Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

tert-Butyl peroxybenzoate mediated formation of 3-alkylated quinolines from *N*-propargylamines via cascade radical addition/cyclization reaction

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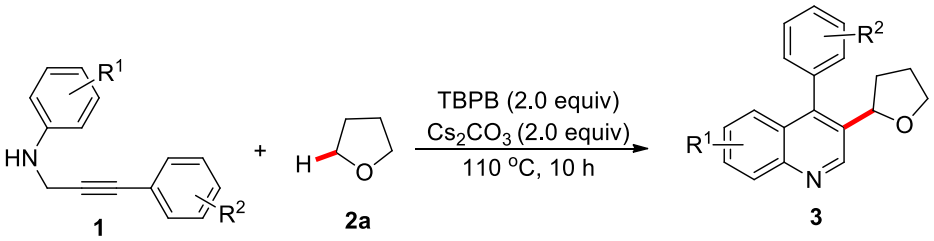
1. General considerations

All ^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 MHz Bruker FT-NMR spectrometers (400 MHz or 100 MHz, respectively). All chemical shifts are given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; q, quartet. The coupling constants, J, are reported in Hertz (Hz). High resolution mass spectroscopy data of the product were collected on a Waters Micromass GCT instrument. High resolution mass spectroscopy data of the product were collected on an Agilent Technologies 6540 UHD Accurate-Mass Q-TOF LC/MS (ESI).

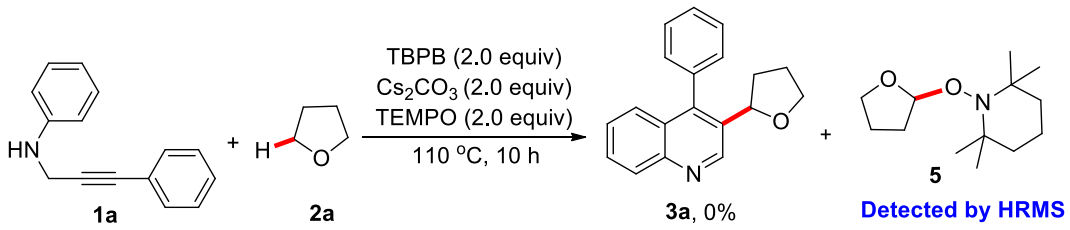
The starting material propargylamine **(1a**–**1o)** were prepared according to the reported method [L. Zhang, S. Chen, Y. Gao, P. Zhang, Y. Wu, G. Tang, and Y. Zhao, *Org. Lett.* 2016, **18**, 1286−1289]. The chemicals and solvents were purchased from commercial suppliers either from Aldrich (USA) or Shanghai Chemical Company (China) without further purification. All the solvents were dried and freshly distilled prior to use. Products were purified by flash chromatography on 200–300 mesh silica gels, SiO_2.

2. General procedure for the reaction



N-(3-Phenyl-2-propynyl)aniline derivative (**1**, 0.30 mmol), tetrahydrofuran (THF, **2a**, 3.0 mL), TBPB (0.60 mmol), and Cs_2CO_3 (0.60 mmol) were sequentially added to a Schlenk tube, and the reaction mixture was heated with stirring under air at 110 ^{o}C for 10 h. Upon completion, the reaction mixture was cooled to room temperature and the solution was concentrated in vacuum. The resulting mixture purified by flash column chromatography (petroleum ether/ethyl acetate = 5:1) to give the desired product (**3**).

3. Free radical-trapping experiment



N-(3-Phenyl-2-propynyl)aniline (**1a**, 0.30 mmol), tetrahydrofuran (THF, **2a**, 3.0 mL), TBPB (0.60 mmol), Cs_2CO_3 (0.60 mmol) and 2,2,6,6-tetramethyl-1-oxylpiperidine (TEMPO, 0.60 mmol) were added to a Schlenk tube, and the reaction mixture was heated with stirring under air at 110 °C for 10 h. After the reaction was completed, no desired product **3a** was detected by TLC and HPLC-HRMS, indicating that the reaction was completely inhibited. Meanwhile, a free radical-trapping adduct of THF with TEMPO was observed through HPLC-HRMS analysis of the reaction solution, shown in Figure S1.

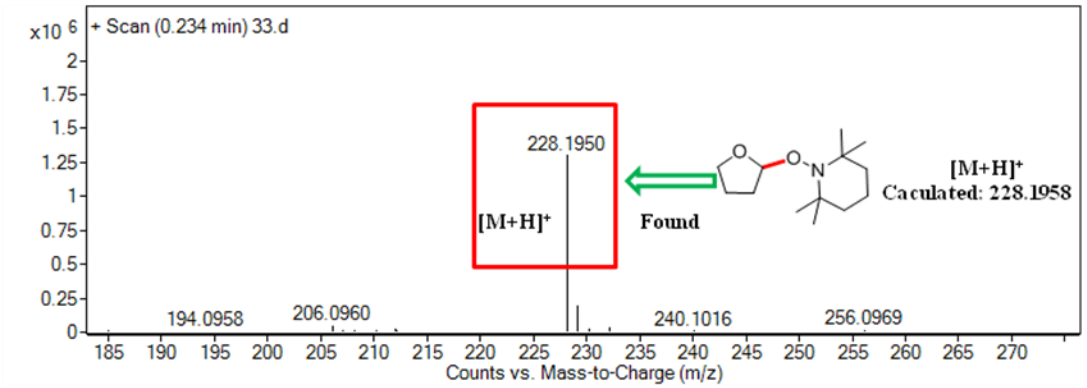
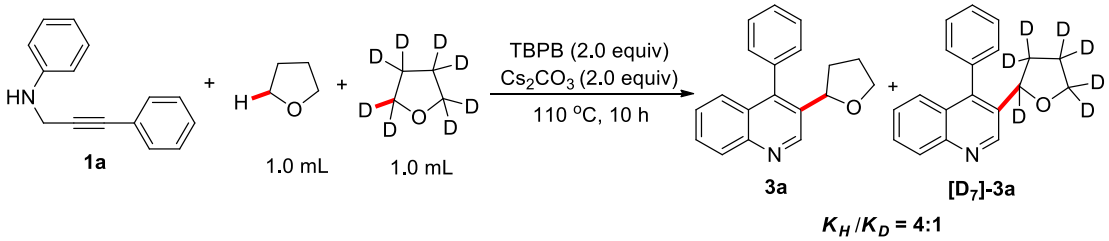
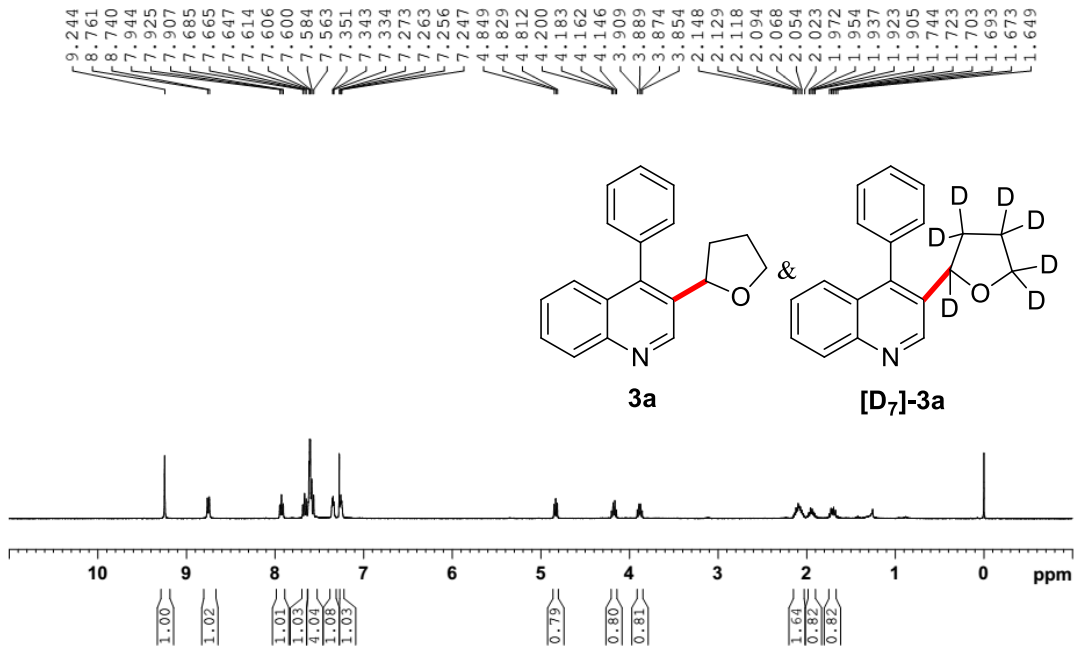


Figure S1 HRMS analysis of the adduct of THF with TEMPO

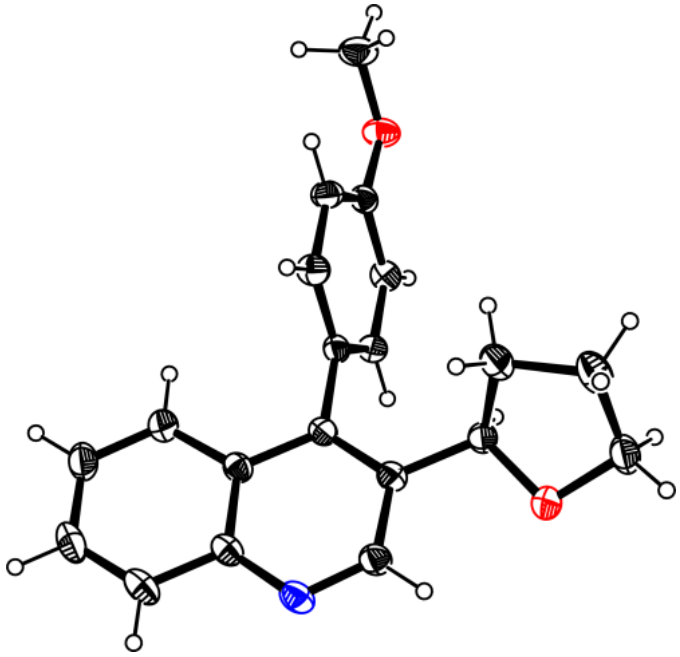
4. Kinetic isotope effect experiment



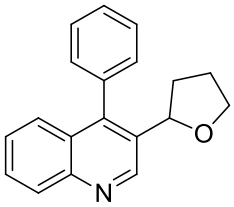
N-(3-Phenyl-2-propynyl)aniline (**1a**, 0.20 mmol), TBPB (0.40 mmol), Cs_2CO_3 (0.40 mmol), THF (1.0 mL) and [D_8]-THF (1.0 mL) were sequentially added to a Schlenk tube, and the reaction mixture was heated with stirring under air at 110 ^oC for 10 h. Upon completion, the reaction mixture was cooled to room temperature and the solution was concentrated in vacuum. The resulting mixture purified by flash column chromatography (petroleum ether/ethyl acetate = 5:1) to give the desired products **3a**/[D_7]-**3a**. The kinetic isotope effect (K_H/K_D) was found to be from the ^{1}H NMR of **3a**/[D_7]-**3a**.



5. The X-ray single crystal analysis of 3c (CCDC: 1576256)

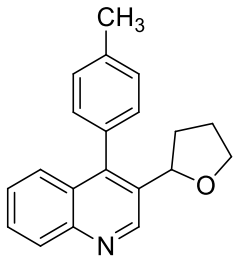


6. Characterization data for the products



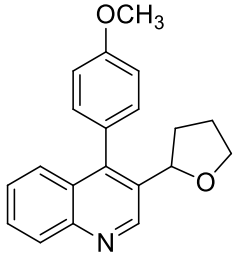
4-phenyl-3-(tetrahydrofuran-2-yl)quinoline (**3a**)

Pale yellow solid (53.7 mg, 65% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.14 (s, 1H), 8.15 (d, *J* = 8.8 Hz, 1H), 7.69–7.65 (m, 1H), 7.53–7.50 (m, 3H), 7.41–7.40 (m, 2H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.23–7.22 (m, 1H), 4.77 (dd, *J* = 8.2 Hz and *J* = 6.8 Hz, 1H), 4.20–4.14 (m, 1H), 3.89–3.84 (m, 1H), 2.15–2.04 (m, 2H), 1.97–1.86 (m, 1H), 1.83–1.75 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.3, 147.3, 145.0, 135.8, 133.1, 129.8, 129.4, 129.1, 128.8, 128.6, 128.2, 128.1, 127.1, 126.5, 126.2, 77.1, 69.1, 35.1, 26.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{19}H_{18}NO$: 276.1383, Found: 276.1386.



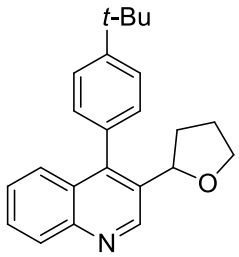
3-(tetrahydrofuran-2-yl)-4-(*p*-tolyl)quinoline (**3b**)

Pale yellow solid (53.8 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.13 (s, 1H), 8.14 (d, *J* = 8.8 Hz, 1H), 7.67–7.63 (m, 1H), 7.44–7.37 (m, 2H), 7.34–7.31 (m, 2H), 7.23–7.21 (m, 1H), 7.12–7.10 (m, 1H), 4.79 (dd, *J* = 8.0 Hz and *J* = 6.7 Hz, 1H), 4.20–4.14 (m, 1H), 3.89–3.84 (m, 1H), 2.47 (s, 3H), 2.16–2.03 (m, 2H), 1.97–1.86 (m, 1H), 1.84–1.75 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.2, 147.3, 145.1, 137.8, 133.2, 132.7, 129.7, 129.3, 129.2, 129.0, 128.9, 128.7, 127.2, 126.4, 126.3, 77.1, 69.0, 35.0, 26.5, 21.3; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{20}H_{20}NO$: 290.1539, Found: 290.1536.



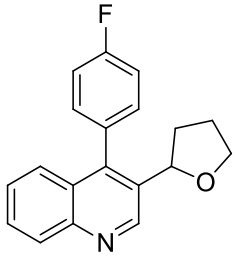
4-(4-methoxyphenyl)-3-(tetrahydrofuran-2-yl)quinoline (**3c**)

Pale yellow solid (55.0 mg, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.12 (s, 1H), 8.13 (d, *J* = 8.8 Hz, 1H), 7.67–7.62 (m, 1H), 7.46–7.37 (m, 2H), 7.26–7.23 (m, 1H), 7.14–7.12 (m, 1H), 7.06–7.02 (m, 2H), 4.80 (dd, *J* = 8.3 Hz and *J* = 4.5 Hz, 1H), 4.19–4.13 (m, 1H), 3.89 (s, 3H), 3.87–3.83 (m, 1H), 2.15–2.02 (m, 2H), 1.97–1.86 (m, 1H), 1.83–1.76 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.3, 149.2, 147.3, 144.8, 133.3, 130.9, 130.2, 129.3, 128.6, 127.7, 127.4, 126.3, 126.2, 113.9, 113.7, 77.1, 68.9, 55.2, 35.0, 26.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{20}H_{20}NO_2$: 306.1489, Found: 306.1502.



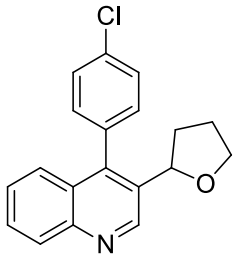
4-(4-(*tert*-butyl)phenyl)-3-(tetrahydrofuran-2-yl)quinoline (**3d**)

Pale yellow solid (67.6 mg, 68% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.13 (s, 1H), 8.14 (d, *J* = 8.8 Hz, 1H), 7.66–7.62 (m, 1H), 7.53–7.49 (m, 2H), 7.45–7.37 (m, 2H), 7.26–7.24 (m, 1H), 7.15–7.13 (m, 1H), 4.80 (dd, *J* = 8.2 Hz and *J* = 6.8 Hz, 1H), 4.19–4.14 (m, 1H), 3.89–3.84 (m, 1H), 2.17–2.03 (m, 2H), 1.98–1.85 (m, 1H), 1.83–1.76 (m, 1H), 1.42 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 150.9, 149.3, 147.3, 145.1, 133.2, 132.6, 129.5, 129.3, 128.8, 128.6, 127.2, 126.4, 126.3, 125.4, 125.0, 77.0, 69.0, 35.1, 34.6, 31.3, 26.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{23}H_{26}NO$: 332.2009, Found: 332.2006.



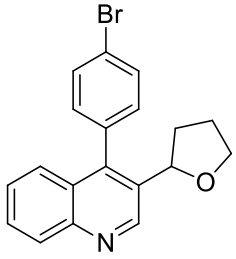
4-(4-fluorophenyl)-3-(tetrahydrofuran-2-yl)quinoline (**3e**)

Pale yellow solid (51.0 mg, 58% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.14 (s, 1H), 8.14 (d, *J* = 8.8 Hz, 1H), 7.67–7.63 (m, 1H), 7.42–7.35 (m, 2H), 7.31–7.28 (m, 1H), 7.23–7.19 (m, 3H), 4.74 (dd, *J* = 8.0 Hz and *J* = 6.9 Hz, 1H), 4.18–4.13 (m, 1H), 3.88–3.83 (m, 1H), 2.14–2.03 (m, 2H), 1.95–1.86 (m, 1H), 1.83–1.74 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.4 (d, *J* = 246.3 Hz), 149.1, 147.2, 143.8, 133.2, 131.5 (d, *J* = 3.5 Hz), 131.4 (d, *J* = 8.0 Hz), 130.8 (d, *J* = 8.0 Hz), 129.3, 128.7, 126.9, 126.5, 125.8, 115.6 (d, *J* = 21.4 Hz), 115.3 (d, *J* = 21.4 Hz), 76.9, 68.9, 34.8, 26.4; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{19}H_{17}FNO$: 294.1289, Found: 294.1292.



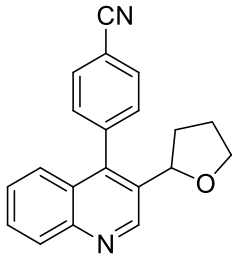
4-(4-chlorophenyl)-3-(tetrahydrofuran-2-yl)quinoline (**3f**)

Pale yellow solid (55.8 mg, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.13 (s, 1H), 8.15 (d, *J* = 8.4 Hz, 1H), 7.69–7.65 (m, 1H), 7.52–7.49 (m, 2H), 7.43–7.40 (m, 1H), 7.36–7.33 (m, 1H), 7.29–7.27 (m, 1H), 7.18–7.15 (m, 1H), 4.73 (dd, *J* = 8.3 Hz and *J* = 6.6 Hz, 1H), 4.18–4.13 (m, 1H), 3.89–3.83 (m, 1H), 2.14–2.03 (m, 2H), 1.96–1.88 (m, 1H), 1.84–1.74 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.2, 147.3, 143.7, 134.3, 134.2, 133.1, 131.2, 130.5, 129.5, 128.9, 128.6, 126.8, 126.7, 125.8, 77.0, 69.0, 34.9, 26.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{19}H_{17}ClNO$: 310.0993, Found: 310.0996.



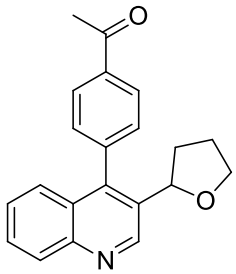
4-(4-bromophenyl)-3-(tetrahydrofuran-2-yl)quinoline (**3g**)

Pale yellow solid (65.9 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.13 (s, 1H), 8.15 (d, *J* = 8.8 Hz, 1H), 7.69–7.64 (m, 3H), 7.44–7.40 (m, 1H), 7.37–7.35 (m, 1H), 7.22 (dd, *J* = 8.7 Hz and *J* = 2.4 Hz, 1H), 7.11 (dd, *J* = 7.9 Hz and *J* = 1.8 Hz, 1H), 4.73 (dd, *J* = 8.4 Hz and *J* = 6.4 Hz, 1H), 4.19–4.14 (m, 1H), 3.90–3.84 (m, 1H), 2.15–2.04 (m, 2H), 1.98–1.88 (m, 1H), 1.84–1.75 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.2, 147.3, 143.6, 134.7, 133.0, 131.9, 131.5, 131.5, 130.8, 129.5, 128.9, 126.7, 126.7, 125.8, 122.4, 77.0, 69.1, 35.0, 26.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{19}H_{17}BrNO$: 354.0488, Found: 354.0487.



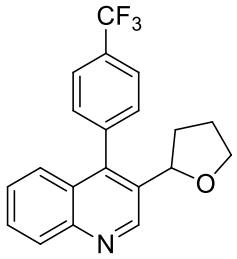
4-(3-(tetrahydrofuran-2-yl)quinolin-4-yl)benzonitrile (**3h**)

Pale yellow solid (60.4 mg, 67% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.14 (s, 1H), 8.16 (d, *J* = 8.8 Hz, 1H), 7.85–7.82 (m, 2H), 7.72–7.68 (m, 1H), 7.50–7.37 (m, 3H), 7.25 (d, *J* = 8.3 Hz, 1H), 4.65 (dd, *J* = 8.4 Hz and *J* = 6.7 Hz, 1H), 4.17–4.12 (m, 1H), 3.89–3.84 (m, 1H), 2.13–2.05 (m, 2H), 1.99–1.89 (m, 1H), 1.86–1.77 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.3, 147.3, 142.8, 141.0, 132.7, 132.4, 132.1, 130.7, 130.2, 129.7, 129.2, 127.1, 126.1, 125.4, 118.3, 112.4, 76.9, 69.1, 34.9, 26.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{20}H_{17}N_2O$: 301.1335, Found: 301.1336.



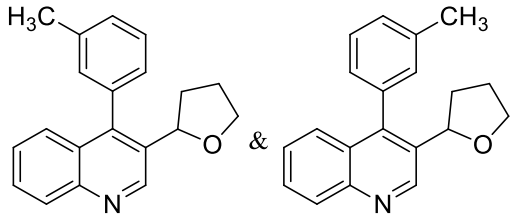
1-(4-(3-(tetrahydrofuran-2-yl)quinolin-4-yl)phenyl)ethanone (**3i**)

Pale yellow solid (60.9 mg, 64% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.13 (s, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 8.11–8.09 (m, 2H), 7.68–7.64 (m, 1H), 7.45–7.38 (m, 2H), 7.36–7.28 (m, 2H), 4.68 (dd, *J* = 8.4 Hz and *J* = 6.6 Hz, 1H), 4.16–4.11 (m, 1H), 3.87–3.81 (m, 1H), 2.68 (s, 3H), 2.12–2.02 (m, 2H), 1.93–1.87 (m, 1H), 1.85–1.77 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.4, 149.2, 147.2, 143.7, 140.9, 136.8, 132.8, 130.2, 129.5, 128.9, 128.6, 128.1, 126.7, 126.4, 125.7, 76.9, 69.0, 35.0, 26.6, 26.4; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{21}H_{20}NO_2$: 318.1489, Found: 318.1491.



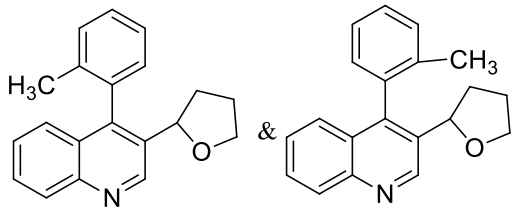
3-(tetrahydrofuran-2-yl)-4-(4-(trifluoromethyl)phenyl)quinoline (**3j**)

Pale yellow solid (71.1 mg, 69% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.15 (s, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 7.82–7.79 (m, 2H), 7.71–7.67 (m, 1H), 7.50–7.48 (m, 1H), 7.45–7.37 (m, 2H), 7.29 (d, *J* = 8.4 Hz, 1H), 4.69 (dd, *J* = 8.5 Hz and *J* = 6.6 Hz, 1H), 4.19–4.14 (m, 1H), 3.90–3.84 (m, 1H), 2.14–2.05 (m, 2H), 1.98–1.91 (m, 1H), 1.87–1.78 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.3, 147.3, 143.3, 139.8, 132.9, 130.5 (q, *J* = 32.6 Hz), 129.7, 129.7 (d, *J* =124.9 Hz), 129.6, 126.9, 126.5, 125.7, 125.7 (q, *J* = 3.7 Hz), 125.3 (q, *J* = 3.7 Hz), 124.0 (q, *J* = 270.7 Hz), 76.9, 69.1, 35.0, 26.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{20}H_{17}F_3NO$: 344.1257, Found: 344.1261.



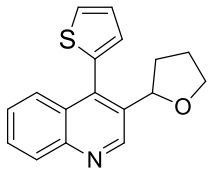
3-(tetrahydrofuran-2-yl)-4-(*m*-tolyl)quinoline (**3k**+**3k'**)

Pale yellow oil (47.7 mg, 55% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.13 (s, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.67–7.63 (m, 1H), 7.42–7.37 (m, 3H), 7.30–7.28 (m, 1H), 7.14–7.12 (m, 1H), 7.03–7.00 (m, 1H), 4.80–4.76 (m, 1H), 4.20–4.14 (m, 1H), 3.90–3.83 (m, 1H), 2.43 (s, 1.5H), 2.42 (s, 1.5H), 2.14–2.04 (m, 2H), 1.95–1.87 (m, 1H), 1.83–1.76 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.2, 147.2, 145.2, 145.1, 138.2, 137.8, 135.6, 133.0, 133.0, 130.4, 129.5, 129.2, 128.7, 128.7, 128.4, 128.1, 127.1, 126.8, 126.4, 126.3, 126.1, 77.0, 69.0, 69.0, 35.1, 35.0, 26.5, 21.4, 21.4; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{20}H_{20}NO$: 290.1539, Found: 290.1533.



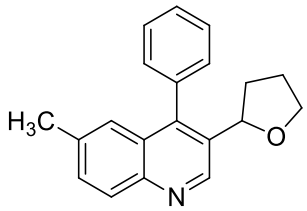
3-(tetrahydrofuran-2-yl)-4-(*o*-tolyl)quinoline (**3l+3l'**)

Pale yellow oil (37.3 mg, 43% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.152 (s, 1H), 9.146 (s, 1H), 8.15 (d, *J* = 8.4 Hz, 2H), 7.67–7.63 (m, 2H), 7.41–7.36 (m, 6H), 7.34–7.30 (m, 2H), 7.25–7.22 (m, 2H), 7.17 (d, *J* = 7.5 Hz, 1H), 7.05 (d, *J* = 7.4 Hz, 1H), 4.75 (dd, *J* = 8.8 Hz and *J* = 6.6 Hz, 1H), 4.57 (dd, *J* = 8.4 Hz and *J* = 6.4 Hz, 1H), 4.19–4.09 (m, 2H), 3.89–3.82 (m, 2H), 2.12–1.99 (m, 4H), 1.96 (s, 3H), 1.90 (s, 3H), 1.88–1.81 (m, 2H), 1.79–1.69 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.4, 149.3, 147.3, 147.2, 144.7, 144.3, 136.4, 135.8, 135.2, 135.2, 133.3, 133.0, 130.2, 130.0, 129.8, 129.4, 129.4, 128.8, 128.8, 128.3, 126.7, 126.6, 126.1, 125.8, 125.7, 125.6, 76.9, 69.1, 68.8, 35.0, 33.9, 26.4, 19.7, 19.6; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{20}H_{20}NO$: 290.1539, Found: 290.1538.



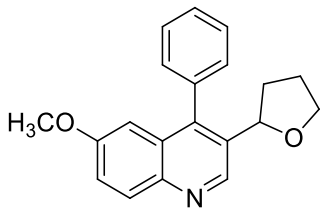
3-(tetrahydrofuran-2-yl)-4-(thiophen-2-yl)quinoline (**3m**)

Pale yellow solid (45.6 mg, 54% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.13 (s, 1H), 8.15 (d, *J* = 8.4 Hz, 1H), 7.71–7.67 (m, 1H), 7.63–7.61 (m, 1H), 7.56 (dd, *J* = 5.2 Hz and *J* = 1.0 Hz, 1H), 7.49–7.45 (m, 1H), 7.24–7.22 (m, 1H), 7.08–7.07 (m, 1H), 4.95 (dd, *J* = 8.2 Hz and *J* = 7.1 Hz, 1H), 4.23–4.18 (m, 1H), 3.95–3.90 (m, 1H), 2.27–2.20 (m, 1H), 2.15–2.06 (m, 1H), 2.03–1.92 (m, 1H), 1.87–1.78 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.0, 147.3, 137.7, 135.4, 135.2, 129.4, 129.0, 128.9, 128.0, 127.3, 127.1, 126.9, 126.0, 77.2, 69.3, 35.4, 26.6; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{17}H_{16}NOS$: 282.0947, Found: 282.0945.



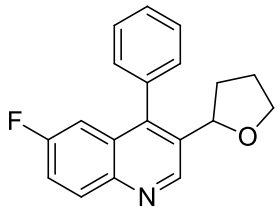
6-methyl-4-phenyl-3-(tetrahydrofuran-2-yl)quinoline (**3n**)

Pale yellow solid (53.0 mg, 61% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.07 (s, 1H), 8.04 (d, *J* = 8.8 Hz, 1H), 7.54–7.49 (m, 4H), 7.34–7.32 (m, 1H), 7.23–7.21 (m, 1H), 7.13 (s, 1H), 4.74 (dd, *J* = 8.2 Hz and *J* = 6.5 Hz, 1H), 4.19–4.14 (m, 1H), 3.89–3.83 (m, 1H), 2.39 (s, 3H), 2.13–2.03 (m, 2H), 1.94–1.86 (m, 1H), 1.84–1.74 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 148.3, 146.0, 144.3, 136.4, 136.0, 133.0, 131.0, 129.8, 129.1, 128.6, 128.2, 128.0, 127.0, 125.0, 77.2, 69.0, 35.0, 26.5, 21.7; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{20}H_{20}NO$: 290.1539, Found: 290.1537.



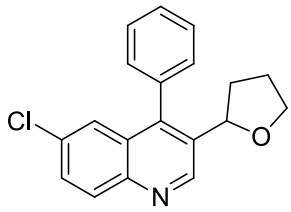
6-methoxy-4-phenyl-3-(tetrahydrofuran-2-yl)quinoline (**3o**)

Pale yellow solid (49.5 mg, 54% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.98 (s, 1H), 8.04 (d, *J* = 9.2 Hz, 1H), 7.54–7.45 (m, 3H), 7.34–7.30 (m, 2H), 7.22–7.21 (m, 1H), 6.63–6.62 (m, 1H), 4.73 (dd, *J* = 8.1 Hz and *J* = 6.6 Hz, 1H), 4.17–4.12 (m, 1H), 3.87–3.82 (m, 1H), 3.66 (s, 3H), 2.12–2.01 (m, 2H), 1.93–1.86 (m, 1H), 1.82–1.75 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.7, 146.7, 143.7, 143.4, 136.0, 133.3, 130.7, 129.7, 128.9, 128.7, 128.3, 128.0, 120.9, 104.4, 77.2, 69.0, 55.2, 35.0, 26.4; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{20}H_{20}NO_2$: 306.1489, Found: 306.1485.



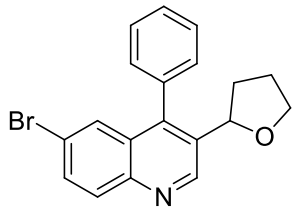
6-fluoro-4-phenyl-3-(tetrahydrofuran-2-yl)quinoline (**3p**)

Pale yellow solid (45.8 mg, 52% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.09 (s, 1H), 8.15–8.11 (m, 1H), 7.53–7.49 (m, 3H), 7.44–7.39 (m, 1H), 7.32–7.30 (m, 1H), 7.21–7.19 (m, 1H), 6.99 (dd, *J* = 10.1 Hz and *J* = 2.8 Hz, 1H), 4.76 (dd, *J* = 8.3 Hz and *J* = 6.5 Hz, 1H), 4.19–4.13 (m, 1H), 3.89–3.83 (m, 1H), 2.12–2.04 (m, 2H), 1.94–1.86 (m, 1H), 1.81–1.76 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 160.6 (d, *J* = 245.7 Hz), 148.6 (d, *J* = 2.7 Hz), 144.5, 144.4, 135.3, 133.9, 131.8 (d, *J* = 9.2 Hz), 129.7, 128.9, 128.8, 128.4, 128.3, 128.0 (d, *J* = 9.4 Hz), 118.9 (d, *J* = 25.6 Hz), 109.6 (d, *J* = 23.1 Hz), 77.0, 69.1, 35.0, 26.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{19}H_{17}FNO$: 294.1289, Found: 294.1287.



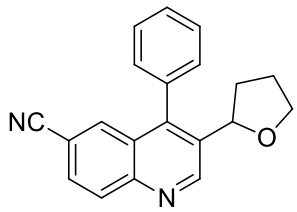
6-chloro-4-phenyl-3-(tetrahydrofuran-2-yl)quinoline (**3q**)

Pale yellow solid (53.9 mg, 58% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.12 (s, 1H), 8.08 (d, *J* = 8.8 Hz, 1H), 7.59 (dd, *J* = 9.0 Hz and *J* = 2.2 Hz, 1H), 7.55–7.52 (m, 3H), 7.35–7.30 (m, 2H), 7.21–7.19 (m, 1H), 4.74 (dd, *J* = 8.2 Hz and *J* = 6.7 Hz, 1H), 4.18–4.13 (m, 1H), 3.89–3.83 (m, 1H), 2.14–2.04 (m, 2H), 1.94–1.88 (m, 1H), 1.82–1.75 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.5, 145.7, 144.2, 135.1, 134.1, 132.5, 131.0, 129.7, 129.7, 129.0, 128.8, 128.5, 128.4, 127.9, 125.0, 69.1, 35.0, 26.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{19}H_{17}ClNO$: 310.0993, Found: 310.0996.



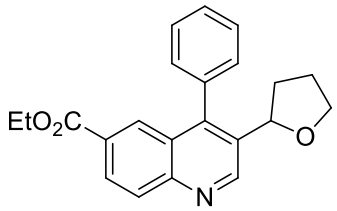
6-bromo-4-phenyl-3-(tetrahydrofuran-2-yl)quinoline (**3r**)

Pale yellow solid (59.5 mg, 56% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.13 (s, 1H), 8.00 (d, *J* = 8.9 Hz, 1H), 7.72 (dd, *J* = 8.9 Hz and *J* = 2.2 Hz, 1H), 7.55–7.50 (m, 4H), 7.32–7.29 (m, 1H), 7.21–7.18 (m, 1H), 4.73 (dd, *J* = 8.4 Hz and *J* = 6.5 Hz, 1H), 4.18–4.12 (m, 1H), 3.88–3.82 (m, 1H), 2.13–2.02 (m, 2H), 1.95–1.85 (m, 1H), 1.81–1.74 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.6, 145.9, 144.0, 134.9, 134.1, 132.2, 131.1, 129.7, 128.9, 128.8, 128.4, 128.4, 128.3, 128.3, 120.7, 76.9, 69.1, 35.0, 26.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{19}H_{17}BrNO$: 354.0488, Found: 354.0485.



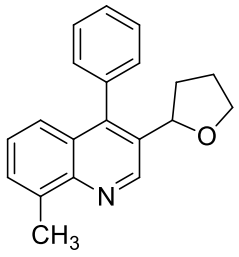
4-phenyl-3-(tetrahydrofuran-2-yl)quinoline-6-carbonitrile (**3s**)

Pale yellow solid (45.1 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.25 (s, 1H), 8.21 (d, *J* = 9.4 Hz, 1H), 7.82–7.79 (m, 2H), 7.58–7.54 (m, 3H), 7.32–7.29 (m, 1H), 7.22–7.19 (m, 1H), 4.77 (dd, *J* = 8.3 Hz and *J* = 6.5 Hz, 1H), 4.20–4.14 (m, 1H), 3.91–3.85 (m, 1H), 2.17–2.06 (m, 2H), 1.99–1.90 (m, 1H), 1.82–1.75 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 152.3, 148.2, 145.3, 135.1, 134.2, 132.8, 130.9, 129.6, 129.4, 129.0, 128.8, 128.7, 126.8, 118.7, 110.2, 76.8, 69.2, 35.0, 26.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{20}H_{17}N_2O$: 301.1335, Found: 301.1333.



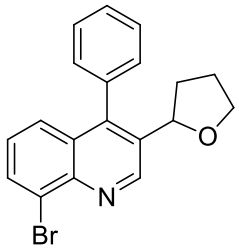
ethyl 4-phenyl-3-(tetrahydrofuran-2-yl)quinoline-6-carboxylate (**3t**)

Pale yellow solid (55.2 mg, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.20 (s, 1H), 8.25 (dd, *J* = 8.9 Hz and *J* = 1.7 Hz, 1H), 8.18–8.16 (m, 2H), 7.57–7.51 (m, 3H), 7.35–7.33 (m, 1H), 7.24–7.21 (m, 1H), 4.77 (dd, *J* = 8.3 Hz and *J* = 6.5 Hz, 1H), 4.34 (q, *J* = 6.8 Hz, 2H), 4.19–4.14 (m, 1H), 3.89–3.84 (m, 1H), 2.15–2.05 (m, 2H), 1.98–1.87 (m, 1H), 1.84–1.77 (m, 1H), 1.34 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3): δ = 166.1, 151.4, 149.1, 146.3, 134.9, 134.0, 129.8, 129.6, 129.3, 129.0, 128.7, 128.4, 128.4, 128.3, 126.4, 76.9, 69.1, 61.1, 35.0, 26.5, 14.2; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{22}H_{22}NO_3$: 348.1594, Found: 348.1590.



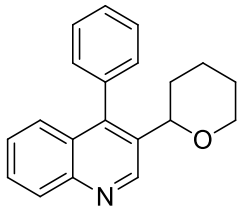
8-methyl-4-phenyl-3-(tetrahydrofuran-2-yl)quinoline (**3u**)

Pale yellow solid (49.5 mg, 57% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.18 (s, 1H), 7.54–7.46 (m, 4H), 7.35–7.28 (m, 2H), 7.25–7.21 (m, 2H), 4.78 (dd, *J* = 8.0 Hz and *J* = 6.7 Hz, 1H), 4.20–4.14 (m, 1H), 3.91–3.85 (m, 1H), 2.88 (s, 3H), 2.14–2.05 (m, 2H), 1.93–1.86 (m, 1H), 1.84–1.77 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 148.0, 146.4, 145.2, 137.0, 136.3, 132.9, 129.9, 129.2, 129.1, 128.5, 128.2, 128.0, 127.0, 126.2, 124.4, 77.2, 69.1, 35.1, 26.6, 18.3; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{20}H_{20}NO$: 290.1539, Found: 290.1535.



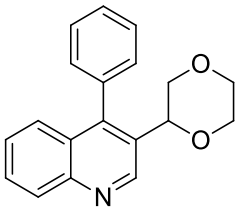
8-bromo-4-phenyl-3-(tetrahydrofuran-2-yl)quinoline (**3v**)

Pale yellow solid (57.4 mg, 54% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.26 (s, 1H), 7.99 (dd, *J* = 7.4 Hz and *J* = 1.1 Hz, 1H), 7.54–7.49 (m, 3H), 7.36 (dd, *J* = 8.4 Hz and *J* = 1.2 Hz, 1H), 7.32–7.29 (m, 1H), 7.25–7.18 (m, 2H), 4.77 (dd, *J* = 7.9 Hz and *J* = 6.7 Hz, 1H), 4.17–4.12 (m, 1H), 3.89–3.84 (m, 1H), 2.14–2.02 (m, 2H), 1.92–1.87 (m, 1H), 1.82–1.75 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 150.1, 145.4, 144.3, 135.4, 134.3, 132.5, 129.7, 129.0, 128.7, 128.6, 128.3, 128.3, 126.7, 126.2, 125.0, 76.9, 69.2, 35.0, 26.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{19}H_{17}BrNO$: 354.0488, Found: 354.0483.



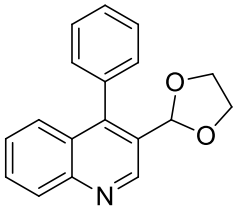
4-phenyl-3-(tetrahydro-2H-pyran-2-yl)quinoline (**4a**)

Pale yellow solid (46.0 mg, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.19 (s, 1H), 8.15 (d, *J* = 8.4 Hz, 1H), 7.69–7.65 (m, 1H), 7.57–7.50 (m, 3H), 7.41–7.35 (m, 3H), 7.24–7.21 (m, 1H), 4.26 (dd, *J* = 10.9 Hz and *J* = 2.6 Hz, 1H), 4.09 (dd, *J* = 11.4 Hz and *J* = 4.5 Hz, 1H), 3.43–3.37 (m, 1H), 1.88–1.84 (m, 1H), 1.76–1.65 (m, 3H), 1.52–1.49 (m, 1H), 1.45–1.35 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.7, 147.3, 144.8, 135.7, 132.8, 129.6, 129.3, 129.2, 128.8, 128.5, 128.2, 128.0, 127.1, 126.5, 126.4, 76.2, 68.9, 33.6, 25.6, 23.8; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{20}H_{20}NO$: 290.1539, Found: 290.1548.



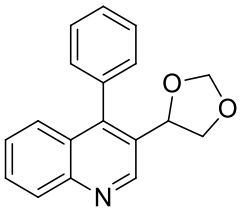
3-(1,4-dioxan-2-yl)-4-phenylquinoline (**4b**)

Pale yellow solid (41.1 mg, 47% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.26 (s, 1H), 8.77 (d, *J* = 8.5 Hz, 1H), 7.97–7.93 (m, 1H), 7.72–7.68 (m, 1H), 7.60–7.54 (m, 4H), 7.30–7.29 (m, 1H), 7.19–7.17 (m, 1H), 4.62 (dd, *J* = 10.0 Hz and *J* = 2.5 Hz, 1H), 3.87–3.84 (m, 1H), 3.73–3.60 (m, 4H), 3.31–3.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 155.8, 142.1, 137.2, 134.0, 132.1, 130.7, 130.1, 130.0, 129.3, 129.0, 128.5, 128.0, 127.4, 127.1, 121.7, 72.4, 70.7, 66.6, 65.9; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{19}H_{18}NO_2$: 292.1332, Found: 292.1334.



3-(1,3-dioxolan-2-yl)-4-phenylquinoline (**4c**)

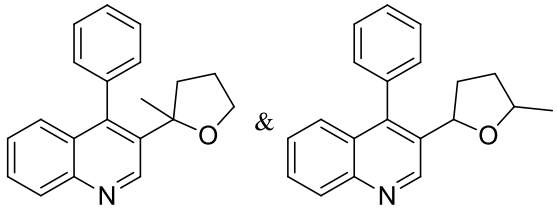
Pale yellow solid (36.6 mg, 44% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.17 (s, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 7.74–7.70 (m, 1H), 7.54–7.50 (m, 4H), 7.47–7.43 (m, 1H), 7.39–7.37 (m, 2H), 5.63 (s, 1H), 4.22–4.19 (m, 2H), 3.96–3.92 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.3, 148.2, 147.6, 134.5, 129.9, 129.6, 129.5, 128.3, 128.1, 127.1, 126.8, 126.6, 126.6, 100.9, 65.7; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{18}H_{16}NO_2$: 278.1176, Found: 278.1178.



3-(1,3-dioxolan-4-yl)-4-phenylquinoline (**4c'**)

Pale yellow solid (19.1 mg, 23% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.18 (s, 1H),

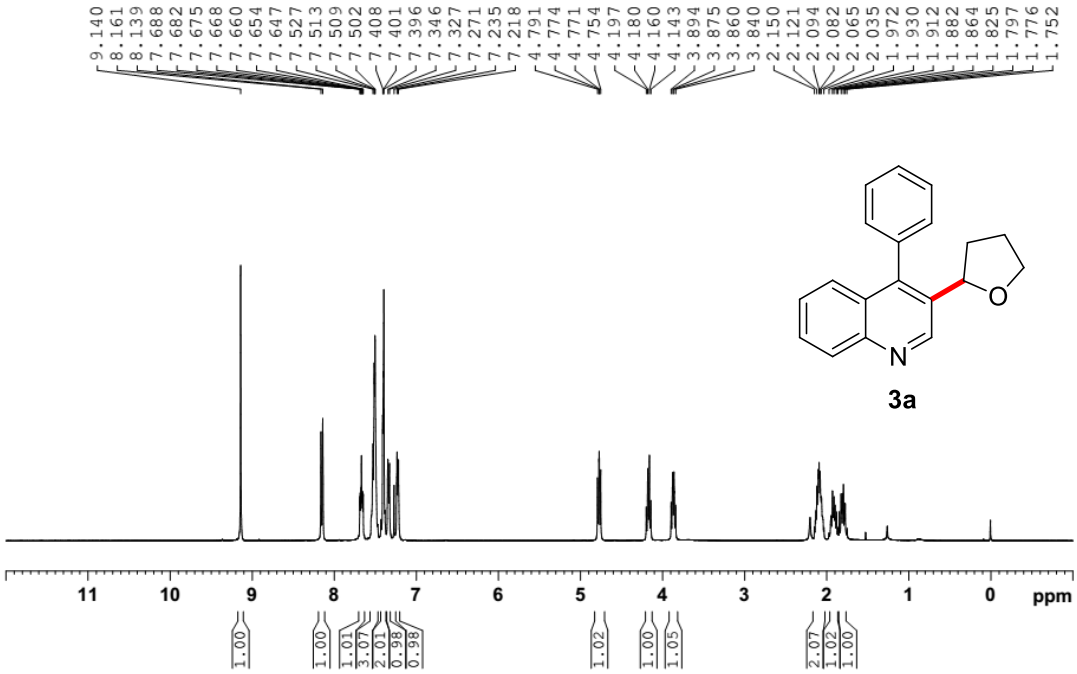
8.18 (d, *J* = 8.4 Hz, 1H), 7.73–7.68 (m, 1H), 7.58–7.50 (m, 3H), 7.46–7.42 (m, 2H), 7.38–7.35 (m, 1H), 7.19–7.16 (m, 1H), 5.34 (s, 1H), 5.00 (s, 1H), 4.96 (t, *J* = 8.0 Hz, 1H), 4.00–3.96 (m, 1H), 3.74–3.70 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 148.8, 147.7, 146.0, 135.3, 129.6, 129.5, 129.4, 129.3, 129.0, 128.8, 128.5, 128.5, 126.8, 126.8, 126.2, 96.1, 74.0, 71.5; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{18}H_{16}NO_2$: 278.1176, Found: 278.1171.

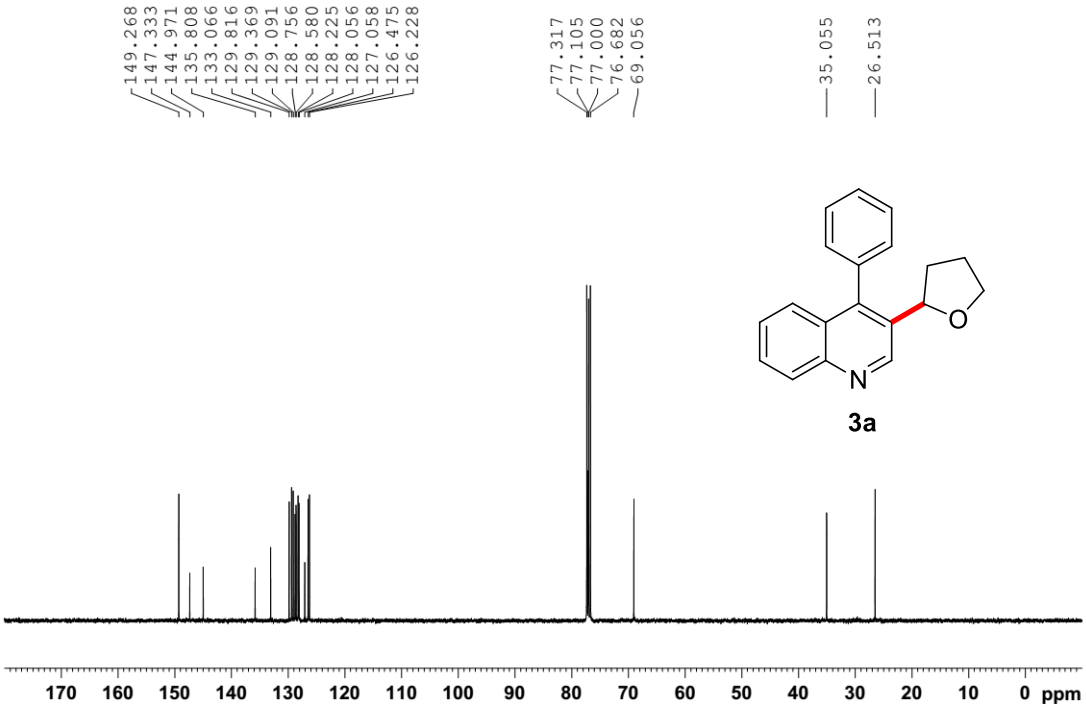


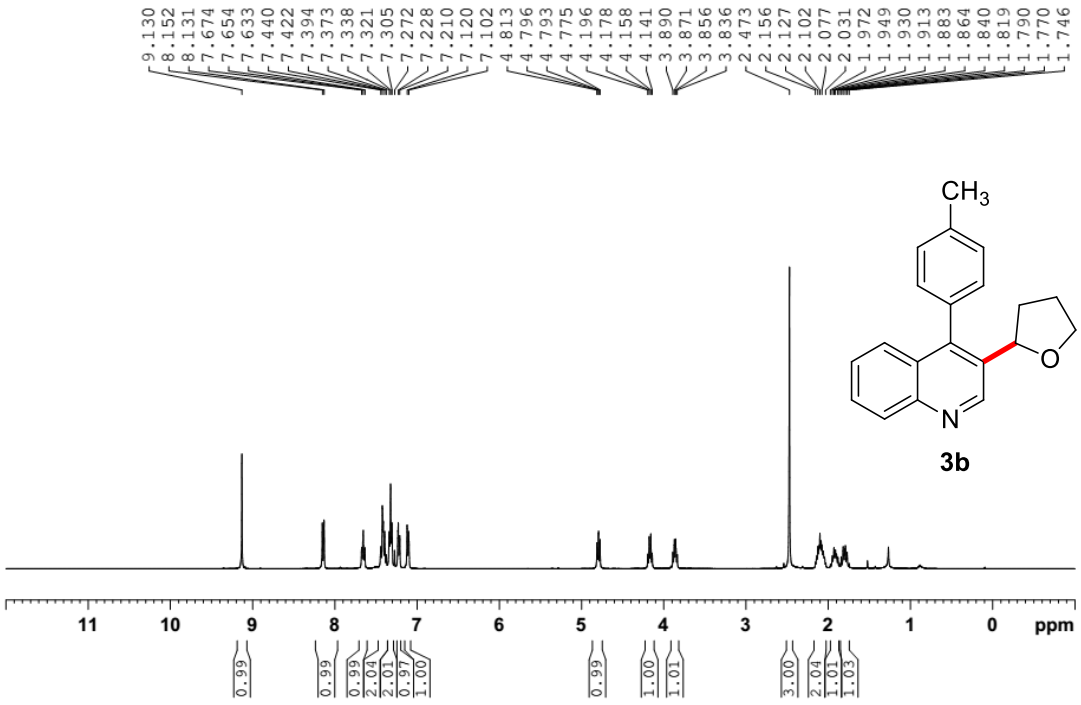
3-(2-methyltetrahydrofuran-2-yl)-4-phenylquinoline (**4d**) and 3-(5-methyltetrahydrofuran-2-yl)-4-phenylquinoline (**4d'**)

Pale yellow solid (59.0 mg, 68% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.39 (s, 1H), 9.15 (s, 0.4H), 8.15–8.12 (m, 1.5H), 7.67–7.61 (m, 1.5H), 7.54–7.47 (m, 4.5H), 7.39–7.32 (m, 2.5H), 7.29–7.24 (m, 2H), 7.22–7.18 (m, 1.5H), 4.97–4.93 (m, 0.4H), 4.49–4.44 (m, 0.4H), 3.96–3.91 (m, 1H), 3.77–3.72 (m, 1H), 2.20–2.13 (m, 1H), 2.06–1.99 (m, 1H), 1.90–1.83 (m, 1.5H), 1.81–1.73 (m, 1H), 1.60–1.54 (m, 1H), 1.28 (s, 3H), 1.27 (d, *J* = 6.0 Hz, 0.4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.9, 149.3, 147.2, 146.9, 144.6, 143.8, 137.6, 137.5, 135.8, 133.8, 130.1, 129.8, 129.7, 129.3, 129.1, 128.6, 128.5, 128.3, 128.2, 128.0, 127.9, 127.7, 127.0, 126.4, 126.4, 126.2, 126.1, 84.0, 76.7, 66.7, 39.4, 36.4, 34.7, 30.0, 25.8, 21.2; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{20}H_{20}NO$: 290.1539, Found: 290.1544.

7. ^{1}H and ^{13}C NMR spectra of the products



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7.272
7.228
7.210
7.120
7.102
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4.793
4.775
4.196
4.178
4.158
4.141
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3.856
3.836
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2.156
2.127
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2.077
2.031
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1.913
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1.840
1.819
1.790
1.770
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O
N
3b
11
10
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6
5
4
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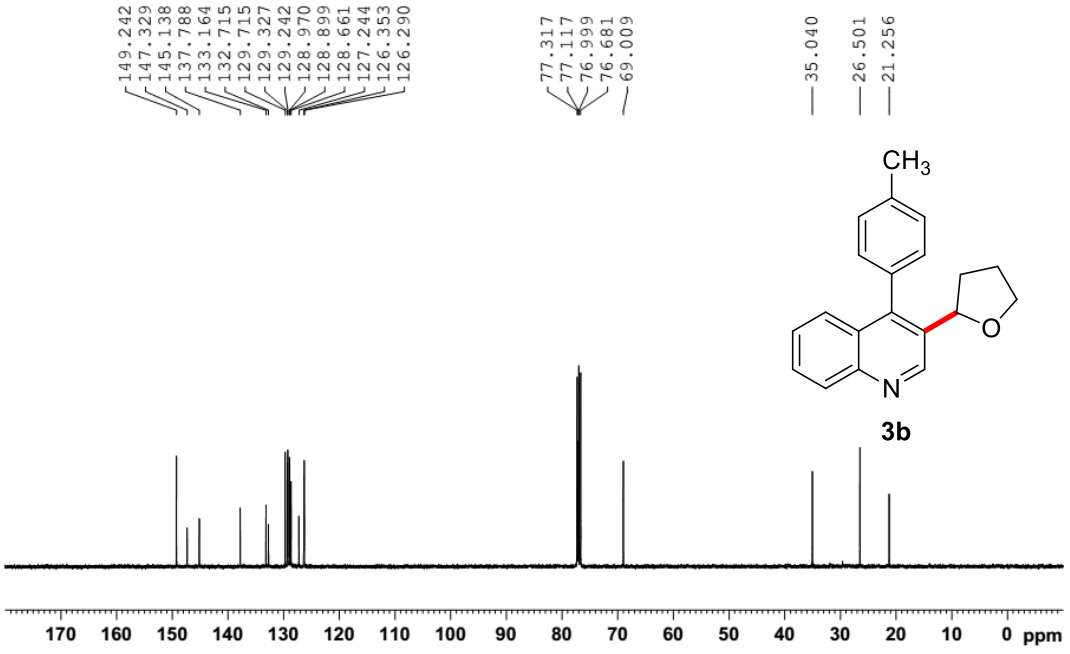
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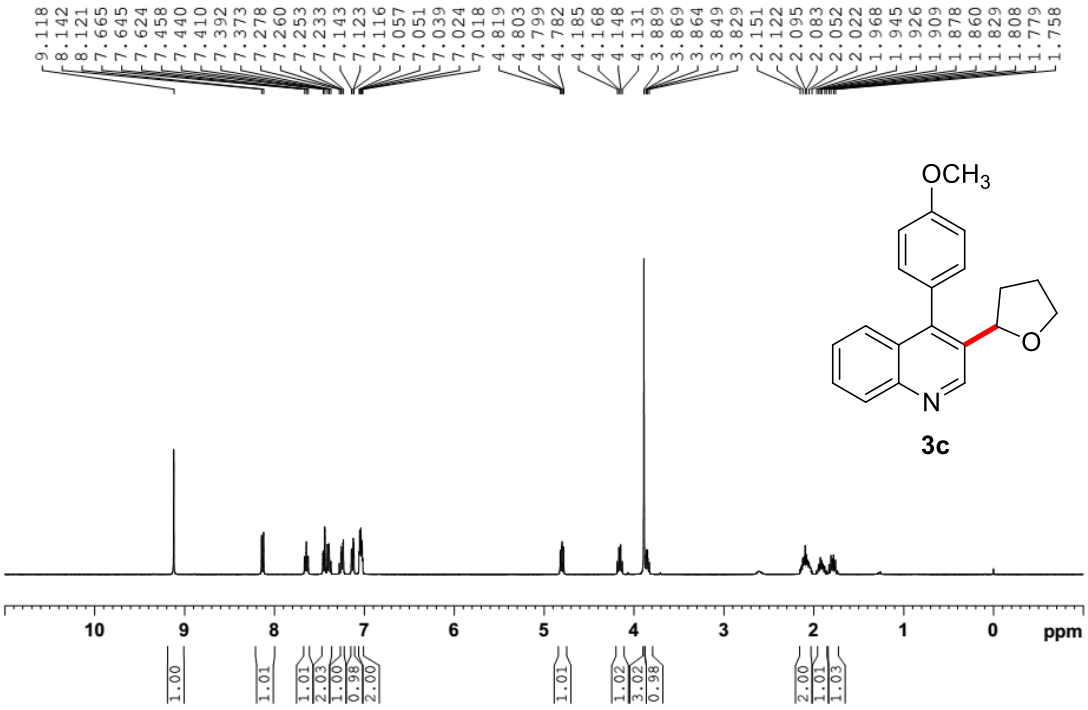
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4.131
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3.869
3.864
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2.122
2.095
2.083
2.052
2.022
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1.945
1.926
1.909
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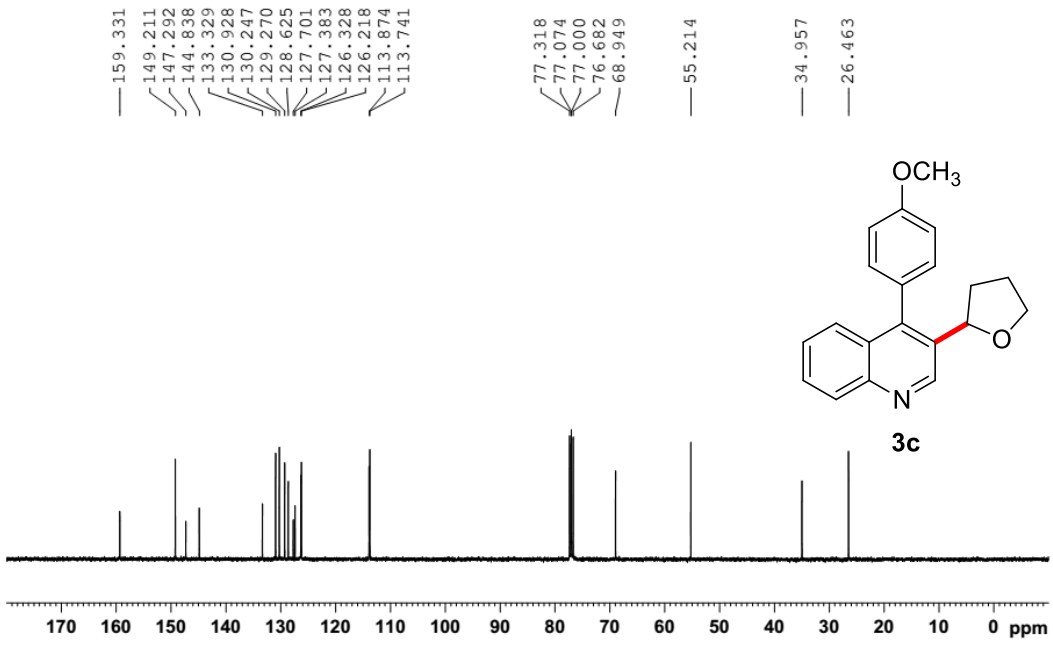
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113.741
77.318
77.074
77.000
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OCH3
O
N
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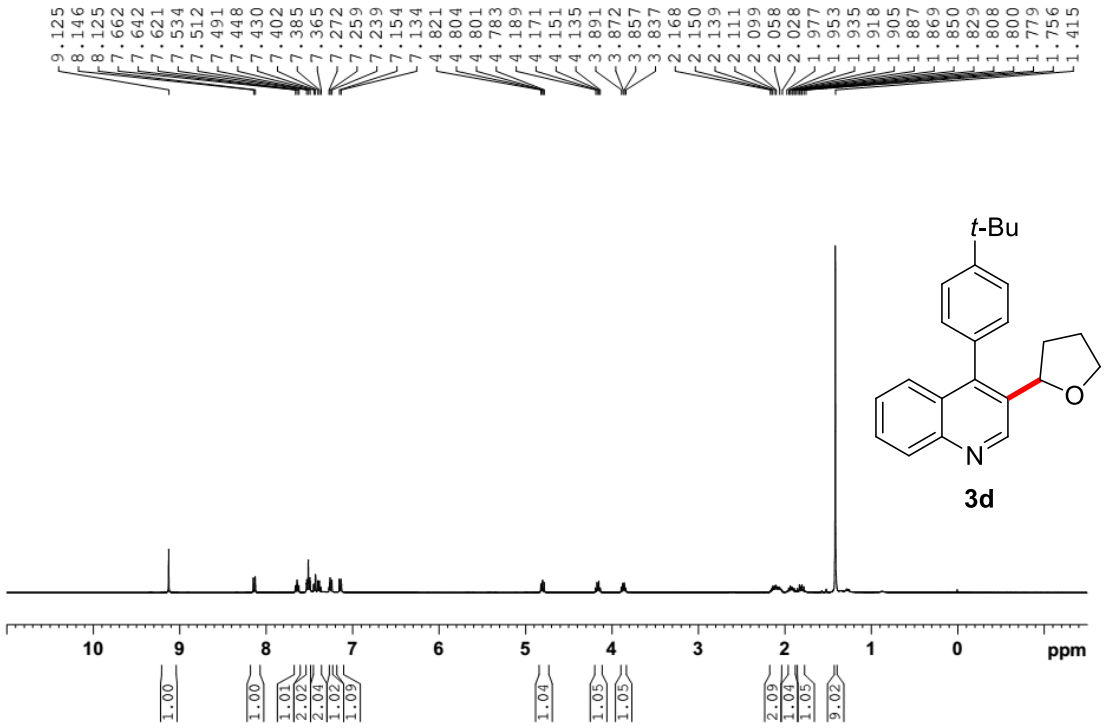
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7.365
7.272
7.259
7.239
7.154
7.134
4.821
4.804
4.801
4.783
4.189
4.171
4.151
4.135
3.891
3.872
3.857
3.837
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2.150
2.139
2.111
2.099
2.058
2.028
1.977
1.953
1.935
1.918
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1.869
1.850
1.829
1.808
1.800
1.779
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1.415
t-Bu
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3d
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8
7
6
5
4
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2
1
0
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1.00
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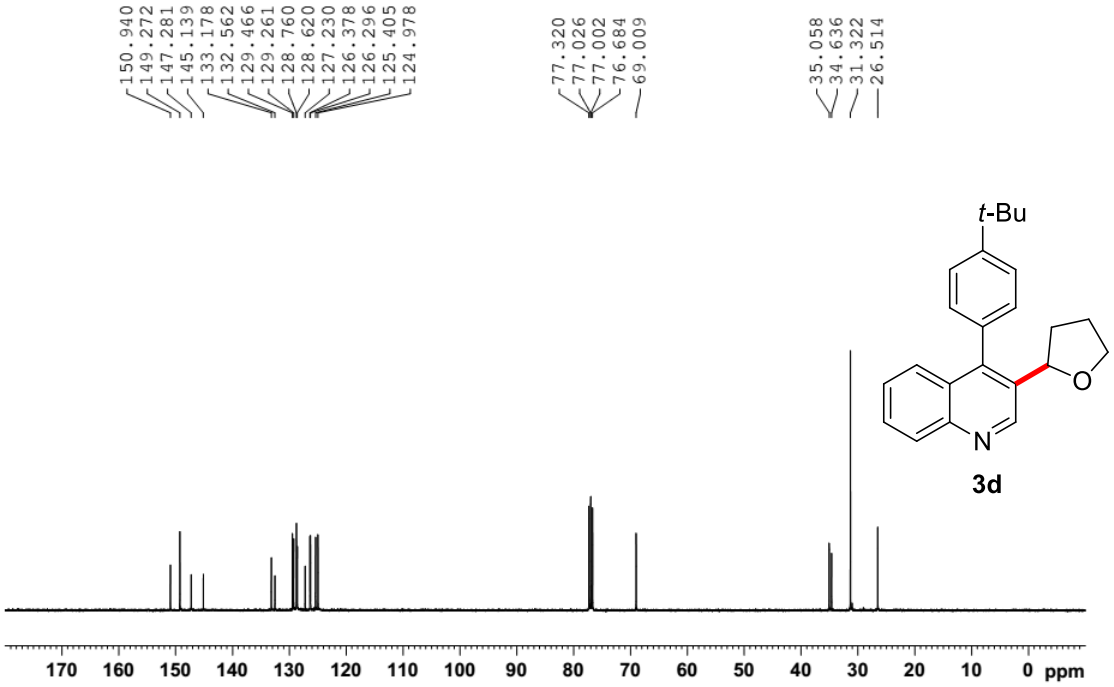
9.02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31.322
26.514
t-Bu
O
N
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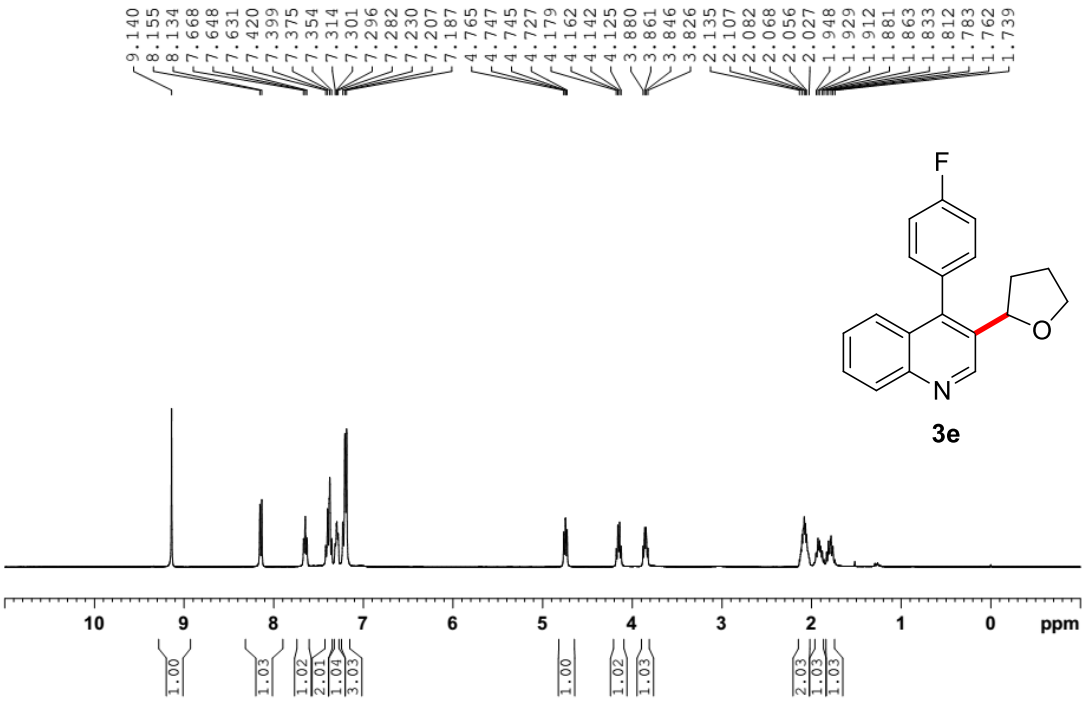
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3.826
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2.082
2.068
2.056
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1.02
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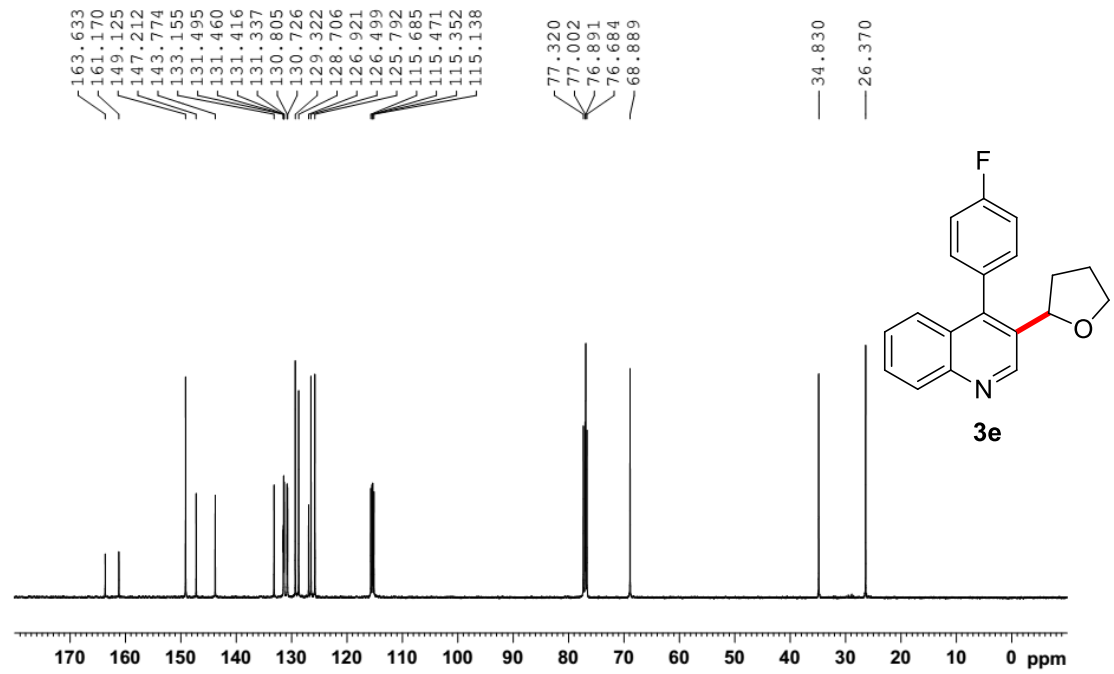
1.03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N
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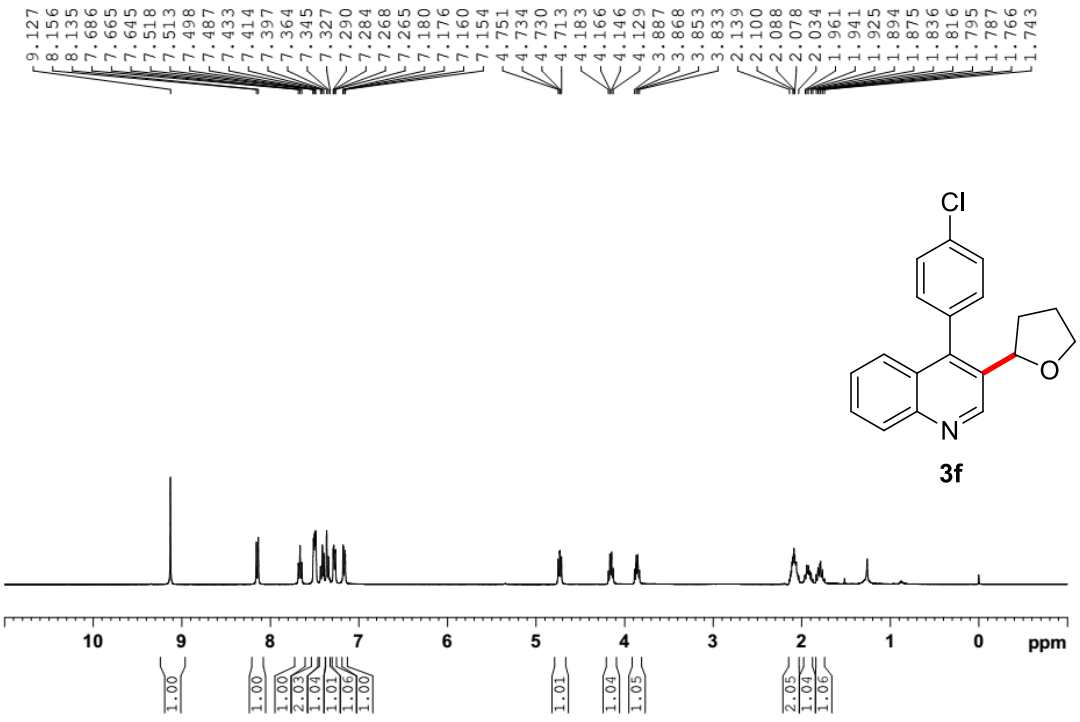
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7
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4
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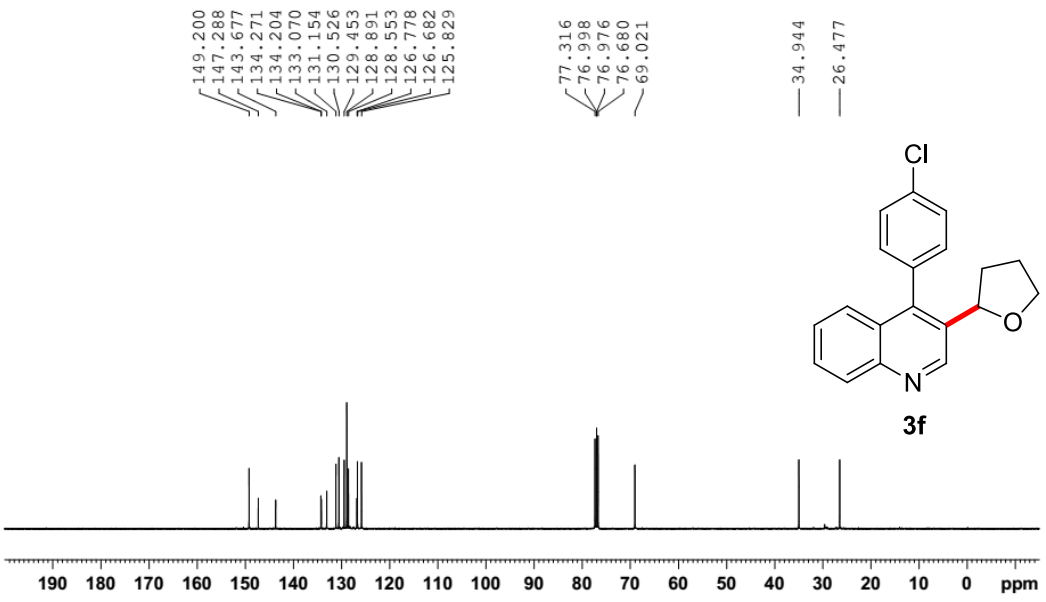
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26.477
Cl
O
N
3f
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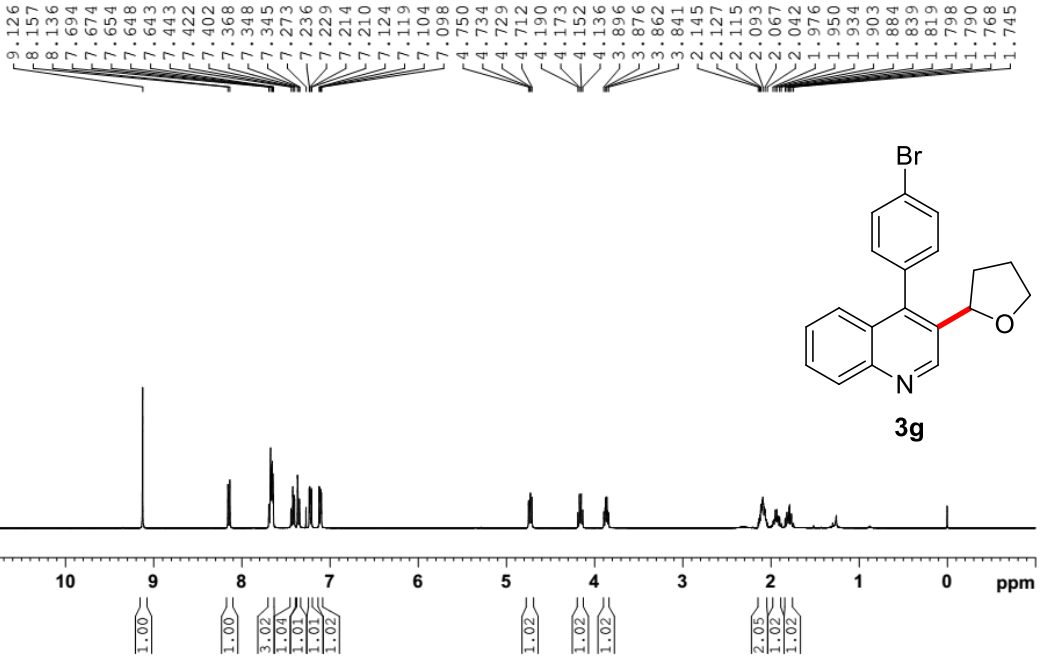
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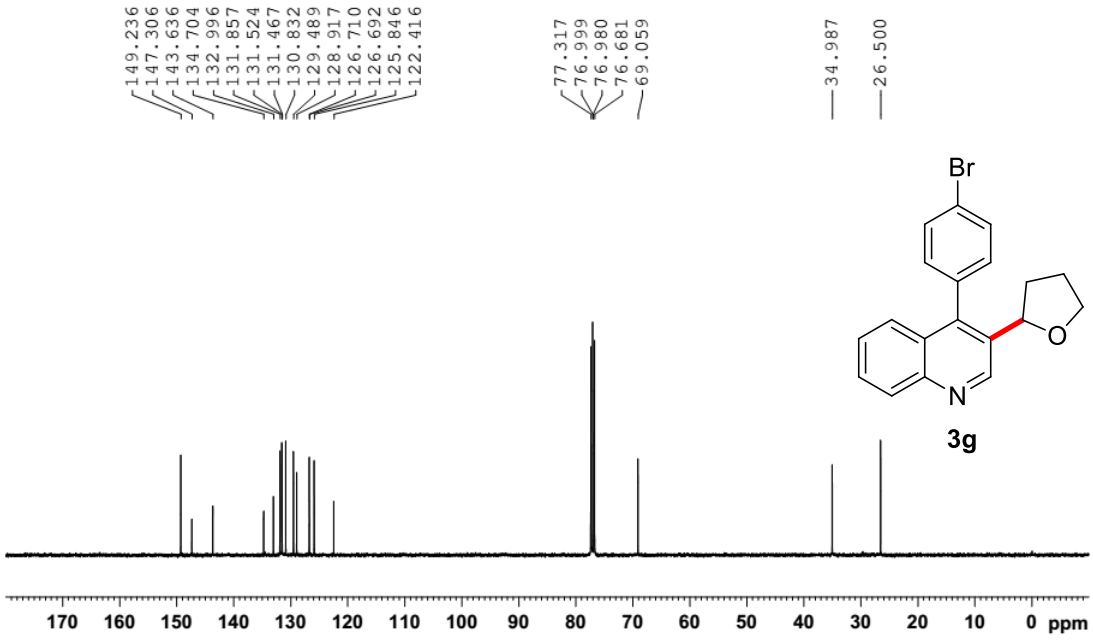
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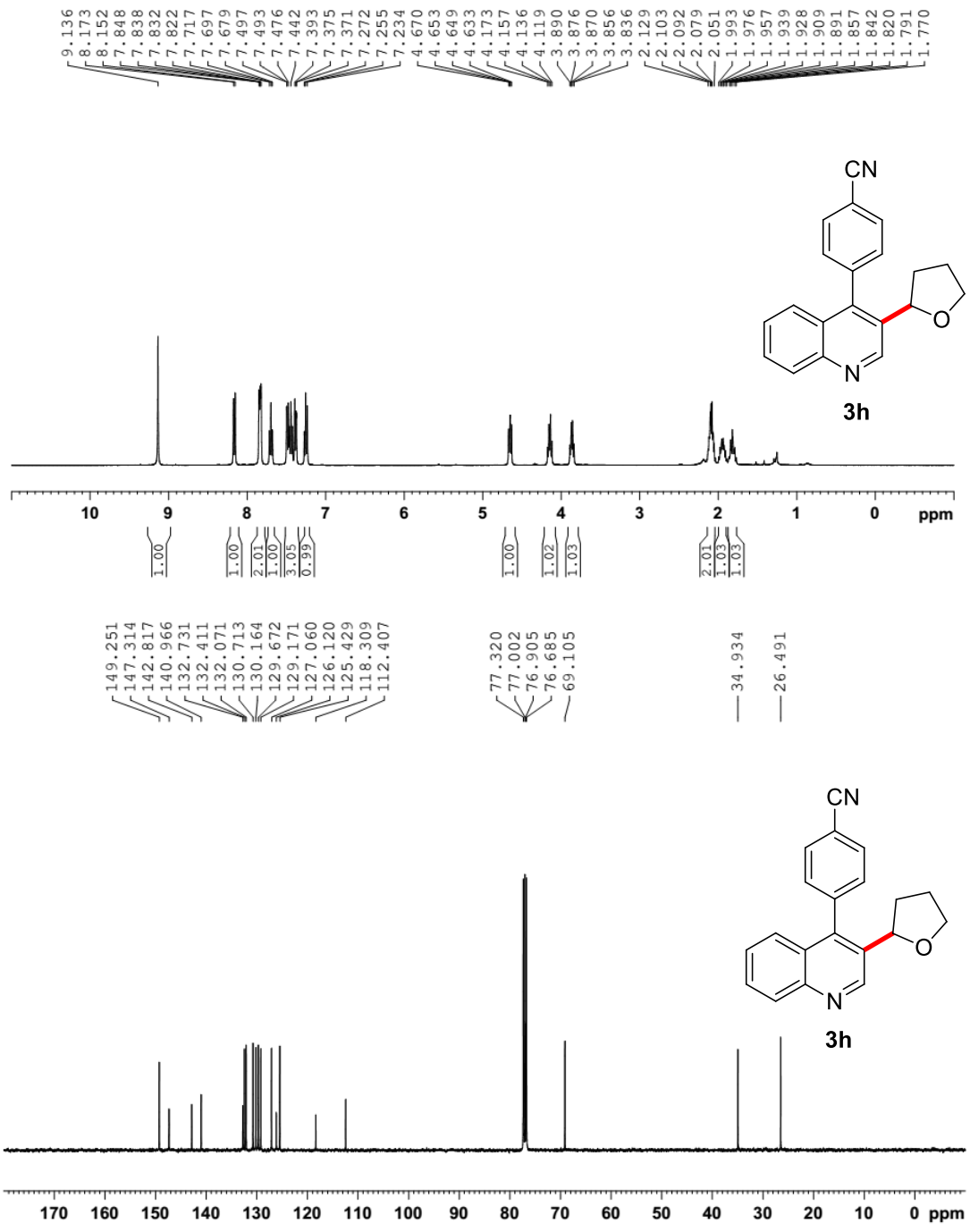
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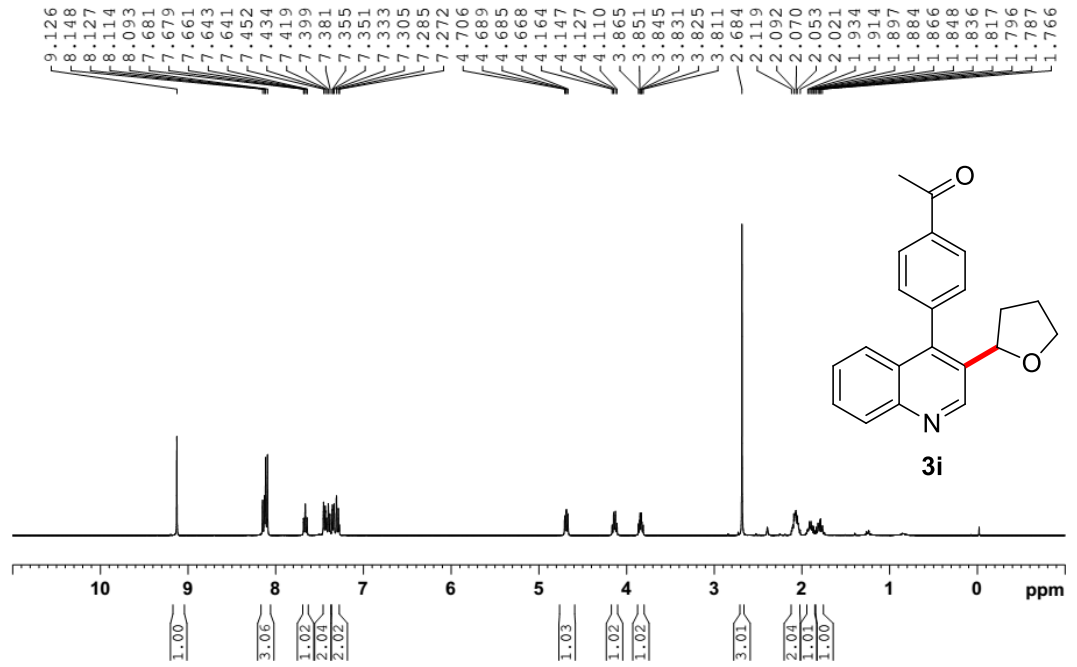
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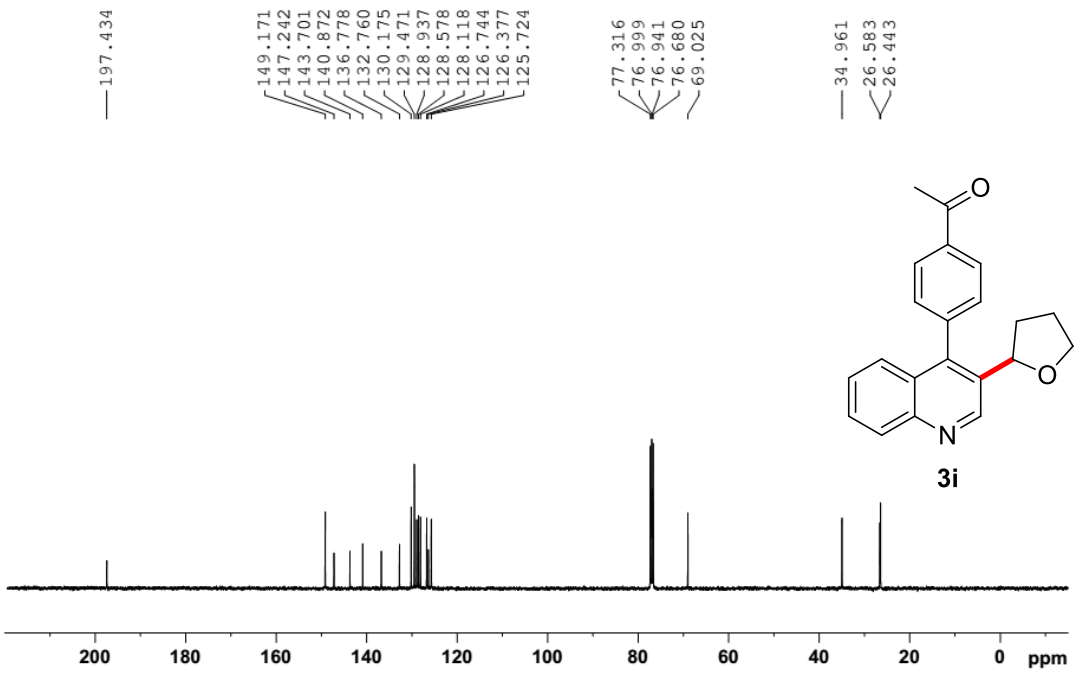
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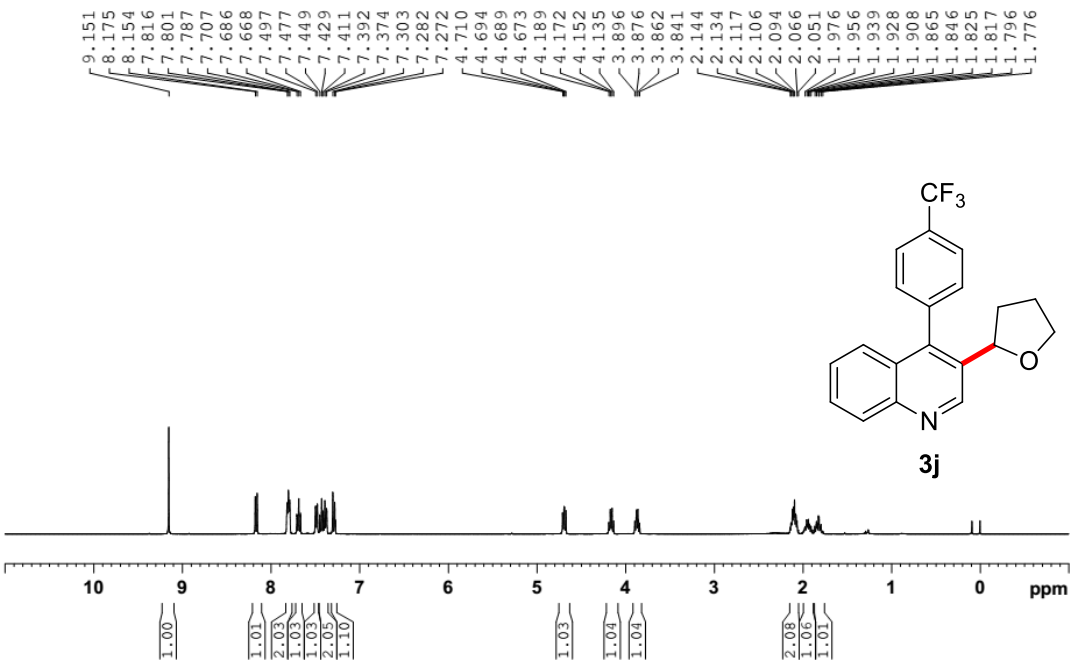
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1.817
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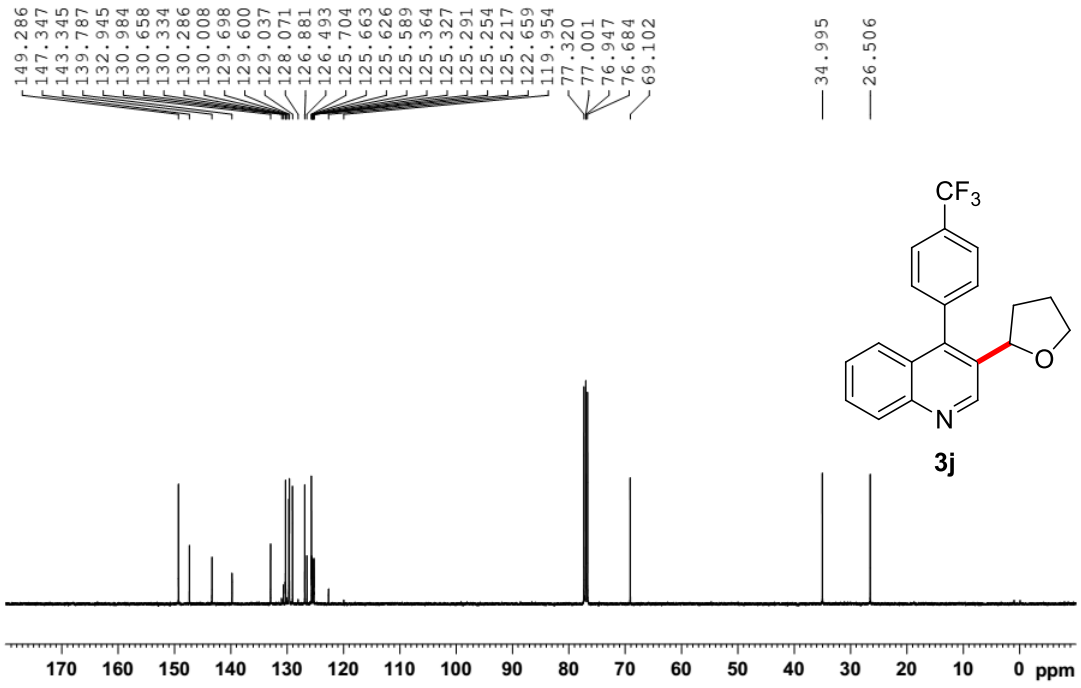
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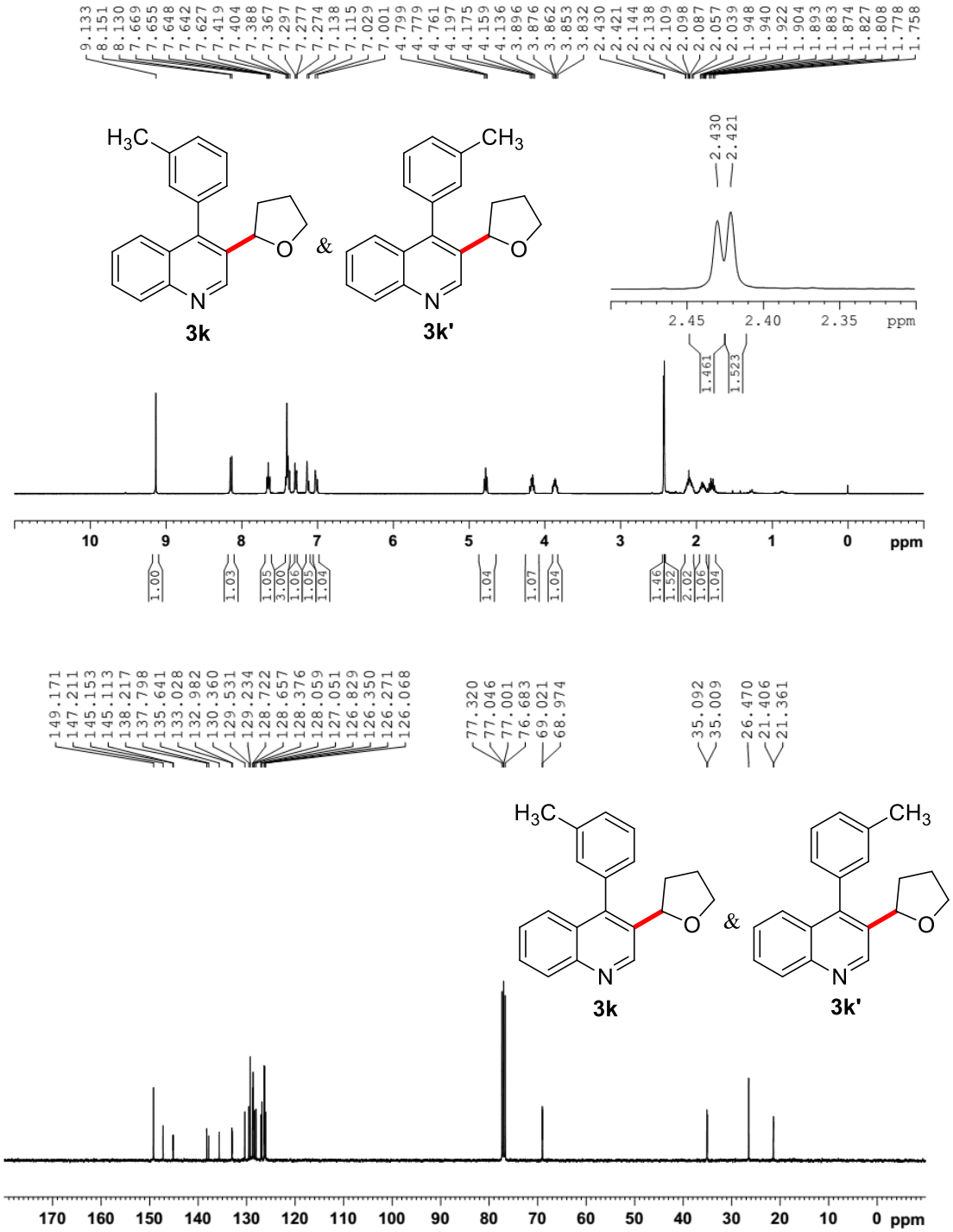
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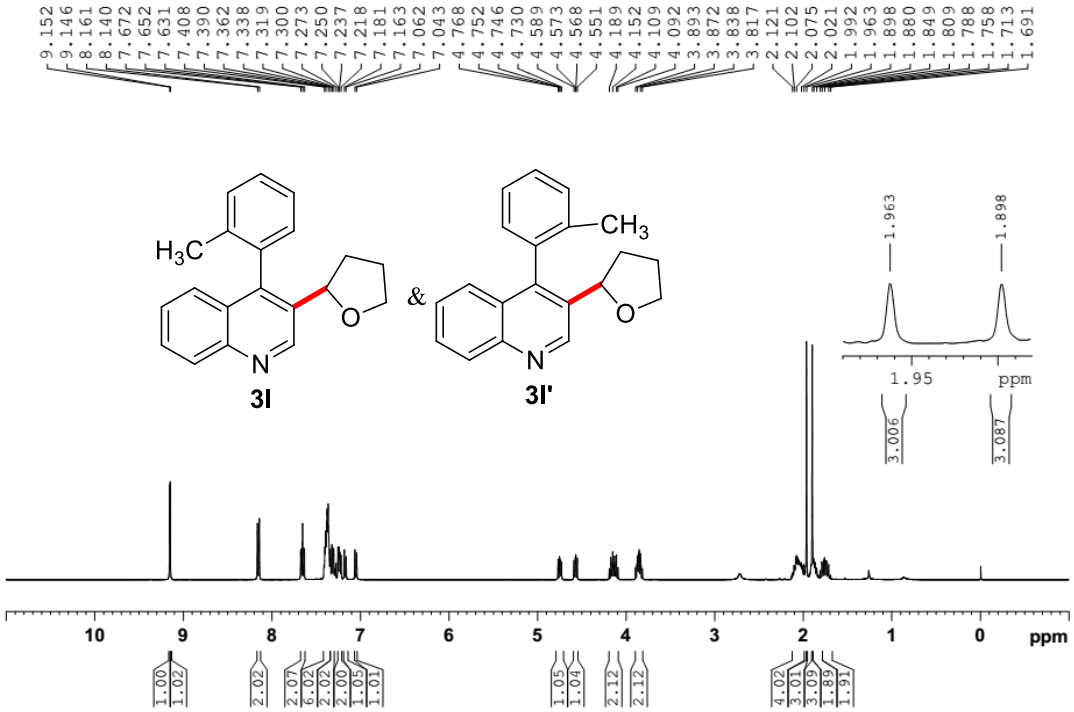
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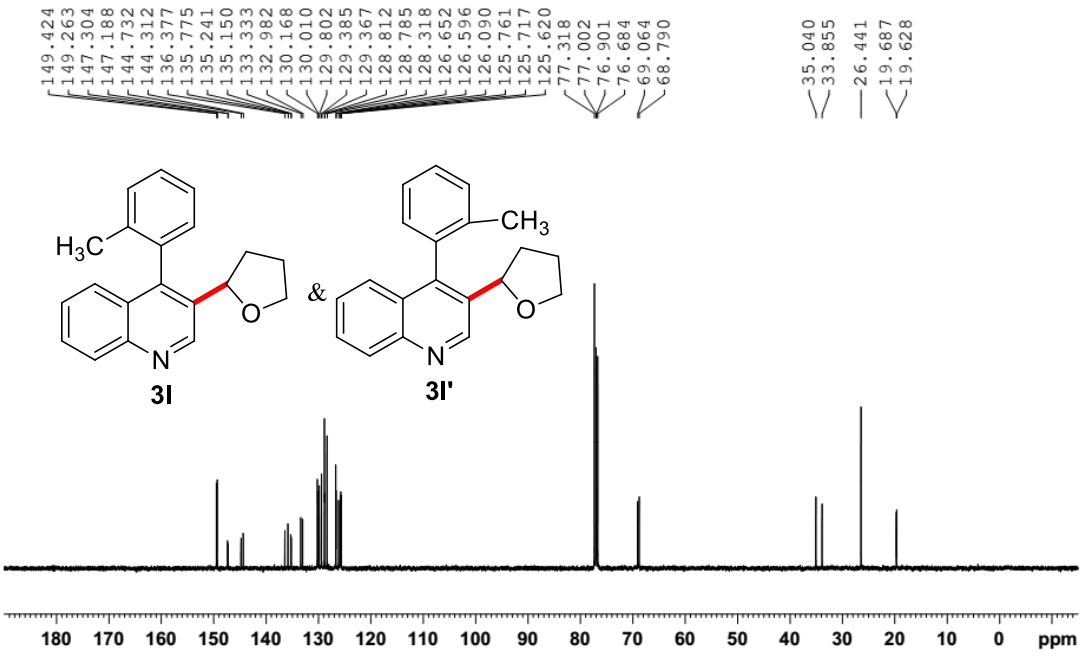
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&
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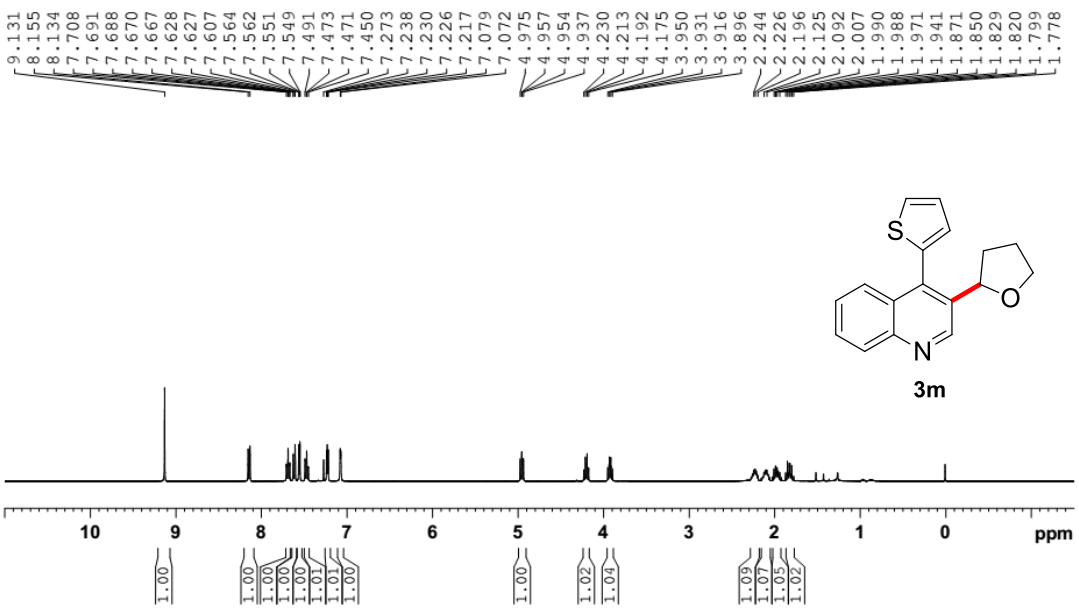
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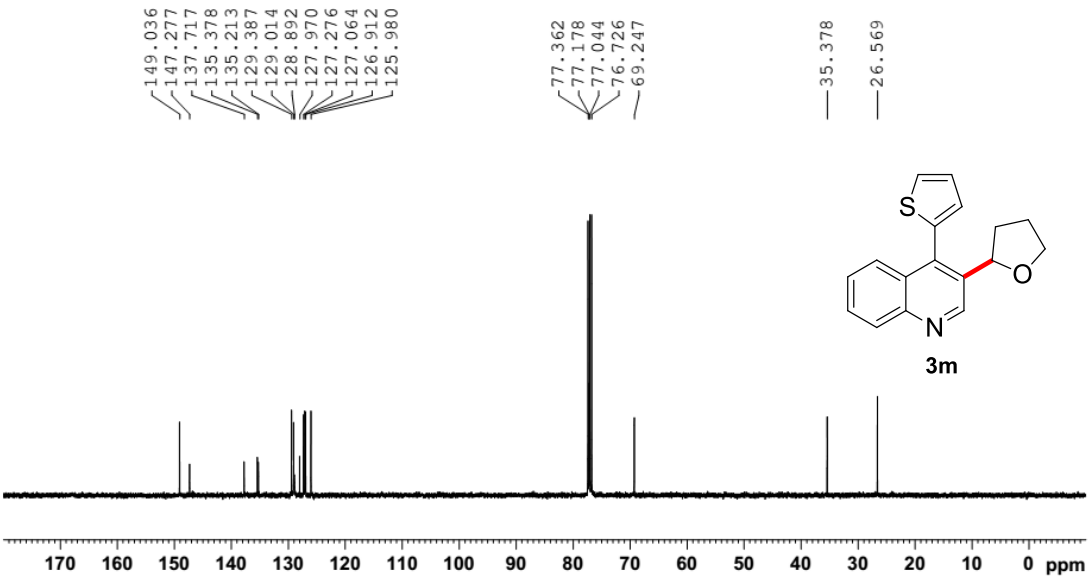
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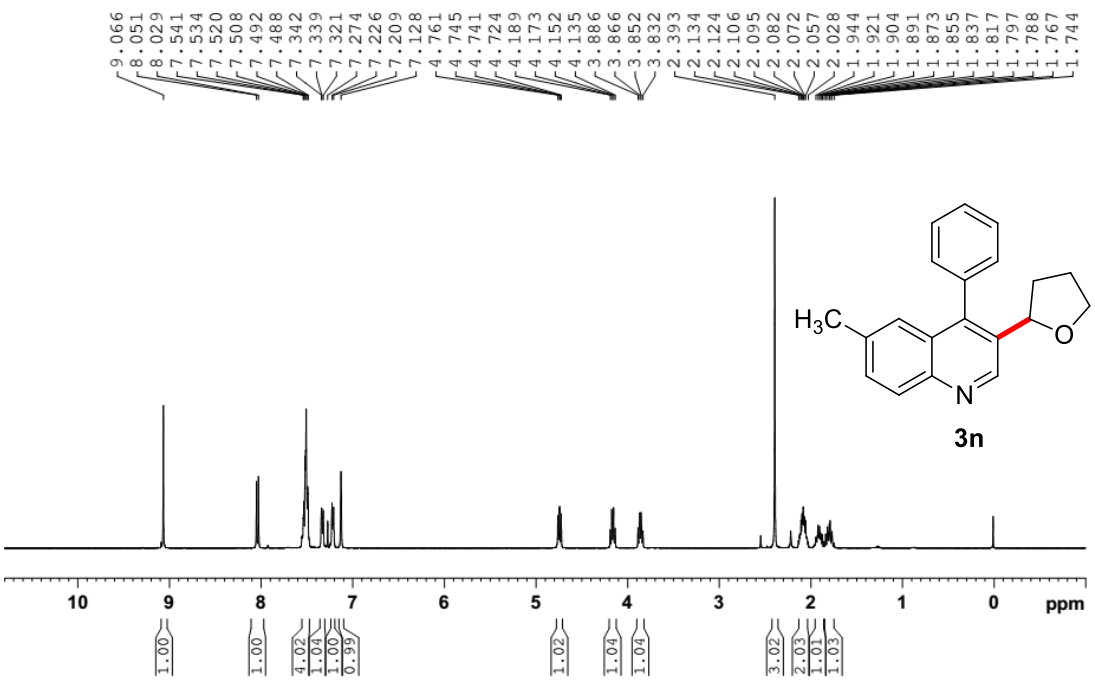
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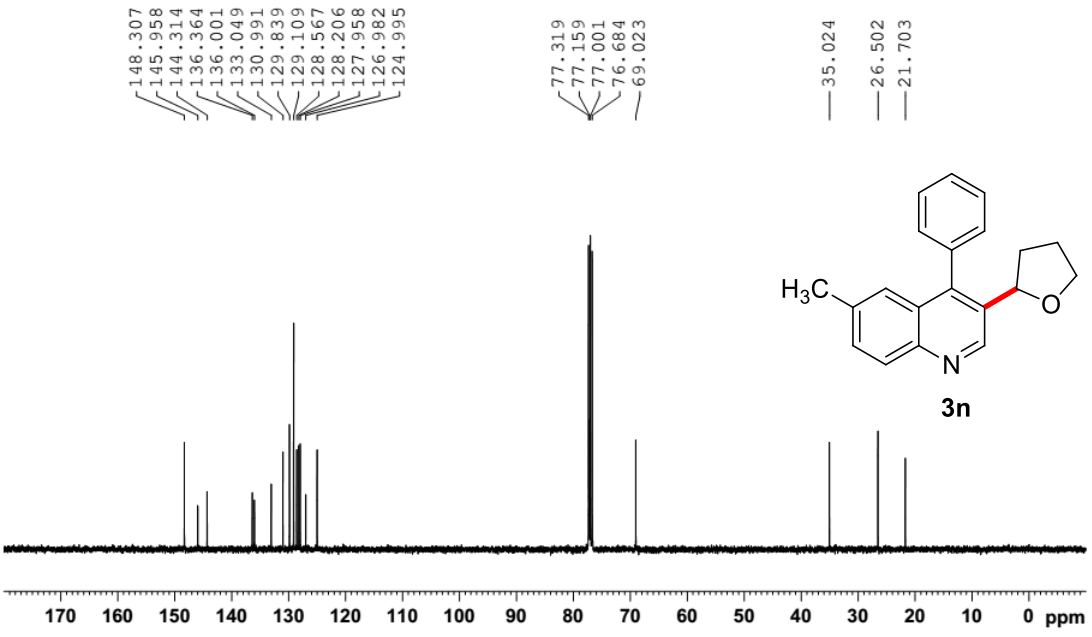
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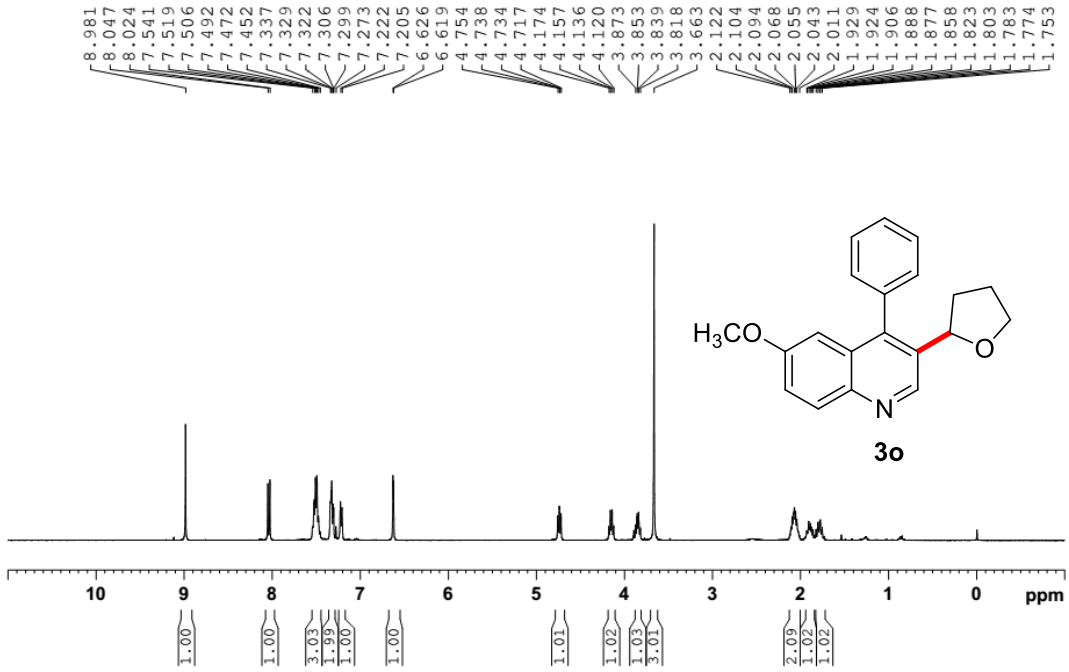
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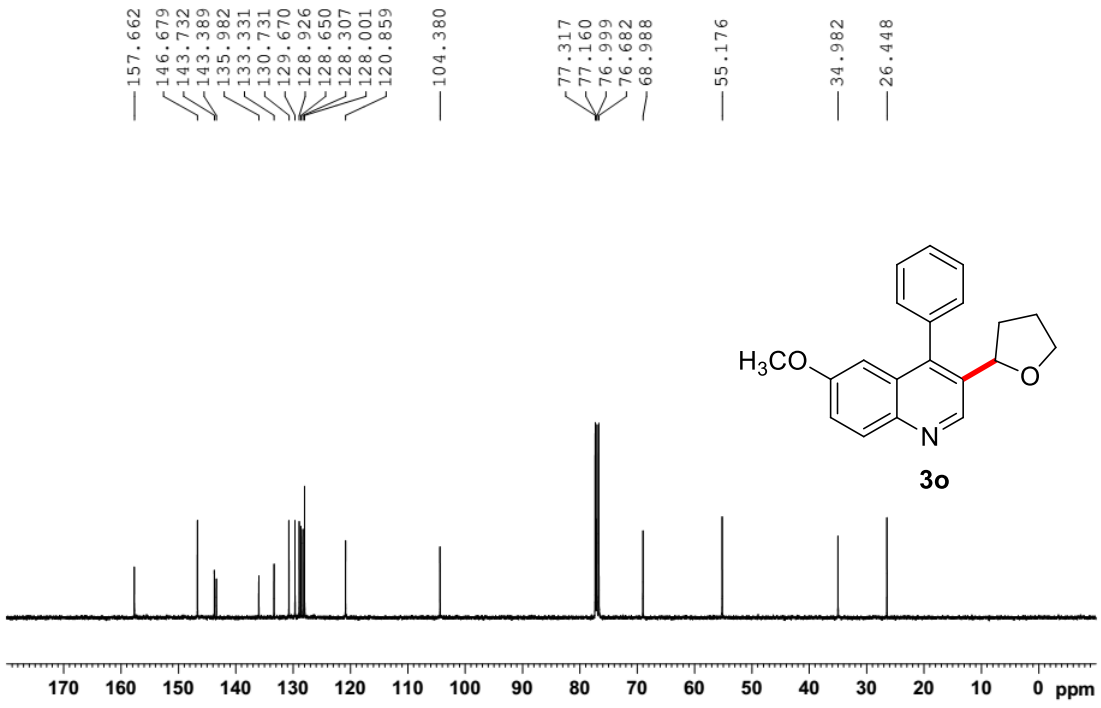
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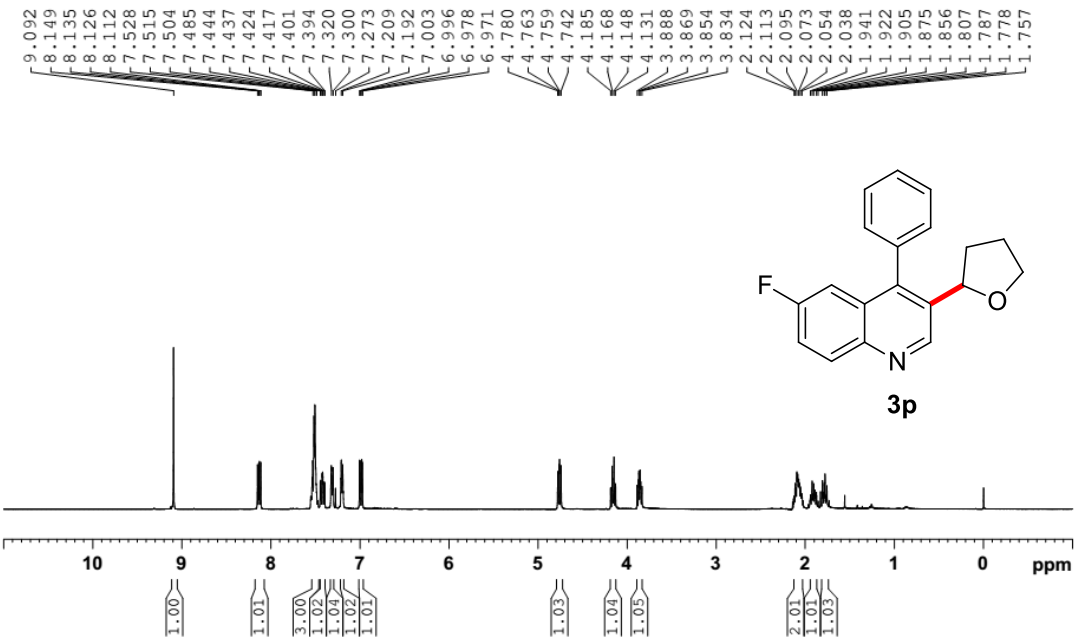
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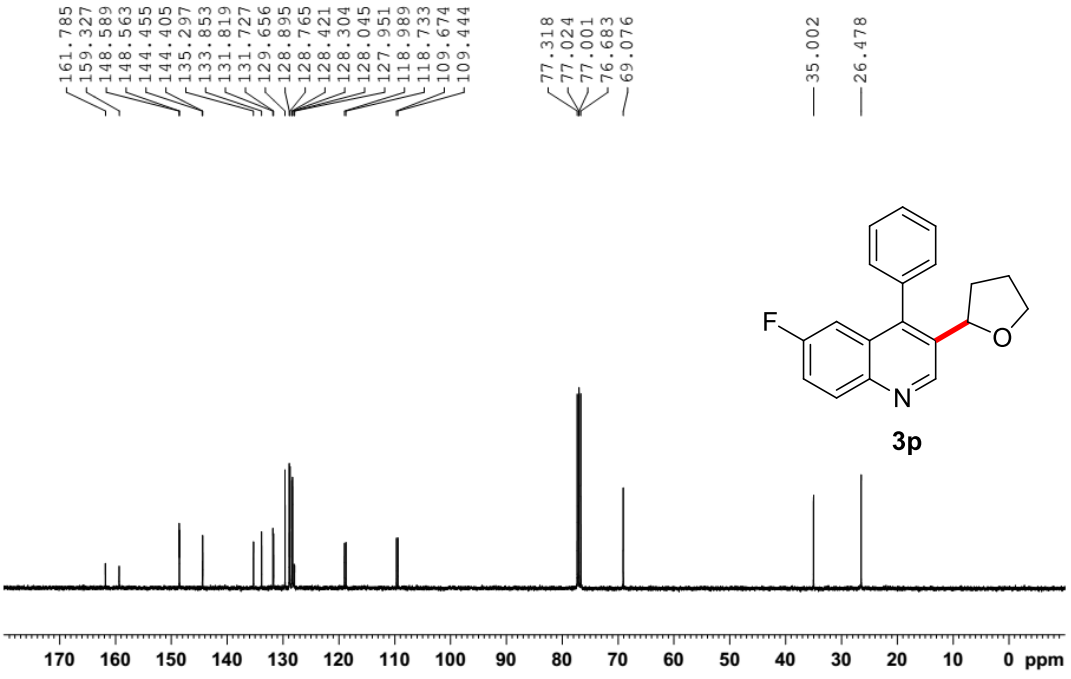
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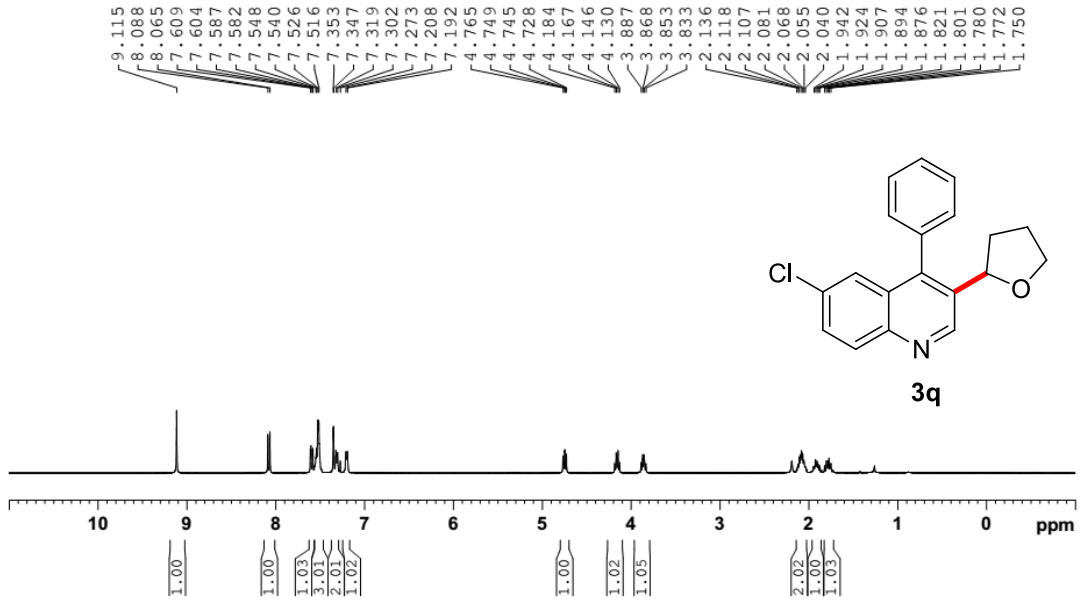
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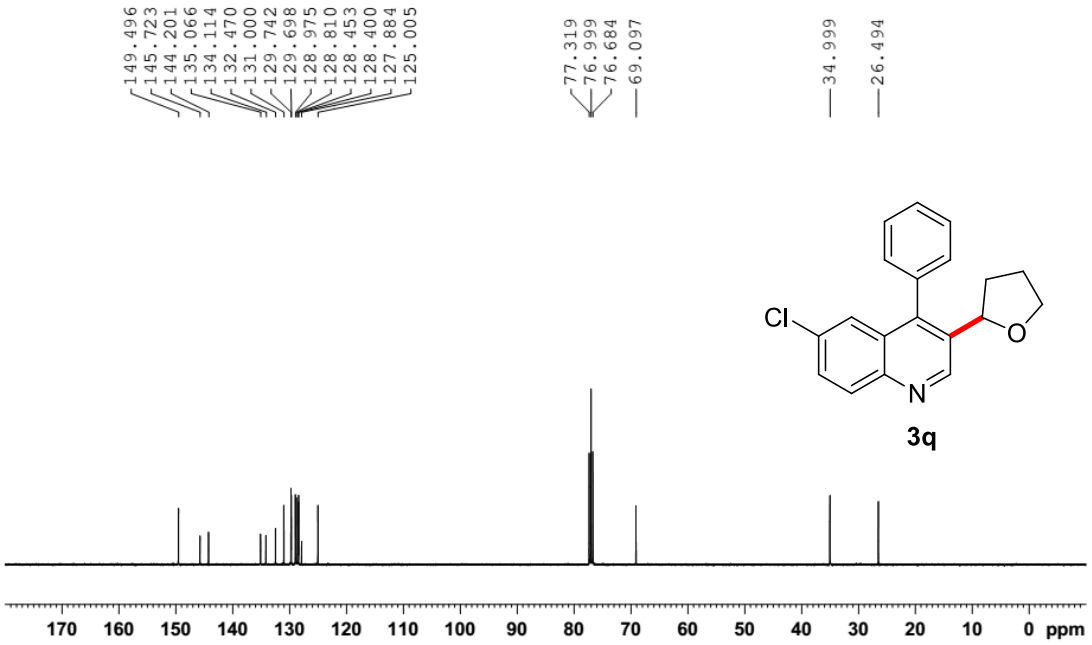
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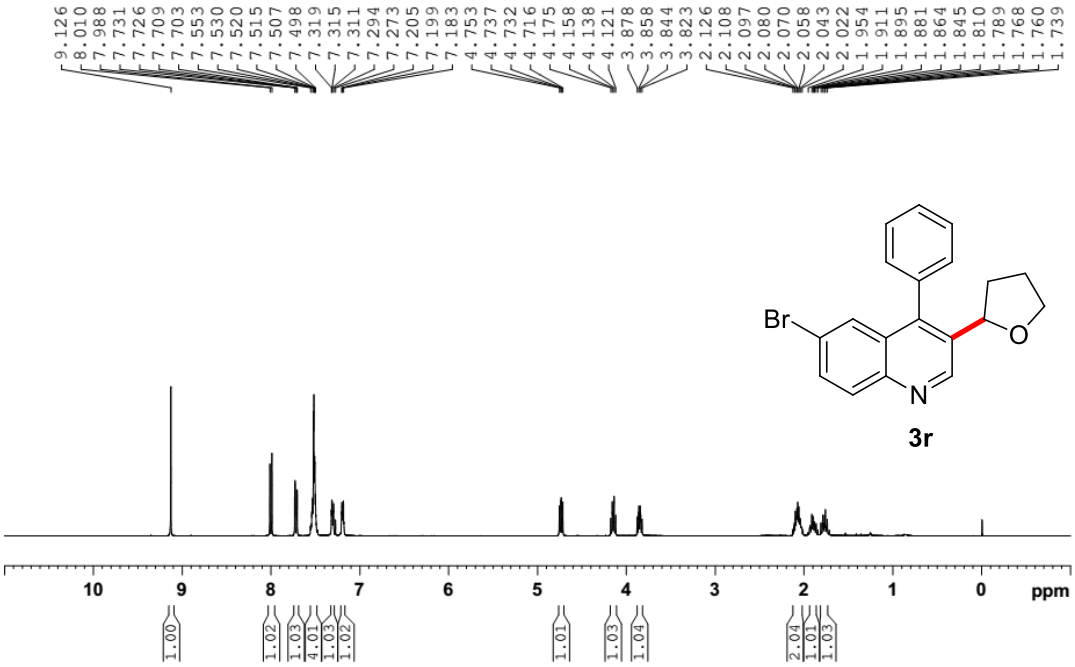
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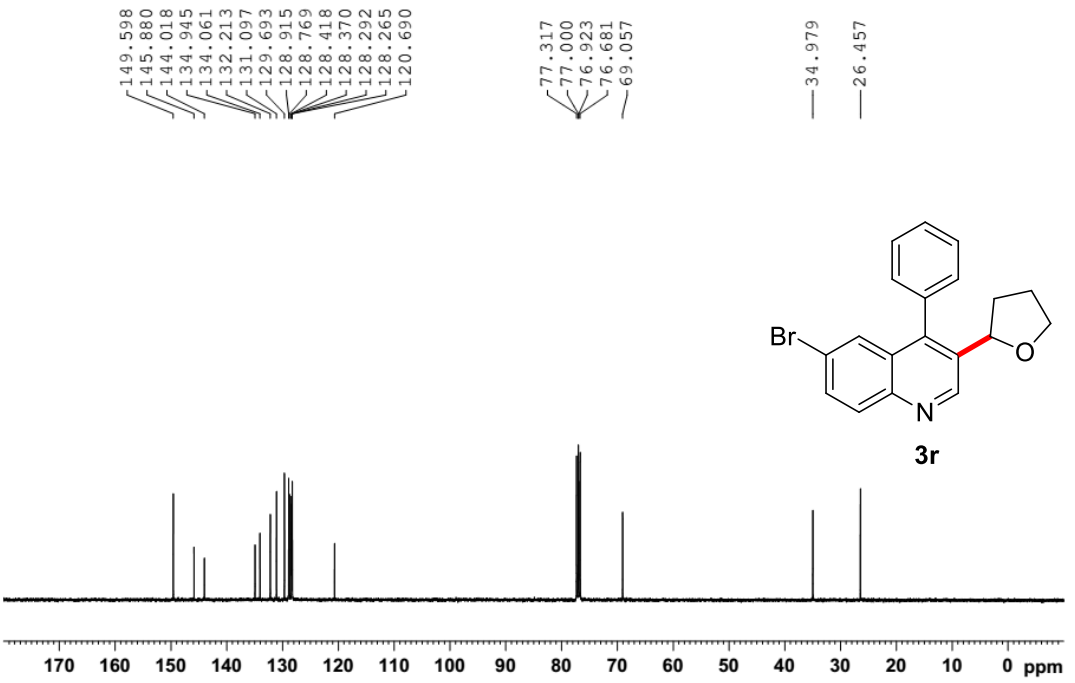
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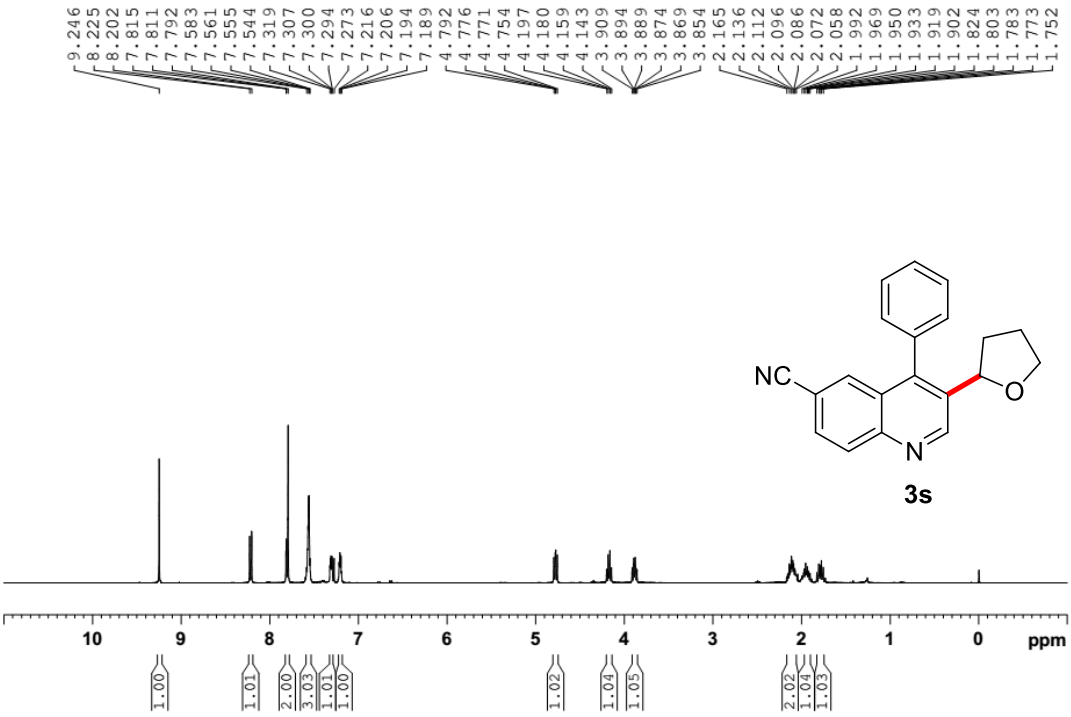
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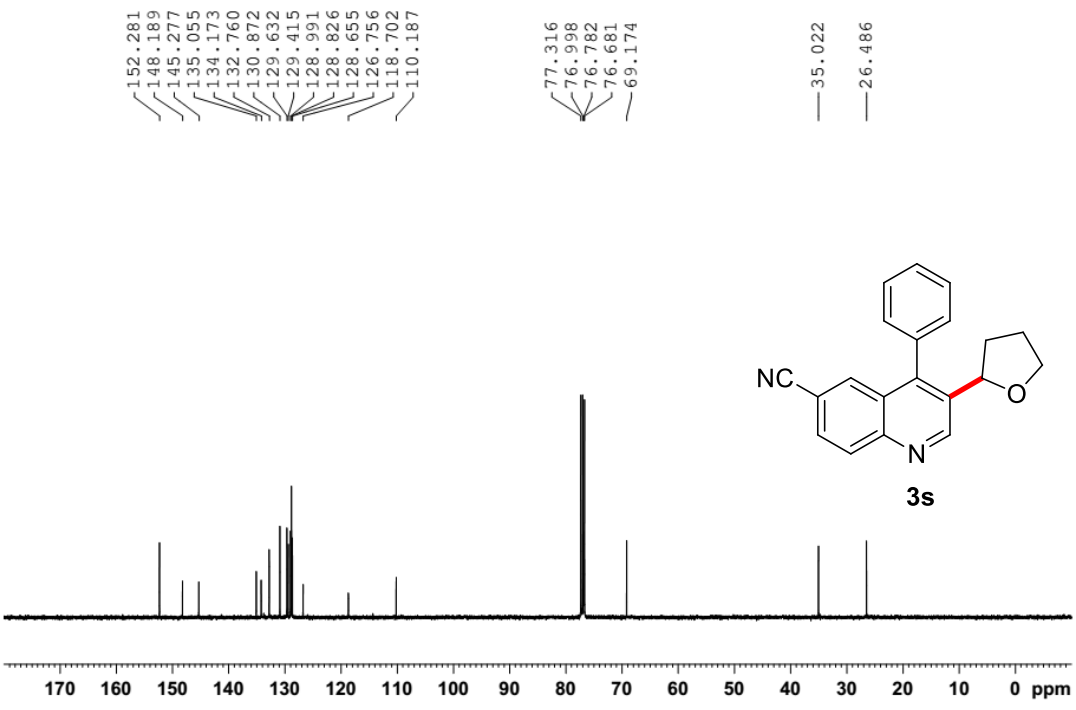
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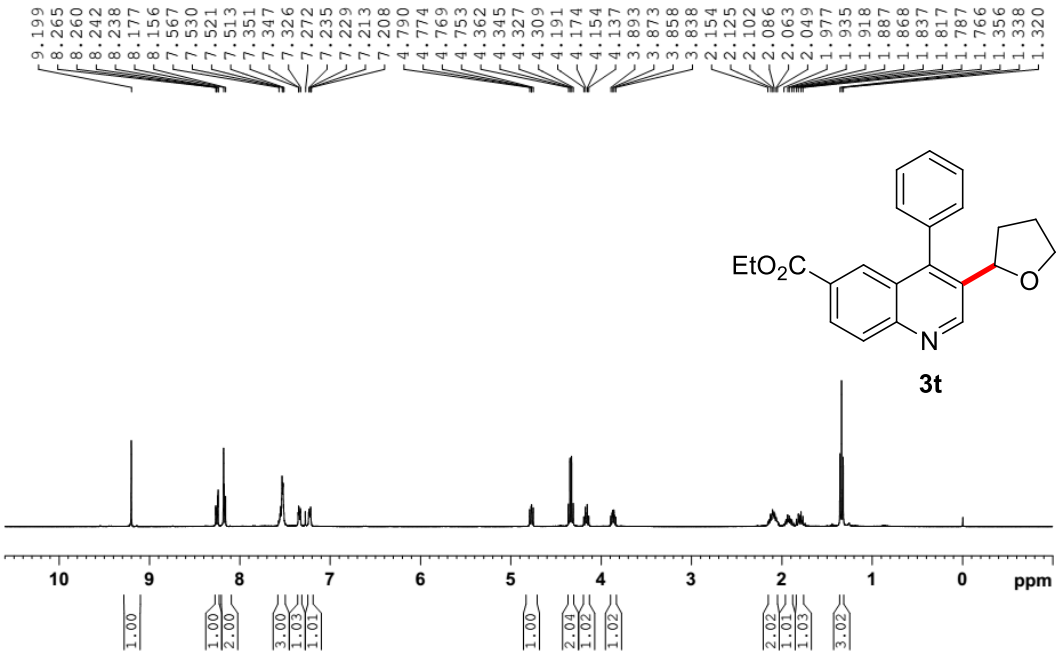
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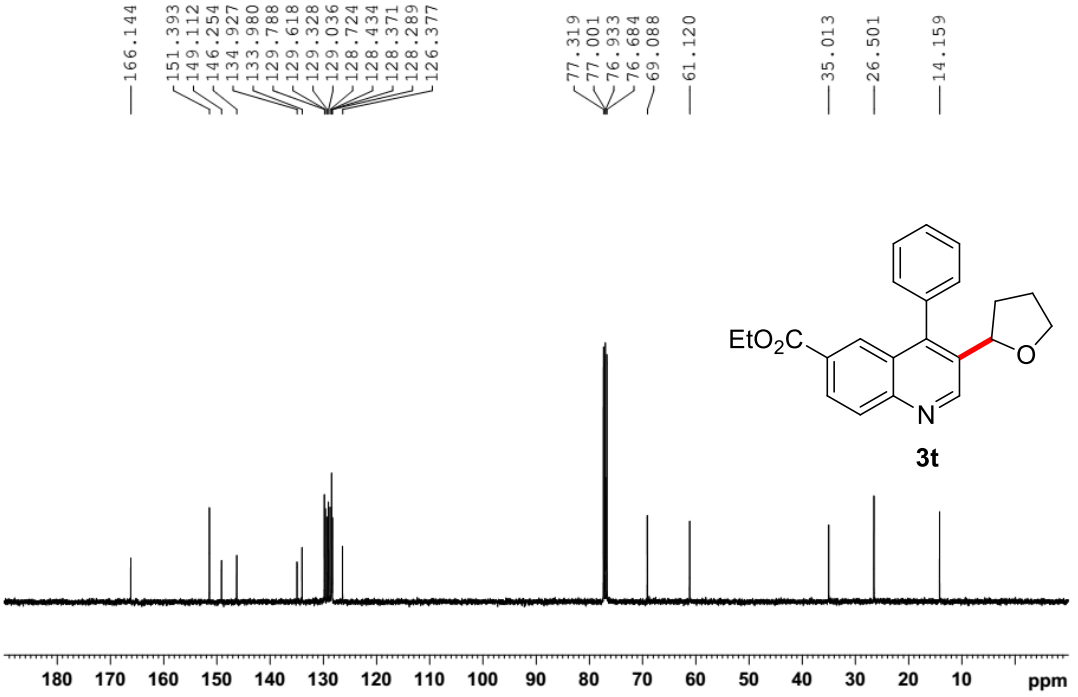
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69.088
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35.013
26.501
14.159
EtO2C
O
N
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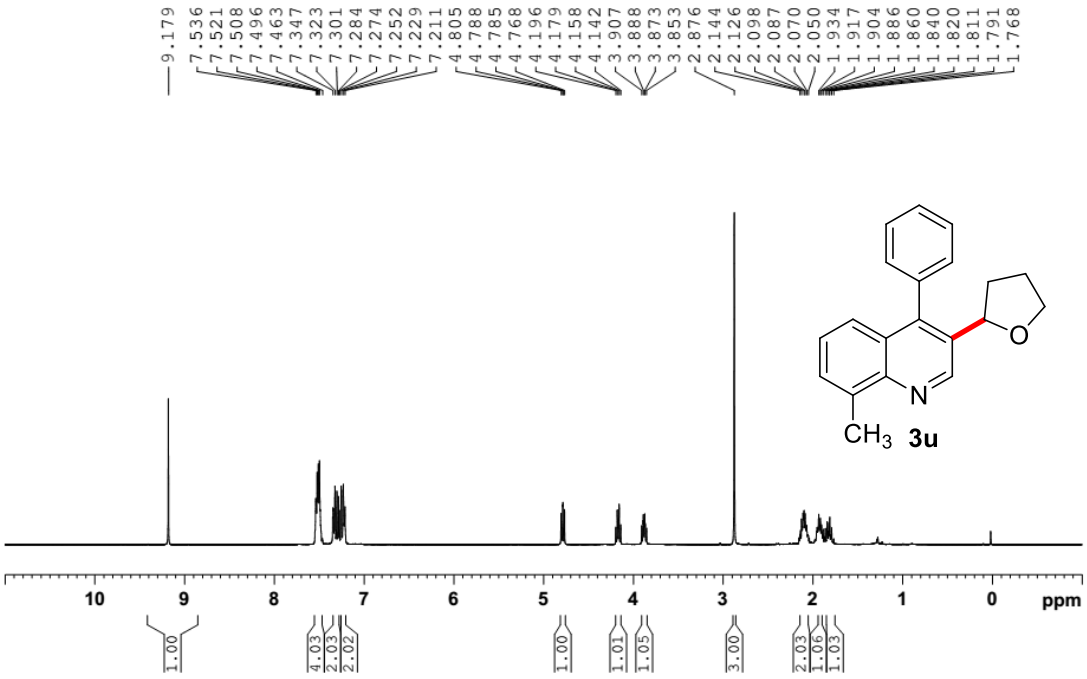
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7.211
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4.788
4.785
4.768
4.196
4.179
4.158
4.142
3.907
3.888
3.873
3.853
2.876
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2.098
2.087
2.070
2.050
1.934
1.917
1.904
1.886
1.860
1.840
1.820
1.811
1.791
1.768
O
N
CH3
3u
10
9
8
7
6
5
4
3
2
1
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2.03
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1.05
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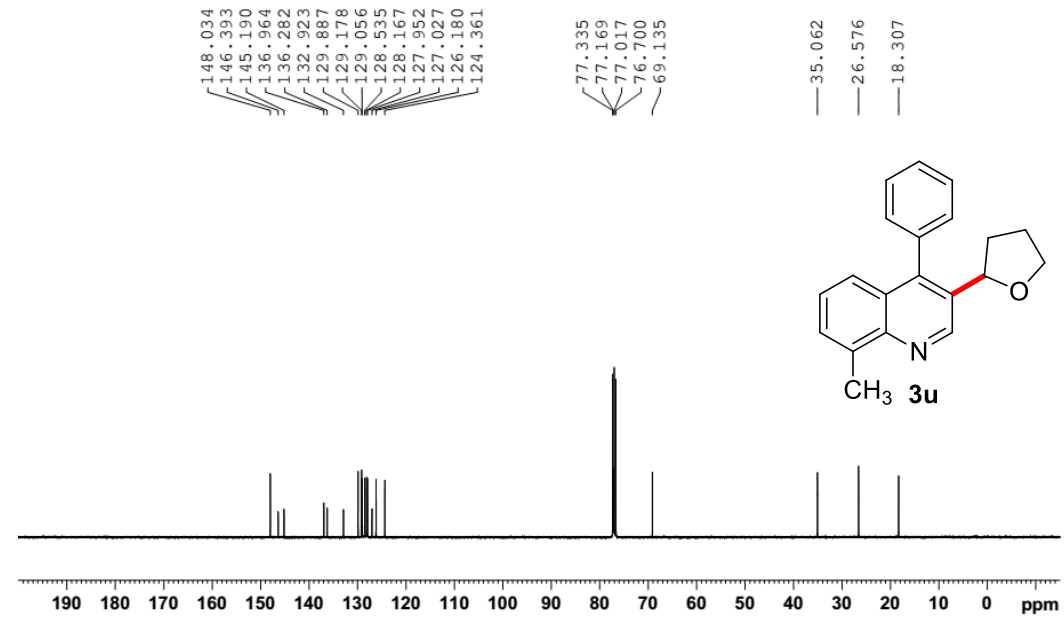
1.03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129.178
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127.952
127.027
126.180
124.361
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77.169
77.017
76.700
69.135
35.062
26.576
18.307
O
N
CH3
3u
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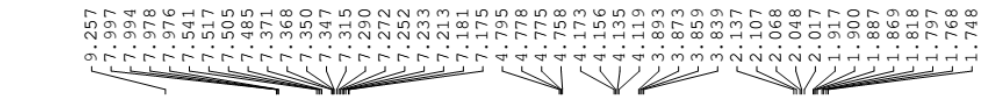
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7.347
7.315
7.290
7.272
7.252
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7.213
7.181
7.175
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4.775
4.758
4.173
4.156
4.135
4.119
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3.873
3.859
3.839
2.137
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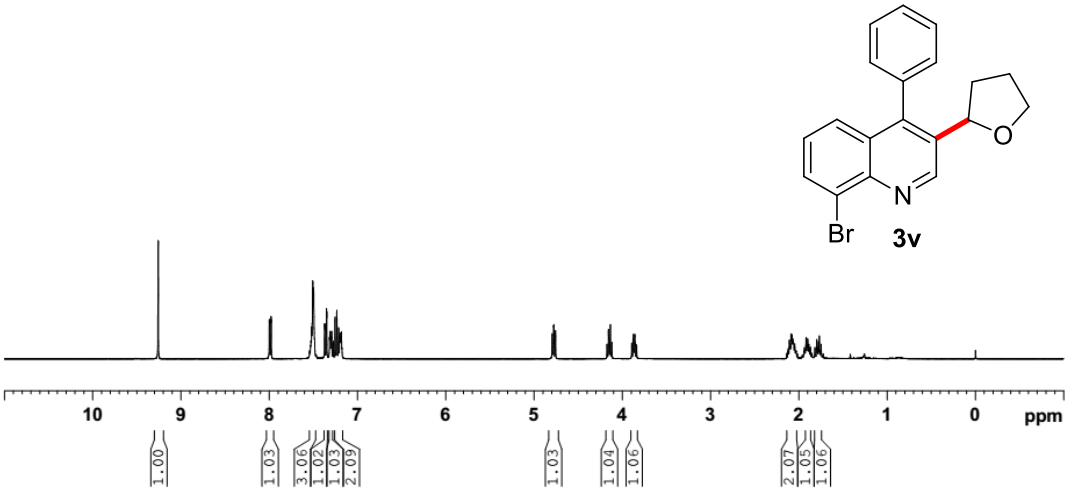
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Br
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1.04
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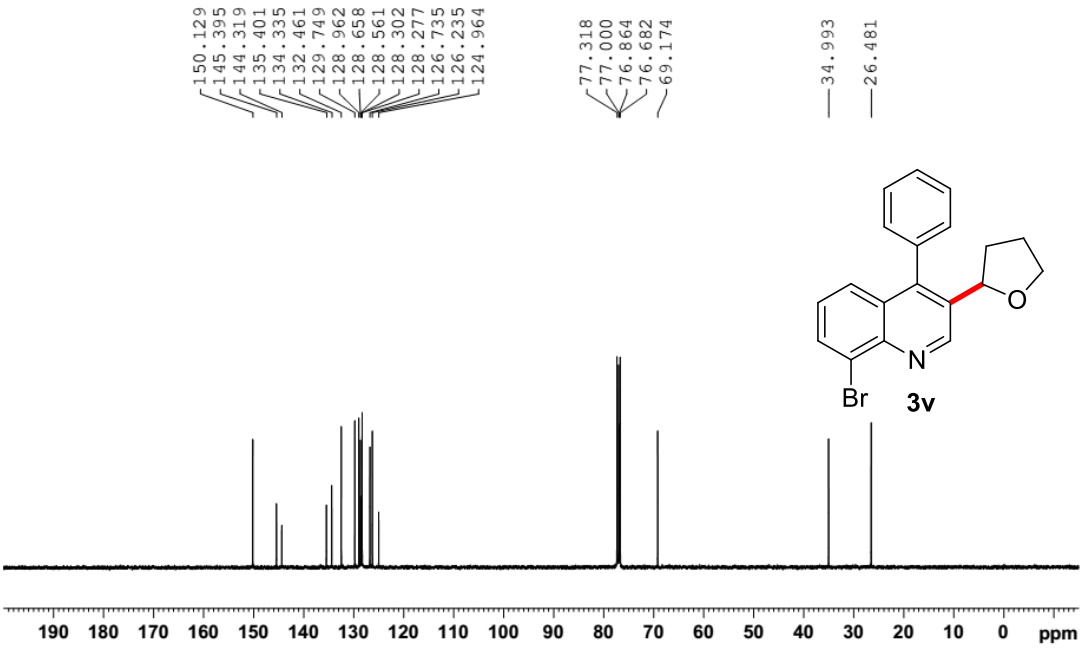
1.05
1.06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128.277
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126.235
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77.318
77.000
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76.682
69.174
34.993
26.481
N
O
Br
3v
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140
130
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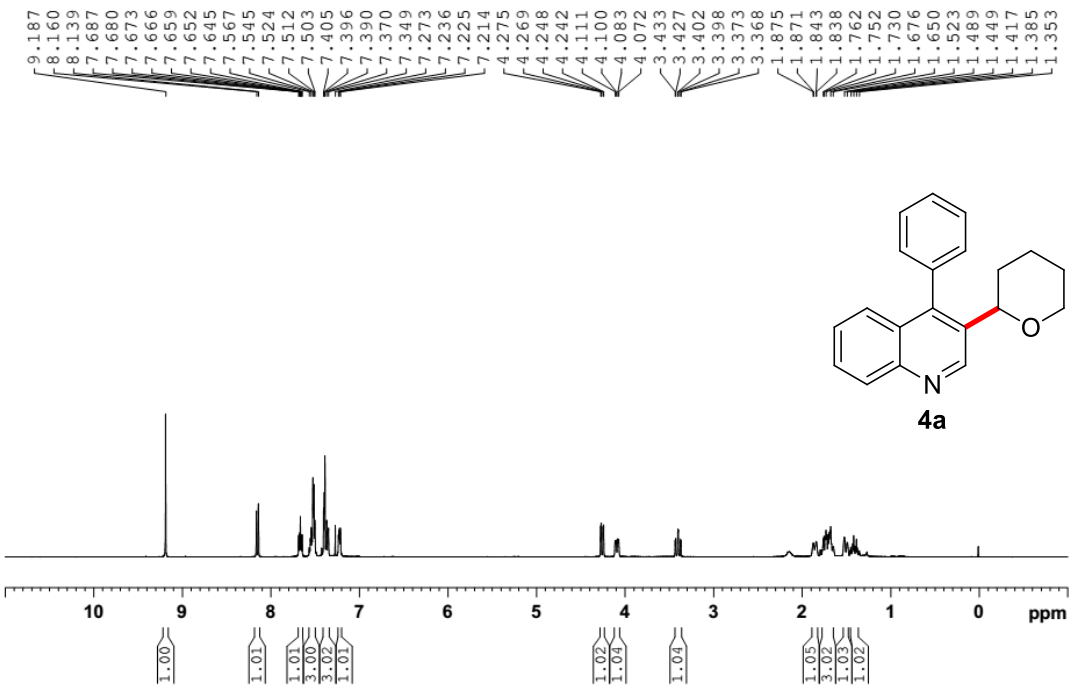
ppm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7.659
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7.567
7.545
7.524
7.512
7.503
7.405
7.396
7.390
7.370
7.349
7.273
7.236
7.225
7.214
4.275
4.269
4.248
4.242
4.111
4.100
4.083
4.072
3.433
3.427
3.402
3.398
3.373
3.368
1.875
1.871
1.843
1.838
1.762
1.752
1.730
1.676
1.650
1.523
1.489
1.449
1.417
1.385
1.353
O
N
4a
10
9
8
7
6
5
4
3
2
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ppm
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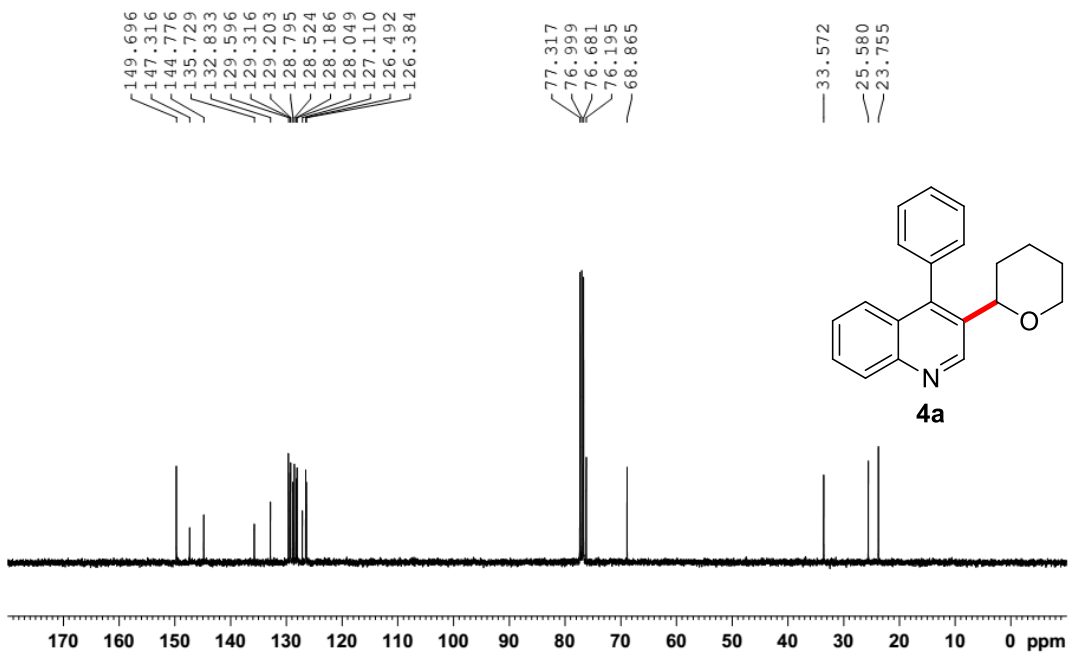
1.04
1.05
3.02
1.03
1.02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126.492
126.384
77.317
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76.681
76.195
68.865
33.572
25.580
23.755
O
N
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130
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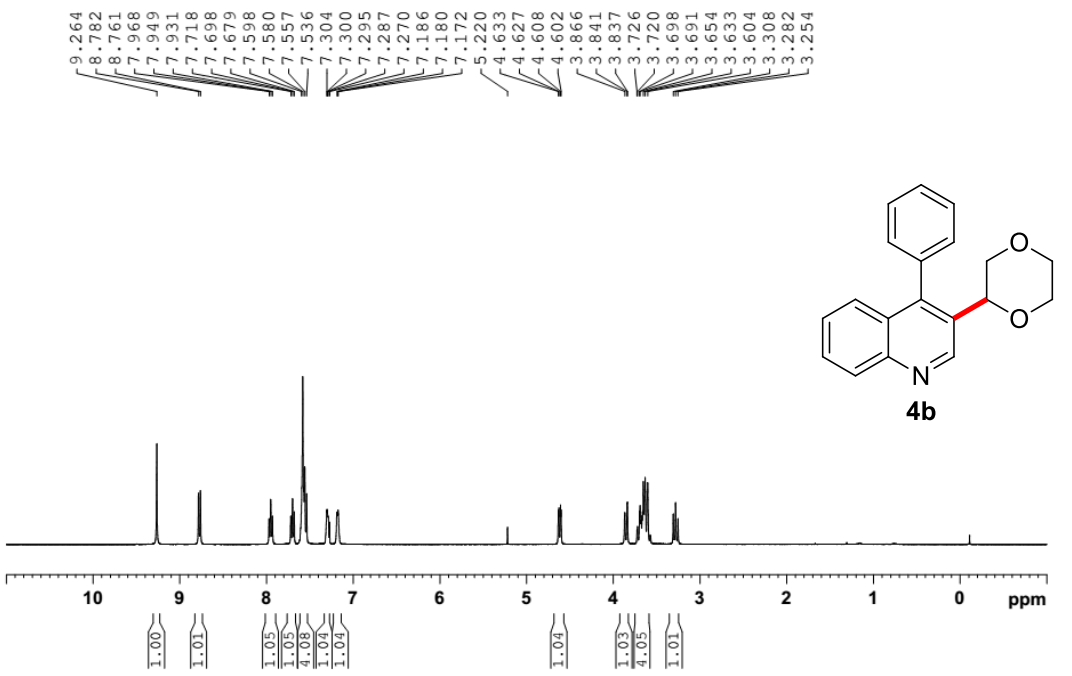
10
0
ppm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7.598
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7.557
7.536
7.304
7.300
7.295
7.287
7.270
7.186
7.180
7.172
5.220
4.633
4.627
4.608
4.602
3.866
3.841
3.837
3.726
3.720
3.698
3.691
3.654
3.633
3.604
3.308
3.282
3.254
O
O
N
4b
10
9
8
7
6
5
4
3
2
1
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1.05
1.05
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1.04
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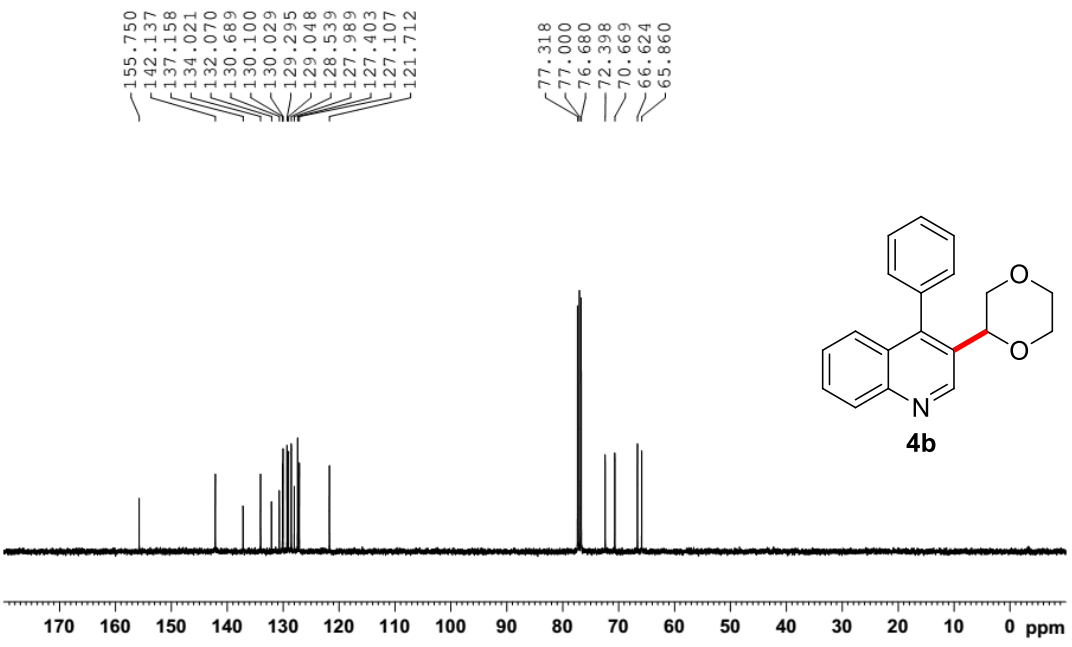
1.03
4.05
1.01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127.107
121.712
77.318
77.000
76.680
72.398
70.669
66.624
65.860
O
O
N
4b
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150
140
130
120
110
100
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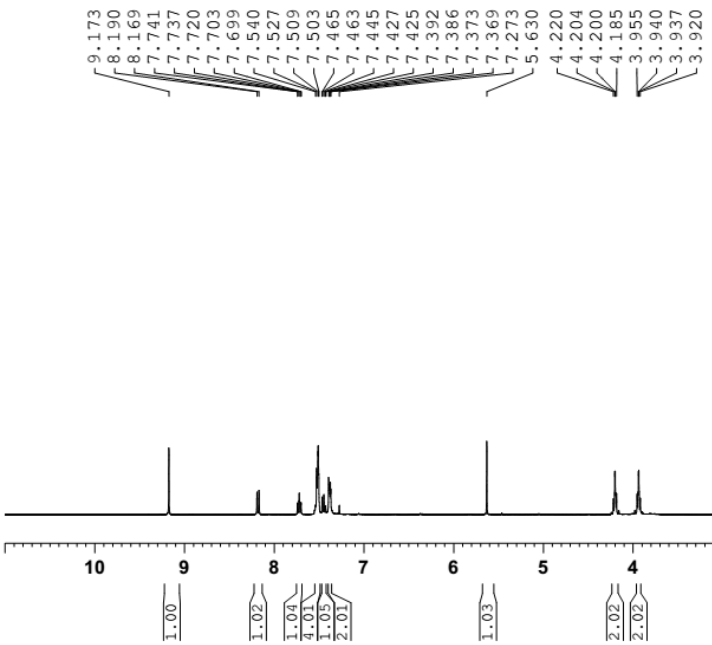
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7.503
7.465
7.463
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7.427
7.425
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7.386
7.373
7.369
7.273
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4.204
4.200
4.185
3.955
3.940
3.937
3.920
O
O
N
4c
10
9
8
7
6
5
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1.05
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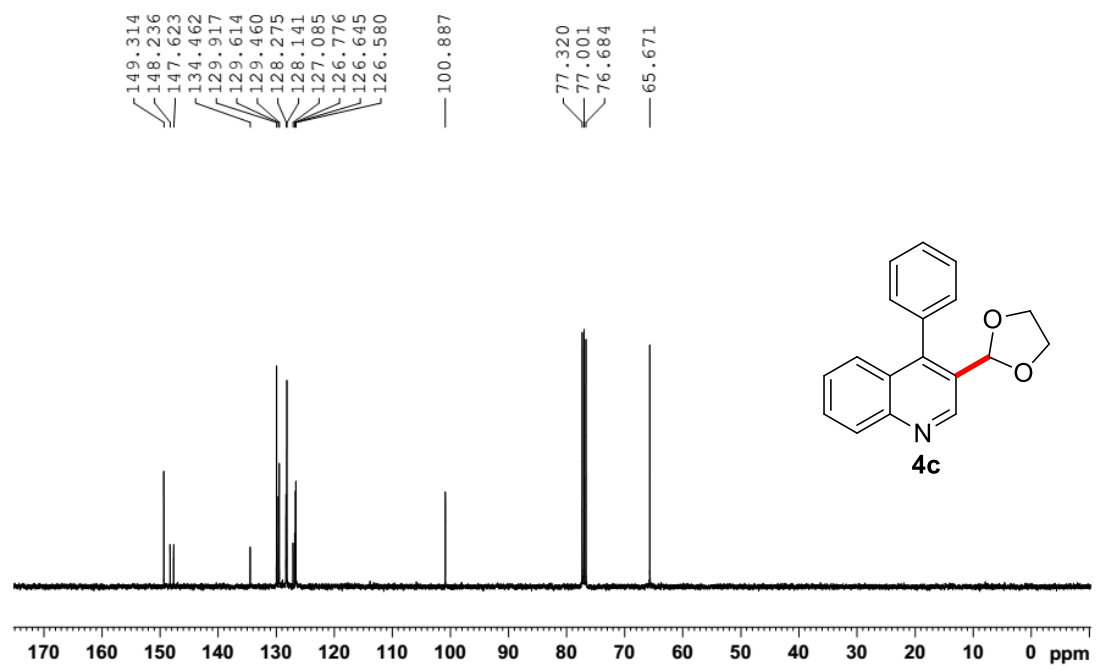
2.02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100.887
77.320
77.001
76.684
65.671
O
O
N
4c
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140
130
120
110
100
90
80
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60
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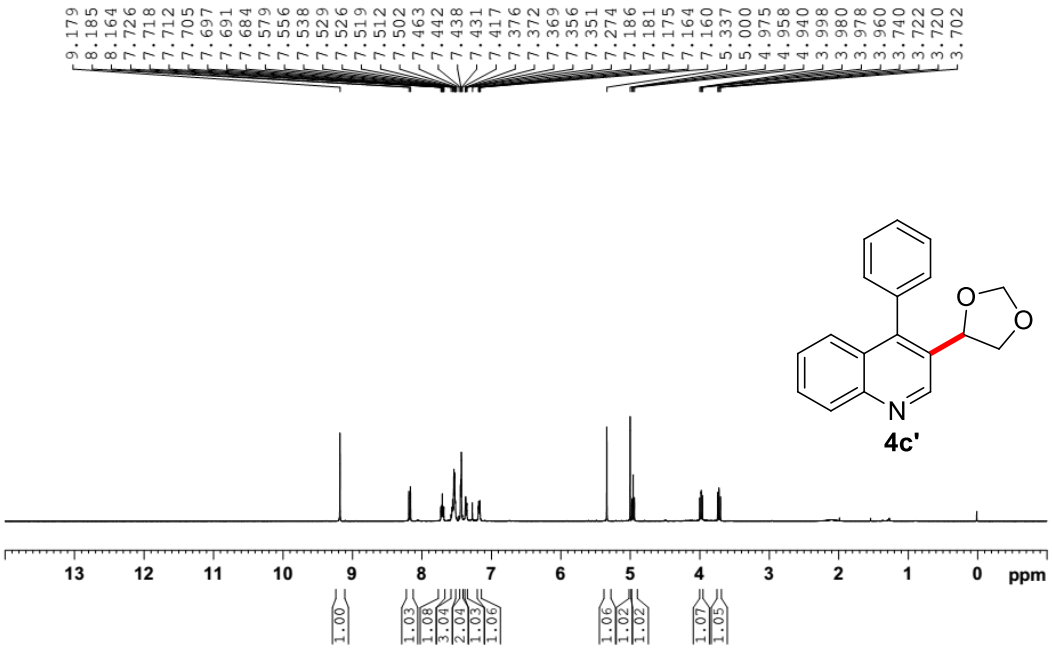
30
20
10
0
ppm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7.684
7.579
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7.538
7.529
7.526
7.519
7.512
7.502
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7.438
7.431
7.417
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7.372
7.369
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7.351
7.274
7.186
7.181
7.175
7.164
7.160
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4.958
4.940
3.998
3.980
3.978
3.960
3.740
3.722
3.720
3.702
O
O
N
4c'
13
12
11
10
9
8
7
6
5
4
3
2
1
0
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1.08
3.04
2.04
1.03
1.06
1.06
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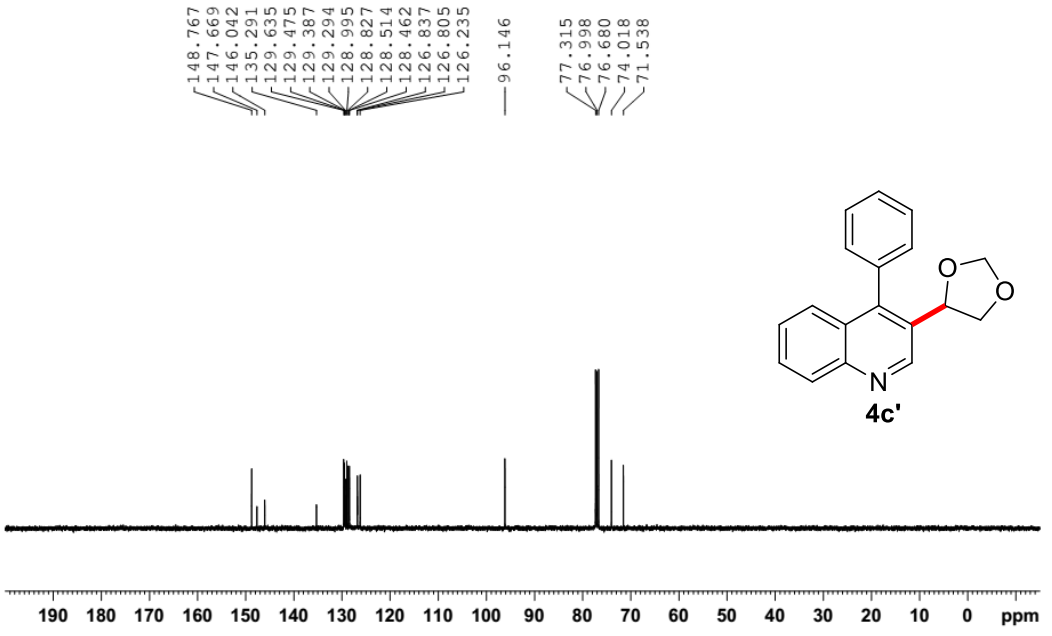
1.07
1.05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126.805
126.235
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76.998
76.680
74.018
71.538
O
O
N
4c'
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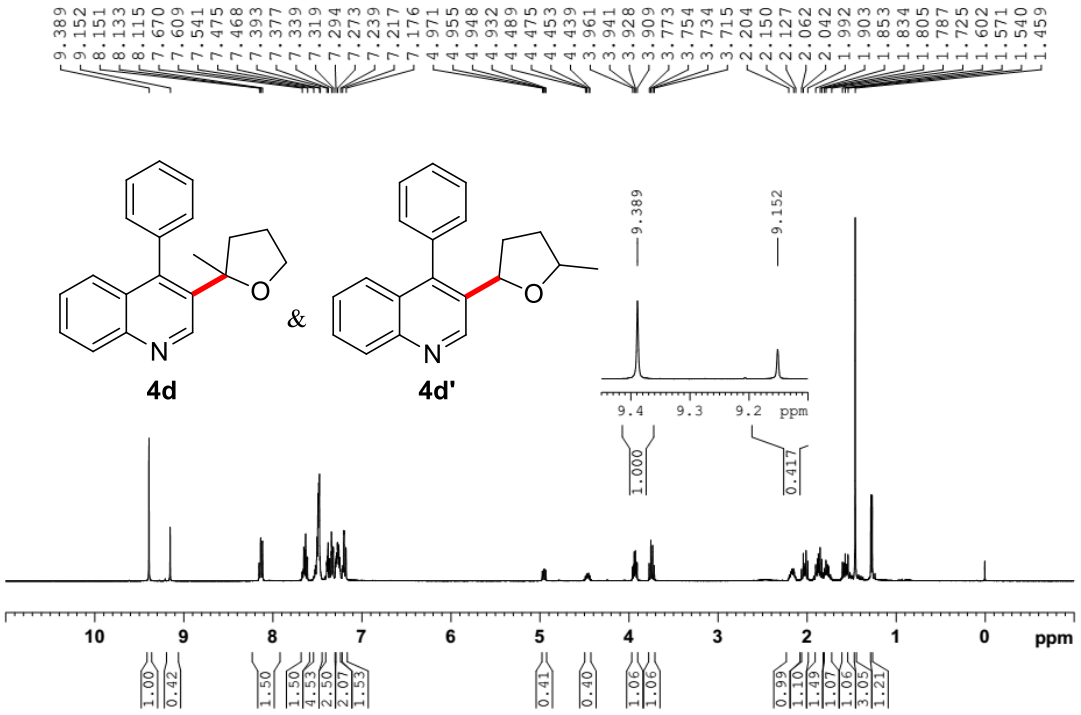
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3.941
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3.773
3.754
3.734
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2.150
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4d
&
4d'
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9.4
9.3
9.2
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10
9
8
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6
5
4
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0
ppm
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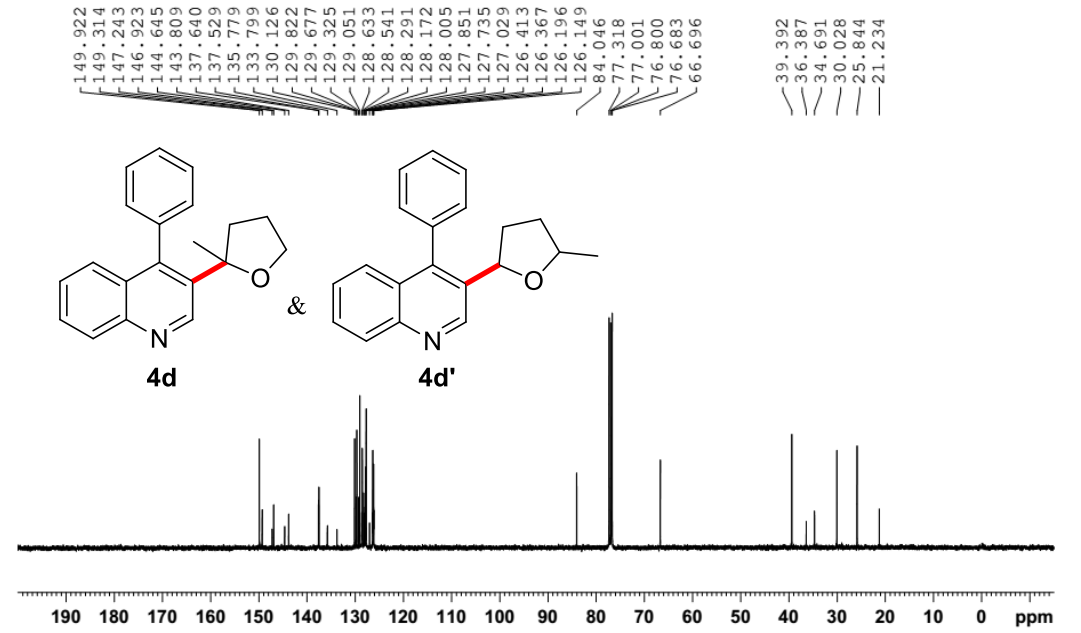
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128.633
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128.172
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77.318
77.001
76.800
76.683
66.696
39.392
36.387
34.691
30.028
25.844
21.234
4d
&
4d'
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm