Supporting Information

Aniline Assisted Dimerization of Phenylalanines: Convenient Synthesis of 2-Aroyl-3-arylquinoline in I_2-DMSO System

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1. General

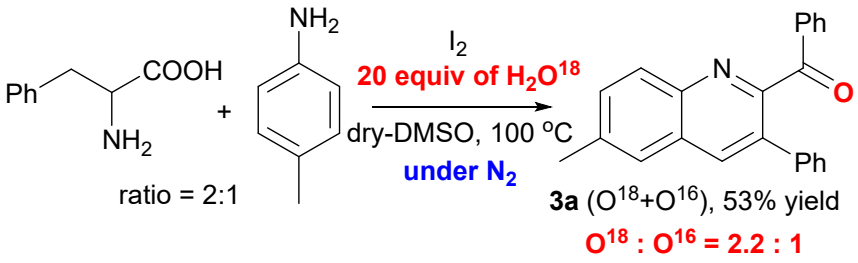
All other substrates and reagents were commercially available and used without further purification. TLC analysis was performed using pre-coated glass plates. Column chromatography was performed using silica gel (200–300 mesh). ^{1}H spectra were recorded in $CDCl_3$/DMSO-d_6 on 400 MHz NMR spectrometers and resonances (δ) are given in parts per million relative to tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz) and integration. ^{13}C spectra were recorded in $CDCl_3$/DMSO-d_6 on 100 MHz NMR spectrometers and resonances (δ) are given in ppm. HRMS were obtained on a Bruker 7-tesla FT-ICR MS equipped with an electrospray source. The X-ray crystal-structure determinations of **3v** were obtained on a Bruker SMART APEX CCD system. Melting points were determined using XT-4 apparatus and not corrected.

2. General procedure for the synthesis of 3 (3a as an example)

To a flame-dried pressure sealed tube charged with aspartate ester or phenylalanine (**1a**) (165.0 mg, 1.0 mmol), *p*-toluidine (**2a**) (53.5 mg, 0.5 mmol), I_2 (190.5mg, 0.75mmol) and DMSO (3.0 mL, *c* 0.17 M) at 100 ^{o}C (heating block) for 12 h till almost completed conversion of the substrates by TLC analysis. When the reaction is completed, the reaction was quenched by slow addition of saturated sodium thiosulfate, water and ethyl acetate. The mixture was then poured into a separating funnel. After the phases were separated, and the aqueous phase was extracted three times with ethyl acetate. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated by rotary evaporation. The crude product can be separated by preparative TLC or silica gel column chromatography to obtain the dichlorination product **3a** (117.9 mg, 73% yield).

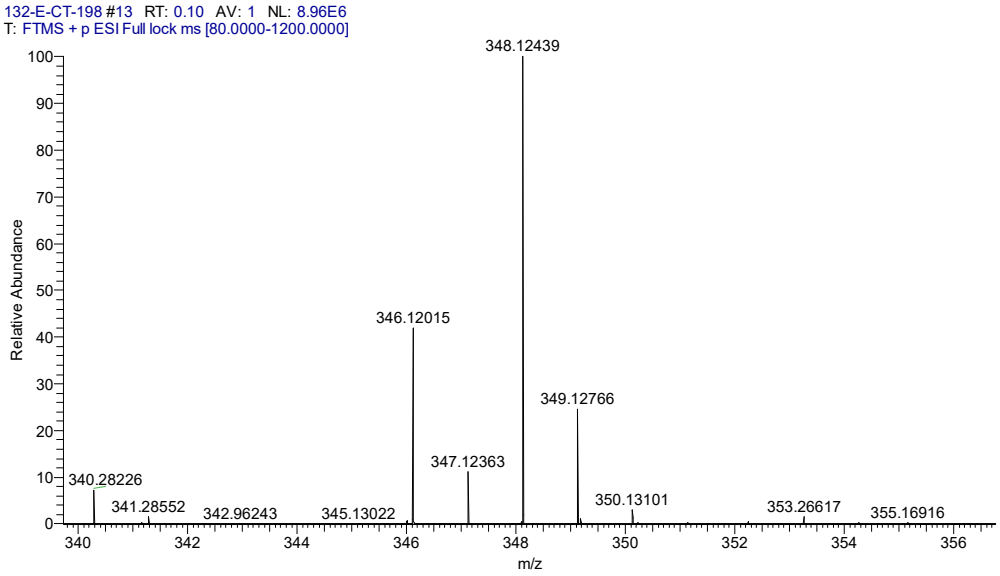
3. Mechanism study

When 20 equiv of H_2O^{18} was added to conduct the reaction under N_2 using a dry-DMSO solvent, both **3a**-O^{18} and **3a**-O^{16} were detected as products. Since it is understandable that O-exchange could happen between 2-aroylpyridines and H_2O, the detection of 3a-O^{16} clearly proved that the oxygen in the product comes from both DMSO and water.

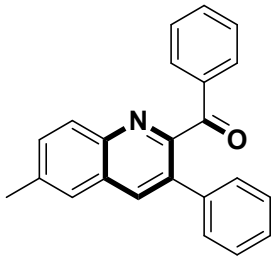


The HRMS Spectra of **3a**-O^{18} is listed below:

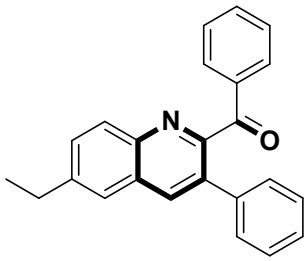
HRMS (ESI) m/z calcd for $C_{23}H_{17}N^{18}ONa^+$ $(M+Na)^+$ 348.12448, found 348.12439.



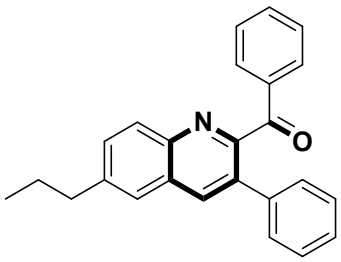
4. Characterization data for compounds 3 and 5ah



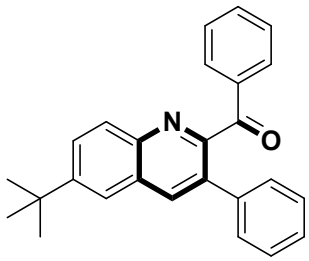
(6-methyl-3-phenylquinolin-2-yl)(phenyl)methanone (3a)[1] Yield 73%; 117.9 mg; yellow solid; mp 96–98 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1676, 1595, 1286, 904, 825, 717, 696 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.17 (s, 1H), 8.07 (d, J = 8.8 Hz, 1H), 7.87 (d, J = 7.6 Hz, 2H), 7.68 (s, 1H), 7.61 (d, J = 8.8 Hz, 1H), 7.53 (t, J = 7.6 Hz, 1H), 7.39 (t, J = 7.6 Hz, 4H), 7.35–7.26 (m, 3H), 2.59 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.2, 155.3, 144.6, 138.1, 137.9, 136.5, 136.2, 134.0, 133.4, 132.5, 130.4, 129.3, 129.0, 128.6, 128.3, 128.1, 127.8, 126.5, 21.7. HRMS (ESI) m/z calcd for $C_{23}H_{18}NO^+$ $(M+H)^+$ 324.1383, found 324.1382.



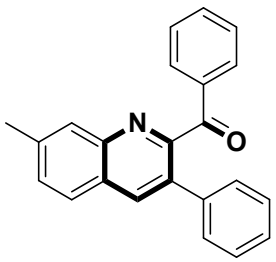
(6-ethyl-3-phenylquinolin-2-yl)(phenyl)methanone (3b) Yield 72%; 120.6 mg; yellow solid; mp 93-95 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr):1670, 1286, 898, 844, 740, 715, 700, 688 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.21 (s, 1H), 8.10 (d, J = 8.8 Hz, 1H), 7.87 (d, J = 7.2 Hz, 2H), 7.70 (s, 1H), 7.65 (d, J = 8.8 Hz, 1H), 7.53 (t, J = 7.6 Hz, 1H), 7.39 (t, J = 7.6 Hz, 4H), 7.35–7.27 (m, 3H), 2.89 (q, J = 7.6 Hz, 2H), 1.38 (t, J = 7.6 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.2, 155.4, 144.8, 144.3, 137.9, 136.7, 136.2, 134.0, 133.4, 131.5, 130.5, 129.4, 129.0, 128.6, 128.4, 128.2, 127.8, 125.2, 29.0, 15.3. HRMS (ESI) m/z calcd for $C_{24}H_{20}NO_2^+$ $(M+H)^+$ 338.1539, found 338.1538.



phenyl(3-phenyl-6-propylquinolin-2-yl)methanone (3c) Yield 65%; 114.1mg; yellow solid; mp 99-101 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1670, 1452, 1284, 1157, 908, 696 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.20 (s, 1H), 8.10 (d, J = 8.8 Hz, 1H), 7.87 (d, J = 7.6 Hz, 2H), 7.68 (s, 1H), 7.63 (d, J = 8.8 Hz, 1H), 7.53 (t, J = 7.6 Hz, 1H), 7.39 (t, J = 7.6 Hz, 4H), 7.35–7.27 (m, 3H), 2.83 (t, J = 7.6 Hz, 2H), 1.78 (dd, J = 15.2, 7.6 Hz, 2H), 1.01 (t, J = 7.2 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.1, 155.3, 144.7, 142.8, 137.9, 136.8, 136.2, 134.0, 133.4, 131.9, 130.5, 129.3, 129.0, 128.6, 128.3, 128.1, 127.8, 126.0, 38.0, 24.3, 13.8. HRMS (ESI) m/z calcd for $C_{25}H_{22}NO^+$ $(M+H)^+$ 352.1696, found 352.1692.

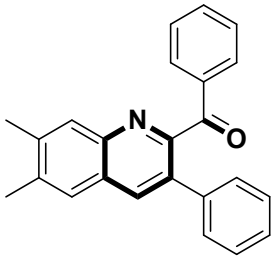


(6-(tert-butyl)-3-phenylquinolin-2-yl)(phenyl)methanone (3d) Yield 61%; 111.9 mg; yellow oil; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr):1676, 1452, 1284, 1157, 908, 696 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.24 (s, 1H), 8.12 (d, J = 8.8 Hz, 1H), 7.90–7.83 (m, 4H), 7.52 (d, J = 7.6 Hz, 1H), 7.41–7.36 (m, 4H), 7.34–7.27 (m, 3H), 1.46 (s, 9H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.2, 155.6, 151.1, 144.6, 137.9, 137.2, 136.3, 134.0, 133.4, 130.5, 129.2, 129.1, 129.0, 128.5, 128.3, 127.9, 127.8, 122.6, 35.1, 31.1. HRMS (ESI) m/z calcd for $C_{26}H_{24}NO^+$ $(M+H)^+$ 366.1852, found 366.1851.

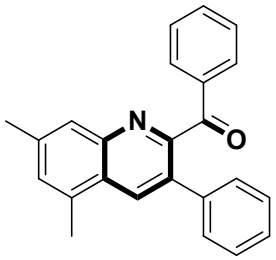


(7-methyl-3-phenylquinolin-2-yl)(phenyl)methanone (3e)[2] Yield 70%; 113.0 mg; yellow solid; mp 89-91 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1676, 1276, 1149, 897, 698 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.23 (s, 1H), 7.97 (s, 1H), 7.88 (d, J = 7.6 Hz, 2H), 7.83 (d, J = 8.4 Hz, 1H), 7.56–7.48 (m, 2H), 7.43–7.36 (m,

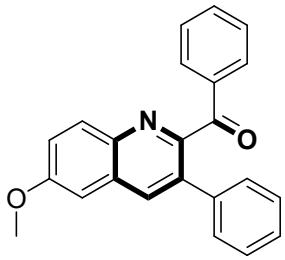
4H), 7.35–7.27 (m, 3H), 2.59 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.2, 156.1, 146.2, 140.6, 137.8, 136.9, 136.2, 133.5, 133.2, 130.5, 130.3, 129.0, 128.6, 128.5, 128.4, 127.8, 127.3, 126.2, 22.0. HRMS (ESI) m/z calcd for $C_{23}H_{18}NO^+$ $(M+H)^+$ 324.1383, found 324.1382.



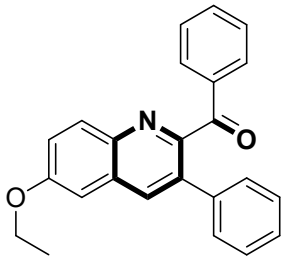
(6,7-dimethyl-3-phenylquinolin-2-yl)(phenyl)methanone (3f)[2] Yield 65%; 110.2 mg; yellow solid; mp 97-99 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1666, 1450, 910, 704 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.14 (s, 1H), 7.94 (s, 1H), 7.87 (d, J = 7.6 Hz, 2H), 7.65 (s, 1H), 7.53 (t, J = 7.6 Hz, 1H), 7.42–7.36 (m, 4H), 7.34–7.26 (m, 3H), 2.49 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.3, 155.2, 145.1, 140.6, 138.2, 138.1, 136.3, 136.1, 133.4, 133.3, 130.5, 128.9, 128.8, 128.5, 128.3, 127.7, 126.8, 126.7, 20.5, 20.2. HRMS (ESI) m/z calcd for $C_{24}H_{20}NO^+$ $(M+H)^+$ 338.1539, found 338.1538.



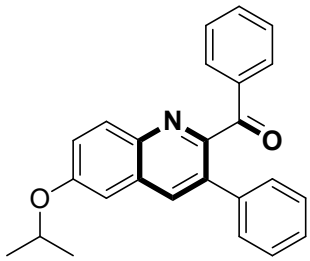
(5,7-dimethyl-3-phenylquinolin-2-yl)(phenyl)methanone (3g) Yield 69%; 117.0 mg; yellow solid; mp 98-100 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1674, 1618, 1458, 1419, 1276, 1213, 1157, 918, 698 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.36 (s, 1H), 7.90–7.81 (m, 3H), 7.53 (t, J = 7.6 Hz, 1H), 7.39 (t, J = 7.6 Hz, 4H), 7.32 (dd, J = 12.8, 5.2 Hz, 4H), 2.72 (s, 3H), 2.54 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.2, 155.5, 146.5, 140.3, 138.2, 136.2, 134.3, 133.8, 133.4, 132.8, 130.8, 130.5, 129.1, 128.6, 128.3, 127.8, 126.6, 125.6, 21.9, 18.6. HRMS (ESI) m/z calcd for $C_{24}H_{20}NO^+$ $(M+H)^+$ 338.1539, found 338.1537.



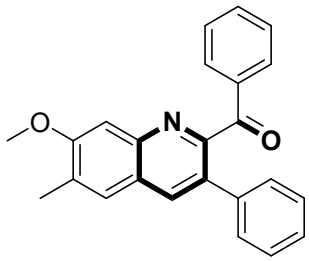
(6-methoxy-3-phenylquinolin-2-yl)(phenyl)methanone (3h)[1] Yield 73%; 123.7 mg; yellow solid; mp 142-144 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:12); IR (KBr): 1676, 1618, 1490, 1276, 1213, 698 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.15 (s, 1H), 8.07 (d, J = 9.2 Hz, 1H), 7.88 (d, J = 7.2 Hz, 2H), 7.53 (t, J = 7.6 Hz, 1H), 7.45–7.35 (m, 5H), 7.35–7.26 (m, 3H), 7.16 (d, J = 2.8 Hz, 1H), 3.97 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.2, 159.0, 153.7, 142.1, 138.0, 136.3, 135.9, 134.5, 133.4, 131.1, 130.5, 129.3, 128.9, 128.5, 128.3, 127.8, 123.1, 104.8, 55.6. HRMS (ESI) m/z calcd for $C_{23}H_{18}NO_2^+$ $(M+H)^+$ 340.1332, found 340.1329.



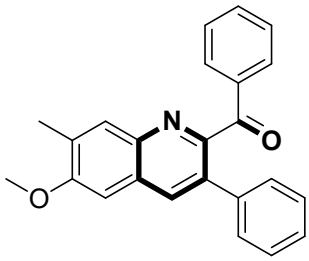
(6-ethoxy-3-phenylquinolin-2-yl)(phenyl)methanone (3i) Yield 72%; 127.1 mg; yellow solid; mp 143-145 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:12); IR (KBr): 1676, 1618, 1597, 1490, 1452, 1309, 1274, 698 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.13 (s, 1H), 8.06 (d, J = 9.2 Hz, 1H), 7.88 (d, J = 7.6 Hz, 2H), 7.52 (d, J = 7.6 Hz, 1H), 7.43–7.37 (m, 5H), 7.34–7.28 (m, 3H), 7.15 (d, J = 2.8 Hz, 1H), 4.20 (q, J = 7.2 Hz, 2H), 1.52 (t, J = 7.2 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.2, 158.3, 153.6, 142.0, 138.1, 136.4, 135.8, 134.5, 133.3, 131.1, 130.5, 129.4, 128.9, 128.5, 128.3, 127.8, 123.4, 105.5, 63.9, 14.7. HRMS (ESI) m/z calcd for $C_{24}H_{20}NO_2^+$ $(M+H)^+$ 354.1489, found 354.1486.



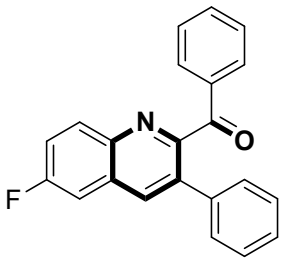
(6-isopropoxy-3-phenylquinolin-2-yl)(phenyl)methanone (3j) Yield 69%; 126.6 mg; yellow solid; mp 146-148 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:12); IR (KBr): 1674, 1618, 1487, 1452, 1288, 1213, 1110, 694 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.12 (s, 1H), 8.06 (d, J = 9.2 Hz, 1H), 7.88 (d, J = 7.2 Hz, 2H), 7.53 (t, J = 7.6 Hz, 1H), 7.39 (dd, J = 9.6, 5.6 Hz, 5H), 7.33–7.27 (m, 3H), 7.16 (d, J = 2.8 Hz, 1H), 4.75 (dt, J = 12.0, 6.0 Hz, 1H), 1.44 (d, J = 6.0 Hz, 6H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.2, 157.2, 153.5, 141.8, 138.1, 136.4, 135.8, 134.4, 133.3, 131.2, 130.5, 129.4, 128.9, 128.5, 128.3, 127.8, 124.0, 107.0, 70.3, 21.9. HRMS (ESI) m/z calcd for $C_{25}H_{22}NO_2^+$ $(M+H)^+$ 368.1645, found 368.1643.



(7-methoxy-6-methyl-3-phenylquinolin-2-yl)(phenyl)methanone (3k) Yield 71%; 125.3 mg; yellow solid; mp 147-159 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:12); IR (KBr): 1674, 1491, 1448, 1238, 1141, 916, 700 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.11 (s, 1H), 7.87 (d, J = 7.6 Hz, 2H), 7.63 (s, 1H), 7.52 (t, J = 7.2 Hz, 1H), 7.44 (s, 1H), 7.42–7.35 (m, 4H), 7.33–7.26 (m, 3H), 3.97 (s, 3H), 2.44 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.5, 160.4, 155.2, 146.8, 138.1, 136.3, 136.0, 133.4, 131.8, 131.4, 130.4, 129.0, 128.5, 128.3, 127.7, 127.6, 123.3, 106.2, 55.7, 17.0. HRMS (ESI) m/z calcd for $C_{24}H_{20}NO_2^+$ $(M+H)^+$ 354.1489, found 354.1487.

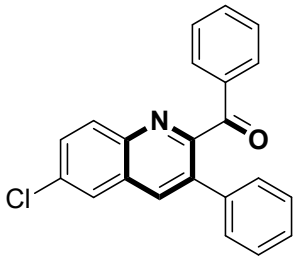


(6-methoxy-7-methyl-3-phenylquinolin-2-yl)(phenyl)methanone (3l) Yield 72%; 127.1 mg; yellow solid; mp 150-152 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:12); IR (KBr): 1672, 1489, 1417, 1228, 1016, 927, 696 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.12 (s, 1H), 7.93–7.86 (m, 3H), 7.52 (d, J = 7.2 Hz, 1H), 7.41–7.36 (m, 4H), 7.33–7.27 (m, 3H), 7.09 (s, 1H), 3.99 (s, 3H), 2.43 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.3, 158.3, 153.3, 141.9, 138.2, 136.5, 135.4, 133.69, 133.65, 133.3, 130.5, 130.3, 129.0, 128.5, 128.3, 128.1, 127.6, 103.3, 55.6, 17.2. HRMS (ESI) m/z calcd for $C_{24}H_{20}NO_2^+$ $(M+H)^+$ 354.1489, found 354.1487.

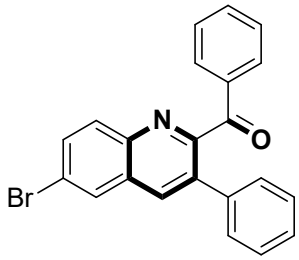


(6-fluoro-3-phenylquinolin-2-yl)(phenyl)methanone (3m) Yield 69%; 112.8 mg; yellow solid; mp 95-97 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1676, 1448, 1284, 1207, 1151, 912, 694 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.22 (s, 1H), 8.19 (dd, *J* = 10.0, 5.5 Hz, 1H), 7.87 (d, *J* = 7.7 Hz, 2H), 7.55 (t, *J* = 7.8 Hz, 3H), 7.40 (dd, *J* = 14.9, 7.0 Hz, 4H), 7.32 (d, *J* = 6.0 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 194.8,

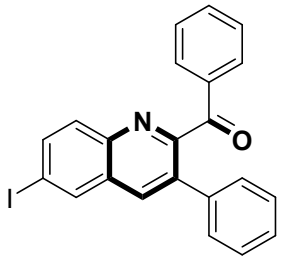
161.4 (d, J = 248.0 Hz, $^{1}J_{CF}$), 155.7, 143.0, 137.3, 136.5 (d, J = 5.0 Hz, $^{3}J_{CF}$), 136.0, 134.9, 133.6, 132.3 (d, J = 9.0 Hz, $^{3}J_{CF}$), 130.4, 128.9, 128.8, 128.7, 128.4, 128.1, 120.5 (d, J = 26.0 Hz, $^{2}J_{CF}$), 110.7 (d, J = 22.0 Hz, $^{2}J_{CF}$). **^{19}F NMR (376 MHz, $CDCl_3$) δ** -110.85. HRMS (ESI) m/z calcd for $C_{22}H_{15}FNO^+$ $(M+H)^+$ 328.1132, found 328.1135.



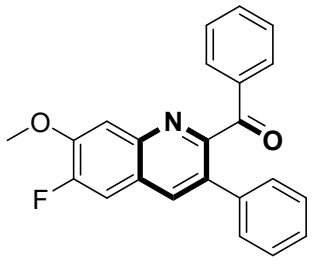
(6-chloro-3-phenylquinolin-2-yl)(phenyl)methanone (3n)[3] Yield 62%; 106.3mg; yellow solid; mp 100-102 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1676, 1448, 1286, 896, 758, 698 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.18 (s, 1H), 8.11 (d, J = 9.2 Hz, 1H), 7.91 (s, 1H), 7.86 (d, J = 8.0 Hz, 2H), 7.71 (d, J = 8.8 Hz, 1H), 7.55 (t, J = 7.2 Hz, 1H), 7.42 (d, J = 7.6 Hz, 2H), 7.38 (d, J = 8.8 Hz, 2H), 7.32 (d, J = 6.0 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ**194.7, 156.5, 144.4, 137.2, 136.1, 135.9, 135.0, 133.8, 133.7, 131.3, 131.1, 130.4, 128.9, 128.7, 128.5, 128.2, 126.3. HRMS (ESI) m/z calcd for $C_{22}H_{15}ClNO^+$ $(M+H)^+$ 344.0837, found 344.0840.



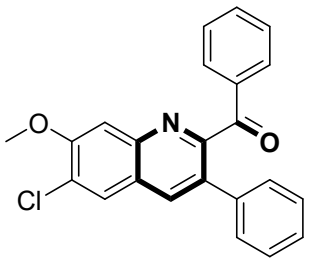
(6-bromo-3-phenylquinolin-2-yl)(phenyl)methanone (3o) Yield 54%; 104.5 mg; yellow solid; mp 123-125 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1680, 1595, 1448, 1286, 1220, 1178, 1153, 694 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.18 (s, 1H), 8.10 (s, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.85 (s, 3H), 7.55 (s, 1H), 7.45–7.29 (m, 7H). **^{13}C NMR (100 MHz, $CDCl_3$) δ**194.7, 156.7, 144.5, 137.2, 136.0, 135.9, 135.0, 133.7, 133.6, 131.3, 130.4, 129.7, 129.2, 128.9, 128.7, 128.5, 128.2, 122.1. HRMS (ESI) m/z calcd for $C_{22}H_{15}BrNO^+$ $(M+H)^+$ 388.0332, found 388.0334.



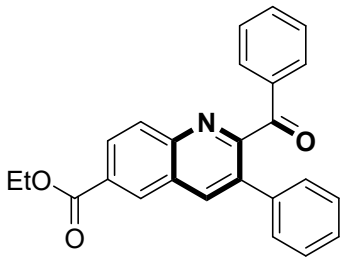
(6-iodo-3-phenylquinolin-2-yl)(phenyl)methanone (3p) Yield 48%; 104.4 mg; yellow solid; mp 129-131 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1678, 1282, 763, 706 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.28 (s, 1H), 8.19 (d, J = 8.4 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.88 (d, J = 7.6 Hz, 2H), 7.78 (t, J = 7.6 Hz, 1H), 7.66 (t, J = 7.6 Hz, 1H), 7.54 (t, J = 7.6 Hz, 1H), 7.40 (t, J = 7.2 Hz, 4H), 7.31 (d, J = 7.2 Hz, 2H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 194.8, 156.8, 144.9, 138.9, 137.2, 136.4, 135.9, 135.8, 134.8, 133.7, 131.2, 130.4, 129.7, 128.9, 128.7, 128.5, 128.2, 93.9. HRMS (ESI) m/z calcd for $C_{22}H_{15}INO^+$ $(M+H)^+$ 436.0193, found 436.0192.



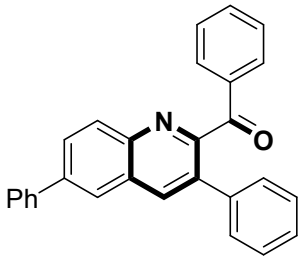
(6-fluoro-7-methoxy-3-phenylquinolin-2-yl)(phenyl)methanone (3q) Yield 68%; 121.4 mg; yellow solid; mp 147-149 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:12); IR (KBr): 1674, 1450, 1236, 1147, 912, 754, 696 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.15 (s, 1H), 7.86 (d, J = 8.0 Hz, 2H), 7.60–7.52 (m, 3H), 7.44–7.35 (m, 4H), 7.34–7.27 (m, 3H), 4.03 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.1, 155.7 (d, J = 2.0 Hz, $^4J_{CF}$), 153.3 (d, J = 253.0 Hz, $^1J_{CF}$), 151.4 (d, J = 13.0 Hz, $^2J_{CF}$), 144.2, 137.5, 136.2 (d, J = 6.0 Hz, $^3J_{CF}$), 133.6, 132.8, 130.4, 129.0, 128.6, 128.4, 127.9, 123.1 (d, J = 9.0 Hz, $^3J_{CF}$), 111.2 (d, J = 19.0 Hz, $^2J_{CF}$), 109.9 (d, J = 3.0 Hz, $^4J_{CF}$), 56.3. **^{19}F NMR (376 MHz, CDCl3) δ** -129.99. HRMS (ESI) m/z calcd for $C_{23}H_{17}FNO_2^+$ $(M+H)^+$ 358.1238, found 358.1235.



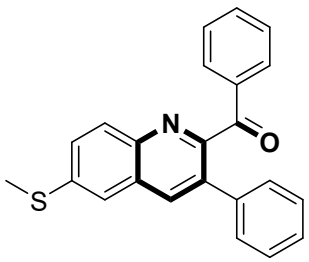
(6-chloro-7-methoxy-3-phenylquinolin-2-yl)(phenyl)methanone (3r) Yield 71%; 132.4 mg; yellow solid; mp 151-153 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:12); IR (KBr): 1678, 1446, 1238, 914, 698 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.13 (s, 1H), 7.94 (s, 1H), 7.86 (d, J = 7.6 Hz, 2H), 7.57–7.52 (m, 2H), 7.43–7.28 (m, 7H), 4.04 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.0, 156.6, 156.5, 146.2, 137.4, 136.0, 135.8, 133.6, 132.8, 130.4, 129.0, 128.6, 128.5, 127.93, 127.86, 126.4, 123.3, 108.7, 56.6. HRMS (ESI) m/z calcd for $C_{23}H_{17}ClNO_2^+$ $(M+H)^+$ 374.0942, found 374.0940.



ethyl 2-benzoyl-3-phenylquinoline-6-carboxylate (3s)[1] Yield 55%; 104.8 mg; yellow solid; mp 96-98 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:12); IR (KBr): 1710, 1678, 1276, 1250, 694 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.70 (s, 1H), 8.40–8.34 (m, 2H), 8.21 (d, J = 8.8 Hz, 1H), 7.87 (d, J = 8.0 Hz, 2H), 7.55 (d, J = 7.6 Hz, 1H), 7.44–7.32 (m, 7H), 4.49 (q, J = 7.2 Hz, 2H), 1.47 (t, J = 7.2 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 194.7, 165.9, 158.3, 147.7, 138.3, 137.1, 135.8, 134.8, 133.7, 130.7, 130.4, 129.9, 129.7, 129.6, 129.0, 128.7, 128.5, 128.2, 127.3, 61.5, 14.3. HRMS (ESI) m/z calcd for $C_{25}H_{20}NO_3^+$ $(M+H)^+$ 382.1438, found 382.1436.

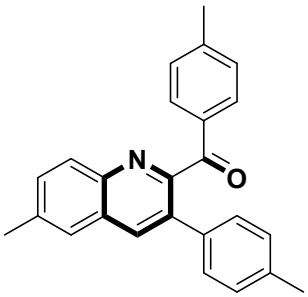


(3,6-diphenylquinolin-2-yl)(phenyl)methanone (3t) Yield 67%; 130.0 mg; yellow solid; mp 131-133 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1674, 1481, 1284, 760, 694 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.31 (s, 1H), 8.24 (d, J = 8.8 Hz, 1H), 8.10 (d, J = 1.6 Hz, 1H), 8.04 (dd, J = 8.8, 2.0 Hz, 1H), 7.89 (d, J = 7.6 Hz, 2H), 7.76 (d, J = 7.2 Hz, 2H), 7.53 (t, J = 8.0 Hz, 3H), 7.44–7.38 (m, 5H), 7.35–7.29 (m, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.1, 156.2, 145.4, 140.8, 140.1, 137.7, 137.3, 136.2, 134.5, 133.5, 130.5, 130.1, 129.9, 129.1, 129.0, 128.6, 128.4, 128.3, 128.0, 127.9, 127.5, 125.3. HRMS (ESI) m/z calcd for $C_{28}H_{20}NO^+$ $(M+H)^+$ 386.1539, found 386.1538.

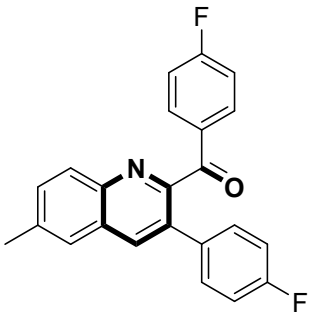


(6-(methylthio)-3-phenylquinolin-2-yl)(phenyl)methanone (3u) Yield 69%; 122.5 mg; yellow solid; mp 119-121 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:12); IR (KBr): 1668, 1446, 1273, 1226, 903, 696 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.15 (s, 1H), 8.05 (d, J = 8.9 Hz, 1H), 7.88 (d, J = 7.4 Hz, 2H), 7.66 – 7.58 (m, 2H), 7.55 (t, J = 7.4

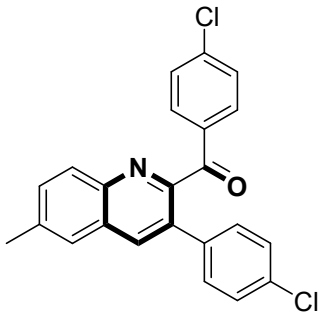
Hz, 1H), 7.44 – 7.36 (m, 4H), 7.35 – 7.28 (m, 3H), 2.64 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.0, 155.1, 144.1, 139.6, 137.7, 136.2, 135.7, 134.8, 133.5, 130.5, 129.7, 129.4, 128.9, 128.6, 128.4, 127.9, 121.5, 15.4. HRMS (ESI) m/z calcd for $C_{23}H_{18}NOS^+$ $(M+H)^+$ 356.1104, found 356.1100.



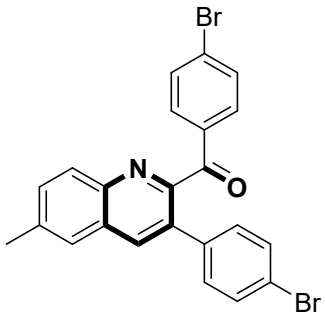
(6-methyl-3-(p-tolyl)quinolin-2-yl)(p-tolyl)methanone (3v) Yield 73%; 128.1 mg; yellow solid; mp 101-103 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr):825, 906, 1290, 1600, 1664 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.15 (s, 1H), 8.06 (d, J = 8.8 Hz, 1H), 7.79 (d, J = 8.0 Hz, 2H), 7.67 (s, 1H), 7.59 (d, J = 8.8 Hz, 1H), 7.28 (d, J = 8.0 Hz, 2H), 7.20 (d, J = 8.0 Hz, 2H), 7.05 (dd, J = 61.6, 7.6 Hz, 2H), 2.59 (s, 3H), 2.39 (s, 3H), 2.32 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.0, 155.7, 144.4, 138.0, 137.7, 136.4, 135.1, 134.0, 133.9, 132.3, 130.7, 129.4, 129.3, 129.2, 128.8, 128.2, 126.5, 21.82, 21.78, 21.2. HRMS (ESI) m/z calcd for $C_{25}H_{22}NO^+$ $(M+H)^+$ 352.1696, found 352.1694.



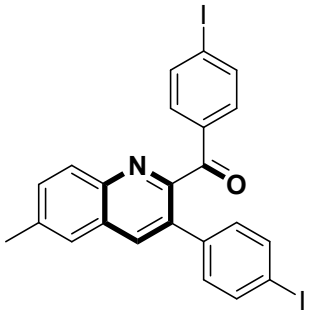
(4-fluorophenyl)(3-(4-fluorophenyl)-6-methylquinolin-2-yl)methanone (3w) Yield 69%; 123.9 mg; yellow solid; mp 101-103 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1666, 1595, 1296, 1224, 1145, 906, 835 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.15 (s, 1H), 8.07 (d, J = 8.8 Hz, 1H), 7.91 (dd, J = 8.4, 5.6 Hz, 2H), 7.69 (s, 1H), 7.63 (d, J = 8.8 Hz, 1H), 7.33 (dd, J = 8.0, 5.6 Hz, 2H), 7.06 (dt, J = 22.4, 8.4 Hz, 4H), 2.60 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 193.5, 166.1 (d, J = 254.0 Hz, $^1J_{CF}$), 162.6 (d, J = 247.0 Hz, $^1J_{CF}$), 154.8, 144.6, 138.5, 136.7, 133.9 (d, J = 3.0 Hz, $^4J_{CF}$), 133.2 (d, J = 9.0 Hz, $^3J_{CF}$), 133.0, 132.8, 132.6 (d, J = 3.0 Hz, $^4J_{CF}$), 130.7 (d, J = 8.0 Hz, $^3J_{CF}$), 129.3, 128.2, 126.5, 115.74 (d, J = 22.0 Hz, $^2J_{CF}$), 115.71 (d, J = 22.0 Hz, $^2J_{CF}$), 21.8. **^{19}F NMR (376 MHz, CDCl3) δ** -103.84, -113.97. HRMS (ESI) m/z calcd for $C_{23}H_{16}F_2NO^+$ $(M+H)^+$ 360.1194, found 360.1193.



(4-chlorophenyl)(3-(4-chlorophenyl)-6-methylquinolin-2-yl)methanone (3x) Yield 62%; 121.2 mg; yellow solid; mp 107-109 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1664, 1583, 1292, 1088, 902, 829 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.14 (s, 1H), 8.05 (d, J = 8.8 Hz, 1H), 7.85 (d, J = 8.4 Hz, 2H), 7.68 (s, 1H), 7.63 (d, J = 8.8 Hz, 1H), 7.40 (d, J = 8.4 Hz, 2H), 7.34-7.27 (m, 4H), 2.60 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 193.6, 154.3, 144.6, 140.2, 138.6, 136.7, 136.3, 134.5, 134.2, 132.95, 132.86, 131.9, 130.2, 129.3, 128.88, 128.86, 128.1, 126.5, 21.8. HRMS (ESI) m/z calcd for $C_{23}H_{16}Cl_2NO^+$ $(M+H)^+$ 392.0603, found 392.0601.

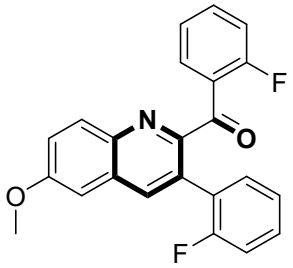


(4-bromophenyl)(3-(4-bromophenyl)-6-methylquinolin-2-yl)methanone (3y) Yield 57%; 136.8 mg; yellow solid; mp 129-131 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1672, 1581, 1286, 904, 831, 744 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.15 (s, 1H), 8.06 (d, J = 8.8 Hz, 1H), 7.77 (d, J = 8.4 Hz, 2H), 7.68 (s, 1H), 7.63 (d, J = 8.8 Hz, 1H), 7.57 (d, J = 8.4 Hz, 2H), 7.47 (d, J = 8.4 Hz, 2H), 7.22 (d, J = 8.4 Hz, 2H), 2.60 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 193.6, 154.1, 144.5, 138.7, 136.8, 134.9, 133.00, 132.96, 132.0, 131.9, 131.8, 130.5, 129.2, 129.1, 128.1, 126.5, 122.5, 21.8. HRMS (ESI) m/z calcd for $C_{23}H_{16}Br_2NO^+$ $(M+H)^+$ 481.9573, found 481.9569.

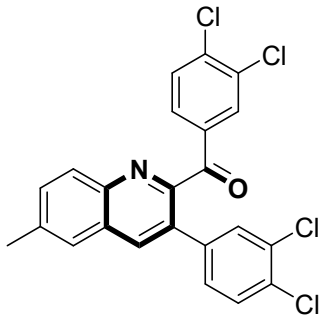


(4-iodophenyl)(3-(4-iodophenyl)-6-methylquinolin-2-yl)methanone (3z) Yield 54%; 155.2 mg; yellow solid; mp 135-137 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15);

IR (KBr):1670, 1576, 1284, 902, 829, 744 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.13 (s, 1H), 8.03 (d, J = 8.8 Hz, 1H), 7.81 (d, J = 8.4 Hz, 2H), 7.65 (dd, J = 19.6, 8.0 Hz, 6H), 7.09 (d, J = 8.0 Hz, 2H), 2.59 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 194.0, 154.1, 144.6, 138.7, 137.84, 137.76, 137.4, 136.6, 135.4, 133.1, 132.9, 131.8, 130.6, 129.3, 128.1, 126.5, 102.2, 94.1, 21.8. HRMS (ESI) m/z calcd for $C_{23}H_{16}I_2NO^+$ $(M+H)^+$ 575.9316, found 575.9311.

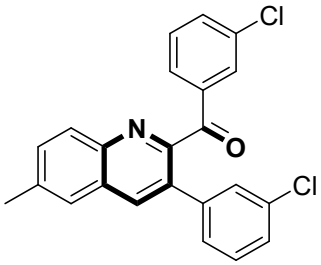


(2-fluorophenyl)(3-(2-fluorophenyl)-6-methoxyquinolin-2-yl)methanone (3aa) Yield 67%; 125.6 mg; yellow solid; mp 118-120 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:12); IR (KBr): 1676, 1614, 1454, 1221, 916, 752 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.13 (s, 1H), 8.00 (d, J = 9.2 Hz, 1H), 7.83 (dd, J = 10.4, 4.4 Hz, 1H), 7.52 (d, J = 7.6 Hz, 1H), 7.48–7.38 (m, 2H), 7.33 (d, J = 7.6 Hz, 1H), 7.22 (td, J = 7.6, 4.4 Hz, 2H), 7.14 (d, J = 2.8 Hz, 1H), 7.06 (dd, J = 18.0, 8.0 Hz, 2H), 3.96 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 192.1, 161.8 (d, J = 255.0 Hz, $^1J_{CF}$), 159.3, 159.2 (d, J = 245.0 Hz, $^1J_{CF}$), 153.0, 142.3, 137.1, 134.4 (d, J = 8.0 Hz, $^3J_{CF}$), 131.9 (d, J = 2.0 Hz, $^4J_{CF}$), 131.5, 131.1 (d, J = 3.0 Hz, $^4J_{CF}$), 129.9 (d, J = 8.0 Hz, $^3J_{CF}$), 129.7, 128.1, 126.2 (d, J = 33.0 Hz, $^2J_{CF}$), 126.1 (d, J = 29.0 Hz, $^2J_{CF}$), 124.5 (d, J = 3.0 Hz, $^4J_{CF}$), 124.0 (d, J = 3.0 Hz, $^4J_{CF}$), 123.3, 116.3 (d, J = 22.0 Hz, $^2J_{CF}$), 115.6 (d, J = 22.0 Hz, $^2J_{CF}$), 104.9, 55.7. **^{19}F NMR (376 MHz, CDCl3) δ** -112.72, -114.99. HRMS (ESI) m/z calcd for $C_{23}H_{16}F_2NO_2^+$ $(M+H)^+$ 376.1144, found 376.1141.

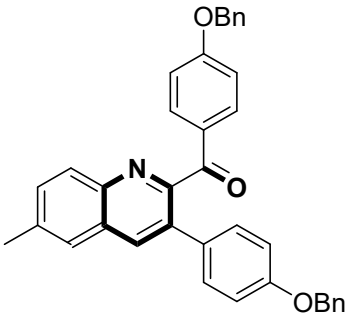


(3,4-dichlorophenyl)(3-(3,4-dichlorophenyl)-6-methylquinolin-2-yl)methanone (3ab) Yield 61%; 140.6 mg; yellow solid; mp 135-137 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1668, 1288, 1151, 1026, 927, 827 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.16 (s, 1H), 8.06 (d, J = 8.8 Hz, 2H), 7.79 (dd, J = 8.4, 2.0 Hz, 1H), 7.70 (s, 1H), 7.67 (d, J = 8.8 Hz, 1H), 7.55 (d, J = 8.4 Hz, 1H), 7.50 (d, J = 2.0 Hz, 1H), 7.42 (d, J = 8.4 Hz, 1H), 7.14 (dd, J = 8.4, 2.0 Hz, 1H), 2.61 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 192.0, 153.1, 144.6, 139.2, 138.4, 137.9, 137.1, 135.7, 133.3, 133.2, 132.9,

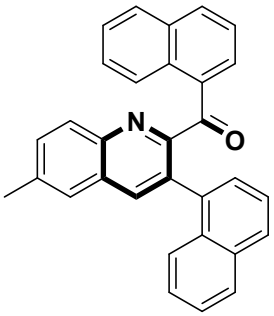
132.5, 132.4, 132.1, 130.70, 130.66, 130.6, 129.6, 129.4, 128.2, 128.1, 126.5, 21.8. HRMS (ESI) m/z calcd for $C_{23}H_{14}Cl_4NO^+$ $(M+H)^+$ 461.9795, found 461.9792.



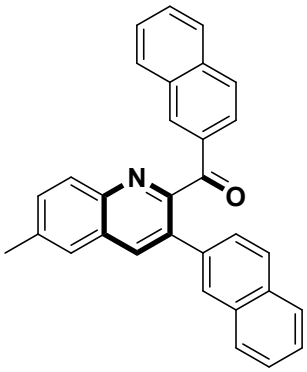
(3-chlorophenyl)(3-(3-chlorophenyl)-6-methylquinolin-2-yl)methanone (3ac) Yield 64%; 125.1 mg; yellow solid; mp 102-104 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1672, 1566, 1209, 1157, 929, 827, 781, 748 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.17 (s, 1H), 8.07 (d, J = 8.8 Hz, 1H), 7.89 (s, 1H), 7.78 (d, J = 7.6 Hz, 1H), 7.69 (s, 1H), 7.65 (d, J = 8.8 Hz, 1H), 7.54 (d, J = 8.0 Hz, 1H), 7.38 (dd, J = 13.2, 4.8 Hz, 2H), 7.30 (d, J = 8.0 Hz, 1H), 7.26 (t, J = 3.6 Hz, 1H), 7.19 (d, J = 7.6 Hz, 1H), 2.60 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 193.3, 153.9, 144.7, 139.7, 138.8, 137.7, 136.9, 134.7, 134.6, 133.5, 133.0, 132.8, 130.3, 129.79, 129.78, 129.4, 128.9, 128.7, 128.1, 128.0, 127.2, 126.5, 21.8. HRMS (ESI) m/z calcd for $C_{23}H_{16}Cl_2NO^+$ $(M+H)^+$ 392.0603, found 392.0598.



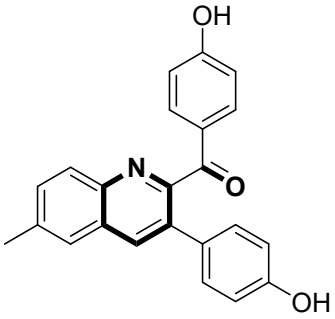
(4-(benzyloxy)phenyl)(3-(4-(benzyloxy)phenyl)-6-methylquinolin-2-yl)methanone (3ad) Yield 63%; 168.5 mg; yellow solid; mp 142-144 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:12); IR (KBr): 1666, 1599, 1510, 1249, 1228, 1149, 993, 908, 831, 738, 696 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.15–8.03 (m, 2H), 7.85 (d, J = 6.8 Hz, 2H), 7.62 (d, J = 26.8 Hz, 2H), 7.37 (d, J = 28.0 Hz, 14H), 6.94 (s, 4H), 5.07 (d, J = 29.6 Hz, 4H), 2.58 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 194.1, 163.0, 158.5, 155.8, 144.4, 137.8, 136.7, 136.1, 133.4, 132.9, 132.2, 130.5, 130.1, 129.5, 129.2, 128.7, 128.6, 128.23, 128.15, 128.0, 127.50, 127.48, 126.4, 114.9, 114.5, 70.1, 69.9, 21.7. HRMS (ESI) m/z calcd for $C_{37}H_{30}NO_3^+$ $(M+H)^+$ 536.2220, found 536.2221.



(6-methyl-3-(naphthalen-1-yl)quinolin-2-yl)(naphthalen-1-yl)methanone (3ae) Yield 69%; 145.9 mg; yellow solid; mp 131-133 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1670, 1288, 902, 777, 752 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.24 (dd, J = 13.2, 8.8 Hz, 2H), 8.18 (s, 1H), 7.67 (t, J = 10.0 Hz, 5H), 7.58 (d, J = 8.4 Hz, 1H), 7.50 (d, J = 7.6 Hz, 2H), 7.40–7.30 (m, 4H), 7.24 (d, J = 7.2 Hz, 1H), 7.17–7.09 (m, 2H), 2.61 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 197.2, 157.4, 145.2, 138.4, 138.1, 135.2, 133.8, 133.4, 133.2, 132.8, 132.7, 132.4, 131.7, 131.3, 130.5, 129.7, 128.1, 128.0, 127.90, 127.88, 127.6, 126.4, 126.2, 126.0, 125.8, 125.7, 125.5, 124.8, 123.6, 21.8. HRMS (ESI) m/z calcd for $C_{31}H_{22}NO^+$ $(M+H)^+$ 424.1696, found 424.1693.



(6-methyl-3-(naphthalen-2-yl)quinolin-2-yl)(naphthalen-2-yl)methanone (3af) Yield 68%; 143.8 mg; yellow solid; mp 137-139 ℃; R_f 0.2 (EtOAc/petroleum ether = 1:15); IR (KBr): 1660, 1294, 904, 825, 746 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.38 (s, 1H), 8.32 (s, 1H), 8.11 (d, J = 8.8 Hz, 1H), 8.04 (dd, J = 8.8, 1.2 Hz, 1H), 7.92 (s, 1H), 7.84 (dd, J = 8.4, 3.6 Hz, 3H), 7.75 (t, J = 8.4 Hz, 4H), 7.64 (d, J = 8.8 Hz, 1H), 7.57 (t, J = 7.6 Hz, 1H), 7.52–7.46 (m, 2H), 7.43 (dd, J = 6.4, 3.2 Hz, 2H), 2.62 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 195.2, 155.6, 144.6, 138.2, 136.9, 135.8, 135.4, 134.1, 133.7, 133.4, 133.2, 132.6, 132.5, 132.3, 129.8, 129.4, 128.7, 128.4, 128.3, 128.2, 128.1, 127.8, 127.6, 126.8, 126.60, 126.56, 126.4, 126.3, 125.1, 21.8. HRMS (ESI) m/z calcd for $C_{31}H_{22}NO^+$ $(M+H)^+$ 424.1696, found 424.1693.



(4-hydroxyphenyl)(3-(4-hydroxyphenyl)-6-methylquinolin-2-yl)methanone (5ah) Yield 37%; 65.7 mg; yellow solid; mp 169-171 ℃; R_f 0.3 (EtOAc/petroleum ether = 1:3); IR (KBr): 3370, 1660, 1591, 1282, 1226, 1153, 831, 756 cm^{-1}; **^{1}H NMR (400 MHz, DMSO-d_6) δ** 10.60 (s, 1H), 9.64 (s, 1H), 8.34 (s, 1H), 7.92 (d, J = 8.8 Hz, 1H), 7.85 (s, 1H), 7.64 (d, J = 8.8 Hz, 1H), 7.60 (d, J = 8.8 Hz, 2H), 7.19 (d, J = 8.4 Hz, 2H), 6.81 (d, J = 8.8 Hz, 2H), 6.73 (d, J = 8.4 Hz, 2H), 2.53 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d_6) δ** 193.5, 162.8, 157.4, 156.0, 143.8, 137.5, 135.9, 133.0, 132.7, 132.3, 130.1, 128.5, 128.2, 128.0, 127.7, 126.8, 115.63, 115.58, 21.4. HRMS (ESI) m/z calcd for $C_{23}H_{18}NO_3^+$ $(M+H)^+$ 356.1281, found 356.1278.

5. References

[1] X. Geng, X. Wu, P. Zhao, J. Zhang, Y. D. Wu and A. X. Wu, *Org. Lett.*, 2017, **19**, 4179-4182.
[2] Z. Y. Li, X. Y. Wang, L. F. Ma and N. Jiao, *Synlett*. 2017, **28**, 1581–1585.
[3] X. Wan, S. Wang, C. Wu, J. Gan and C. Wang, *Org. Lett.*, 2021, **23**, 8799-8803.

6. Crystallographic data and molecular structure of 3v

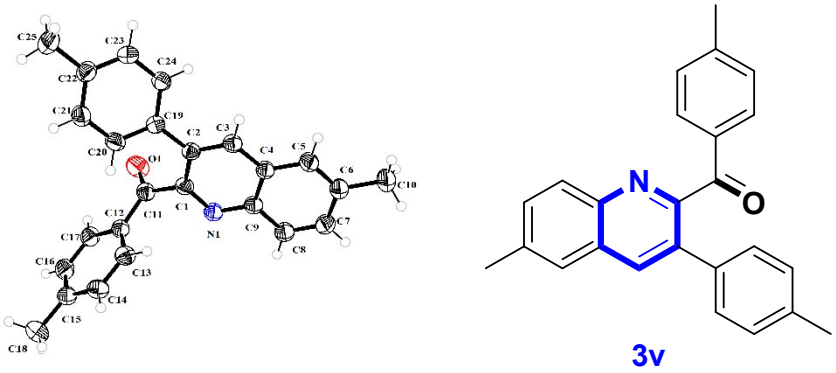


Figure S1. X-ray crystal structure of **3v**, thermal ellipsoids shown at 50% probability level. Sample preparation: 35 mg of **3v** was dissolved in 6 ml CH_2Cl_2 and 1 ml CH_3OH at room temperature for slow evaporation about a week. The crystals were mounted on a glass fiber for diffraction experiments. Intensity data were collected on a Bruker SMART APEX CCD diffractometer with Mo Kα radiation (0.71073 Å) at room temperature. Crystal Data for Compound **3v**: CCDC 2227223 contains the supplementary crystallographic data for this paper. These data could be obtained free of charge from The Cambridge Crystallographic.

Bond precision: C-C = 0.0019 A Wavelength=0.71073

Cell: a=8.2419(15) b=10.5399(19) c=11.222(2)
alpha=99.154(3) beta=93.011(3) gamma=102.359(3)
Temperature: 296 K

	Calculated	Reported
Volume	936.3(3)	936.3(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C25 H21 N O	C25 H21 N O
Sum formula	C25 H21 N O	C25 H21 N O
Mr	351.43	351.43
Dx,g cm-3	1.247	1.246
Z	2	2
Mu (mm-1)	0.075	0.075
F000	372.0	372.0
F000'	372.14	
h,k,lmax	11,14,15	11,14,15
Nref	5644	5497
Tmin,Tmax	0.985,0.993	0.645,0.746
Tmin'	0.985	

Correction method= # Reported T Limits: Tmin=0.645 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.974 Theta(max)= 30.374

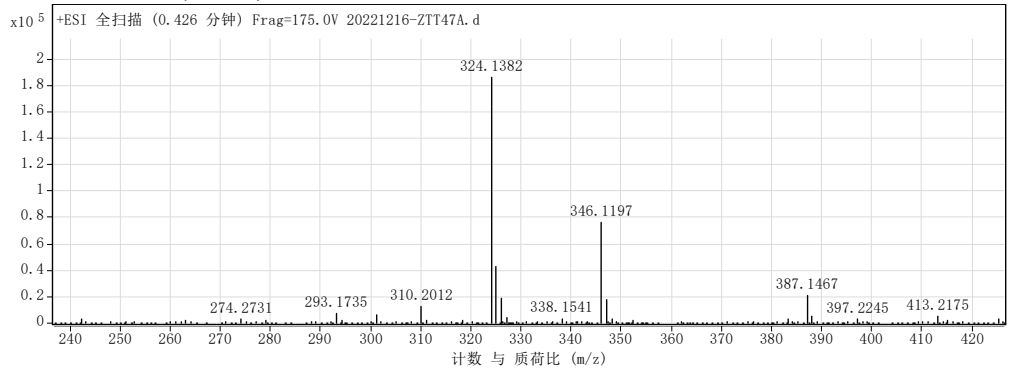
R(reflections)= 0.0567(4130) wR2(reflections)= 0.1870(5497)

S = 1.040 Npar= 247

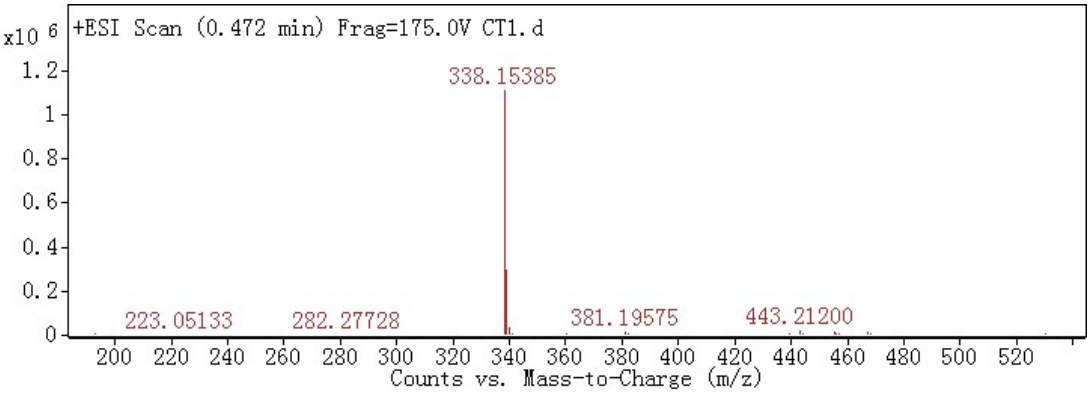
The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

5. HRMS spectra for compounds 3 and 5ah

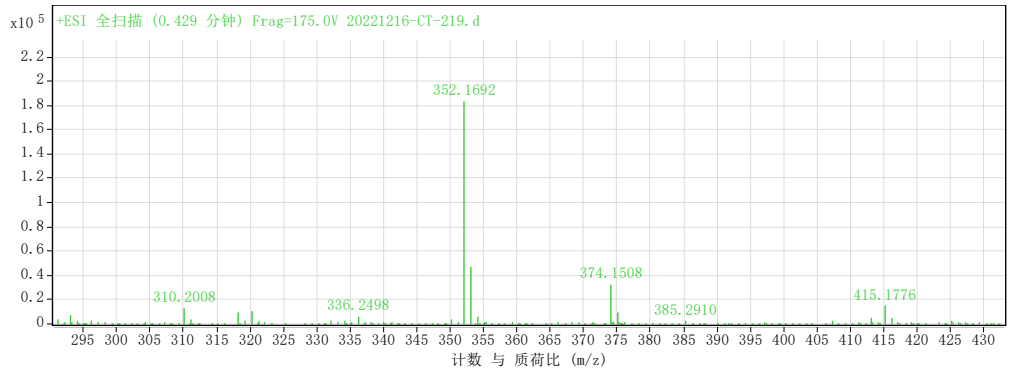
(6-methyl-3-phenylquinolin-2-yl)(phenyl)methanone (3a) HRMS (ESI) m/z calcd for $C_{23}H_{18}NO^+$ $(M+H)^+$ 324.1383, found 324.1382.



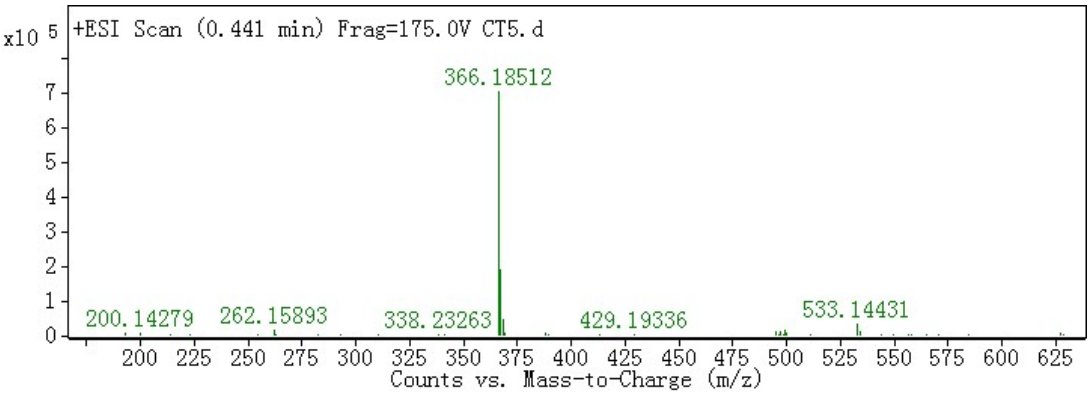
(6-ethyl-3-phenylquinolin-2-yl)(phenyl)methanone (3b) HRMS (ESI) m/z calcd for $C_{24}H_{20}NO_2^+$ $(M+H)^+$ 338.1539, found 338.1538.



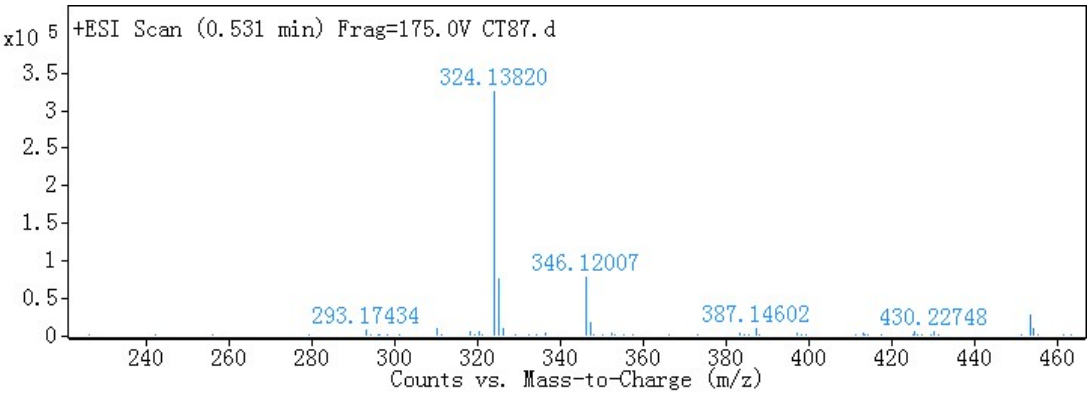
phenyl(3-phenyl-6-propylquinolin-2-yl)methanone (3c) HRMS (ESI) m/z calcd for $C_{25}H_{22}NO^+$ $(M+H)^+$ 352.1696, found 352.1692.



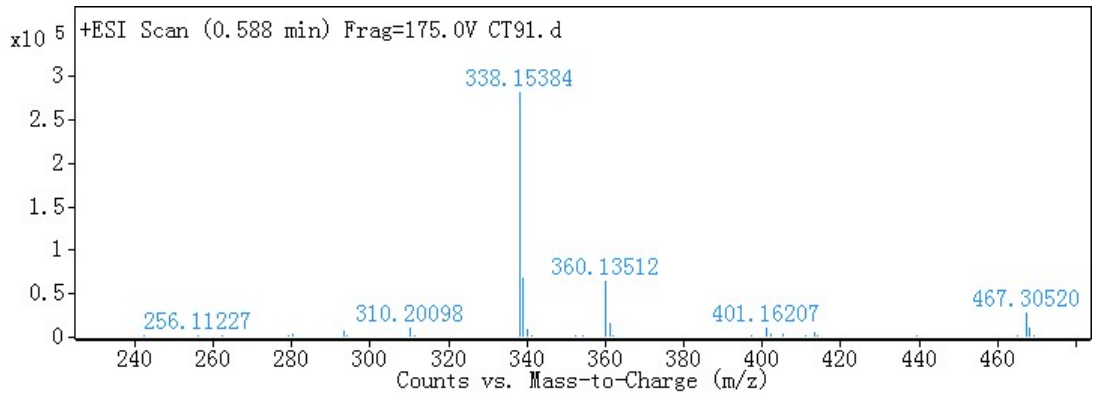
(6-(tert-butyl)-3-phenylquinolin-2-yl)(phenyl)methanone (3d) HRMS (ESI) m/z calcd for $C_{26}H_{24}NO^+$ $(M+H)^+$ 366.1852, found 366.1851.



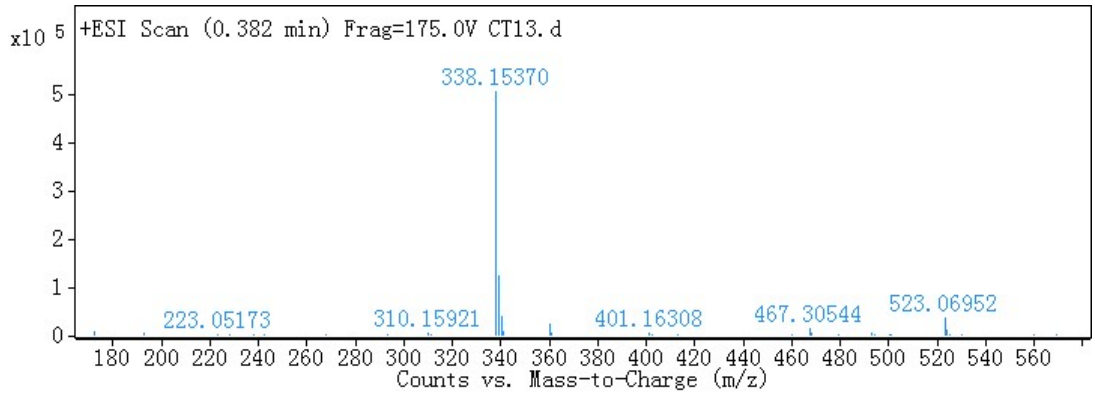
(7-methyl-3-phenylquinolin-2-yl)(phenyl)methanone (3e) HRMS (ESI) m/z calcd for $C_{23}H_{18}NO^+$ $(M+H)^+$ 324.1383, found 324.1382.



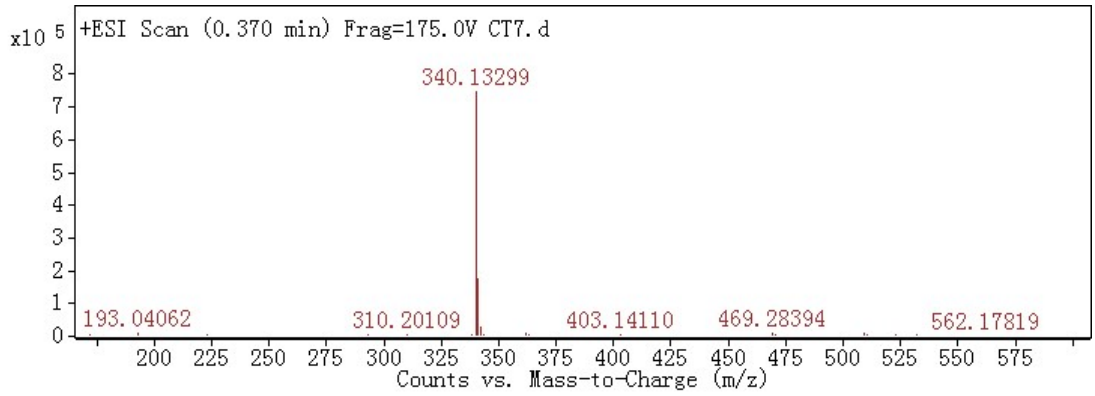
(6,7-dimethyl-3-phenylquinolin-2-yl)(phenyl)methanone (3f) HRMS (ESI) m/z calcd for $C_{24}H_{20}NO^+$ $(M+H)^+$ 338.1539, found 338.1538.



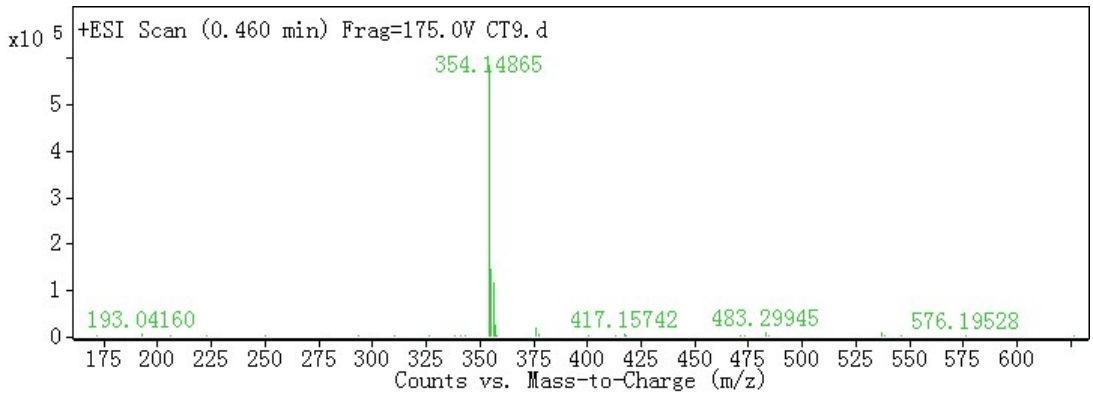
(5,7-dimethyl-3-phenylquinolin-2-yl)(phenyl)methanone (3g) HRMS (ESI) m/z calcd for $C_{24}H_{20}NO^+$ $(M+H)^+$ 338.1539, found 338.1537.



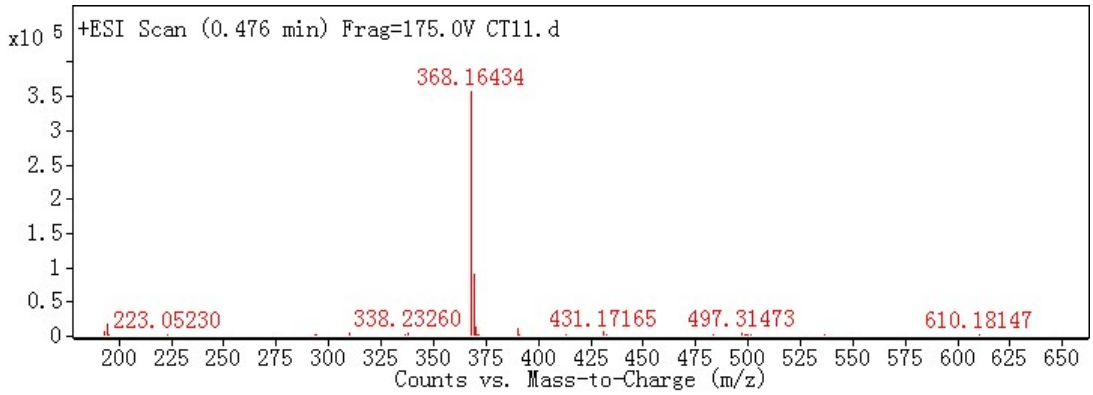
(6-methoxy-3-phenylquinolin-2-yl)(phenyl)methanone (3h) HRMS (ESI) m/z calcd for $C_{23}H_{18}NO_2^+$ $(M+H)^+$ 340.1332, found 340.1329.



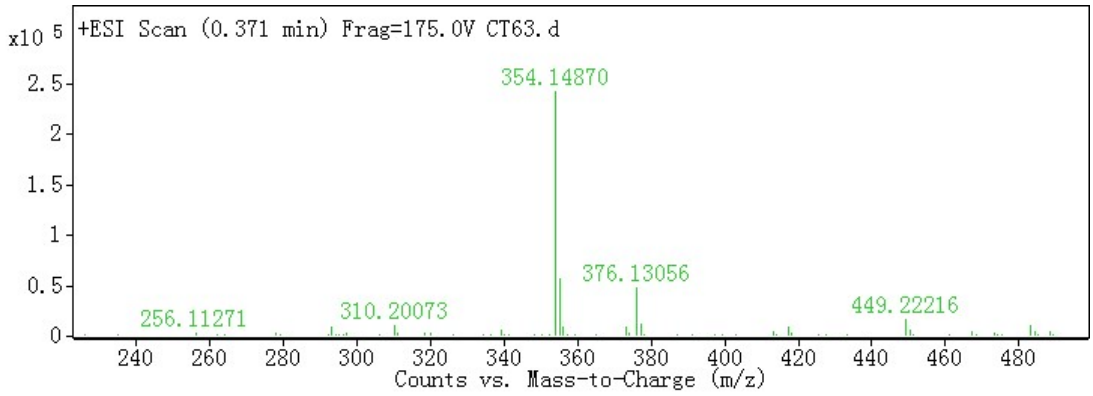
(6-ethoxy-3-phenylquinolin-2-yl)(phenyl)methanone (3i) HRMS (ESI) m/z calcd for $C_{24}H_{20}NO_2^+$ $(M+H)^+$ 354.1489, found 354.1486.



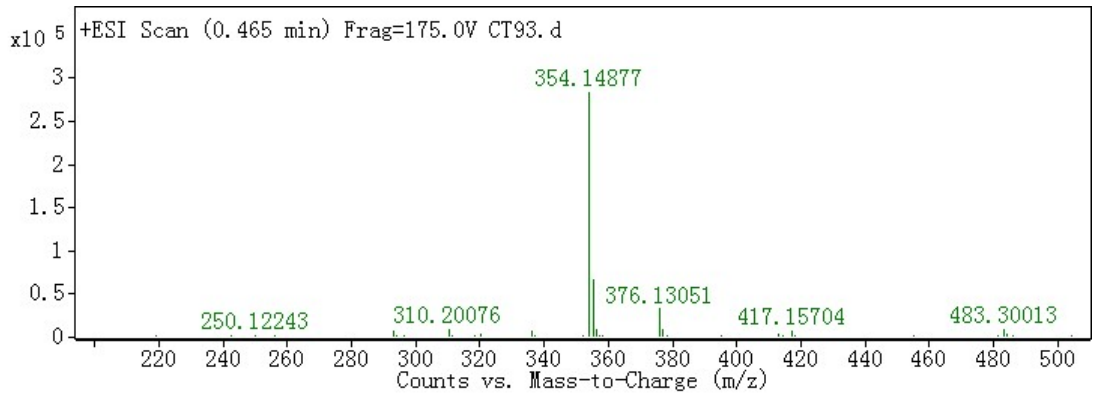
(6-isopropoxy-3-phenylquinolin-2-yl)(phenyl)methanone (3j) HRMS (ESI) m/z calcd for $C_{25}H_{22}NO_2^+$ $(M+H)^+$ 368.1645, found 368.1643.



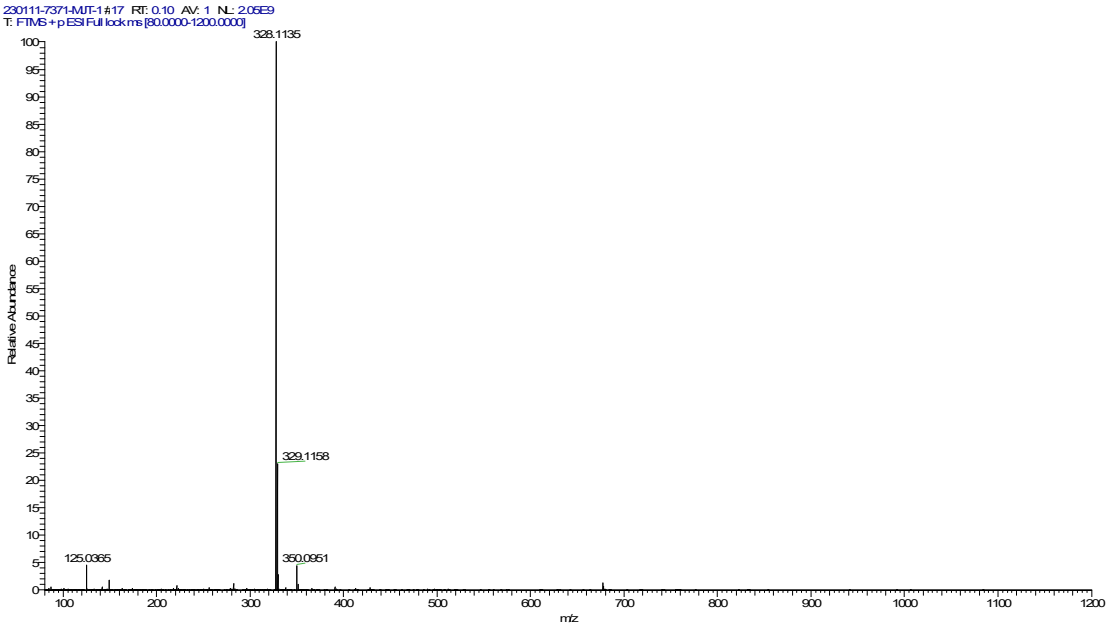
(7-methoxy-6-methyl-3-phenylquinolin-2-yl)(phenyl)methanone (3k) HRMS (ESI) m/z calcd for $C_{24}H_{20}NO_2^+$ $(M+H)^+$ 354.1489, found 354.1487.



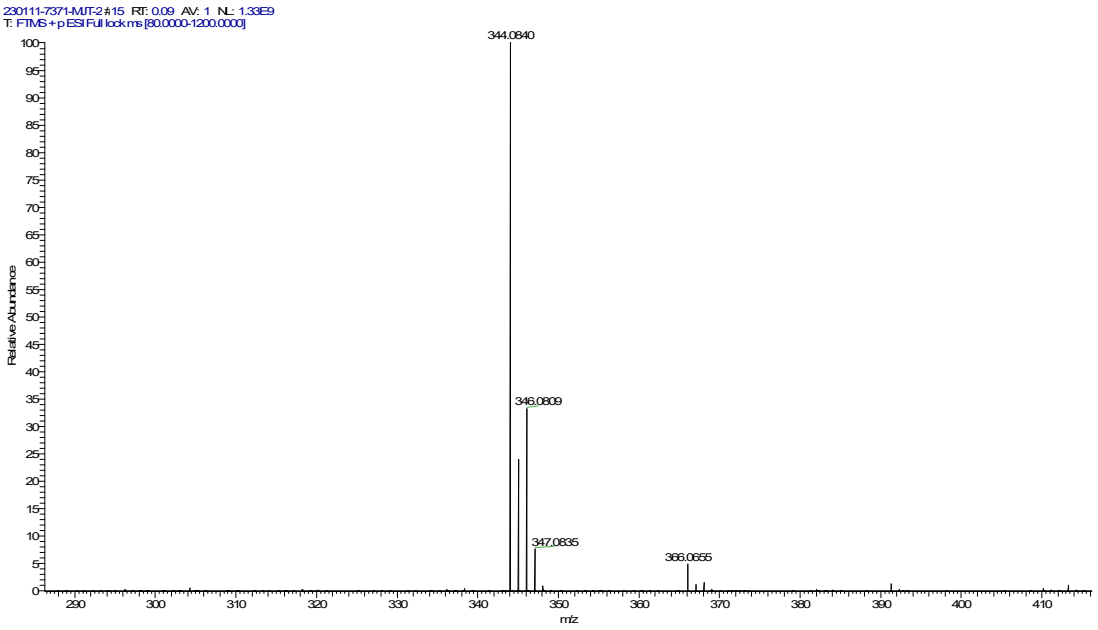
(6-methoxy-7-methyl-3-phenylquinolin-2-yl)(phenyl)methanone (3l) HRMS (ESI) m/z calcd for $C_{24}H_{20}NO_2^+$ $(M+H)^+$ 354.1489, found 354.1487.



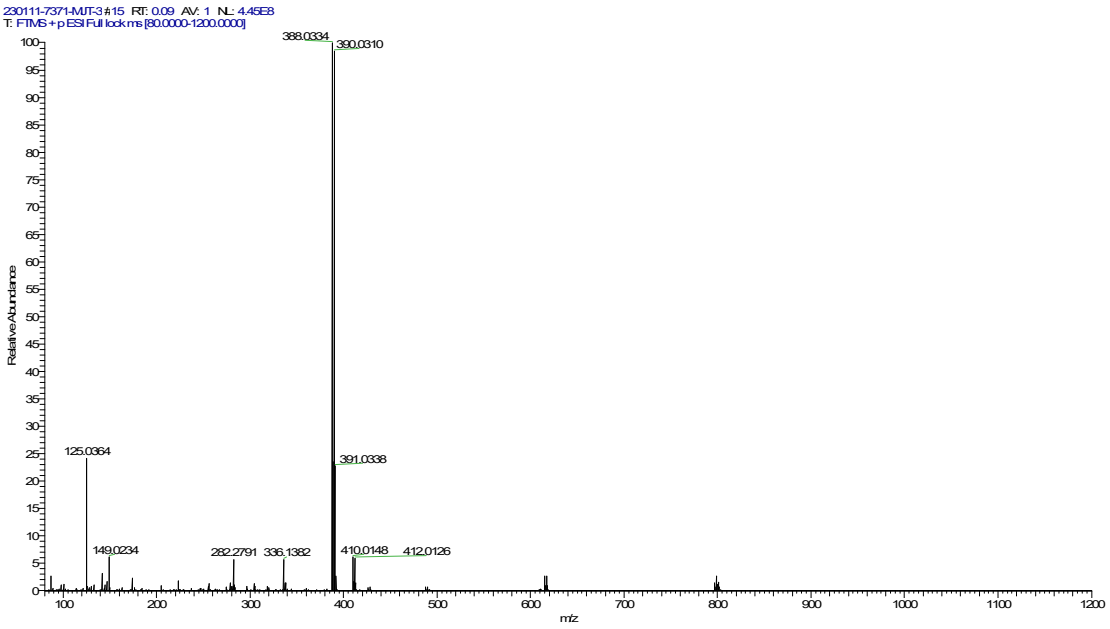
(6-fluoro-3-phenylquinolin-2-yl)(phenyl)methanone (3m) HRMS (ESI) m/z calcd for $C_{22}H_{15}FNO^+$ $(M+H)^+$ 328.1132, found 328.1135.



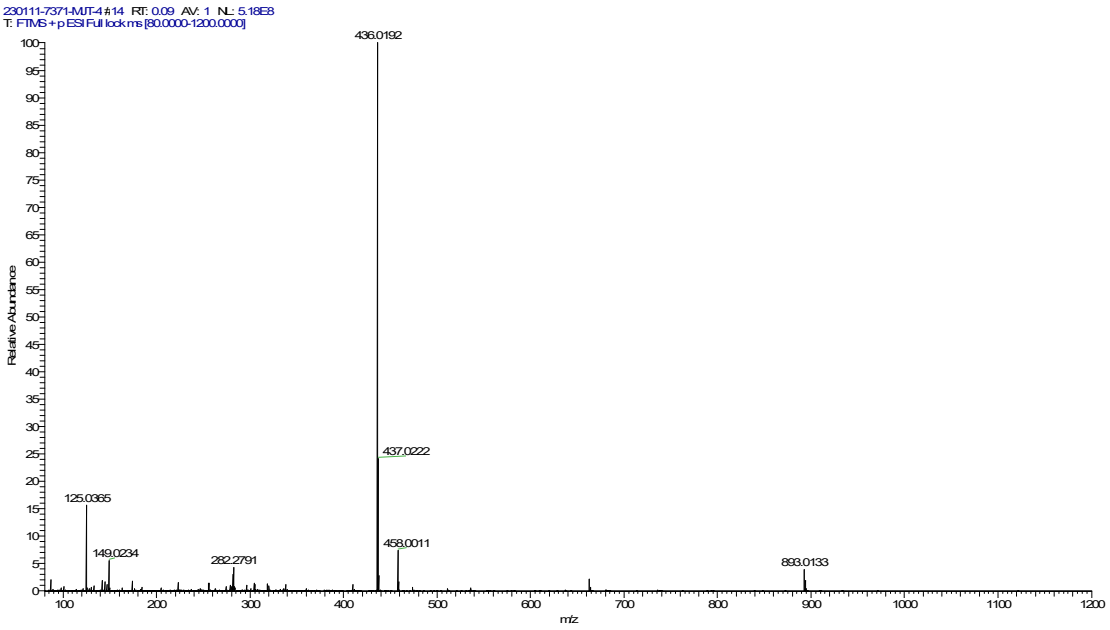
(6-chloro-3-phenylquinolin-2-yl)(phenyl)methanone (3n) HRMS (ESI) m/z calcd for $C_{22}H_{15}ClNO^+$ $(M+H)^+$ 344.0837, found 344.0840.



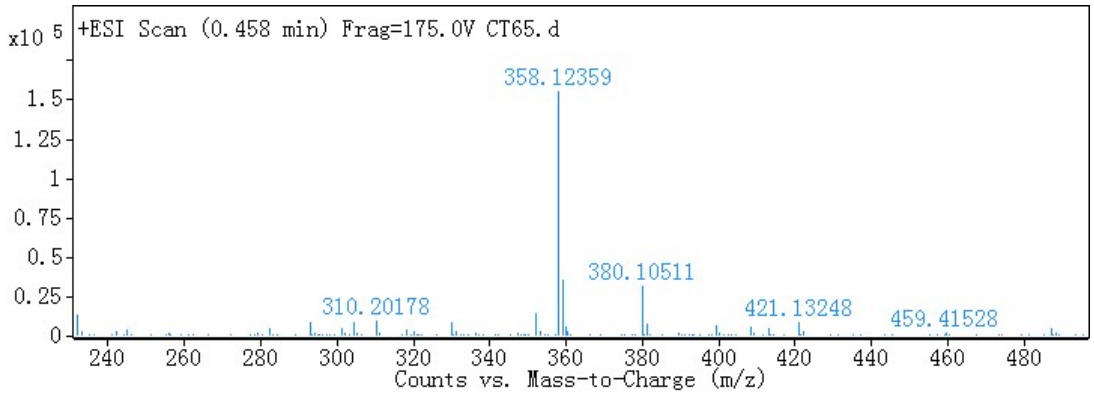
(6-bromo-3-phenylquinolin-2-yl)(phenyl)methanone (3o) HRMS (ESI) m/z calcd for $C_{22}H_{15}BrNO^+$ $(M+H)^+$ 388.0332, found 388.0334.



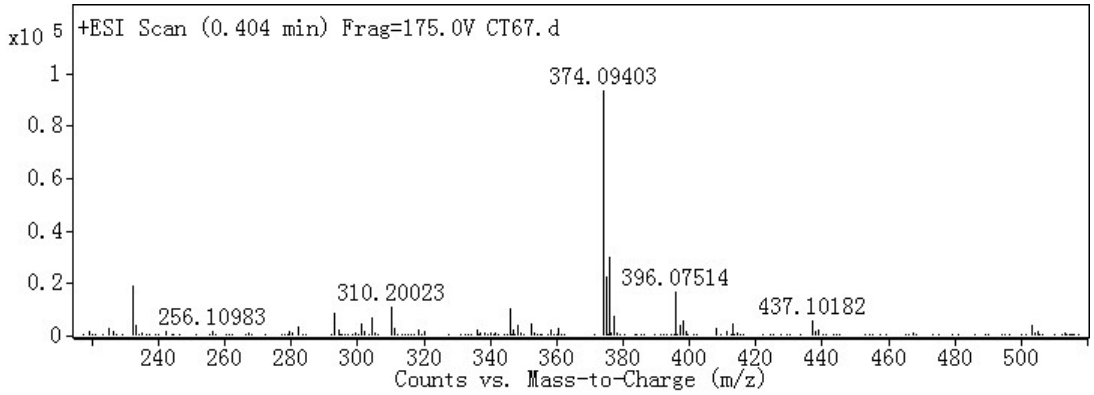
(6-iodo-3-phenylquinolin-2-yl)(phenyl)methanone (3p) HRMS (ESI) m/z calcd for $C_{22}H_{15}INO^+$ $(M+H)^+$ 436.0193, found 436.0192.



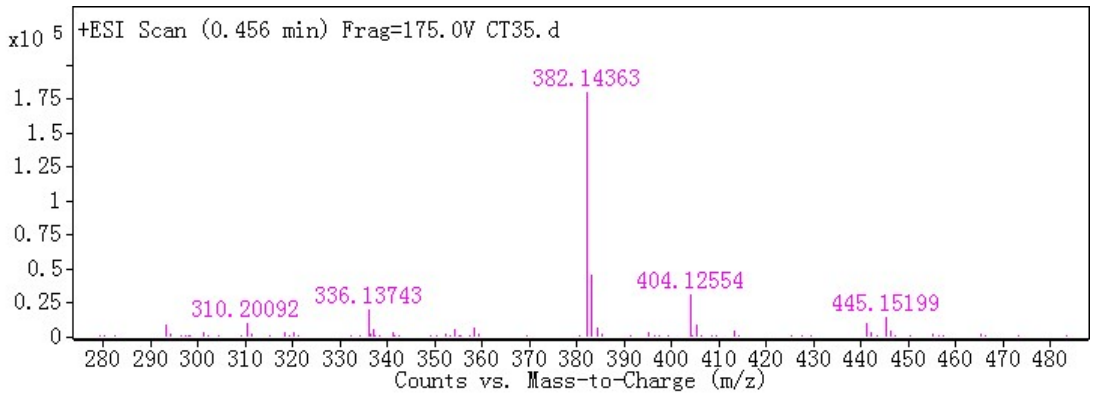
(6-fluoro-7-methoxy-3-phenylquinolin-2-yl)(phenyl)methanone (3q) HRMS (ESI) m/z calcd for $C_{23}H_{17}FNO_2^+$ $(M+H)^+$ 358.1238, found 358.1235.



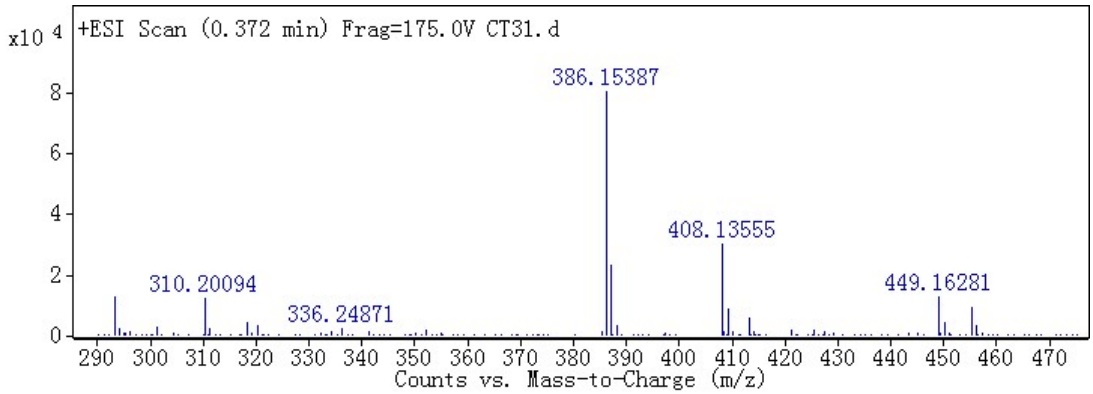
(6-chloro-7-methoxy-3-phenylquinolin-2-yl)(phenyl)methanone (3r) HRMS (ESI) m/z calcd for $C_{23}H_{17}ClNO_2^+$ $(M+H)^+$ 374.0942, found 374.0940.



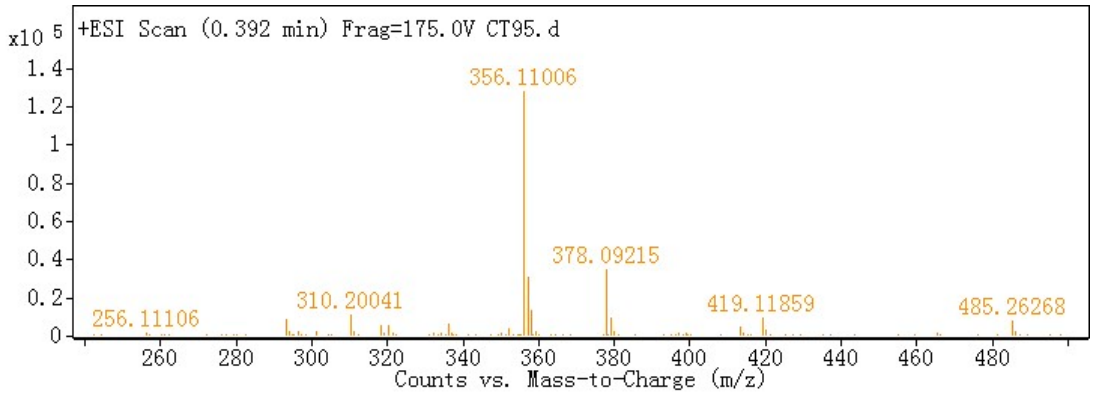
ethyl 2-benzoyl-3-phenylquinoline-6-carboxylate (3s) HRMS (ESI) m/z calcd for $C_{25}H_{20}NO_3^+$ $(M+H)^+$ 382.1438, found 382.1436.



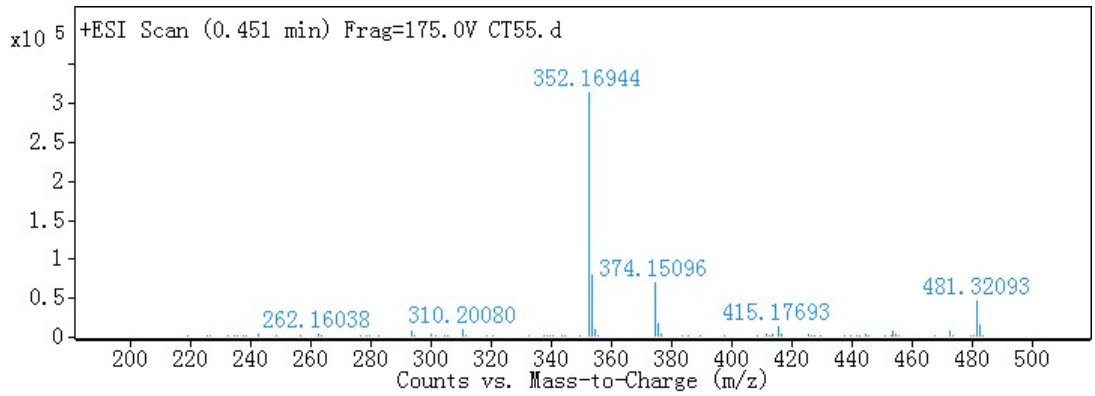
(3,6-diphenylquinolin-2-yl)(phenyl)methanone (3t) HRMS (ESI) m/z calcd for $C_{28}H_{20}NO^+$ $(M+H)^+$ 386.1539, found 386.1538.



(6-(methylthio)-3-phenylquinolin-2-yl)(phenyl)methanone (3u) HRMS (ESI) m/z calcd for $C_{23}H_{18}NOS^+$ $(M+H)^+$ 356.1104, found 356.1100.

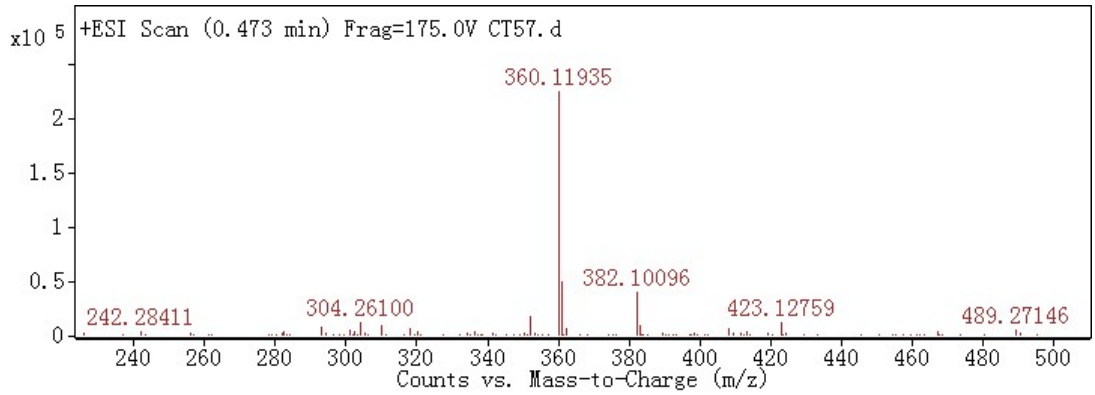


(6-methyl-3-(p-tolyl)quinolin-2-yl)(p-tolyl)methanone (3v) HRMS (ESI) m/z calcd for $C_{25}H_{22}NO^+$ $(M+H)^+$ 352.1696, found 352.1694.



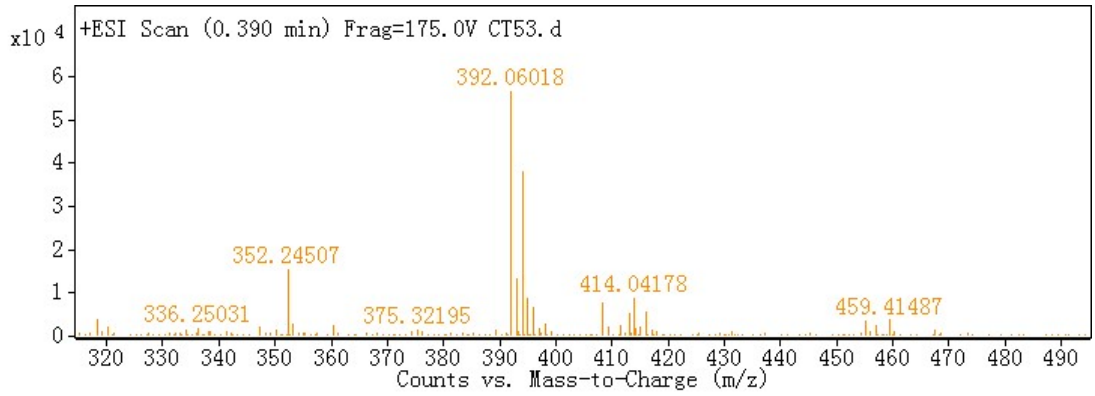
(4-fluorophenyl)(3-(4-fluorophenyl)-6-methylquinolin-2-yl)methanone (3w)

HRMS (ESI) m/z calcd for $C_{23}H_{16}F_2NO^+$ $(M+H)^+$ 360.1194, found 360.1193.



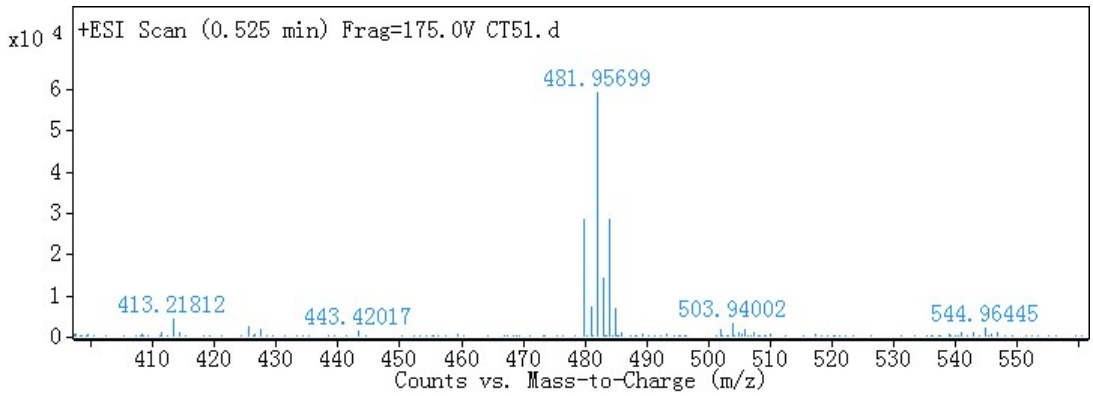
(4-chlorophenyl)(3-(4-chlorophenyl)-6-methylquinolin-2-yl)methanone (3x)

HRMS (ESI) m/z calcd for $C_{23}H_{16}Cl_2NO^+$ $(M+H)^+$ 392.0603, found 392.0601.

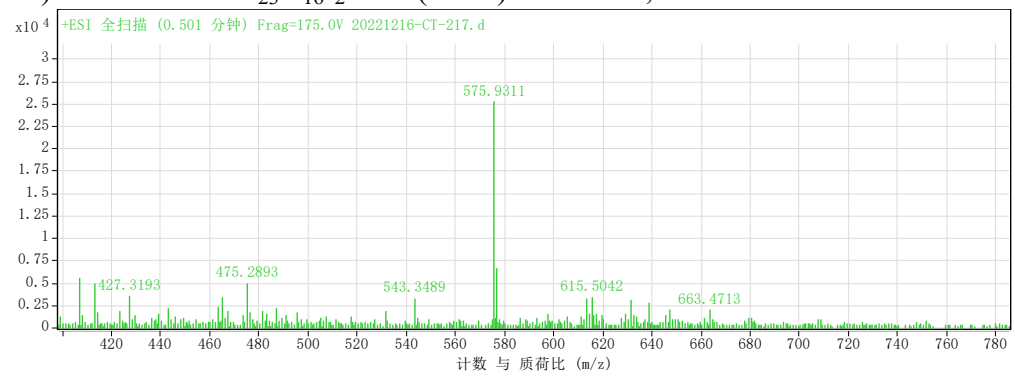


(4-bromophenyl)(3-(4-bromophenyl)-6-methylquinolin-2-yl)methanone (3y)

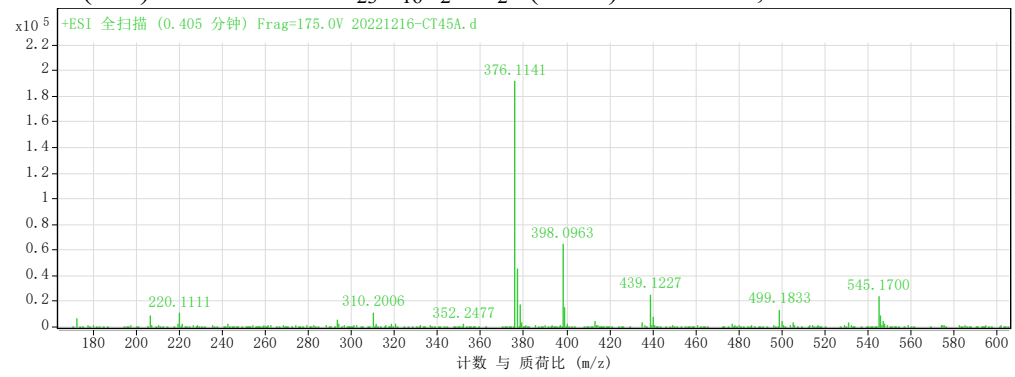
HRMS (ESI) m/z calcd for $C_{23}H_{16}Br_2NO^+$ $(M+H)^+$ 481.9573, found 481.9569.



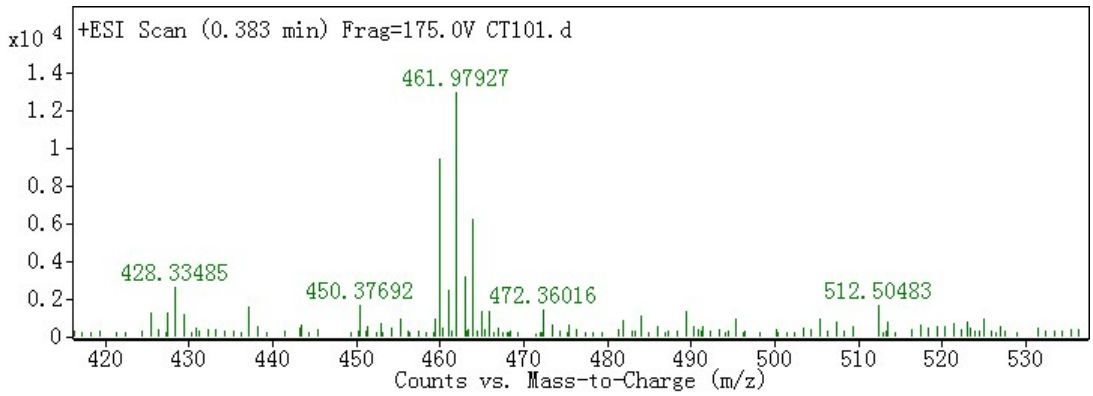
(4-iodophenyl)(3-(4-iodophenyl)-6-methylquinolin-2-yl)methanone (3z) HRMS (ESI) m/z calcd for $C_{23}H_{16}I_2NO^+$ $(M+H)^+$ 575.9316, found 575.9311.



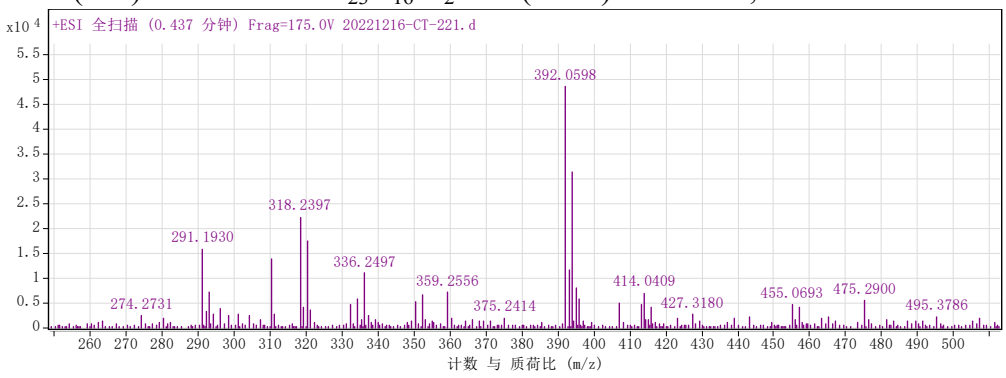
(2-fluorophenyl)(3-(2-fluorophenyl)-6-methoxyquinolin-2-yl)methanone (3aa) HRMS (ESI) m/z calcd for $C_{23}H_{16}F_2NO_2^+$ $(M+H)^+$ 376.1144, found 376.1141.



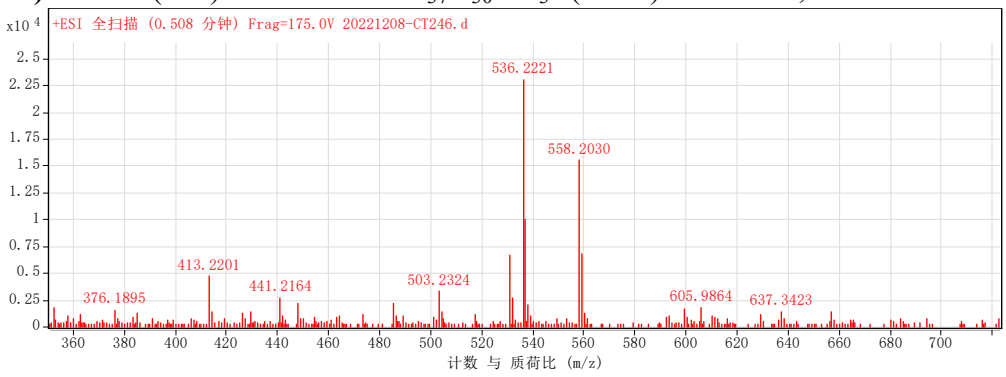
(3,4-dichlorophenyl)(3-(3,4-dichlorophenyl)-6-methylquinolin-2-yl)methanone (3ab) HRMS (ESI) m/z calcd for $C_{23}H_{14}Cl_4NO^+$ $(M+H)^+$ 461.9795, found 461.9792.



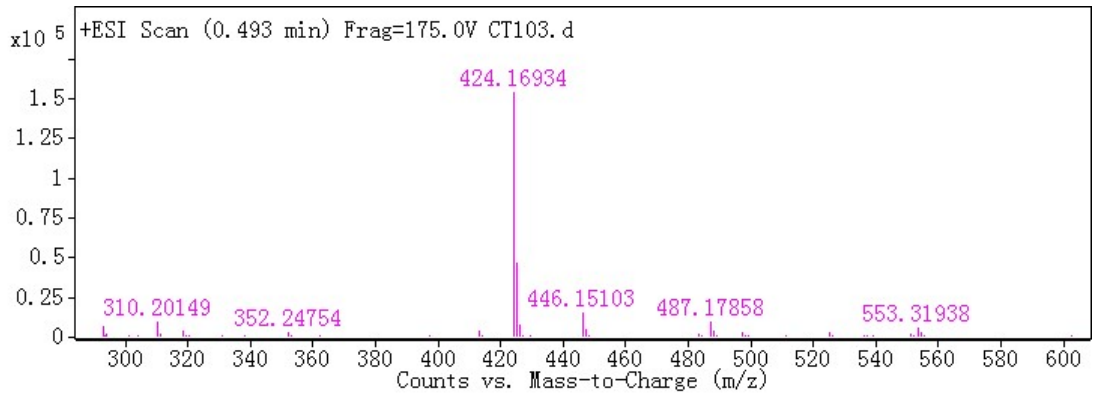
(3-chlorophenyl)(3-(3-chlorophenyl)-6-methylquinolin-2-yl)methanone (3ac) HRMS (ESI) m/z calcd for $C_{23}H_{16}Cl_2NO^+$ $(M+H)^+$ 392.0603, found 392.0598.



(4-(benzyloxy)phenyl)(3-(4-(benzyloxy)phenyl)-6-methylquinolin-2-yl)methanone (3ad) HRMS (ESI) m/z calcd for $C_{37}H_{30}NO_3^+$ $(M+H)^+$ 536.2220, found 536.2221.

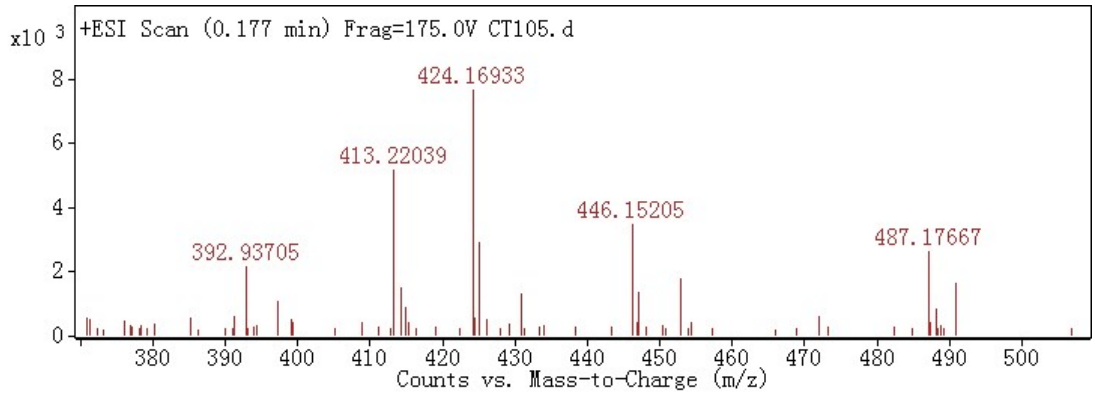


(6-methyl-3-(naphthalen-1-yl)quinolin-2-yl)(naphthalen-1-yl)methanone (3ae) HRMS (ESI) m/z calcd for $C_{31}H_{22}NO^+$ $(M+H)^+$ 424.1696, found 424.1693.



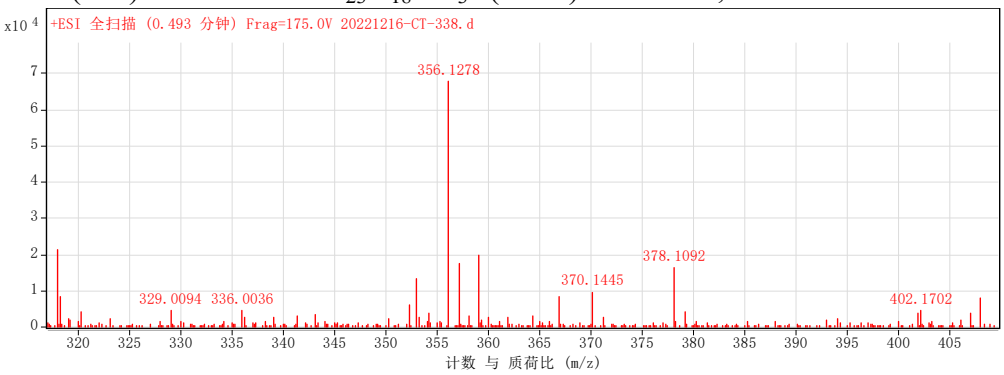
(6-methyl-3-(naphthalen-2-yl)quinolin-2-yl)(naphthalen-2-yl)methanone (3af)

HRMS (ESI) m/z calcd for $C_{31}H_{22}NO^+$ $(M+H)^+$ 424.1696, found 424.1693.

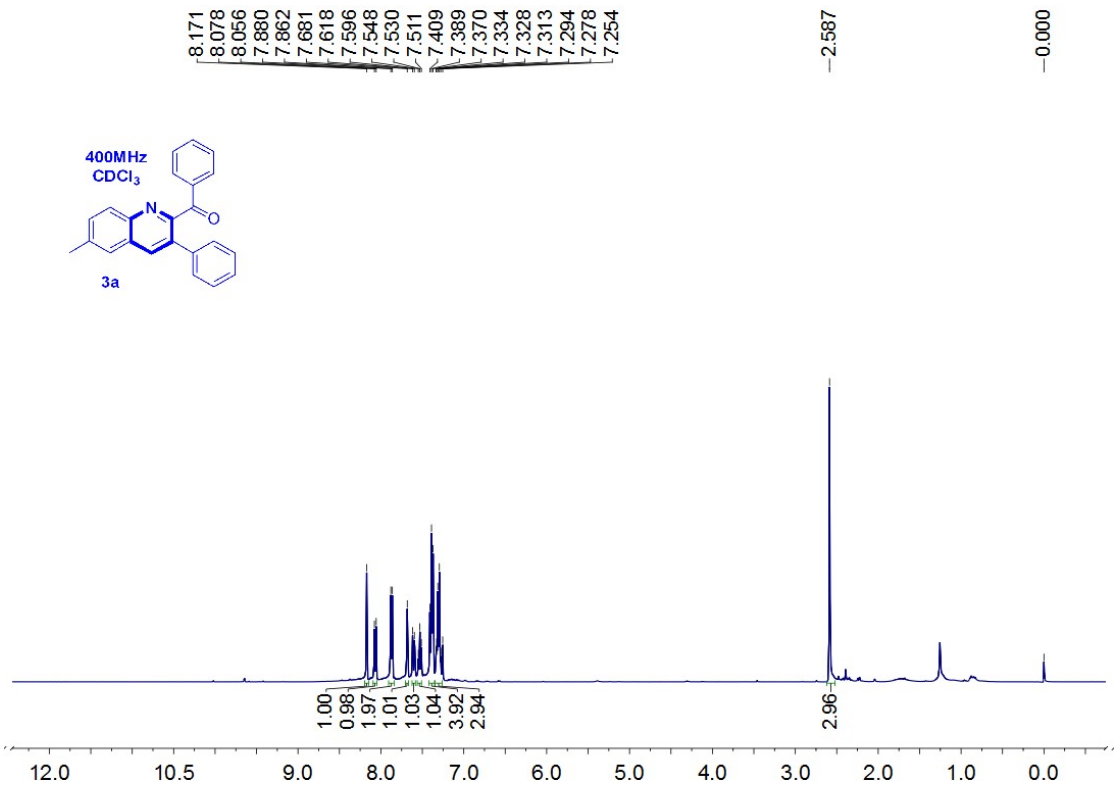


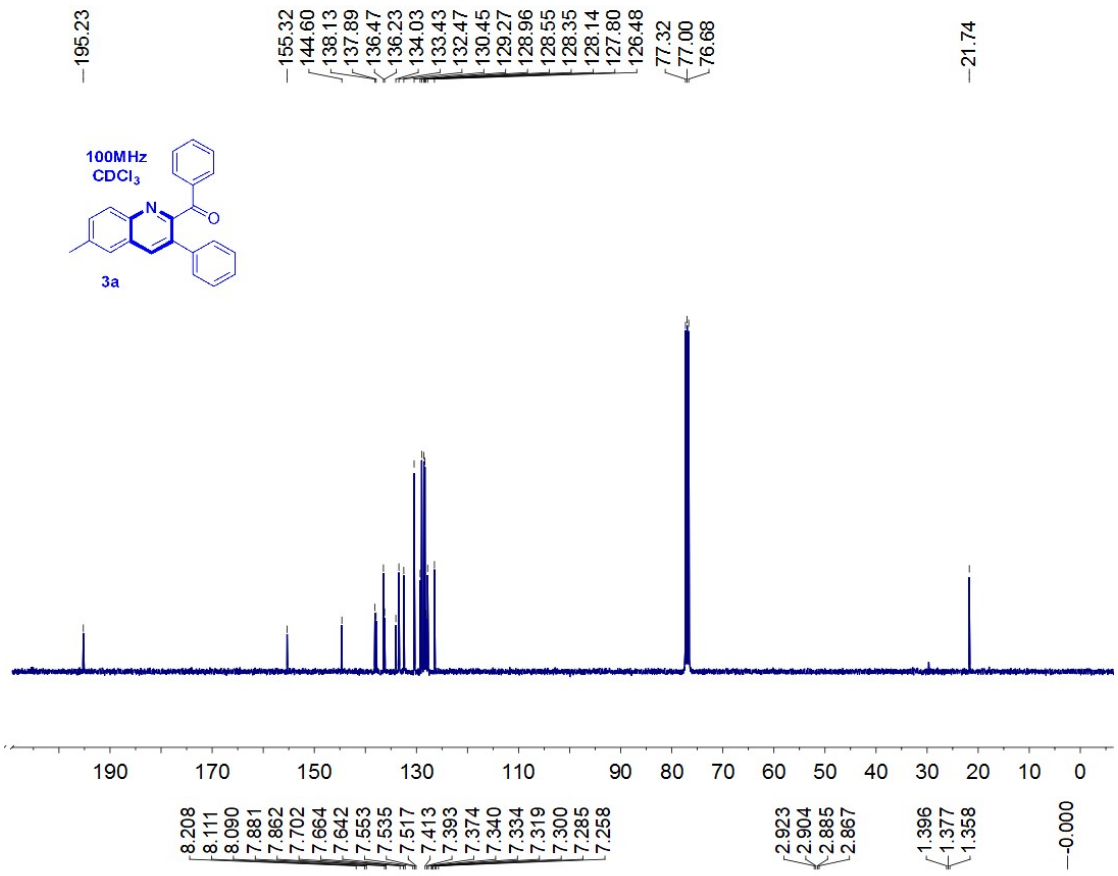
(4-hydroxyphenyl)(3-(4-hydroxyphenyl)-6-methylquinolin-2-yl)methanone (5ah)

HRMS (ESI) m/z calcd for $C_{23}H_{18}NO_3^+$ $(M+H)^+$ 356.1281, found 356.1278.



7. ^{1}H and ^{13}C NMR spectra of compounds 3 and 5ah

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136.23
134.03
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132.47
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128.55
128.35
128.14
127.80
126.48
77.32
77.00
76.68
21.74
100MHz
CDCl3
3a
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
8.208
8.111
8.090
7.881
7.862
7.702
7.664
7.642
7.553
7.535
7.517
7.413
7.393
7.374
7.340
7.334
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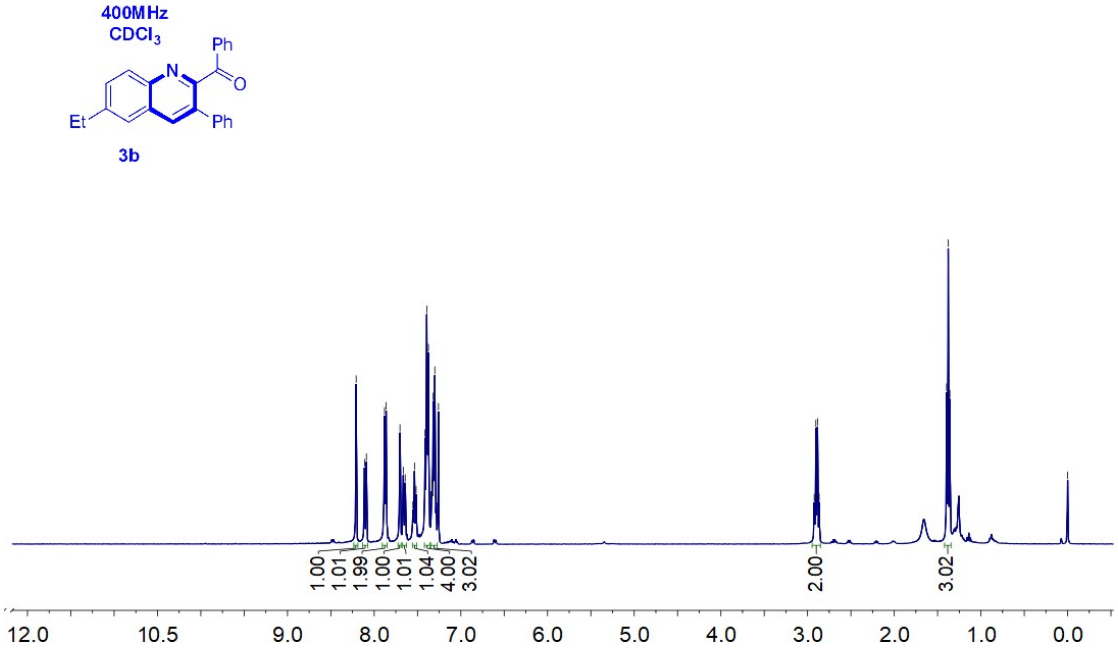
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Et
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3.02
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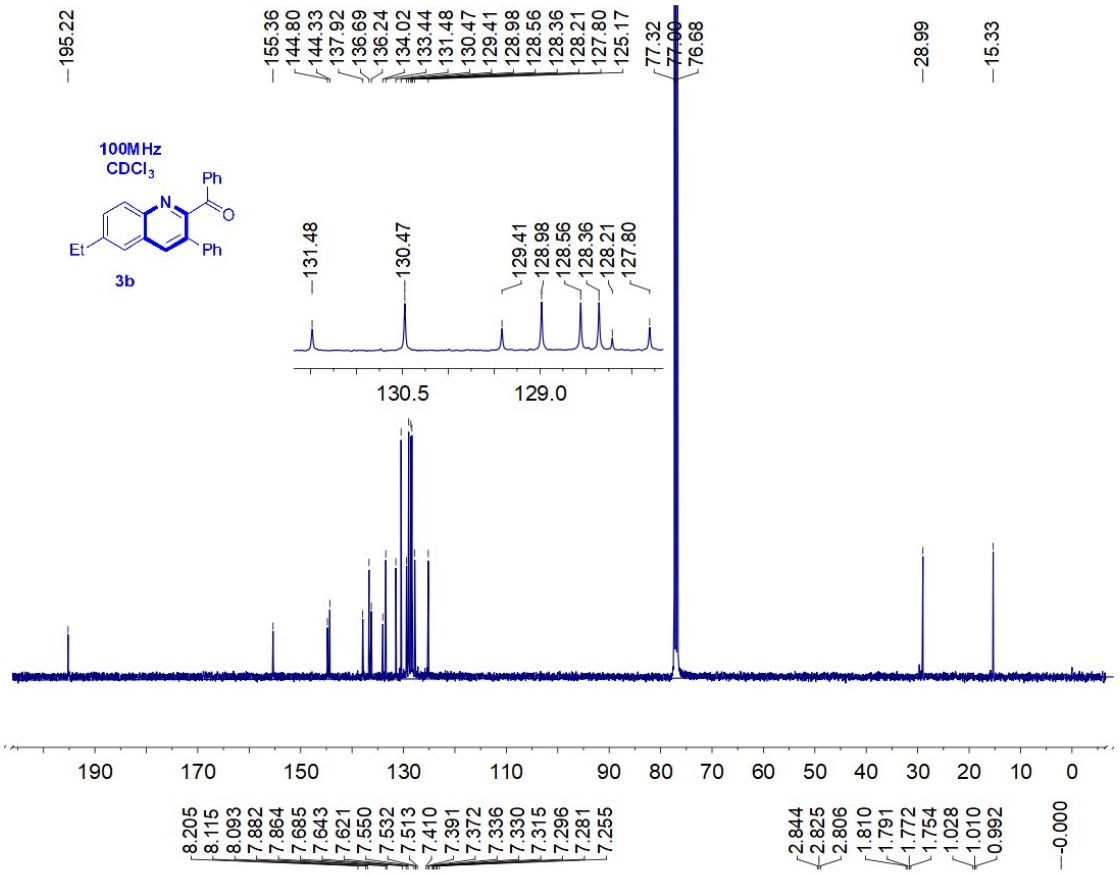
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133.44
131.48
130.47
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128.21
127.80
125.17
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77.00
76.68
28.99
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131.48
130.47
129.41
128.98
128.56
128.36
128.21
127.80
130.5
129.0
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
8.205
8.115
8.093
7.882
7.864
7.685
7.643
7.621
7.550
7.532
7.513
7.410
7.391
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7.315
7.296
7.281
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2.806
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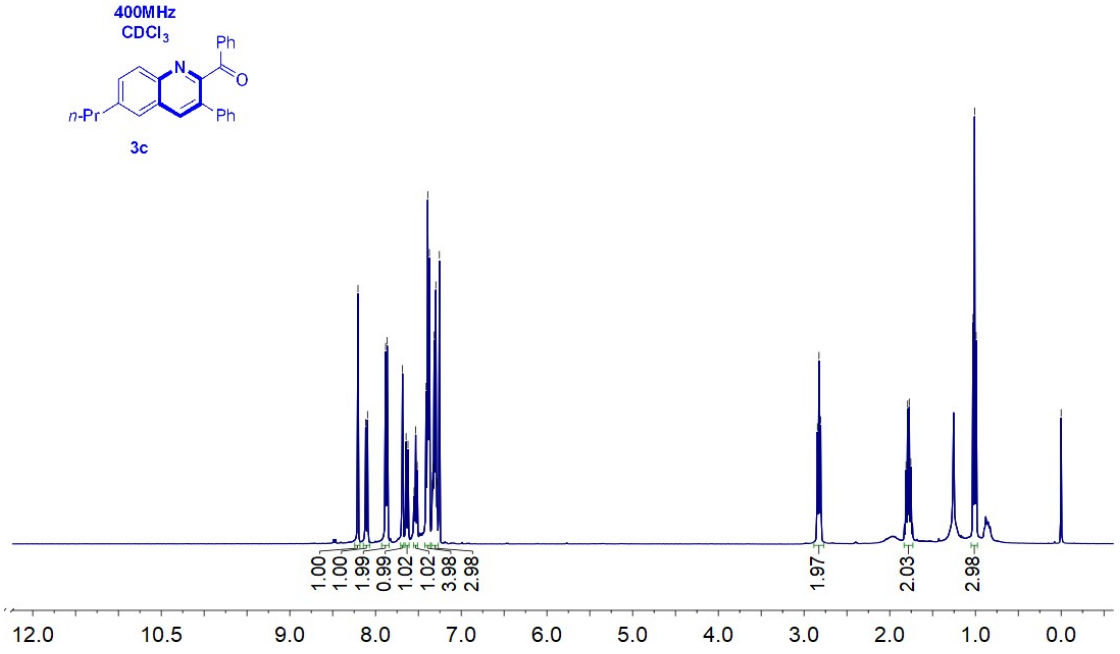
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Ph
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1.97
2.03
2.98
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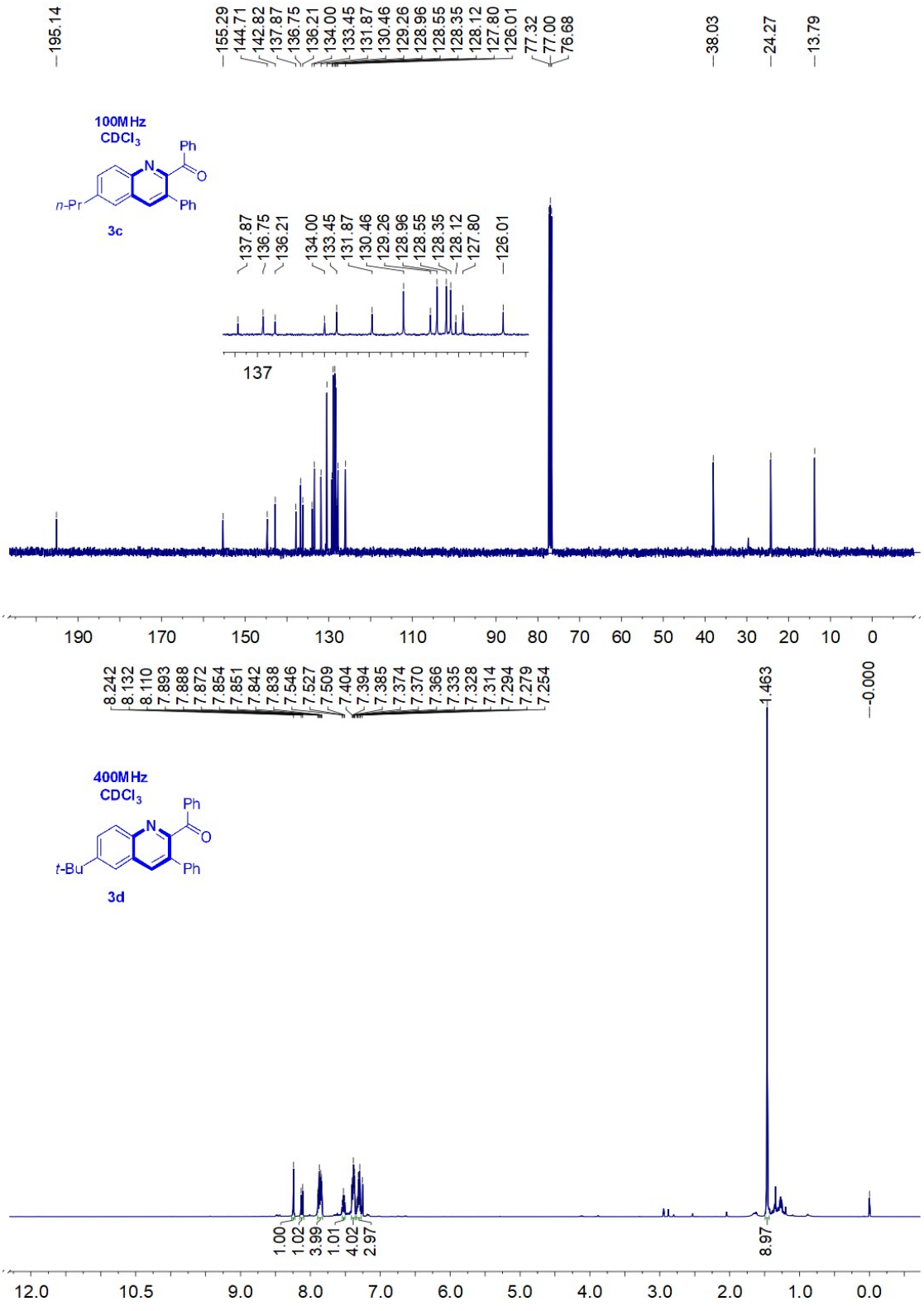
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77.00
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38.03
24.27
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100MHz
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Ph
N
O
n-Pr
Ph
3c
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131.87
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128.12
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137
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170
150
130
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90
80
70
60
50
40
30
20
10
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8.132
8.110
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7.888
7.872
7.854
7.851
7.842
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7.385
7.374
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O
t-Bu
Ph
3d
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4.02
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8.97
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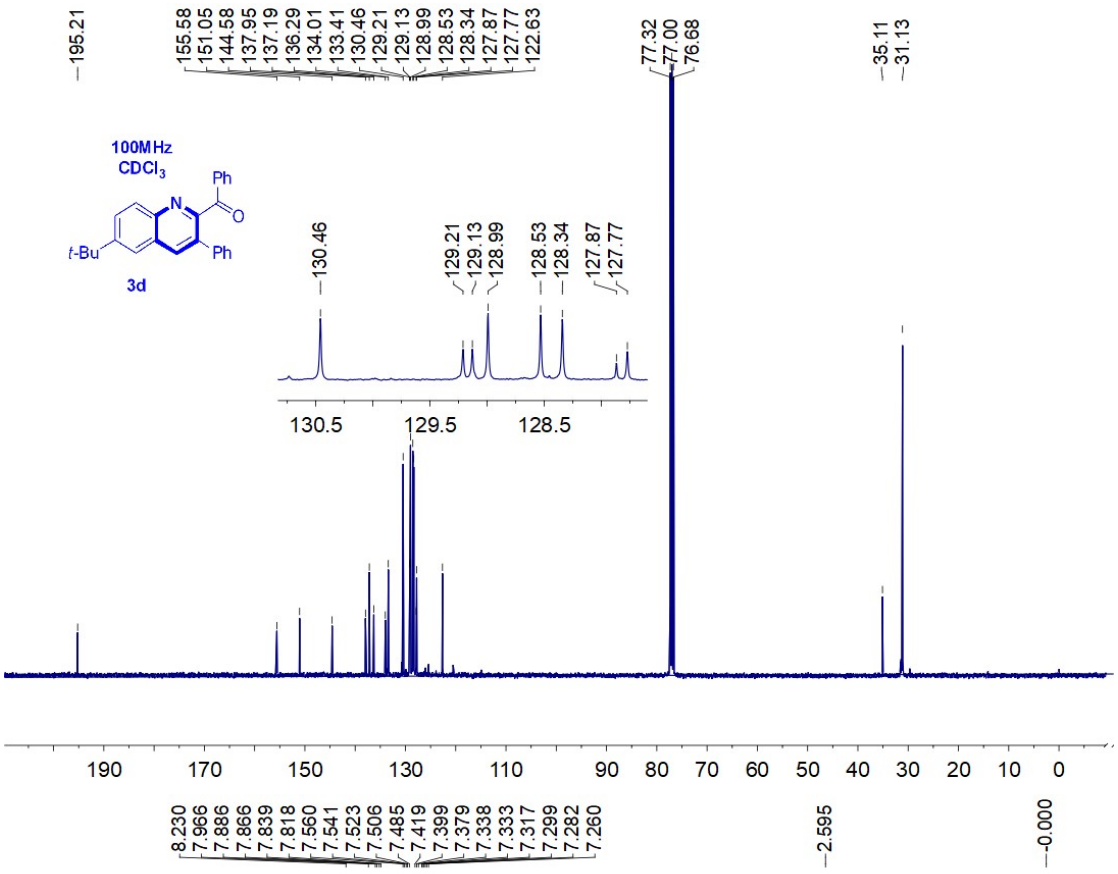
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129.13
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77.32
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31.13
100MHz
CDCl3
Ph
N
O
t-Bu
Ph
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128.34
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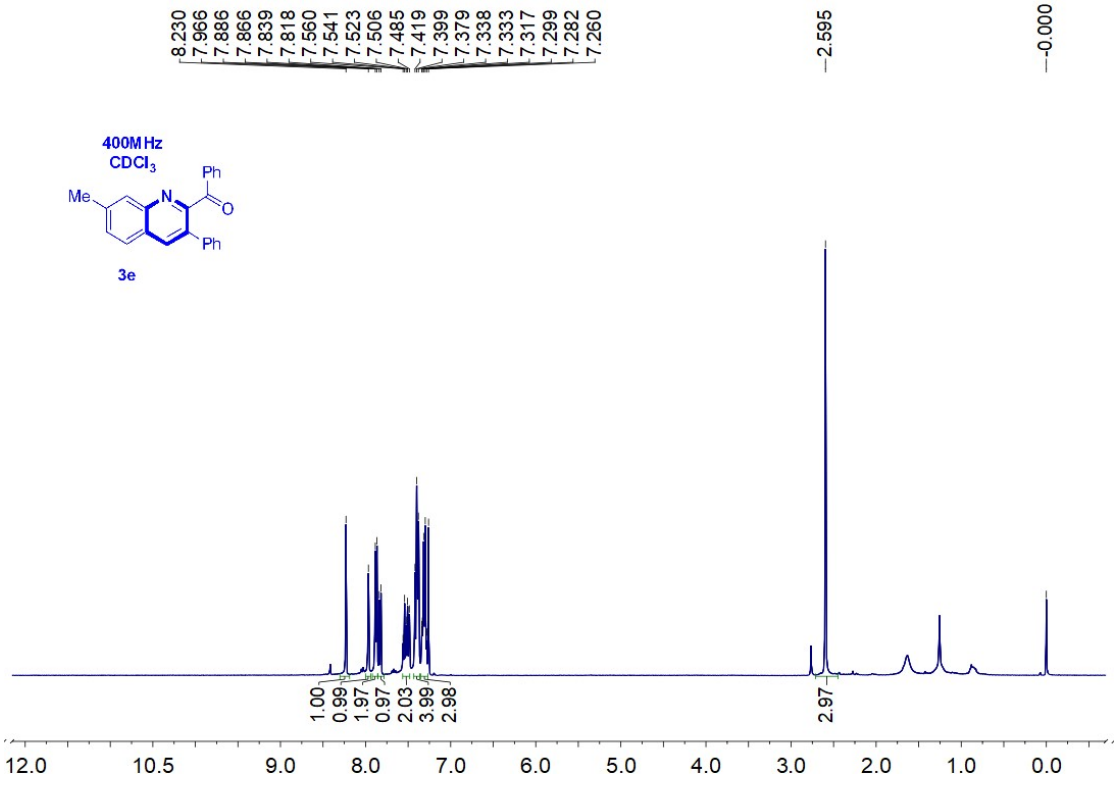
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7.523
7.506
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7.419
7.399
7.379
7.338
7.333
7.317
7.299
7.282
7.260
2.595
0.000
400MHz
CDCl3
Ph
Me
N
O
Ph
3e
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0.99
1.97
0.97
2.03
3.99
2.98
2.97
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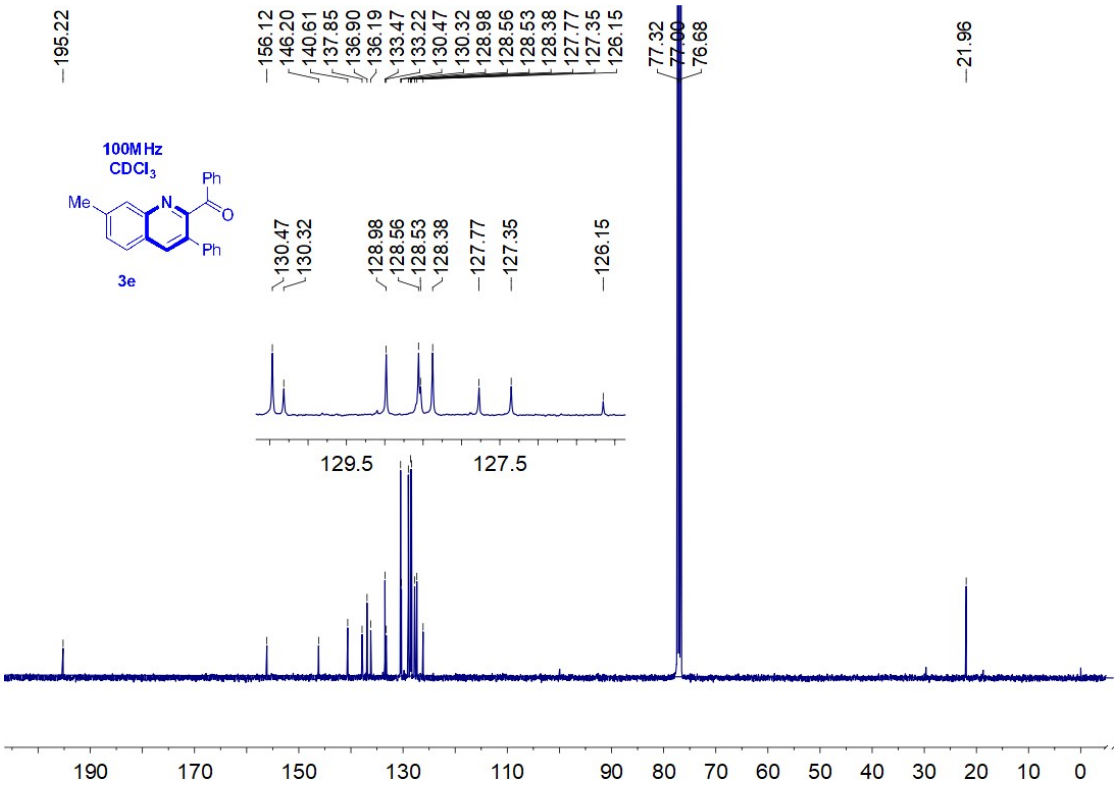
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O
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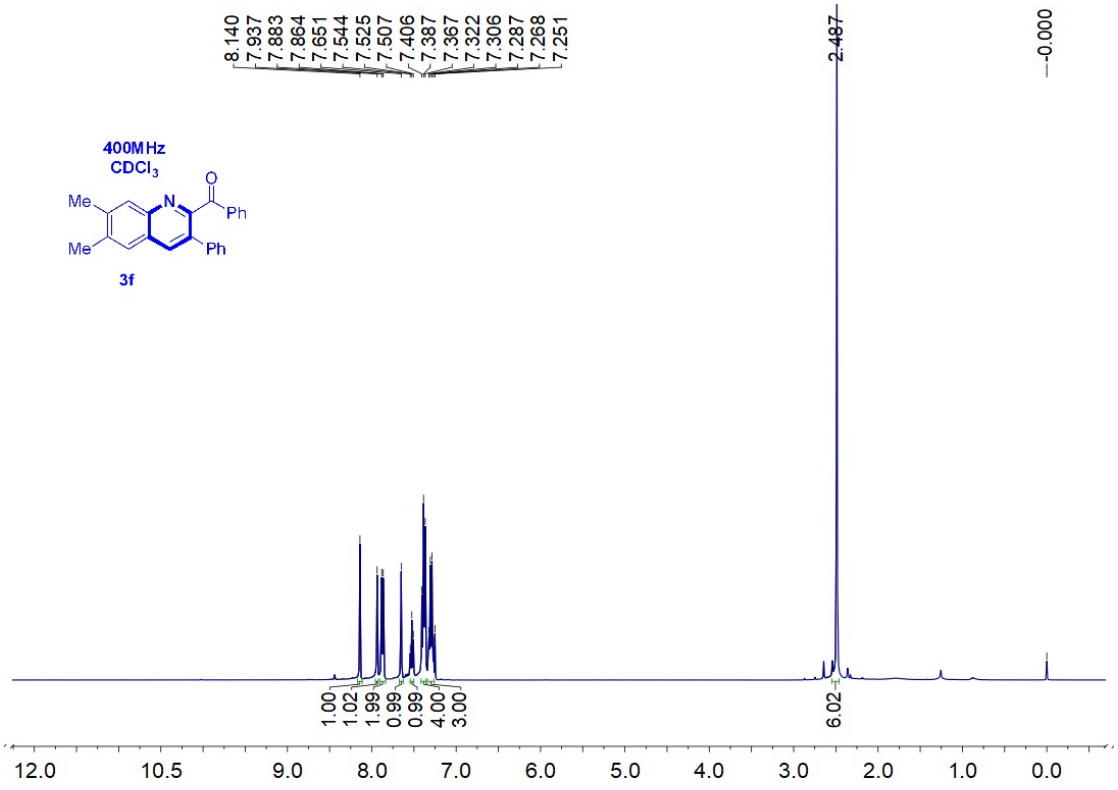
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0.99
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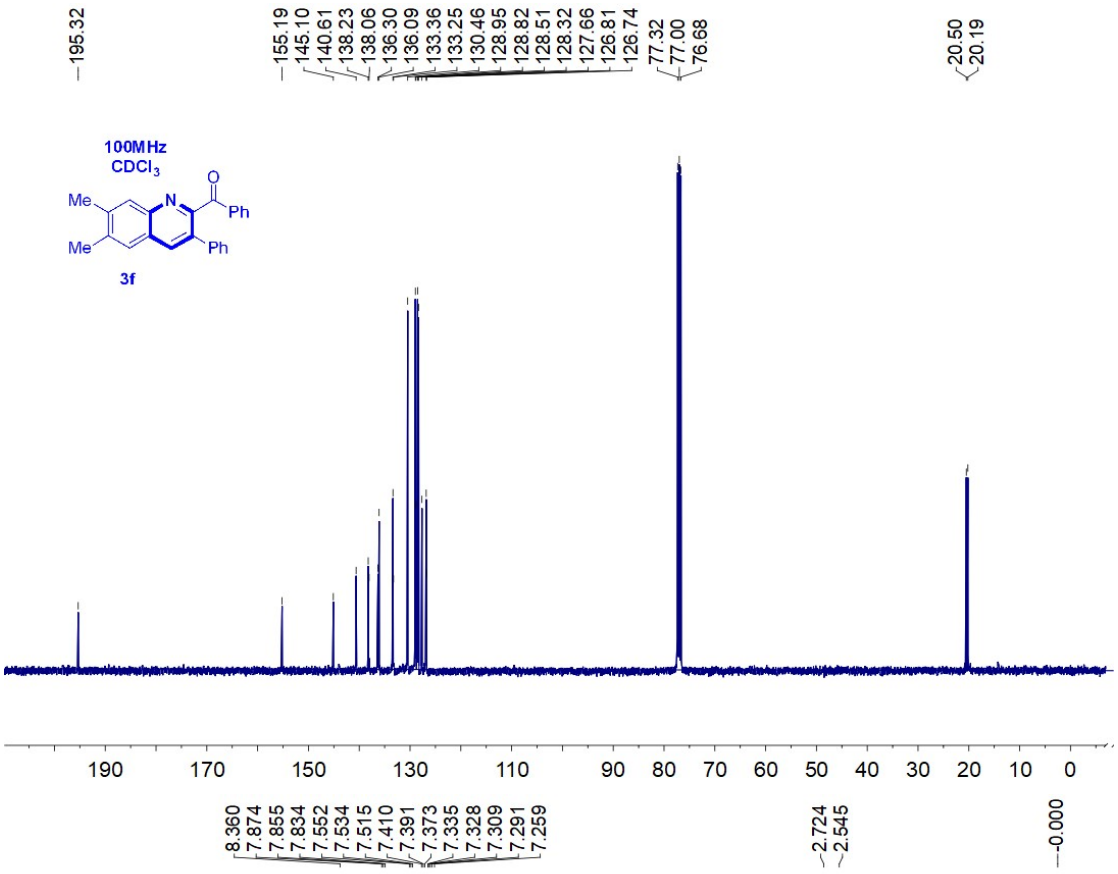
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126.74
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77.00
76.68
20.50
20.19
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Me
Me
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10
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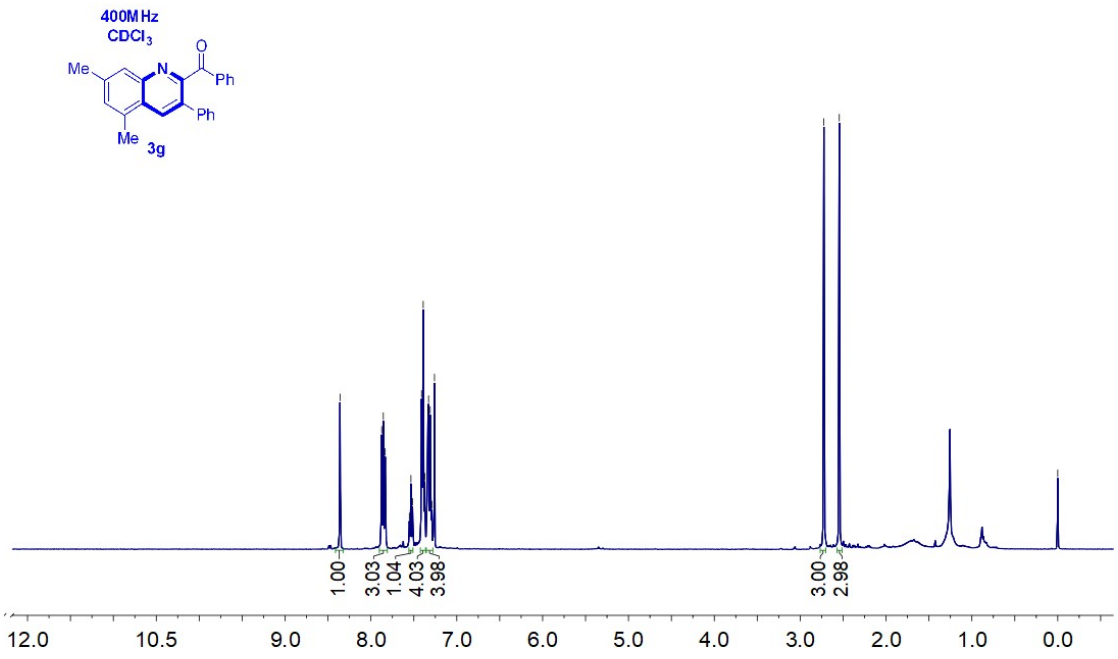
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4.03
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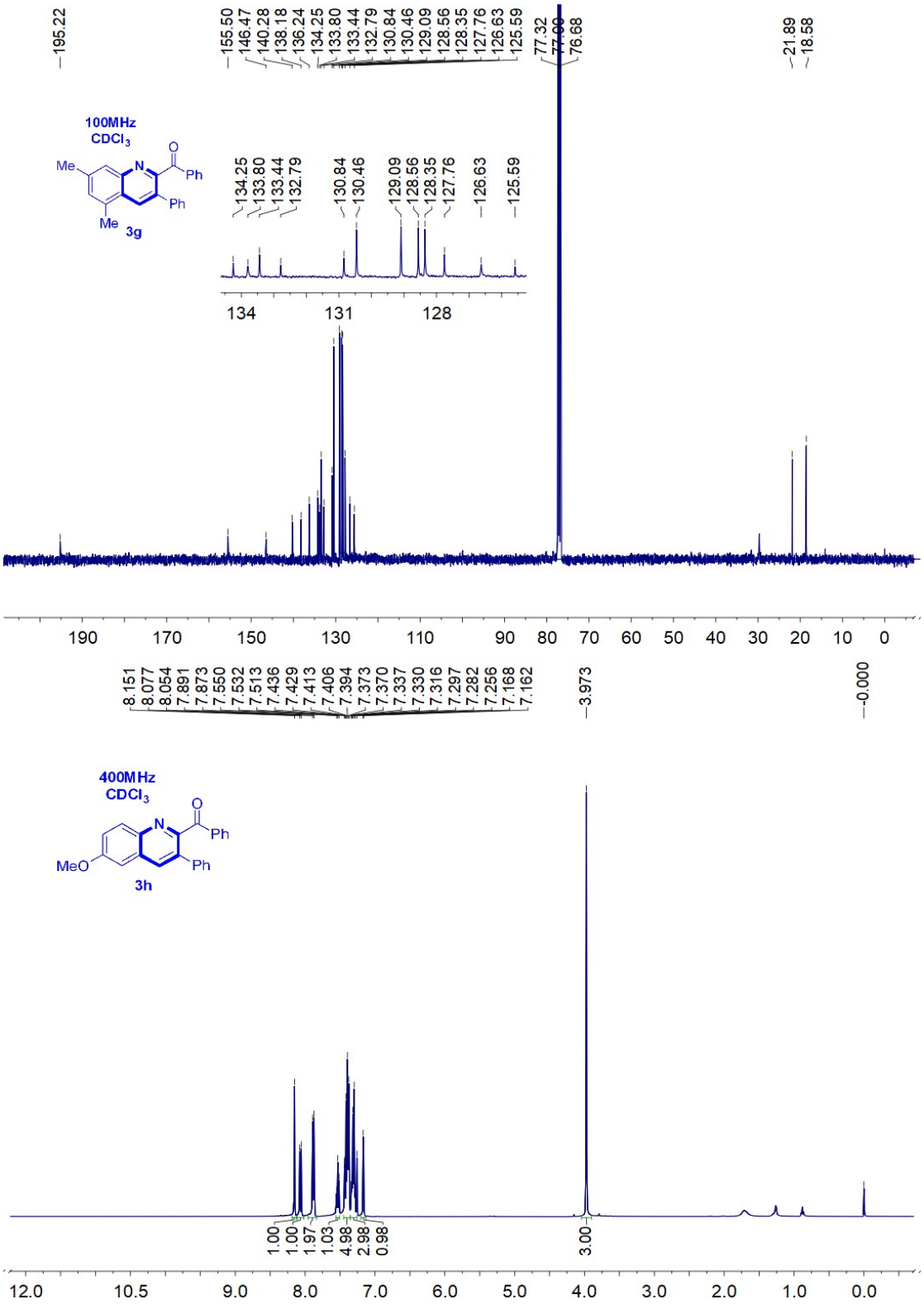
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Ph
Ph
3h
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1.00
1.97
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0.98
3.00
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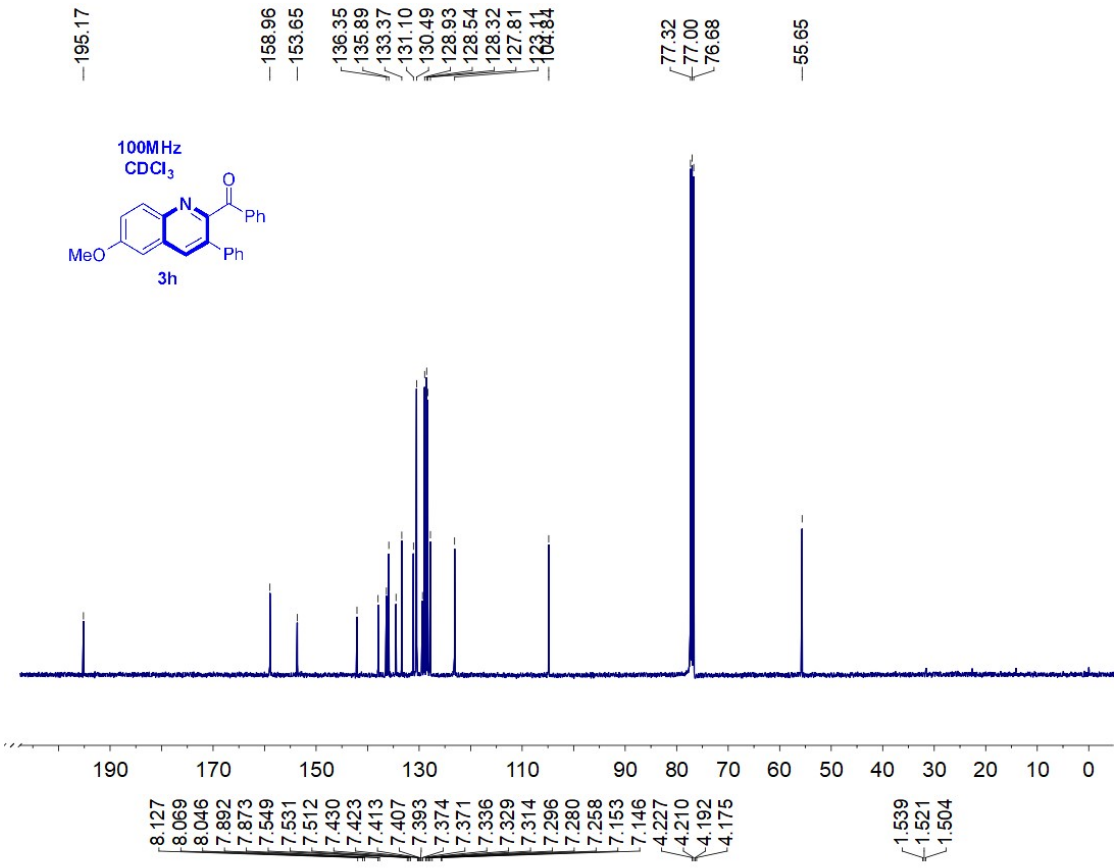
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55.65
100MHz
CDCl3
MeO
Ph
Ph
3h
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
8.127
8.069
8.046
7.892
7.873
7.549
7.531
7.512
7.430
7.423
7.413
7.407
7.393
7.374
7.371
7.336
7.329
7.314
7.296
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7.258
7.153
7.146
4.227
4.210
4.192
4.175
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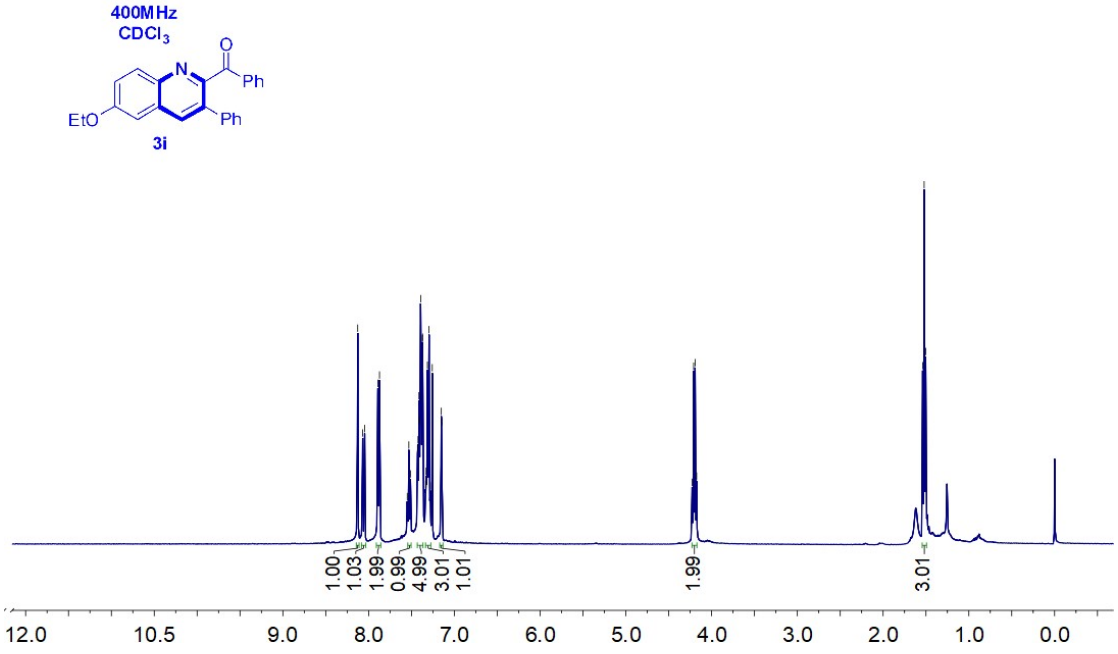
1.521
1.504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CDCl3
EtO
Ph
Ph
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1.03
1.99
0.99
4.99
3.01
1.01
1.99
3.01
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8.0
7.0
6.0
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4.0
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2.0
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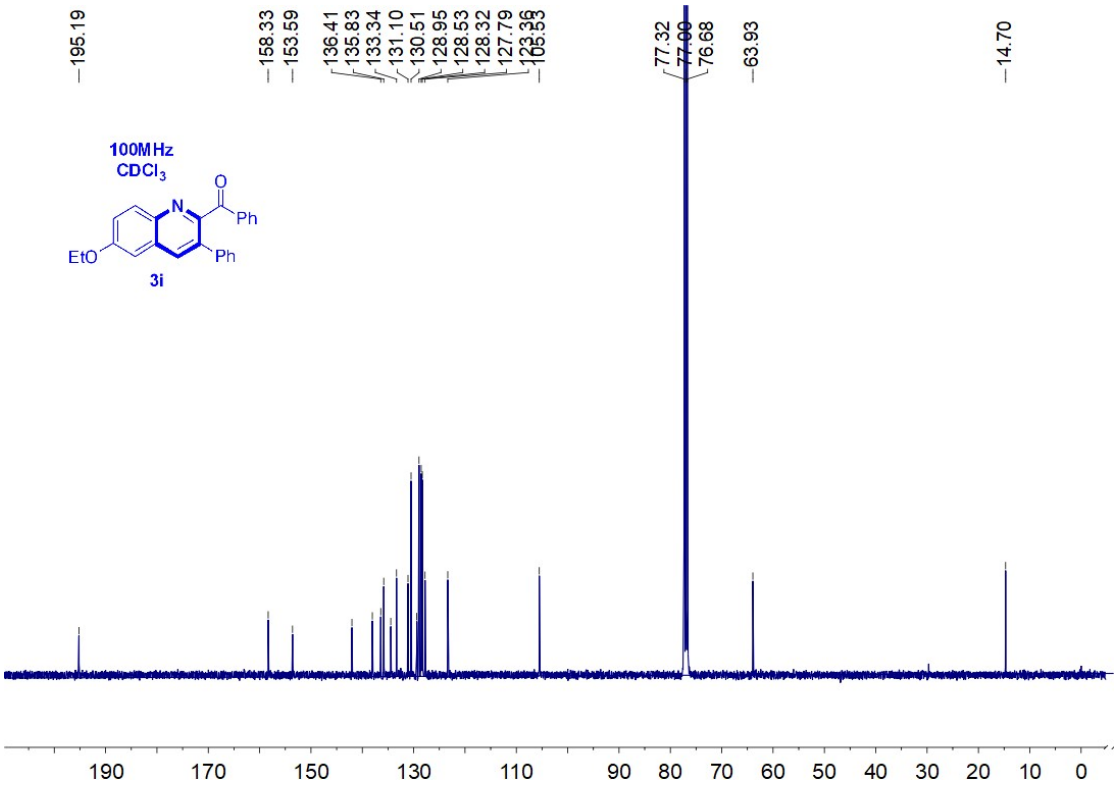
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130.51
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128.53
128.32
127.79
77.32
77.00
76.68
63.93
14.70
100MHz
CDCl3
EtO
Ph
Ph
3i
190
170
150
130
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80
70
60
50
40
30
20
10
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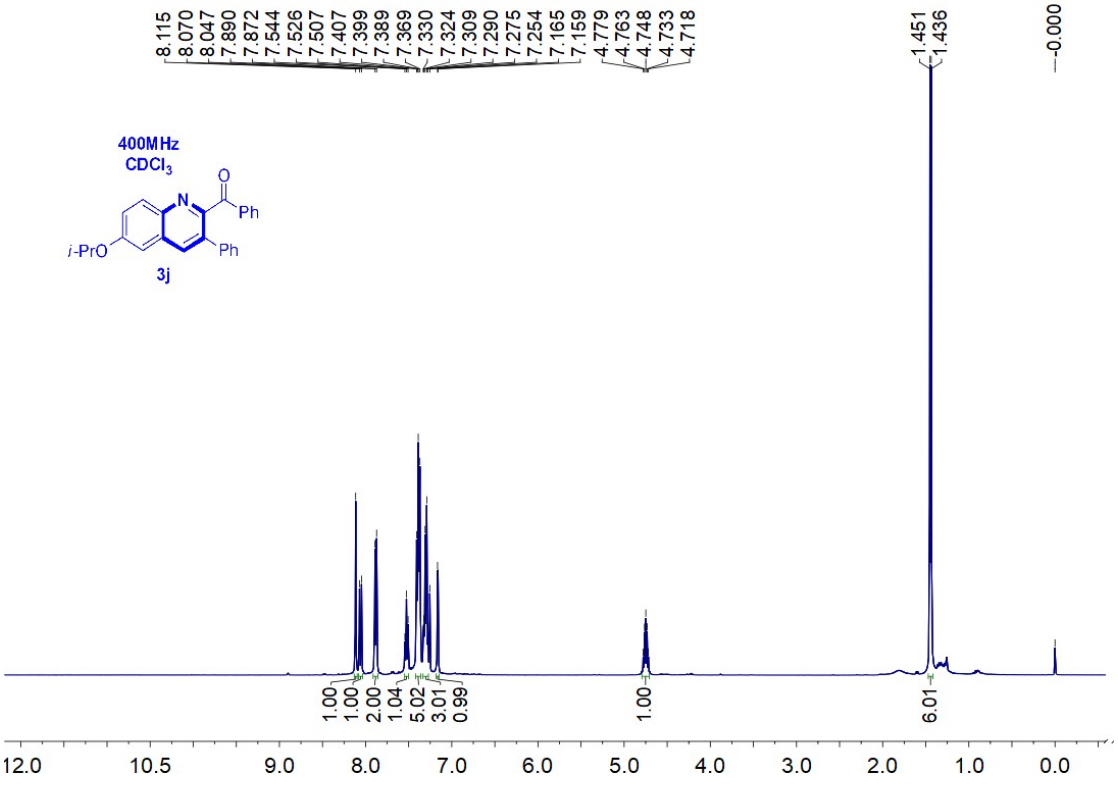
8.115
8.070
8.047
7.890
7.872
7.544
7.526
7.507
7.407
7.399
7.389
7.369
7.330
7.324
7.309
7.290
7.275
7.254
7.165
7.159
4.779
4.763
4.748
4.733
4.718
1.451
1.436
0.000
400MHz
CDCl3
i-PrO
Ph
Ph
3j
1.00
1.00
2.00
1.04
5.02
3.01
0.99
1.00
6.01
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10.5
9.0
8.0
7.0
6.0
5.0
4.0
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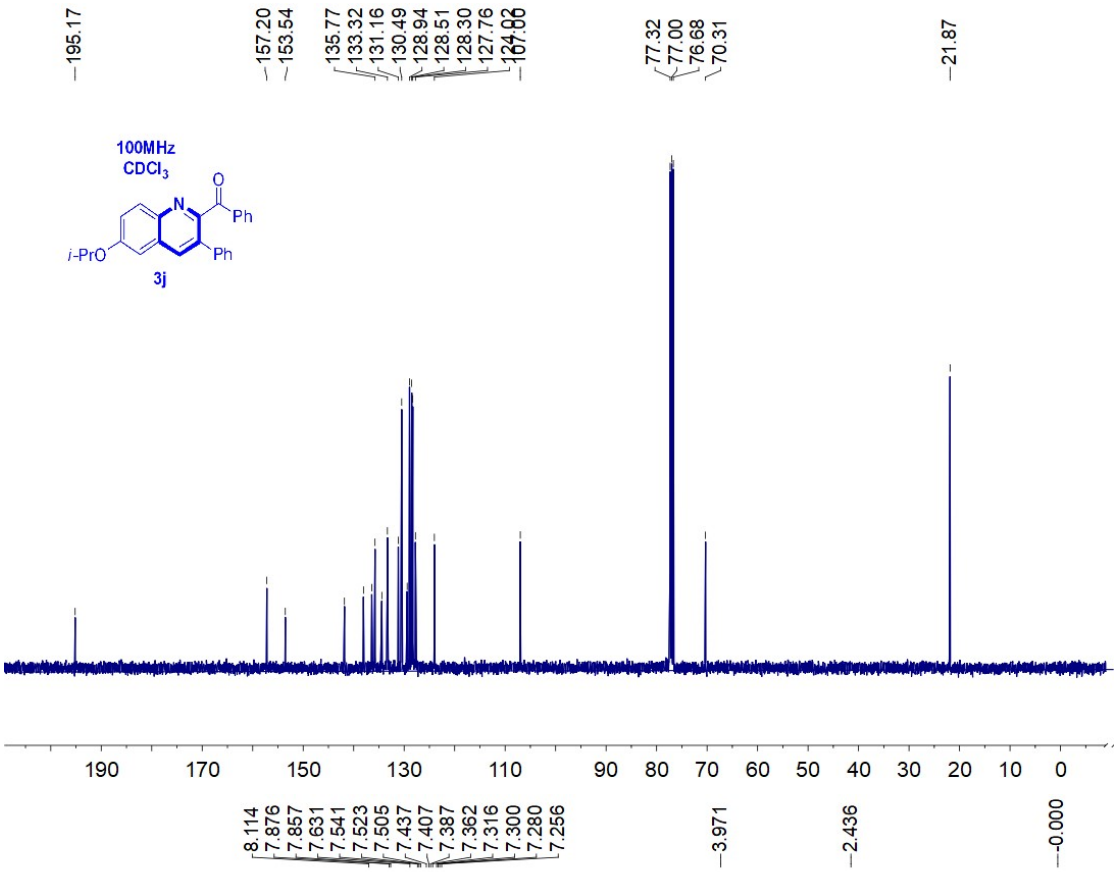
0.0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131.16
130.49
128.94
128.51
128.30
127.76
77.32
77.00
76.68
70.31
21.87
100MHz
CDCl3
i-PrO
Ph
Ph
3j
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
8.114
7.876
7.857
7.631
7.541
7.523
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7.387
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7.316
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7.280
7.256
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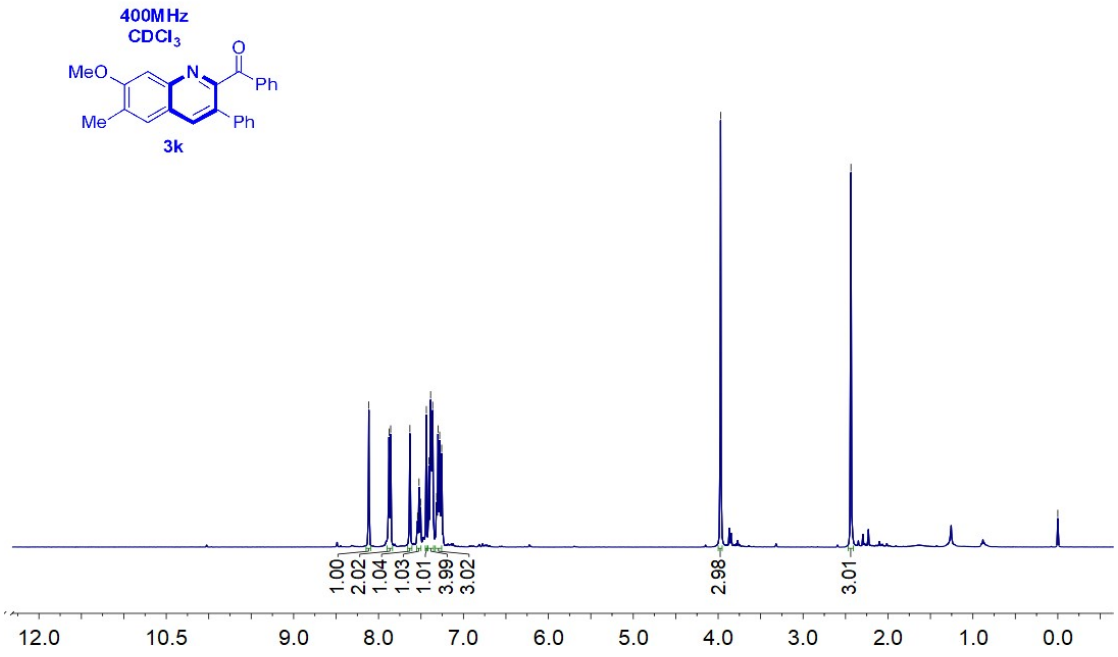
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Me
Ph
Ph
3k
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1.04
1.03
1.01
3.99
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2.98
3.01
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
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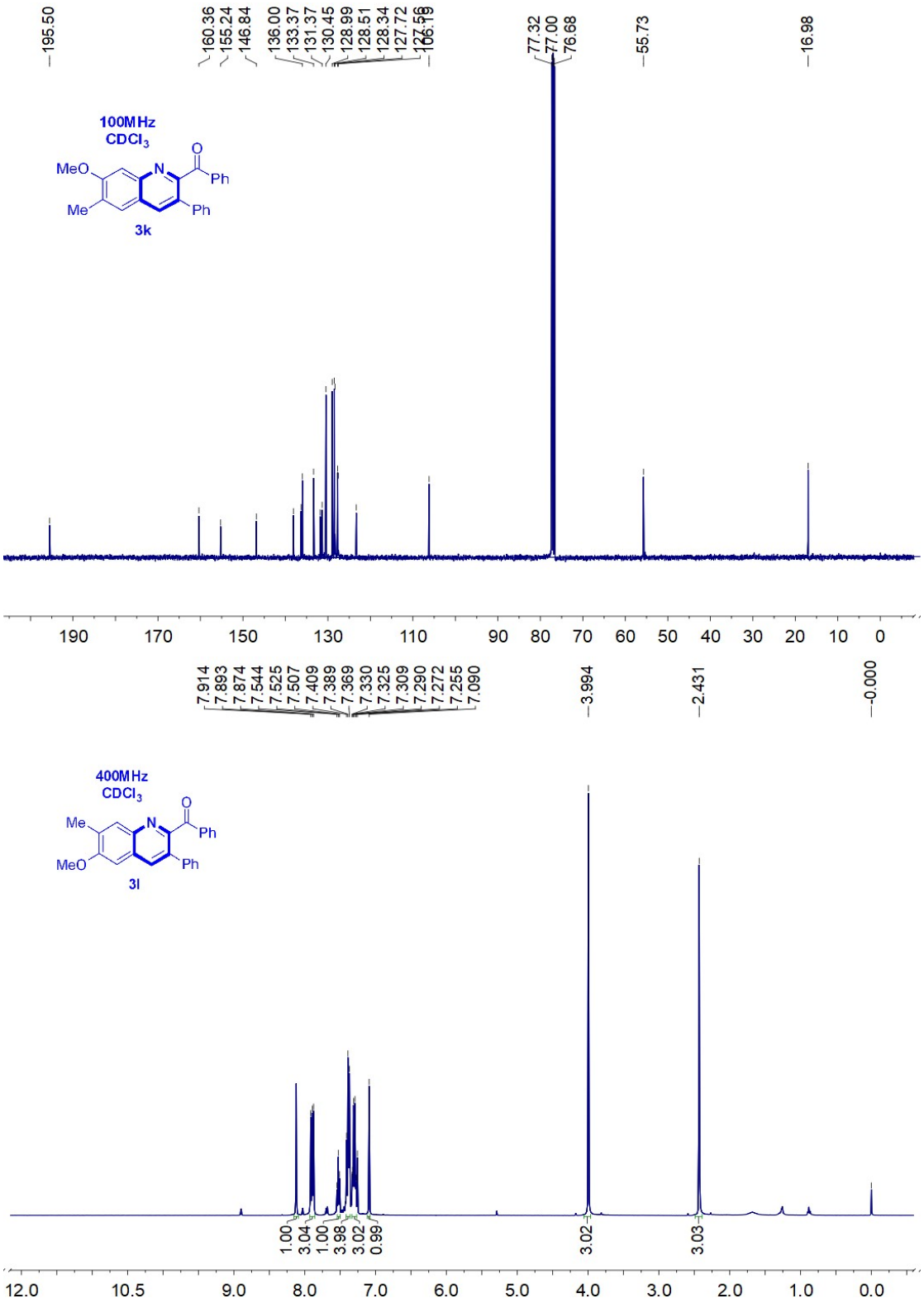
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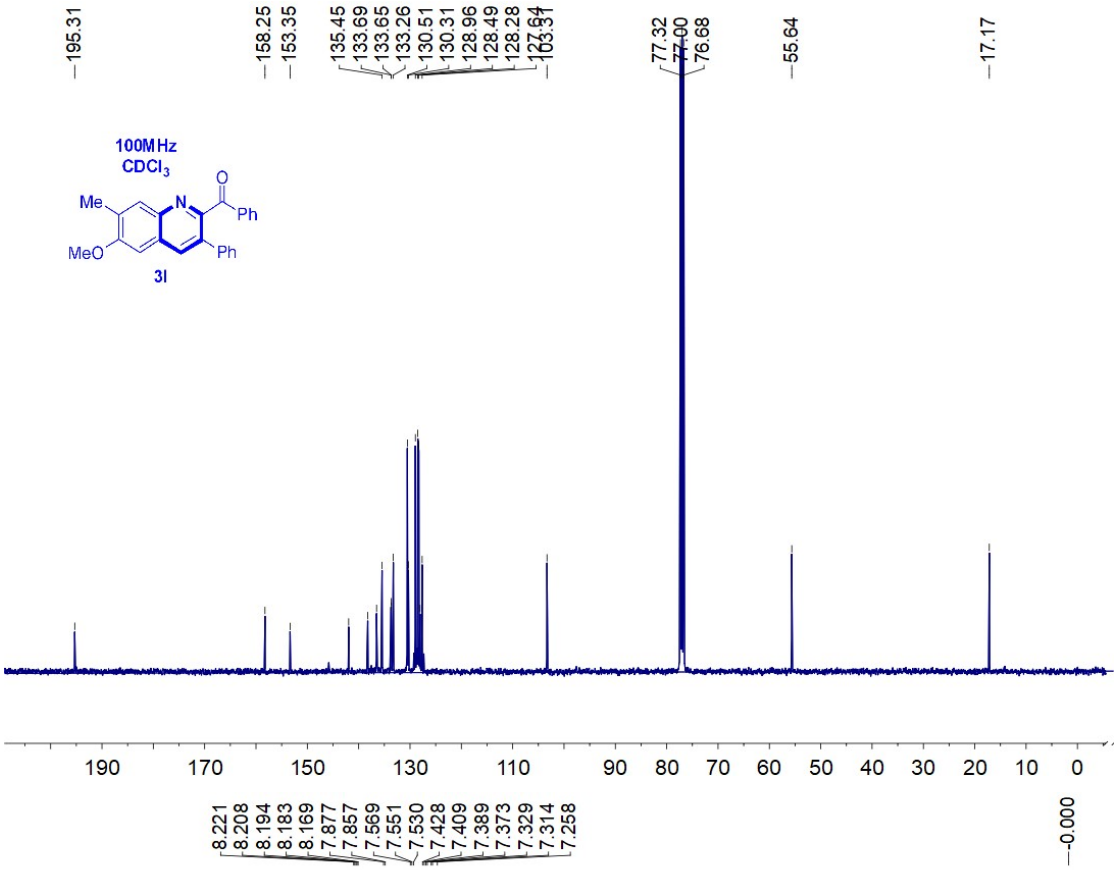
146.84
136.00
133.37
131.37
130.45
128.99
128.51
128.34
127.72
77.32
77.00
76.68
55.73
16.98
100MHz
CDCl3
MeO
Me
N
O
Ph
Ph
3k
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
7.914
7.893
7.874
7.544
7.525
7.507
7.409
7.389
7.369
7.330
7.325
7.309
7.290
7.272
7.255
7.090
3.994
2.431
0.000
400MHz
CDCl3
Me
MeO
N
O
Ph
Ph
3l
1.00
3.04
1.00
3.98
3.02
0.99
3.02
3.03
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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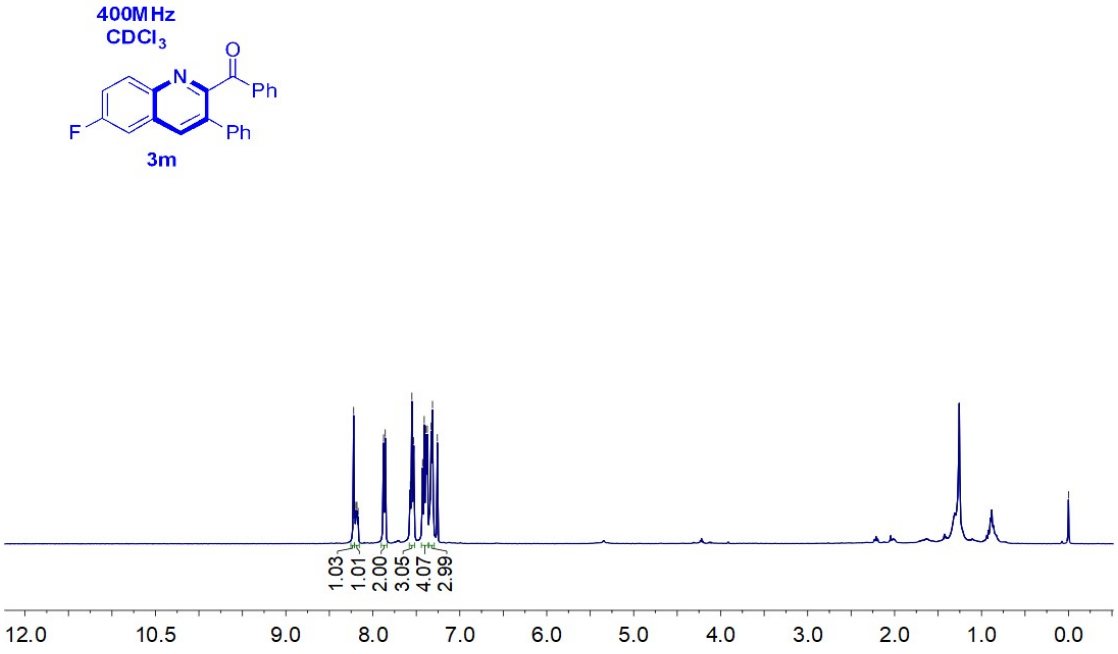
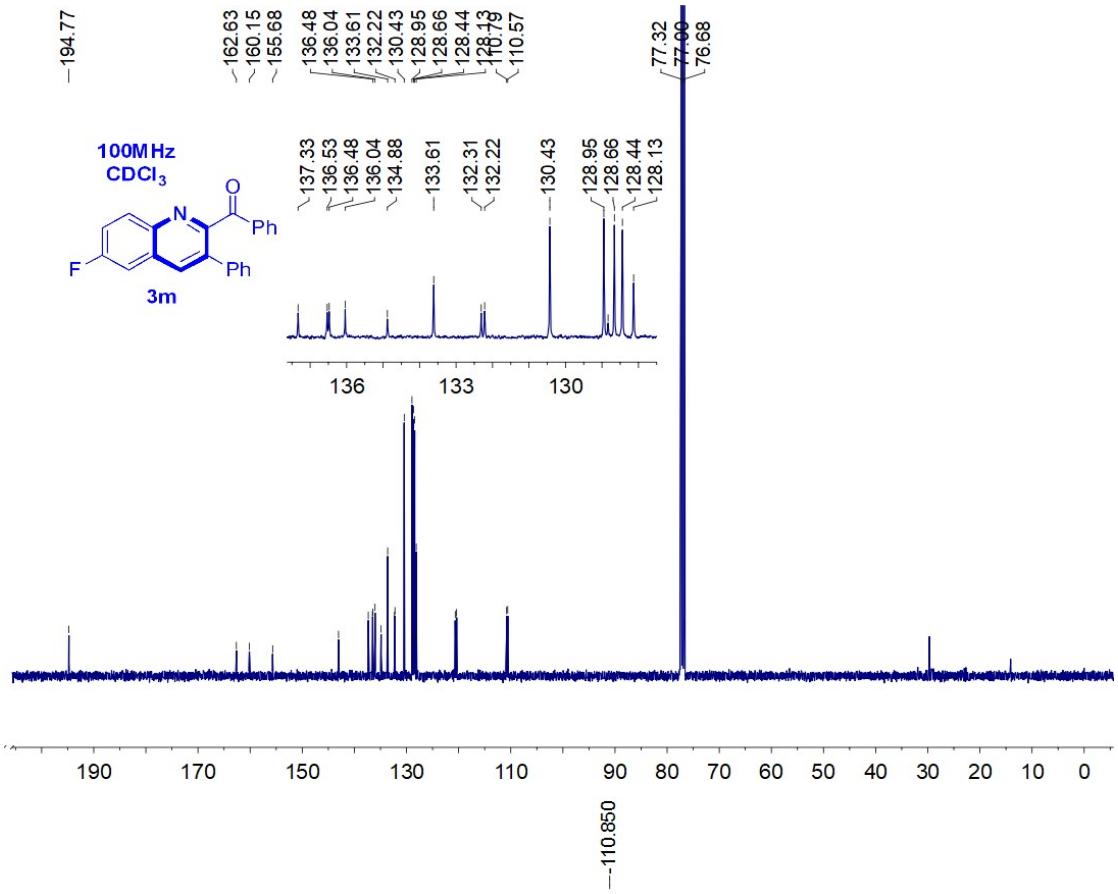
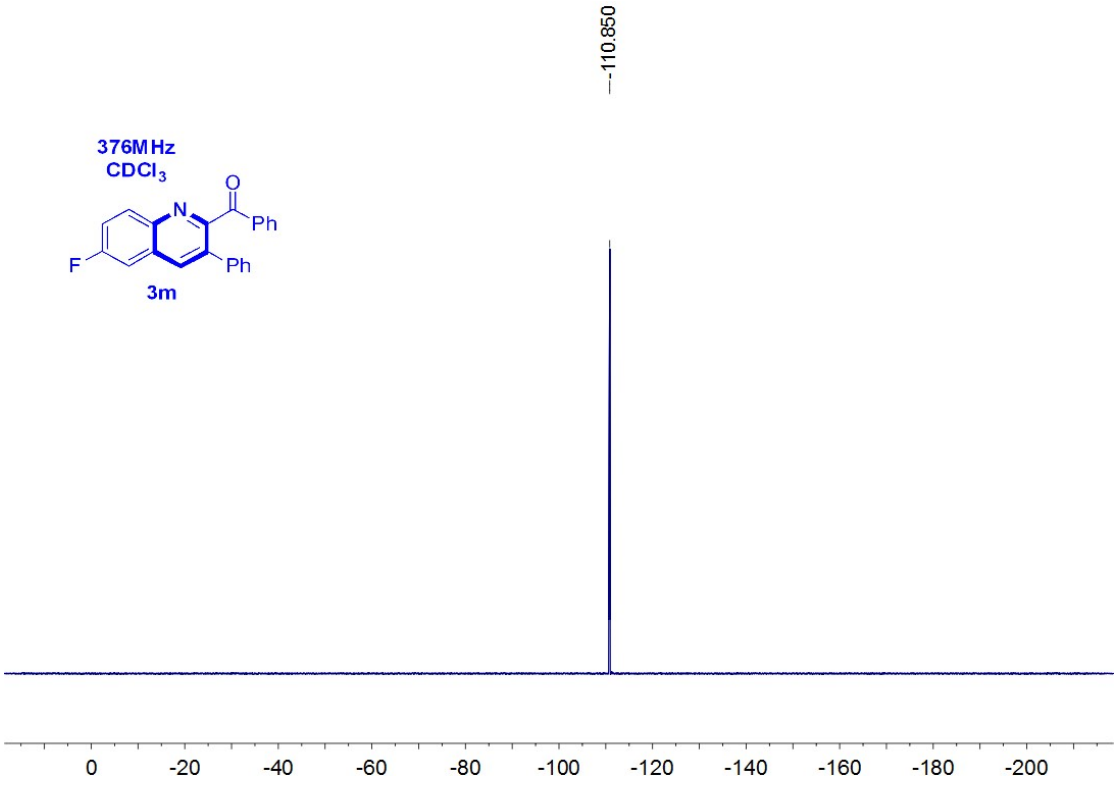
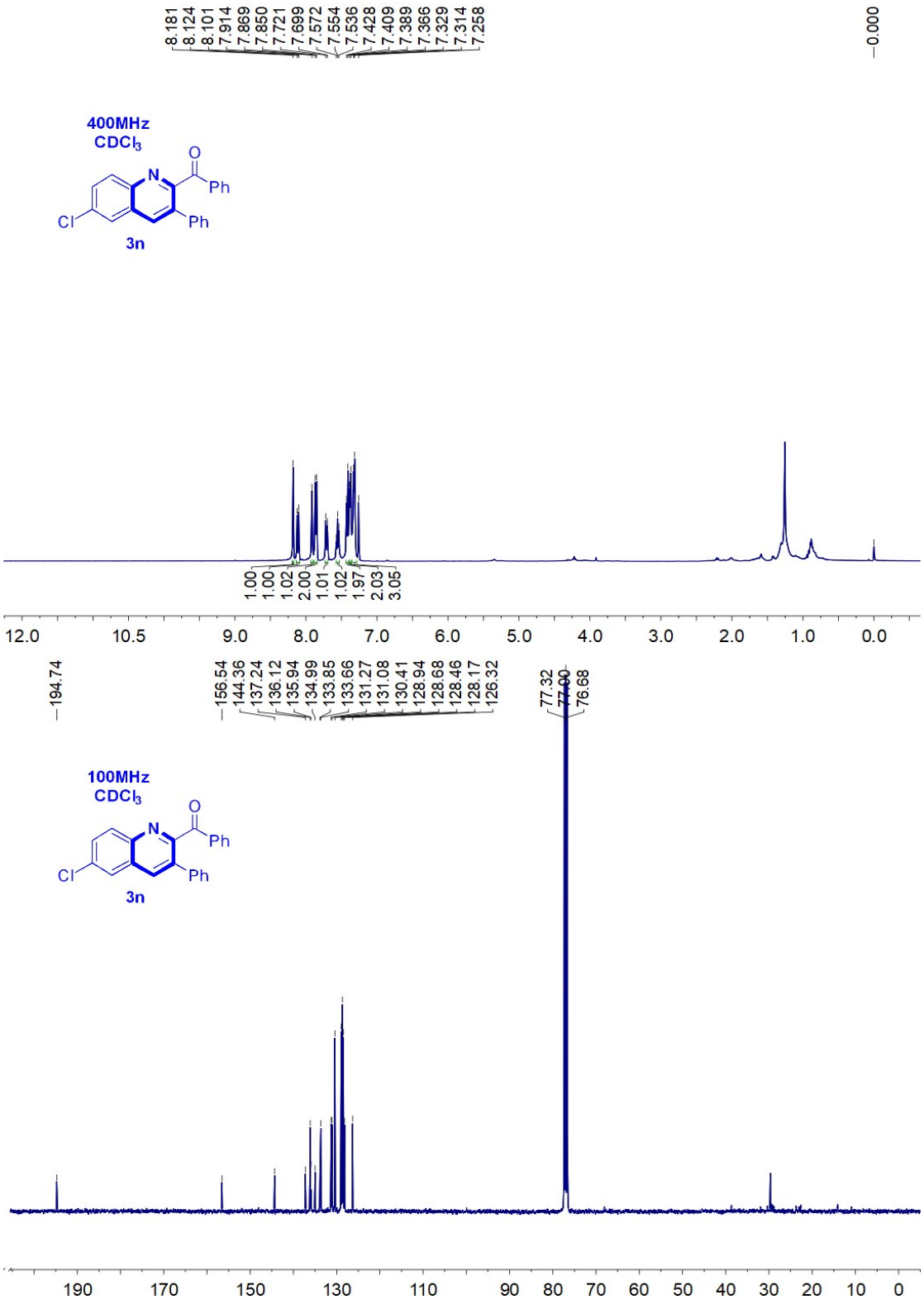
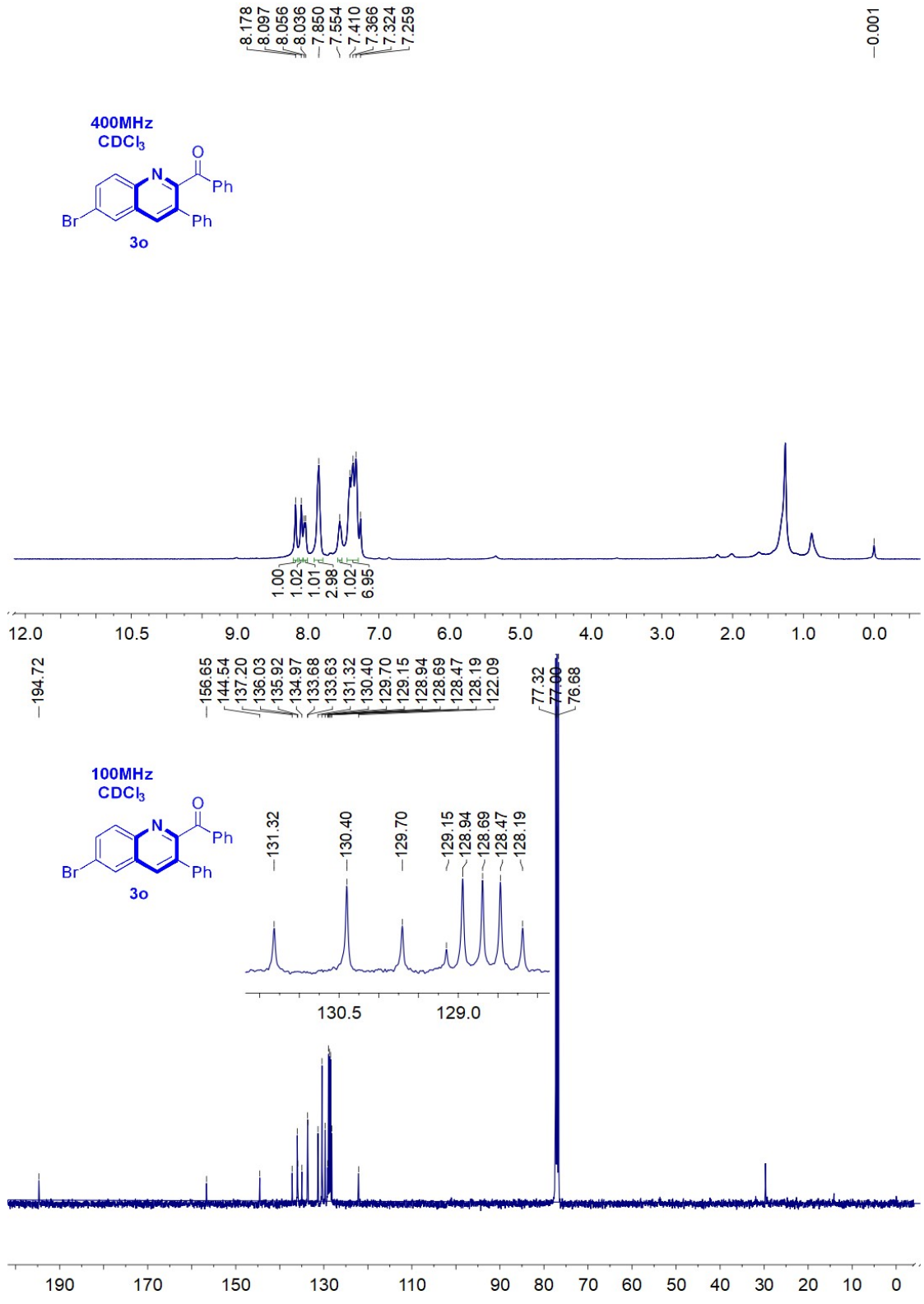
153.35
135.45
133.69
133.65
133.26
130.51
130.31
128.96
128.49
128.28
77.32
77.00
76.68
55.64
17.17
100MHz
CDCl3
Me
MeO
N
O
Ph
Ph
3l
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
8.221
8.208
8.194
8.183
8.169
7.877
7.857
7.569
7.551
7.530
7.428
7.409
7.389
7.373
7.329
7.314
7.258
0.000


400MHz
CDCl3
F
N
O
Ph
Ph
3m
1.03
1.01
2.00
3.05
4.07
2.99
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


194.77
162.63
160.15
155.68
136.48
136.04
133.61
132.22
130.43
128.95
128.66
128.44
110.57
77.32
77.00
76.68
100MHz
CDCl3
O
N
Ph
F
Ph
3m
137.33
136.53
136.48
136.04
134.88
133.61
132.31
132.22
130.43
128.95
128.66
128.44
128.13
136
133
130
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0


-110.850
376MHz
CDCl3
O
N
Ph
F
Ph
3m
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200


8.181
8.124
8.101
7.914
7.869
7.850
7.721
7.699
7.572
7.554
7.536
7.428
7.409
7.389
7.366
7.329
7.314
7.258
0.000
400MHz
CDCl3
O
N
Ph
Cl
Ph
3n
1.00
1.00
1.02
2.00
1.01
1.02
1.97
2.03
3.05
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
194.74
156.54
144.36
137.24
136.12
135.94
134.99
133.85
133.66
131.27
131.08
130.41
128.94
128.68
128.46
128.17
126.32
77.32
77.00
76.68
100MHz
CDCl3
O
N
Ph
Cl
Ph
3n
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0


8.178
8.097
8.056
8.036
7.850
7.554
7.410
7.366
7.324
7.259
0.001
400MHz
CDCl3
O
N
Ph
Br
Ph
3o
1.00
1.02
1.01
2.98
1.02
6.95
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
194.72
156.65
144.54
137.20
136.03
135.92
134.97
133.68
133.63
131.32
130.40
129.70
129.15
128.94
128.69
128.47
128.19
122.09
77.32
77.00
76.68
100MHz
CDCl3
131.32
130.40
129.70
129.15
128.94
128.69
128.47
128.19
130.5
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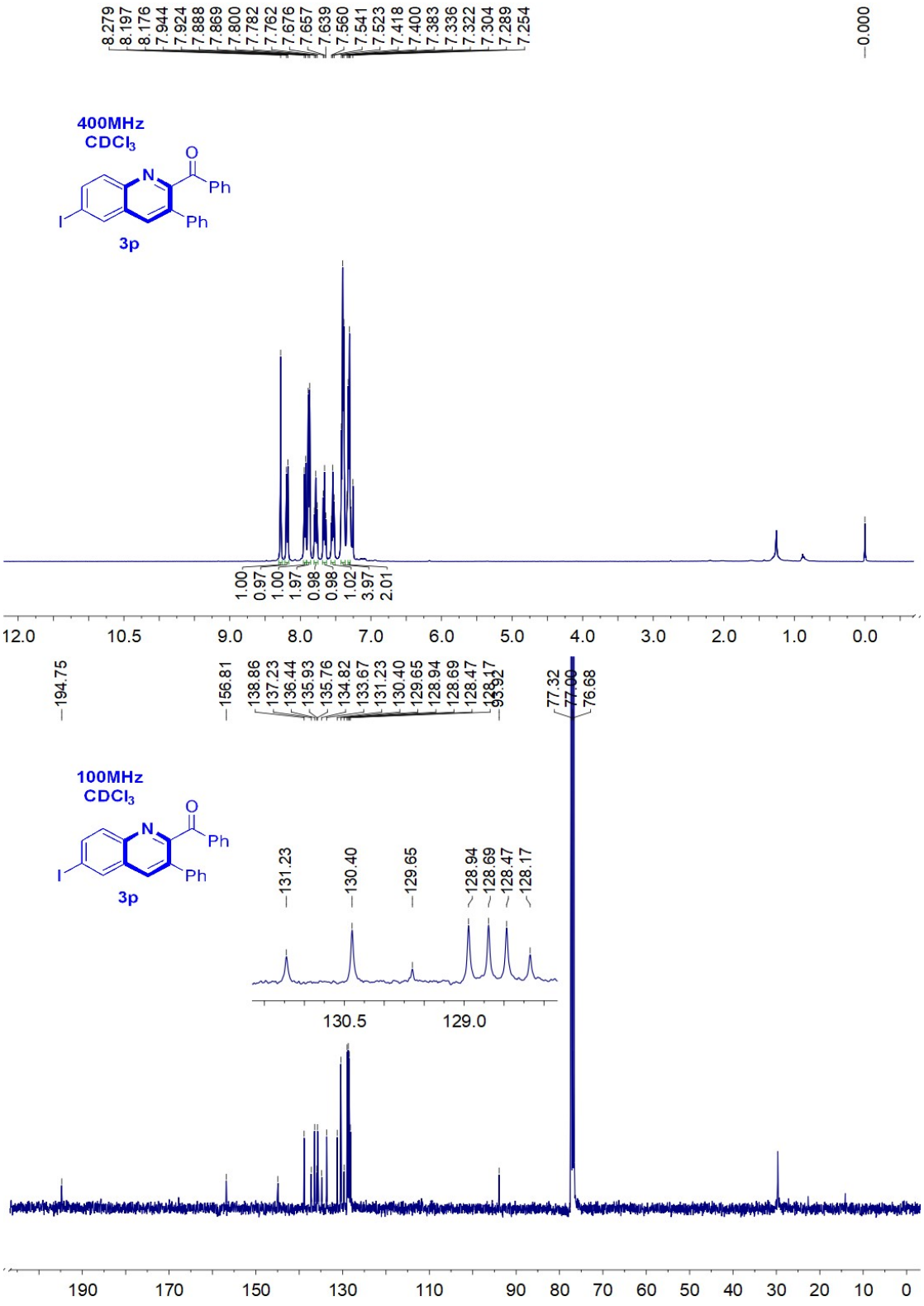
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0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8.197
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7.888
7.869
7.800
7.782
7.762
7.676
7.657
7.639
7.560
7.541
7.523
7.418
7.400
7.383
7.336
7.322
7.304
7.289
7.254
0.000
400MHz
CDCl3
O
N
Ph
I
Ph
3p
1.00
0.97
1.00
1.97
0.98
0.98
1.02
3.97
2.01
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
194.75
156.81
138.86
137.23
136.44
135.93
135.76
134.82
133.67
131.23
130.40
129.65
128.94
128.69
128.47
128.17
77.32
77.00
76.68
100MHz
CDCl3
3p
131.23
130.40
129.65
128.94
128.69
128.47
128.17
130.5
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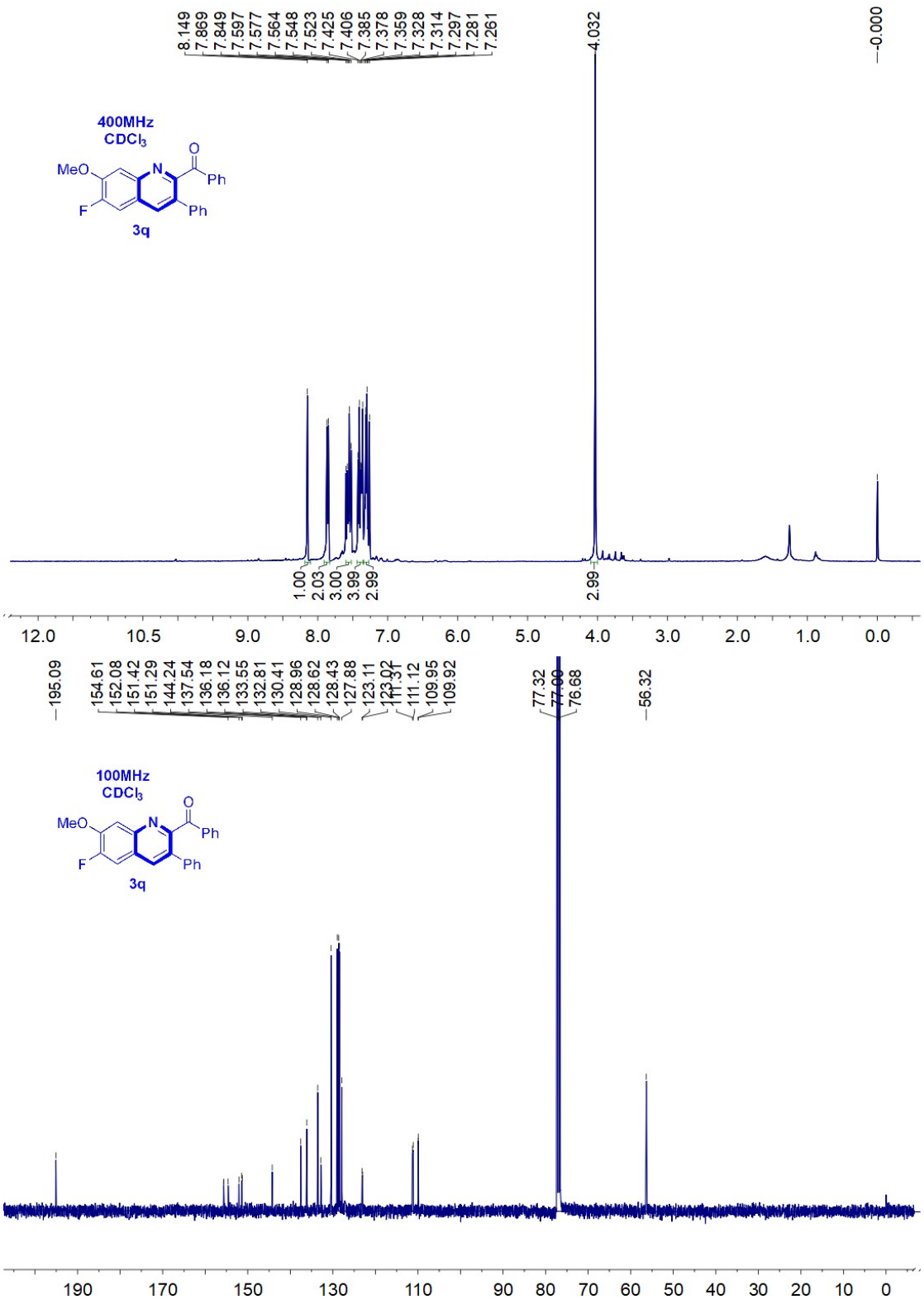
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0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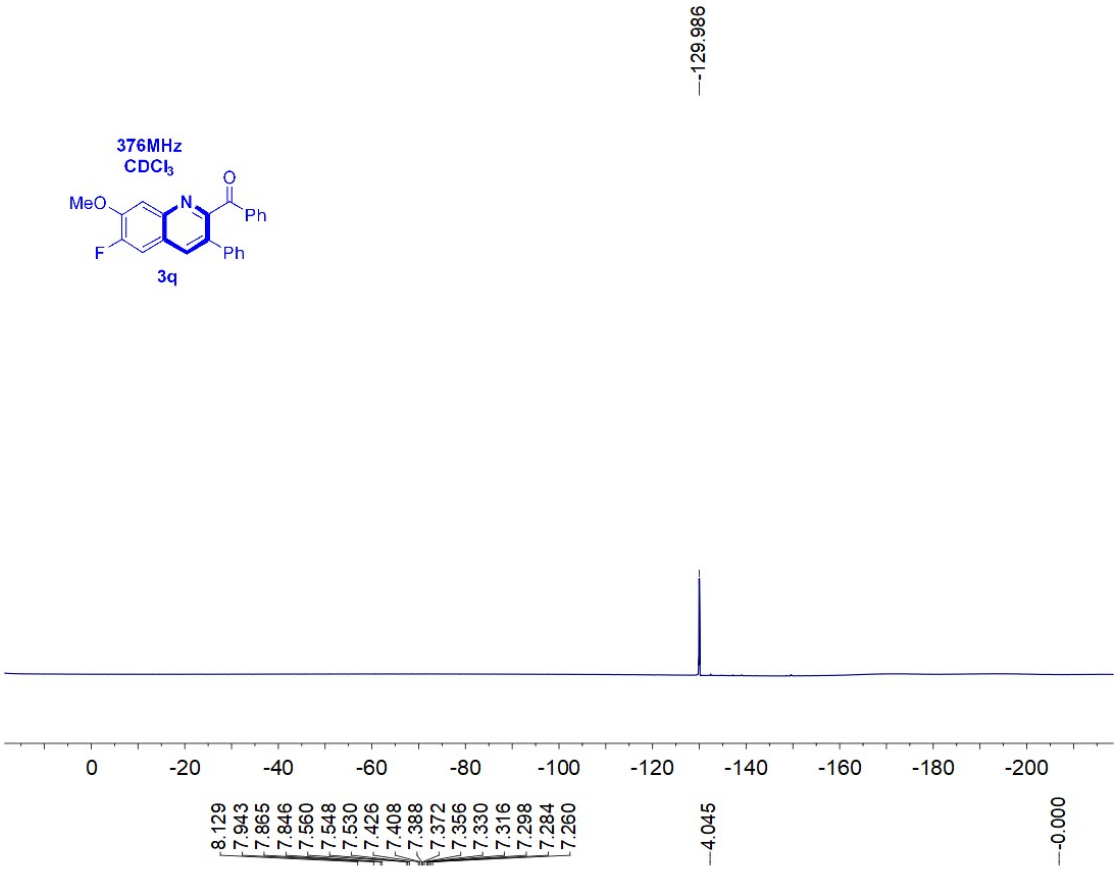
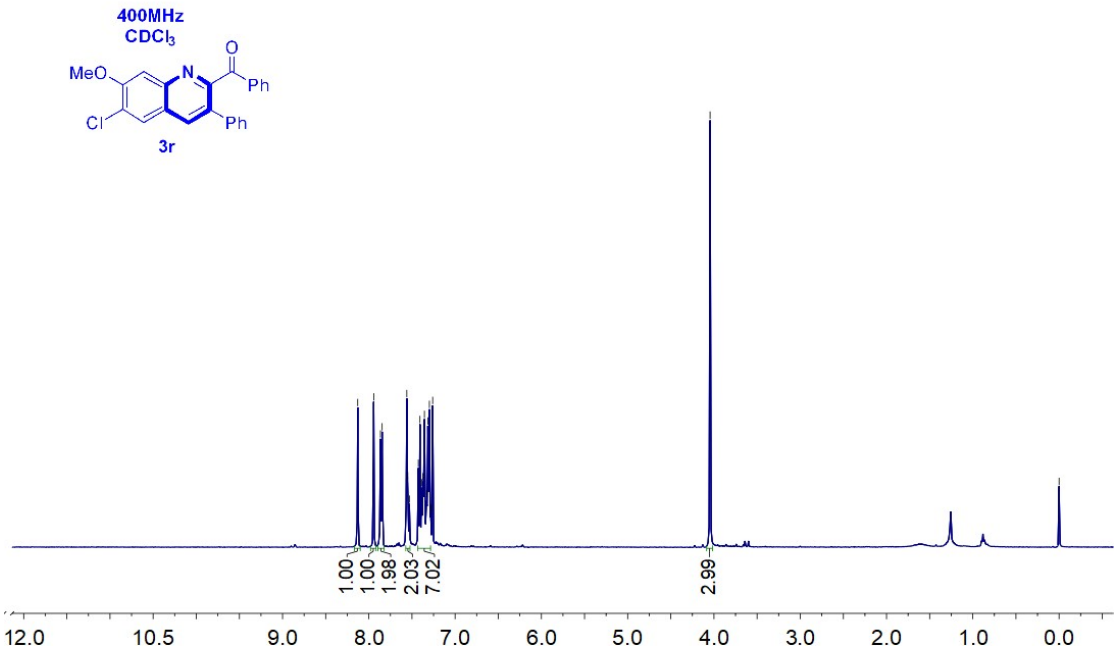
7.548
7.523
7.425
7.406
7.385
7.378
7.359
7.328
7.314
7.297
7.281
7.261
4.032
0.000
400MHz
CDCl3
MeO
F
N
O
Ph
Ph
3q
1.00
2.03
3.00
3.99
2.99
2.99
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
195.09
154.61
152.08
151.42
151.29
144.24
137.54
136.18
136.12
133.55
132.81
130.41
128.96
128.62
128.43
127.88
123.11
123.02
111.31
111.12
109.95
109.92
77.32
77.00
76.68
56.32
100MHz
CDCl3
MeO
F
N
O
Ph
Ph
3q
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0


376MHz
CDCl3
MeO
F
N
O
Ph
Ph
3q
-129.986
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
8.129
7.943
7.865
7.846
7.560
7.548
7.530
7.426
7.408
7.388
7.372
7.356
7.330
7.316
7.298
7.284
7.260
4.045
0.000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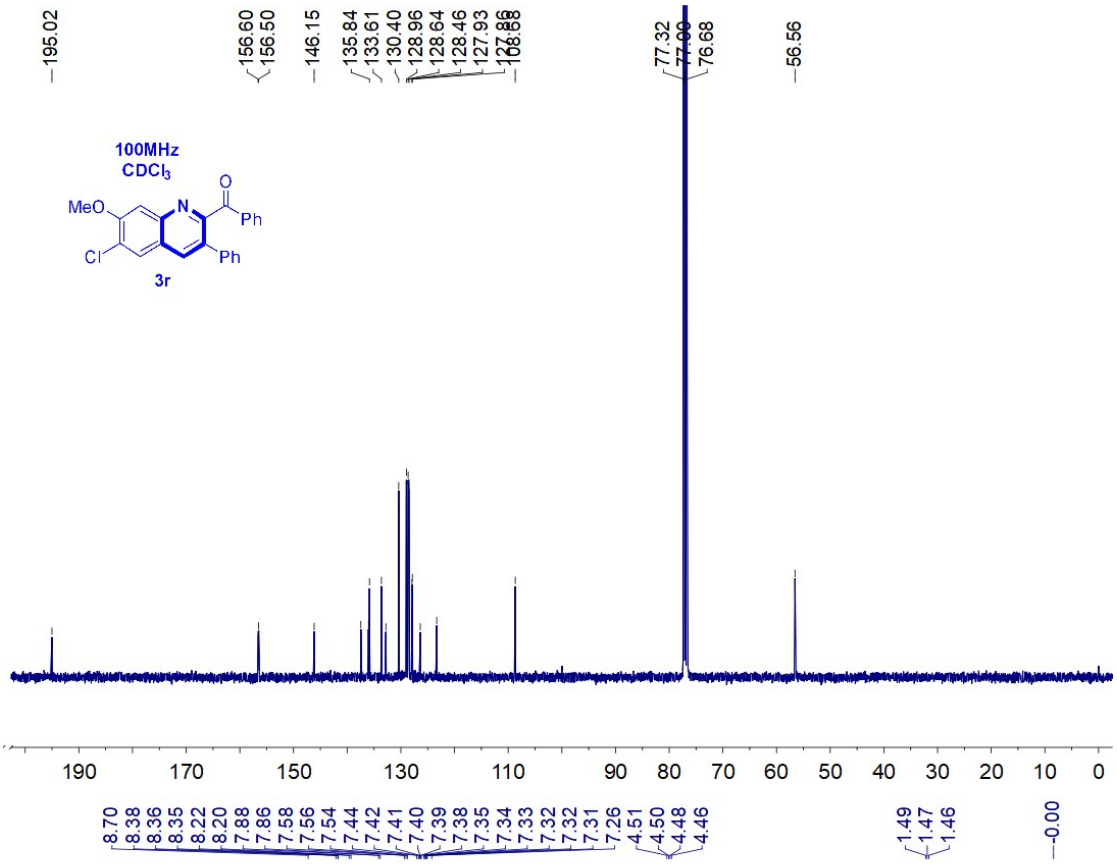
MeO
Cl
N
O
Ph
Ph
3r
1.00
1.00
1.98
2.03
7.02
2.99
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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133.61
130.40
128.96
128.64
128.46
127.93
77.32
77.00
76.68
56.56
100MHz
CDCl3
MeO
Cl
N
O
Ph
Ph
3r
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
8.70
8.38
8.36
8.35
8.22
8.20
7.88
7.86
7.58
7.56
7.54
7.44
7.42
7.41
7.40
7.39
7.38
7.35
7.34
7.33
7.32
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7.31
7.26
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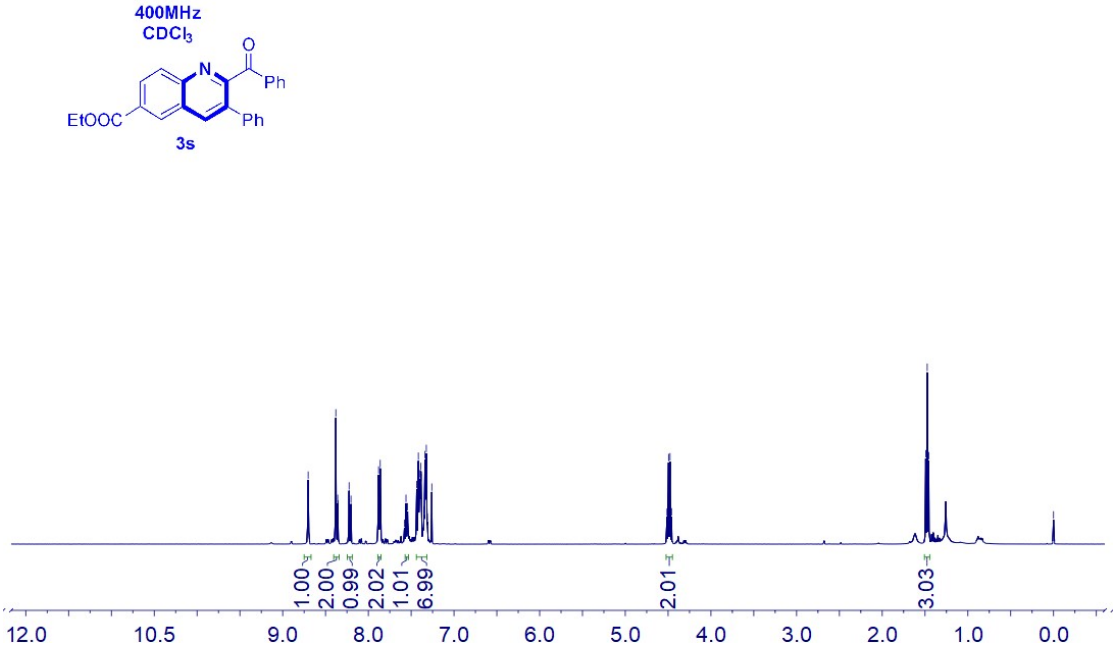
4.46
1.49
1.47
1.46
0.00


400MHz
CDCl3
EtOOC
N
O
Ph
Ph
3s
1.00
2.00
0.99
2.02
1.01
6.99
2.01
3.03
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9.0
8.0
7.0
6.0
5.0
4.0
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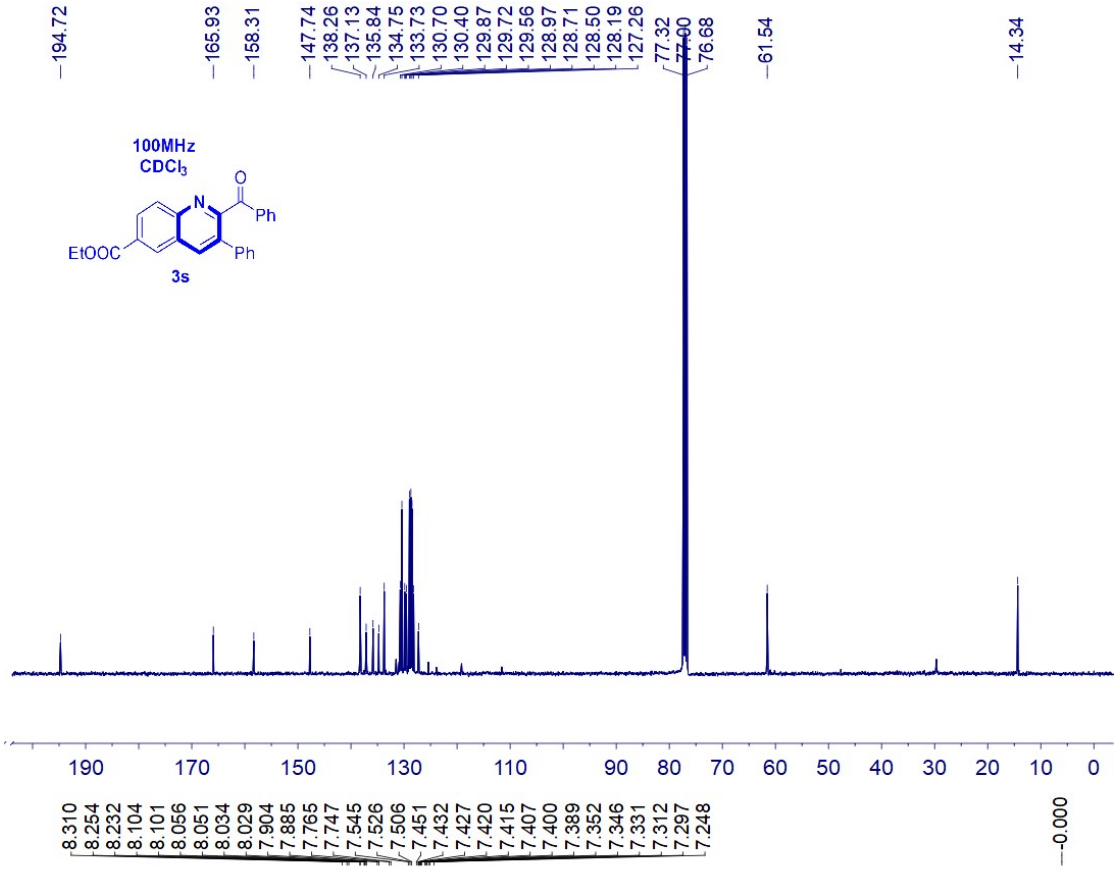
2.0
1.0
0.0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130.70
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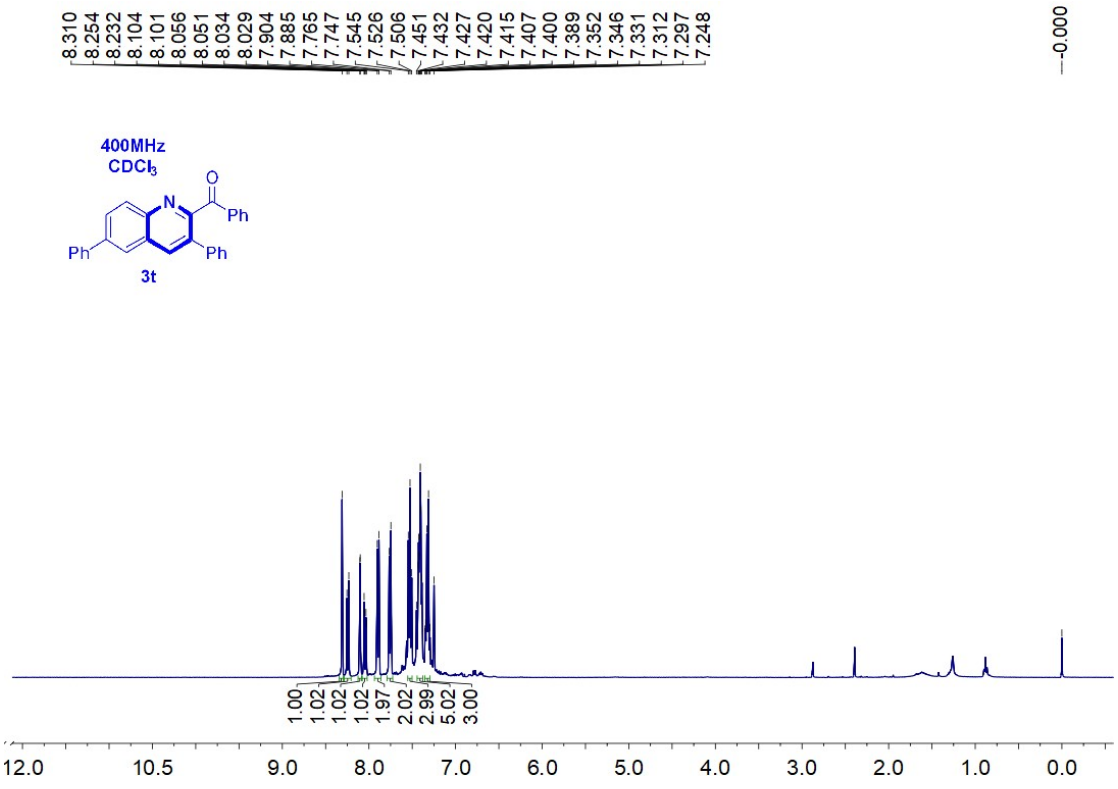
129.87
129.72
129.56
128.97
128.71
128.50
128.19
127.26
77.32
77.00
76.68
61.54
14.34
100MHz
CDCl3
O
N
Ph
EtOOC
Ph
3s
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0


8.310
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8.232
8.104
8.101
8.056
8.051
8.034
8.029
7.904
7.885
7.765
7.747
7.545
7.526
7.506
7.451
7.432
7.427
7.420
7.415
7.407
7.400
7.389
7.352
7.346
7.331
7.312
7.297
7.248
0.000
400MHz
CDCl3
O
N
Ph
Ph
Ph
3t
1.00
1.02
1.02
1.02
1.97
2.02
2.99
5.02
3.00
12.0
10.5
9.0
8.0
7.0
6.0
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4.0
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1.0
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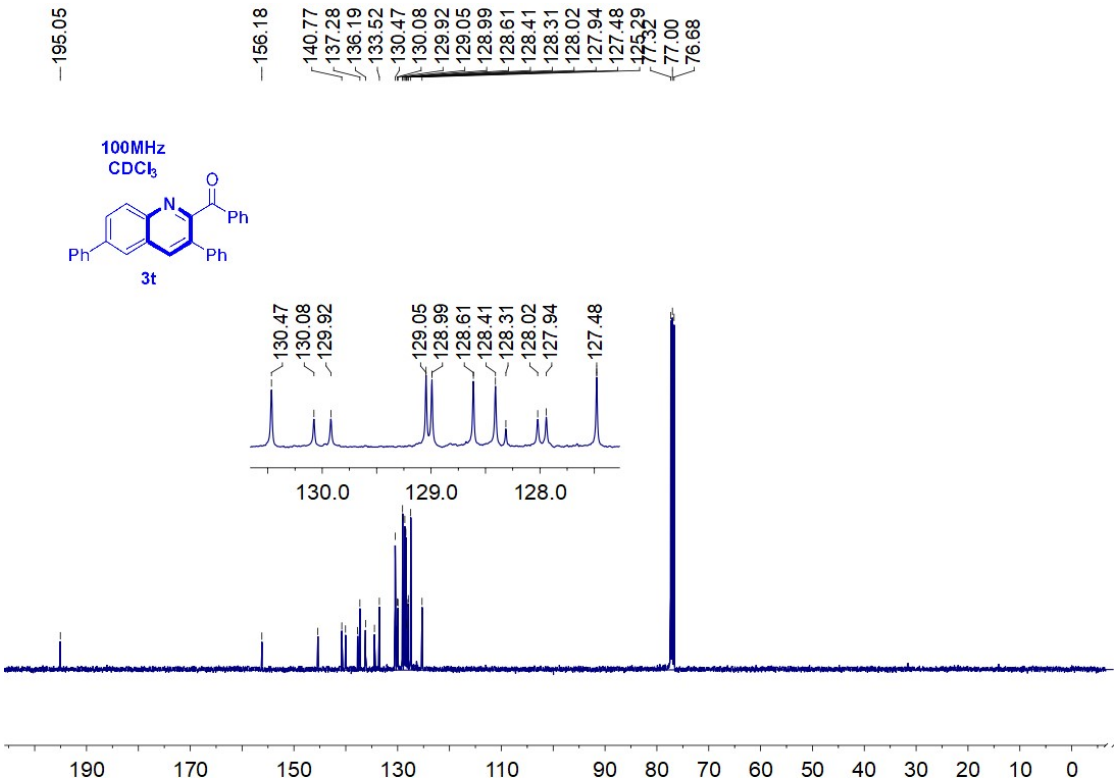
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133.52
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130.08
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129.05
128.99
128.61
128.41
128.31
128.02
127.94
127.48
125.29
77.32
77.00
76.68
100MHz
CDCl3
Ph
Ph
Ph
3t
130.47
130.08
129.92
129.05
128.99
128.61
128.41
128.31
128.02
127.94
127.48
130.0
129.0
128.0
190
170
150
130
110
90
80
70
60
50
40
30
20
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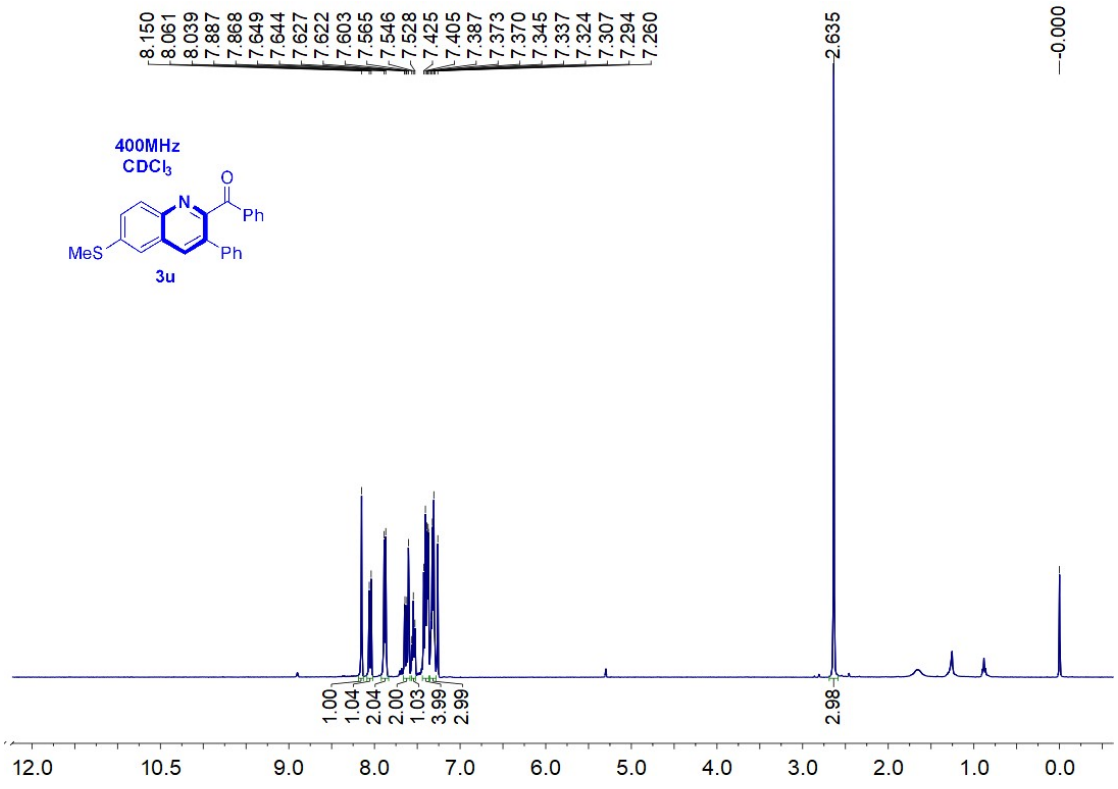
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MeS
Ph
Ph
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2.99
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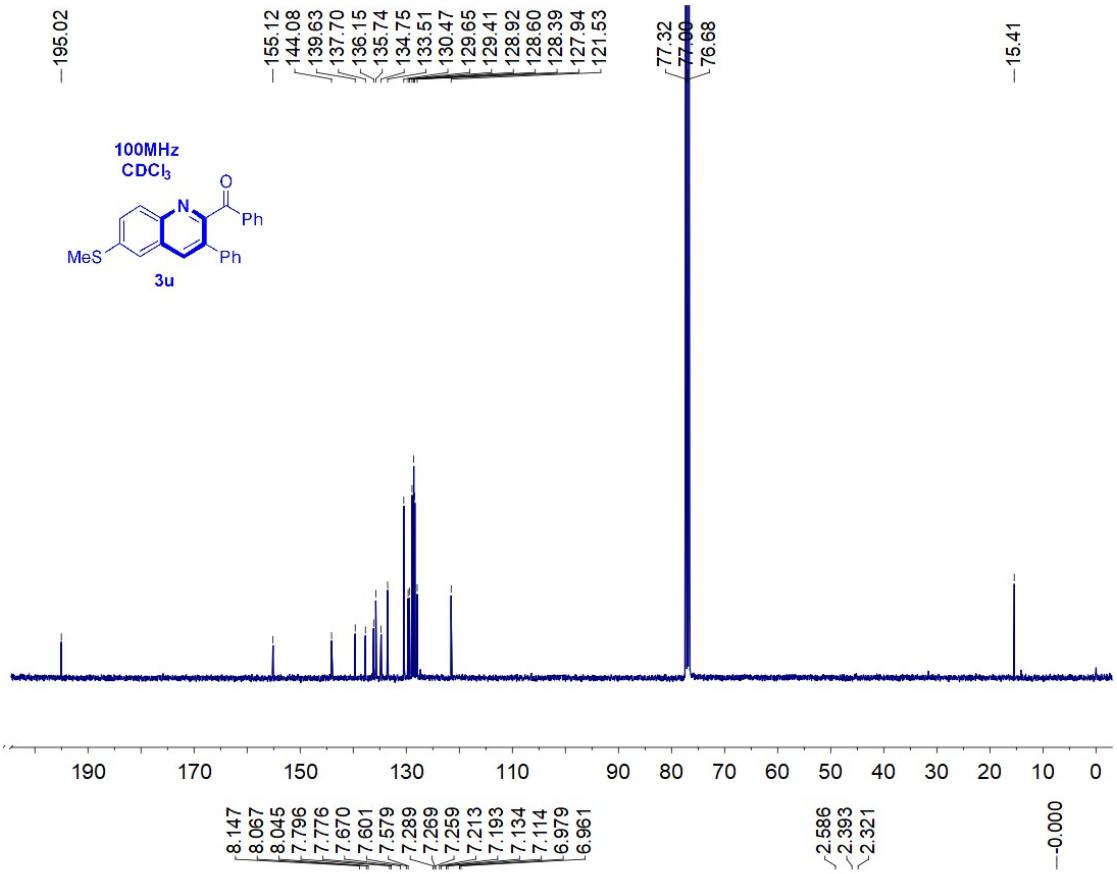
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127.94
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15.41
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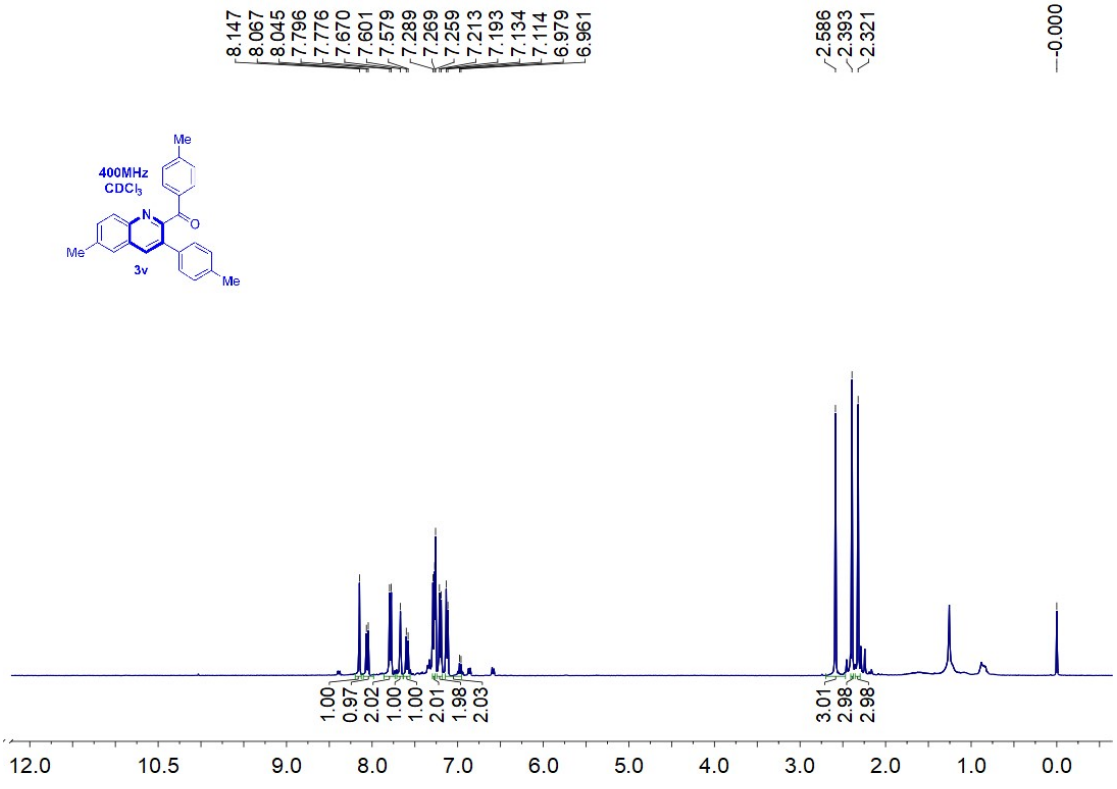
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O
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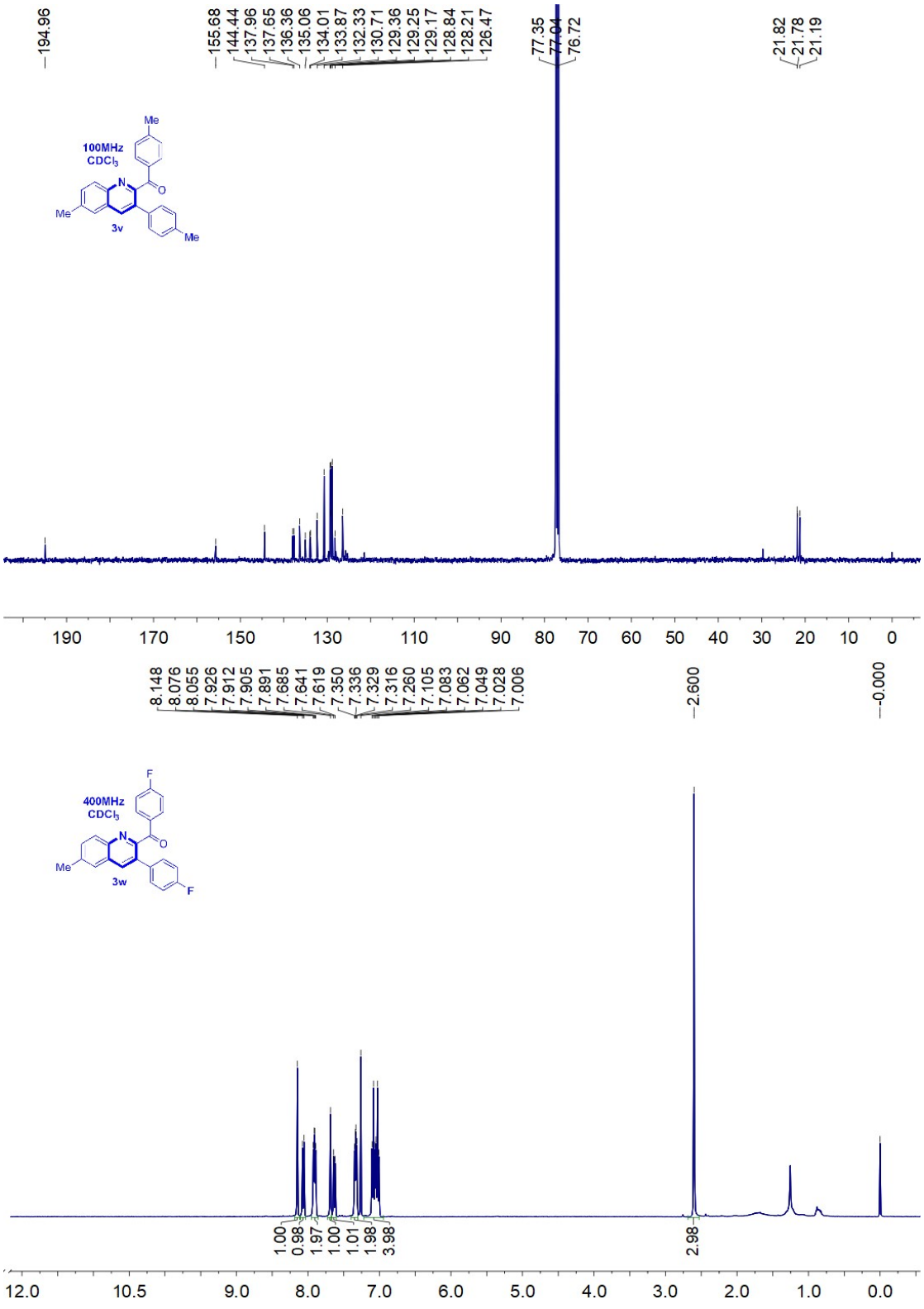
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128.84
128.21
126.47
77.35
77.04
76.72
21.82
21.78
21.19
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Me
Me
Me
3v
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170
150
130
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7.049
7.028
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F
Me
F
3w
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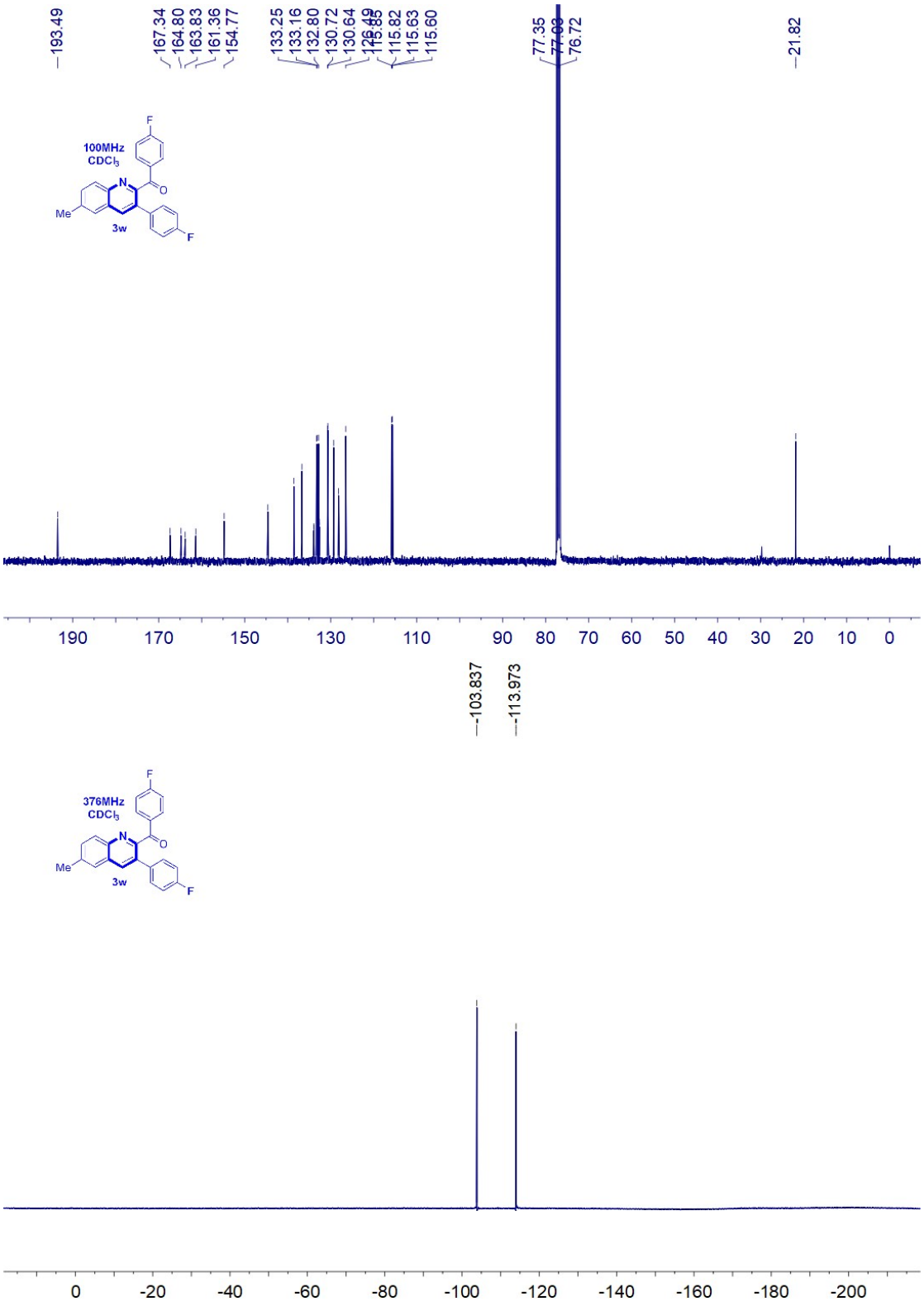
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115.63
115.60
77.35
77.00
76.72
21.82
100MHz
CDCl3
3w
190
170
150
130
110
90
80
70
60
50
40
30
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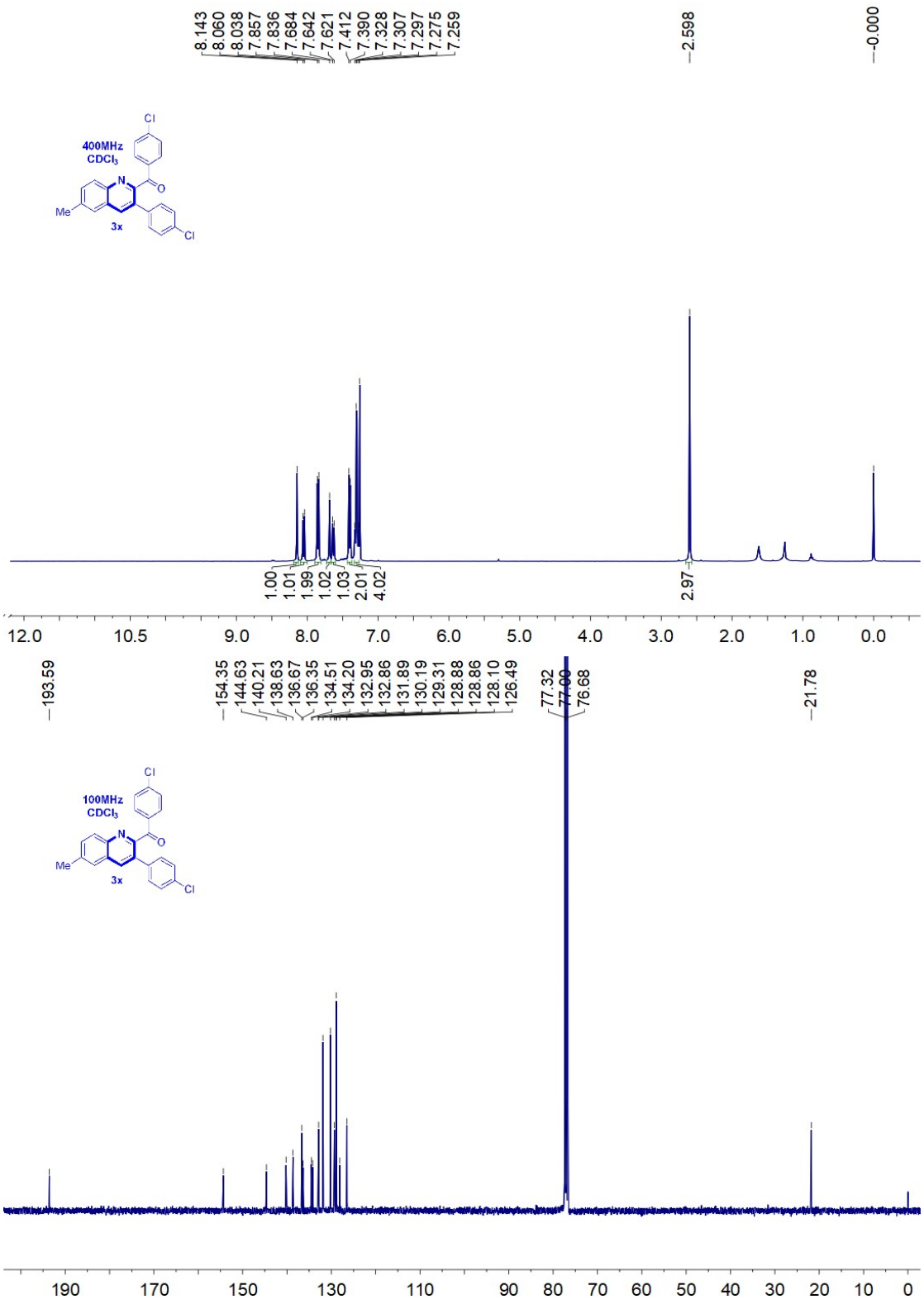
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1.99
1.02
1.03
2.01
4.02
2.97
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5.0
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136.67
136.35
134.51
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128.88
128.86
128.10
126.49
77.32
77.00
76.68
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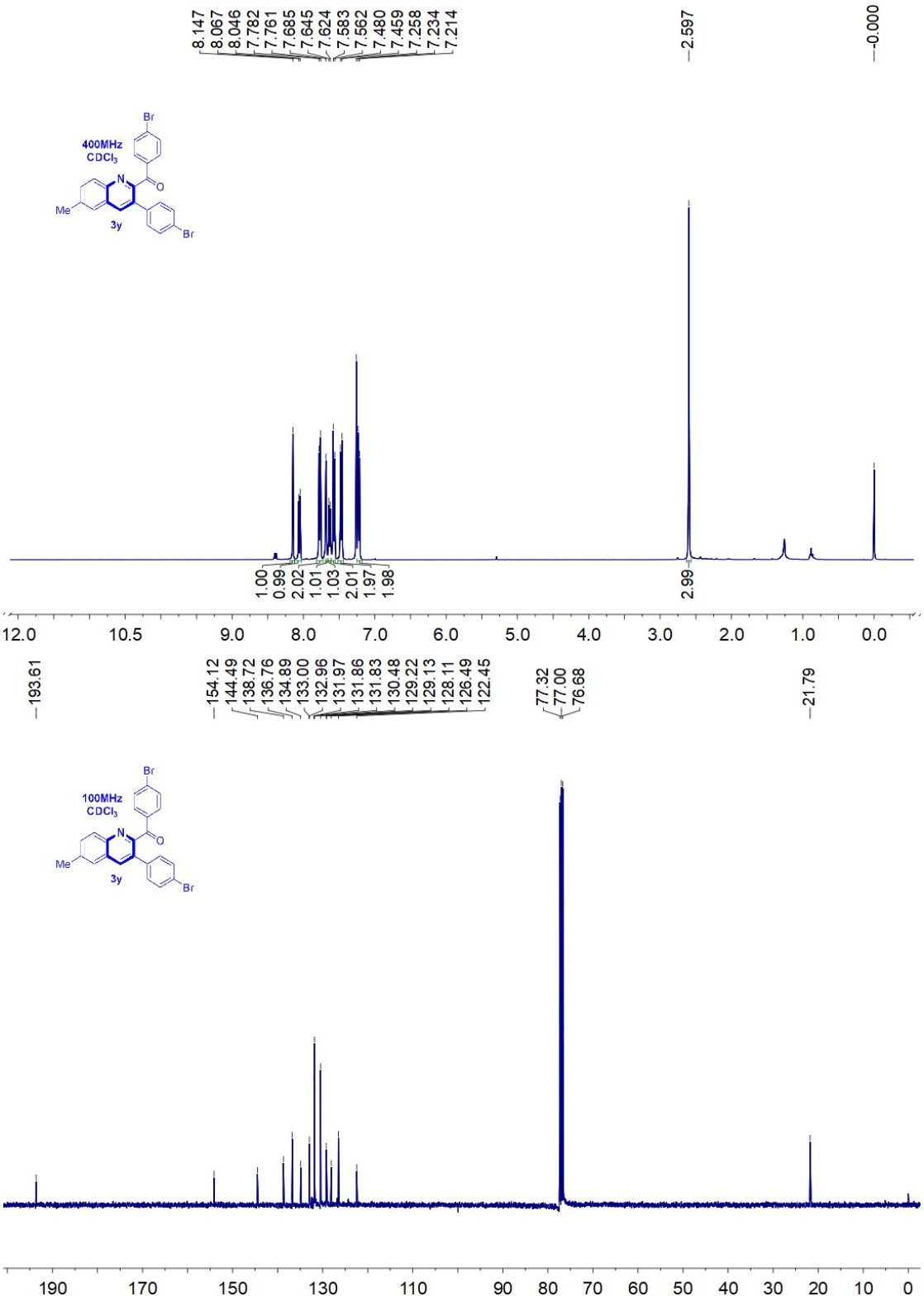
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1.01
1.03
2.01
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1.98
2.99
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9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
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77.00
76.68
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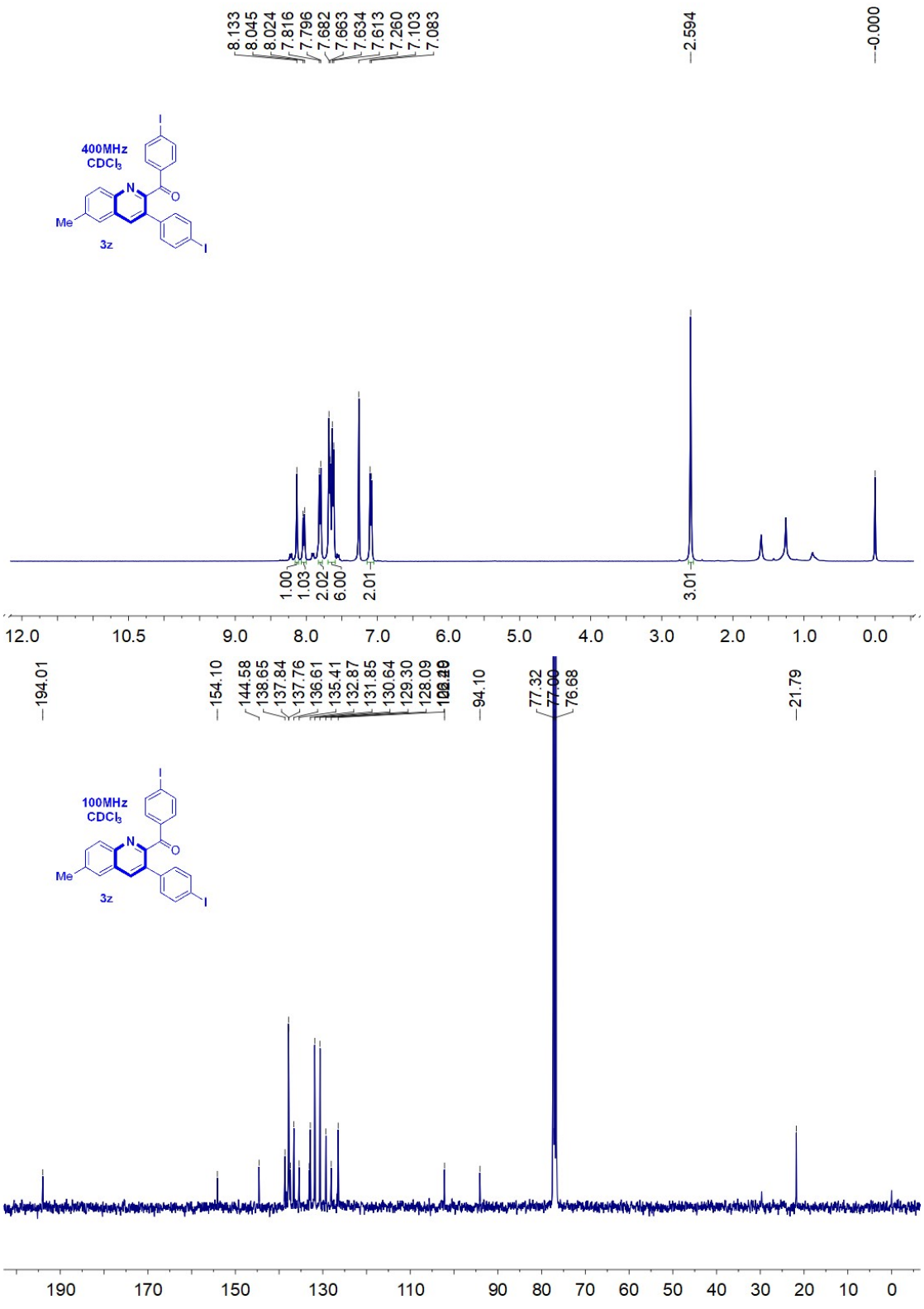
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7.103
7.083
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2.01
3.01
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7.0
6.0
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129.30
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77.32
77.00
76.68
21.79
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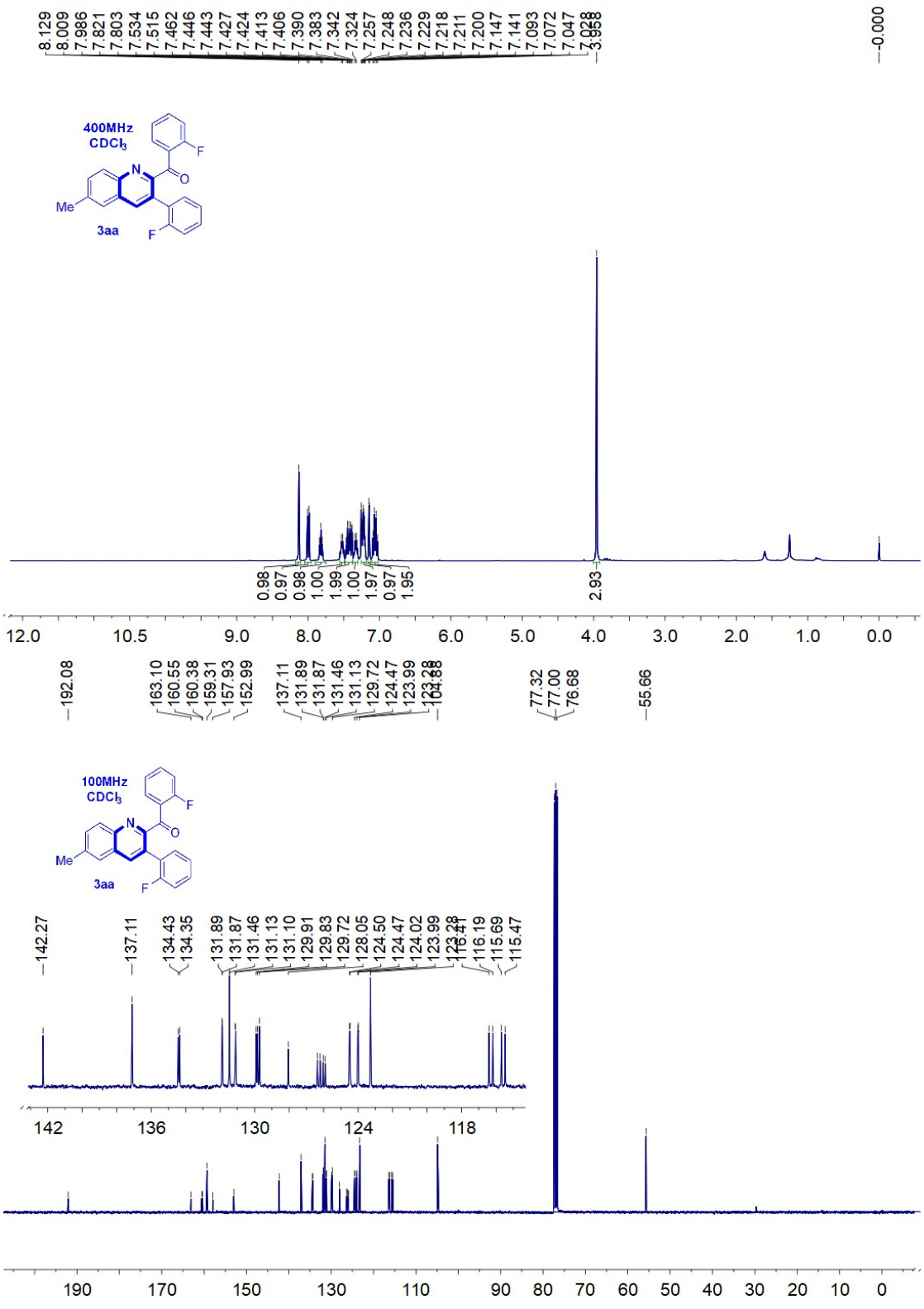
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7.413
7.406
7.390
7.383
7.342
7.324
7.257
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7.229
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1.99
1.00
1.97
0.97
1.95
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9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
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163.10
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160.38
159.31
157.93
152.99
137.11
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131.46
131.13
129.72
124.47
123.99
77.32
77.00
76.68
55.66
100MHz
CDCl3
Me
3aa
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131.10
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124.47
124.02
123.99
116.19
115.69
115.47
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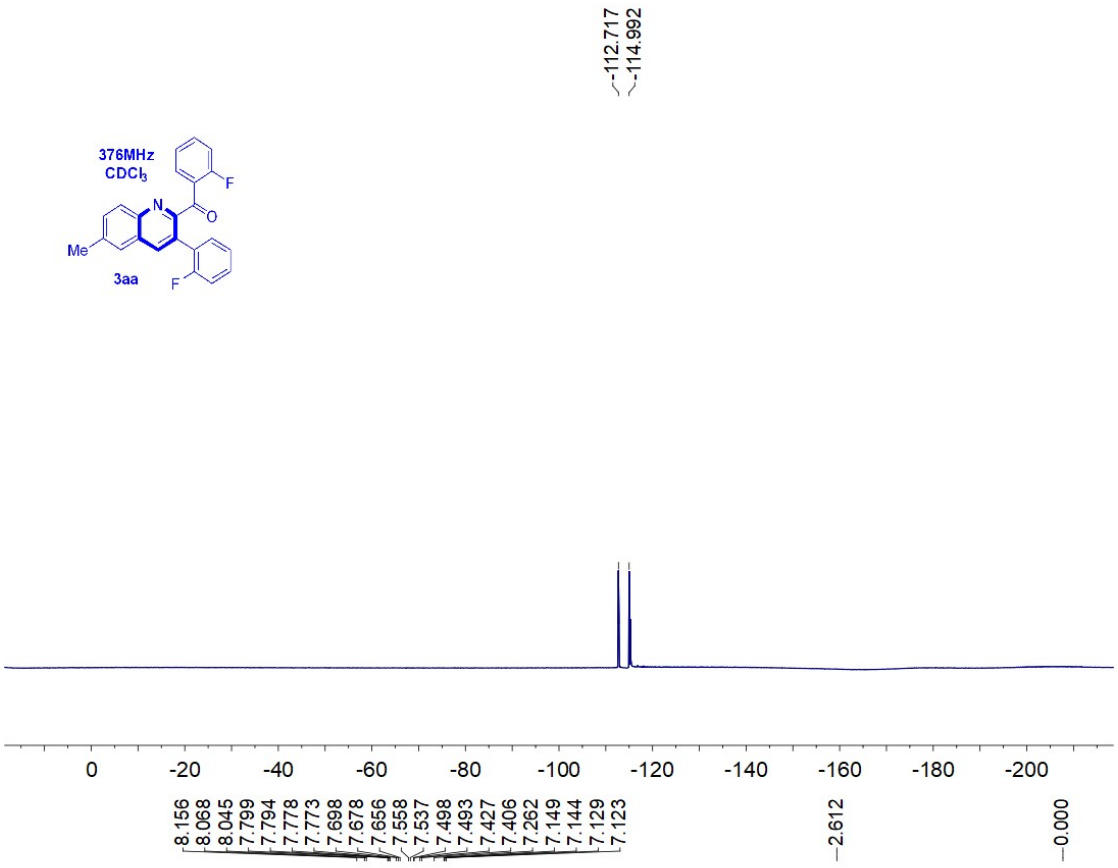
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-114.992
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F
N
O
Me
F
3aa
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-40
-60
-80
-100
-120
-140
-160
-180
-200
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8.068
8.045
7.799
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7.778
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7.678
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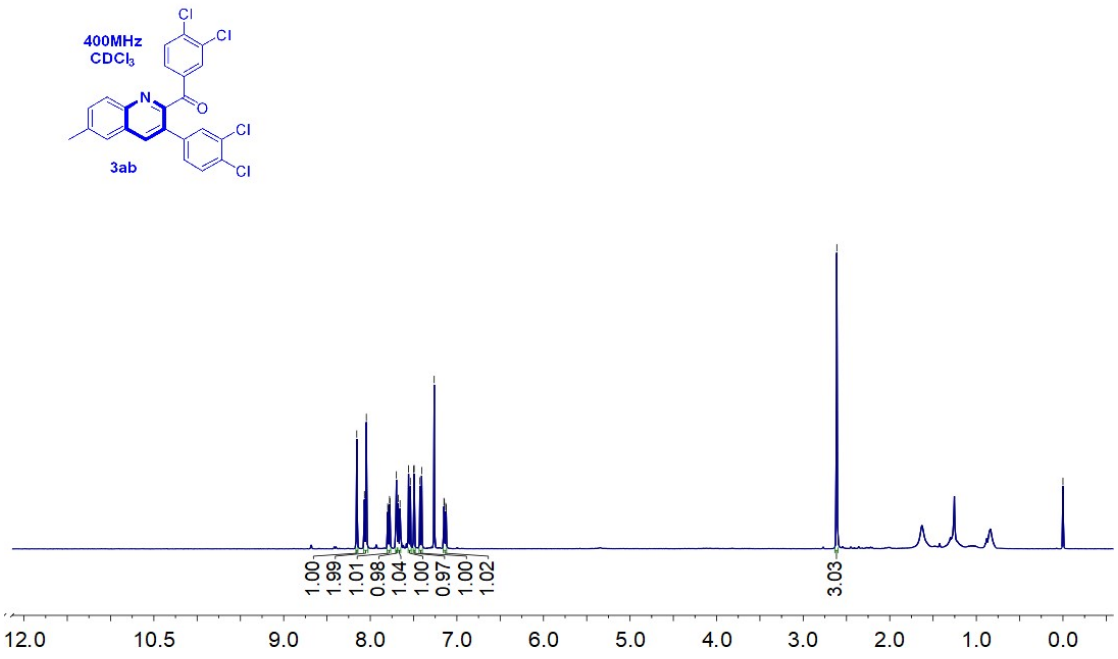
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Cl
Cl
N
O
Cl
Cl
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1.99
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0.98
1.04
1.00
0.97
1.00
1.02
3.03
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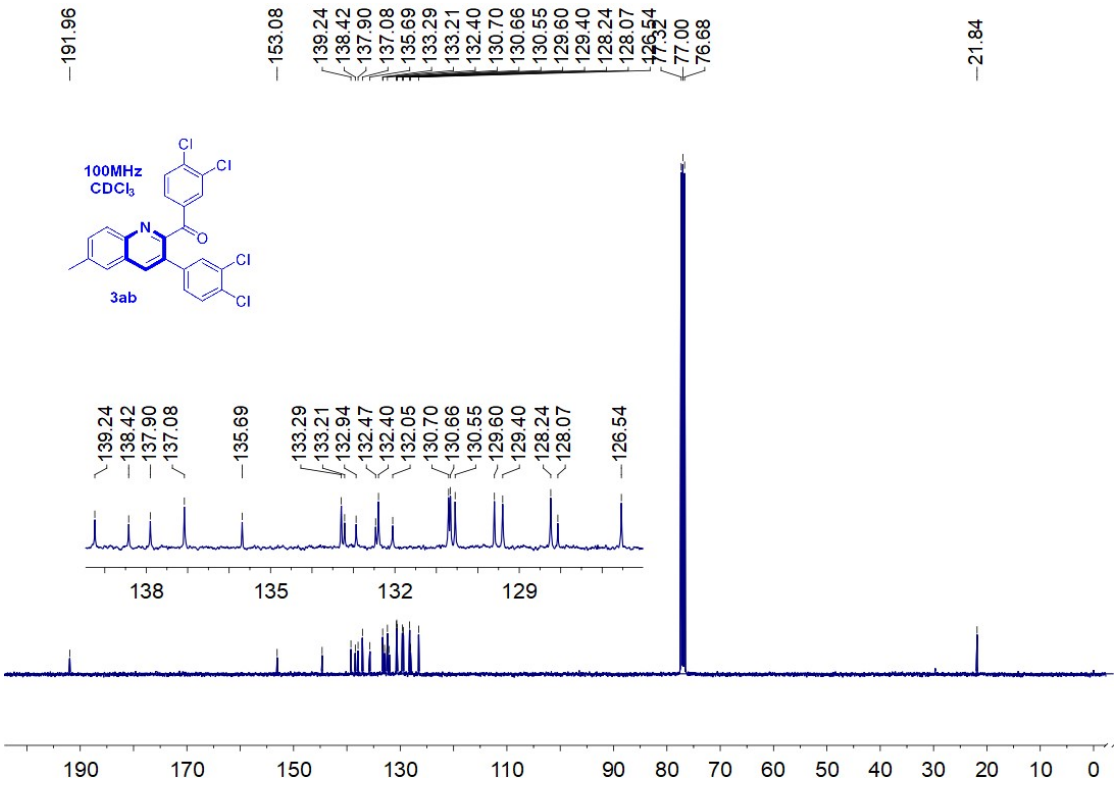
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128.24
128.07
126.54
77.32
77.00
76.68
21.84
100MHz
CDCl3
3ab
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138.42
137.90
137.08
135.69
133.29
133.21
132.94
132.47
132.40
132.05
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130.66
130.55
129.60
129.40
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128.07
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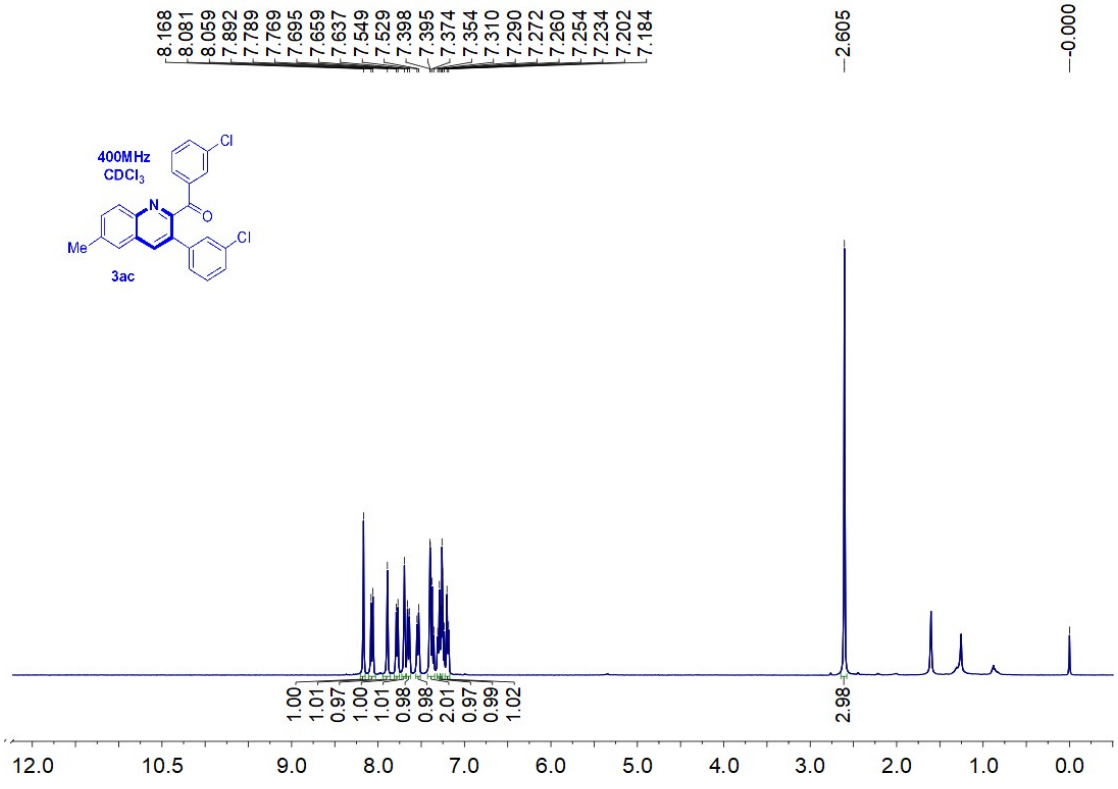
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7.395
7.374
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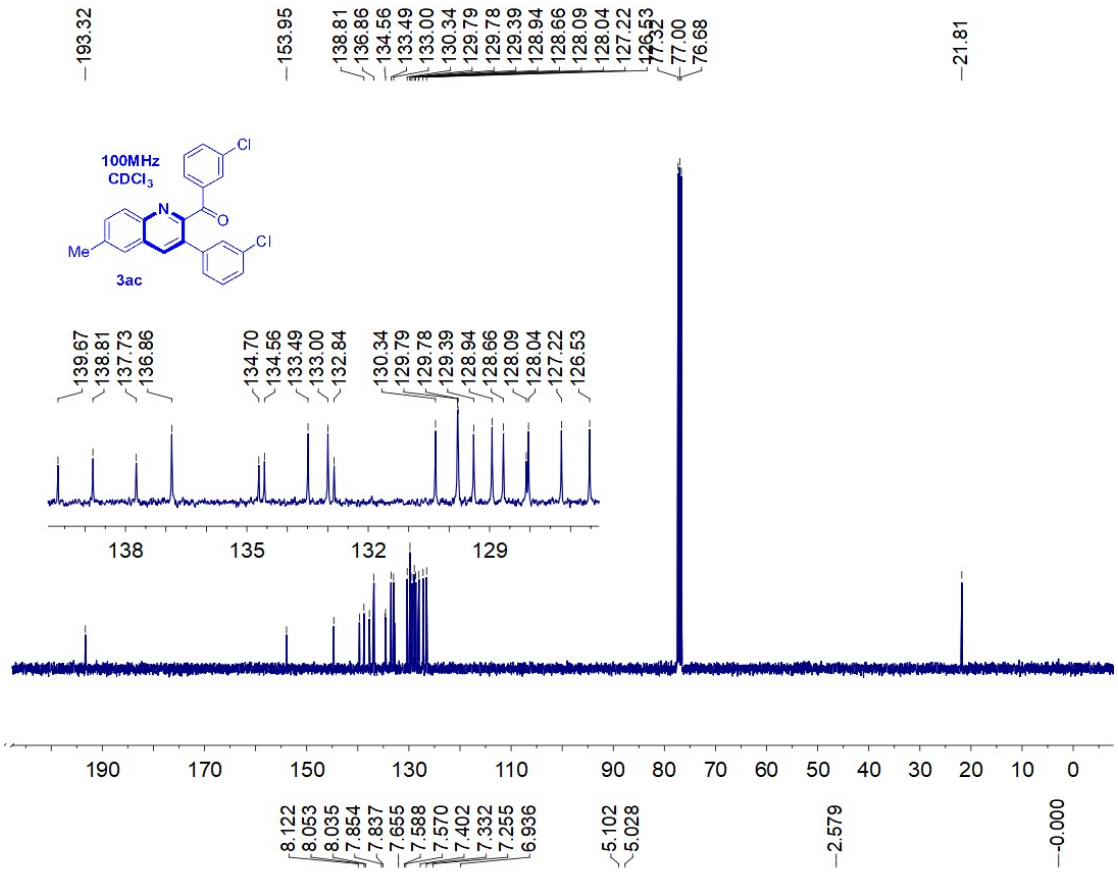
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128.04
127.22
126.53
77.32
77.00
76.68
21.81
100MHz
CDCl3
Cl
N
O
Cl
Me
3ac
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133.49
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128.94
128.66
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132
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150
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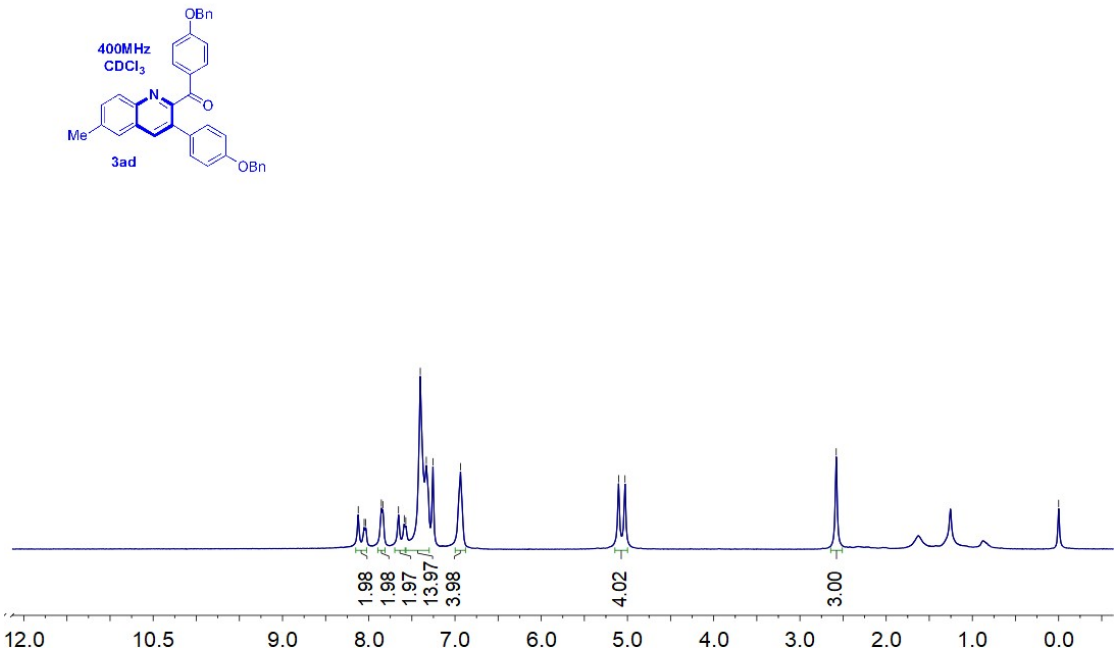
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3.00
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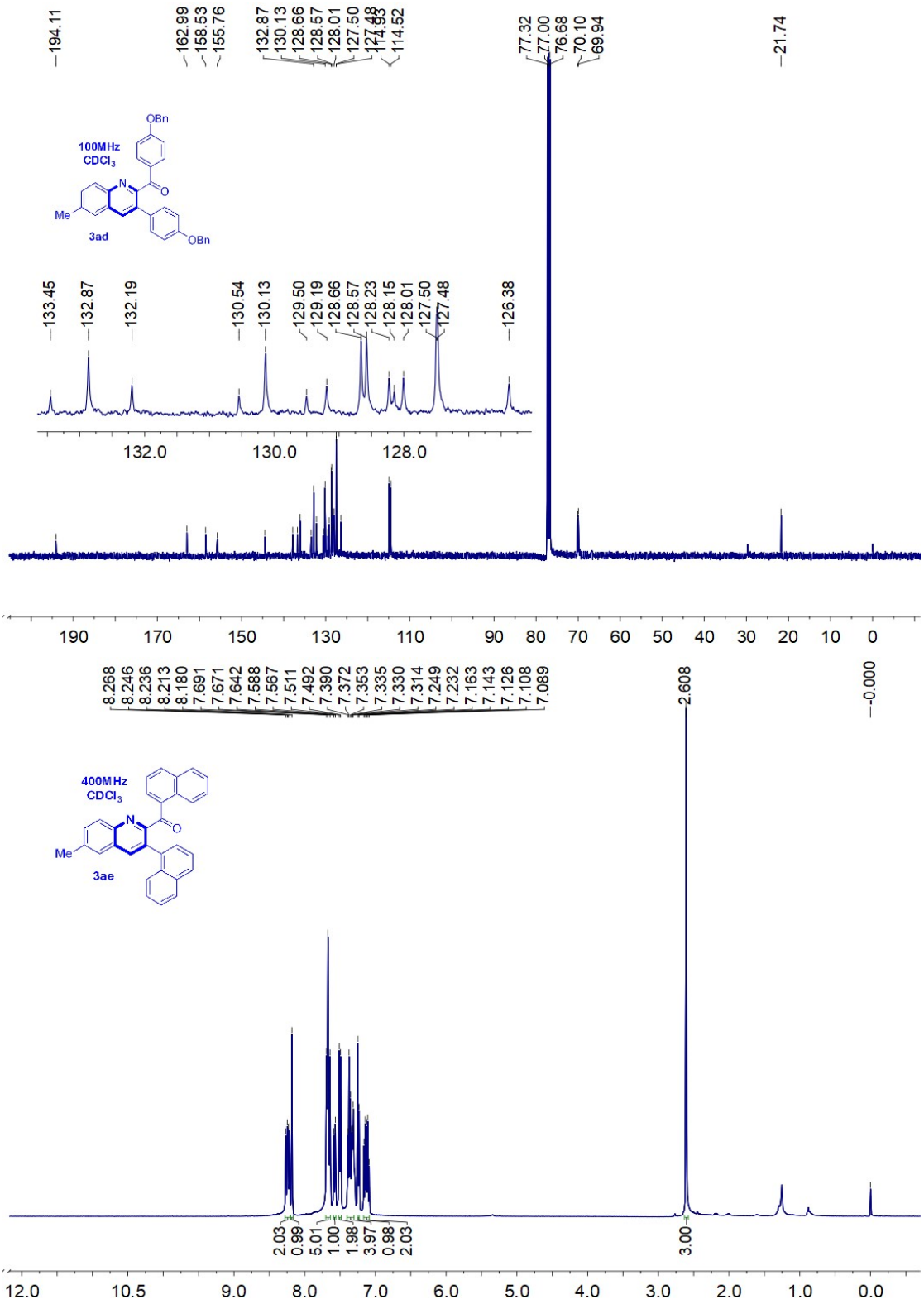
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69.94
21.74
100MHz
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OBn
Me
3ad
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150
130
110
90
80
70
60
50
40
30
20
10
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7.390
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7.330
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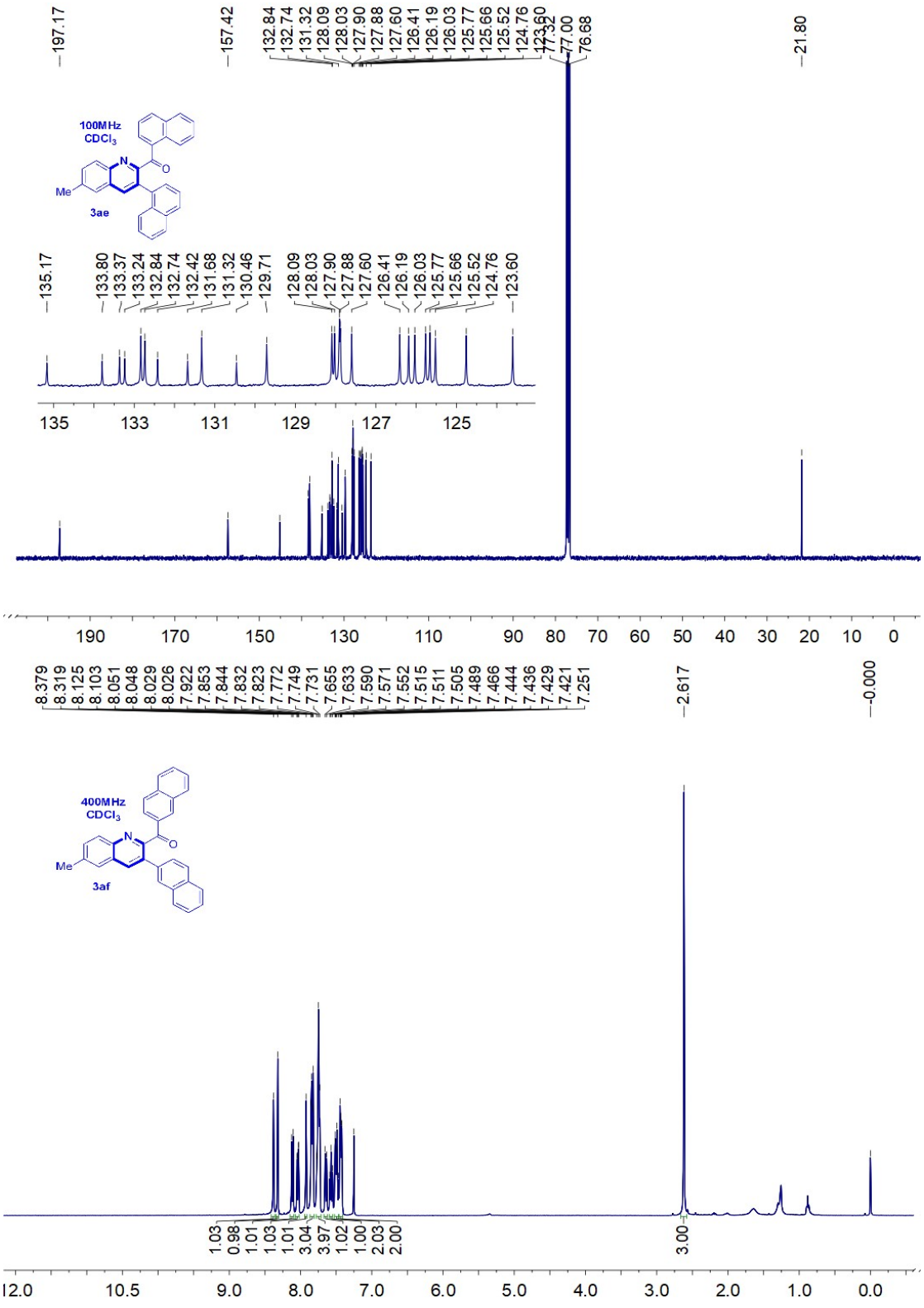
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8.103
8.051
8.048
8.029
8.026
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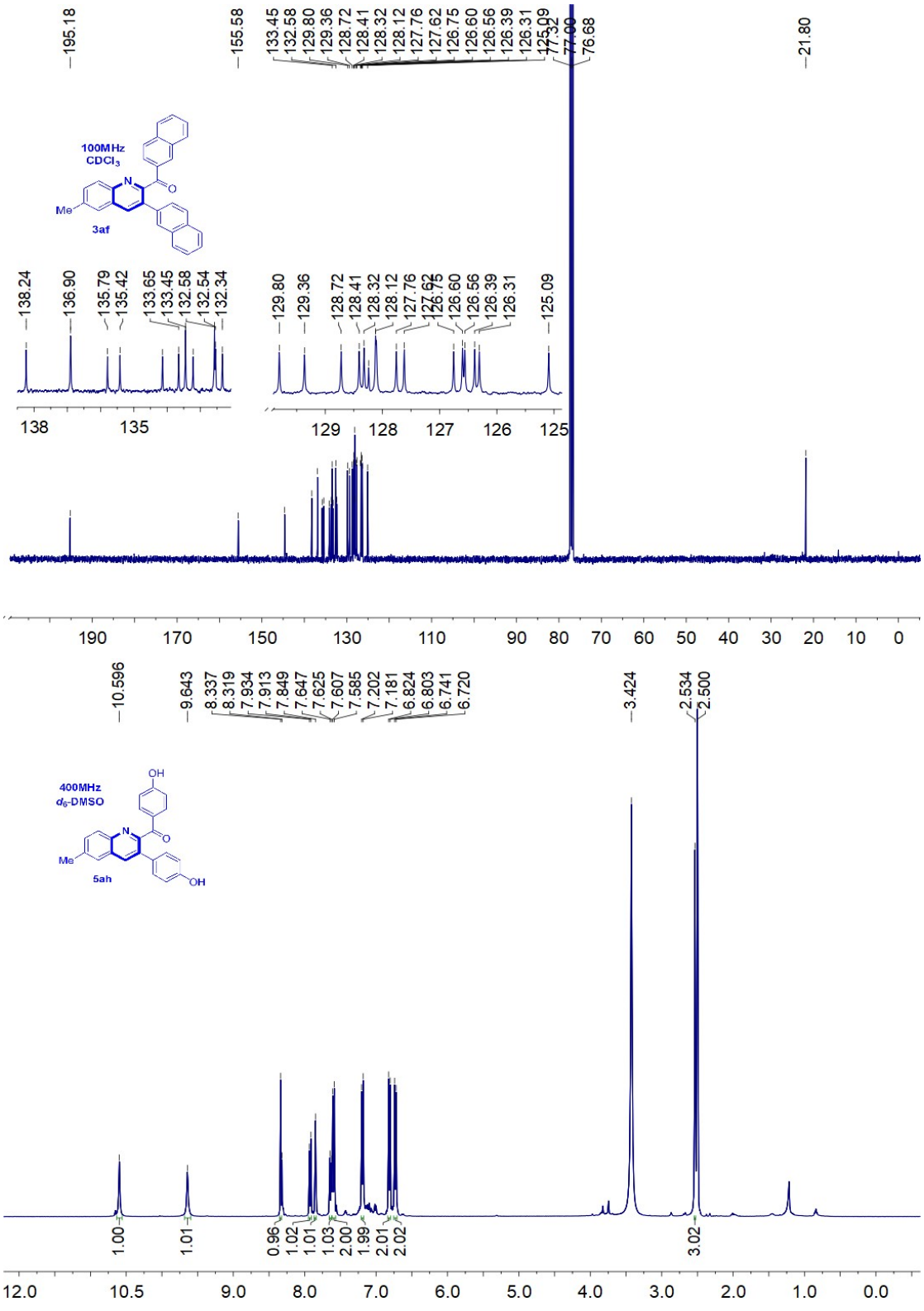
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126.39
126.31
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77.00
76.68
21.80
100MHz
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6.741
6.720
3.424
2.534
2.500
400MHz
d6-DMSO
OH
Me
5ah
OH
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1.01
0.96
1.02
1.01
1.03
2.00
1.99
2.01
2.02
3.02
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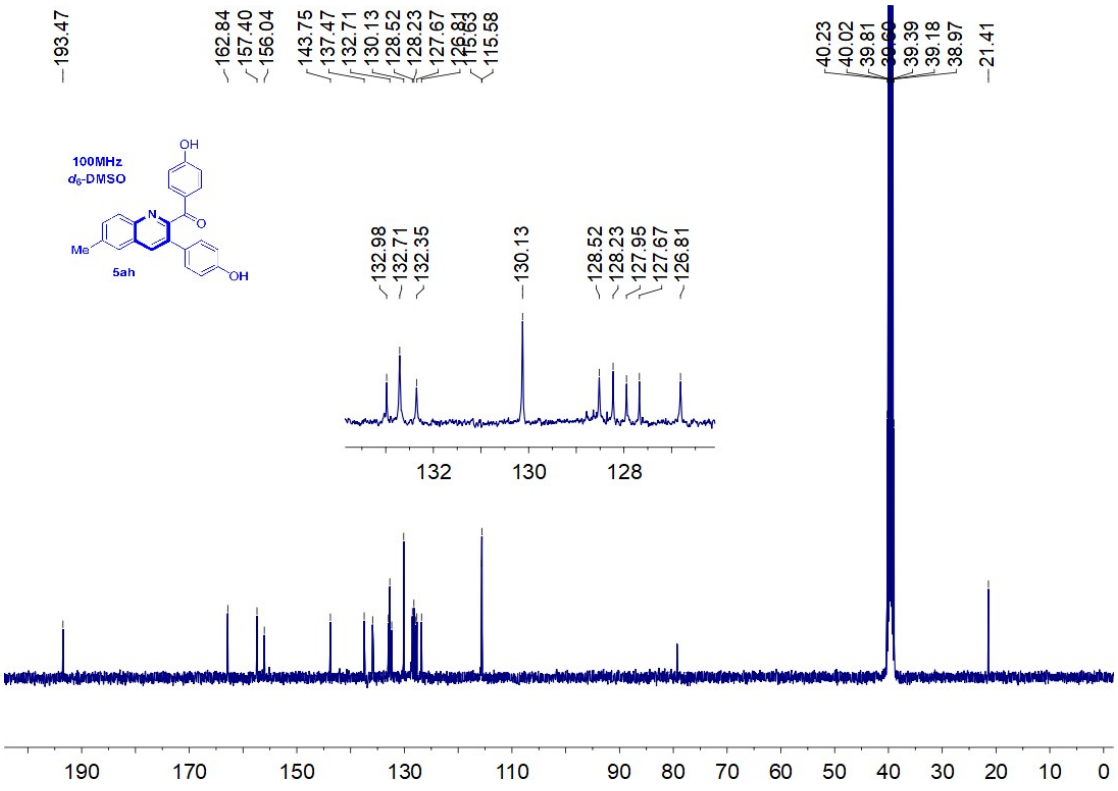
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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156.04
143.75
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132.71
130.13
128.52
128.23
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115.58
40.23
40.02
39.81
39.39
39.18
38.97
21.41
100MHz
d_6-DMSO
OH
N
O
Me
OH
5ah
132.98
132.71
132.35
130.13
128.52
128.23
127.95
127.67
126.81
132
130
128
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0