – 7.52 (m, 1H), 7.28 – 7.18 (m, 2H), 2.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1 (d, J = 249.9 Hz), 163.1, 153.1, 149.1, 145.39, 133.4 (d, J = 2.9 Hz), 133.0, 131.5 (d, J = 8.4 Hz), 130.0, 128.9, 126.9, 120.0, 115.59 (d, J = 21.5 Hz), 115.56, 14.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.3. HRMS (TOF MS CI$^+$) calculated for $C_{17}H_{12}FN_2O^+$ $[M+H]^+$: 279.0934, found 279.0936.



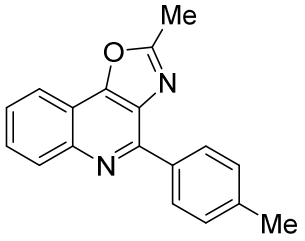
4-(4-Chlorophenyl)-2-methyloxazolo[4,5-*c*]quinoline (3j). 49.5 mg, 84% yield. Yellow solid; mp: 173-175 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.70 – 8.63 (m, 2H), 8.22 (d, J = 8.5 Hz, 1H), 8.10 – 8.07 (m, 1H), 7.73 – 7.69 (m, 1H), 7.61 – 7.57 (m, 1H), 7.56 – 7.50 (m, 2H), 2.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.2, 153.1, 148.9, 145.4, 136.1, 135.7, 133.1, 130.7, 130.1, 129.0, 128.8, 127.1, 120.0, 115.7, 14.7. HRMS (TOF MS CI$^+$) calculated for $C_{17}H_{12}ClN_2O^+$ $[M+H]^+$: 295.0638, found 295.0642.



4-(4-Bromophenyl)-2-methyloxazolo[4,5-*c*]quinoline (3k). 55.6 mg, 82% yield. White solid; mp: 191-193 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.62 – 8.57 (m, 2H), 8.25 – 8.20 (m, 1H), 8.11– 8.09 (m, 1H), 7.74 – 7.66 (comp, 3H), 7.62– 7.59 (m, 1H), 2.78 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3, 153.2, 149.0, 145.5, 136.1, 133.2, 131.9, 131.0, 130.2, 129.1, 127.1, 124.7, 120.1, 115.8, 14.7. HRMS (TOF MS CI^{+}) calculated for $C_{17}H_{12}BrN_2O^{+}$ $[M+H]^{+}$: 339.0133, found 339.0125.

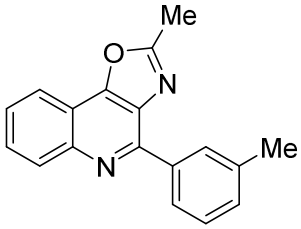


4-(4-Methoxyphenyl)-2-methyloxazolo[4,5-*c*]quinoline (3l). 29.0mg, 50% yield. White solid; mp: 132-134 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.72 – 8.64 (m, 2H), 8.23 – 8.21(m, 1H), 8.07 – 8.04 (m, 1H), 7.70 – 7.56 (m, 1H), 7.56 – 7.52 (m, 1H), 7.10 – 7.07 (m, 2H), 3.89 (s, 3H), 2.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ162.9, 161.2, 153.0, 150.0, 145.5, 133.0, 131.0, 129.9, 129.8, 128.8, 126.4, 119.9, 115.4, 114.0, 55.4, 14.6. HRMS (TOF MS CI^{+}) calculated for $C_{18}H_{15}N_2O_2^{+}$ $[M+H]^{+}$: 291.1128, found 291.1132.

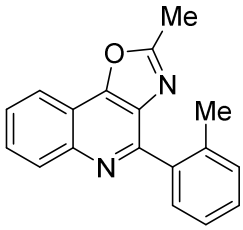


2-Methyl-4-(*p*-tolyl)oxazolo[4,5-*c*]quinoline (3m). 52.1 mg, 95% yield. Yellow solid;

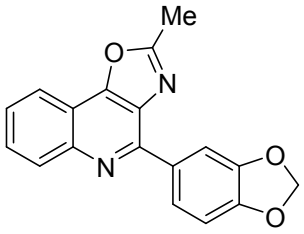
mp: 140-142 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.64 – 8.55 (m, 2H), 8.26 – 8.24 (m, 1H), 8.09 – 8.06 (m, 1H), 7.72 – 7.67 (m, 1H), 7.58 –7.54 (m, 1H), 7.42 – 7.36 (m, 2H), 2.76 (s, 3H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9, 153.0, 150.5, 145.5, 140.0, 134.5, 133.2, 130.0, 129.4, 129.3, 128.8, 126.6, 119.9, 115.6, 21.6, 14.6. HRMS (TOF MS CI$^+$) calculated for $C_{18}H_{15}N_2O^+$ $[M+H]^+$: 275.1184, found 275.1178.



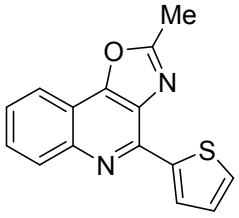
2-Methyl-4-(*m*-tolyl)oxazolo[4,5-*c*]quinoline (3n). 41.1 mg, 75% yield. White solid; mp: 114-116 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.51 – 8.42 (m, 2H), 8.30 –8.27 (m, 1H), 8.13 – 8.11 (m, 1H), 7.74 – 7.70 (m, 1H), 7.62 – 7.58 (m, 1H), 7.49 – 7.45 (t, *J* = 7.6 Hz, 1H), 7.33 – 7.30 (m, 1H), 2.79 (s, 3H), 2.52 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 153.1, 150.8, 145.5, 138.3, 137.2, 133.4, 130.8, 130.2, 129.8, 128.9, 128.6, 126.9, 126.8, 120.0, 115.7, 21.8, 14.7. HRMS (TOF MS CI$^+$) calculated for $C_{18}H_{15}N_2O^+$ $[M+H]^+$: 275.1184, found 275.1185.



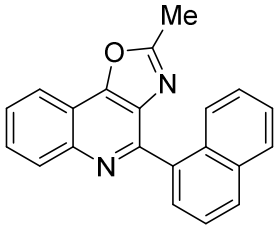
2-Methyl-4-(*o*-tolyl)oxazolo[4,5-*c*]quinoline (3o). 34.0 mg, 62% yield. Yellow solid; mp: 139-141 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.32 – 8.29 (m, 1H), 8.20 – 8.18 (m, 1H), 7.77 – 7.73 (m, 1H), 7.68 – 7.60 (m, 2H), 7.41 – 7.34 (comp, 3H), 2.76 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 153.9, 152.5, 145.4, 136.9, 136.7, 134.2, 131.0, 130.3, 130.1, 129.3, 128.9, 127.1, 126.0, 120.0, 115.6, 20.4, 14.7. HRMS (TOF MS CI$^+$) calculated for $C_{18}H_{15}N_2O^+$ $[M+H]^+$: 275.1184, found 275.1188.



4-(Benzo[*d*][1,3]dioxol-5-yl)-2-methyloxazolo[4,5-*c*]quinoline (3p). 26.2 mg, 43% yield. Yellow solid; mp: 190-192 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.36 – 8.33 (m, 1H), 8.26 – 8.17 (m, 2H), 8.08 – 8.06 (m, 1H), 7.71 – 7.66 (m, 1H), 7.58 – 7.54 (m, 1H), 6.99 (d, *J* = 8.2 Hz, 1H), 6.04 (s, 2H), 2.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ162.9, 153.0, 149.6, 149.2, 148.1, 145.4, 132.9, 131.6, 129.9, 128.8, 126.6, 124.4, 119.9, 115.5, 109.5, 108.4, 101.4, 14.6. HRMS (TOF MS CI$^+$) calculated for $C_{18}H_{13}N_2O_3^+$ $[M+H]^+$: 305.0926, found 305.0920.

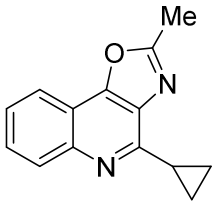


2-Methyl-4-(thiophen-2-yl)oxazolo[4,5-*c*]quinoline (3q). 44.2 mg, 83% yield. Yellow solid; mp: 114-115 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.61 – 8.57 (m, 1H), 8.17 (d, *J* = 8.5 Hz, 1H), 8.04 – 8.01 (m, 1H), 7.69 – 7.65 (m, 1H), 7.55 – 7.51(m, 2H), 7.24 – 7.22 (m, 1H), 2.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4, 152.7, 145.6, 145.5, 142.2, 131.8, 130.8, 129.6, 129.2, 128.9, 128.5, 126.6, 119.9, 115.5, 14.7. HRMS (TOF MS CI$^+$) calculated for $C_{15}H_{11}N_2OS^+$ $[M+H]^+$: 267.0587, found 267.0570.

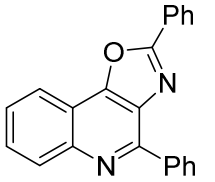


2-Methyl-4-(naphthalen-1-yl)oxazolo[4,5-*c*]quinoline (3r). 39.1 mg, 63% yield. Yellow solid; mp: 188-190 °C. ^{1}H NMR (400 MHz, $CDCl_3$) 8.35 (d, *J* = 8.5 Hz, 1H),

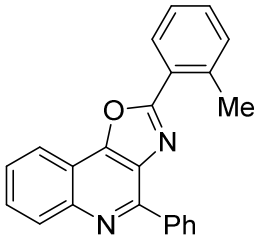
8.25 (d, J = 8.0 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H), 8.01 (d, J = 8.2 Hz, 1H), 7.93 (t, J = 6.3 Hz, 2H), 7.81 –7.77 (m, 1H), 7.73 – 7.64 (m, 2H), 7.53 – 7.49 (m, 1H), 7.47 – 7.42 (m, 1H), 2.76 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 152.9, 152.8, 145.5, 134.8, 134.4, 134.3, 131.6, 130.3, 129.9, 129.1, 128.9, 128.5, 127.3, 126.6, 126.0, 125.3, 120.1, 115.8, 14.7. HRMS (TOF MS CI$^+$) calculated for $C_{21}H_{15}N_2O^+$ $[M+H]^+$: 311.1184, found 311.1179.



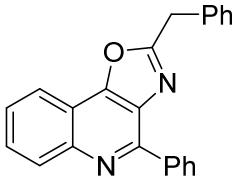
4-Cyclopropyl-2-methyloxazolo[4,5-*c*]quinoline (3s). 30.5 mg, 68% yield. White solid; mp: 94-96 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.07 – 8.01 (m, 2H), 7.64 – 7.60 (m, 1H), 7.52 – 7.48 (m, 1H), 2.80 – 2.72 (comp, 4H), 1.51 – 1.45 (m, 2H), 1.20 – 1.14 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0, 157.4, 151.5, 145.6, 133.9, 129.2, 128.5, 125.8, 120.0, 115.2, 14.6, 14.3, 10.4. HRMS (TOF MS CI$^+$) calculated for $C_{14}H_{13}N_2O^+$ $[M+H]^+$: 225.1028, found 225.1027.



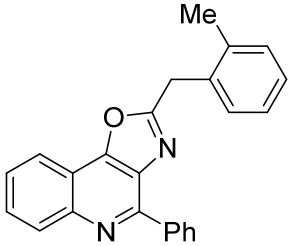
2,4-Diphenyloxazolo[4,5-*c*]quinolinev (3A). 47.1 mg, 73% yield. Yellow solid; mp: 167-169 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.84 – 8.81 (m, 2H), 8.37– 8.35 (m, 2H), 8.29– 8.27 (d, J = 8.5 Hz, 1H), 8.22– 8.20 (m, 1H), 7.75– 7.63 (m, 1H), 7.63– 7.60 (comp, 3H), 7.57 – 7.52 (comp, 4H). ^{13}C NMR (100MHz, $CDCl_3$) δ 162.5, 152.9, 150.7, 145.8, 137.2, 134.1, 131.8, 130.3, 130.0, 129.7, 129.1, 128.7, 127.8, 126.9, 126.8, 120.2, 115.8. HRMS (TOF MS CI$^+$) calculated for $C_{22}H_{15}N_2O^+$ $[M+H]^+$: 323.1179, found 323.1185.



4-Phenyl-2-(*o*-tolyl)oxazolo[4,5-*c*]quinoline (3B). 41.7 mg, 62% yield. White solid; mp: 189-191 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.90 – 8.84 (m, 2H), 8.31 – 8.28 (m, 2H), 8.21 – 8.19 (m, 1H), 7.75 – 7.70 (m, 1H), 7.63 – 7.58 (comp, 3H), 7.55 – 7.51(m, 1H), 7.45 – 7.35 (comp, 3H), 2.90 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.5, 152.3, 150.5, 145.7, 139.2, 137.2, 134.0, 132.1, 131.3, 130.3, 130.0, 129.8, 129.6, 129.0, 128.6, 126.9, 126.3, 125.6, 120.3, 115.7, 22.6. HRMS (TOF MS CI$^+$) calculated for $C_{23}H_{17}N_2O^+$ $[M+H]^+$: 337.1335, found 337.1333.

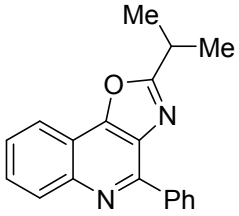


2-Benzyl-4-phenyloxazolo[4,5-*c*]quinoline (3C). 43.7 mg, 65% yield. Yellow solid; mp: 94-96 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.75 – 8.67 (m, 2H), 8.30 (d, J = 8.5 Hz, 1H), 8.15 –8.12 (m, 1H), 7.75 – 7.71 (m, 1H), 7.63 – 7.57 (comp, 3H), 7.55 – 7.49 (m, 1H), 7.48 – 7.44 (m, 2H), 7.41 – 7.35 (m, 2H), 7.34 – 7.28 (m, 1H), 4.46 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 153.5, 150.8, 145.6, 137.1, 134.8, 133.3, 130.12, 130.07, 129.6, 129.13, 129.09, 129.0, 128.8, 127.6, 127.0, 120.2, 115.7, 35.3. HRMS (TOF MS CI$^+$) calculated for $C_{23}H_{17}N_2O^+$ $[M+H]^+$: 337.1341, found 337.1342.

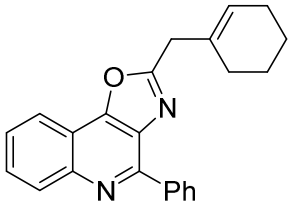


2-(2-Methylbenzyl)-4-phenyloxazolo[4,5-*c*]quinoline (3D). 40.6 mg, 58% yield. Yellow solid; mp: 120-122 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.78 (d, J = 7.6

Hz, 2H), 8.32 (d, *J* = 8.5 Hz, 1H), 8.13 (d, *J* = 8.1 Hz, 1H), 7.79 – 7.72 (m, 1H), 7.67 – 7.55(comp, 4H), 7.41 – 7.39 (m, 1H), 7.30 – 7.25 (comp, 3H), 4.47 (s, 2H), 2.58 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ164.3, 153.3, 150.6, 145.6, 137.2, 136.9, 133.4, 133.2, 130.7, 130.1, 130.0, 129.9, 129.6, 129.0, 128.7, 127.8, 126.8, 126.5, 120.1, 115.7, 33.1, 19.9. HRMS (TOF MS CI$^+$) calculated for $C_{24}H_{19}N_2O^+$ $[M+H]^+$: 351.1497, found 351.1490.

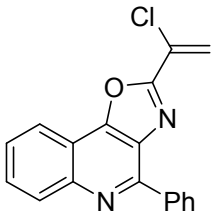


2-Isopropyl-4-phenyloxazolo[4,5-*c*]quinoline (3E). 49.6 mg, 86% yield. Yellow solid; mp: 88-90 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.78 – 8.75 (m, 2H), 8.29 (d, *J* = 8.5 Hz, 1H), 8.18 – 8.16 (m, 1H), 7.75 – 7.70 (m, 1H), 7.67 – 7.56 (comp, 3H), 7.56 – 7.49 (m, 1H), 3.44 (hept, *J* = 7.0 Hz, 1H), 1.58 (d, *J* = 7.0 Hz, 6H).^{13}C NMR (100 MHz, $CDCl_3$) δ170.6, 153.0, 150.6, 145.5, 137.3, 133.2, 130.2, 129.9, 129.6, 128.8, 128.7, 126.8, 120.1, 115.8, 29.2, 20.7. HRMS (TOF MS CI$^+$) calculated for $C_{19}H_{17}N_2O^+$ $[M+H]^+$: 289.1341, found 289.1350.

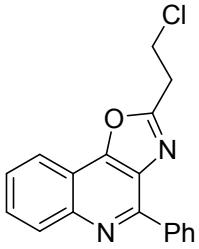


2-(Cyclohex-1-en-1-ylmethyl)-4-phenyloxazolo[4,5-*c*]quinoline (3F). 42.9 mg, 63% yield. Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.72 – 8.69 (m, 2H), 8.30 (d, *J* = 8.5 Hz, 1H), 8.20 – 8.17 (m, 1H), 7.76 – 7.71 (m, 1H), 7.64 – 7.56 (comp, 3H), 7.54 – 7.48 (m, 1H), 5.71 – 5.68 (m, 1H), 3.75 (d, *J* = 1.9 Hz, 2H), 2.18 – 2.03 (m, 4H), 1.64 (comp, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 150.7, 145.5, 137.2, 133.3, 131.9, 130.1, 130.0, 129.6, 129.0, 128.7, 126.9, 125.9, 120.2, 115.8, 37.5, 28.5, 25.4, 22.8, 22.1. HRMS (TOF MS CI$^+$) calculated for $C_{23}H_{21}N_2O^+$ $[M+H]^+$: 341.1648,

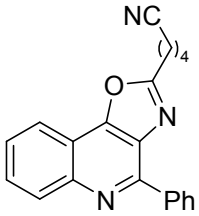
found 341.1650.



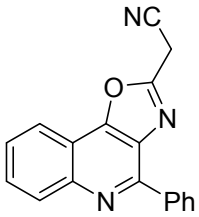
2-(1-Chlorovinyl)-4-phenyloxazolo[4,5-*c*]quinoline (3G). 39.8 mg, 65% yield. Yellow solid; mp: 130-132 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.76 – 8.73 (m, 2H), 8.28 – 8.25 (m, 1H), 8.18 – 8.14 (m, 1H), 7.76 – 7.72 (m, 1H), 7.63 – 7.56 (comp, 3H), 7.55 – 7.51 (m, 1H), 6.74 (d, J = 2.1 Hz, 1H), 6.09 (d, J = 2.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 153.2, 150.9, 146.1, 136.8, 133.5, 130.29, 130.26, 129.7, 129.6, 128.7, 127.2, 126.8, 122.1, 120.3, 115.4. HRMS (TOF MS CI$^+$) calculated for $C_{18}H_{11}ClN_2ONa^+$ $[M+Na]^+$: 329.0458, found 329.0443.



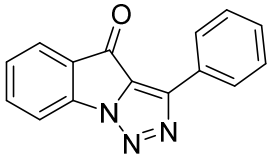
2-(2-Chloroethyl)-4-phenyloxazolo[4,5-*c*]quinoline (3H). 46.3 mg, 75% yield. Yellow solid; mp: 145-147 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.72 – 8.67 (m, 2H), 8.28 (d, J = 8.5 Hz, 1H), 8.14 – 8.12 (m, 1H), 7.76 – 7.72 (m, 1H), 7.65 – 7.55 (comp, 3H), 7.55 – 7.48 (m, 1H), 4.09 (t, J = 7.0 Hz, 2H), 3.56 (t, J = 7.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ162.5, 153.1, 150.6, 145.7, 137.1, 133.0, 130.2, 130.1, 129.5, 129.2, 128.7, 127.0, 120.1, 115.6, 40.2, 32.3. HRMS (TOF MS CI$^+$) calculated for $C_{18}H_{14}ClN_2O^+$ $[M+H]^+$: 309.0795, found 309.0799.



5-(4-Phenyloxazolo[4,5-*c*]quinolin-2-yl)pentanenitrile (3I). 43.2 mg, 66% yield. Yellow solid; mp: 101-103 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.72 – 8.66 (m, 2H), 8.27 (d, *J* = 8.5 Hz, 1H), 8.10 – 8.05 (m, 1H), 7.73 – 7.69 (m, 1H), 7.69 – 7.56 (comp, 3H), 7.52 – 7.49 (m, 1H), 3.07 (t, *J* = 7.4 Hz, 2H), 2.42 (t, *J* = 7.0 Hz, 2H), 2.12 – 2.06 (m, 2H), 1.88 – 1.78 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 152.9, 150.3, 145.4, 137.0, 132.90, 132.87, 130.0, 129.4, 129.0, 128.6, 126.9, 120.0, 119.3, 115.5, 27.8, 25.7, 24.8, 17.0. HRMS (TOF MS CI$^+$) calculated for $C_{21}H_{18}N_3O^+$ $[M+H]^+$: 328.1450, found328.1443.

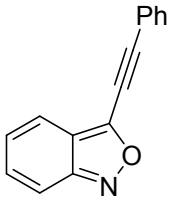


2-(4-Phenyloxazolo[4,5-*c*]quinolin-2-yl)acetonitrile (3J). 46.8 mg, 82% yield. Red solid; mp: 180-182 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.68 – 8.59 (m, 2H), 8.26 (d, *J* = 8.5 Hz, 1H), 8.10 (d, *J* = 8.1 Hz, 1H), 7.80 – 7.72 (m, 1H), 7.66 – 7.49 (comp, 4H), 4.21 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.4, 153.6, 150.5, 145.9, 136.5, 132.6, 130.4, 130.2, 129.8, 129.4, 128.8, 127.4, 120.1, 115.3, 112.9, 18.9. HRMS (TOF MS CI$^+$) calculated for $C_{18}H_{11}N_3ONa^+$ $[M+H]^+$: 286.0980, found 286.0980.



3-Phenyl-4*H*-[1,2,3]triazolo[1,5-*a*]indol-4-one (4a). Yellow solid; mp: 241-243 ^{o}C.

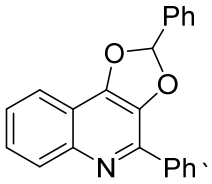
^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.39 – 8.34 (m, 2H), 7.84 – 7.77 (m, 2H), 7.71 – 7.66 (m, 1H), 7.54 – 7.42 (comp, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.0, 146.9, 140.6, 135.8, 130.9, 129.91, 129.87, 129.2, 128.9, 128.4, 127.8, 126.1, 113.1. HRMS (TOF MS CI^+) calculated for $C_{15}H_{10}N_3O^+$ $[M+H]^+$: 248.0818, found 248.0823.



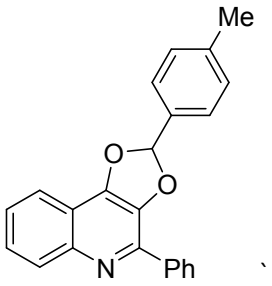
3-(Phenylethynyl)benzo[*c*]isoxazole (5a). Yellow solid; mp: 68-70 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.67 – 7.62 (comp, 4H), 7.47 – 7.39 (comp, 3H), 7.36 – 7.30 (m, 1H), 7.12 – 7.06 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 149.4, 132.0, 131.2, 130.2, 128.8, 125.3, 121.1, 120.4, 119.9, 115.8, 103.6, 75.9. HRMS (TOF MS CI^+) calculated for $C_{15}H_{10}NO^+$ $[M+H]^+$: 220.0757, found 220.0762.

Reactions of Aldehydes with Azide Alkynes

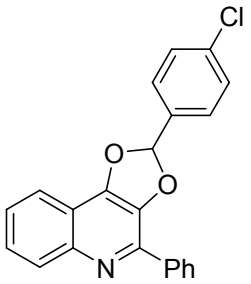
To a 10-mL oven-dried vial containing a magnetic stirring bar, azide alkynes **1** (0.20 mmol), $AuCl_3$ (2.3 mg, 5.0 mol %), and aldehydes **6** (0.24 mmol) were added in sequence at room temperature under argon atmosphere. The resulting reaction mixture was stirred for 4 h under these conditions. When the reaction was completed (monitored by TLC). Then the solvent was evaporated *in vacuo* and the residue was purified by flash column chromatography on silica gel without additional treatment (hexanes/ethyl acetate = 80:1 to 20:1) to afford the pure products **7** in good yields.



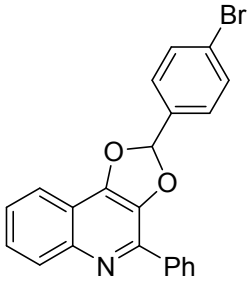
2,4-Diphenyl-[1,3]dioxolo[4,5-*c*]quinoline (7a). 40.3 mg, 62% yield. Yellow solid; mp: 156 -158 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.41 (d, *J* = 7.3 Hz, 2H), 8.14 (d, *J* = 8.6 Hz, 1H), 7.87 – 7.85 (d, *J* = 8.3 Hz, 1H), 7.71 – 7.68 (m, 2H), 7.64 – 7.57 (m, 1H), 7.55 – 7.45 (comp, 7H), 7.35 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.8, 145.8, 142.1, 139.2, 136.2, 135.7, 130.9, 129.8, 129.7, 129.0, 128.7, 128.5, 128.3, 126.8, 126.2, 120.2, 115.7, 112.5. HRMS (TOF MS CI^{+}) calculated for $C_{22}H_{16}NO_2^{+}$ $[M+H]^{+}$: 326.1181, found 326.1187.



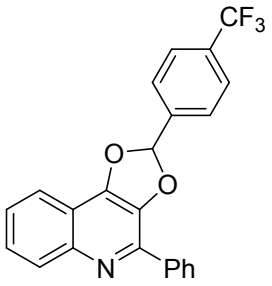
4-Phenyl-2-(*p*-tolyl)-[1,3]dioxolo[4,5-*c*]quinoline (7b). 35.2 mg, 52% yield. Yellow solid; mp: 215-217 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.44 – 8.38 (m, 2H), 8.14 (d, *J* = 8.7 Hz, 1H), 7.87 – 7.84 (m, 1H), 7.63 – 7.55 (comp, 3H), 7.55 – 7.50 (m, 2H), 7.50 – 7.43 (m, 2H), 7.34 – 7.28 (comp, 3H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.9, 145.8, 142.1, 141.1, 139.3, 136.3, 132.8, 129.8, 129.6, 128.7, 128.5, 128.2, 126.8, 126.1, 120.2, 115.7, 112.7, 21.6. HRMS (TOF MS CI^{+}) calculated for $C_{23}H_{18}NO_2^{+}$ $[M+H]^{+}$: 340.1332, found 340.1338.



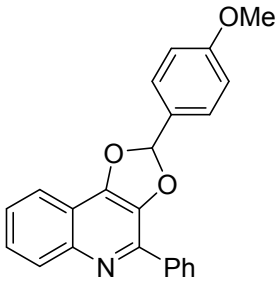
2-(4-Chlorophenyl)-4-phenyl-[1,3]dioxolo[4,5-*c*]quinoline (7c). 42.5 mg, 59% yield. Yellow solid; mp: 212-214 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.42 – 8.35 (m, 2H), 8.15 (d, *J* = 8.6 Hz, 1H), 7.85 – 7.83 (m, 1H), 7.63 – 7.59 (comp, 3H), 7.55 – 7.43 (comp, 6H), 7.32 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ149.7, 145.8, 139.0, 136.9, 136.0, 134.2, 129.80, 129.76, 129.3, 128.8, 128.5, 128.1, 126.3, 120.1, 115.6, 111.7. HRMS (TOF MS CI$^+$) calculated for $C_{22}H_{15}ClNO_2^+$ $[M+H]^+$: 360.0791, found 360.0801.



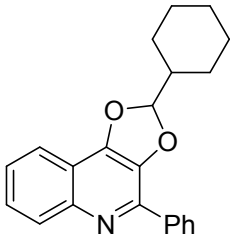
2-(4-Bromophenyl)-4-phenyl-[1,3]dioxolo[4,5-*c*]quinoline (7d). 50.1 mg, 62% yield. Yellow solid; mp: 135-137 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.41 – 8.36 (m, 2H), 8.13 (m, 1H), 7.84 (m, 1H), 7.64 – 7.58 (comp, 3H), 7.57 – 7.50 (comp, 4H), 7.49 – 7.44 (m, 2H), 7.29 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.5, 145.9, 142.1, 139.0, 136.1, 134.7, 132.2, 129.9, 129.7, 128.7, 128.41, 128.36, 126.3, 125.2, 120.1, 115.6, 111.6. HRMS (TOF MS CI$^+$) calculated for $C_{22}H_{15}BrNO_2^+$ $[M+H]^+$: 404.0281, found 404.0285.



4-Phenyl-2-[4-(trifluoromethyl)phenyl]-[1,3]dioxolo[4,5-*c*]quinoline (7e). 31.3 mg, 40% yield. Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.41 – 8.36 (m, 2H), 8.15 (d, *J* = 8.7 Hz, 1H), 7.89 – 7.79 (comp, 3H), 7.75 (d, *J* = 8.2 Hz, 2H), 7.62 (m, 1H), 7.51 (comp, 4H), 7.39 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.5, 145.9, 142.2, 139.4, 138.9, 136.0, 132.9(d, *J* = 32.7 Hz), 129.9, 129.8, 128.9, 128.54, 128.45, 127.2, 126.4, 126.0 (q, *J* = 3.8 Hz), 123.84 (d, *J* = 272.5 Hz), 120.0, 115.6, 111.2. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9. HRMS (TOF MS CI$^+$) calculated for $C_{23}H_{15}F_3NO_2^+$ $[M+H]^+$: 394.1055, found 394.1047.

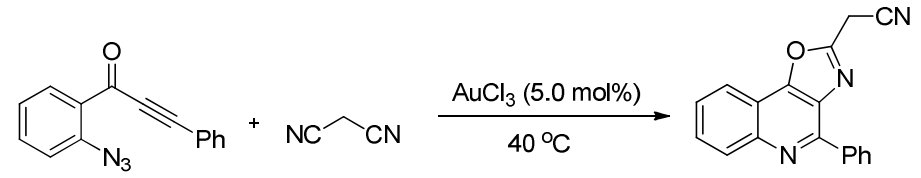


2-(4-Methoxyphenyl)-4-phenyl-[1,3]dioxolo[4,5-*c*]quinoline (7f). 48.3 mg, 68% yield. Yellow solid; mp: 227-229 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.42 – 8.36 (m, 2H), 8.12 (d, *J* = 8.6 Hz, 1H), 7.85 – 7.83 (m, 1H), 7.64 – 7.57 (comp, 3H), 7.51 (t, *J* = 7.3 Hz, 2H), 7.48 – 7.41 (m, 2H), 7.30 (s, 1H), 7.02 – 6.97 (m, 2H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.7, 149.9, 145.8, 142.0, 139.3, 136.3, 129.7, 128.7, 128.5, 128.4, 128.2, 127.8, 126.1, 120.2, 115.7, 114.4, 112.7, 55.5. HRMS (TOF MS CI$^+$) calculated for $C_{23}H_{18}NO_3^+$ $[M+H]^+$: 356.1281, found 356.1288.



2-Cyclohexyl-4-phenyl-[1,3]dioxolo[4,5-*c*]quinoline (7g). 39.8 mg, 60% yield. Yellow solid; mp: 103-105 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.40 – 8.34 (m, 2H), 8.09 (d, *J* = 8.6 Hz, 1H), 7.81 – 7.84 (m, 1H), 7.60 – 7.50 (comp, 3H), 7.49 – 7.40 (m, 2H), 6.28 (d, *J* = 4.6 Hz, 1H), 2.11 – 1.95 (m, 3H), 1.88 – 1.81 (m, 2H), 1.74 (d, *J* = 10.3 Hz, 1H), 1.35 – 1.26 (comp, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.2, 145.5, 141.8, 139.5, 136.4, 129.8, 129.5, 128.7, 128.4, 128.0, 125.9, 120.1, 117.1, 115.6, 42.7, 26.34, 26.27, 25.53, 25.51. HRMS (TOF MS CI$^+$) calculated for $C_{22}H_{22}NO_2^+$ $[M+H]^+$: 332.1651, found 332.1649.

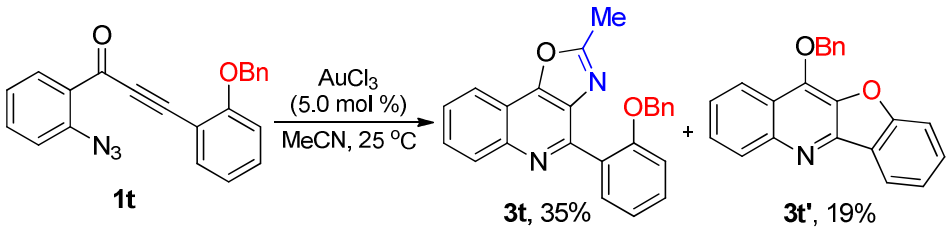
General Procedure for the Scale Up.



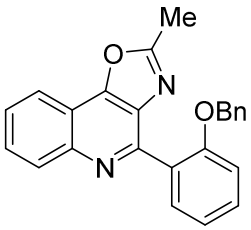
1a, 1.236 g, 5.0 mmol **2j** **3J**, 1.083 g, 76% yield

To a 50-mL oven-dried round-bottom flask with a magnetic stirring bar, **1a** (1.236 g, 5.0 mmol), $AuCl_3$ (58.1 mg, 5.0 mol %), and malononitrile **2j** (20.0 mL) were added in sequence under atmosphere of argon at 40 °C, and the reaction mixture was stirred for 12 h under these conditions. When the reaction was completed (monitored by TLC), H_2O (5.0 mL) was added to quench the reaction, and the aqueous layer was extracted with DCM (2 × 10 mL), the combined organic layer was washed with brine (20 mL) and dried over anhydrous Na_2SO_4. Then the solvent was evaporated in vacuo after filtration, and the residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate = 15:1 to 5:1) to give 1.083 g of pure **3J** (76% yield).

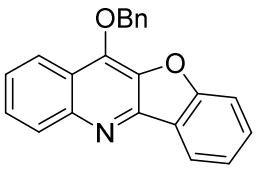
Control Experiment.



To a 10-mL oven-dried vial containing a magnetic stirring bar, **1t** (0.2 mmol), $AuCl_3$ (2.3 mg, 5.0 mol %), and acetonitrile (1.0 mL) were added in sequence under atmosphere of argon at 25 °C, and the reaction mixture was stirred for 12 h under these conditions. When the reaction was completed (monitored by TLC), the solvent was evaporated *in vacuo* and the residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate = 40:1 to 15:1) to give pure products **3t** and **3t'**.



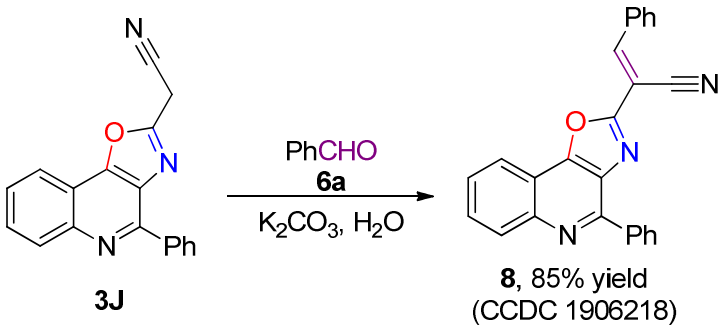
4-[2-(Benzyloxy)phenyl]-2-methyloxazolo[4,5-*c*]quinoline (3t). 25.6 mg, 35% yield. Yellow solid; mp: 128-130 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.35 (d, J = 8.5 Hz, 1H), 8.18 (m, 1H), 7.74 (m, 1H), 7.70 (m, 1H), 7.65 (m, 1H), 7.45 (m, 1H), 7.30 – 7.25 (m, 2H), 7.24 – 7.11 (comp, 5H), 5.16 (s, 2H), 2.70 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 156.9, 152.2, 151.6, 145.6, 137.4, 134.8, 131.5, 131.0, 130.0, 128.9, 128.8, 128.3, 127.5, 127.0, 127.0, 121.5, 120.1, 115.9, 113.4, 70.6, 14.5. HRMS (TOF MS CI$^+$) calculated for $C_{24}H_{18}N_2O_2^+$ $[M+H]^+$: 366.1447, found 366.1444.



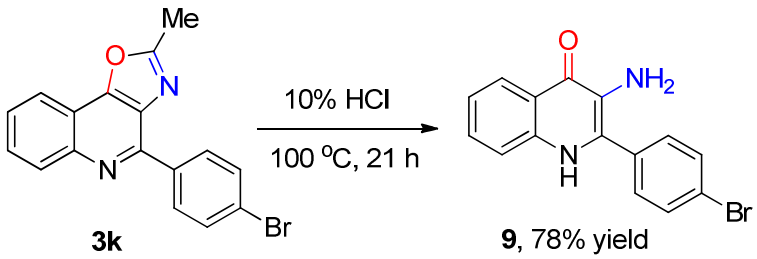
11-(Benzyloxy)benzofuro[3,2-*b*]quinoline (3t'). 12.4 mg, 19% yield. Yellow solid;

mp: 154-156 °C. ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.38 (d, J = 8.3 Hz, 2H), 8.21 (d, J = 8.5 Hz, 1H), 7.74 – 7.67 (m, 1H), 7.66 – 7.58 (comp, 4H), 7.54 – 7.34 (comp, 5H), 6.00 (d, J = 1.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 149.2, 147.5, 143.8, 136.8, 134.7, 130.8, 128.8, 128.7, 128.6, 128.6, 128.0, 125.1, 123.7, 123.2, 122.6, 122.4, 121.5, 112.1, 74.4. HRMS (TOF MS CI$^+$) calculated for $C_{22}H_{16}NO_2^+$ $[M+H]^+$: 326.1181, found 326.1174.

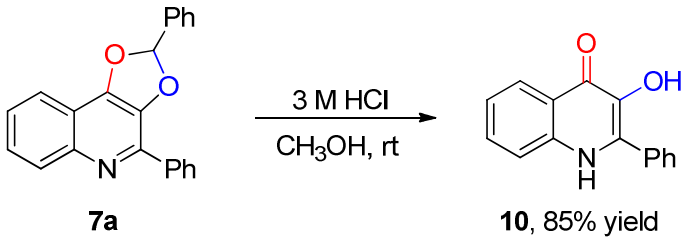
Derivatizations:



Synthesis of 8:[2] To a 10-mL oven-dried vial with a magnetic stirring bar, **3J** (28.5 mg, 0.1 mmol) , **6a** (10.6 mg, 1.0 equiv.), K_2CO_3 (13.8 mg, 5.0 equiv.) and H_2O (1.0 mL) were added in sequence, and the reaction mixture was stirred at room temperature for 10 mins during which time the yellow crystals appeared. The crystalline product was filtered, washed with ethanol, dried and recrystallization in DCM and hexane. The solid product filtrated and dried under vacuum to give the pure product **8** in 85% yield as red solid, mp = 188-190 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.80 – 8.74 (m, 2H), 8.41 (s, 1H), 8.27 (d, J = 8.5 Hz, 1H), 8.22 (m, 1H), 8.13 – 8.07 (m, 2H), 7.76 (m, 1H), 7.65 (t, J = 7.5 Hz, 1H), 7.59 (comp, 5H), 7.55 – 7.50 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 153.0, 150.6, 149.6, 146.1, 136.8, 133.6, 133.1, 132.2, 130.8, 130.4, 130.3, 129.8, 129.6, 129.5, 128.8, 127.4, 120.4, 115.3, 114.8, 99.1. HRMS (TOF MS ESI$^+$) calculated for $C_{24}H_{16}N_3O^+$ $[M+H]^+$: 374.1288, found 374.1290.



Synthesis of 9:[3] To a 10-mL oven-dried round-bottom flask with a magnetic stirring bar, **3k** (33.9 mg, 0.1 mmol), MeOH (1.0 mL), and 10% HCl aqueous solution (1.0 mL) were added in sequence, and the resulting reaction mixture was stirred at 100 °C for 21 h. Then the reaction mixture was diluted with CH_2Cl_2 (10.0 mL), followed by addition of saturated $NaHCO_3$ aqueous solution (10.0 mL) slowly. The aqueous layer was extracted with CH_2Cl_2 (3 × 10.0 mL), the combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was evaporated in *vacuo* after filtration, and the residue was purified by recrystallization in DCM and hexane to give 24.6 mg pure product **9** in 78% yield as yellow solid, mp = 127-129 °C; ^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm) 11.44 (s, 1H), 8.11 (d, J = 8.1 Hz, 1H), 7.79 (d, J = 8.2 Hz, 2H), 7.68 (d, J = 8.1 Hz, 2H), 7.60 (d, J = 8.5 Hz, 1H), 7.55 – 7.48 (m, 1H), 7.20 (t, J = 7.5 Hz, 1H), 4.37 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 170.3, 138.2, 133.4, 132.3, 131.5, 130.4, 128.9, 128.6, 125.1, 122.9, 121.9, 121.0, 118.6. HRMS (TOF MS CI$^+$) calculated for $C_{15}H_{12}BrN_2O$ $[M+H]^+$: 315.0128, found 315.0125.



Synthesis of 10: To a 10-mL oven-dried vial with a magnetic stirring bar, **7a** (32.5 mg, 0.1 mmol) , CH_3OH (1.0 mL), and 3 M HCl (0.5 mL) were added in sequence, and the reaction mixture was stirred at room temperature for 2 h. Then the reaction

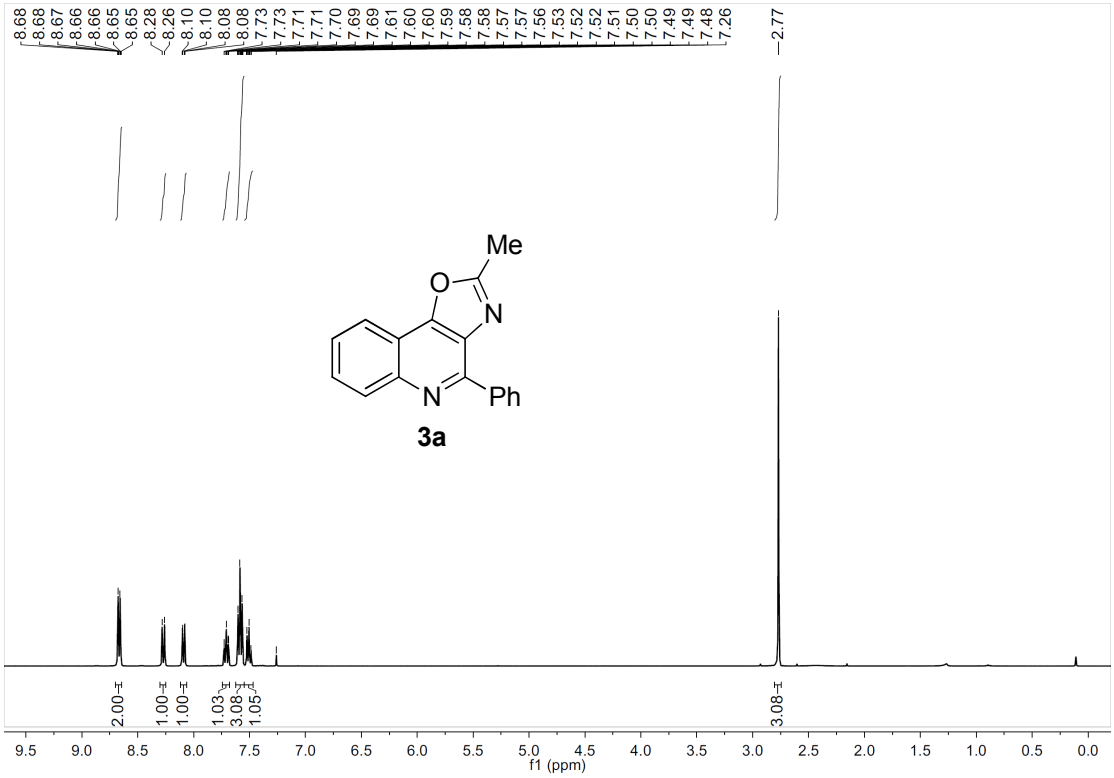
mixture was diluted with CH_2Cl_2 (10.0 mL), followed by addition of saturated $NaHCO_3$ aqueous solution (10.0 mL) slowly. The aqueous layer was extracted with CH_2Cl_2 (3 × 10.0 mL), the combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo after filtration, and the residue was purified by recrystallization in DCM and hexane to give 20.1 mg pure product **10** in 85% yield as yellow solid, mp = 273-275 ^oC; ^1H NMR (400 MHz, DMSO-d_6) (δ, ppm) 11.58 (s, 1H), 8.16 (d, J = 8.0 Hz, 1H), 7.87 – 7.70 (comp, 3H), 7.61 – 7.49 (comp, 5H), 7.27 (t, J = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 170.0, 138.0, 137.9, 132.4, 131.5, 130.5, 129.3, 129.2, 128.3, 124.5, 121.9, 121.8, 118.5. HRMS (TOF MS ESI$^+$) calculated for $C_{15}H_{12}NO_2^+$ $[M+H]^+$: 238.0863, found 238.0865.

References:

1 Y. Jeong, B. Kim, J. K. Lee and J.-S. Ryu, *J. Org. Chem.,* 2014, **79**, 6444.

2 C. Youssef, H. B. Ammar, M. Belhouchet, K. Beydoun, R. B. Salem, H. Doucet and P. H. Dixneuf, *J. Heterocyclic Chem.,* 2011, **48**, 1126.

3 Y. Nakao, N. Kashihara, K. S. Kanyiva and T. Hiyama, *Angew. Chem. Int. Ed.*, 2010, **49**, 4451.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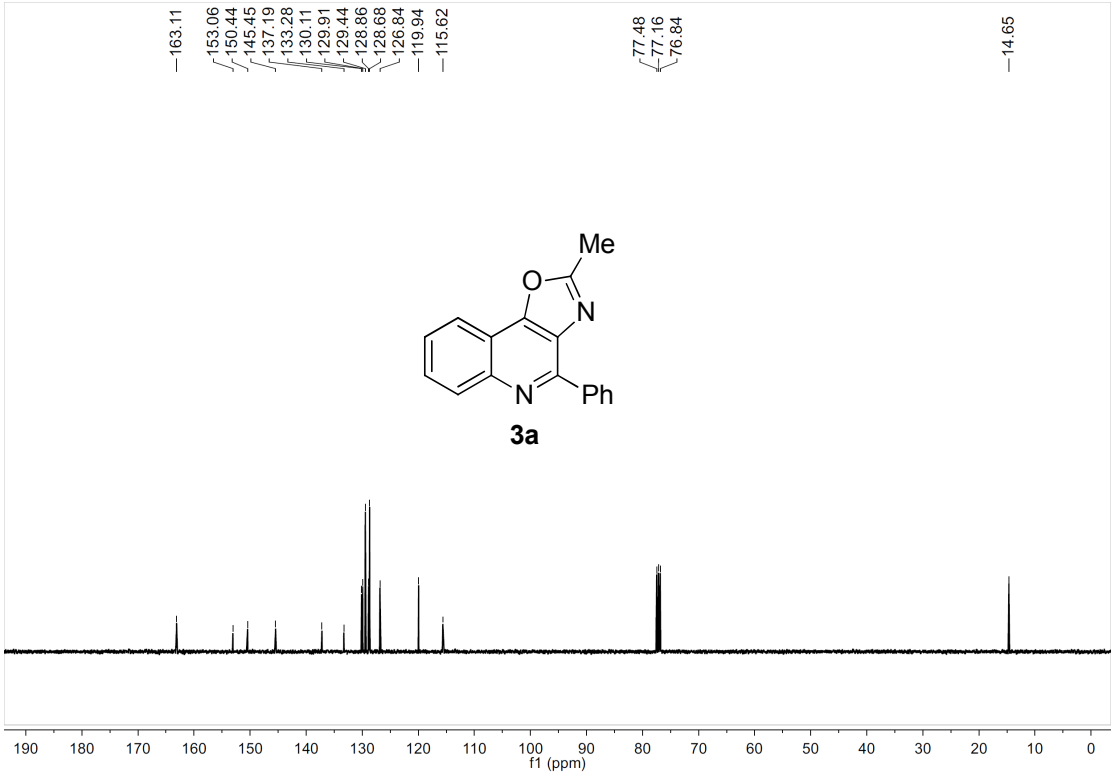
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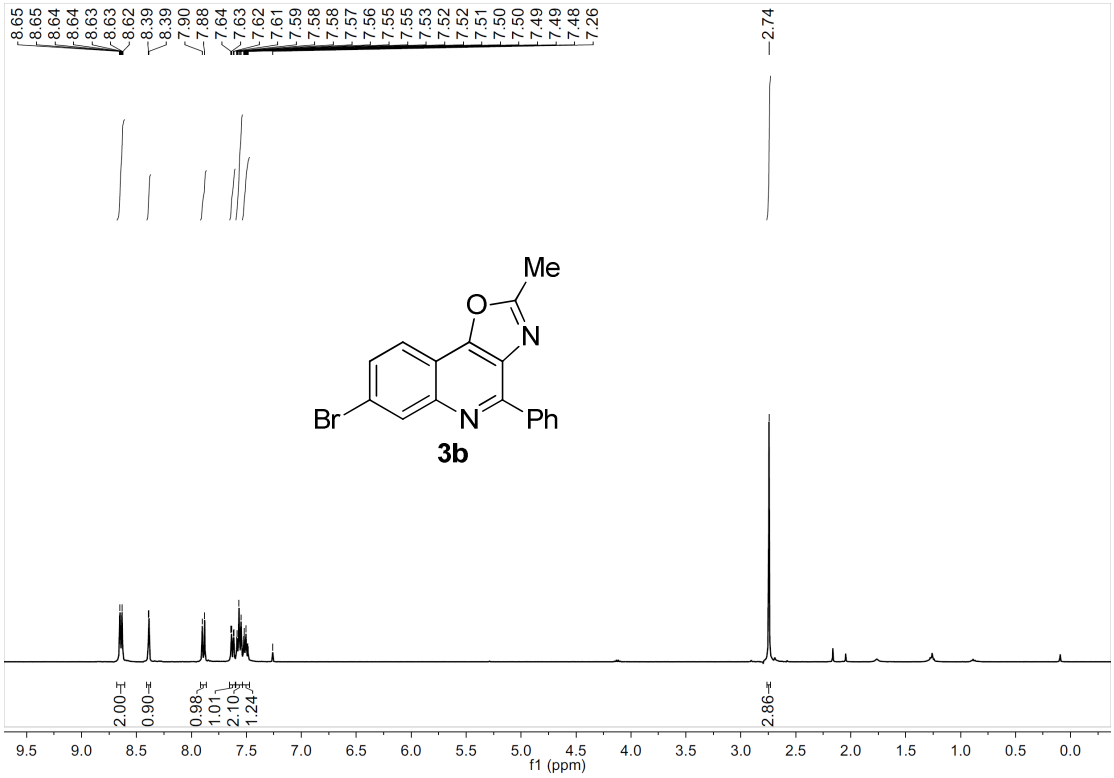
f1 (ppm)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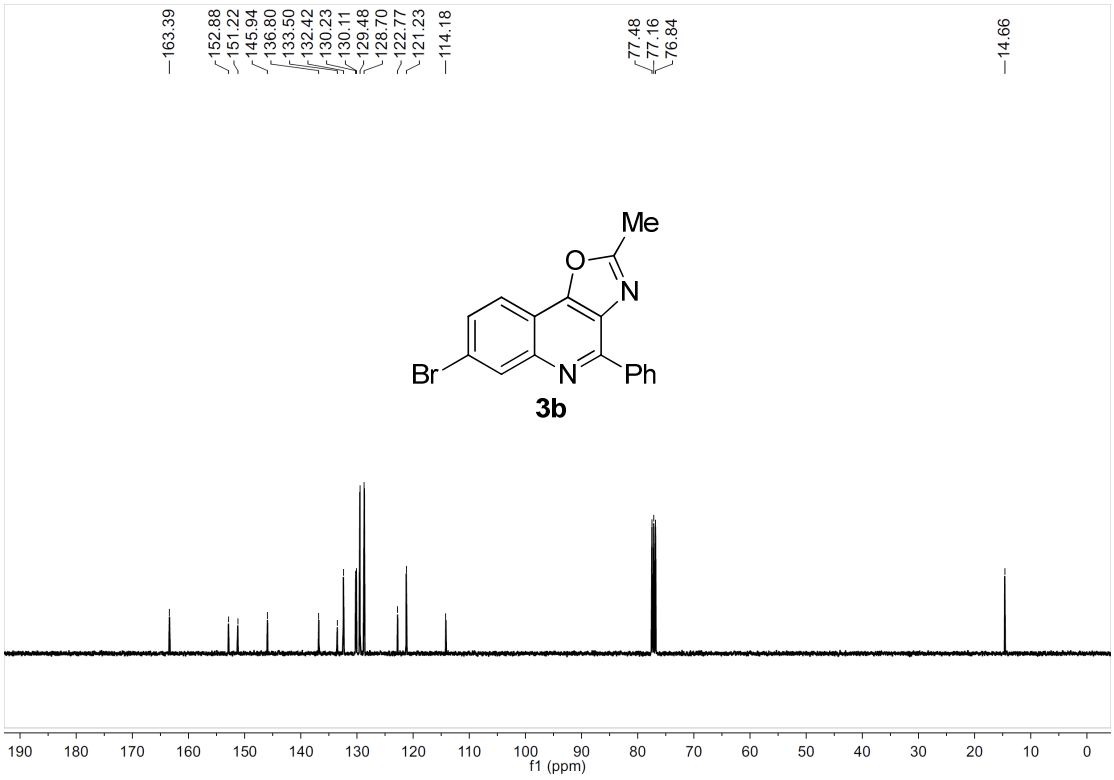
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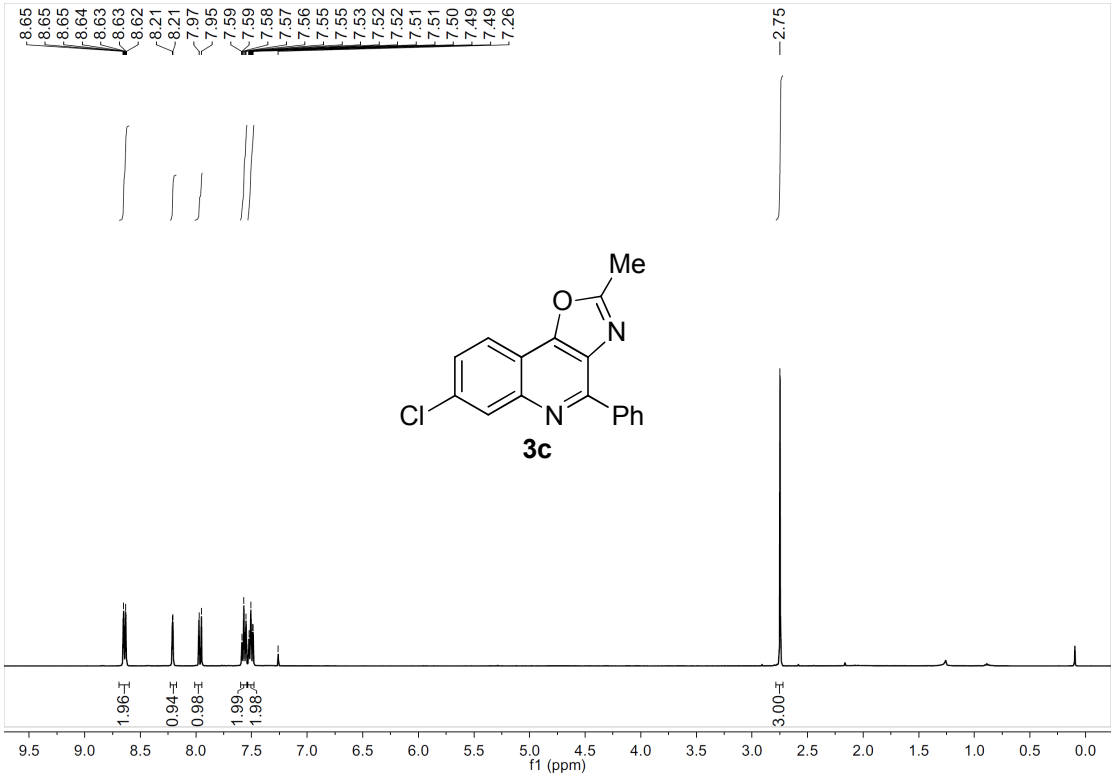
f1 (ppm)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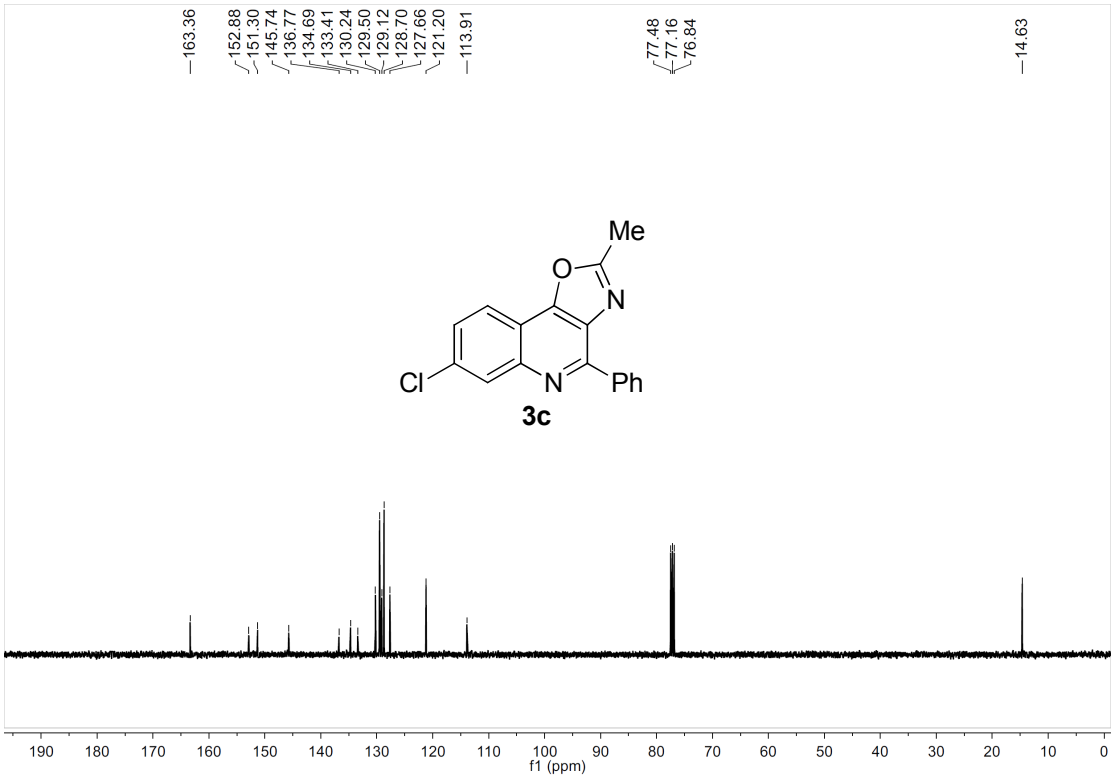
f1 (ppm)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152.88
151.30
145.74
136.77
134.69
133.41
130.24
129.50
129.12
128.70
127.66
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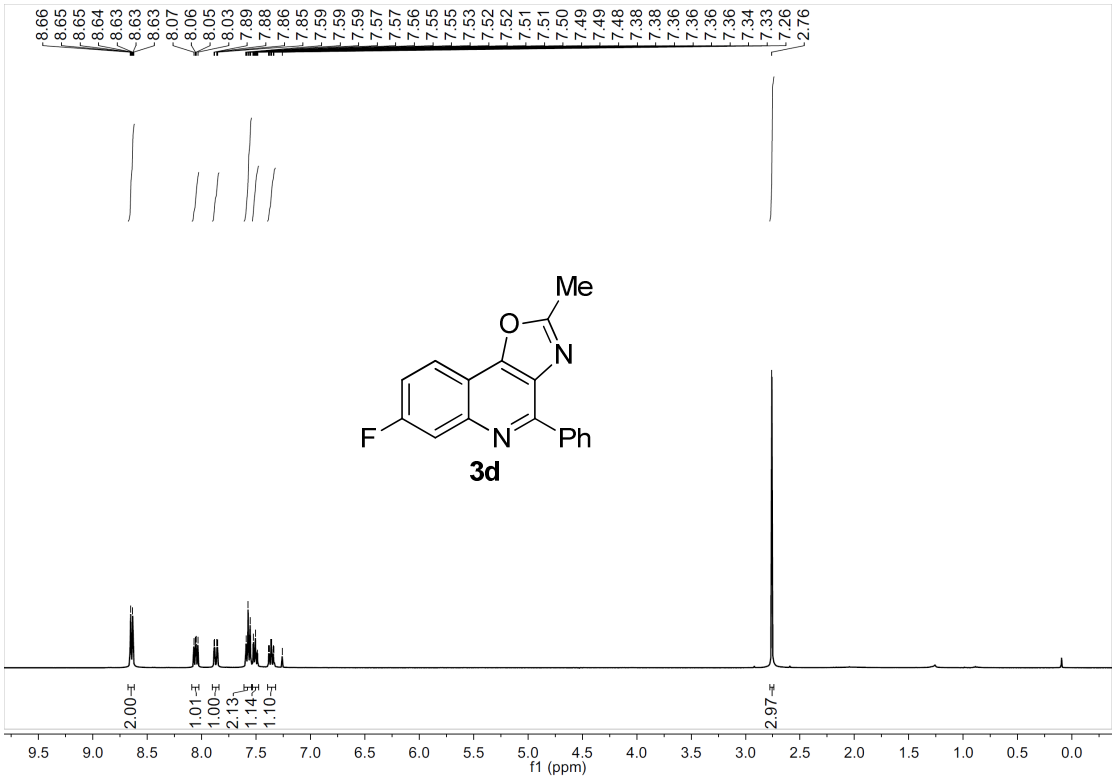
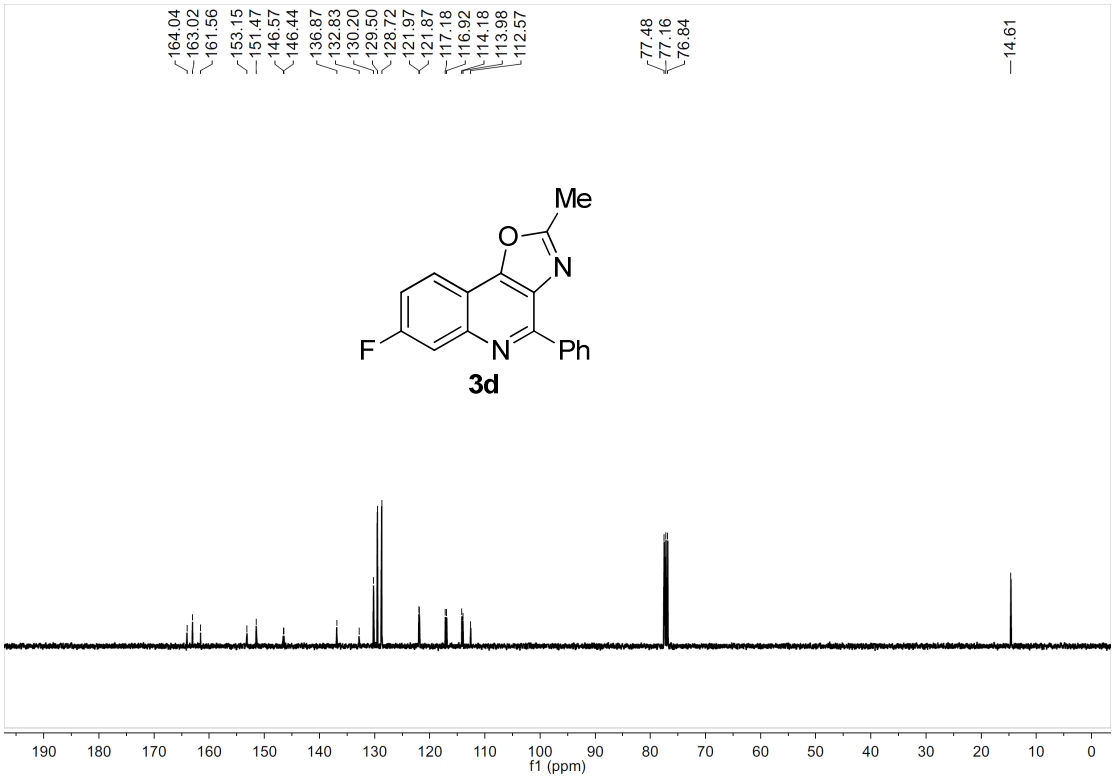
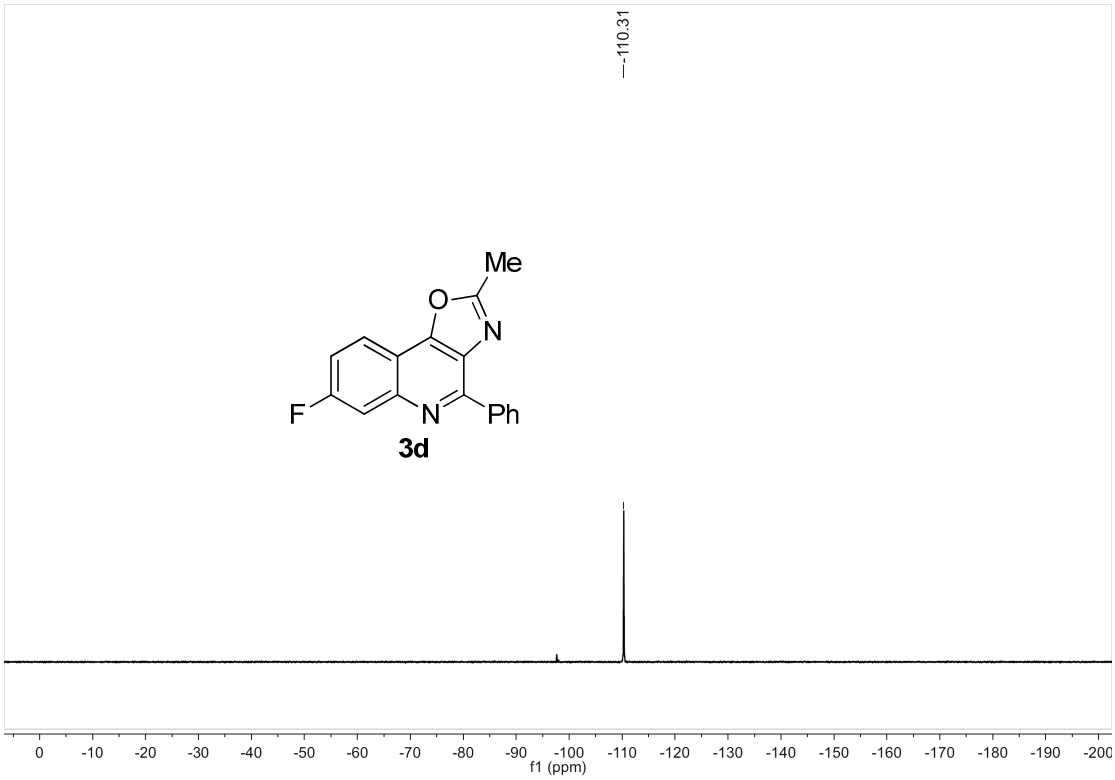
O
N
Cl
N
Ph
3c
f1 (ppm)


8.66 8.65 8.65 8.64 8.63 8.63 8.63 8.07 8.06 8.05 8.03 7.89 7.88 7.86 7.85 7.59 7.59 7.59 7.57 7.57 7.56 7.55 7.55 7.53 7.52 7.52 7.51 7.51 7.50 7.49 7.49 7.48 7.38 7.38 7.36 7.36 7.36 7.34 7.33 7.26 2.76
Me
O
N
F
N
Ph
3d
2.00
1.01
1.00
2.13
1.14
1.10
2.97
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)


164.04 163.02 161.56 153.15 151.47 146.57 146.44 136.87 132.83 130.20 129.50 128.72 121.97 121.87 117.18 116.92 114.18 113.98 112.57
77.48 77.16 76.84
14.61
Me
O
N
F
N
Ph
3d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-110.31
Me
O
N
F
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Ph
3d
0
-10
-20
-30
-40
-50
-60
-70
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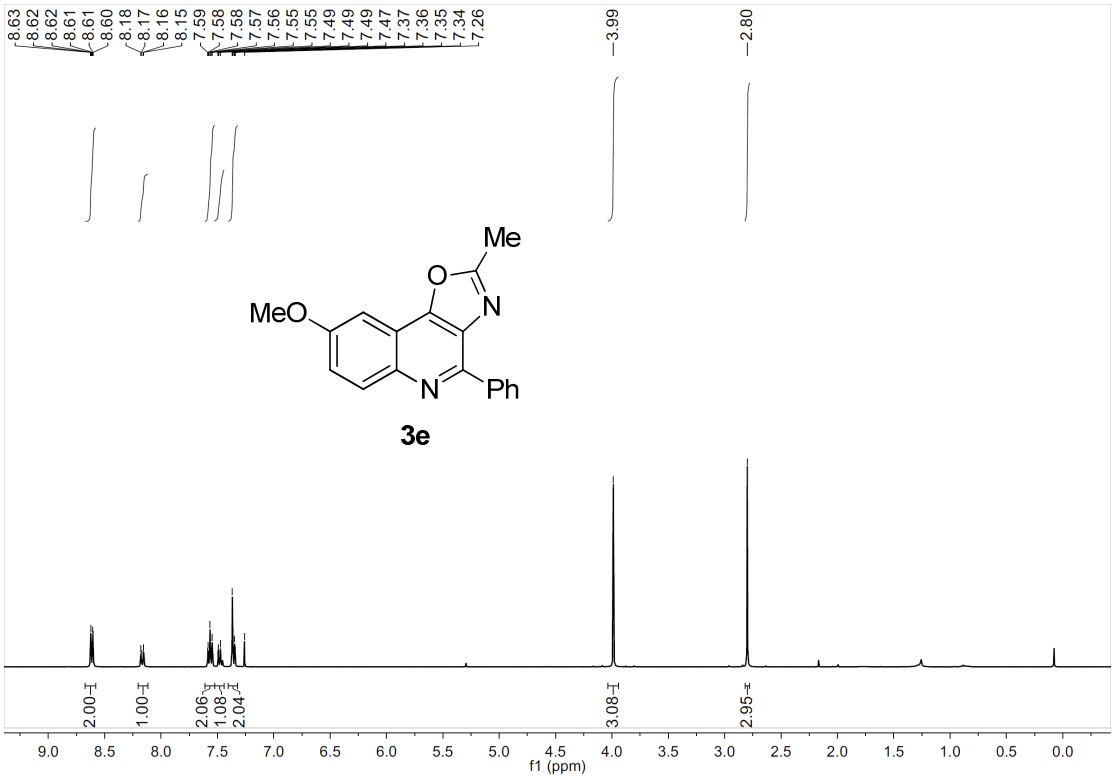
-160
-170
-180
-190
-200
f1 (ppm)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8.62
8.62
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8.17
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7.59
7.58
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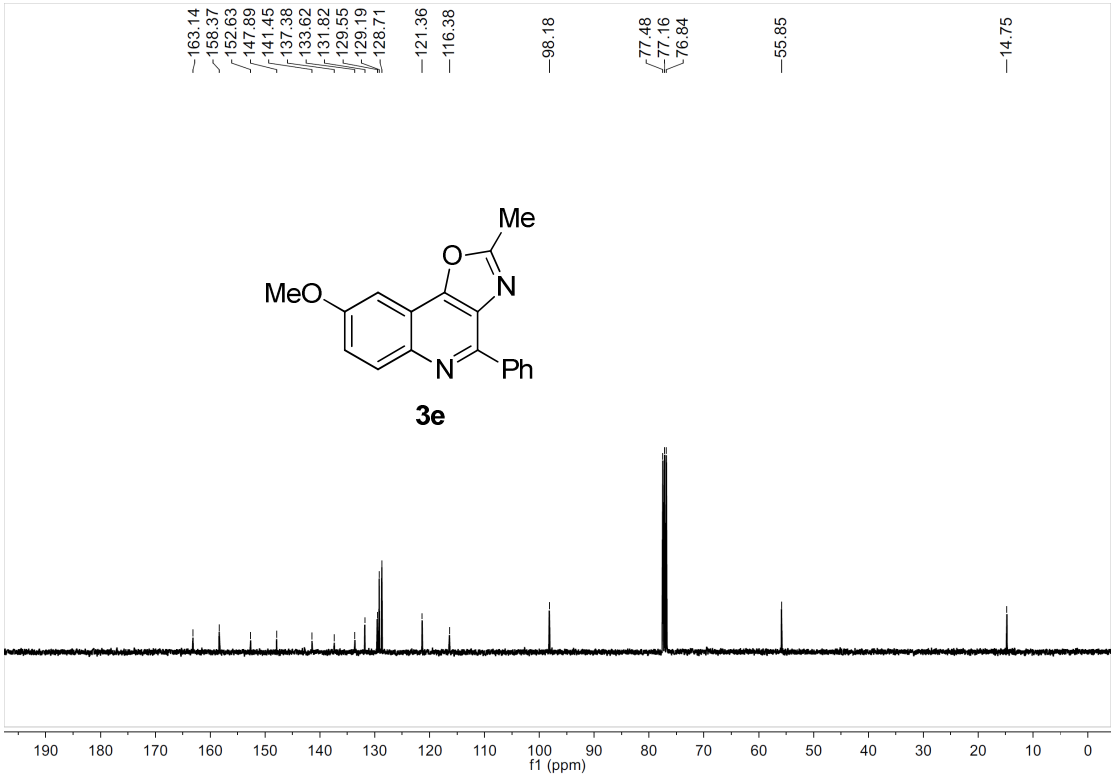
7.57
7.56
7.55
7.55
7.49
7.49
7.49
7.47
7.37
7.36
7.35
7.34
7.26
3.99
2.80
Me
O
N
MeO
N
Ph
3e
2.00
1.00
2.06
1.08
2.04
3.08
2.95
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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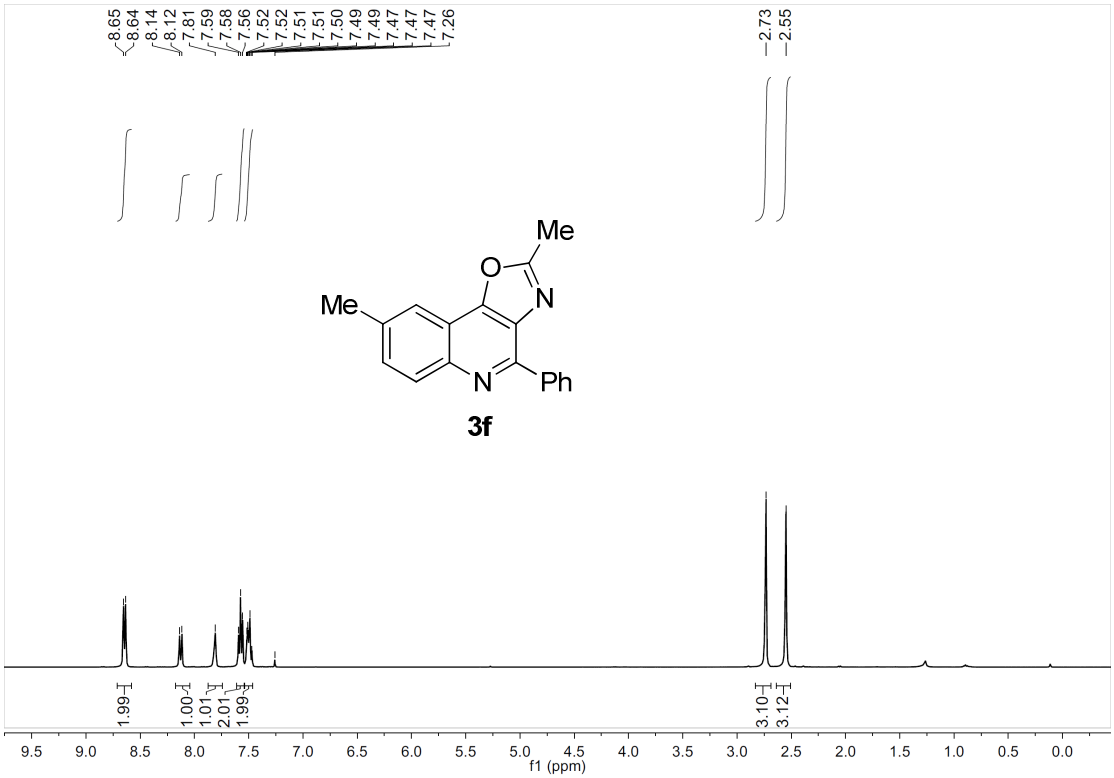
158.37
152.63
147.89
141.45
137.38
133.62
131.82
129.55
129.19
128.71
121.36
116.38
98.18
77.48
77.16
76.84
55.85
14.75
Me
O
N
MeO
N
Ph
3e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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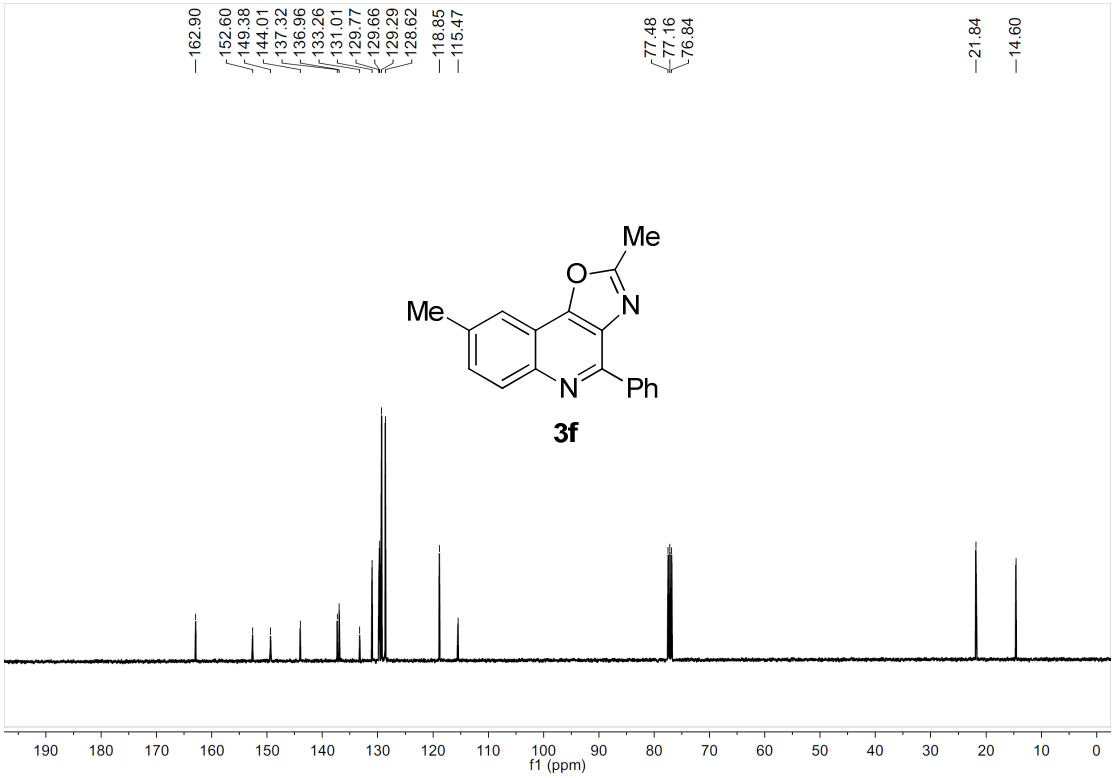
8.64
8.14
8.12
7.81
7.59
7.58
7.56
7.52
7.52
7.51
7.51
7.50
7.49
7.49
7.47
7.47
7.47
7.26
2.73
2.55
Me
O
N
Me
N
Ph
3f
1.99
1.00
1.01
2.01
1.99
3.10
3.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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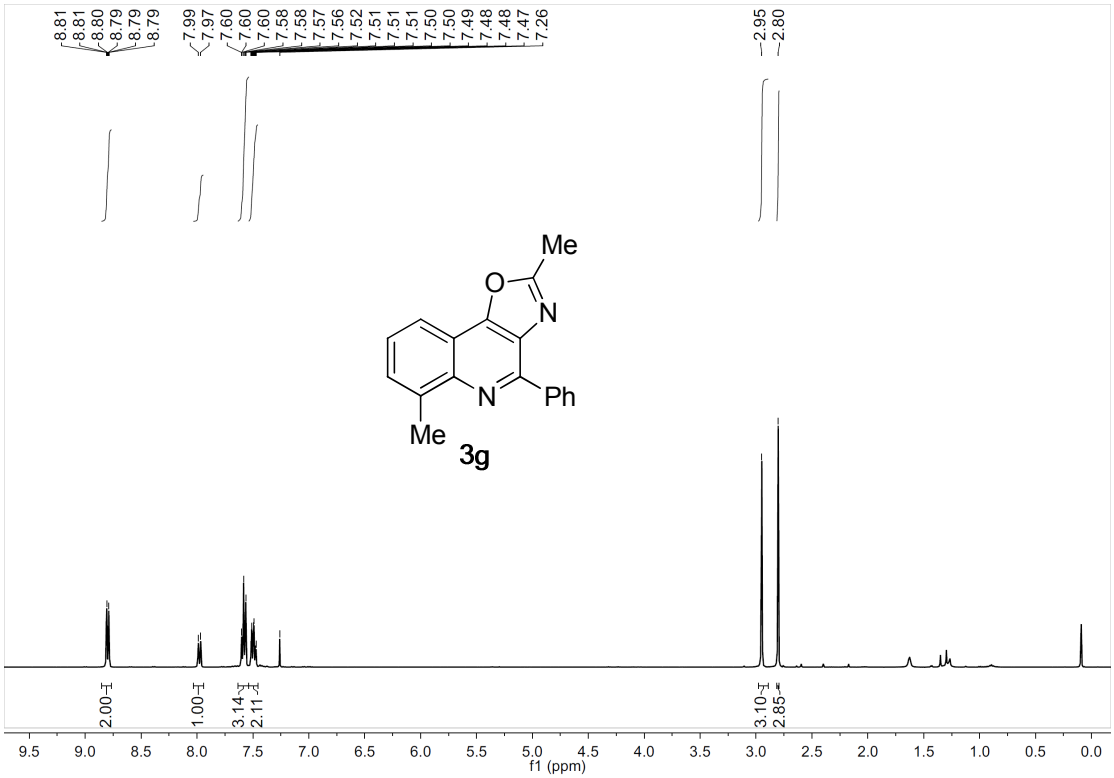
152.60
149.38
144.01
137.32
136.96
133.26
131.01
129.77
129.66
129.29
128.62
118.85
115.47
77.48
77.16
76.84
21.84
14.60
Me
O
N
Me
N
Ph
3f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.81
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8.80
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8.79
7.99
7.97
7.60
7.60
7.58
7.58
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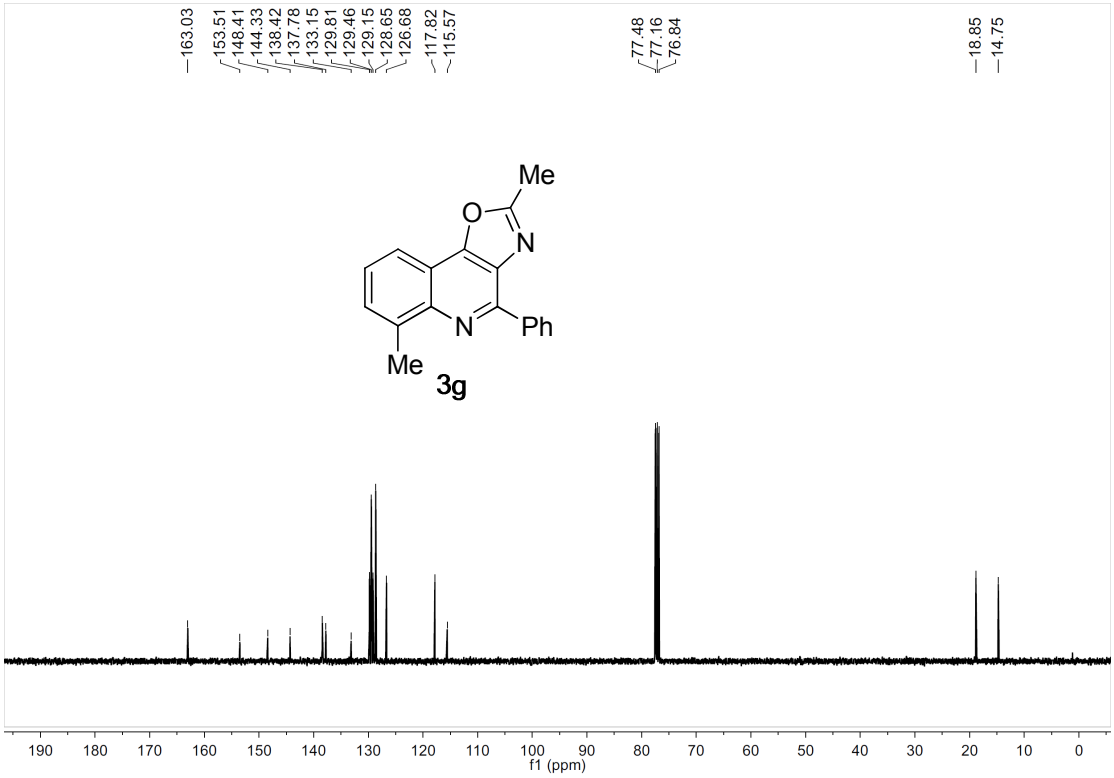
7.56
7.52
7.51
7.51
7.51
7.50
7.50
7.49
7.48
7.48
7.47
7.26
2.95
2.80
Me
O
N
N
Ph
Me
3g
2.00
1.00
3.14
2.11
3.10
2.85
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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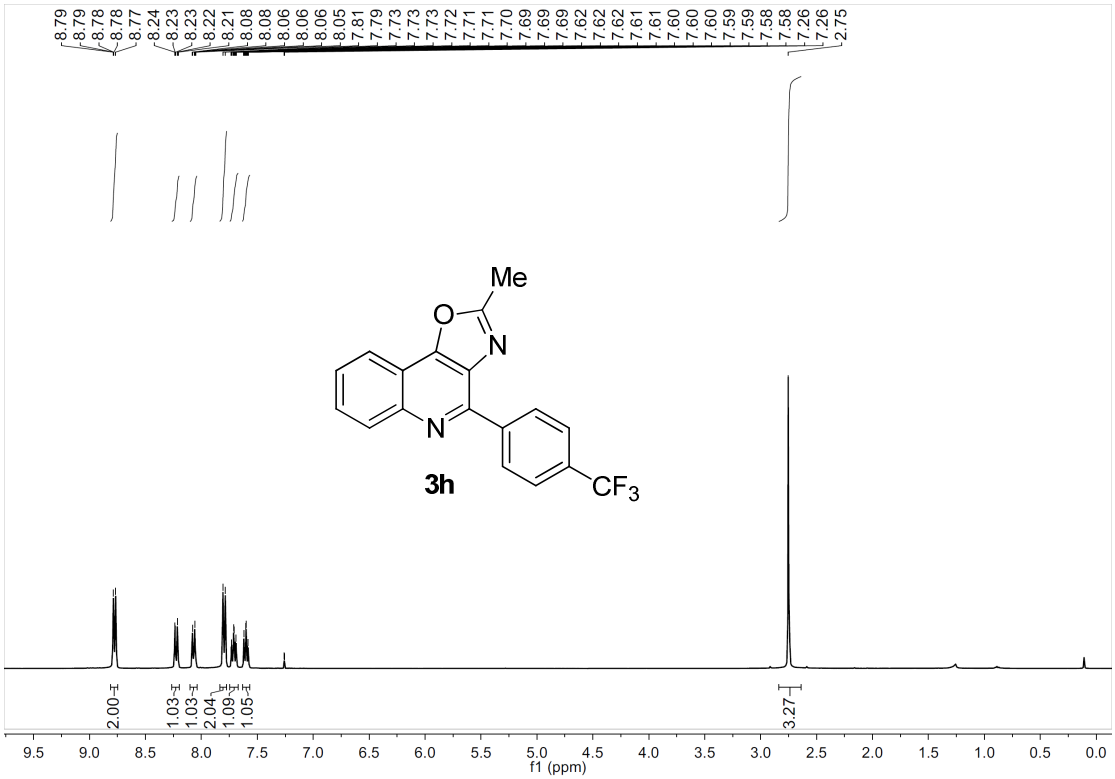
153.51
148.41
144.33
138.42
137.78
133.15
129.81
129.46
129.15
128.65
126.68
117.82
115.57
77.48
77.16
76.84
18.85
14.75
Me
O
N
N
Ph
Me
3g
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.78
8.78
8.77
8.24
8.23
8.23
8.22
8.21
8.08
8.08
8.06
8.06
8.06
8.05
7.81
7.79
7.73
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7.71
7.70
7.69
7.69
7.69
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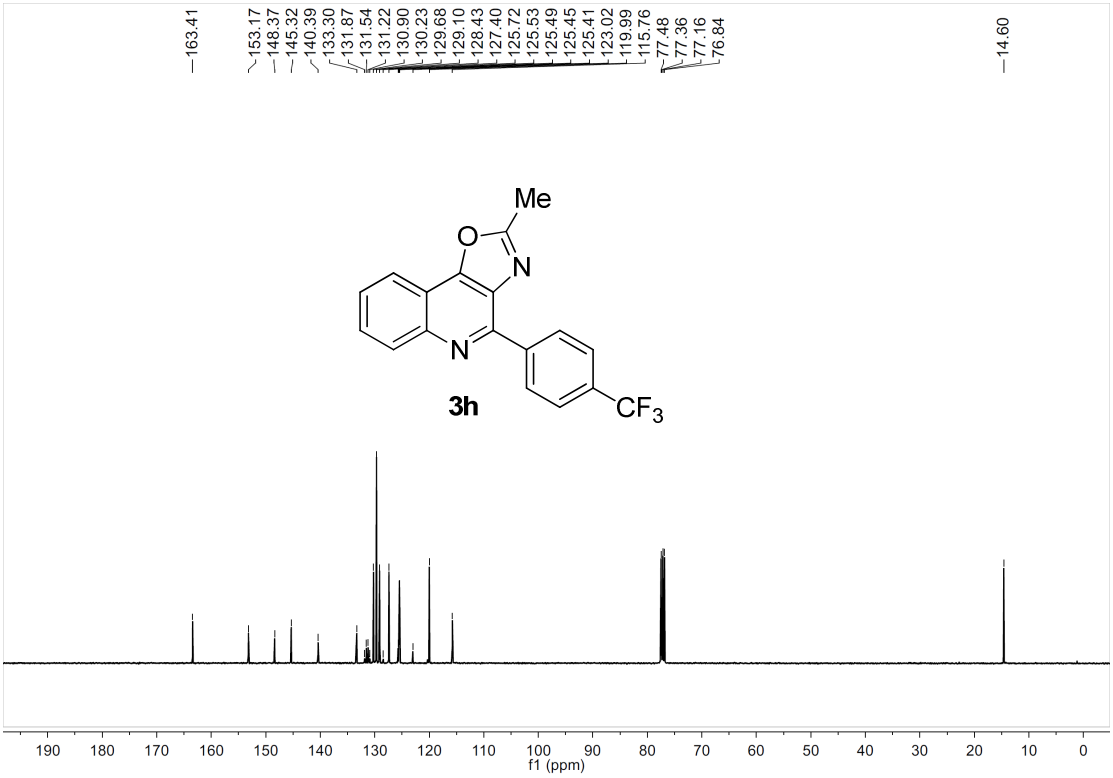
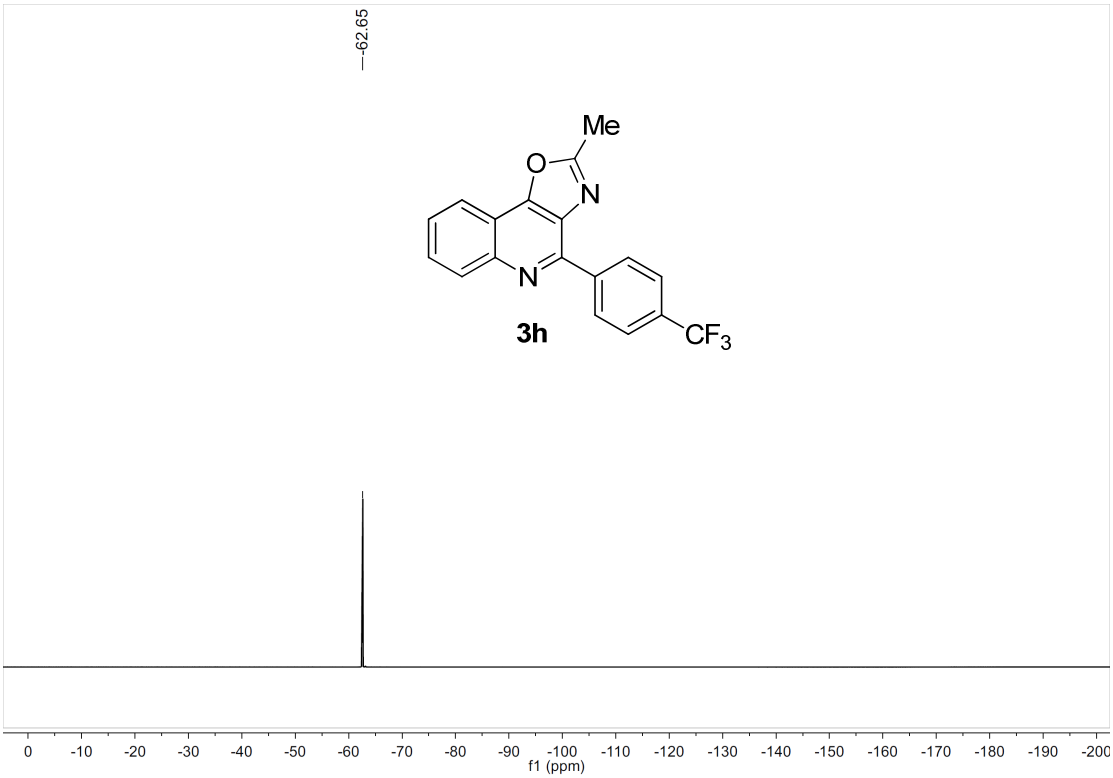
7.62
7.62
7.61
7.61
7.60
7.60
7.60
7.59
7.59
7.58
7.58
7.26
7.26
2.75
Me
O
N
N
3h
CF3
2.00
1.03
1.03
2.04
1.09
1.05
3.27
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


163.41
153.17
148.37
145.32
140.39
133.30
131.87
131.54
131.22
130.90
130.23
129.68
129.10
128.43
127.40
125.72
125.53
125.49
125.45
125.41
123.02
119.99
115.76
77.48
77.36
77.16
76.84
14.60
Me
O
N
N
3h
CF3
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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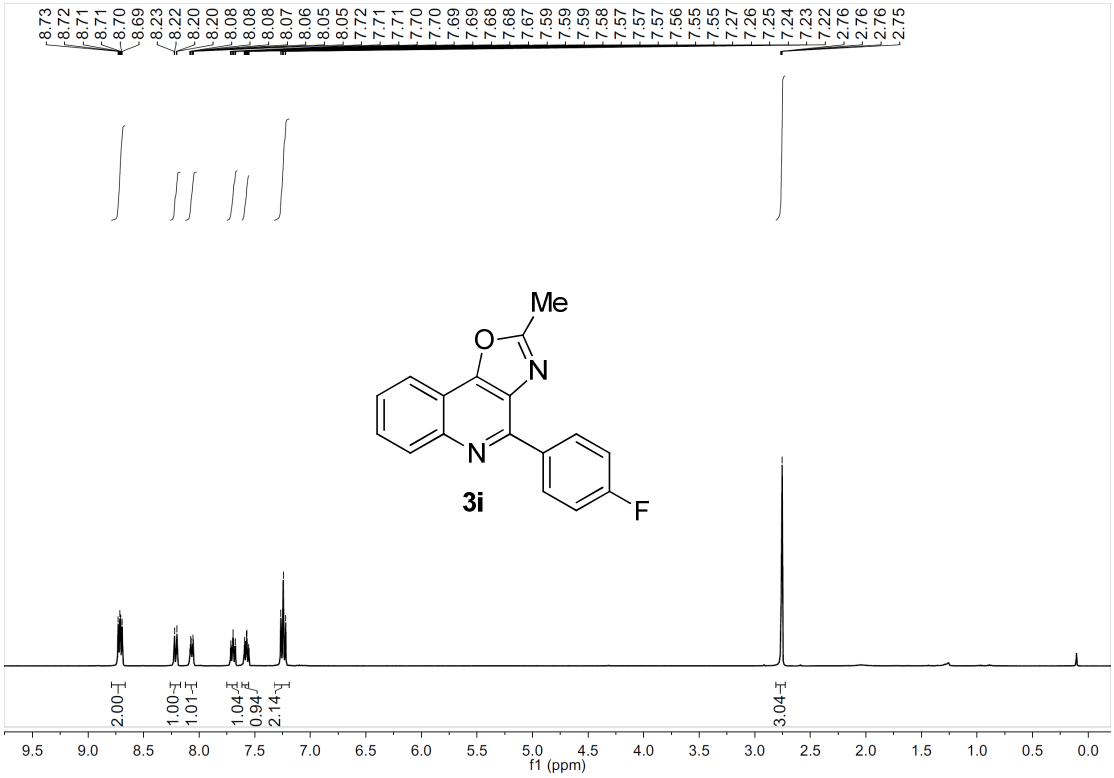
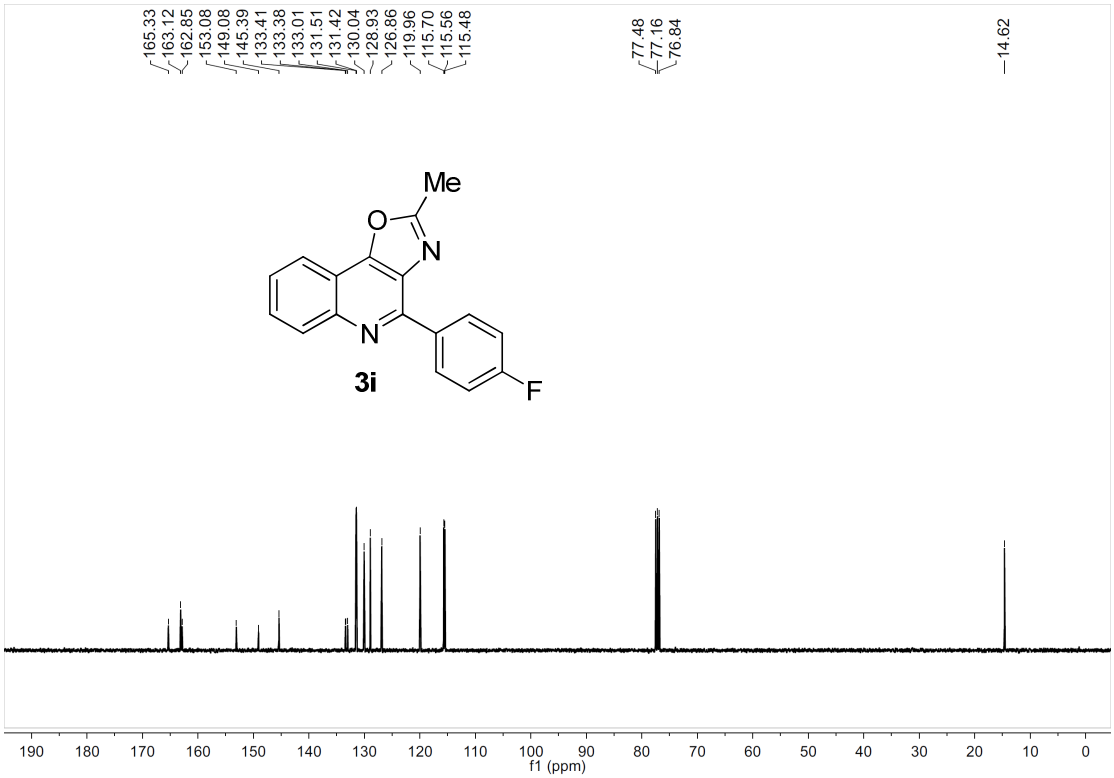
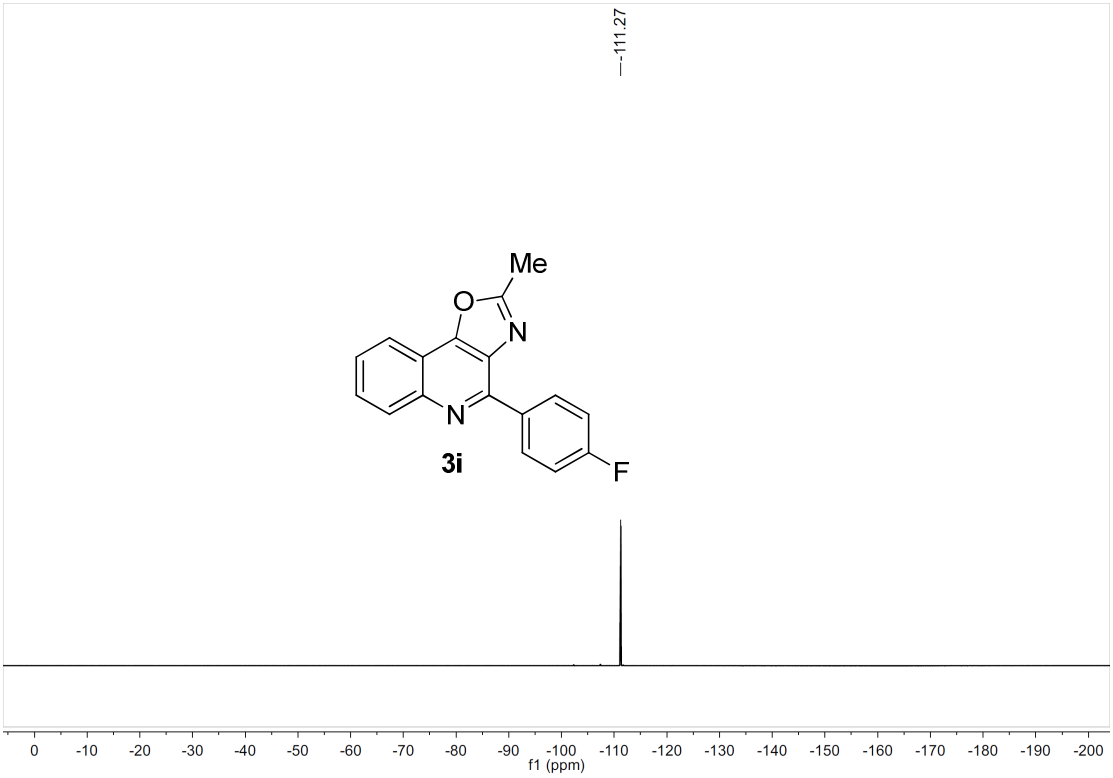
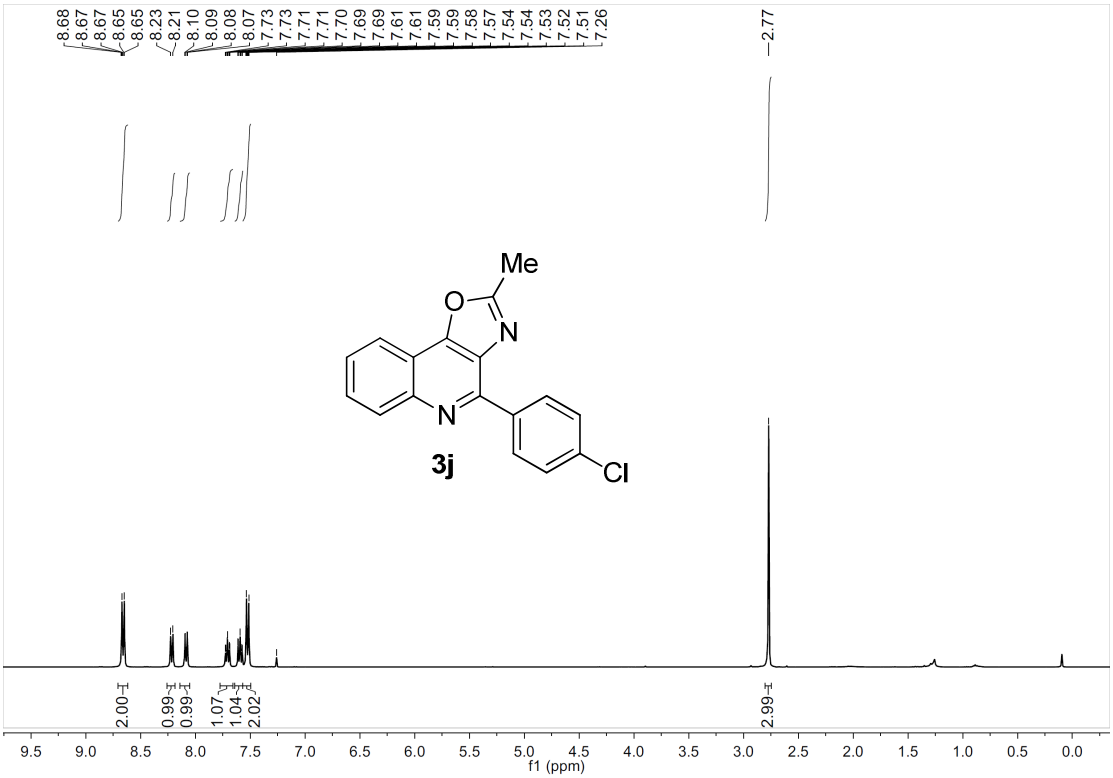
Me
O
N
N
3h
CF3
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


8.73 8.72 8.71 8.71 8.70 8.69 8.23 8.22 8.20 8.20 8.08 8.08 8.08 8.07 8.06 8.05 8.05 7.72 7.71 7.71 7.70 7.70 7.69 7.69 7.68 7.68 7.67 7.59 7.59 7.59 7.58 7.57 7.57 7.57 7.56 7.55 7.55 7.27 7.26 7.25 7.24 7.23 7.22 2.76 2.76 2.75
Me
O
N
N
F
3i
2.00 1.00 1.01 1.04 0.94 2.14 3.04
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)


165.33 163.12 162.85 153.08 149.08 145.39 133.41 133.38 133.01 131.51 131.42 130.04 128.93 126.86 119.96 115.70 115.56 115.48
77.48 77.16 76.84
14.62
Me
O
N
N
F
3i
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-111.27
Me
O
N
N
F
3i
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)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7.69
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7.59
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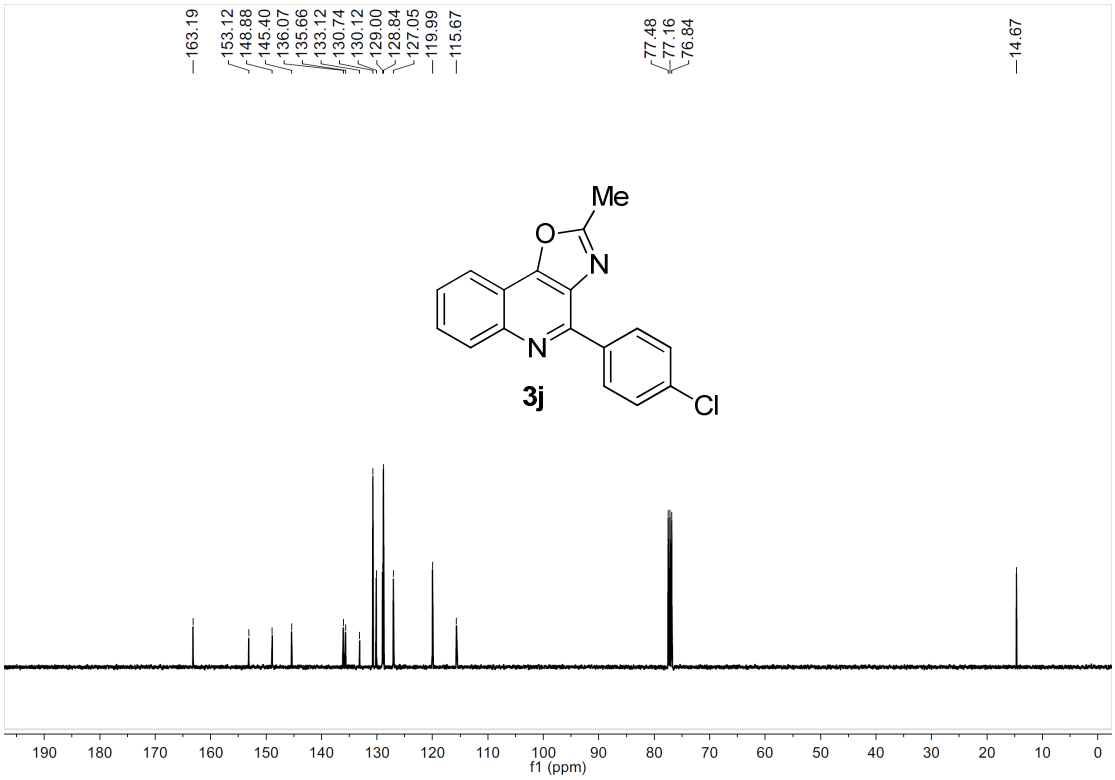
7.57
7.54
7.54
7.53
7.52
7.51
7.26
2.77
Me
O
N
N
Cl
3j
2.00
0.99
0.99
1.07
1.04
2.02
2.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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133.12
130.74
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129.00
128.84
127.05
119.99
115.67
77.48
77.16
76.84
14.67
Me
O
N
N
Cl
3j
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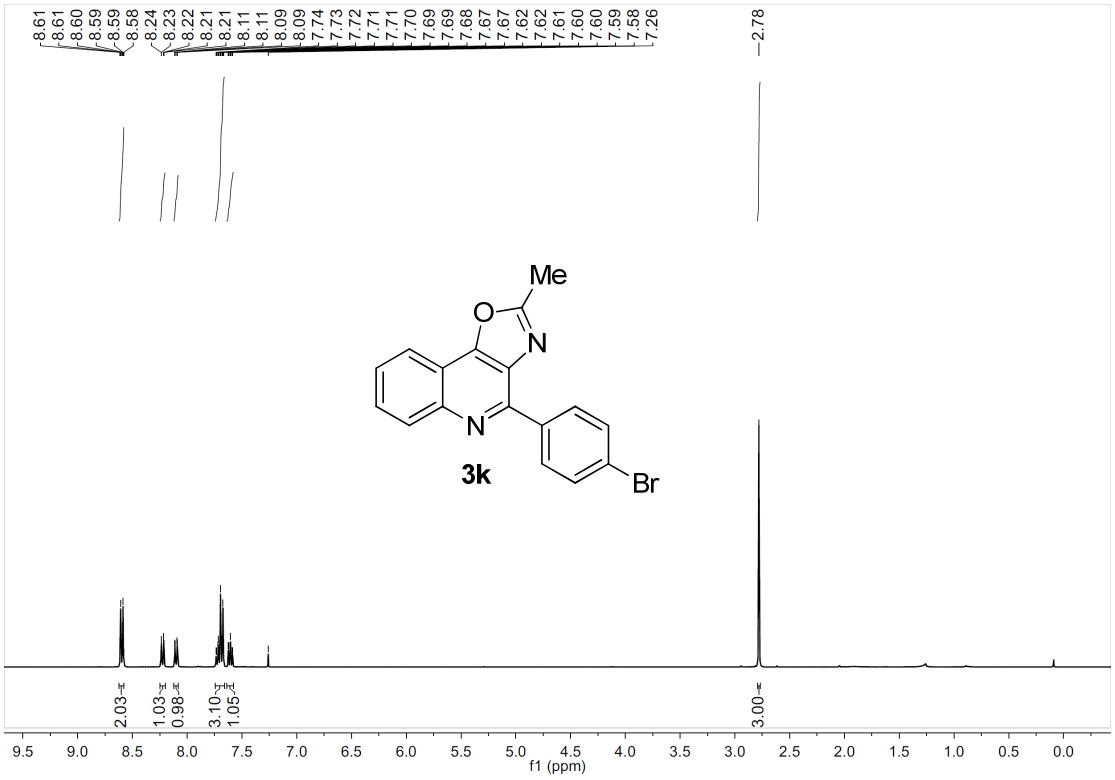
f1 (ppm)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8.11
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8.09
8.09
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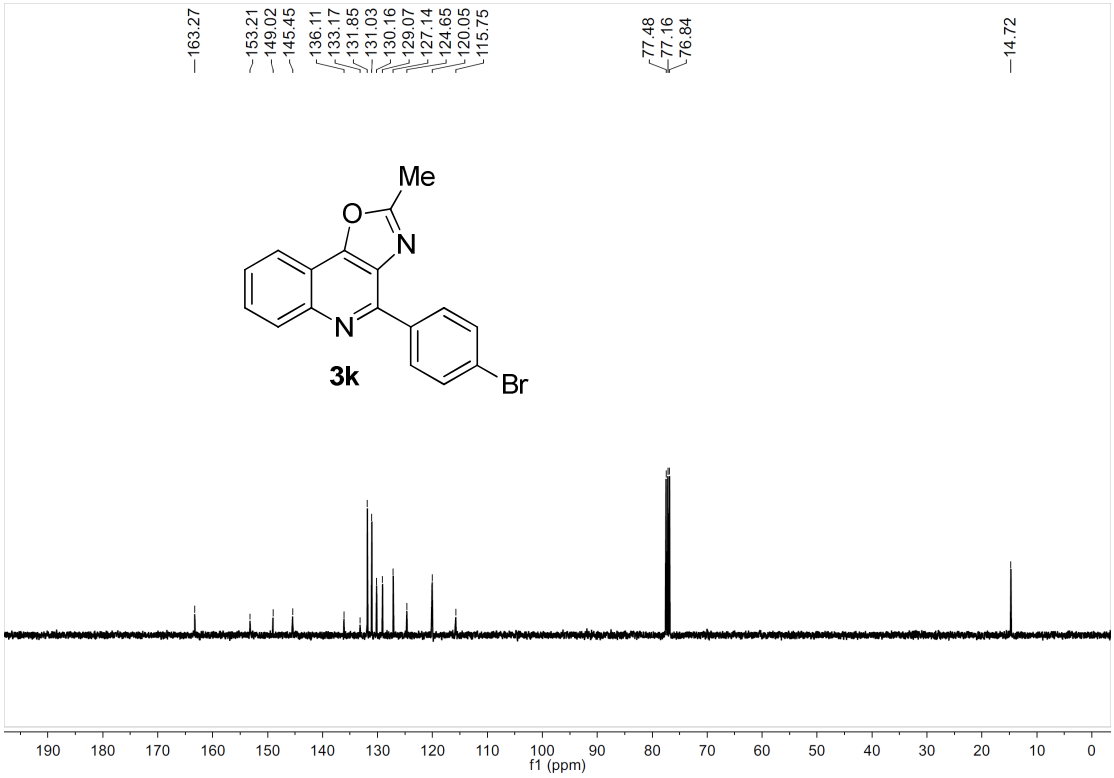
7.69
7.68
7.67
7.67
7.62
7.62
7.61
7.60
7.60
7.59
7.58
7.26
2.78
Me
O
N
N
Br
3k
2.03
1.03
0.98
3.10
1.05
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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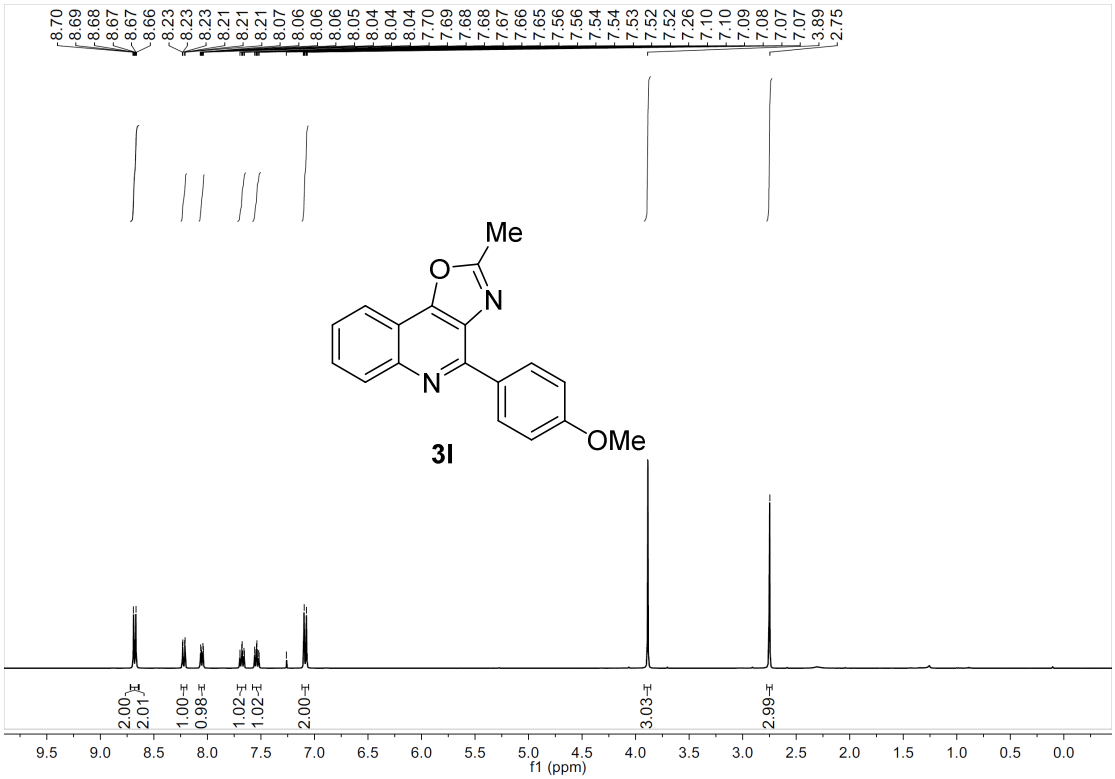
136.11
133.17
131.85
131.03
130.16
129.07
127.14
124.65
120.05
115.75
77.48
77.16
76.84
14.72
Me
O
N
N
Br
3k
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.26
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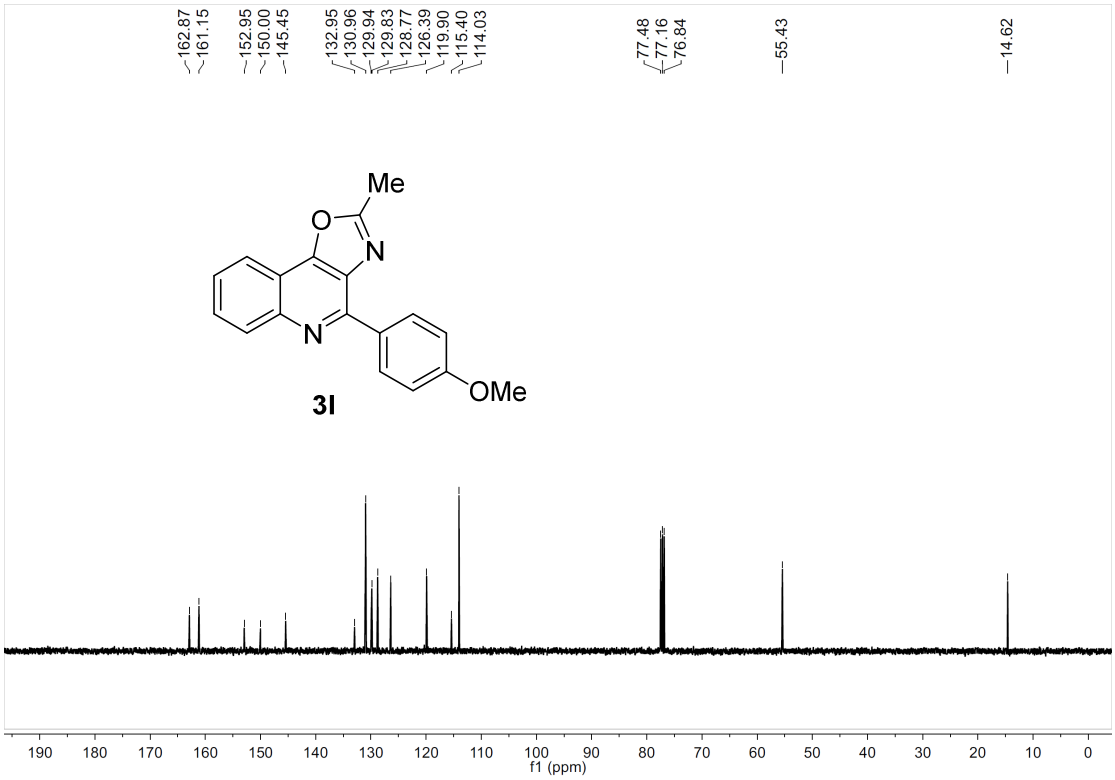
7.10
7.09
7.08
7.07
7.07
3.89
2.75
Me
O
N
N
OMe
3l
2.00
2.01
1.00
0.98
1.02
1.02
2.00
3.03
2.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.94
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128.77
126.39
119.90
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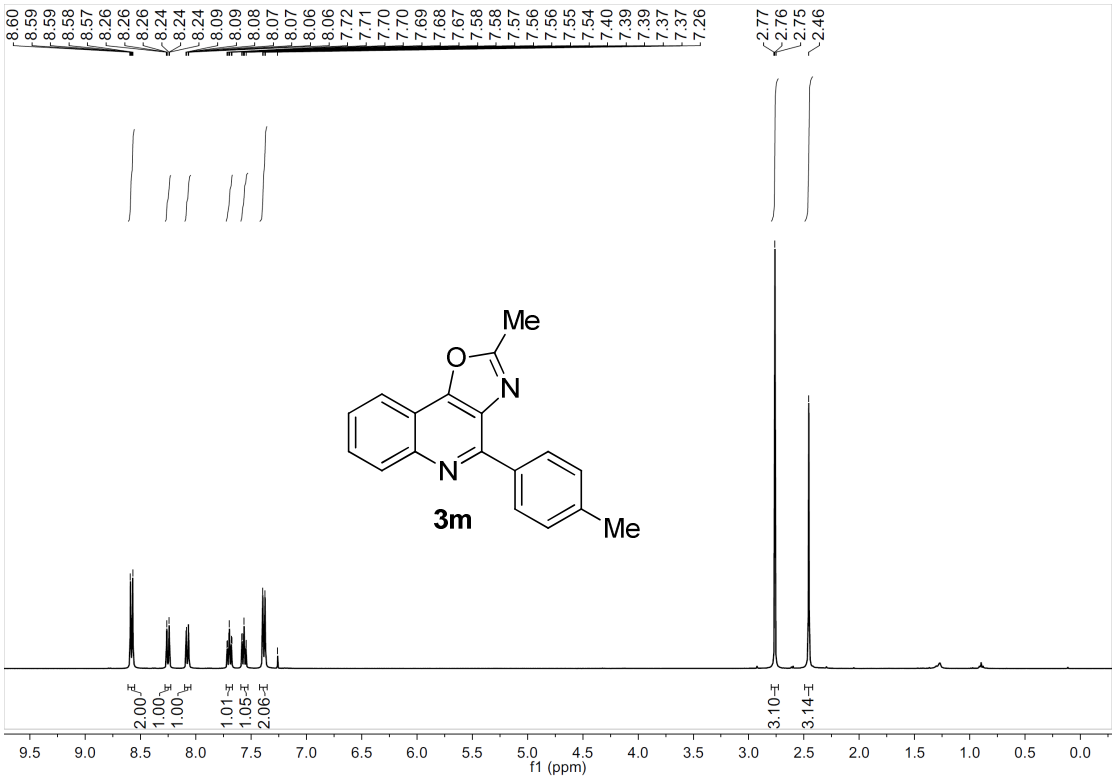
Me
O
N
N
OMe
3l
f1 (ppm)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8.59
8.58
8.57
8.26
8.26
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8.09
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8.07
8.07
8.06
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7.54
7.40
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7.39
7.37
7.37
7.26
2.77
2.76
2.75
2.46
Me
O
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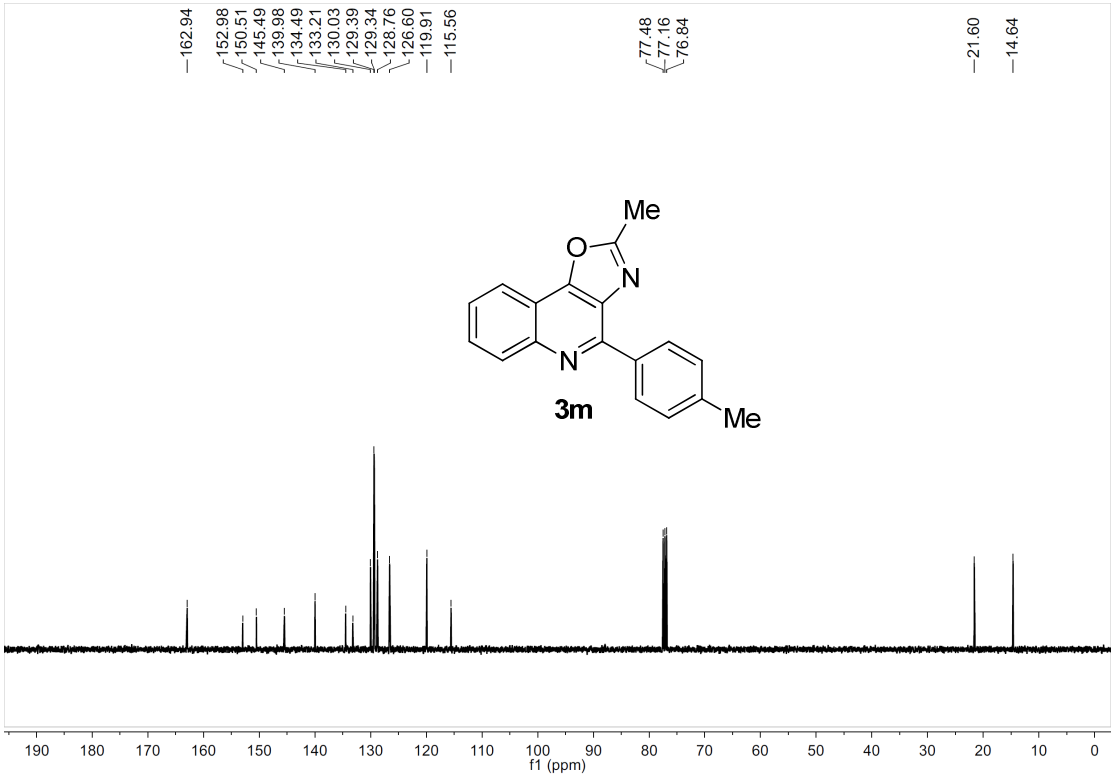
Me
2.00
1.00
1.00
1.01
1.05
2.06
3.10
3.14
f1 (ppm)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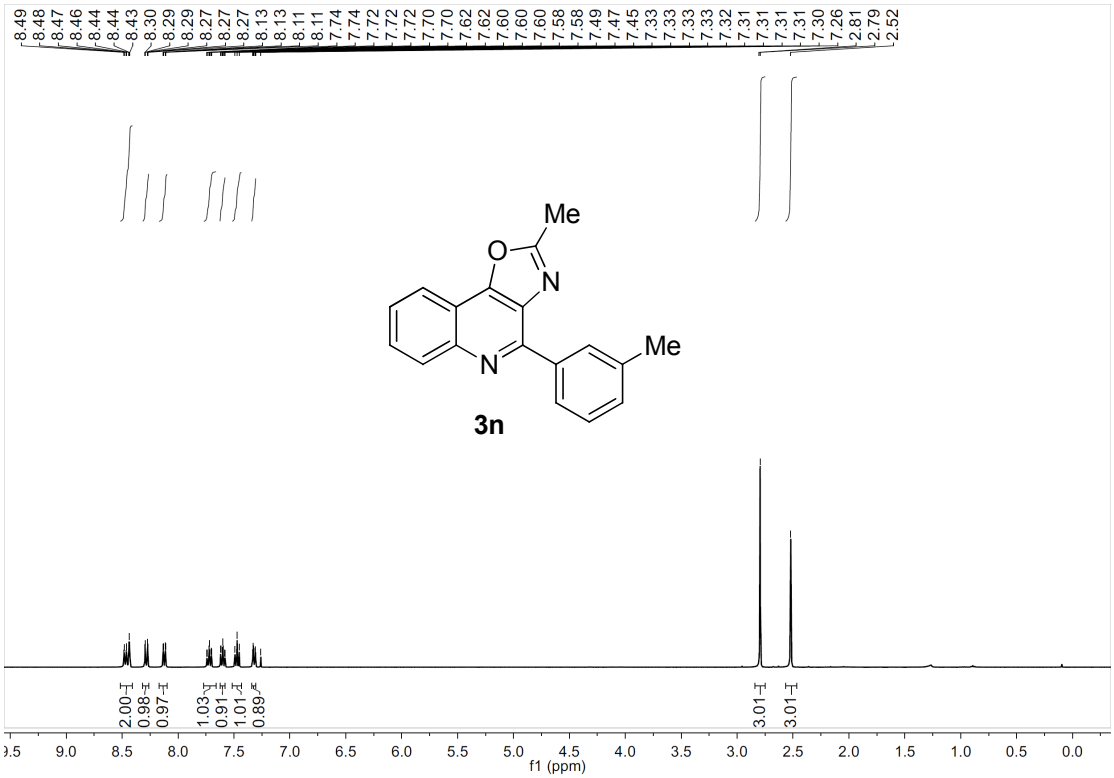
129.34
128.76
126.60
119.91
115.56
77.48
77.16
76.84
21.60
14.64
Me
O
N
N
Me
3m
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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Me
O
N
N
Me
3n
2.00
0.98
0.97
1.03
0.91
1.01
0.89
3.01
3.01
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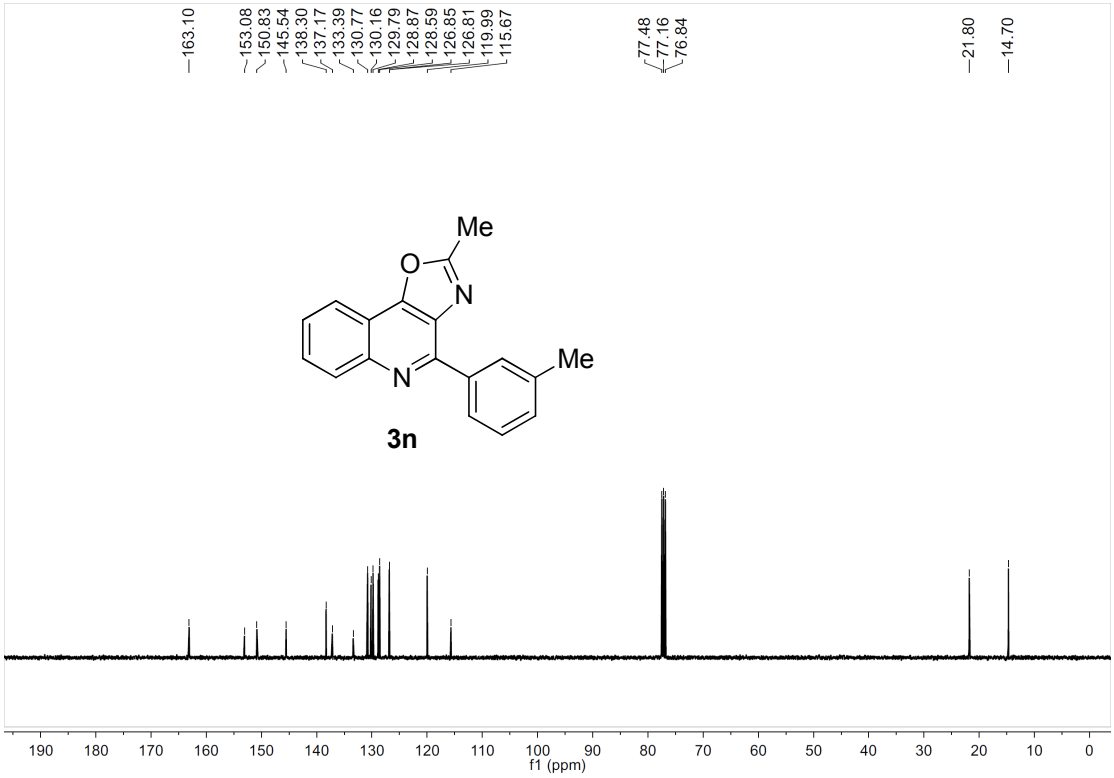
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115.67
77.48
77.16
76.84
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Me
O
N
N
Me
3n
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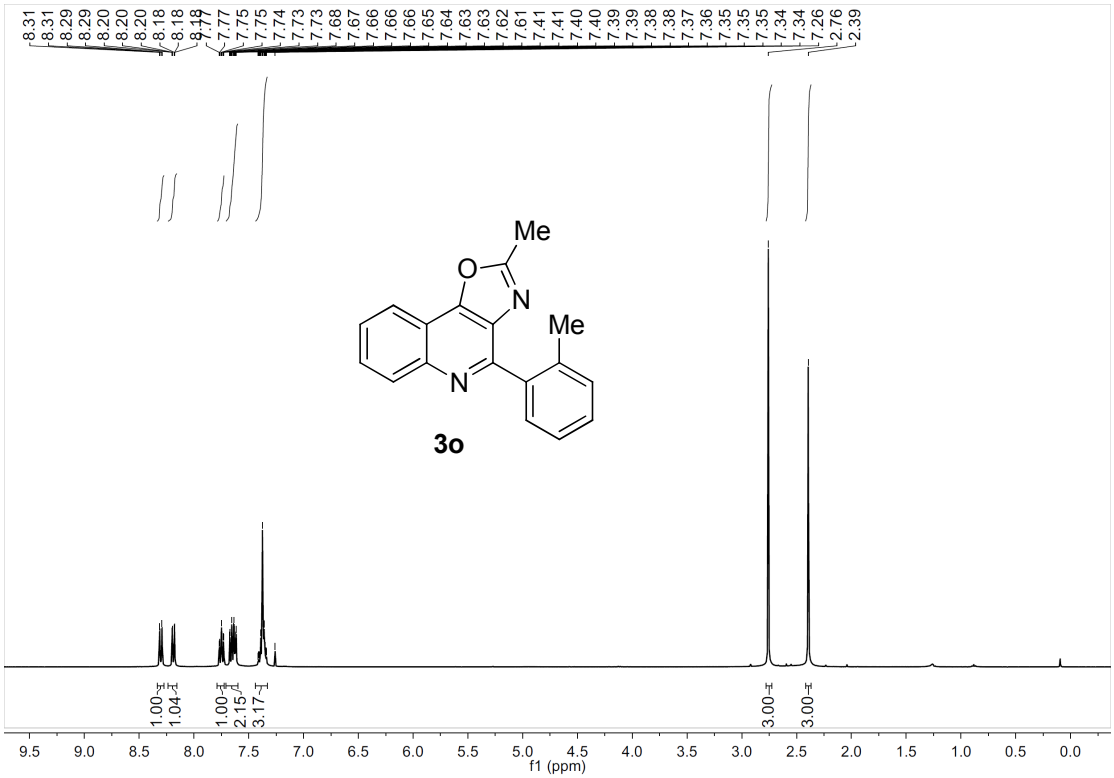
f1 (ppm)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7.66
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7.38
7.37
7.36
7.35
7.35
7.35
7.34
7.34
7.26
2.76
2.39
Me
O
N
Me
N
3o
1.00
1.04
1.00
2.15
3.17
3.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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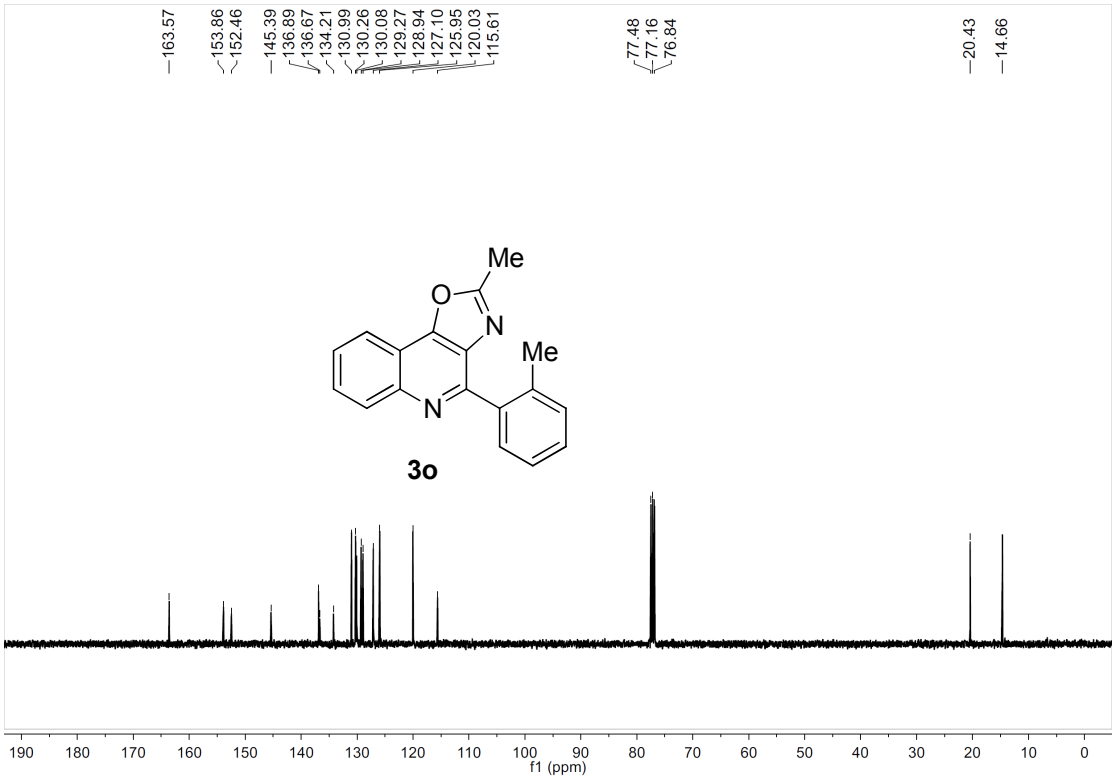
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77.16
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Me
N
3o
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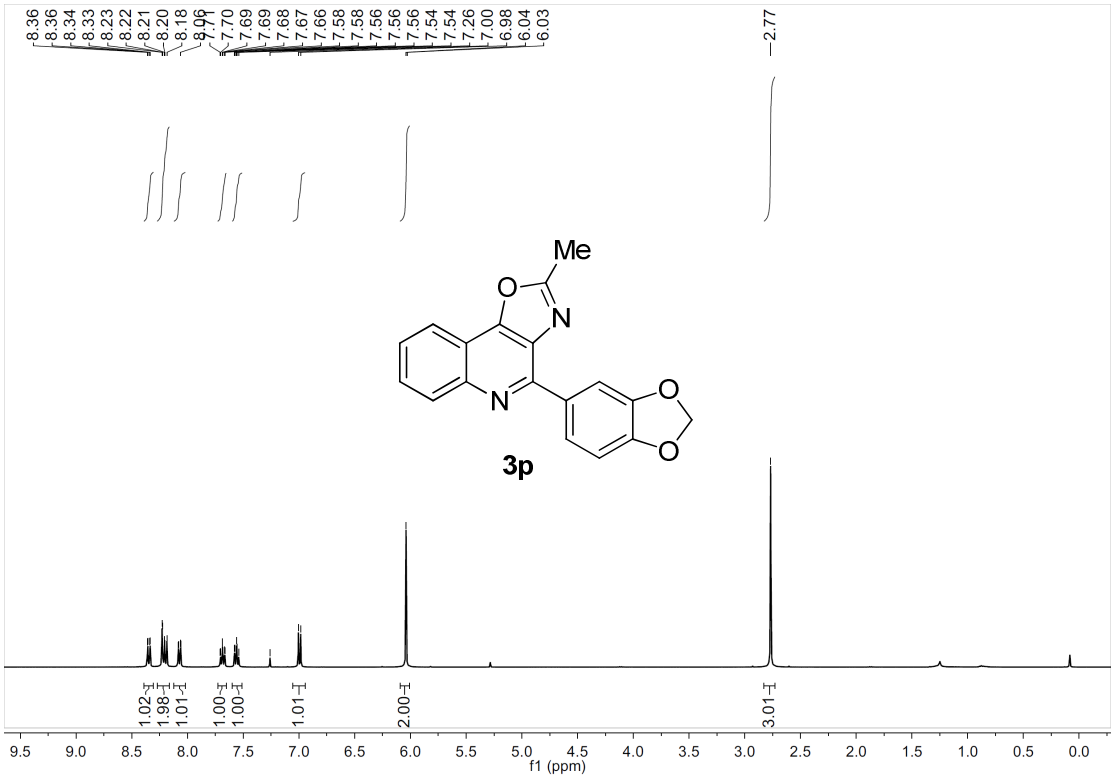
f1 (ppm)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7.58
7.58
7.56
7.56
7.56
7.54
7.54
7.26
7.00
6.98
6.04
6.03
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Me
O
N
N
O
O
3p
1.02
1.98
1.01
1.00
1.00
1.01
2.00
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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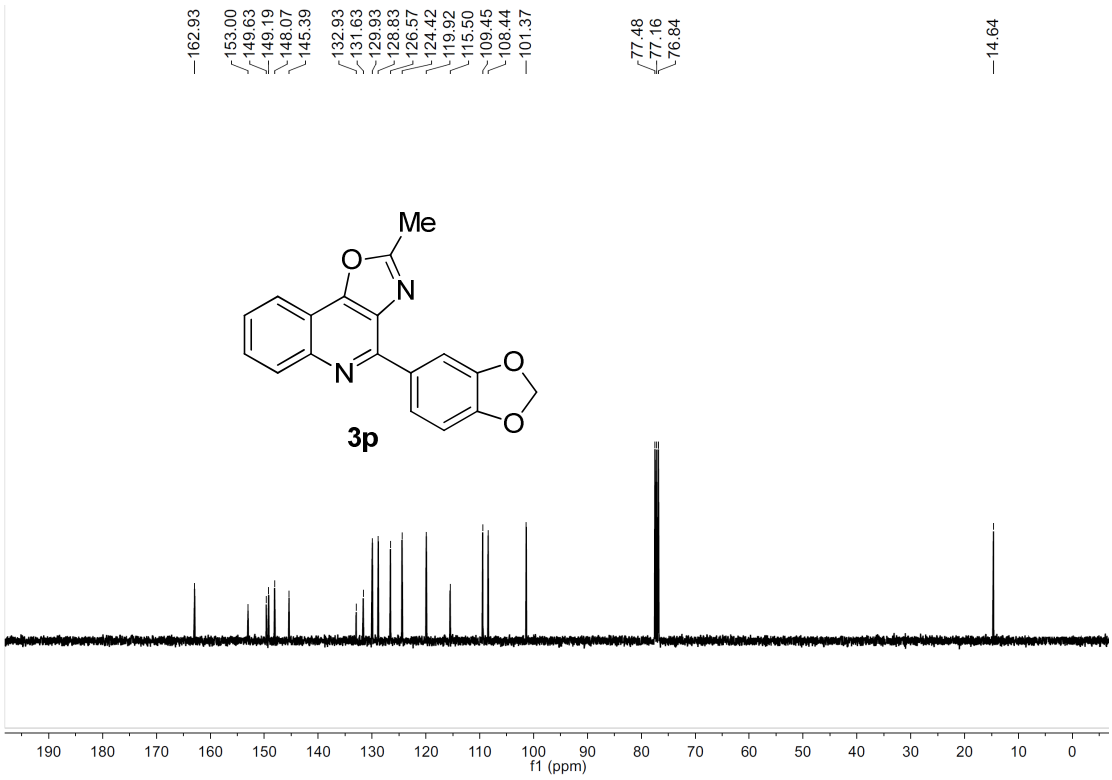
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109.45
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101.37
77.48
77.16
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N
N
O
O
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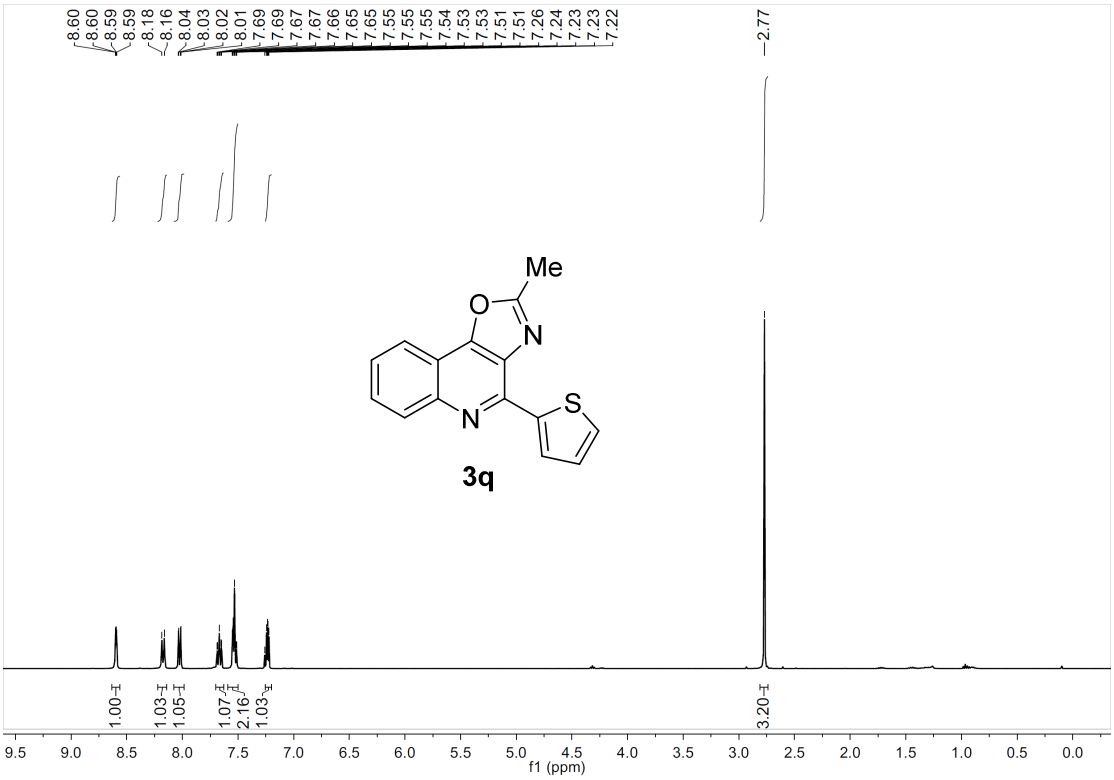
f1 (ppm)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7.23
7.22
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N
S
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1.03
1.05
1.07
2.16
1.03
3.20
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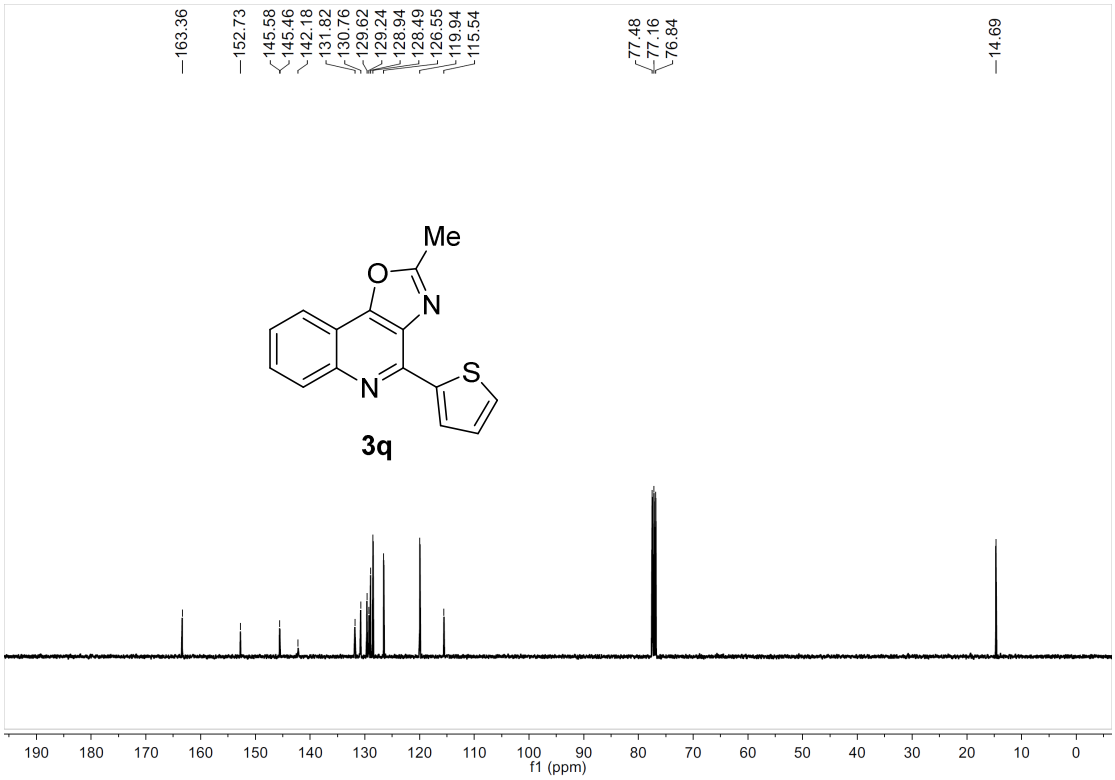
f1 (ppm)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77.48
77.16
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Me
O
N
N
S
3q
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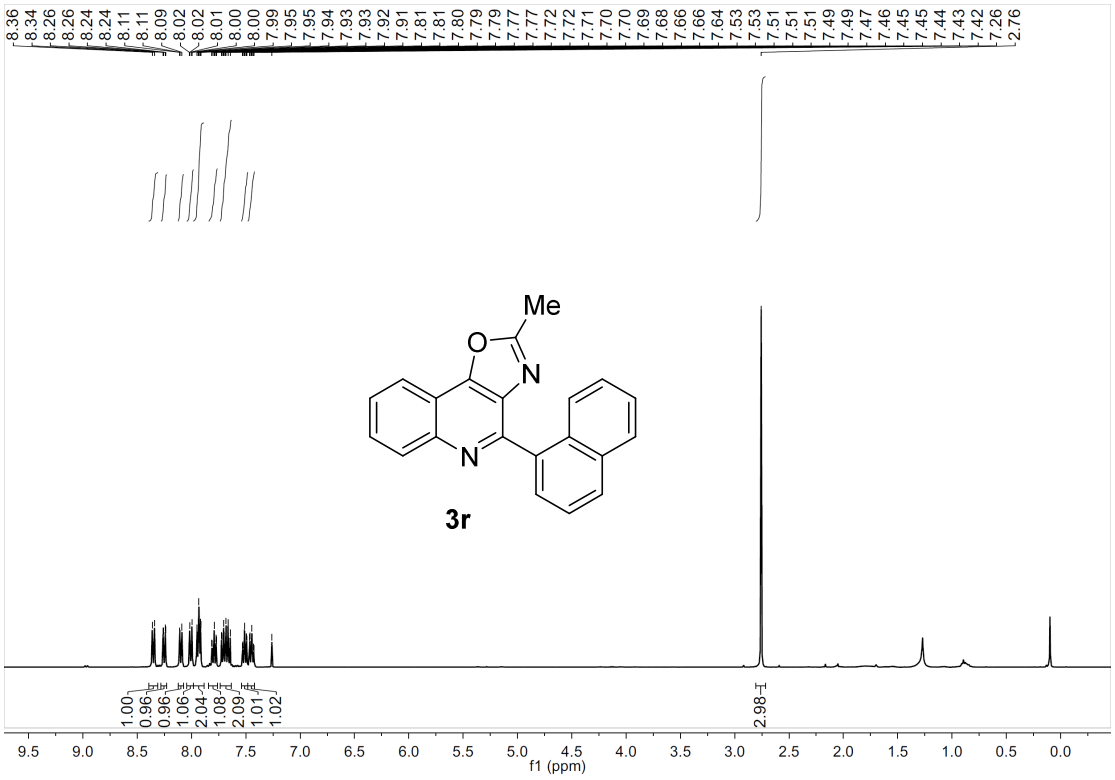
f1 (ppm)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Me
O
N
N
3r
1.00 0.96 0.96 1.06 2.04 1.08 2.09 1.01 1.02
2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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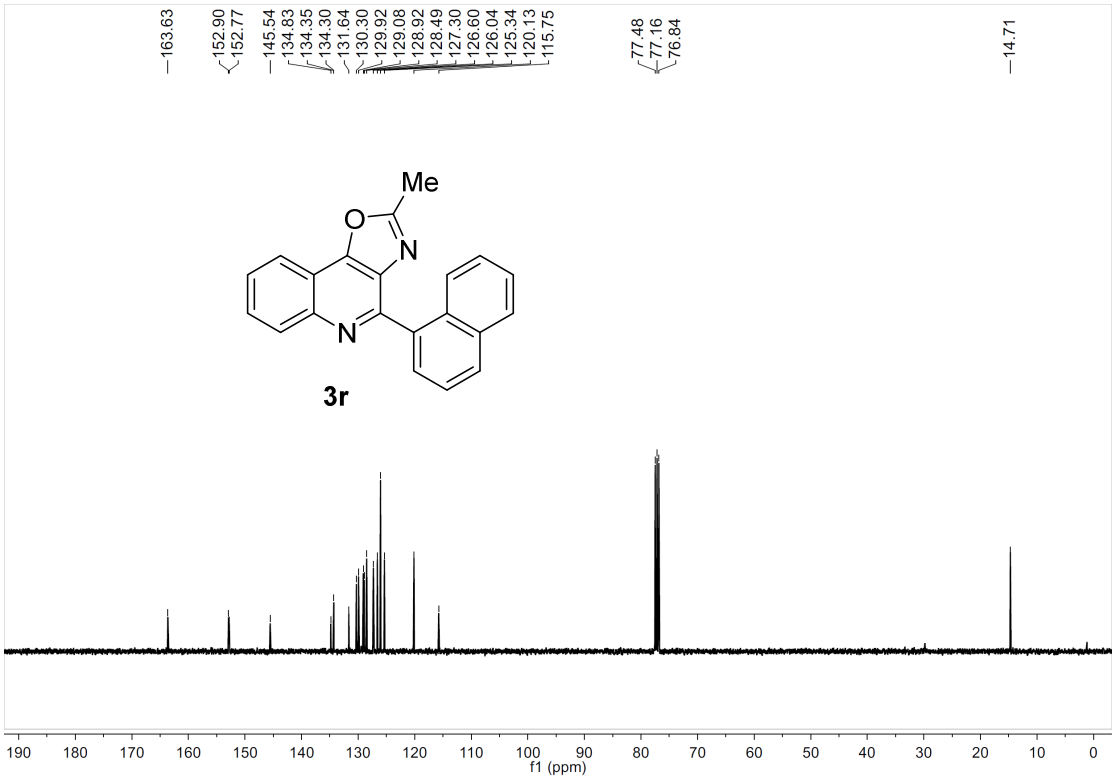
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126.60
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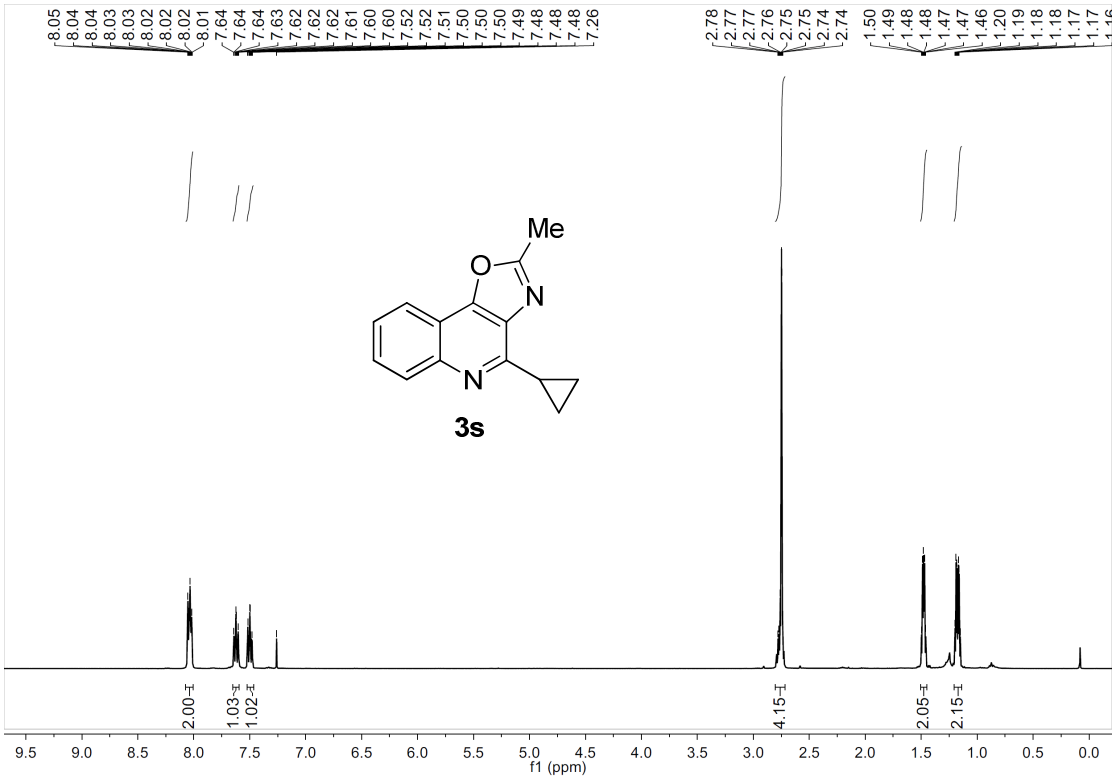
115.75
77.48
77.16
76.84
14.71
Me
O
N
N
3r
f1 (ppm)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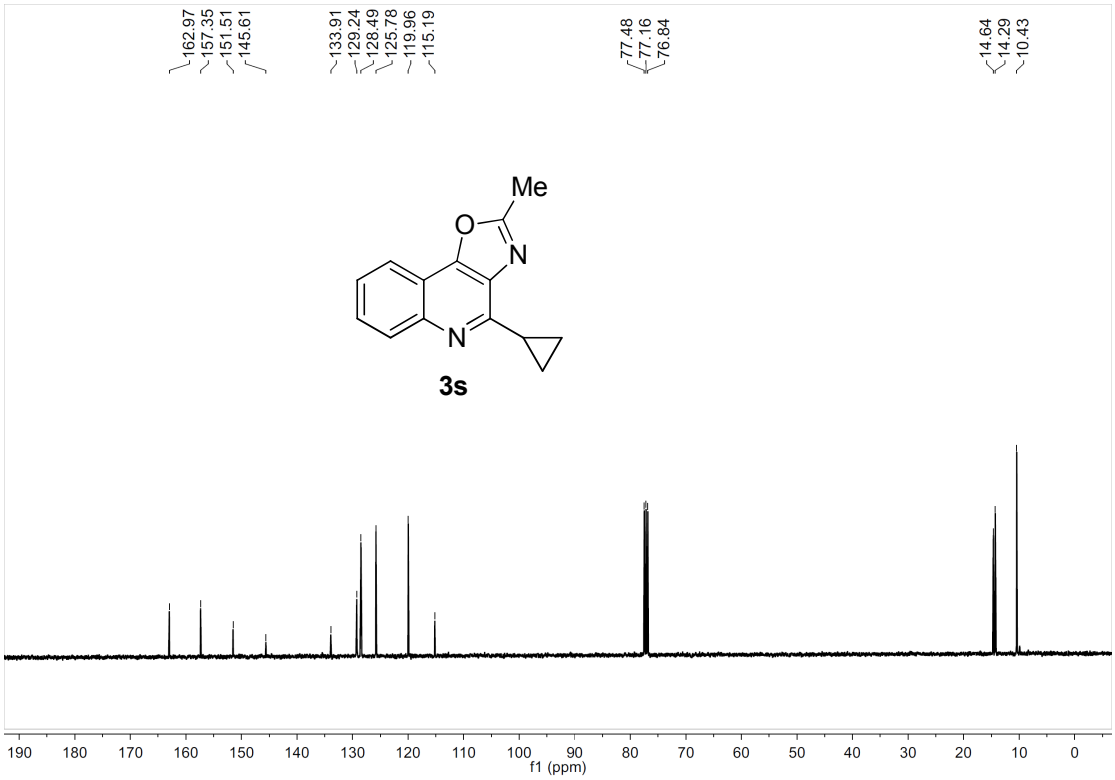
2.15
f1 (ppm)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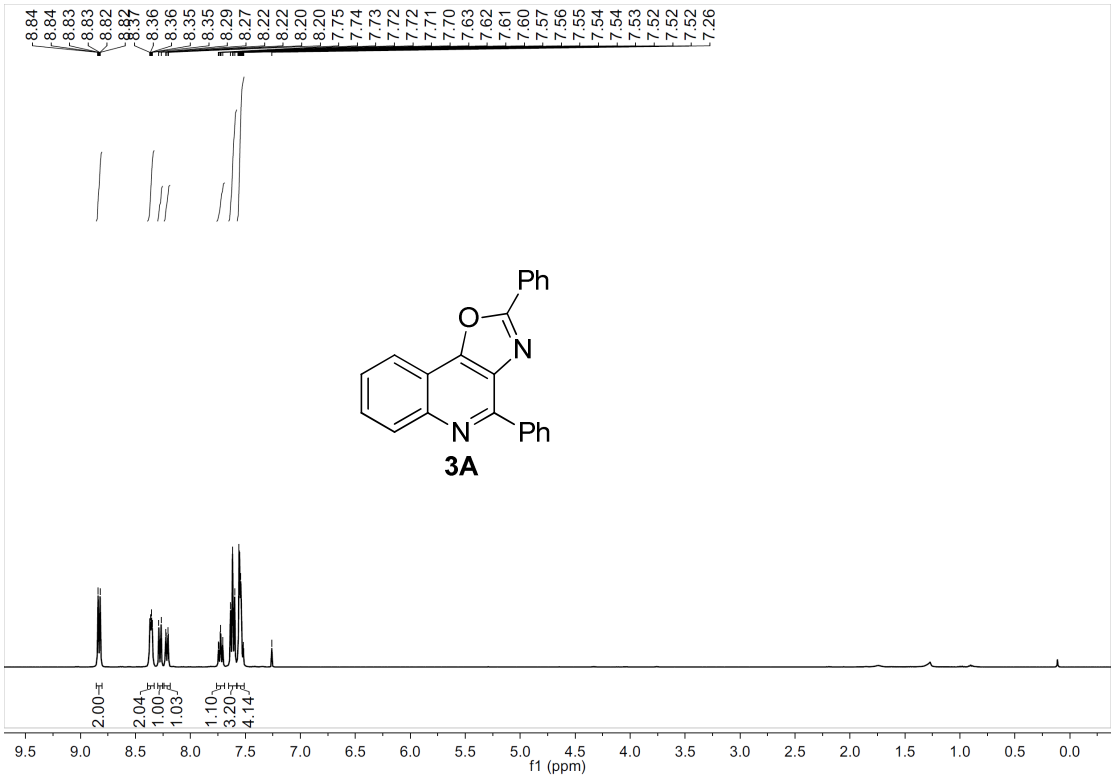
N
3s
f1 (ppm)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7.71
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7.62
7.61
7.60
7.57
7.56
7.55
7.54
7.54
7.53
7.52
7.52
7.52
7.26
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Ph
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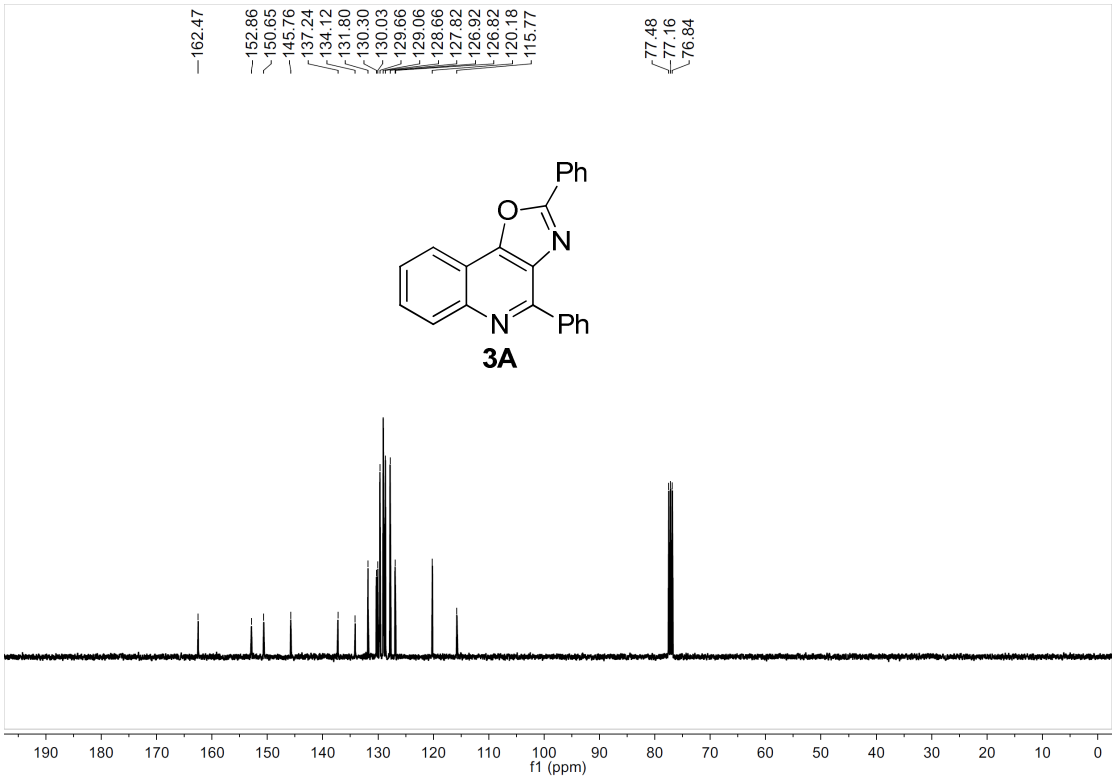
1.10
3.20
4.14
f1 (ppm)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Ph
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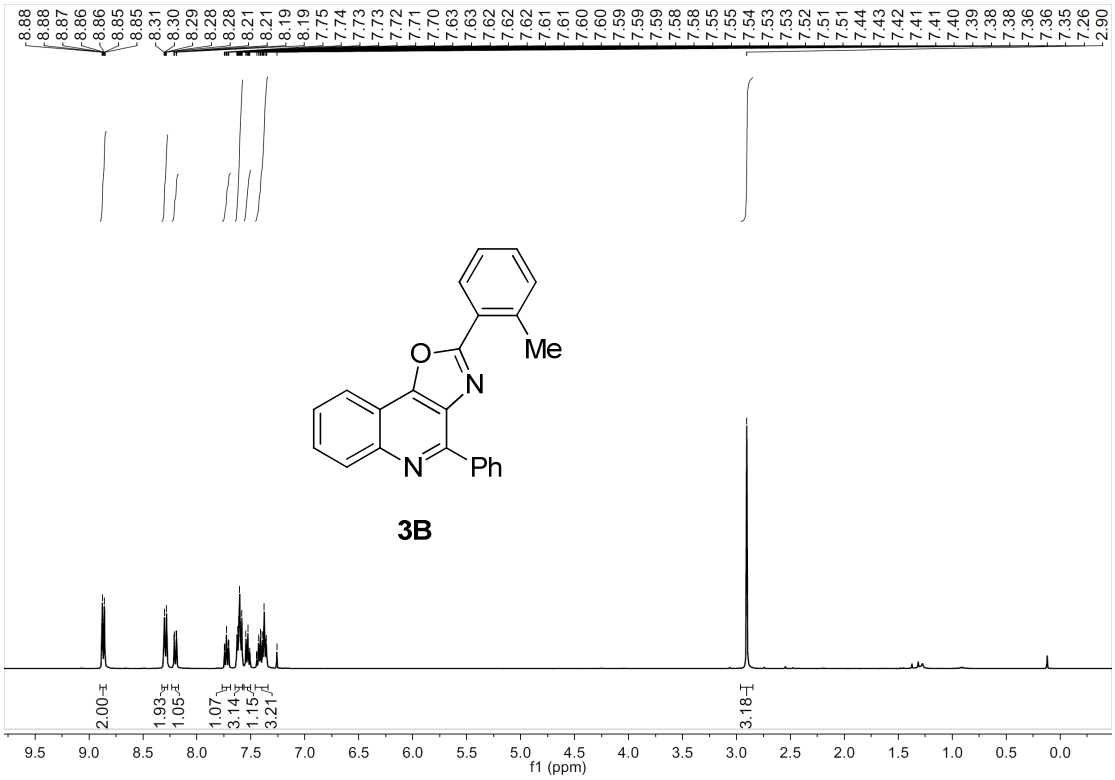
N
Ph
3A
f1 (ppm)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1.05
1.07
3.14
1.15
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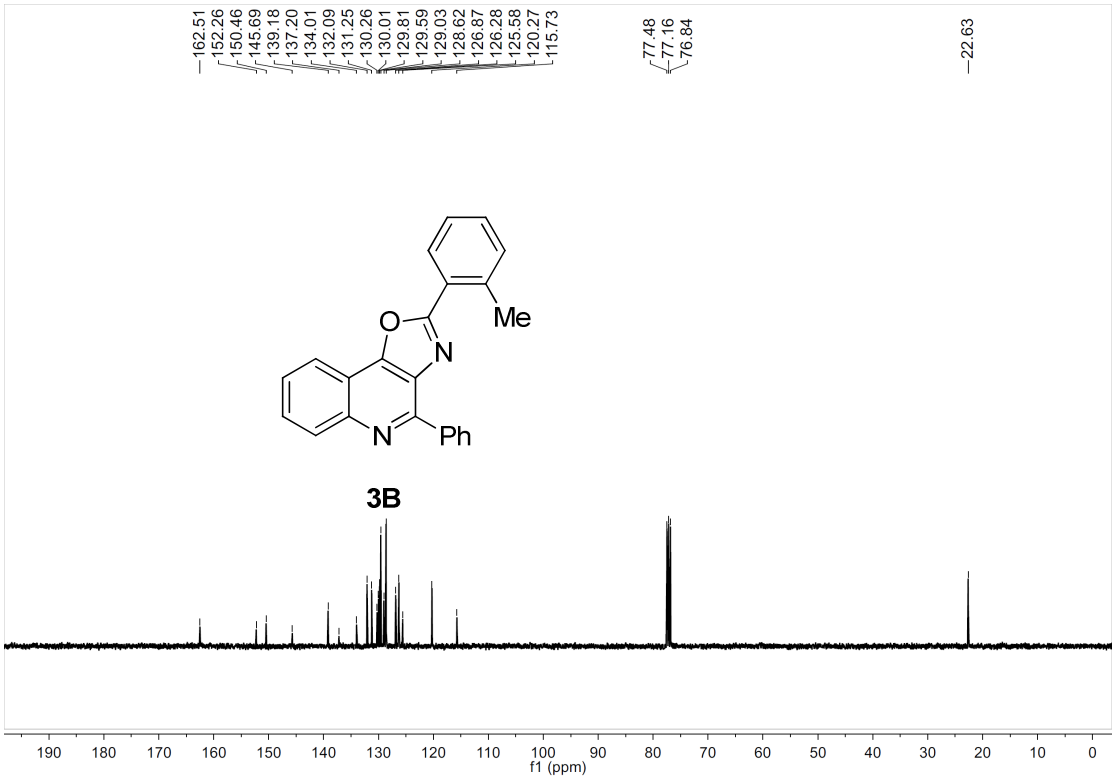
3.18
f1 (ppm)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120.27
115.73
77.48
77.16
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O
N
N
Ph
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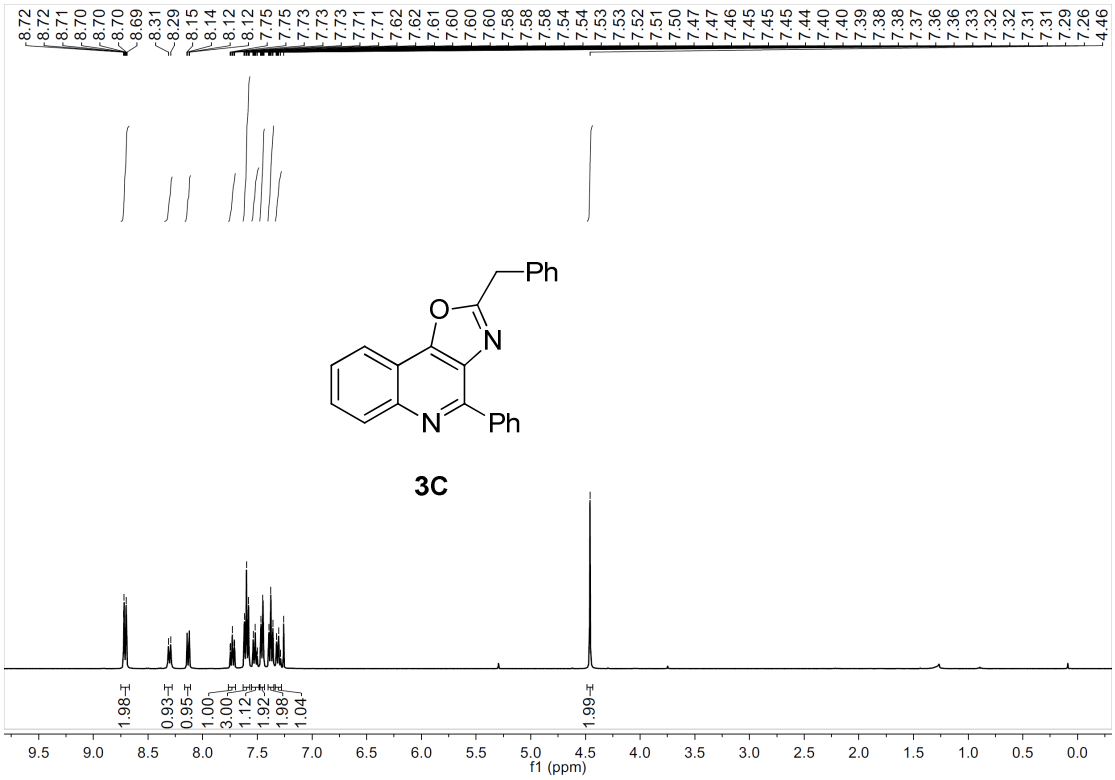
f1 (ppm)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7.26
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Ph
O
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N
Ph
3C
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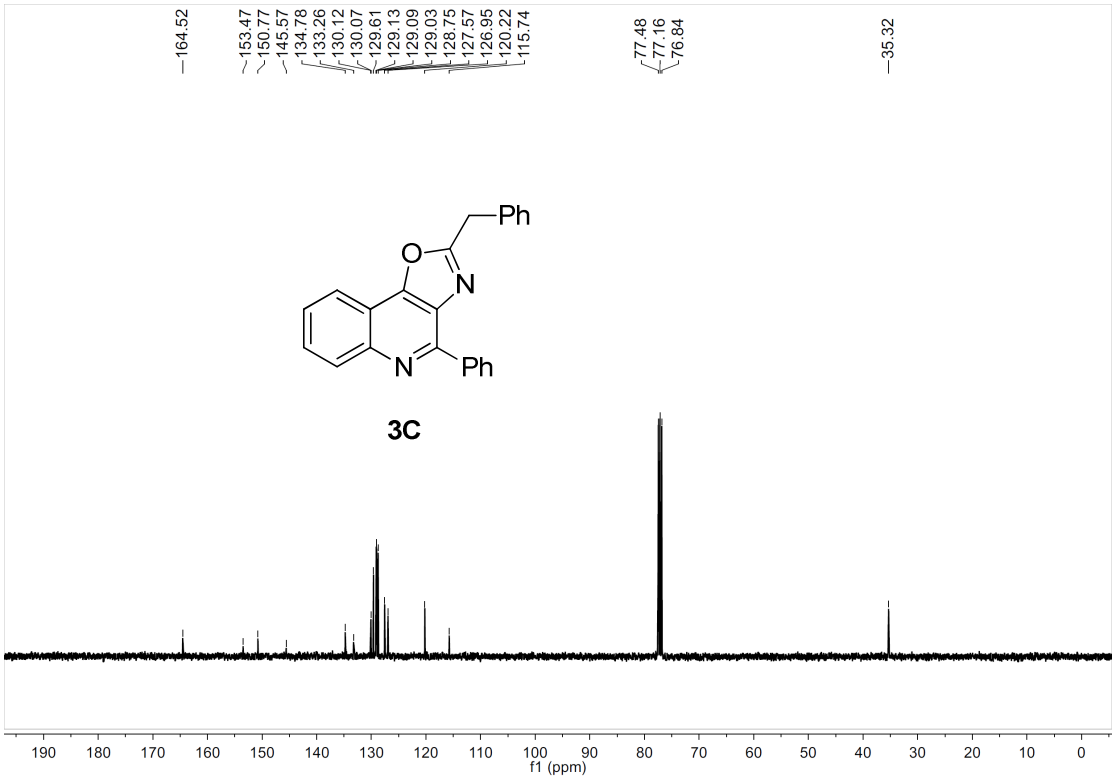
0.95
1.00
3.00
1.12
1.92
1.98
1.04
1.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.57
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76.84
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Ph
O
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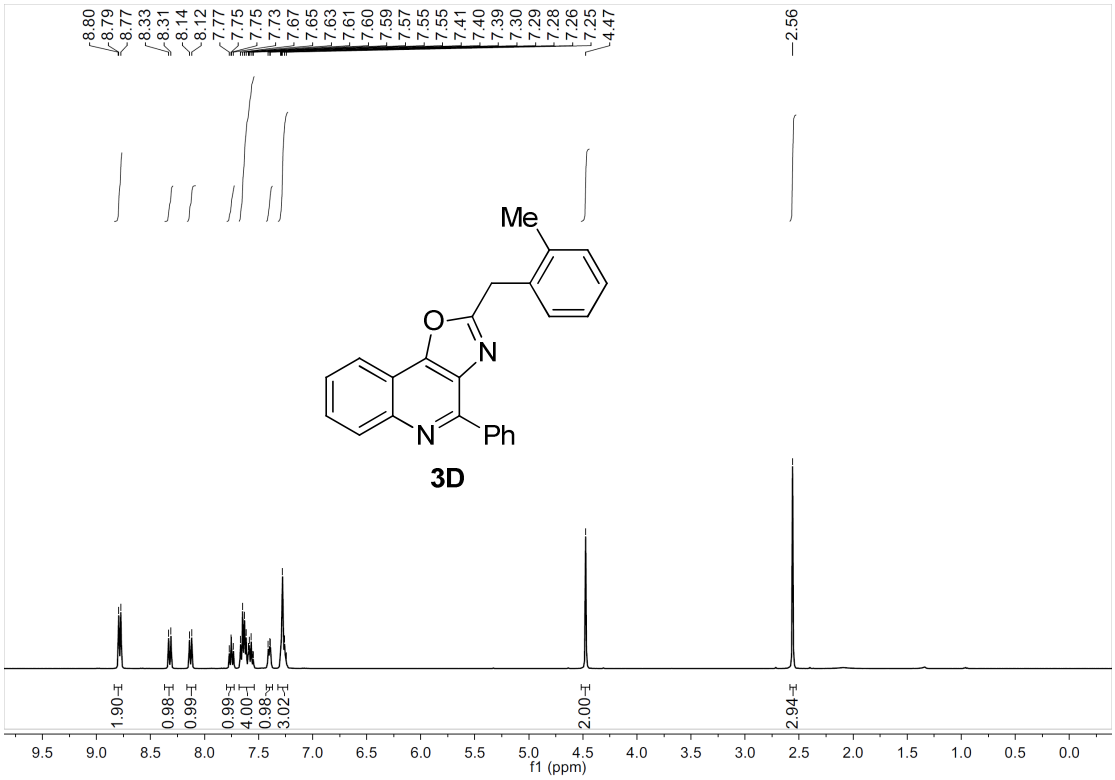
N
Ph
3C
f1 (ppm)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7.28
7.26
7.25
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Me
O
N
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0.99
0.99
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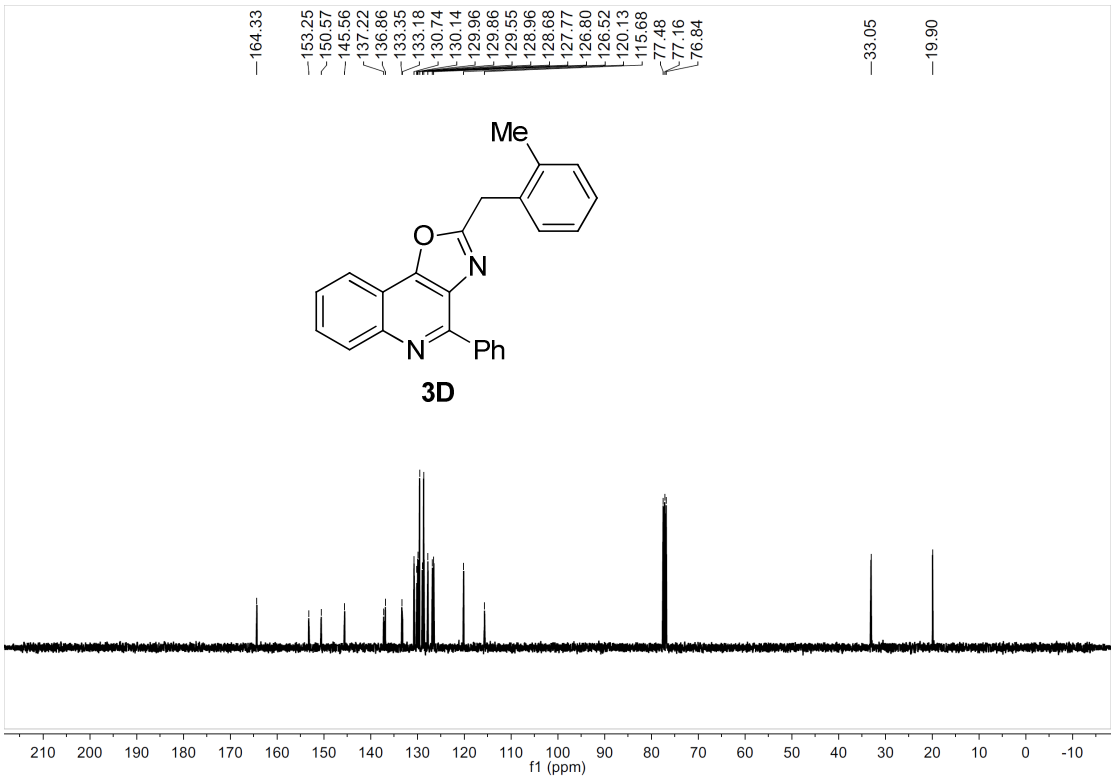
0.98
3.02
2.00
2.94
f1 (ppm)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O
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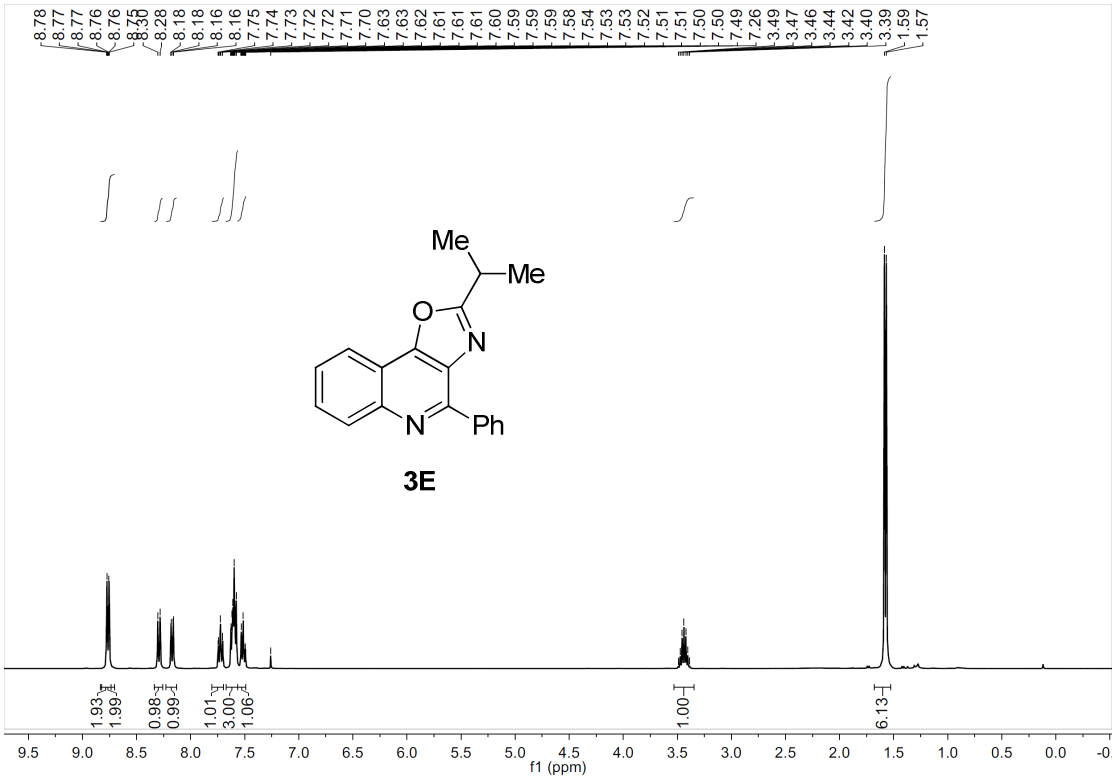
Ph
3D
f1 (ppm)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Me
O
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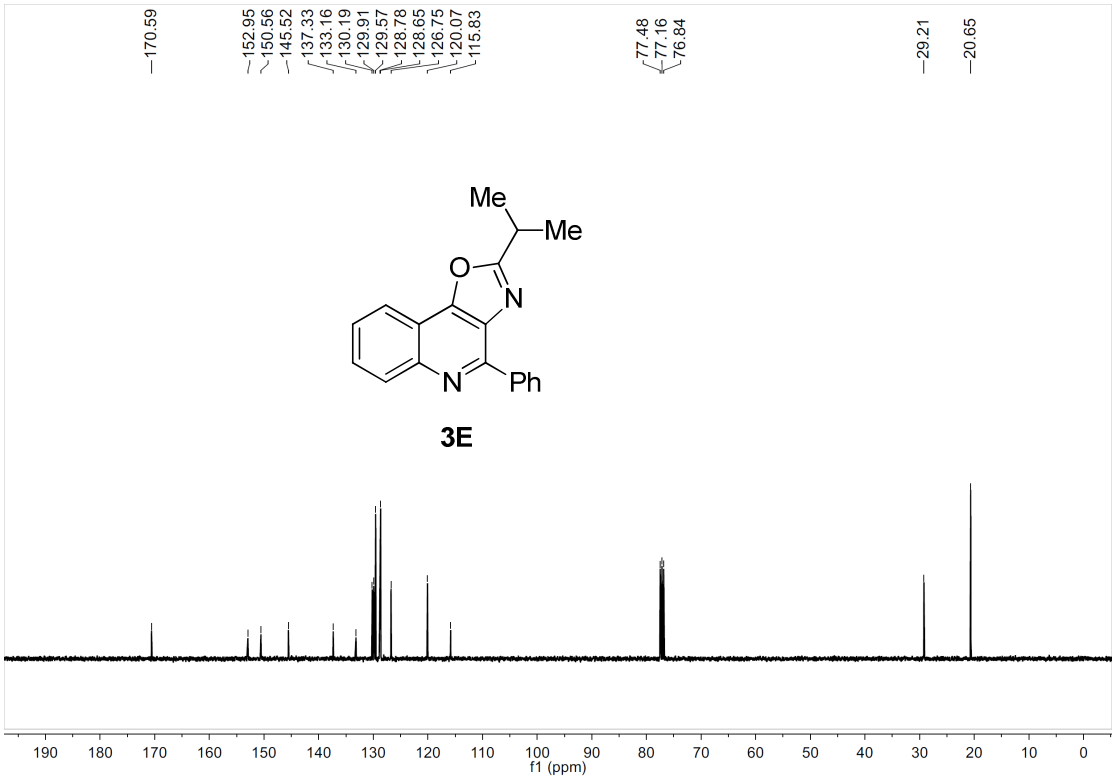
1.06
1.00
6.13
f1 (ppm)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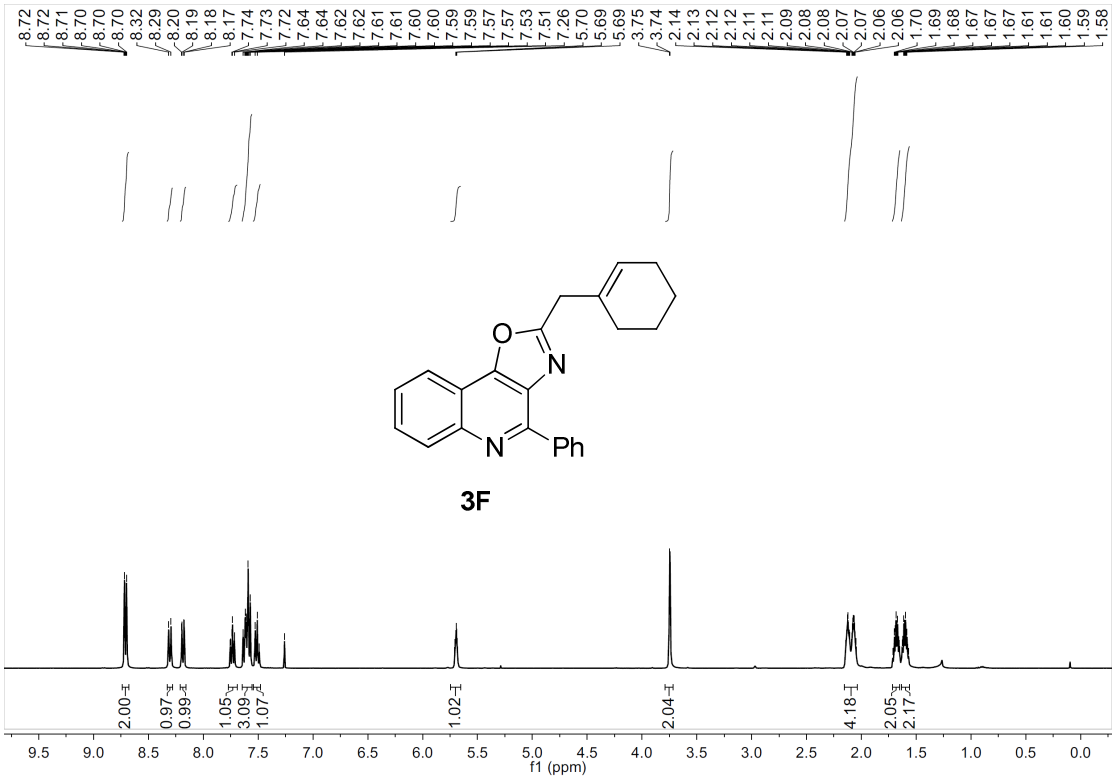
128.65
126.75
120.07
115.83
77.48
77.16
76.84
29.21
20.65
Me
Me
O
N
N
Ph
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3E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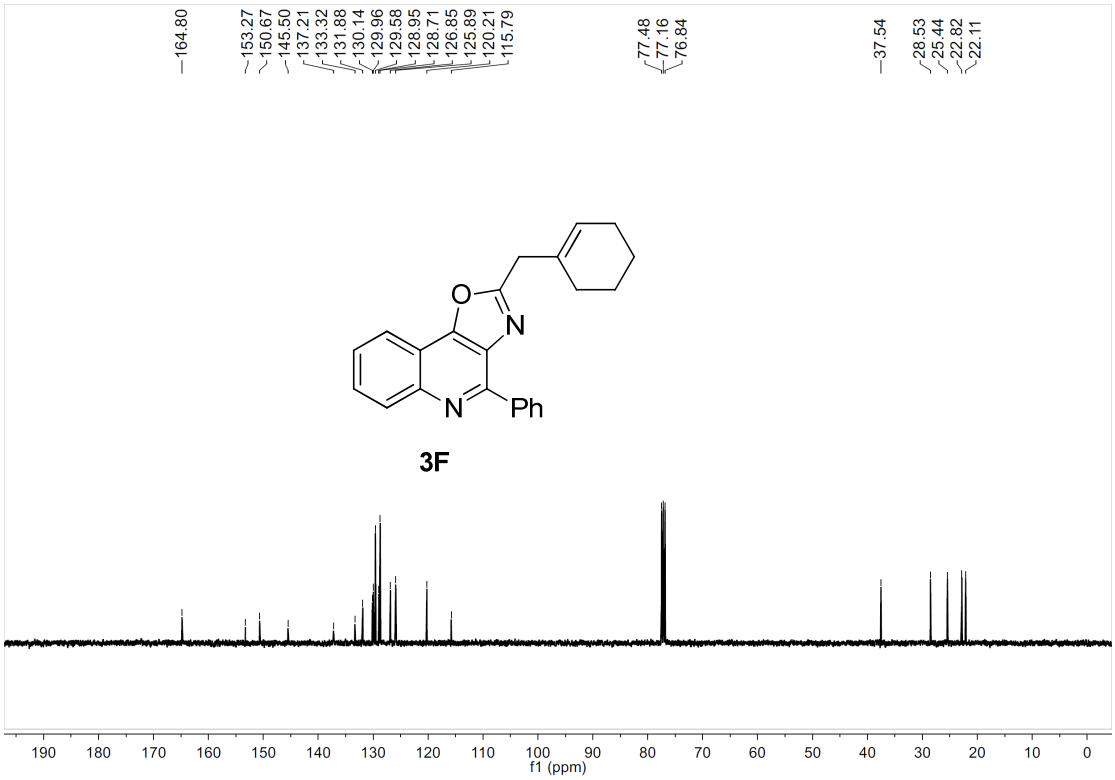
2.17
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3F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129.58
128.95
128.71
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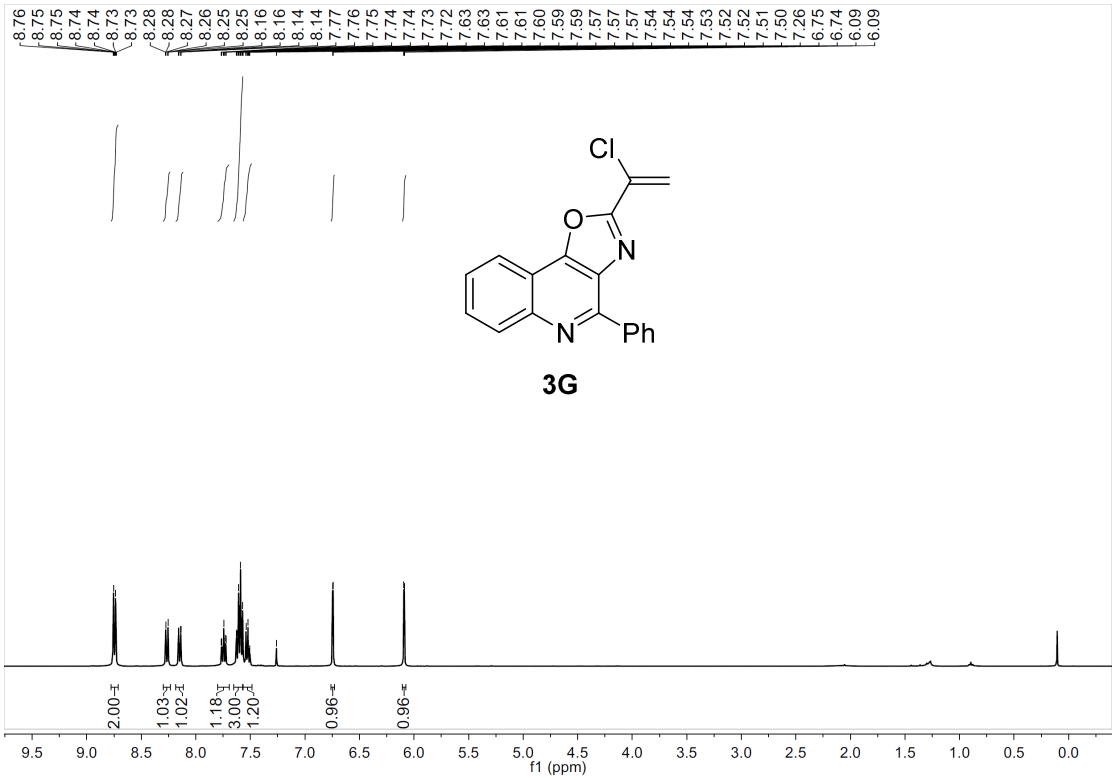
125.89
120.21
115.79
77.48
77.16
76.84
37.54
28.53
25.44
22.82
22.11
O
N
N
Ph
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3F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8.16
8.16
8.14
8.14
7.77
7.76
7.75
7.74
7.74
7.73
7.72
7.63
7.63
7.61
7.61
7.60
7.59
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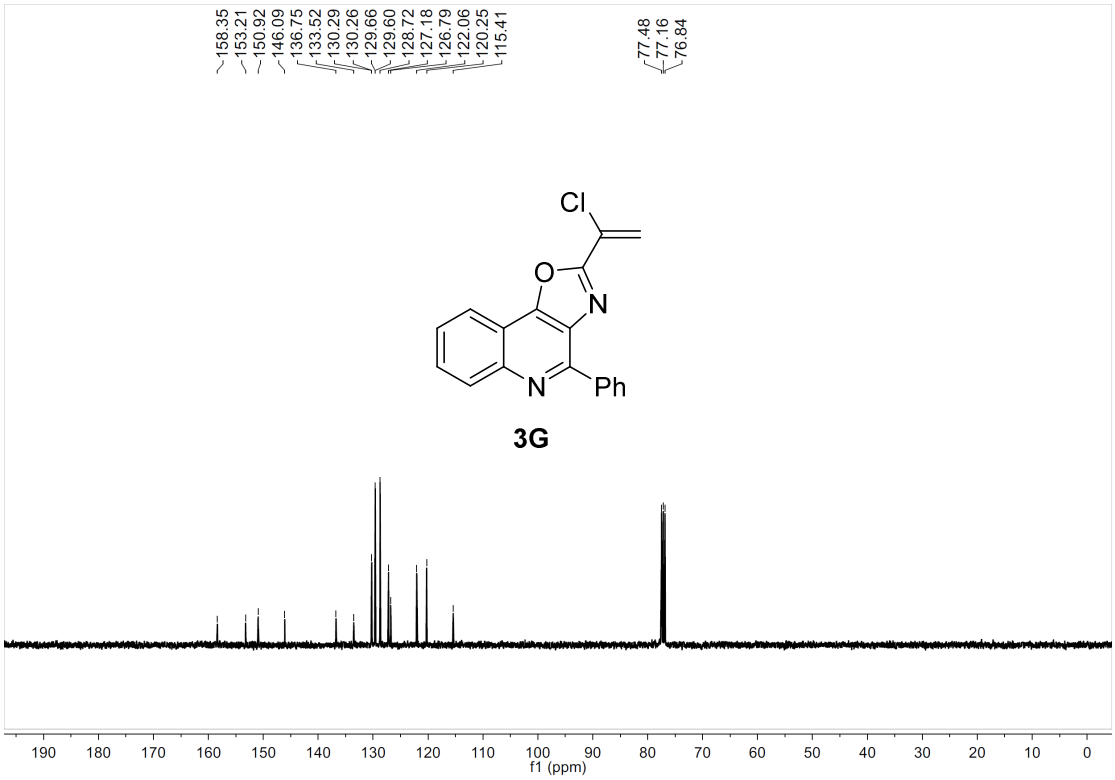
7.57
7.57
7.57
7.54
7.54
7.54
7.53
7.52
7.52
7.51
7.50
7.26
6.75
6.74
6.09
6.09
Cl
O
N
N
Ph
2.00
1.03
1.02
1.18
3.00
1.20
0.96
0.96
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3G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130.26
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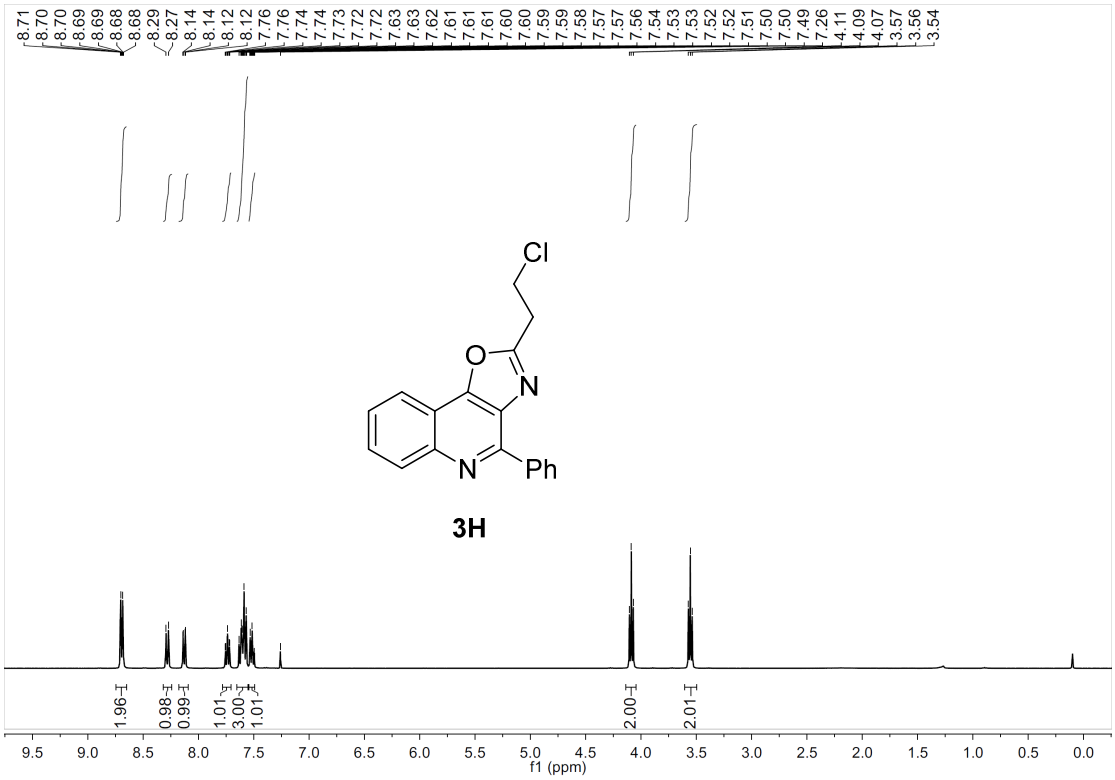
129.60
128.72
127.18
126.79
122.06
120.25
115.41
77.48
77.16
76.84
Cl
O
N
N
Ph
3G
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.12
8.12
7.76
7.76
7.74
7.74
7.73
7.72
7.72
7.63
7.63
7.62
7.61
7.61
7.60
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7.59
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7.58
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7.56
7.54
7.53
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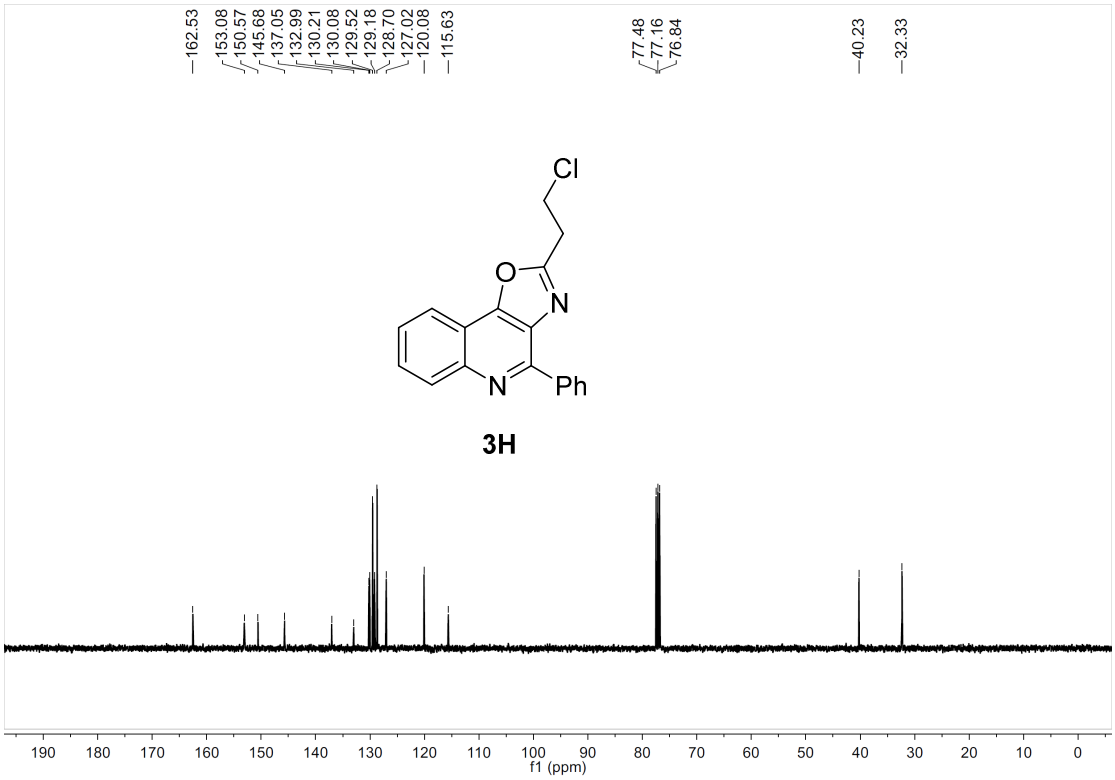
7.51
7.50
7.50
7.49
7.26
4.11
4.09
4.07
3.57
3.56
3.54
Cl
O
N
N
Ph
3H
1.96
0.98
0.99
1.01
3.00
1.01
2.00
2.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.18
128.70
127.02
120.08
115.63
77.48
77.16
76.84
40.23
32.33
Cl
O
N
N
Ph
3H
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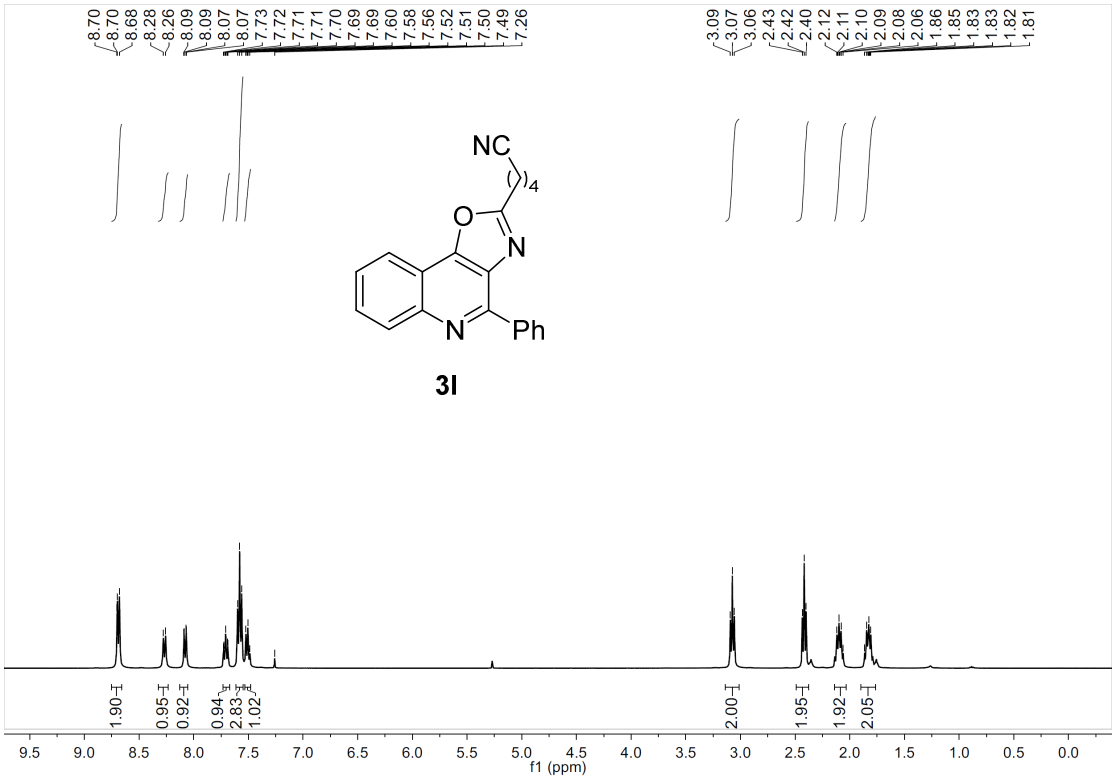
f1 (ppm)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8.07
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7.71
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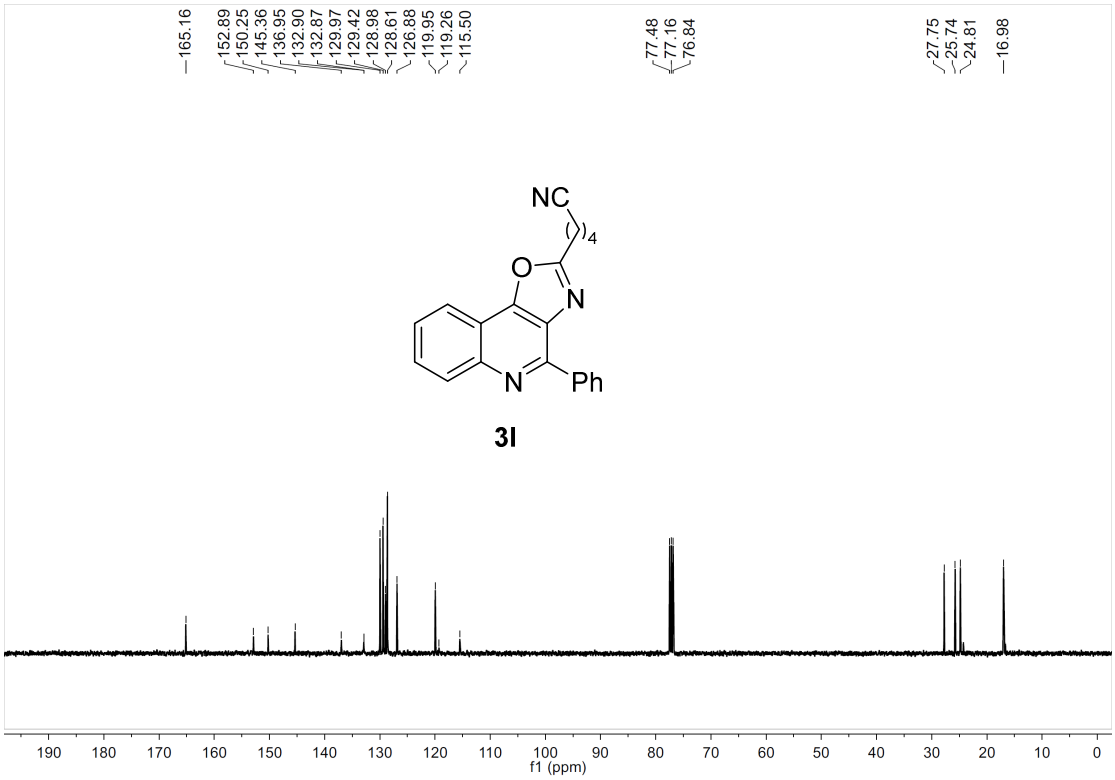
7.69
7.69
7.60
7.58
7.56
7.52
7.51
7.50
7.49
7.26
3.09
3.07
3.06
2.43
2.42
2.40
2.12
2.11
2.10
2.09
2.08
2.06
1.86
1.85
1.83
1.83
1.82
1.81
NC
4
O
N
N
Ph
3I
1.90
0.95
0.92
0.94
2.83
1.02
2.00
1.95
1.92
2.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.97
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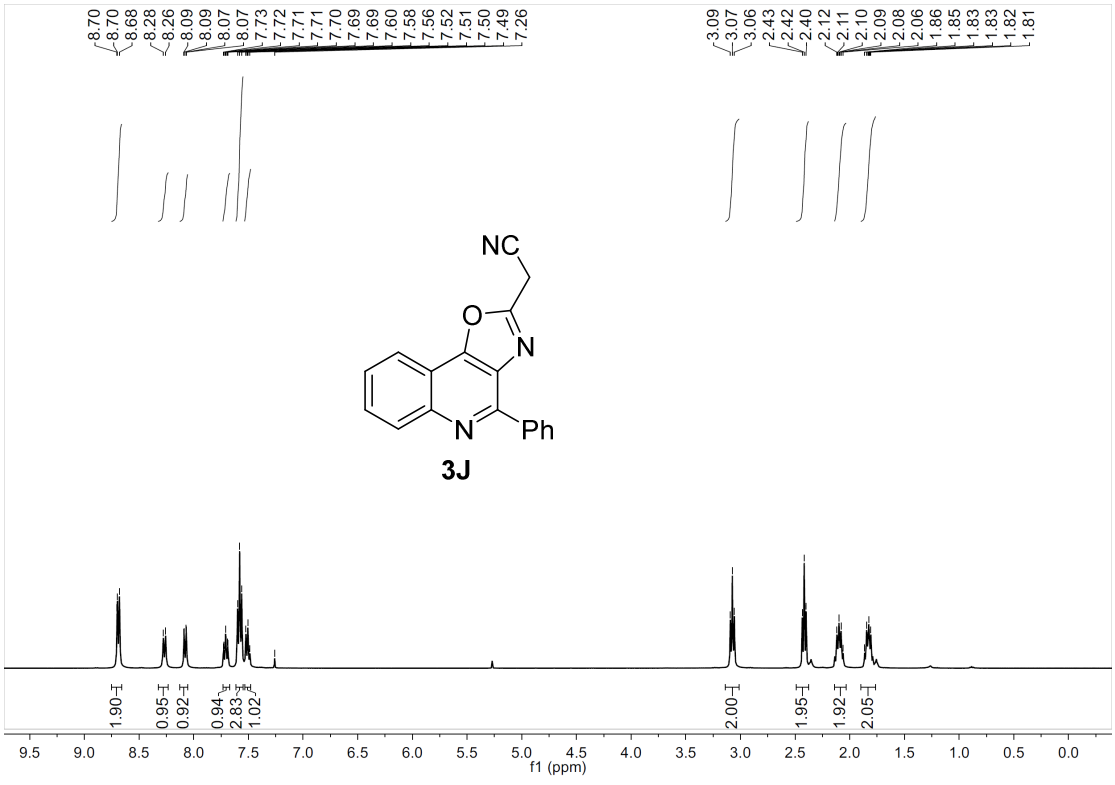
128.98
128.61
126.88
119.95
119.26
115.50
77.48
77.16
76.84
27.75
25.74
24.81
16.98
NC
4
O
N
N
Ph
3I
f1 (ppm)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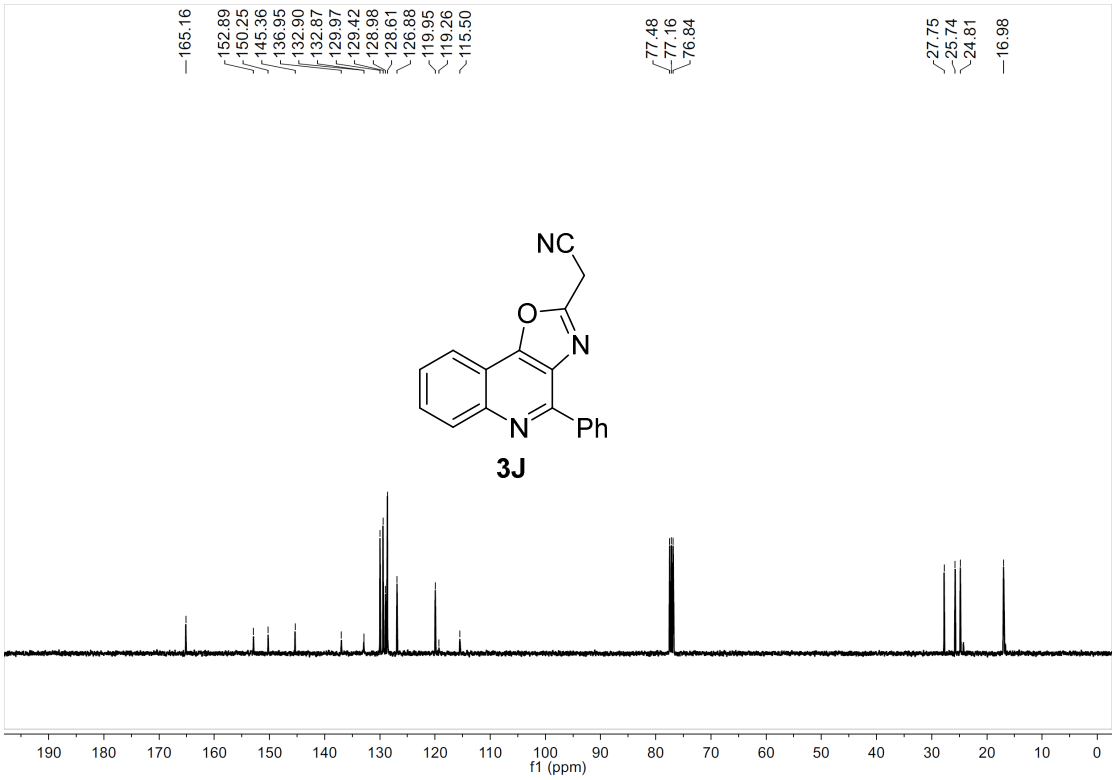
8.68
8.28
8.26
8.09
8.09
8.07
8.07
7.73
7.72
7.71
7.71
7.70
7.69
7.69
7.60
7.58
7.56
7.52
7.51
7.50
7.49
7.26
3.09
3.07
3.06
2.43
2.42
2.40
2.12
2.11
2.10
2.09
2.08
2.06
1.86
1.85
1.83
1.83
1.82
1.81
NC
O
N
N
Ph
3J
1.90
0.95
0.92
0.94
2.83
1.02
2.00
1.95
1.92
2.05
f1 (ppm)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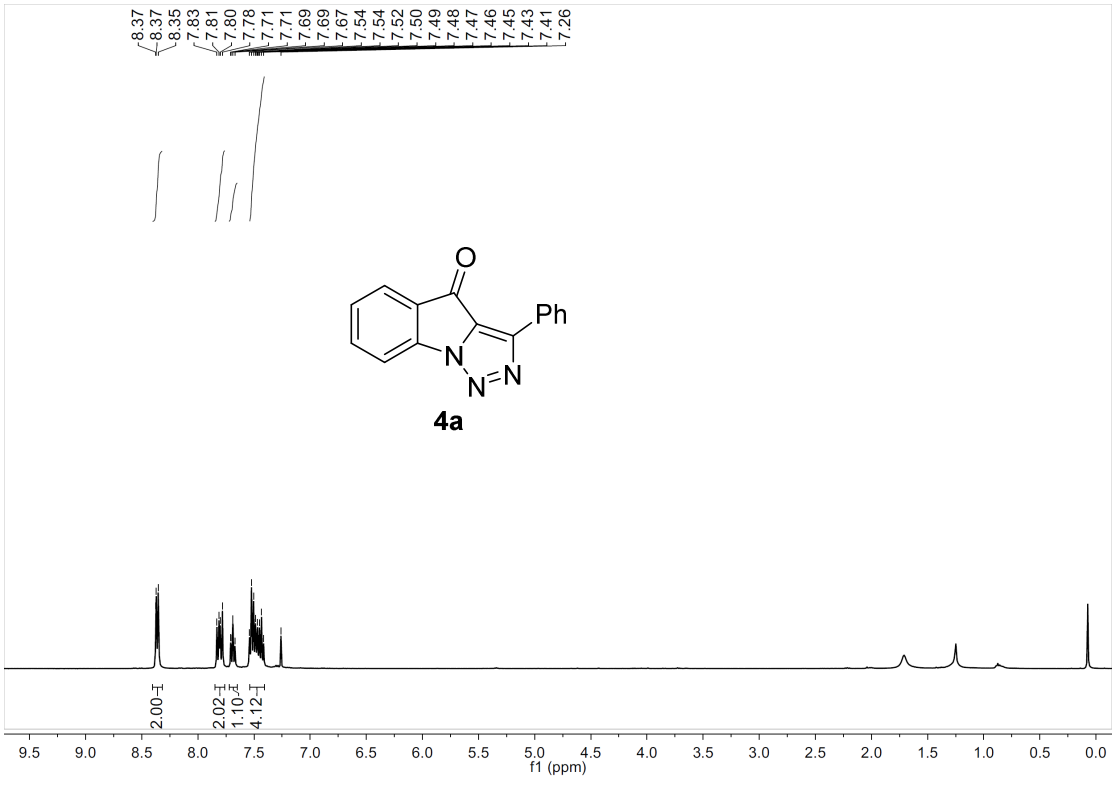
150.25
145.36
136.95
132.90
132.87
129.97
129.42
128.98
128.61
126.88
119.95
119.26
115.50
77.48
77.16
76.84
27.75
25.74
24.81
16.98
NC
O
N
N
Ph
3J
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.80
7.78
7.71
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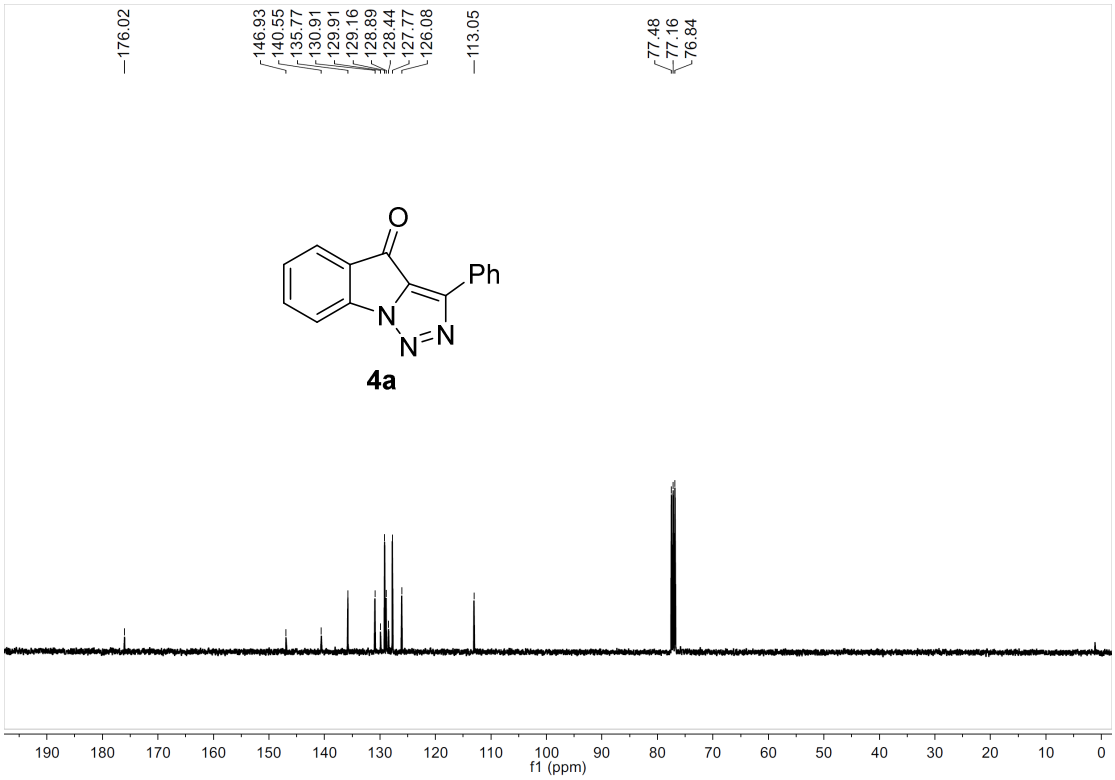
7.69
7.69
7.67
7.54
7.54
7.52
7.50
7.49
7.48
7.47
7.46
7.45
7.43
7.41
7.26
O
Ph
N
N
N
4a
2.00
2.02
1.10
4.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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130.91
129.91
129.16
128.89
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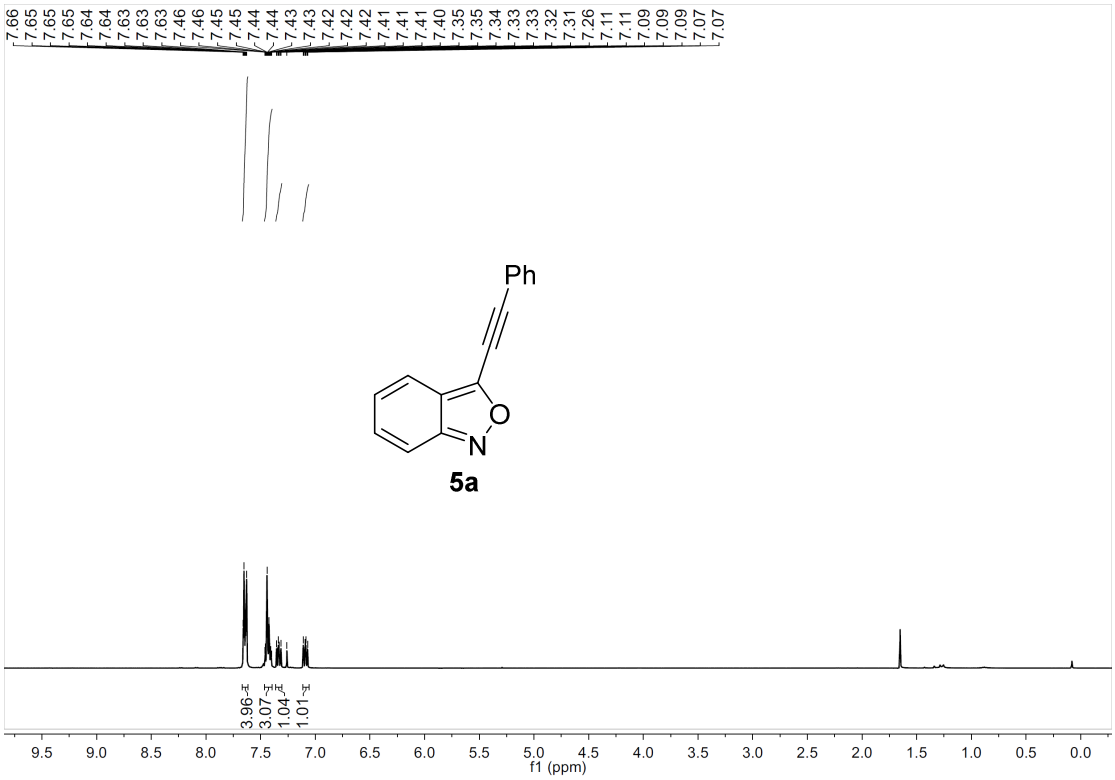
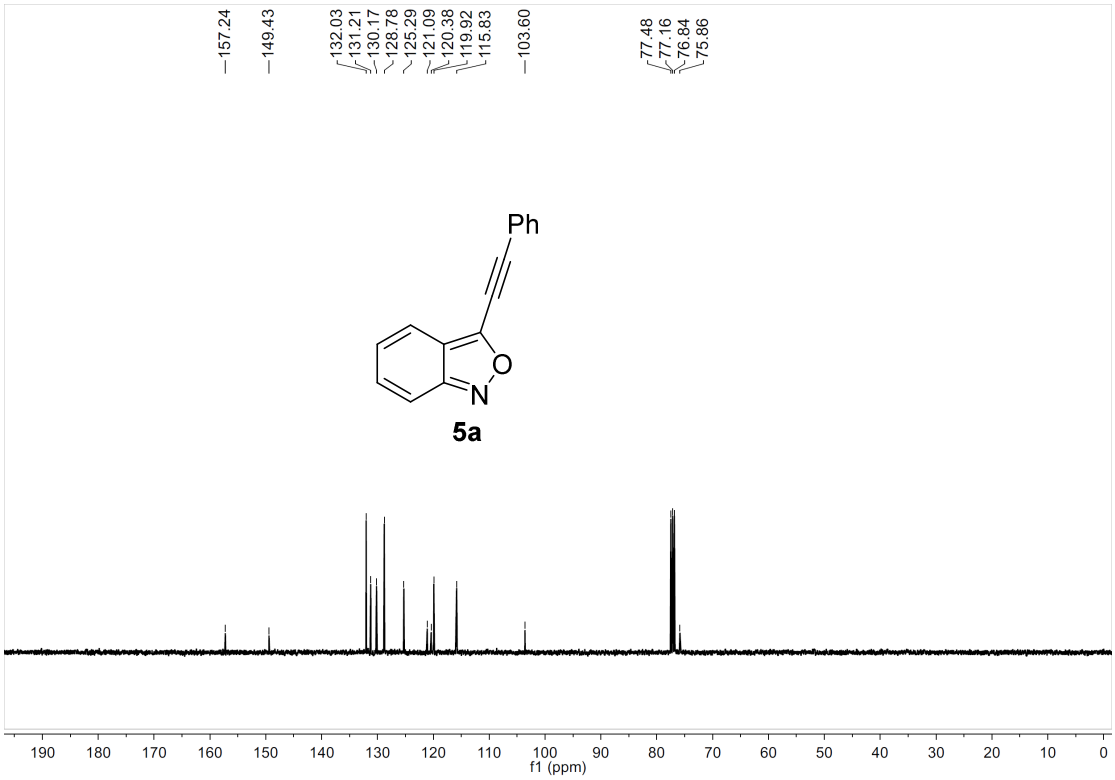
127.77
126.08
113.05
77.48
77.16
76.84
O
Ph
N
N
N
4a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.66 7.65 7.65 7.65 7.64 7.64 7.63 7.63 7.63 7.46 7.46 7.45 7.45 7.44 7.44 7.43 7.43 7.42 7.42 7.42 7.41 7.41 7.41 7.40 7.35 7.35 7.34 7.33 7.33 7.32 7.31 7.26 7.11 7.11 7.09 7.09 7.09 7.07 7.07
Ph
O
N
5a
3.96
3.07
1.04
1.01
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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128.78
125.29
121.09
120.38
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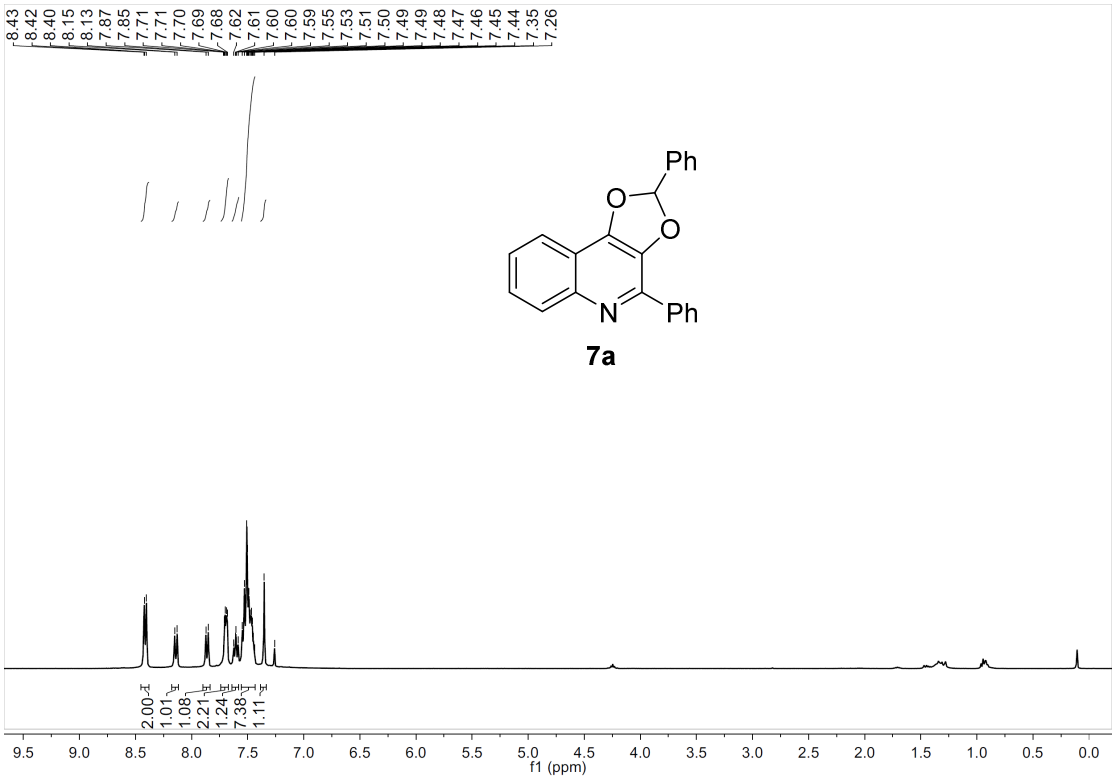
103.60
77.48
77.16
76.84
75.86
Ph
O
N
5a
f1 (ppm)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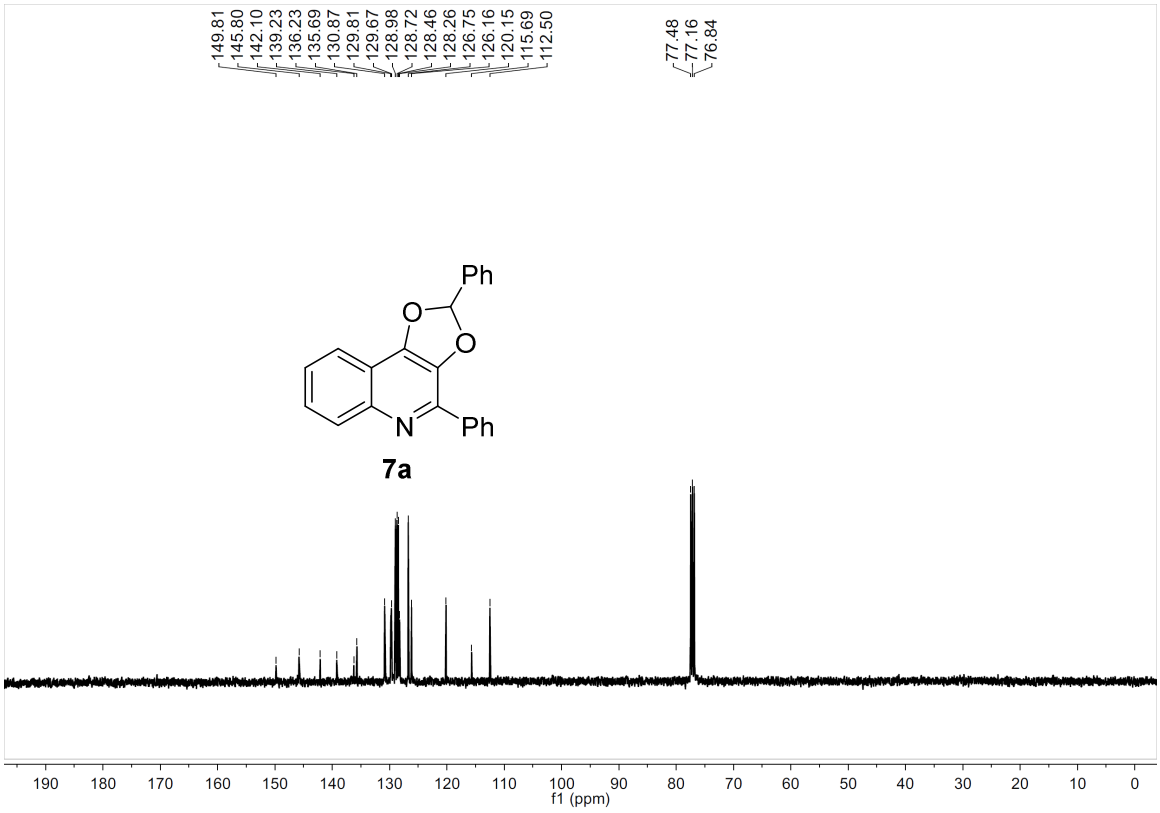
7.85
7.71
7.71
7.70
7.69
7.68
7.62
7.61
7.60
7.60
7.59
7.55
7.53
7.51
7.50
7.49
7.49
7.48
7.47
7.46
7.45
7.44
7.35
7.26
Ph
O
O
N
Ph
7a
2.00
1.01
1.08
2.21
1.24
7.38
1.11
f1 (ppm)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129.81
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128.72
128.46
128.26
126.75
126.16
120.15
115.69
112.50
77.48
77.16
76.84
Ph
O
O
N
Ph
7a
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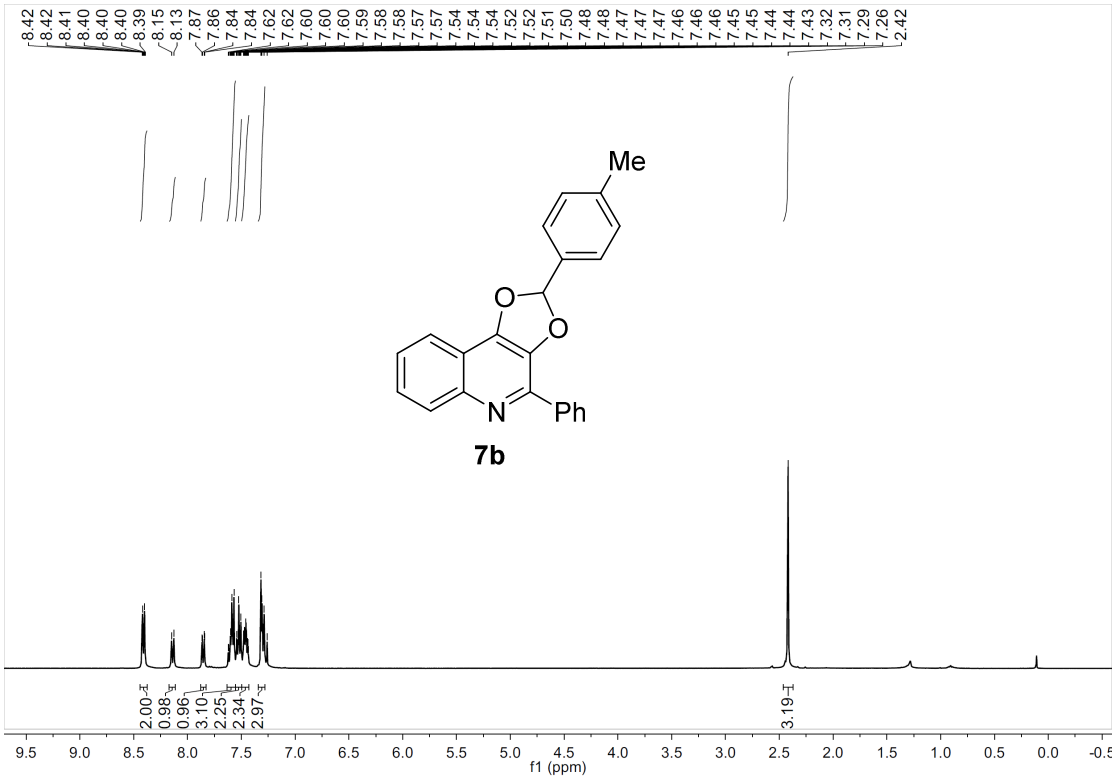
f1 (ppm)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7.44
7.43
7.32
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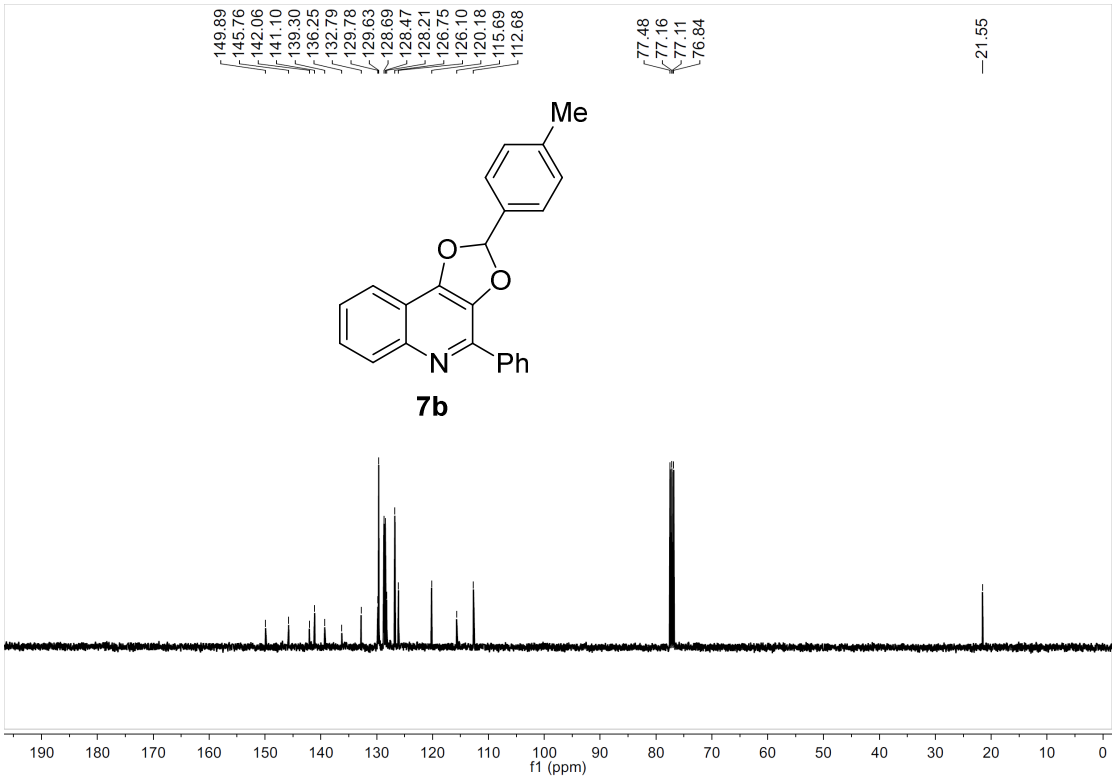
7.29
7.26
2.42
Me
O
O
N
Ph
7b
2.00
0.98
0.96
3.10
2.25
2.34
2.97
3.19
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.69
128.47
128.21
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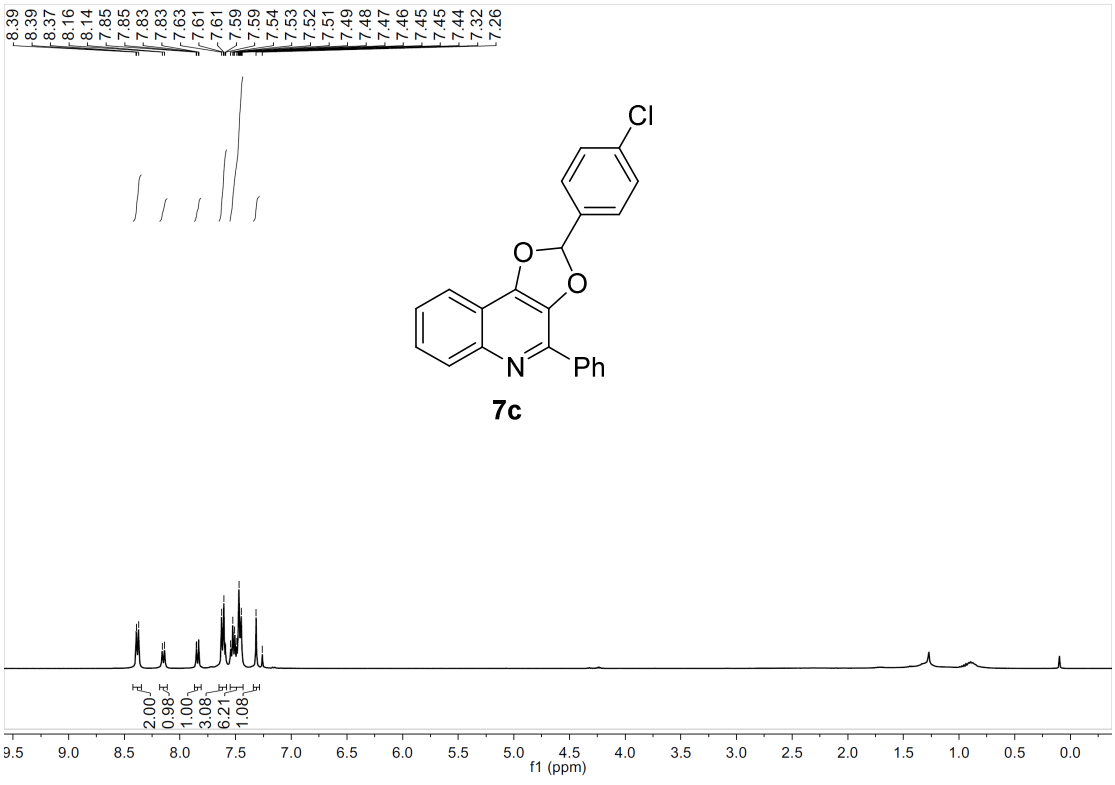
126.10
120.18
115.69
112.68
77.48
77.16
77.11
76.84
21.55
Me
O
O
N
Ph
7b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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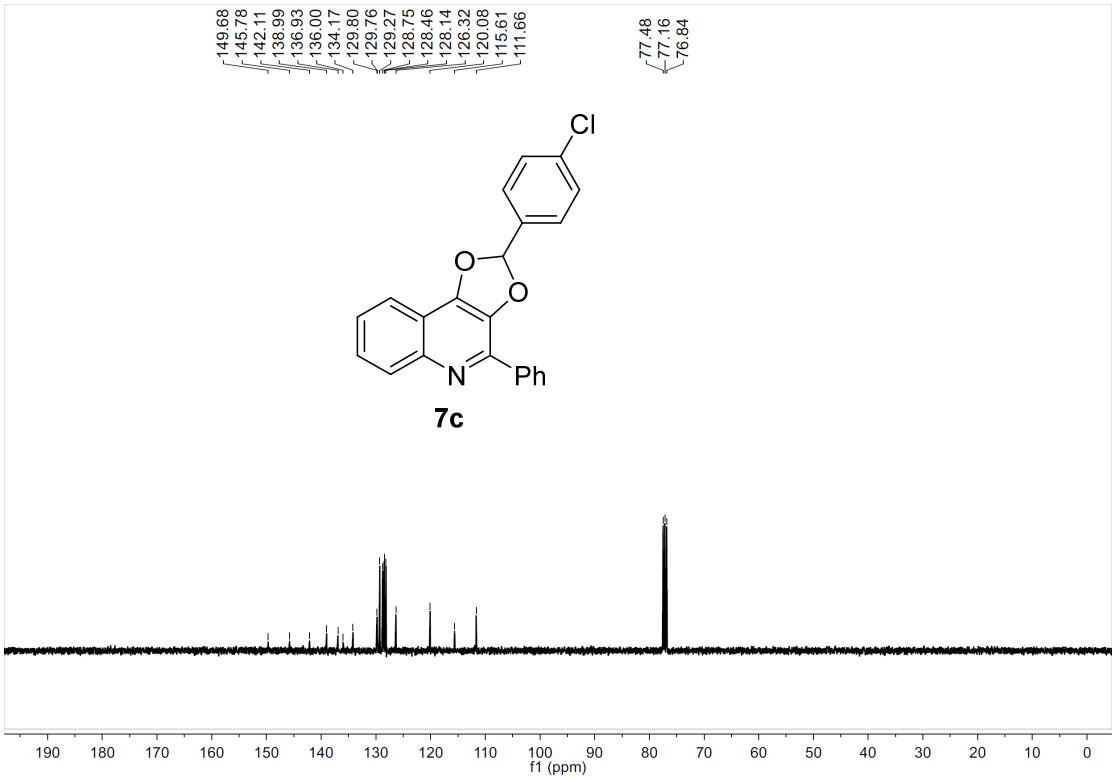
7.61
7.59
7.59
7.54
7.53
7.52
7.51
7.49
7.48
7.47
7.46
7.45
7.45
7.44
7.32
7.26
Cl
O
O
N
Ph
7c
2.00
0.98
1.00
3.08
6.21
1.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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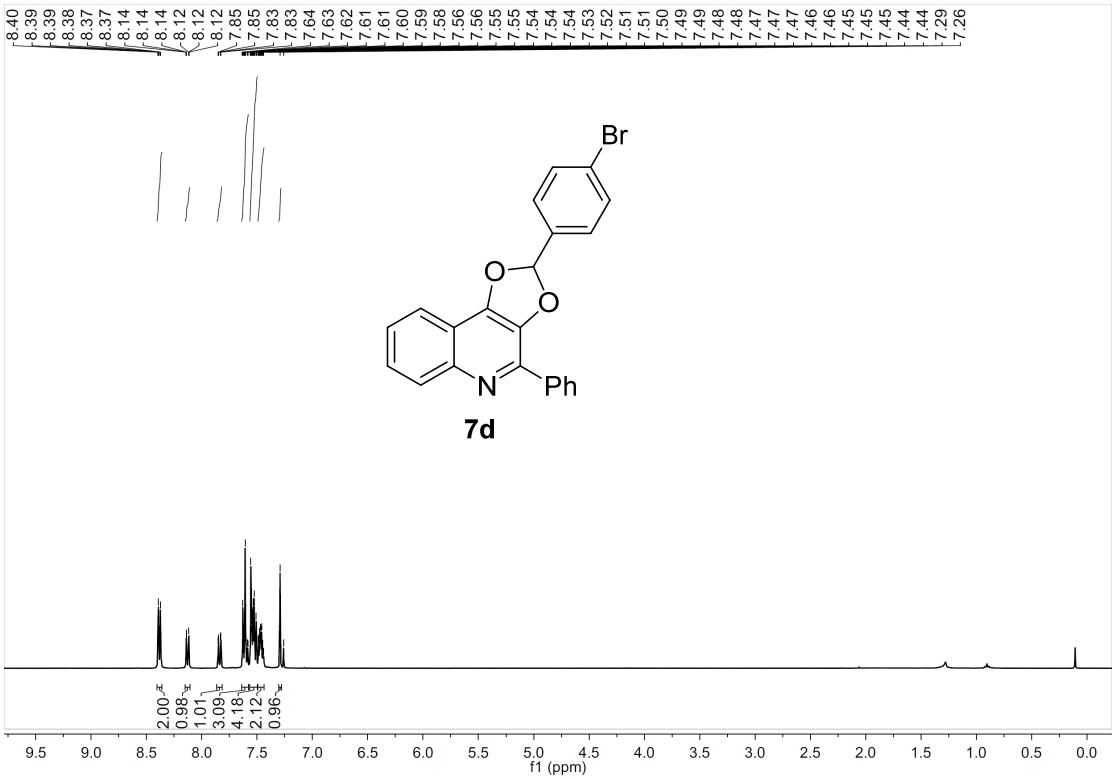
129.27
128.75
128.46
128.14
126.32
120.08
115.61
111.66
77.48
77.16
76.84
Cl
O
O
N
Ph
7c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.37
8.14
8.14
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8.12
7.85
7.85
7.83
7.83
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7.63
7.62
7.61
7.61
7.60
7.59
7.58
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7.55
7.55
7.54
7.54
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7.45
7.45
7.45
7.44
7.44
7.29
7.26
Br
O
O
N
Ph
7d
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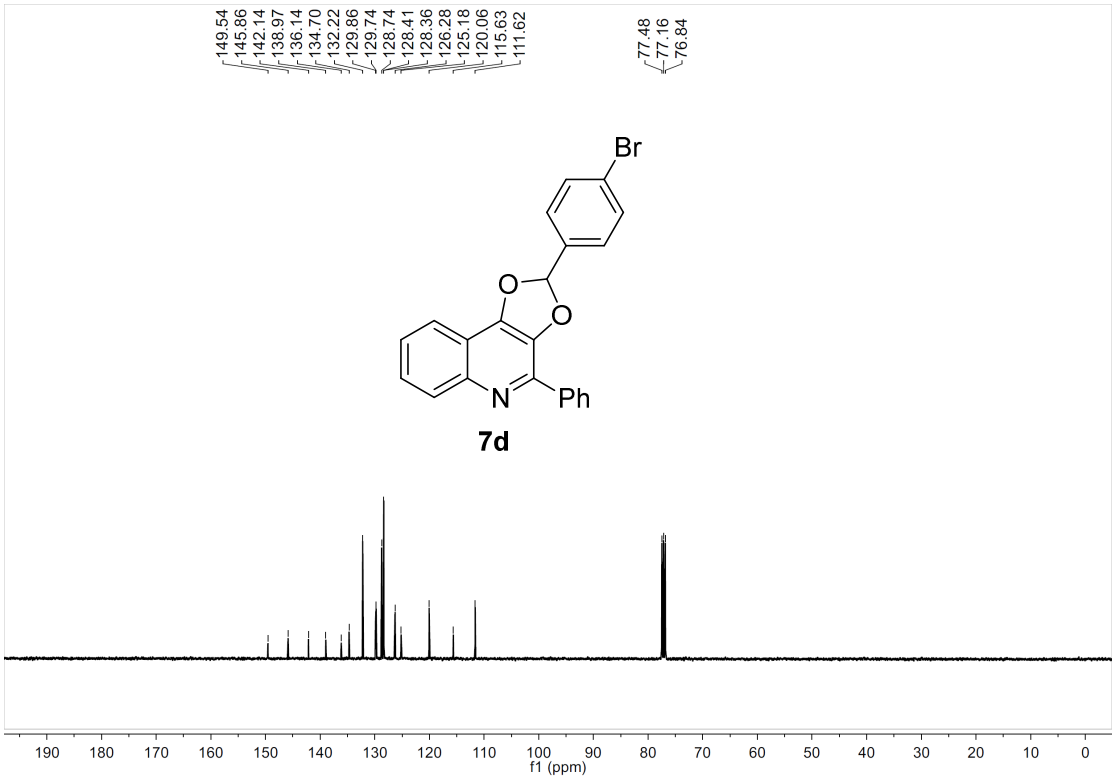
0.98
1.01
3.09
4.18
2.12
0.96
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.74
128.41
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126.28
125.18
120.06
115.63
111.62
77.48
77.16
76.84
Br
O
O
N
Ph
7d
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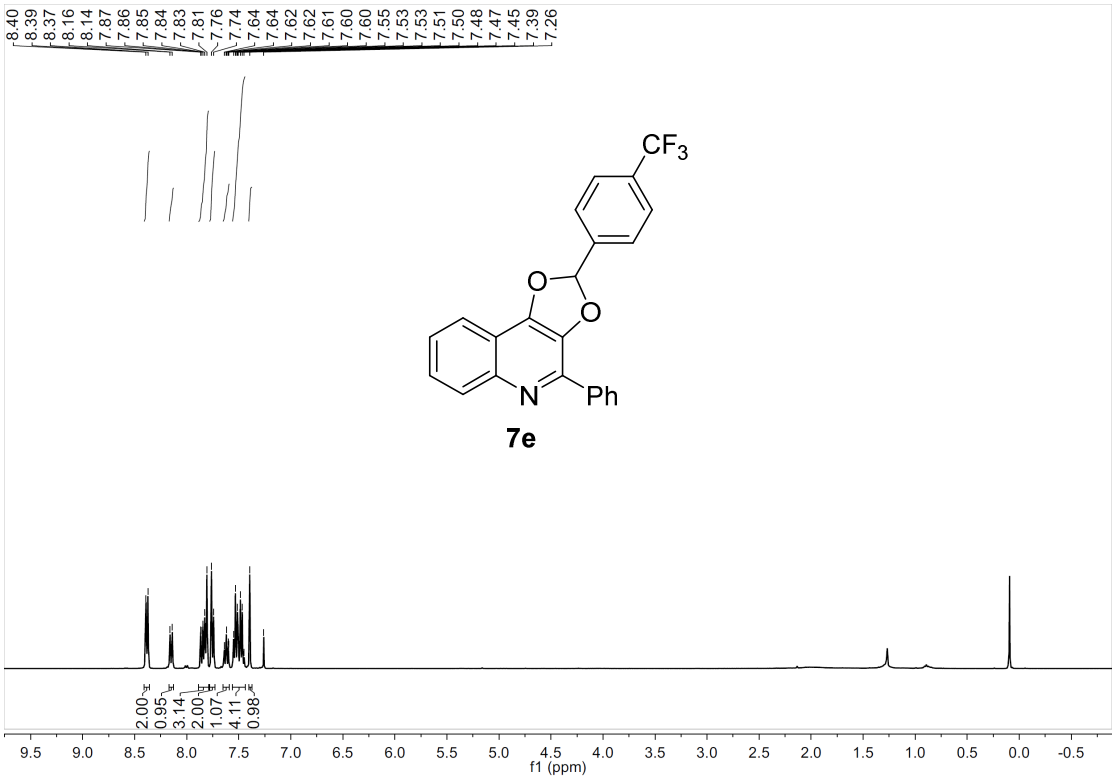
f1 (ppm)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7.87
7.86
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7.83
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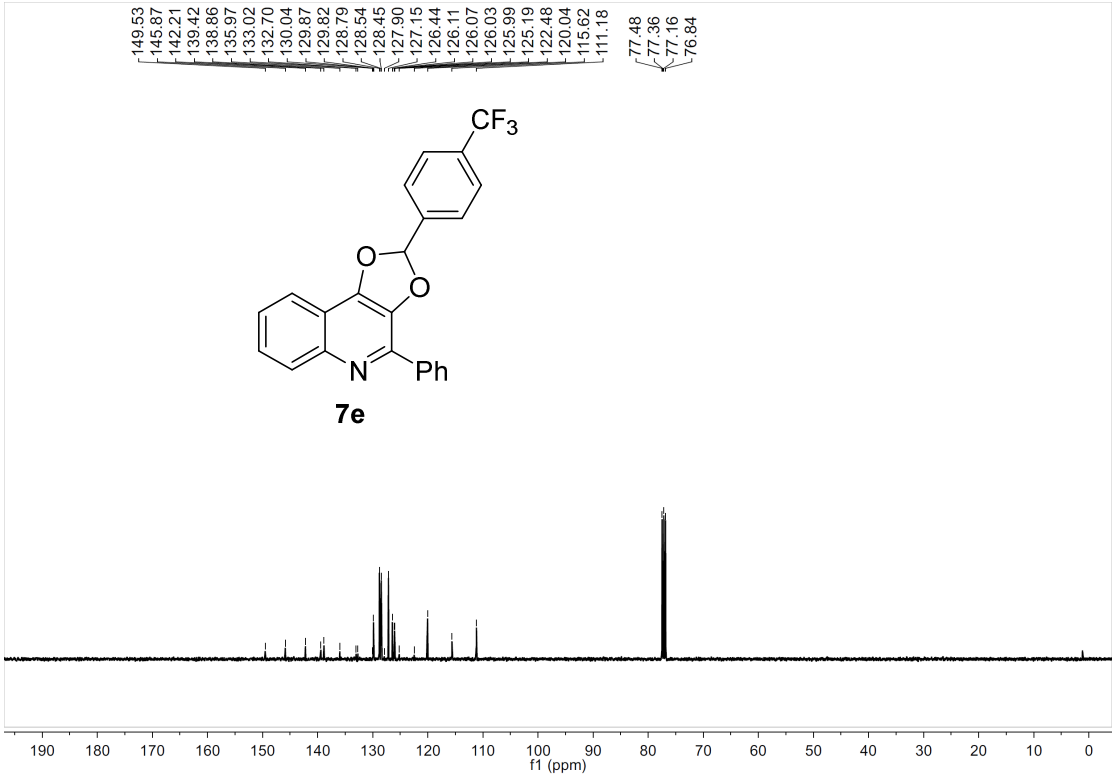
7.74
7.64
7.64
7.62
7.62
7.61
7.60
7.60
7.55
7.53
7.53
7.51
7.50
7.48
7.47
7.45
7.39
7.26
CF3
O
O
N
Ph
7e
2.00
0.95
3.14
2.00
1.07
4.11
0.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


149.53
145.87
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139.42
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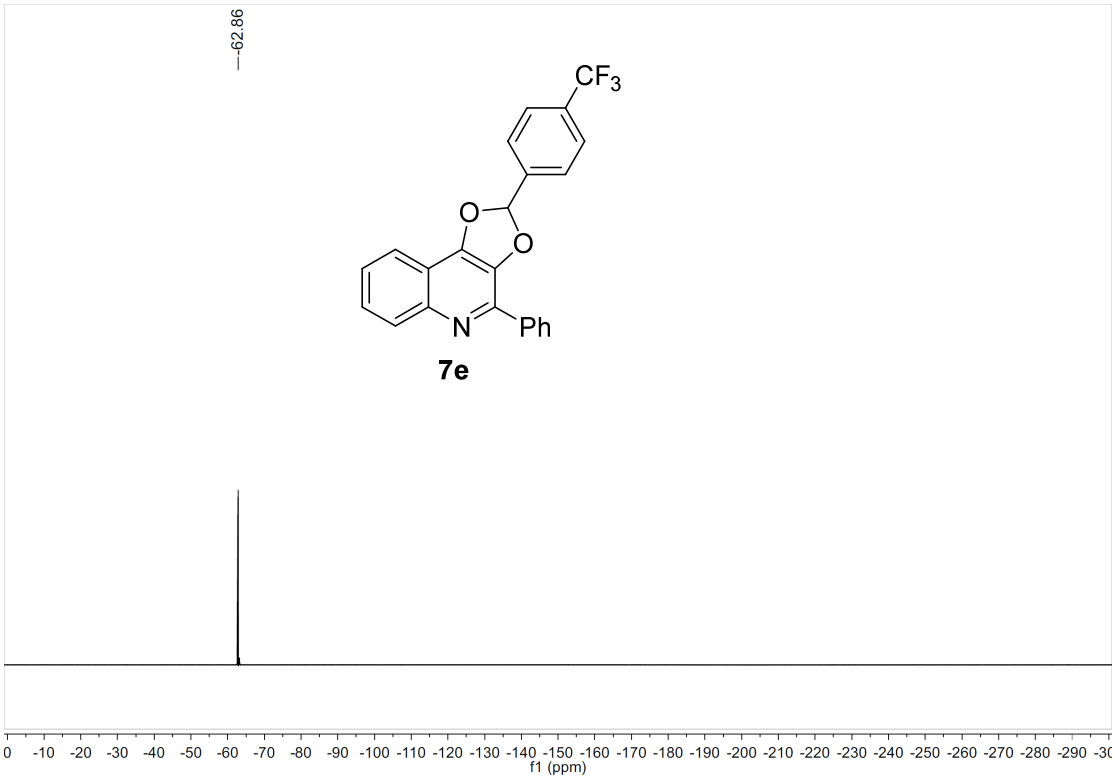
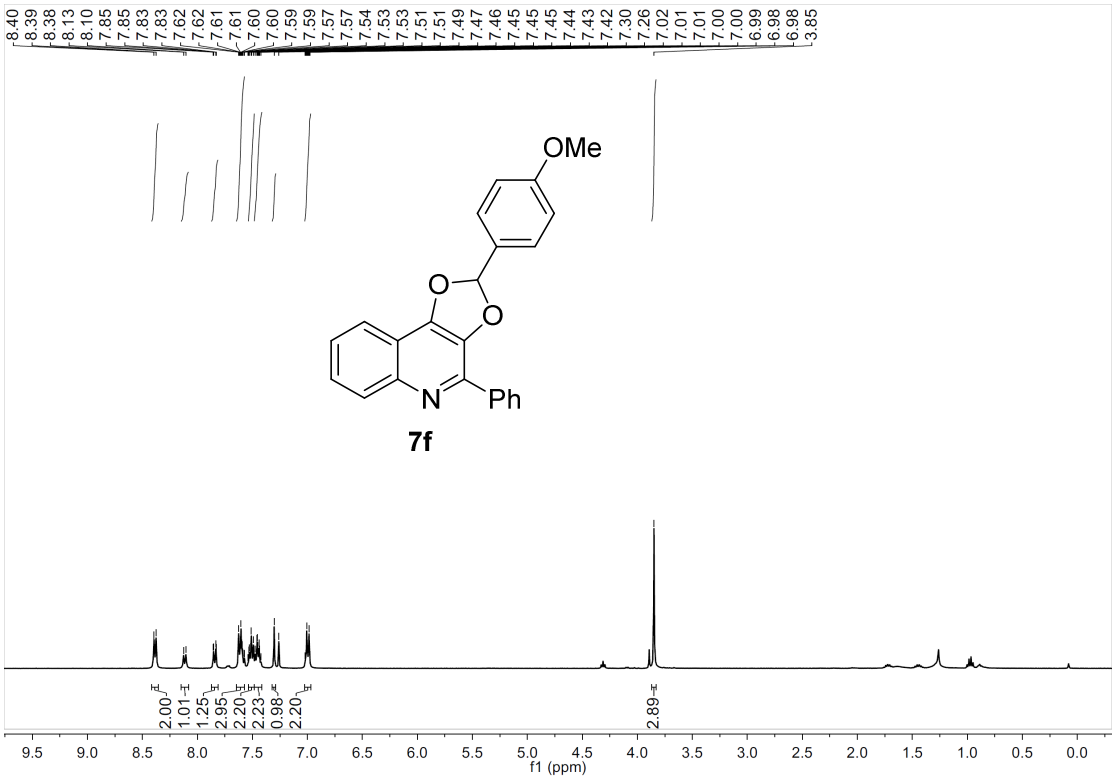
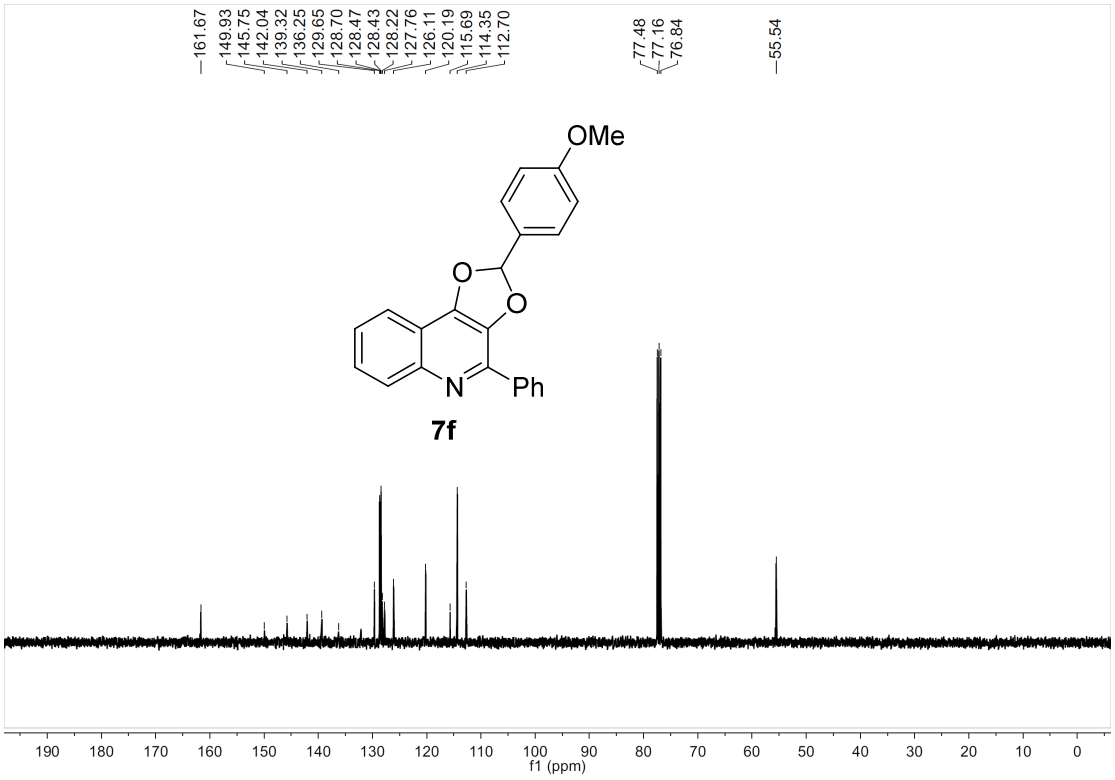
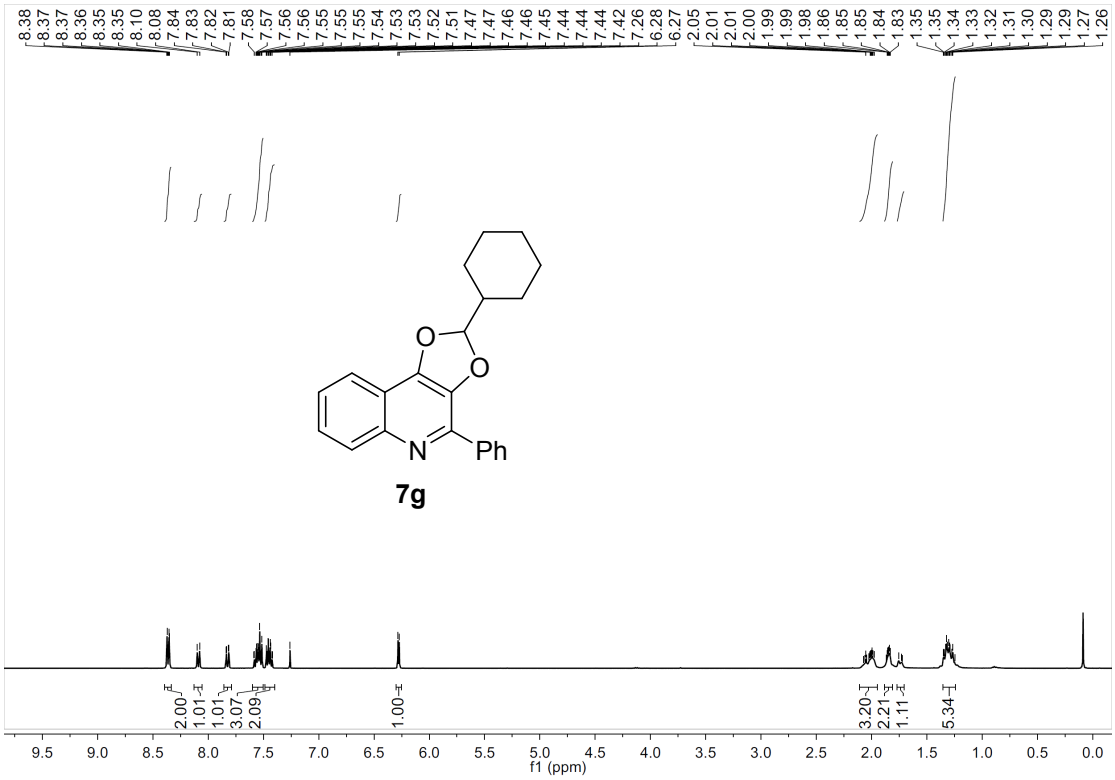
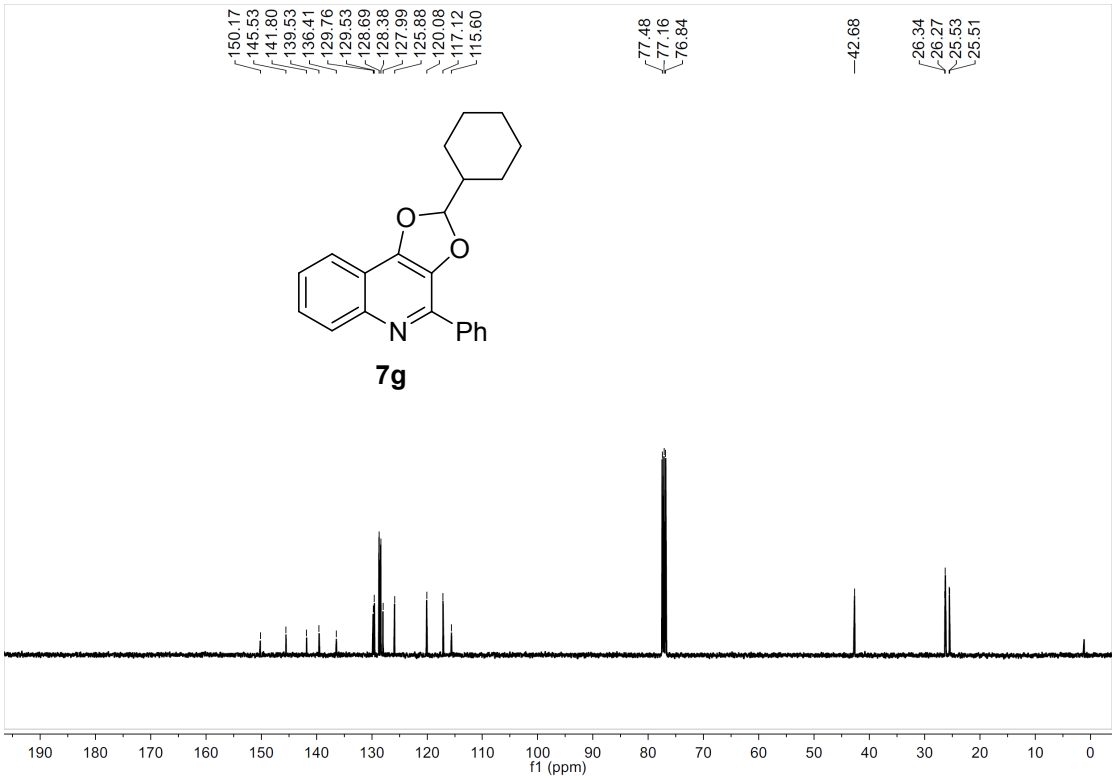
135.97
133.02
132.70
130.04
129.87
129.82
128.79
128.54
128.45
127.90
127.15
126.44
126.11
126.07
126.03
125.99
125.19
122.48
120.04
115.62
111.18
77.48
77.36
77.16
76.84
CF3
O
O
N
Ph
7e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

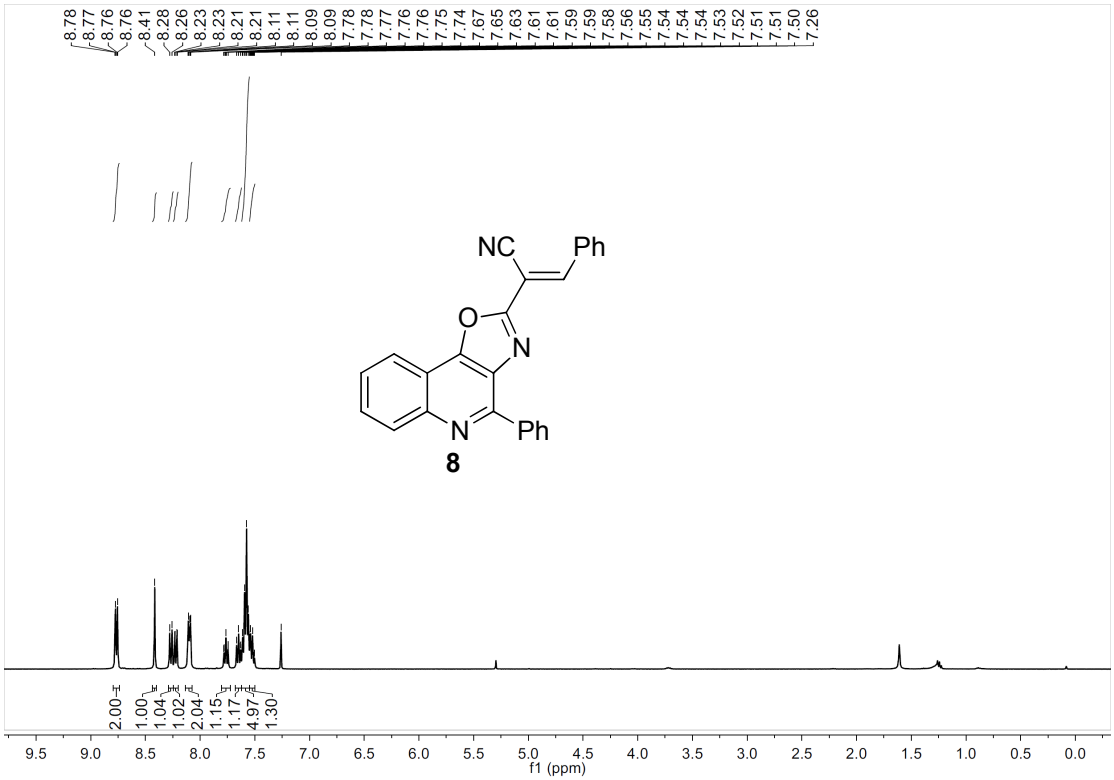

-62.86
CF3
O
O
N
Ph
7e
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260 -270 -280 -290 -30
f1 (ppm)

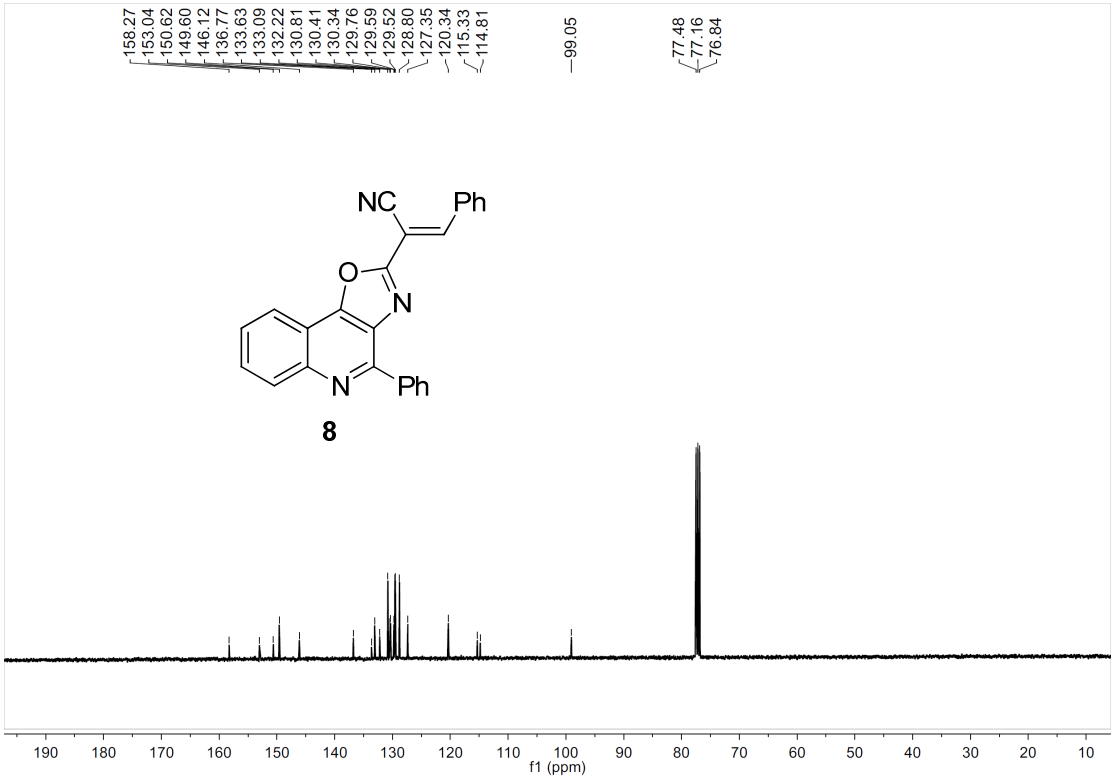

8.40
8.39
8.38
8.13
8.10
7.85
7.85
7.83
7.83
7.62
7.62
7.61
7.61
7.60
7.60
7.59
7.59
7.57
7.57
7.54
7.53
7.53
7.51
7.51
7.49
7.47
7.46
7.45
7.45
7.44
7.43
7.42
7.30
7.26
7.02
7.01
7.01
7.00
7.00
6.99
6.98
6.98
3.85
OMe
O
O
N
Ph
7f
2.00
1.01
1.25
2.95
2.20
2.23
0.98
2.20
2.89
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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)

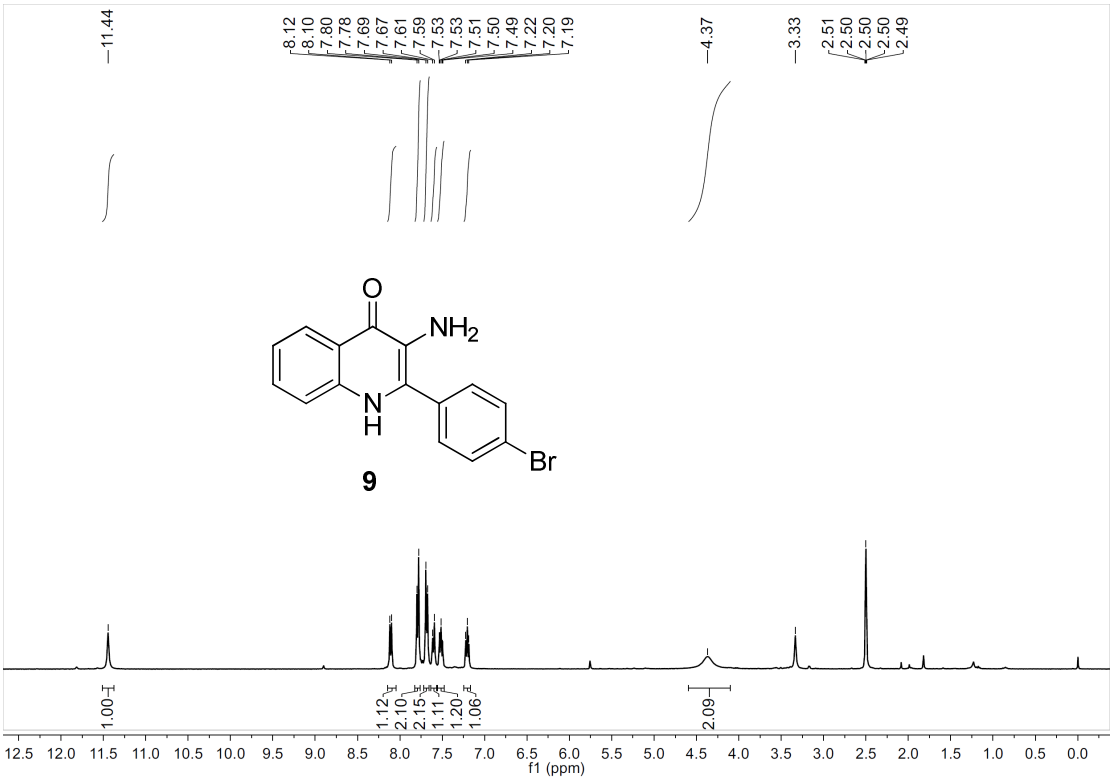

161.67
149.93
145.75
142.04
139.32
136.25
129.65
128.70
128.47
128.43
128.22
127.76
126.11
120.19
115.69
114.35
112.70
77.48
77.16
76.84
55.54
OMe
O
O
N
Ph
7f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

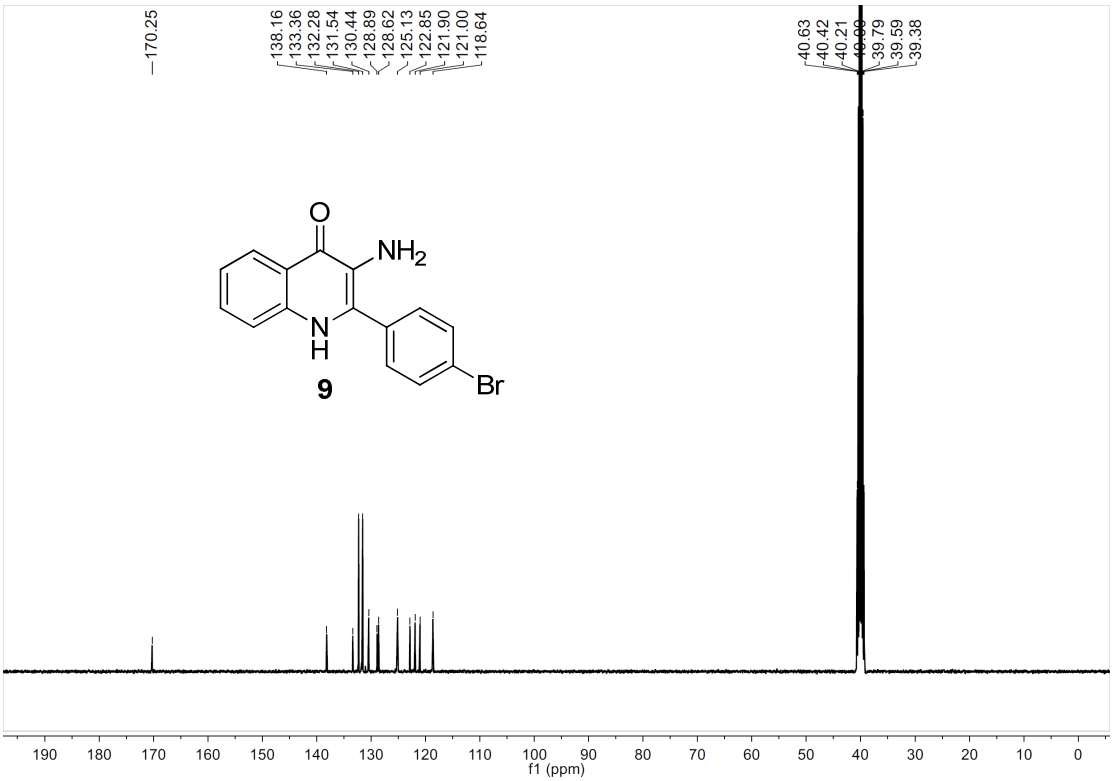

8.38 8.37 8.37 8.36 8.35 8.35 8.10 8.08 7.84 7.83 7.82 7.81 7.58 7.57 7.56 7.56 7.55 7.55 7.55 7.54 7.53 7.53 7.52 7.51 7.47 7.47 7.46 7.46 7.45 7.44 7.44 7.44 7.42 7.26 6.28 6.27 2.05 2.01 2.01 2.00 1.99 1.99 1.98 1.86 1.85 1.85 1.84 1.83 1.35 1.35 1.34 1.33 1.32 1.31 1.30 1.29 1.29 1.27 1.26
O
O
N
Ph
7g
2.00 1.01 1.01 3.07 2.09 1.00 3.20 2.21 1.11 5.34
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)

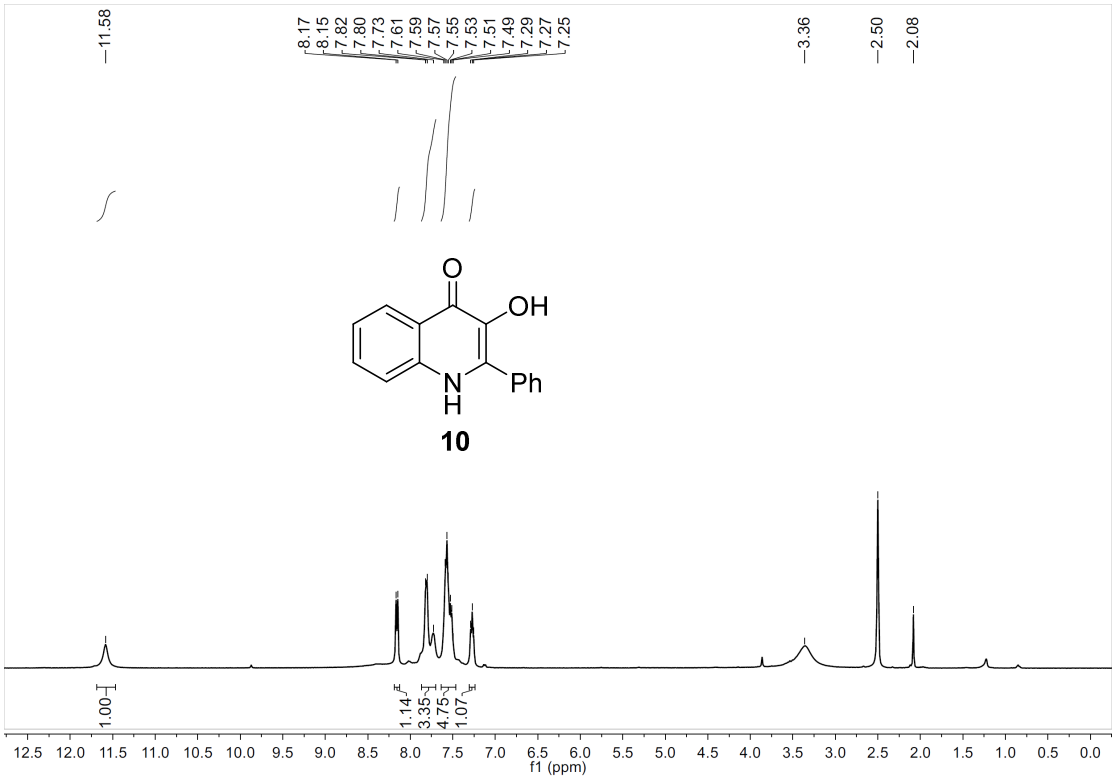

150.17 145.53 141.80 139.53 136.41 129.76 129.53 128.69 128.38 127.99 125.88 120.08 117.12 115.60
77.48 77.16 76.84
42.68
26.34 26.27 25.53 25.51
O
O
N
Ph
7g
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

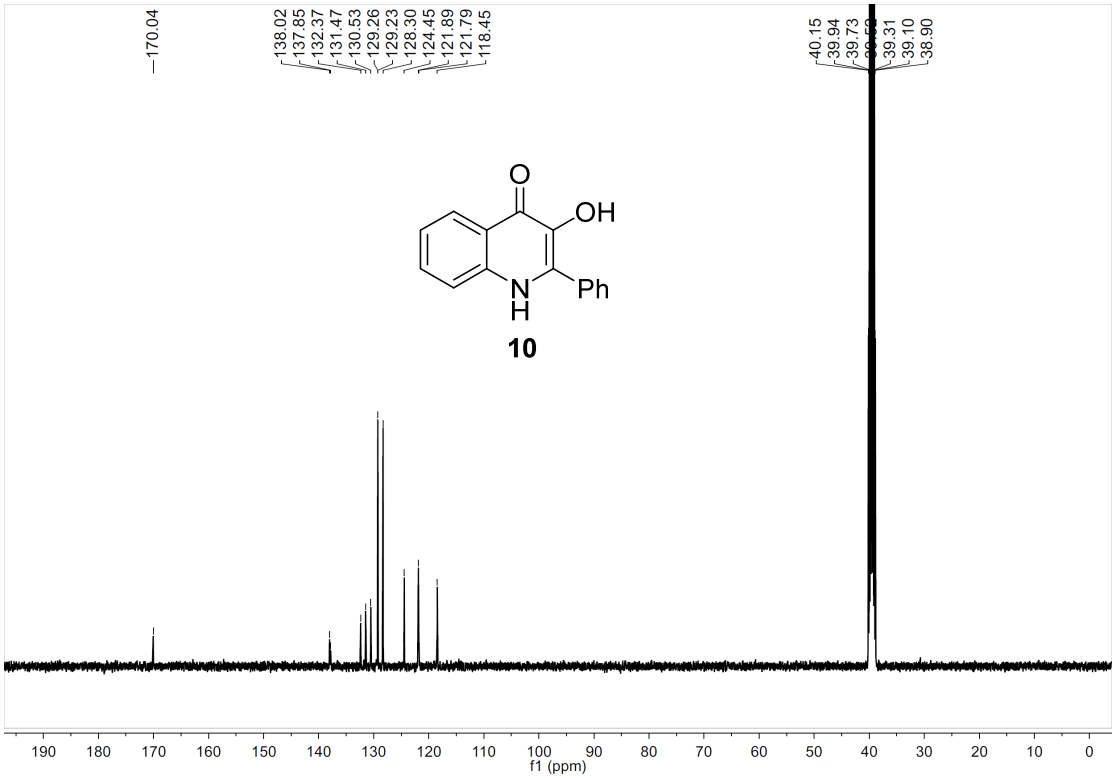

8.78
8.77
8.76
8.76
8.41
8.28
8.26
8.23
8.23
8.21
8.21
8.11
8.11
8.09
8.09
7.78
7.78
7.77
7.76
7.76
7.75
7.74
7.67
7.65
7.63
7.61
7.61
7.59
7.59
7.58
7.56
7.55
7.54
7.54
7.54
7.53
7.52
7.51
7.51
7.50
7.26
NC
Ph
O
N
N
Ph
8
2.00
1.00
1.04
1.02
2.04
1.15
1.17
4.97
1.30
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


158.27
153.04
150.62
149.60
146.12
136.77
133.63
133.09
132.22
130.81
130.41
130.34
129.76
129.59
129.52
128.80
127.35
120.34
115.33
114.81
99.05
77.48
77.16
76.84
NC
Ph
O
N
N
Ph
8
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

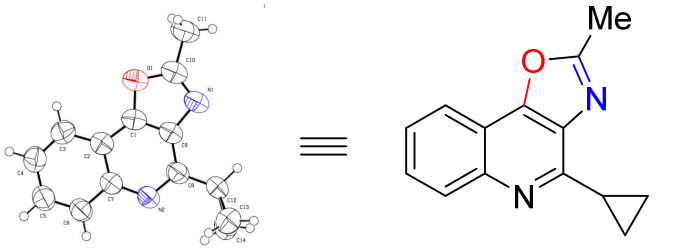

11.44
8.12
8.10
7.80
7.78
7.69
7.67
7.61
7.59
7.53
7.53
7.51
7.50
7.49
7.22
7.20
7.19
4.37
3.33
2.51
2.50
2.50
2.50
2.49
O
NH2
N
H
Br
9
1.00
1.12
2.10
2.15
1.11
1.20
1.06
2.09
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


170.25
138.16
133.36
132.28
131.54
130.44
128.89
128.62
125.13
122.85
121.90
121.00
118.64
40.63
40.42
40.21
39.79
39.59
39.38
O
NH2
N
H
Br
9
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


11.58
8.17
8.15
7.82
7.80
7.73
7.61
7.59
7.57
7.55
7.53
7.51
7.49
7.29
7.27
7.25
3.36
2.50
2.08
O
OH
N
H
Ph
10
1.00
1.14
3.35
4.75
1.07
f1 (ppm)


170.04
138.02
137.85
132.37
131.47
130.53
129.26
129.23
128.30
124.45
121.89
121.79
118.45
40.15
39.94
39.73
39.31
39.10
38.90
O
OH
N
H
Ph
10
f1 (ppm)

Crystallographic Data for Compound 3s.



X-ray of **3s** CCDC 1888665

Bond precision: C-C = 0.0023 A Wavelength=0.71073

Cell: a=7.2536(6) b=9.2341(9) c=9.3515(10)
alpha=85.065(8) beta=81.059(8) gamma=68.355(8)
Temperature: 293 K

	Calculated	Reported
Volume	574.85(10)	574.85(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C14 H12 N2 O	C14 H12 N2 O
Sum formula	C14 H12 N2 O	C14 H12 N2 O
Mr	224.26	224.26
Dx,g cm-3	1.296	1.296
Z	2	2
Mu (mm-1)	0.084	0.084
F000	236.0	236.0
F000'	236.09	
h,k,lmax	10,13,13	10,12,13
Nref	3469	3111
Tmin,Tmax	0.985,0.992	0.869,1.000
Tmin'	0.983	

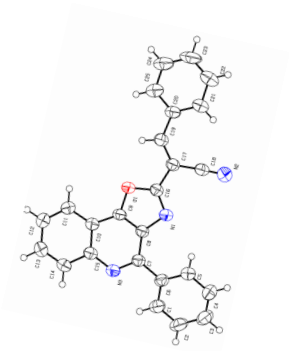
Correction method= # Reported T Limits: Tmin=0.869 Tmax=1.000
AbsCorr = MULTI-SCAN

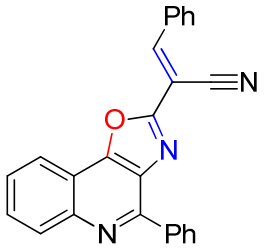
Data completeness= 0.897 Theta(max)= 30.351

R(reflections)= 0.0533(1816) wR2(reflections)= 0.1669(3111)

S = 1.016 Npar= 155

Crystallographic Data for Compound 8.





X-ray of **8** CCDC 1906218

Bond precision: C-C = 0.0027 A Wavelength=0.71073

Cell: a=9.8811(7) b=14.4238(7) c=13.7948(9)
alpha=90 beta=109.258(7) gamma=90
Temperature: 279 K

	Calculated	Reported
Volume	1856.1(2)	1856.1(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2ybc (x-
Moiety formula	C25 H15 N3 O	C25 H15 N3 O
Sum formula	C25 H15 N3 O	C25 H15 N3 O
Mr	373.40	373.42
Dx,g cm-3	1.336	1.336
Z	4	4
Mu (mm-1)	0.084	0.084
F000	776.0	776.3
F000'	776.30	
h,k,lmax	12,18,17	12,18,17
Nref	3788	3785
Tmin,Tmax	0.966,0.973	0.607,1.000
Tmin'	0.949	

Correction method= # Reported T Limits: Tmin=0.607 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.370

R(reflections)= 0.0468(2608) wR2(reflections)= 0.1255(3785)

S = 1.066 Npar= 262
