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Metal-free Regioselective Formation of C-N and C-O Bonds with the Utilization of Diaryliodonium Salts in Water: Facile Synthesis of *N*-Arylquinolones and Aryloxyquinolines

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Supplementary Information

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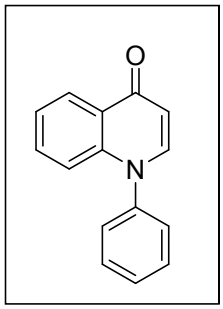
1. General Informations

All the reagents, catalysts, and solvents are commercially available and were used as such purchased without further purification. Required *m*-CPBA for the synthesis of diaryliodonium salts was procured commercially from spectrochem and then dried under vacuum. Reactions were monitored by thin-layer chromatography (TLC) on pre-coated silica gel plates from Merck (silica gel 60, F 254, 0.25mm). Reaction products were purified by column chromatography using 100-200 mesh silica gel and eluting with n-hexane/ethyl acetate mixtures. Microwave (MW) reactions were performed in CEM DISCOVER instrument (power = 50 watt, pressure = 50 psi). Melting points of synthesized compounds were recorded on *E-Z* melting point apparatus and are reported uncorrected. All prepared *N*-arylquinolones and 4-aryloxyquinolines were characterized by NMR (^{1}H & ^{13}C) and mass spectral datas. NMR spectra were recorded using a Bruker AVANCE II spectrometer at 400 MHz (^{1}H NMR) and 100 MHz (^{13}C NMR) in deuterated solvents $CDCl_3$ and DMSO. Chemical shifts are given in ppm relative to the residual solvent peak (^{1}H NMR: $CDCl_3$ δ 7.28; DMSO-d_6 2.50; ^{13}C NMR: $CDCl_3$ δ 77.0; DMSO-d_6 39.52) with multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (in Hz) and integration. Mass spectra were obtained from WATERS XEVO TQD mass spectrometer. Infrared spectra were recorded on Shimadzu IR Prestige-21 FT-IR spectrophotometer. Required symmetrical and unsymmetrical diaryliodonium salts **5** were prepared from the reaction of iodoarenes and arenes in the presence of an oxidant as described in the literature.[1] Quinolin-4(1*H*)-one (**4a**) and 4-methylquinolin-2(1*H*)-one (**4b**) were synthesized from the reaction of aniline with diethyl-(ethoxymethylene)malonate and ethylacetoacetate, respectively.[2]

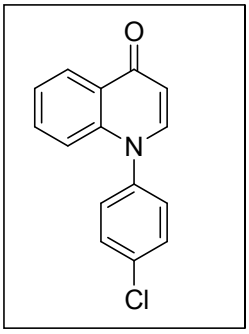
2. Experimental Procedure

Representative procedure for the synthesis of *N*-phenyllquinolin-4(1*H*)-one (6aa): A mixture of quinolin-4(1*H*)-one (**4a**, 100 mg, 0.68 mmol), diphenyliodonium triflate (**5a**, 0.68 mmol) and NaOH (2.04 mmol) in water (1 mL) was irradiated in a CEM Discover MW reactor (100 W power) for 30 min at 80 °C. After completion of reaction as indicated by TLC, organic phase was extracted with CH_2Cl_2 (2 × 3 mL), dried over anhydrous Na_2SO_4 and concentrated in *vaccuo*. The obtained crude product was purified through column chromatography using (hexane : ethylacetate, 2 : 3) as an eluent and afforded pure *N*-phenyl-quinolin-4(1*H*)-one (**6aa**) in 91% yield. Similarly, *N*-arylquinolones **6ab-ak, 6ba-bi**, 10-phenylacridin-9(10*H*)-one **8a**, 3-methyl-1-phenylquinoxalin-2(1*H*)-one **8b**, 1,3-diphenyl-1*H*-benzo[*d*]imidazol-2(3*H*)-one **8c** and 4-aryloxyquinolines **9a-e** were synthesized.

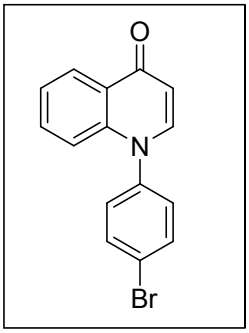
3. Characterization Data of *N*-arylquinolones (6aa-al, 8a-c) and 4-aryloxyquinolines (9a-e, 7aa)



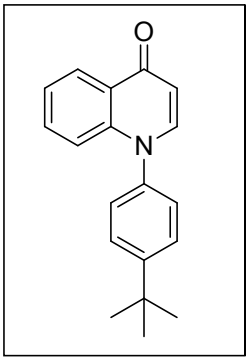
1-Phenylquinolin-4(1*H*)-one (6aa):[3] Yield 91% (138.6 mg); yellowish solid; mp 120−121 °C (lit. mp 118-123 °C); ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.32 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 7.7 Hz, 1H), 7.57 – 7.50 (m, 3H), 7.45 (dd, *J* = 8.6, 7.0 Hz, 1H), 7.35 (d, *J* = 7.9 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 6.96 (d, *J* = 8.6 Hz, 1H), 6.26 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 178.0, 143.0, 141.3, 141.2, 131.9, 130.4, 129.6, 127.5, 126.4, 126.2, 123.9, 117.5, 110.0; IR (KBr,cm^{-1}): 1629, 1595, 1489, 1420, 1389, 1304, 1211, 771; HRMS (ESI) *m/z* calcd for $C_{15}H_{12}NO$: 222.0841 $(M + H)^+$, found: 222.0851



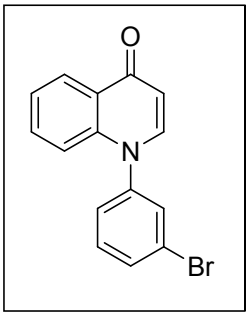
1-(4-Chlorophenyl)quinolin-4(1*H*)-one (6ab): Yield 88% (155.2 mg); yellowish solid; mp 106−108 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.62 – 7.55 (m, 3H), 7.52 (m, 1H), 7.39 (dd, *J* = 8.2, 5.9 Hz, 3H), 7.00 (t, *J* = 8.2 Hz, 1H), 6.38 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.2, 142.4, 141.2, 139.8, 135.6, 132.1, 131.4, 130.6, 129.0, 128.1, 126.7, 126.0, 124.1, 117.0, 110.5; IR (KBr,cm^{-1}): 1622, 1606, 1597, 1489, 1420, 1389, 1304, 1211, 1088, 849; HRMS (ESI) *m/z* calcd for $C_{15}H_{11}ClNO$: 256.0451 $(M + H)^+$, found: 256.0447



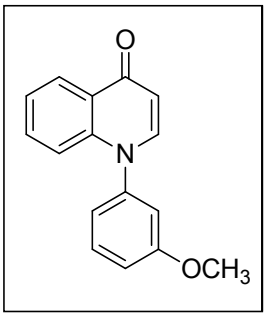
1-(4-Bromophenyl)quinolin-4(1*H*)-one (6ac): Yield 86% (177.9 mg); yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 7.9 Hz, 1H), 7.75 (d, *J* = 8.6 Hz, 2H), 7.61 – 7.48 (m, 3H), 7.39 (d, *J* = 7.9 Hz, 1H), 7.32 (d, *J* = 8.6 Hz, 1H), 7.00 (dd, *J* = 8.4, 4.5 Hz, 1H), 6.38 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.2, 142.4, 141.1, 140.3, 133.6, 132.8, 132.1, 131.6, 130.9, 129.3, 126.7, 124.1, 123.6, 117.0, 110.5; IR (KBr,cm^{-1}): 1628, 1594, 1482, 1413, 1369, 1197, 1071, 812, 746; HRMS (ESI) *m/z* calcd for $C_{15}H_{11}BrNO$: 299.9946 $(M + H)^+$, found: 299.9941



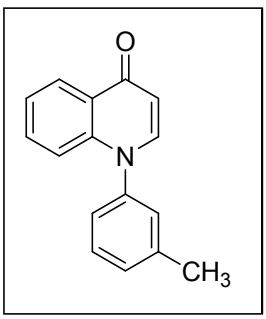
1-(4-(tert-Butyl)phenyl)quinolin-4(1H)-one (6ad): Yield 68% (130.0 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 8.1 Hz, 1H), 7.67 – 7.59 (m, 2H), 7.53 (dd, *J* = 15.4, 7.4 Hz, 2H), 7.42 – 7.33 (m, 2H), 7.29 – 7.21 (m, 1H), 7.09 – 7.00 (m, 1H), 6.40 (dd, *J* = 7.6, 6.1 Hz, 1H), 1.39 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.3, 154.2, 142.9, 141.2, 131.8, 129.9, 127.2, 127.0, 126.5, 124.5, 123.8, 117.4, 110.1, 35.1, 31.3; IR (KBr,cm^{-1}): 1624, 1602, 1591, 1420, 1389, 1257 1211, 833, 764; HRMS (ESI) *m/z* calcd for $C_{19}H_{20}NO$: 278.1467 $(M + H)^+$, found: 278.1462



1-(3-Bromophenyl)quinolin-4(1*H*)-one (6af): Yield 75% (155.1 mg); off white solid; mp 152−154 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.74 – 7.71 (m, 1H), 7.61 (t, *J* = 1.9 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.55 – 7.52 (m, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.42 – 7.37 (m, 2H), 7.01 (d, *J* = 8.4 Hz, 1H), 6.39 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, CDCl3) δ 178.2, 142.4, 142.3, 141.0, 132.8, 132.1, 131.6, 130.9, 127.7, 126.5, 126.4, 124.2, 123.6, 117.0, 110.5; IR (KBr, cm^{-1}): 1625, 1608, 1587, 1425, 1371, 1199, 1081, 823; HRMS (ESI) *m/z* calcd for $C_{15}H_{11}BrNO$: 299.9946 $(M + H)^+$, found: 299.9941

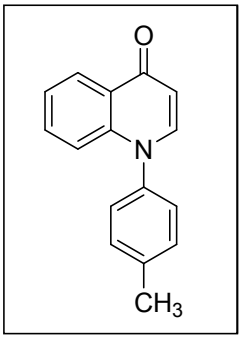


1-(3-Methoxyphenyl)quinolin-4(1*H*)-one (6ag): Yield 78% (135.1 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 – 8.44 (m, 1H), 7.61 (d, *J* = 7.7 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.37 (d, *J* = 7.9 Hz, 1H), 7.12 – 7.04 (m, 2H), 6.99 (dd, *J* = 7.8, 1.0 Hz, 1H), 6.93 (t, *J* = 2.1 Hz, 1H), 6.36 (d, *J* = 7.7 Hz, 1H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 178.3, 160.9, 142.7, 142.3, 141.3, 131.9, 131.0, 126.5, 123.9, 119.6, 117.4, 115.2, 113.2, 110.1, 55.7; IR (KBr,cm^{-1}): 1633, 1589, 1497, 1389, 1250, 1203, 1041, 887, 841, 771; HRMS (ESI) *m/z* calcd for $C_{16}H_{14}NO_2$: 252.0946 $(M + H)^+$, found: 252.0948

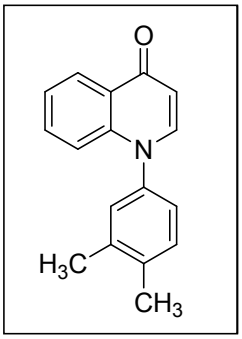


1-(3-Methylphenyl)quinolin-4(1*H*)-one (6ah): Yield 71% (115.0 mg); pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 7.9 Hz, 1H), 7.62 (d, *J* = 7.7 Hz, 1H), 7.50 (d, *J* = 7.2 Hz, 3H), 7.39 (d, *J* = 6.6 Hz, 2H), 7.29 (d, *J* = 4.3 Hz, 1H), 7.04 (d, *J* = 8.6 Hz, 1H), 6.41 (dd, *J* = 12.5, 7.7 Hz, 1H), 2.47 (s, 3H)·; ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.3, 142.8, 140.7, 132.1, 131.8,

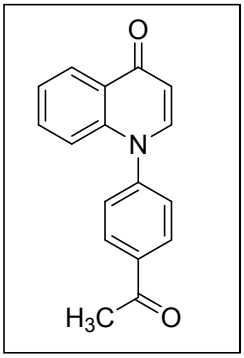
130.8, 130.2, 130.0, 128.1, 127.3, 126.5, 124.5, 123.9, 117.4, 110.1, 21.3; IR (KBr,cm^{-1}): 1632, 1589, 1566, 1504, 1420, 1396, 1257, 1157; HRMS (ESI) *m/z* calcd for $C_{16}H_{14}NO$: 236.0997 $(M+H)^+$, found 236.0995



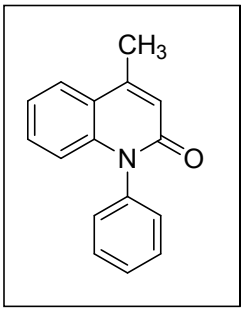
1-(*p*-Tolyl)quinolin-4(1*H*)-one (6ai): Yield 67% (108.5 mg); yellow semi solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.1 Hz, 1H), 7.62 (dd, *J* = 7.7, 3.2 Hz, 1H), 7.50 (d, *J* = 7.0 Hz, 1H), 7.40 (t, *J* = 6.1 Hz, 3H), 7.29 (d, *J* = 8.2 Hz, 1H), 7.22 (s, 1H), 7.04 ((dd, *J* = 8.6, 3.1 Hz, 1H), 6.39 (d, *J* = 7.7 Hz, 1H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.3, 142.8, 131.9, 130.8, 130.3, 130.0, 129.6, 127.5, 127.2, 126.5, 123.9, 117.3, 110.1, 21.3; IR (KBr,cm^{-1}): 1625, 1589, 1566, 1504, 1420, 1396, 1257, 1157; HRMS (ESI) *m/z* calcd for $C_{16}H_{14}NO$: 236.0997 $(M+H)^+$, found : 236.0994



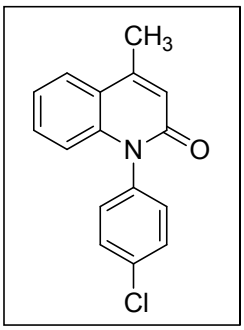
1-(3,4-Dimethylphenyl)quinolin-4(1*H*)-one (6aj): Yield 65% (111.7 mg); grey solid; mp 189−190 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 7.7 Hz, 1H), 7.62 (d, *J* = 7.6 Hz, 1H), 7.55 – 7.48 (m, 1H), 7.40 – 7.34 (m, 2H), 7.20 – 7.11 (m, 2H), 7.06 (d, *J* = 8.4 Hz, 1H), 6.41 (d, *J* = 7.5 Hz, 1H), 2.40 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.4, 143.1, 141.5, 139.0, 138.3, 131.8, 131.2, 128.3, 127.2, 126.5, 125.8, 124.6, 123.8, 117.5, 110.0, 19.9, 19.6; IR (KBr,cm^{-1}): 1622, 1604, 1587, 1430, 1396, 1257, 1157, 943; HRMS (ESI) *m/z* calcd for $C_{17}H_{16}NO$: 249.1154 $(M+H)^+$, found : 249.1159



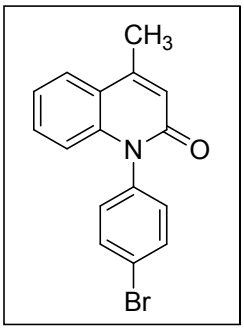
1-(4-Acetylphenyl)quinolin-4(1*H*)-one (6ak): Yield 79% (143.2 mg); brown solid; mp 134−136 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 5.1 Hz, 1H), 8.31 (d, *J* = 9.4 Hz, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 8.09 (d, *J* = 8.8 Hz, 2H), 7.83 –7.79 (m, 1H), 7.62 (t, *J* = 8.0 Hz, 1H), 7.29 – 7.24 (m, 2H), 6.71 (d, *J* = 5.0 Hz, 1H), 2.66 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) 196.7, 178.2, 151.0, 150.0, 147.2, 134.1, 130.9, 130.4, 129.2, 126.6, 121.7, 121.6, 120.2, 105.9, 26.6; ; IR (KBr,cm^{-1}): 1682, 1623, 1604, 1596, 1460, 1416, 1397; HRMS (ESI) *m/z* calcd for $C_{17}H_{14}NO_2$: 264.0946 $(M+H)^+$, found : 264.0939



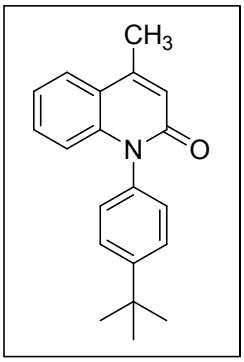
4-Methyl-1-phenylquinolin-2(1*H*)-one (6ba):[4] Yield 85% (141.8 mg); white solid; mp 130−131 °C (lit. mp 125.2 °C) ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.35 (dd, *J* = 12.1, 5.0 Hz, 1H), 7.32 – 7.22 (m, 3H), 6.73 – 6.66 (m, 2H), 2.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 147.4, 140.9, 137.7, 130.2, 130.0, 129.0, 128.9, 124.8, 122.2, 121.5, 121.1, 116.3, 19.2 ; IR (KBr,cm^{-1}): 1655, 1594, 1512, 1481, 1381, 1342, 1219, 756; HRMS (ESI) *m/z* calcd for $C_{16}H_{14}NO$: 236.0997 $(M + H)^+$, found: 236.0991



1-(4-Chlorophenyl)-4-methylquinolin-2(1*H*)-one (6bb): Yield 81% (137.3 mg); off white solid; mp 131−132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.61 – 7.52 (m, 2H), 7.36 – 7.40 (m, 1H), 7.32 – 7.19 (m, 3H), 6.69 (q, *J* = 6.0 Hz, 2H), 2.56 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0, 147.7, 140.6, 136.2, 134.8, 131.1, 130.5, 130.2, 129.5, 129.3, 127.5, 125.0, 122.4, 121.3, 121.1, 19.2; IR (KBr,cm^{-1}): 1652, 1582, 1489, 1481, 1342, 1219, 825; HRMS (ESI) *m/z* calcd for $C_{16}H_{13}ClNO$: 270.0607 $(M + H)^+$, found: 270.0611

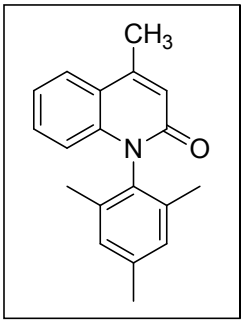


1-(4-Bromophenyl)-4-methylquinolin-2(1*H*)-one (6bc): Yield 80% (158.0 mg); brown solid; mp 83−86 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (t, *J* = 8.3 Hz, 3H), 7.57 – 7.43 (m, 1H), 7.37 (d, *J* = 7.1 Hz, 1H), 7.26 (d, *J* = 9.0 Hz, 1H), 7.19 (d, *J* = 8.6 Hz, 1H), 6.71 – 6.66 (m, 2H), 2.56 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9, 147.8, 140.5, 136.7, 133.5, 132.3, 131.4, 130.8, 130.2, 127.9, 125.0, 122.4, 121.3, 116.1, 19.3; IR (KBr,cm^{-1}): 1652, 1574, 1481, 1342, 1227, 825; HRMS (ESI) *m/z* calcd for $C_{16}H_{13}BrNO$: 314.0102 $(M + H)^+$, found: 314.0108

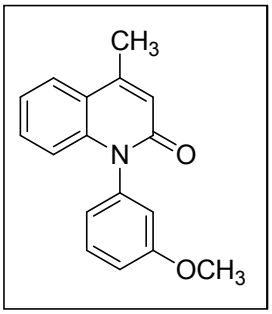


1-(4-(tert-Butyl)phenyl)-4-methylquinolin-2(1*H*)-one (6bd): Yield 45% (82.4 mg); pale yellow semi solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.3 Hz, 1H), 7.61 (d, *J* = 8.3 Hz, 1H), 7.55 (d, *J* = 6.7 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.28 – 7.10 (m, 3H), 6.73 – 6.66 (m, 2H), 2.56 (s, 3H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 153.5, 147.2, 141.1, 137.4, 130.0, 128.3, 127.1, 125.8, 124.8, 121.6, 121.1, 116.5, 34.9, 31.3, 19.2; IR (KBr,cm^{-}

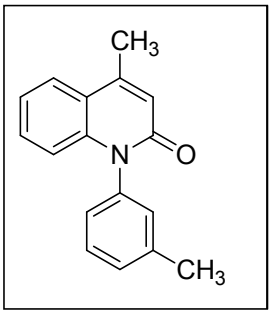
[1]): 1654, 1586, 1476, 1325, 1182, 1025, 824; HRMS (ESI) *m/z* calcd for $C_{20}H_{22}NO$: 292.1623 $(M + H)^+$, found: 292.1629



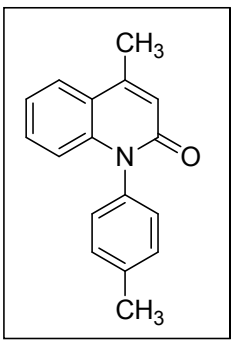
1-Mesityl-4-methylquinolin-2(1*H*)-one (6be): Yield 56% (97.7 mg); yellow semi solid; ^1H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 9.3 Hz, 1H), 7.40 – 7.33 (m, 1H), 7.26 (t, *J* = 8.1 Hz, 1H), 7.08 (s, 2H), 6.75 (s, 1H), 6.61 (d, *J* = 9.2 Hz, 1H), 2.58 (s, 3H), 2.39 (s, 3H), 1.94 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 147.5, 139.4, 138.6, 135.6, 132.9, 130.5, 129.8, 125.0, 122.2, 121.7, 121.3, 115.0, 21.2, 19.2, 17.5; IR (KBr,cm^{-1}): 1645, 1592, 1481, 1342, 1203, 856; HRMS (ESI) *m/z* calcd for $C_{19}H_{20}NO$: 278.1467 $(M + H)^+$, found: 278.1470



1-(3-Methoxyphenyl)-4-methylquinolin-2(1*H*)-one (6bg): Yield 60% (96.4 mg); pale yellow solid; mp 103-104 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.39 – 7.35 (m, 1H), 7.28 – 7.23 (m, 1H), 7.08 (dd, *J* = 8.9, 3.0 Hz, 1H), 6.90 – 6.87 (m, 1H), 6.84 – 6.81 (m, 1H), 6.76 – 6.70 (m, 2H), 3.85 (s, 3H), 2.56 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0, 161.0, 147.4, 140.8, 138.8, 130.9, 130.0, 124.8, 122.1, 121.5, 121.0, 116.4, 115.0, 114.3, 55.4, 19.2; IR (KBr,cm^{-1}): 1656, 1582, 1481, 1219, 829, 796; HRMS (ESI) *m/z* calcd for $C_{17}H_{16}NO_2$: 266.1103 $(M + H)^+$, found: 266.1109

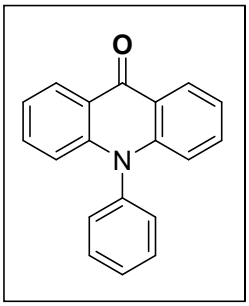


4-Methyl-1-(*m*-tolyl)quinolin-2(1*H*)-one (6bh): Yield 51% (75.4 mg); off white solid; mp 180-181 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.50 (t, *J* = 7.7 Hz, 1H), 7.37 – 7.33 (m, 2H), 7.26 – 7.22 (m, 1H), 7.10 (d, *J* = 9.1 Hz, 2H), 6.71 (t, *J* = 4.6 Hz, 2H), 2.55 (d, *J* = 1.2 Hz, 3H), 2.45 (s, 3H).); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 147.3, 140.9, 140.2, 137.7, 130.0, 129.7 , 129.4, 125.9, 124.8, 122.1, 121.5, 121.0, 116.4, 21.4, 19.2; IR (KBr,cm^{-1}): 1652, 1581, 1476, 1325, 1025, 834, 759; HRMS (ESI) *m/z* calcd for $C_{17}H_{16}NO$: 250.1154 $(M + H)^+$, found: 250.1158

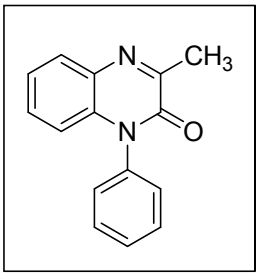


4-Methyl-1-(*p*-tolyl)quinolin-2(1*H*)-one (6bi): Yield 42% (62.1 mg); off white solid; mp 184-186 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 8.6 Hz, 1H), 7.24 (t, *J* = 8.1 Hz,

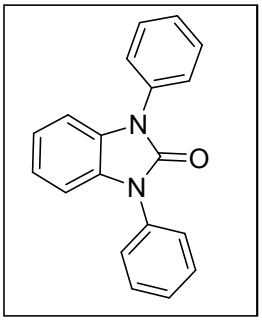
1H), 7.17 (d, *J* = 8.2 Hz, 2H), 6.75 – 6.69 (m, 2H), 2.55 (s, 3H), 2.48 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 147.2, 141.0, 138.8, 135.0, 130.9, 129.9, 128.6, 124.8, 122.0, 121.5, 121.0, 116.4, 21.3, 19.2; IR (KBr,cm^{-1}): 1647, 1584, 1476, 1325, 1186, 1031, 826,; HRMS (ESI) *m/z* calcd for $C_{17}H_{16}NO$: 250.1154 $(M + H)^+$, found: 250.1159



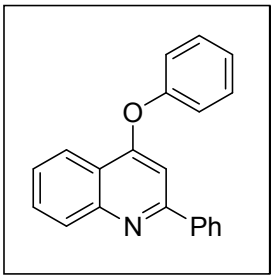
10-Phenylacridin-9(10*H*)-one (8a):[5] Yield 62% (85.7 mg); yellow solid; mp 270−271 °C (lit. mp 271−273 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (dd, *J* = 8.2, 1.7 Hz, 2H), 7.78 – 7.67 (m, 3H), 7.55 – 7.51 (m, 2H), 7.41 (t, *J* = 4.4 Hz, 2H), 7.33 – 7.29 (m, 2H), 6.78 (d, *J* = 9.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.2, 143.1, 139.0, 133.3, 131.1, 130.1, 129.6, 127.3, 121.8, 121.6, 116.8; IR (KBr,cm^{-1}): 1631, 1597, 1481, 1458, 1357, 1176; HRMS (ESI) *m/z* calcd for $C_{19}H_{14}NO$: 272.0997 $(M + H)^+$, found: 272.0992



3-Methyl-1-phenylquinoxalin-2(1*H*)-one (8b):[6] Yield 72% (86.7 mg); yellow solid; mp 198 °C (lit. mp 198−199 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (dd, *J* = 6.2, 3.5 Hz, 1H), 7.73 (dd, *J* = 6.2, 3.5 Hz, 1H), 7.59 (dd, *J* = 6.3, 3.4 Hz, 2H), 7.52 – 7.47 (m, 2H), 7.32 (d, *J* = 9.3 Hz, 3H), 2.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.0, 152.9, 148.1, 139.4, 129.6, 129.1, 128.0, 127.3, 125.3, 121.7, 20.7; IR (KBr,cm^{-1}): 1650, 1598, 1460, 1374, 1284, 1159; HRMS (ESI) *m/z* calcd for $C_{15}H_{13}N_2O$: 237.0950 $(M + H)^+$, found: 237.0954

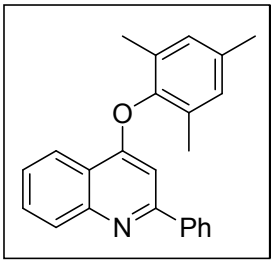


1,3-Diphenyl-1*H*-benzo[*d*]imidazol-2(3*H*)-one (8c):[7] Yield 70% (102.2 mg); pale yellow solid; mp 101−102 °C (lit. mp 100-101 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 8.5, 1.2 Hz, 4H), 7.61 – 7.55 (m, 4H), 7.49 – 7.44 (m, 2H), 7.22 – 7.10 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 134.5, 129.6, 127.8, 126.2, 122.2, 109.0; IR (KBr,cm^{-1}): 1707, 1596,1558, 1498, 1244, 1101; HRMS (ESI) *m/z* calcd for $C_{19}H_{15}N_2O$: 287.1106 $(M + H)^+$, found: 287.1101

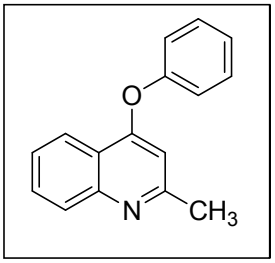


4-Phenoxy-2-phenylquinoline (9a):[8] Yield 91% (121.7 mg); off-white solid; mp 69-71 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.2 Hz, 1H), 8.20 (d, *J* = 8.5 Hz, 1H), 7.98 (d, *J* = 7.0 Hz, 2H), 7.80 (t, *J* = 7.4 Hz, 1H),

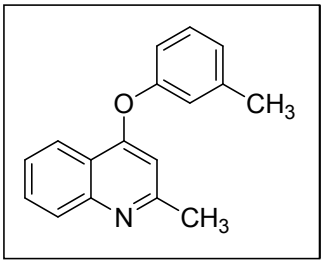
7.59 (t, *J* = 7.5 Hz, 1H), 7.54–7.44 (m, 6H), 7.34 (t, *J* = 7.3 Hz, 1H), 7.26 (s, 1H), 7.06 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 158.6, 154.6, 149.8, 139.8, 130.4, 130.3, 129.4, 129.3, 128.7, 127.5, 125.9, 125.5, 121.7, 121.0, 120.6, 102.5, IR (KBr,cm^{-1}): 1589, 1481, 1412, 1350, 1211, 918, 764, 694; MS (ESI) *m/z* calcd for $C_{21}H_{16}NO$: 298.1, found: 298.1



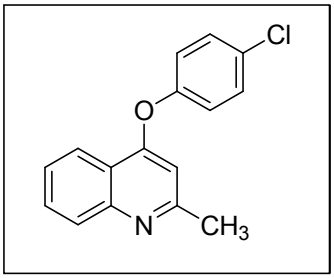
4-(Mesityloxy)-2-phenylquinoline (9b): Yield 90% (137.4 mg); off-white solid; mp 81-82 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 9.2 Hz, 1H), 8.23 (d, *J* = 8.3 Hz, 1H), 7.96 (dd, *J* = 8.1, 1.5 Hz, 2H), 7.82 (t, *J* = 8.4 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.52 – 7.42 (m, 3H), 7.03 (s, 2H), 6.77 (s, 1H), 2.40 (s, 3H), 2.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 158.9, 149.8, 147.9, 140.0, 135.4, 130.5, 130.3, 129.9, 129.3, 129.2, 128.7, 127.6, 125.7, 121.8, 119.9, 99.8, 20.9, 16.1; IR (KBr,cm^{-1}): 1578, 1472, 1402, 1340, 1201, 915, 760; HRMS (ESI) *m/z* calcd for $C_{24}H_{22}NO$: 340.1623, found: 340.1628



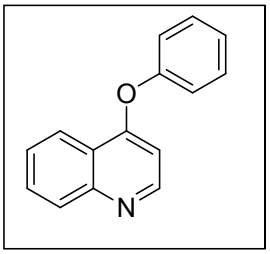
2-Methyl-4-phenoxyquinoline (9c):[9] Yield 80% (116.7 mg); brown solid; mp 71-72 °C (lit. mp 73 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.3 Hz, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.75 (t, *J* = 8.4 Hz, 1H), 7.57 – 7.47 (m, 3H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.23 – 7.18 (m, 2H), 6.45 (s, 1H), 2.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9, 160.0, 154.5, 149.3, 130.2, 130.1, 128.2, 125.5, 125.3, 121.7, 121.1, 120.0, 104.8, 25.7; IR (KBr,cm^{-1}): 1590, 1468, 1389, 1191, 895; HRMS (ESI) *m/z* calcd for $C_{16}H_{14}NO$: 236.0997, found: 236.0987



2-Methyl-4-(*m*-tolyloxy)quinoline (9d): Yield 60% (92.7 mg); off-white; mp 90-92 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.3 Hz, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.74 (t, *J* = 8.4 Hz, 1H), 7.53 (t, *J* = 8.1 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.16 (d, *J* = 13.6 Hz, 1H), 7.06 – 6.97 (m, 2H), 6.45 (s, 1H), 2.62 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0, 160.0, 154.4, 149.3, 140.6, 130.1, 129.9, 128.1, 126.3, 125.2, 121.7, 121.6, 120.0, 118.0, 104.8, 25.7, 21.4; IR (KBr,cm-1): 1589, 1497, 1250, 1203, 1041, 841, 771; HRMS (ESI) *m/z* calcd for $C_{17}H_{16}NO$: 250.1154 $(M + H)^+$, found: 250.1158



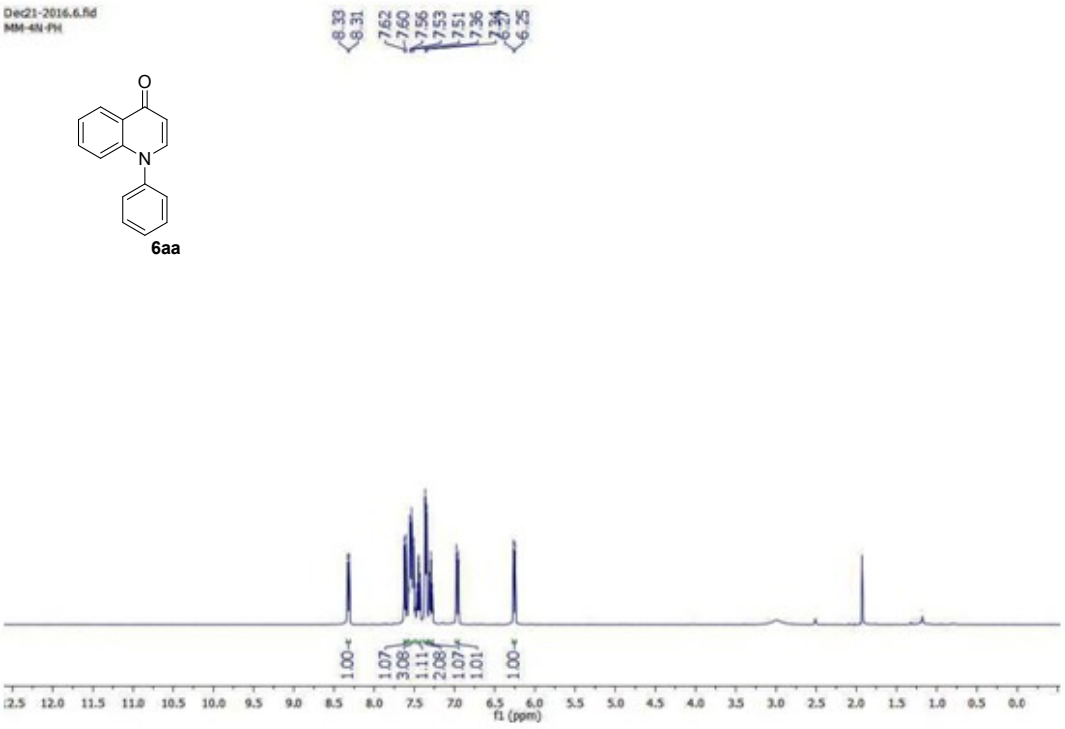
4-(4-Chlorophenoxy)-2-methylquinoline (**9e)**: Yield 72% (120.3 mg); off-white solid; mp 138-139 °C ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 9.3 Hz, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.77 – 7.72 (m, 1H), 7.55 – 7.51 (m, 1H), 7.48 – 7.43 (m, 2H), 7.18 – 7.12 (m, 2H), 6.44 (s, 1H), 2.62 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.6, 160.0, 153.1, 149.4, 130.8, 130.4, 130.3, 128.3, 125.4, 122.4, 121.5, 119.8, 104.9, 25.7; IR (KBr,cm^{-1}): 1589, 1498, 1253, 1214, 1053, 851, 779; HRMS (ESI) *m/z* calcd for $C_{16}H_{13}ClNO$: 270.0607 $(M + H)^+$, found: 270.0601

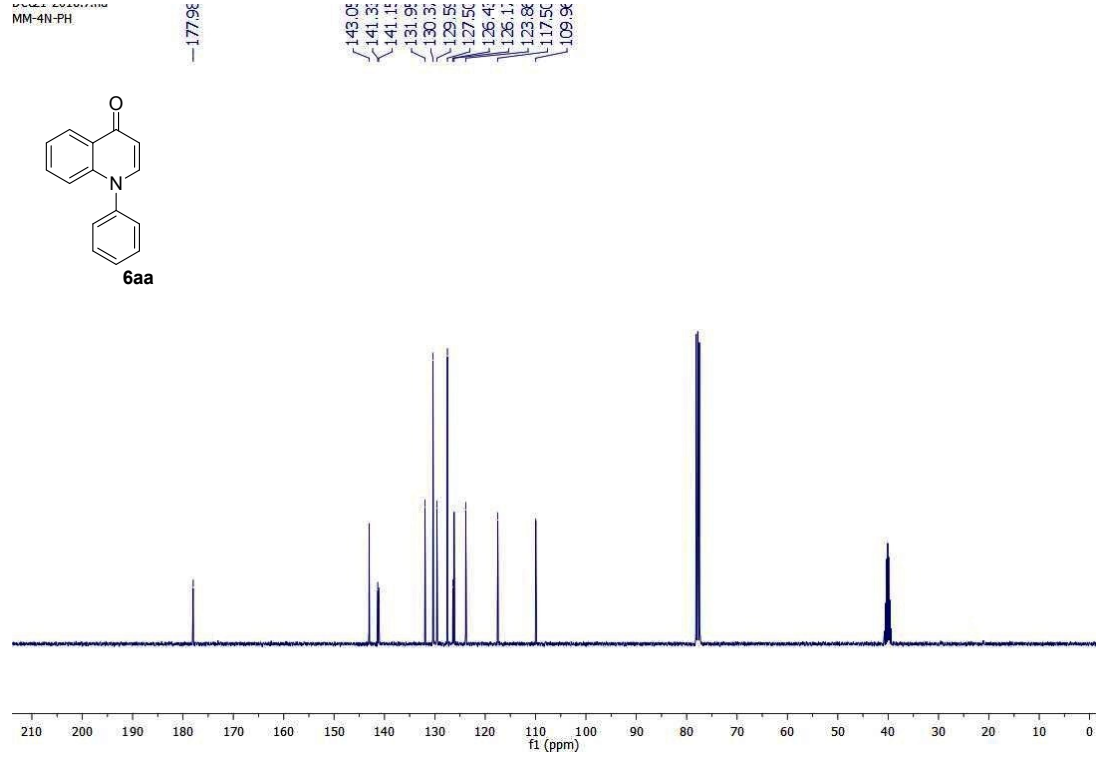


4-Phenoxyquinoline (7aa):[8] Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.2 Hz, 1H), 8.44–8.33 (m, 1H), 8.12 (d, *J* = 8.5 Hz, 1H), 7.78–7.73 (m, 1H), 7.59–7.55 (m, 1H), 7.49–7.44 (m, 2H), 7.33–7.27 (m, 1H), 7.22–7.16 (m, 2H), 6.55 (d, *J* = 5.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9, 154.4, 151.1, 149.7, 130.3, 130.1, 129.0, 126.1, 125.6, 121.8, 121.5, 121.1, 104.3; IR (KBr,cm^{-1}): 1566, 1489, 1420, 1389, 1304, 1211, 771

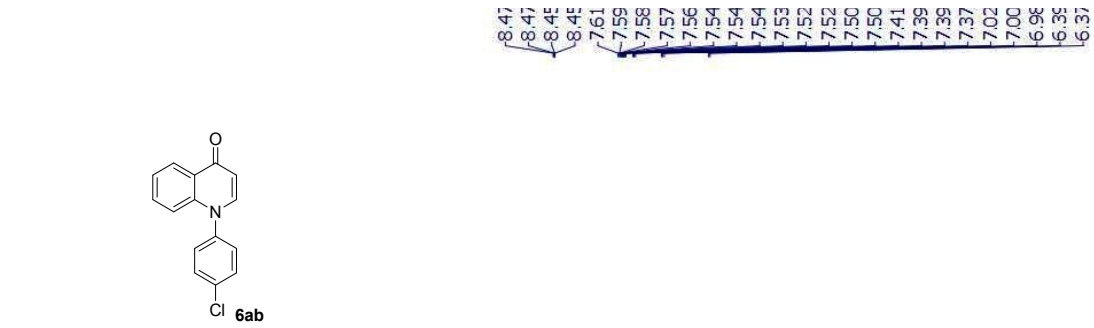
4. Copies of ^{1}H & ^{13}C NMR spectra of *N*-arylquinolones (6aa-al, 8a-c) and 4-aryloxyquinolines (9a-e, 7aa)

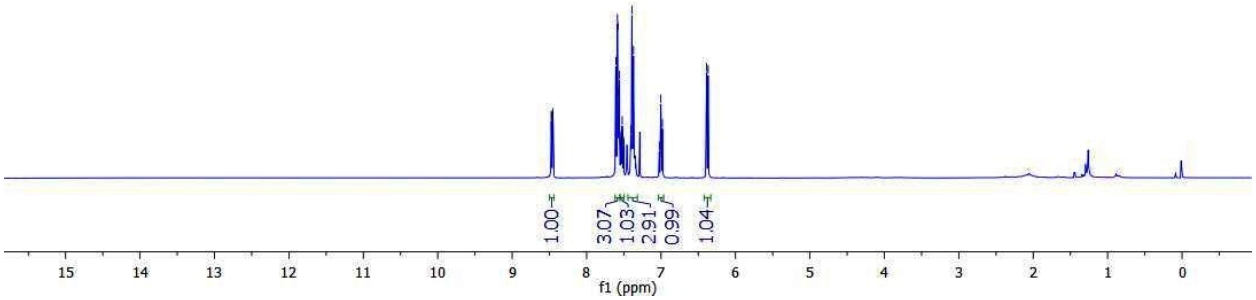
^{1}H & ^{13}C NMR spectra of 1-phenylquinolin-4(1*H*)-one (6aa)

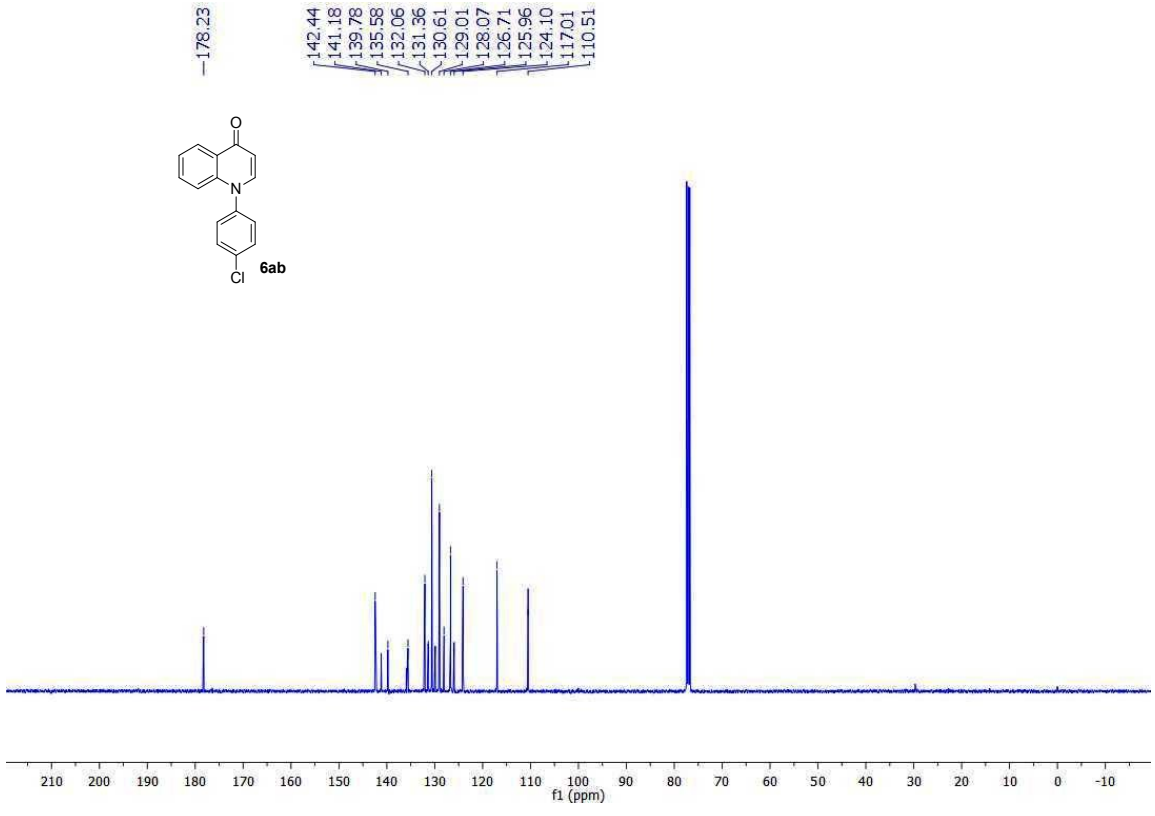




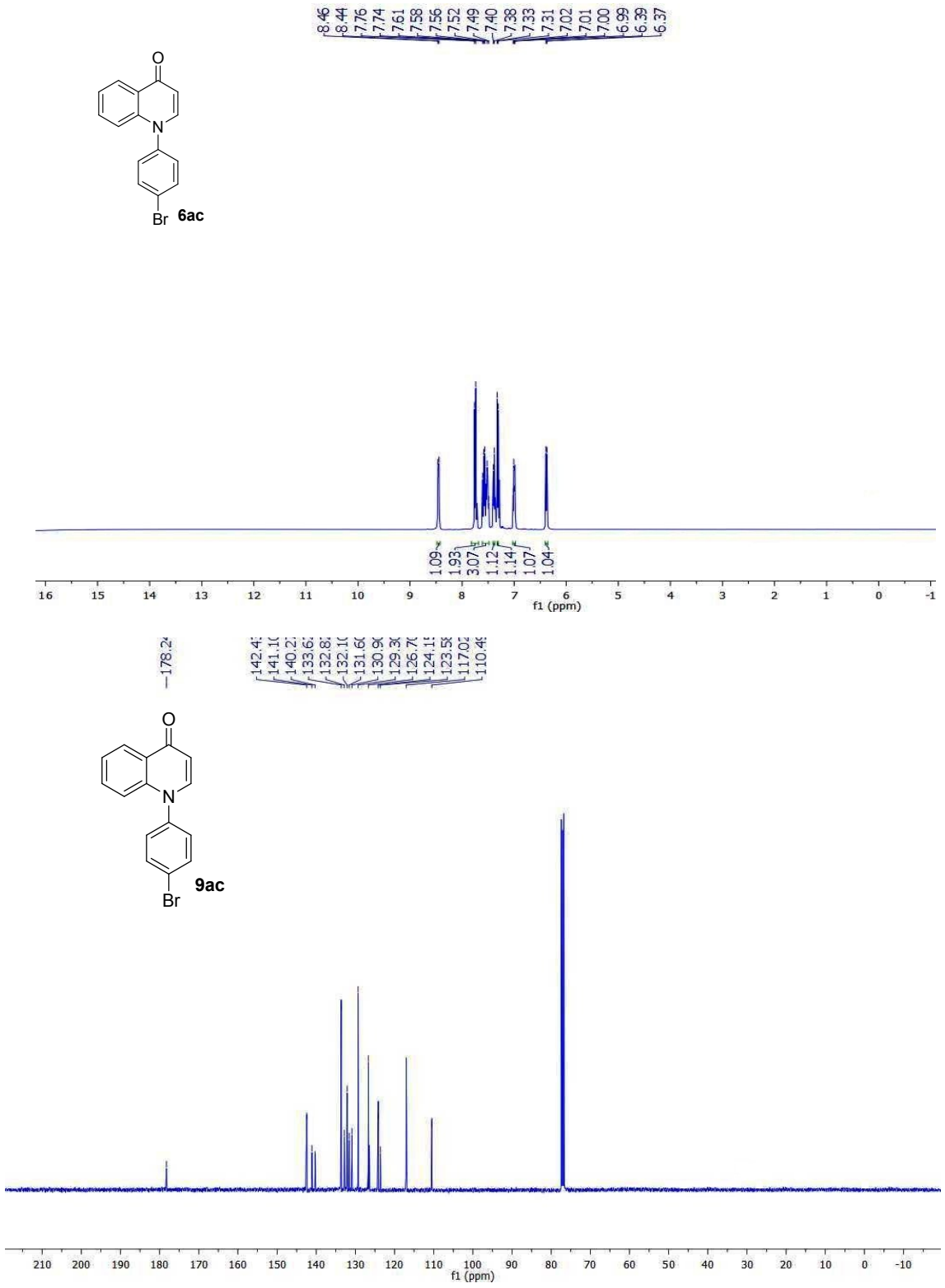
^{1}H & ^{13}C NMR spectra of 1-(4-chlorophenyl)quinolin-4(1*H*)-one (6ab)



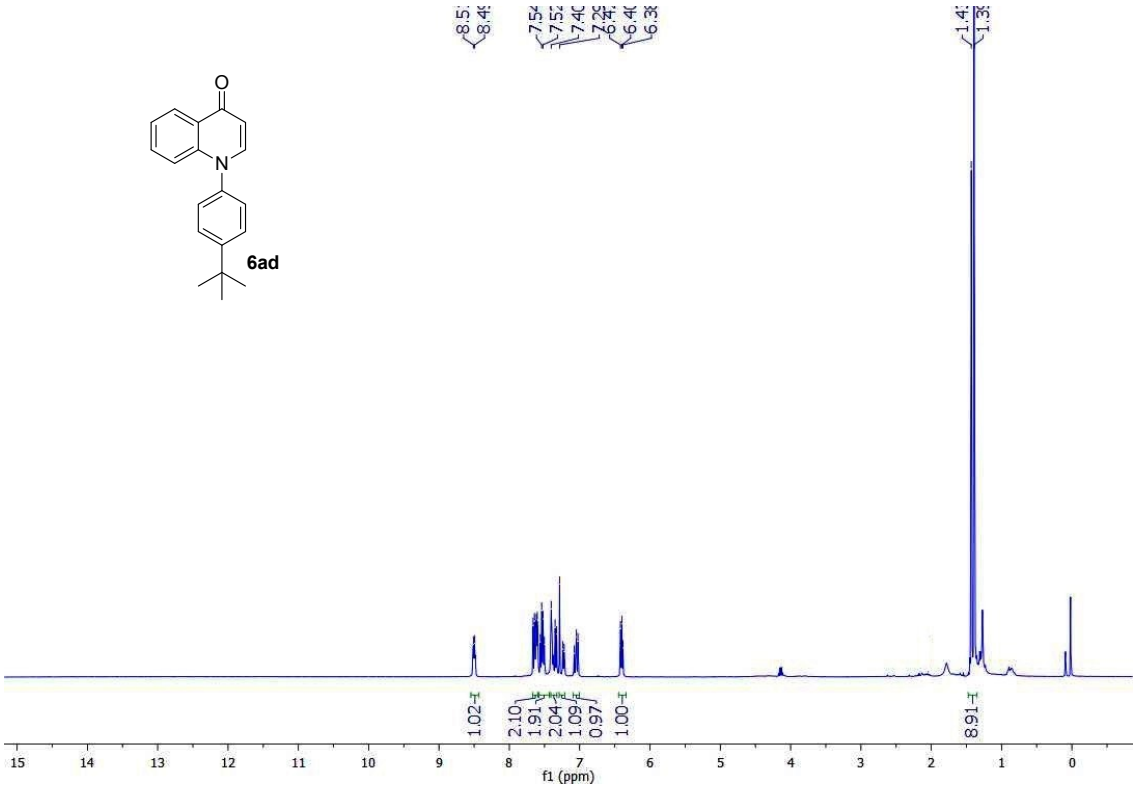


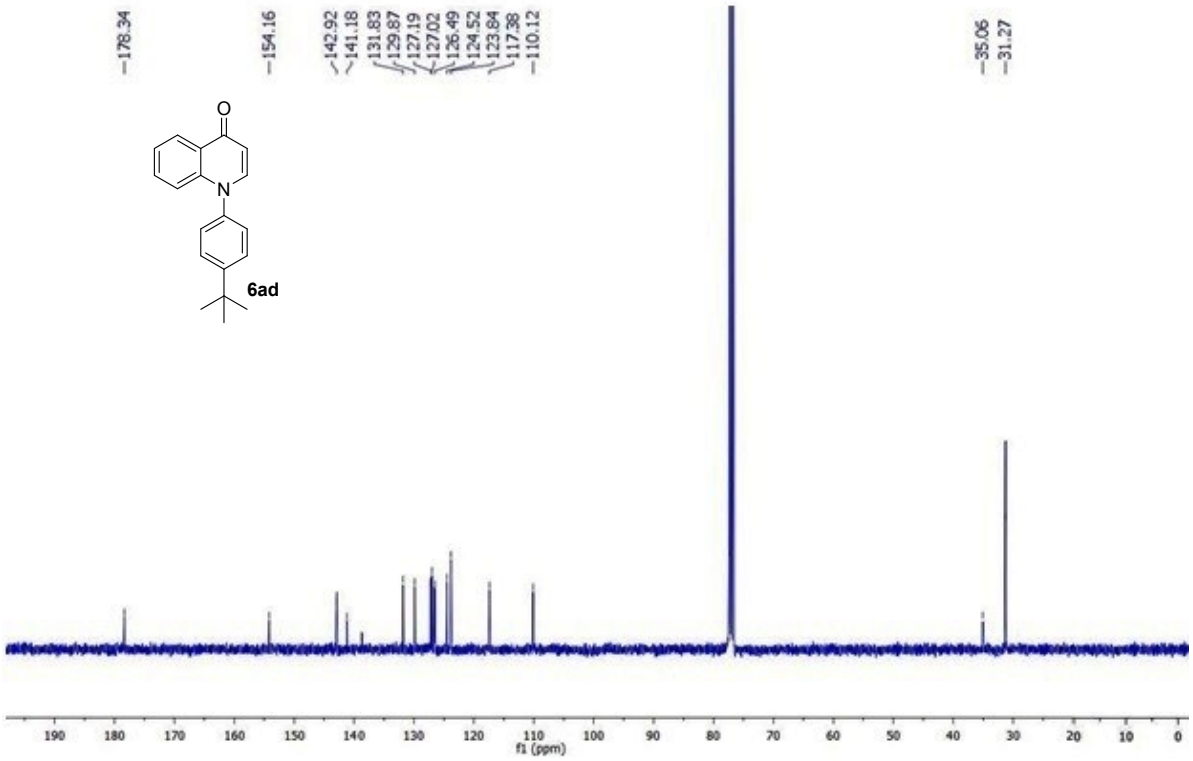


^{1}H & ^{13}C NMR spectra of 1-(4-bromophenyl)quinolin-4(1*H*)-one (6ac)

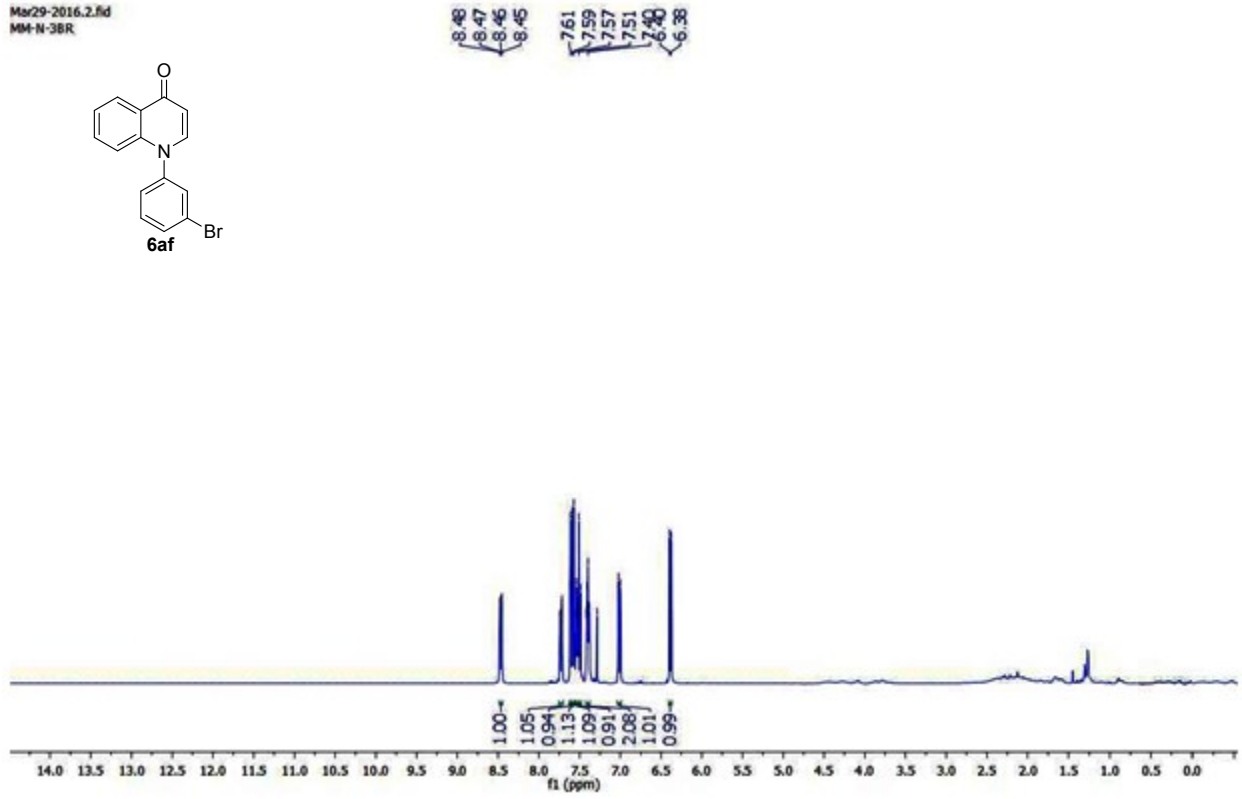


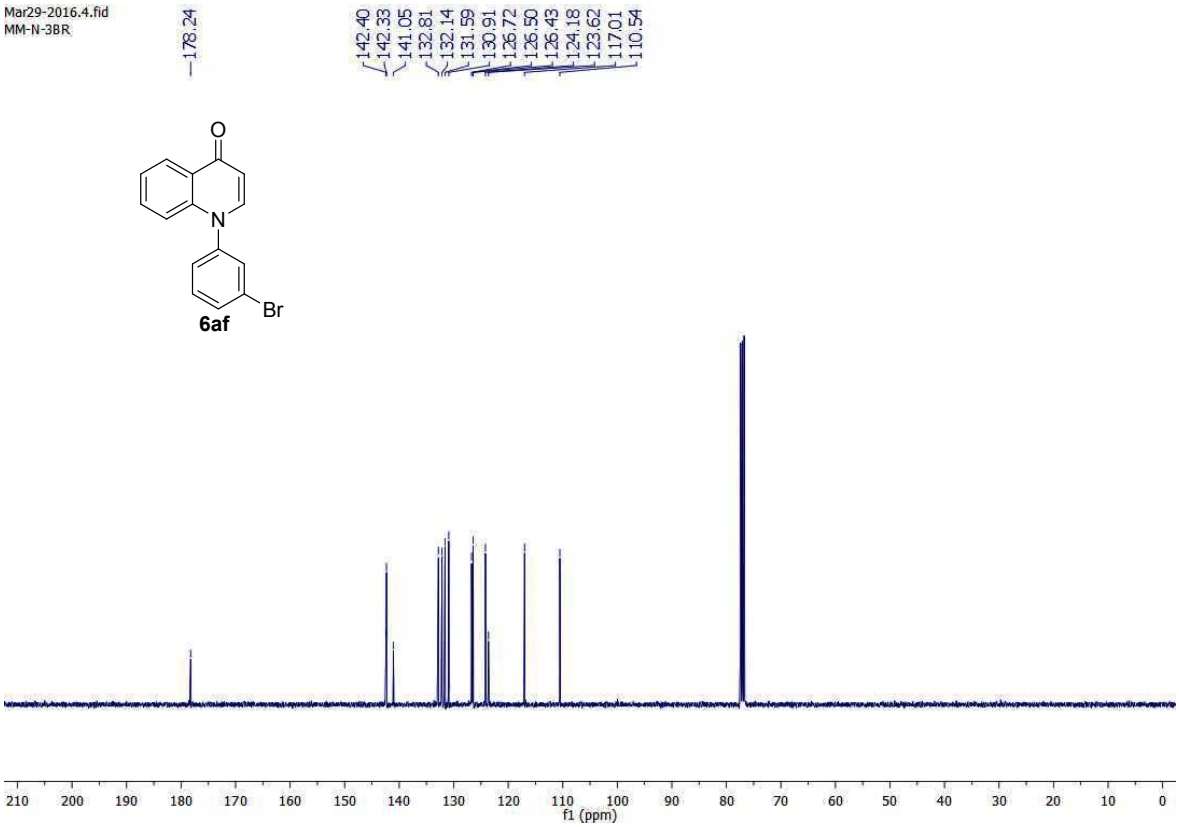
^{1}H & ^{13}C NMR spectra of 1-(4-(tert-butyl)phenyl)quinolin-4(1*H*)-one (6ad)



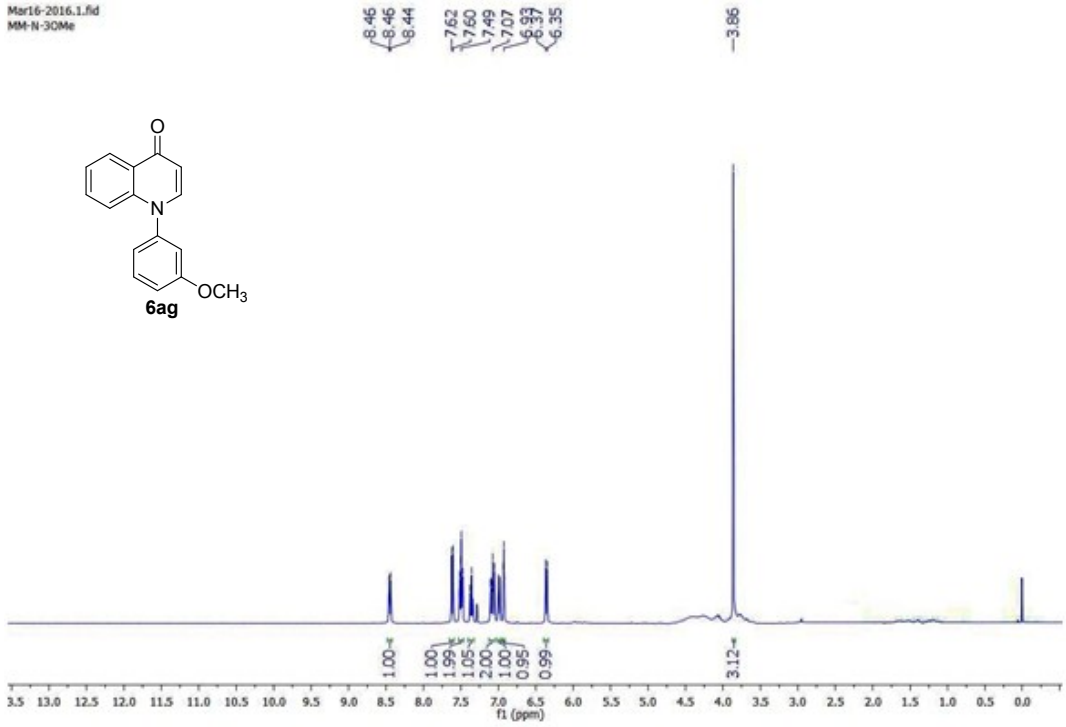


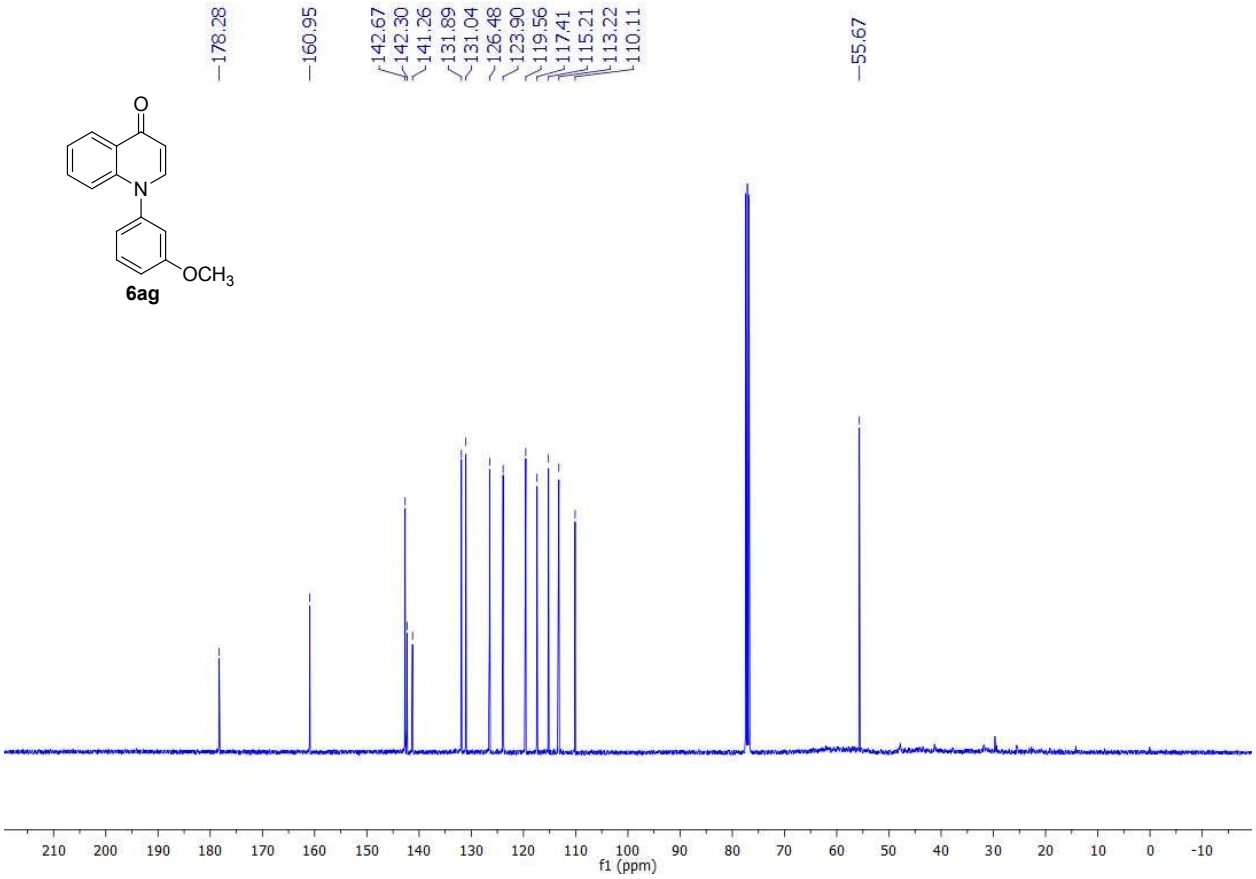
^{1}H & ^{13}C NMR spectra of 1-(3-bromophenyl)quinolin-4(1*H*)-one (6af)



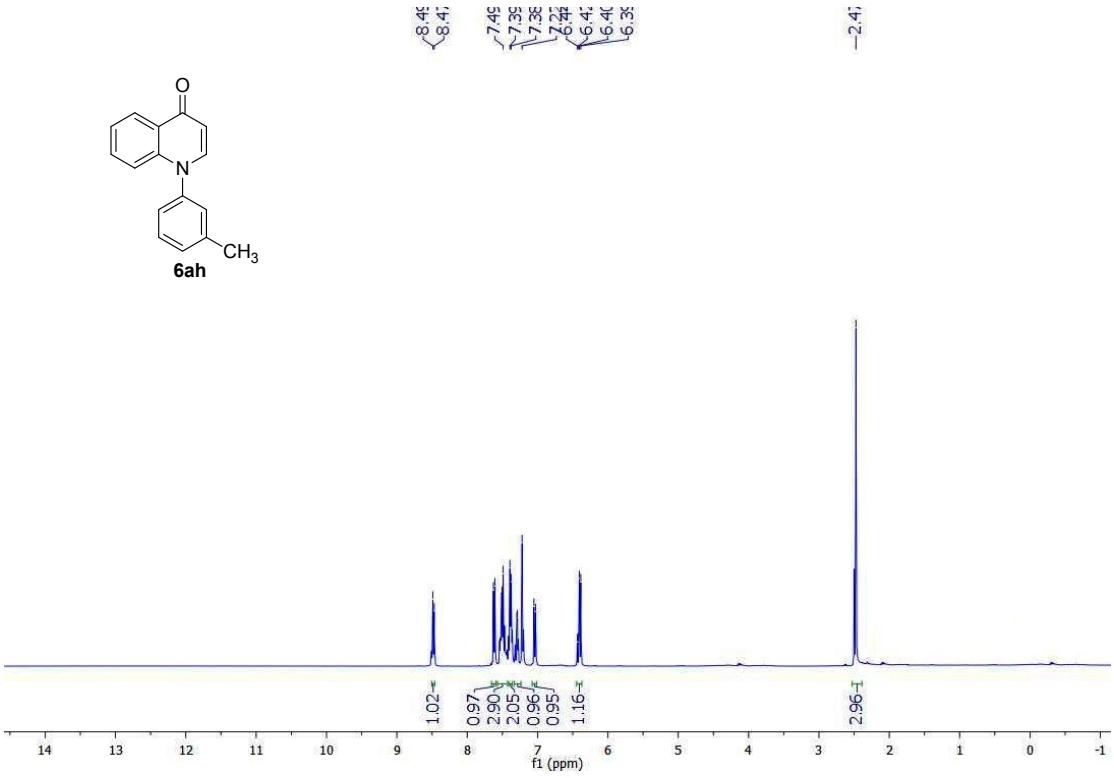


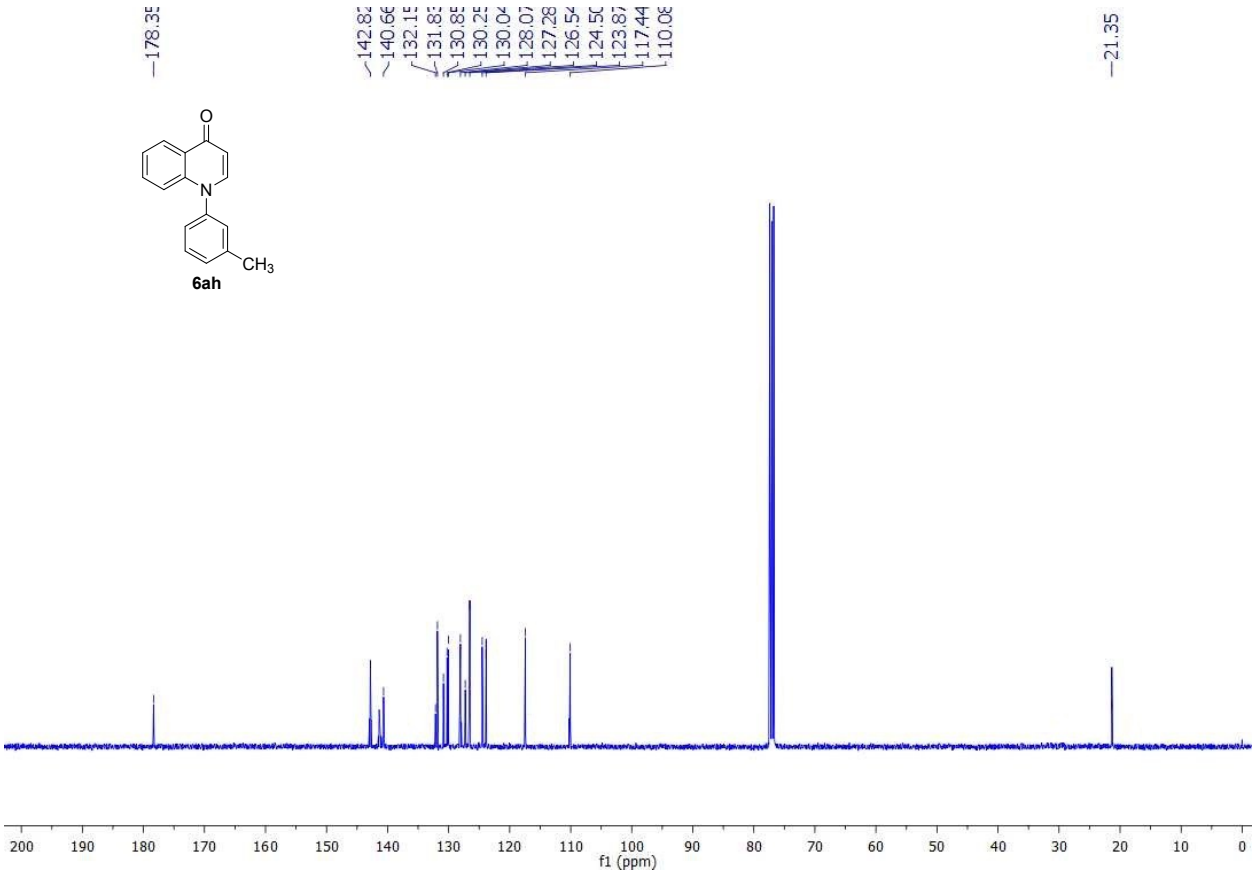
^{1}H & ^{13}C NMR spectra of 1-(3-methoxyphenyl)quinolin-4(1*H*)-one (6ag)



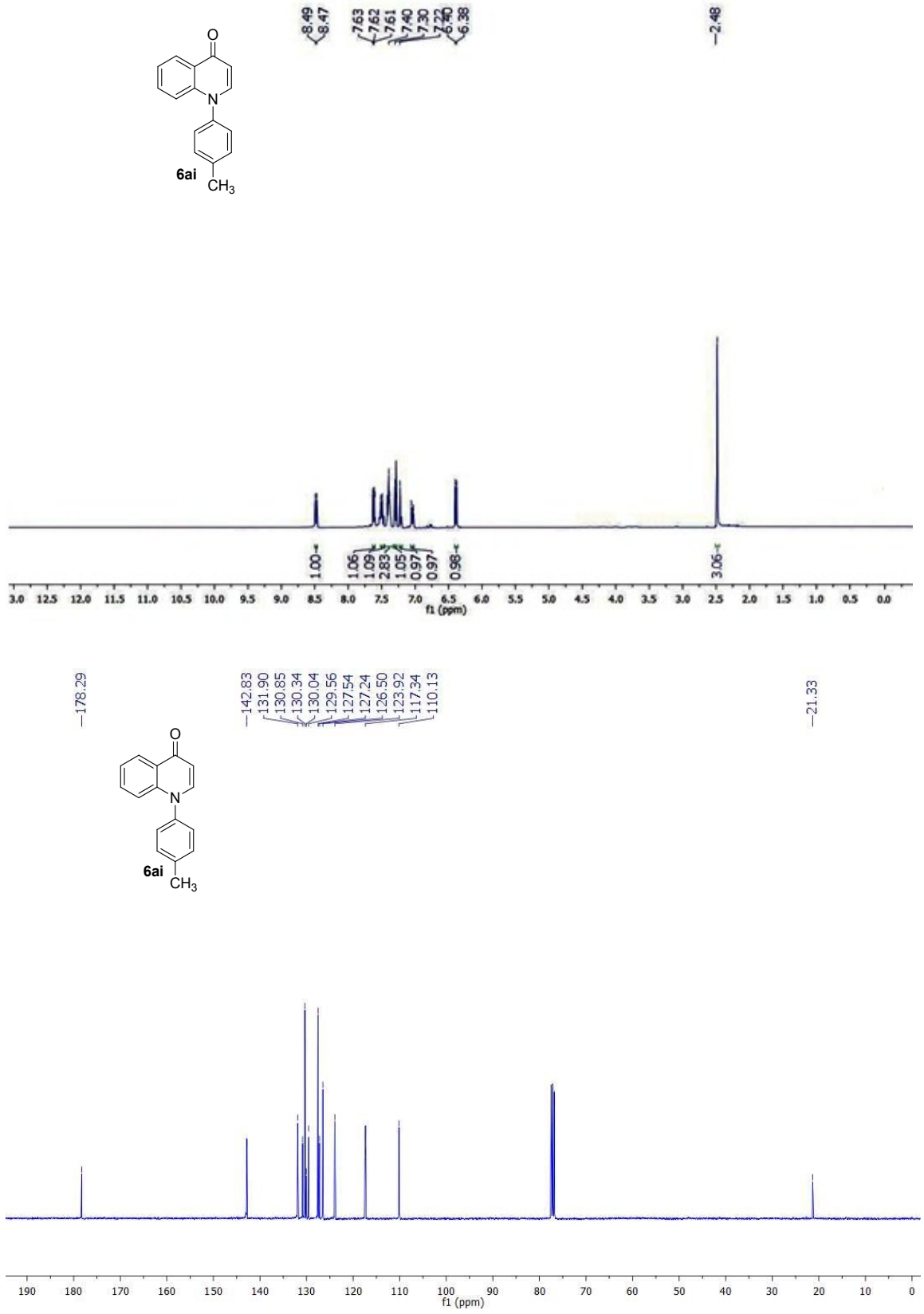


^{1}H & ^{13}C NMR spectra of 1-(*m*-tolyl)quinolin-4(1*H*)-one (6ah)

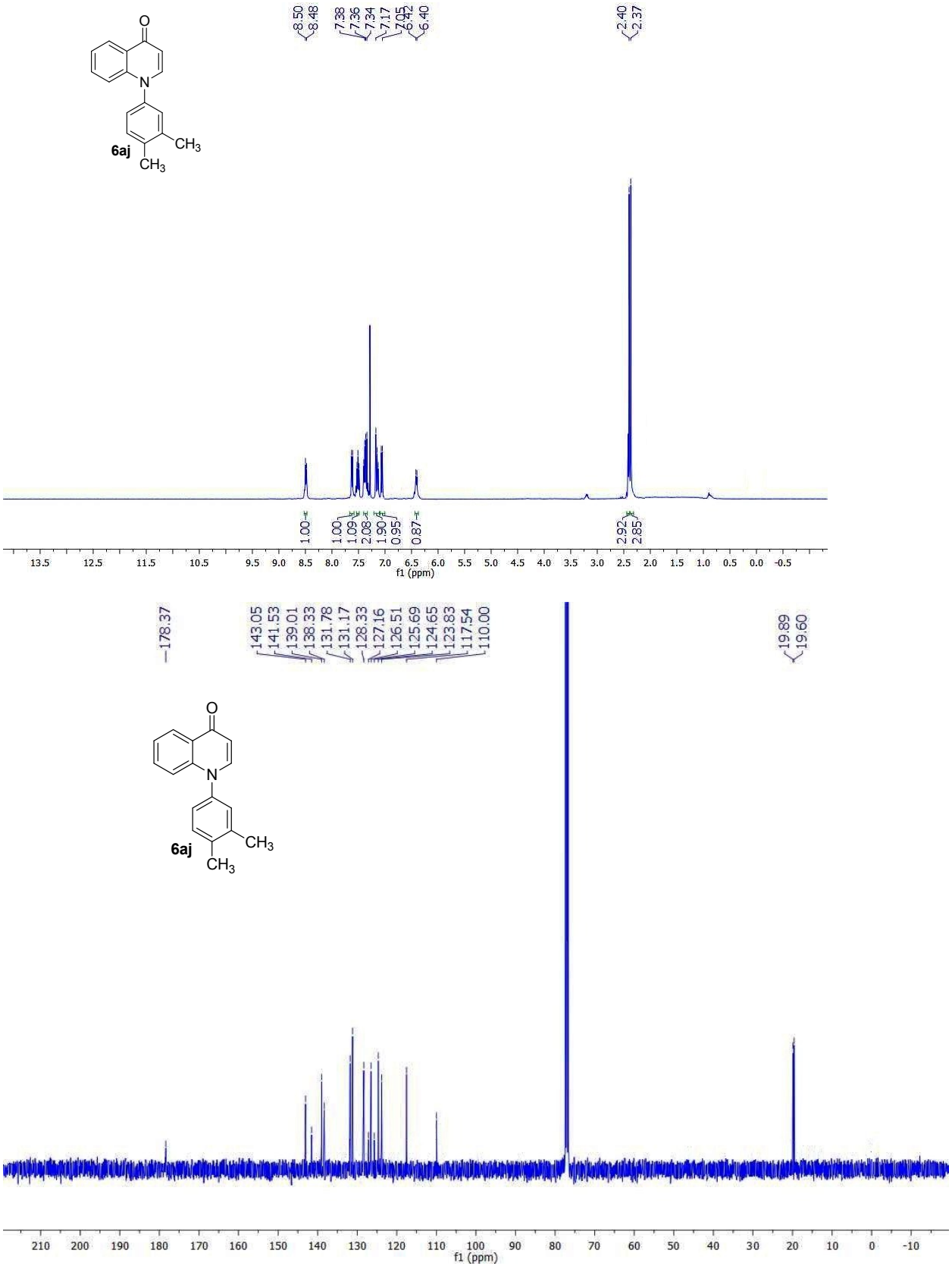




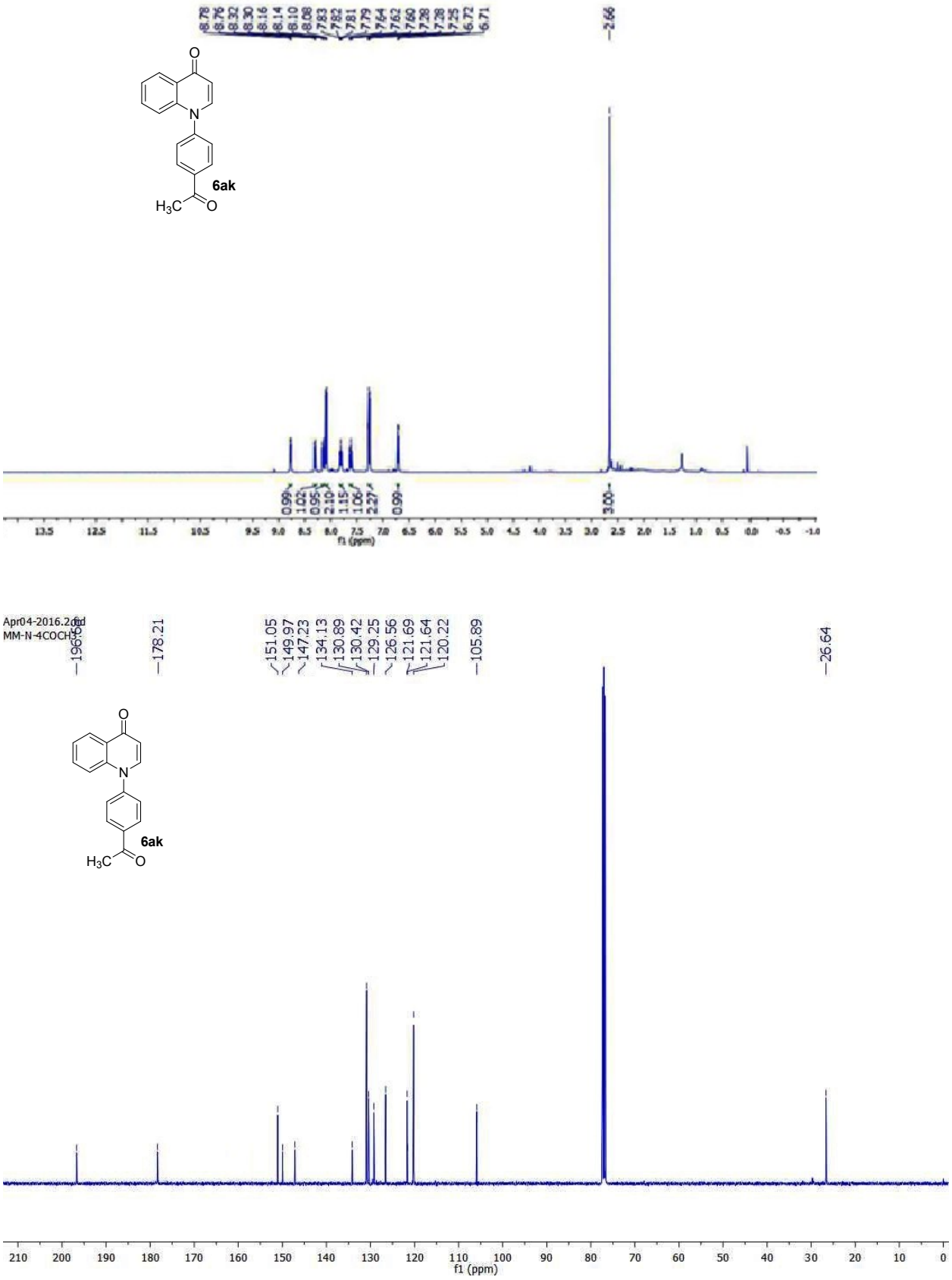
^{1}H & ^{13}C NMR spectra of 1-(*p*-tolyl)quinolin-4(1*H*)-one (6ai)



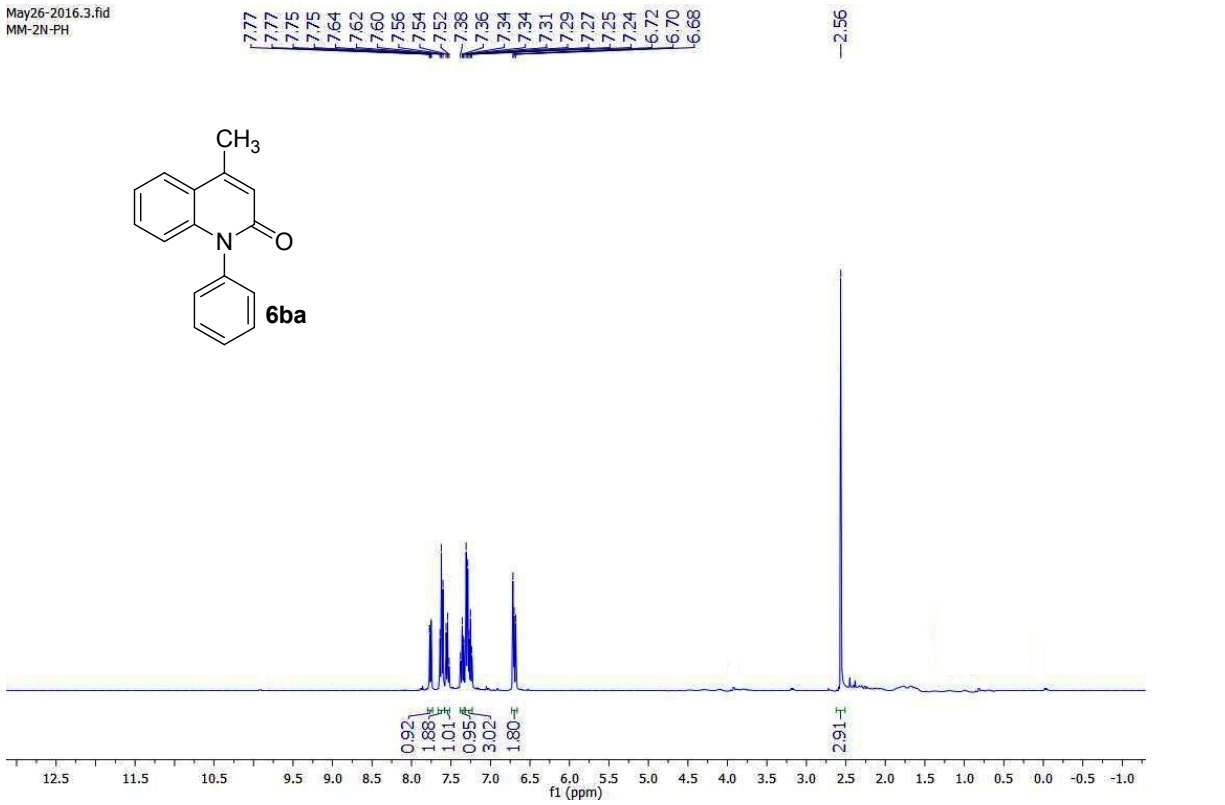
^{1}H & ^{13}C NMR spectra of 1-(3,4-dimethylphenyl)quinolin-4(1*H*)-one (6aj)

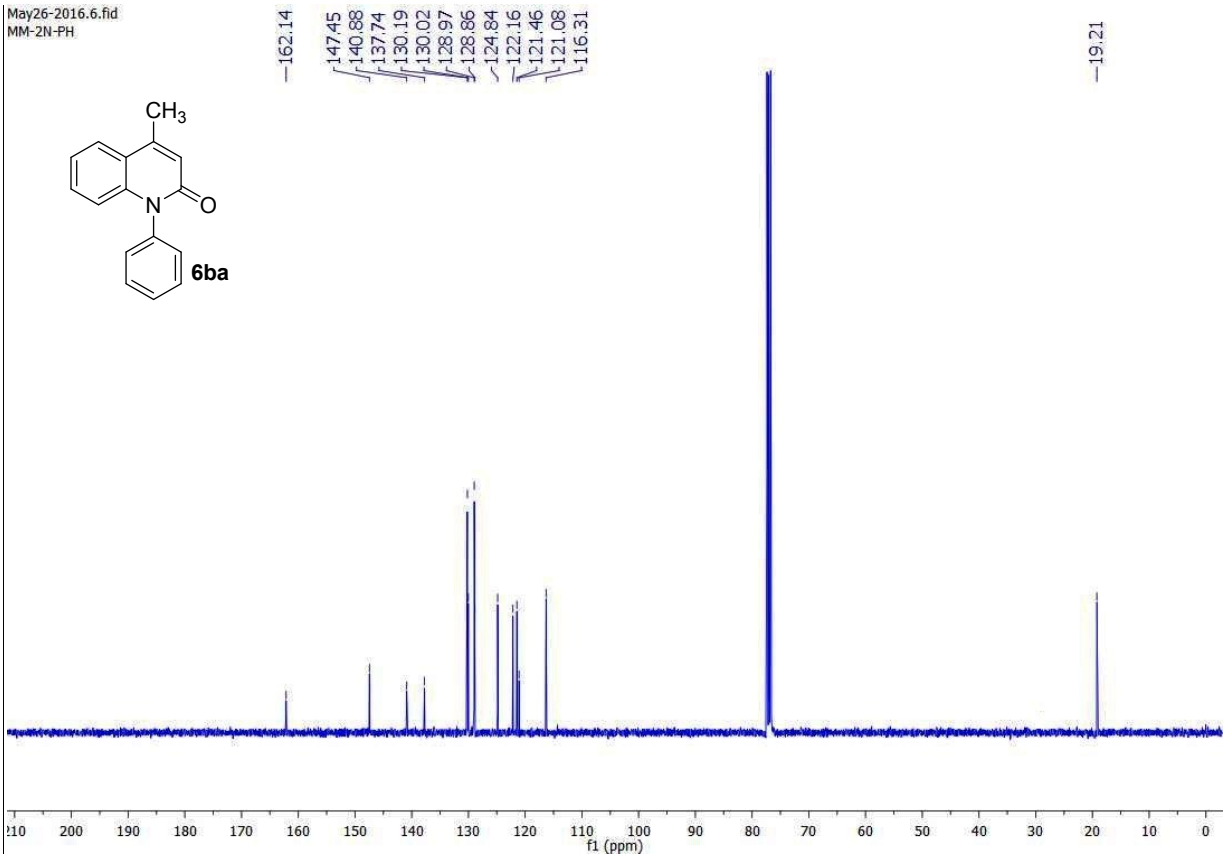


^{1}H & ^{13}C NMR spectra of 1-(4-acetylphenyl)quinolin-4(1*H*)-one (6ak)

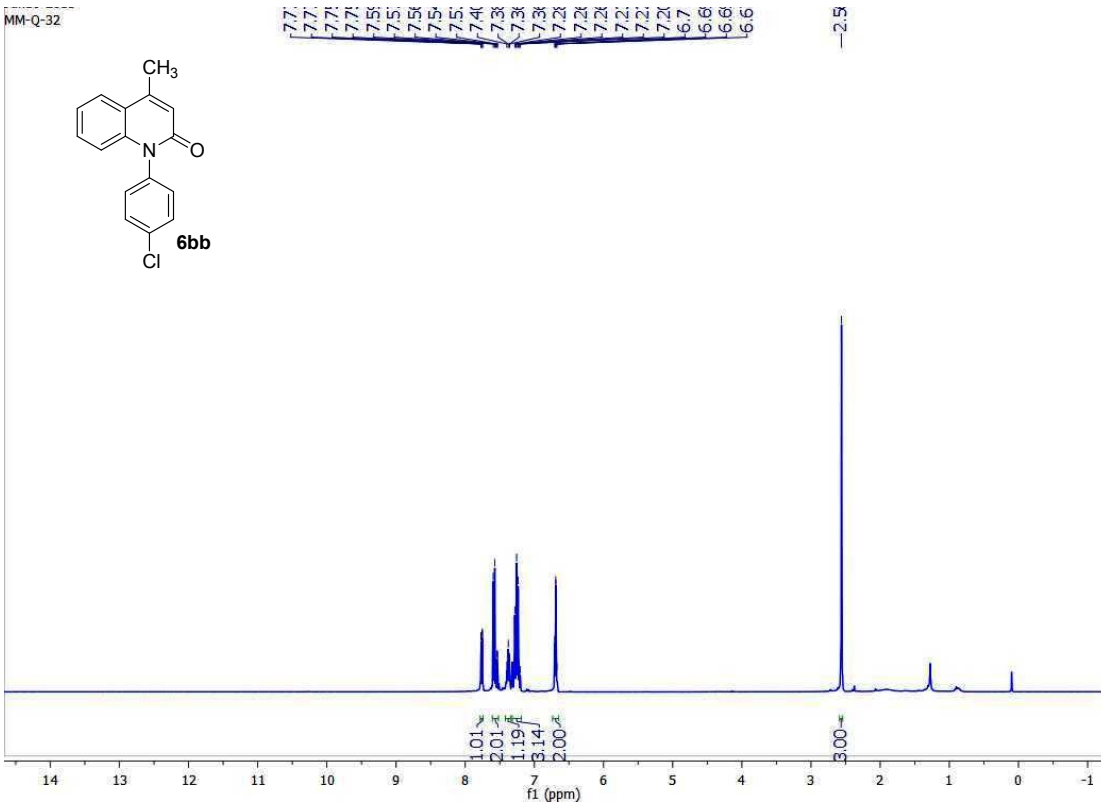


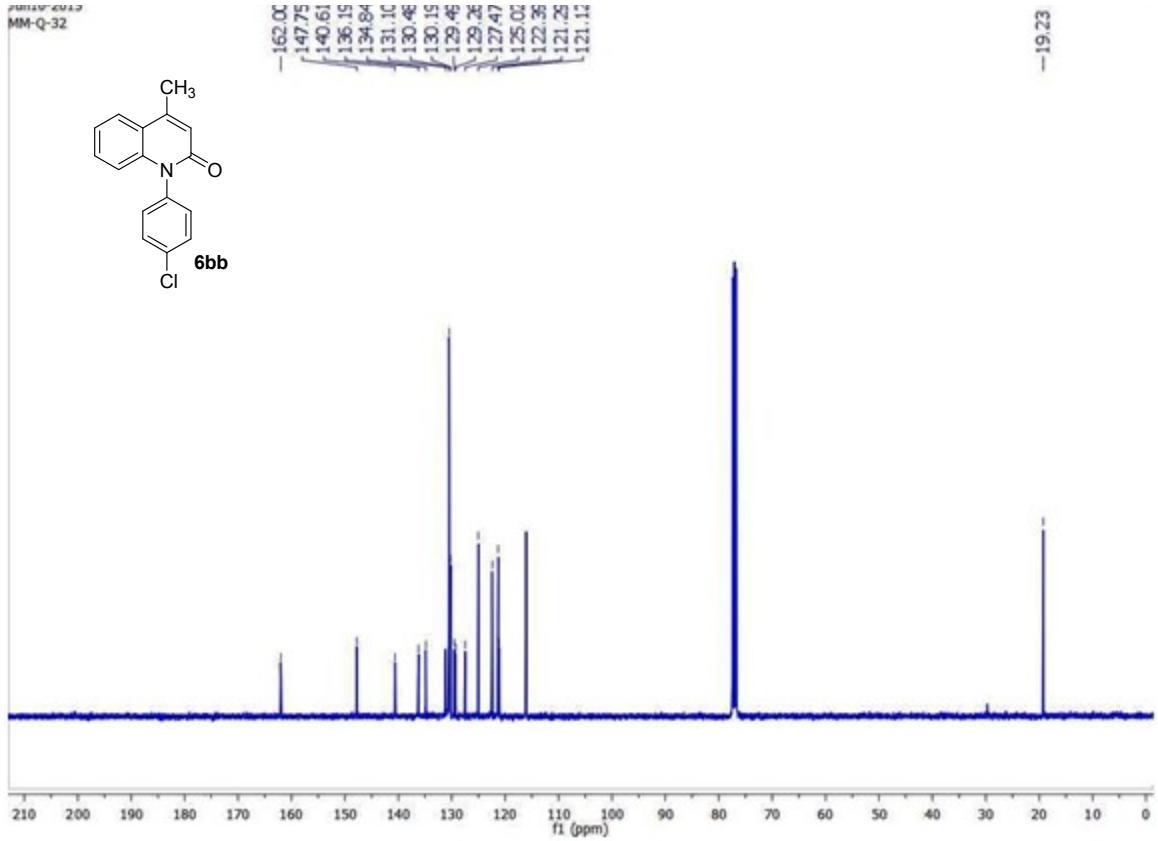
^{1}H & ^{13}C NMR spectra of 4-methyl-1-phenylquinolin-2(1*H*)-one (6aa)



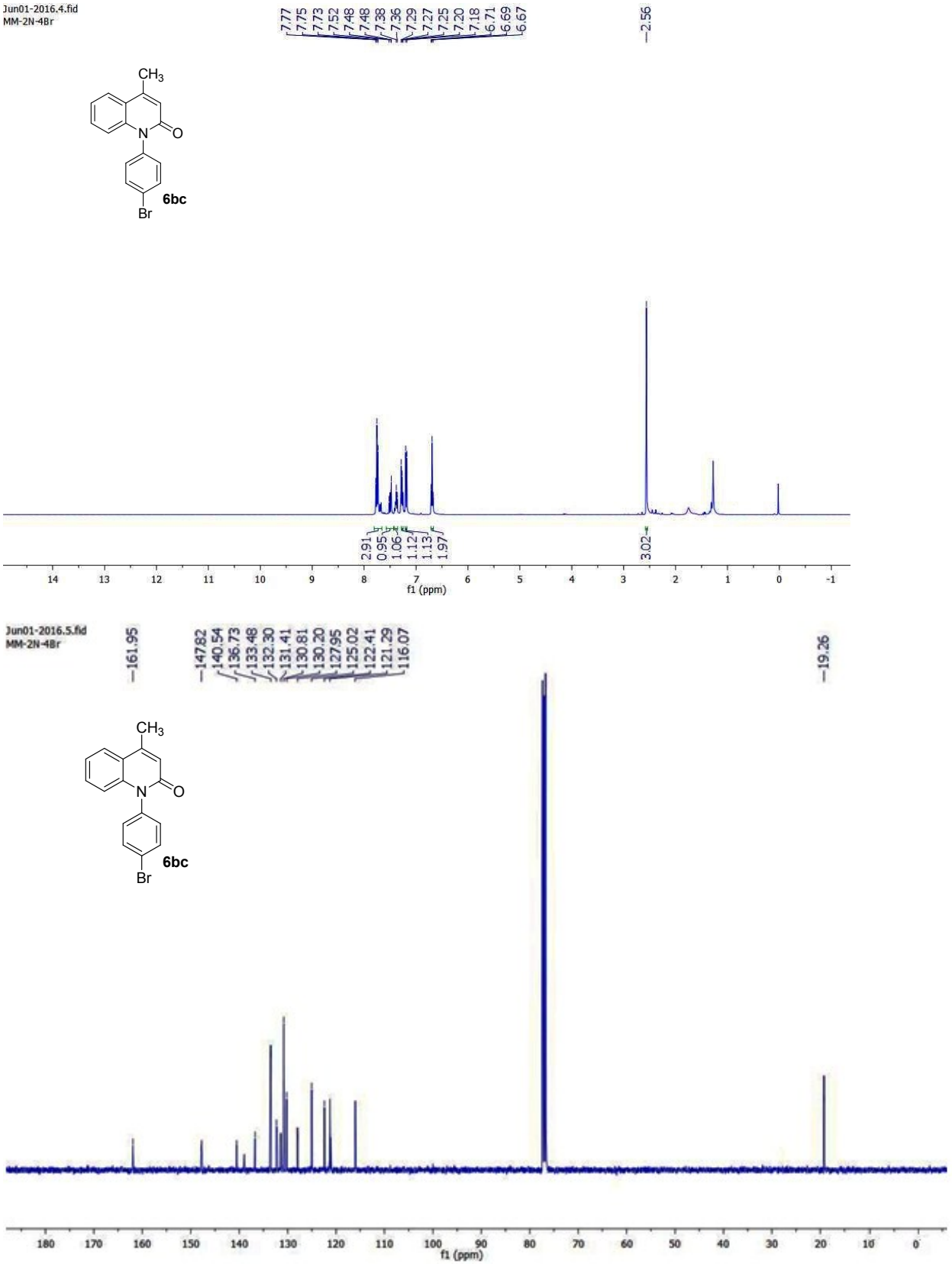


^{1}H & ^{13}C NMR spectra of 1-(4-chlorophenyl)-4-methylquinolin-2(1*H*)-one (6bb)

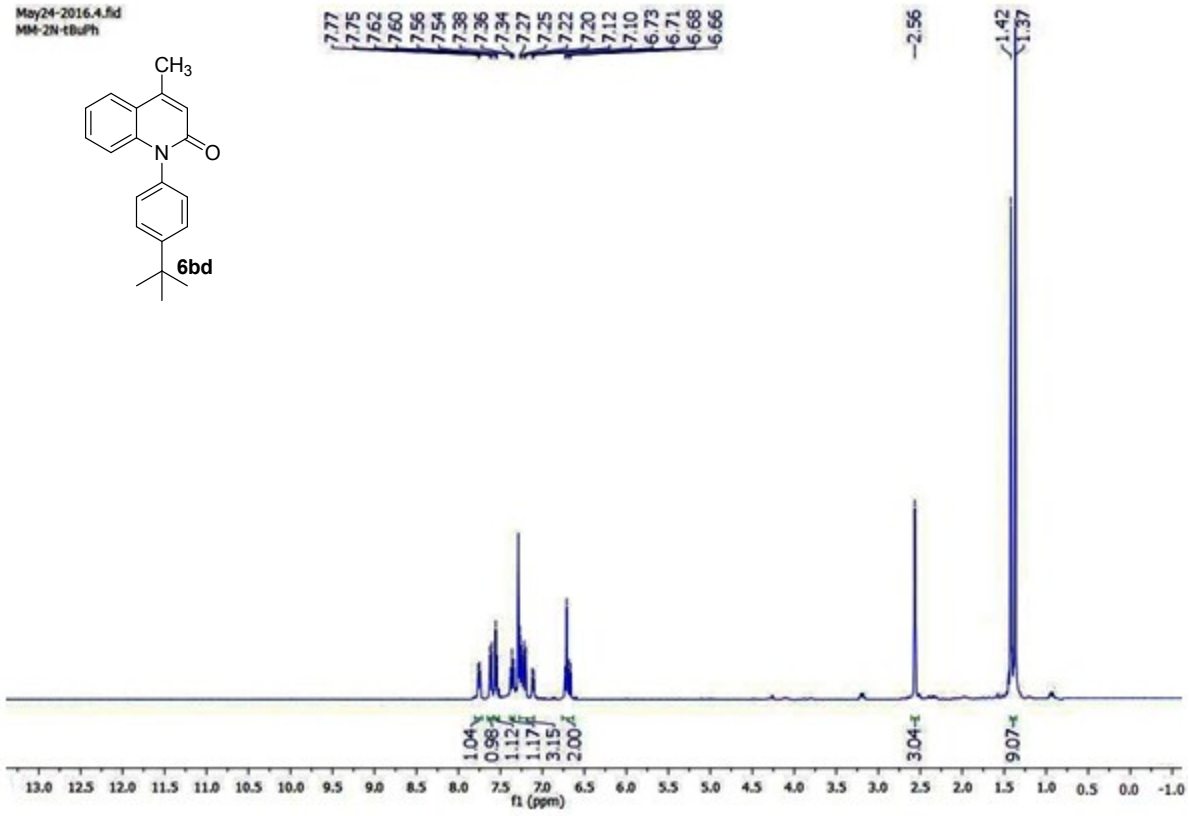


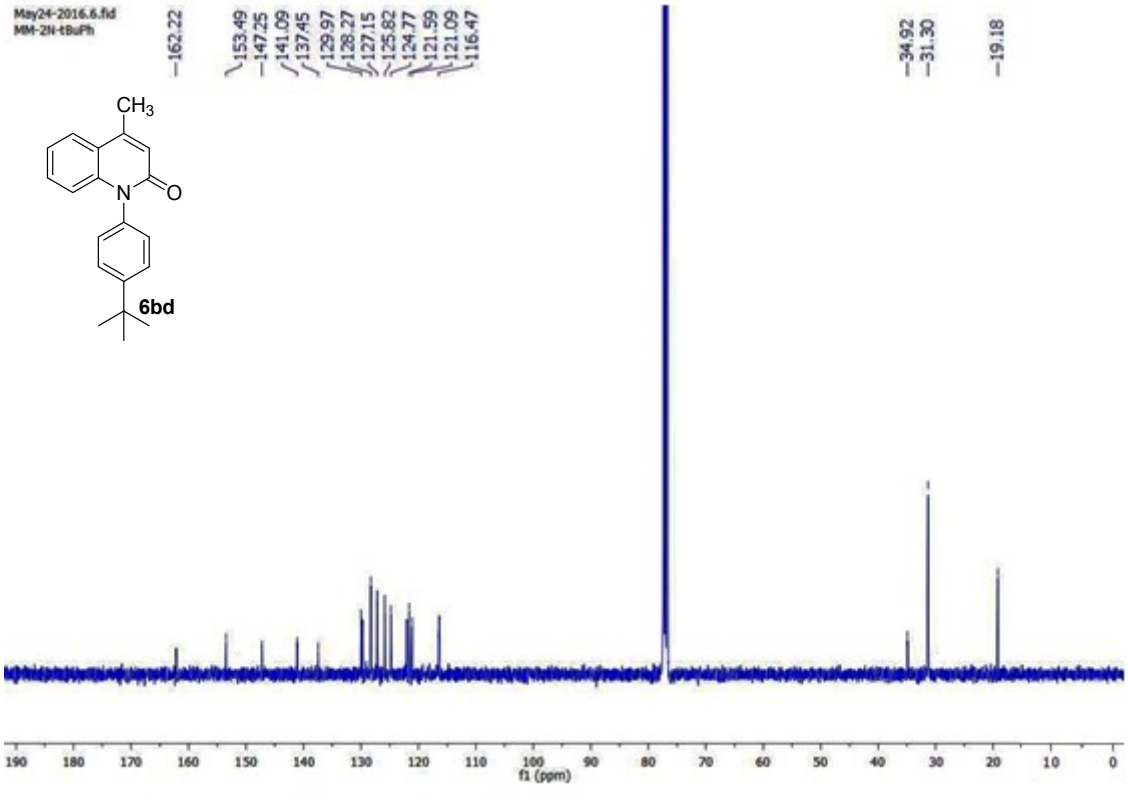


^{1}H & ^{13}C NMR spectra of 1-(4-bromophenyl)-4-methylquinolin-2(1*H*)-one (6bc)

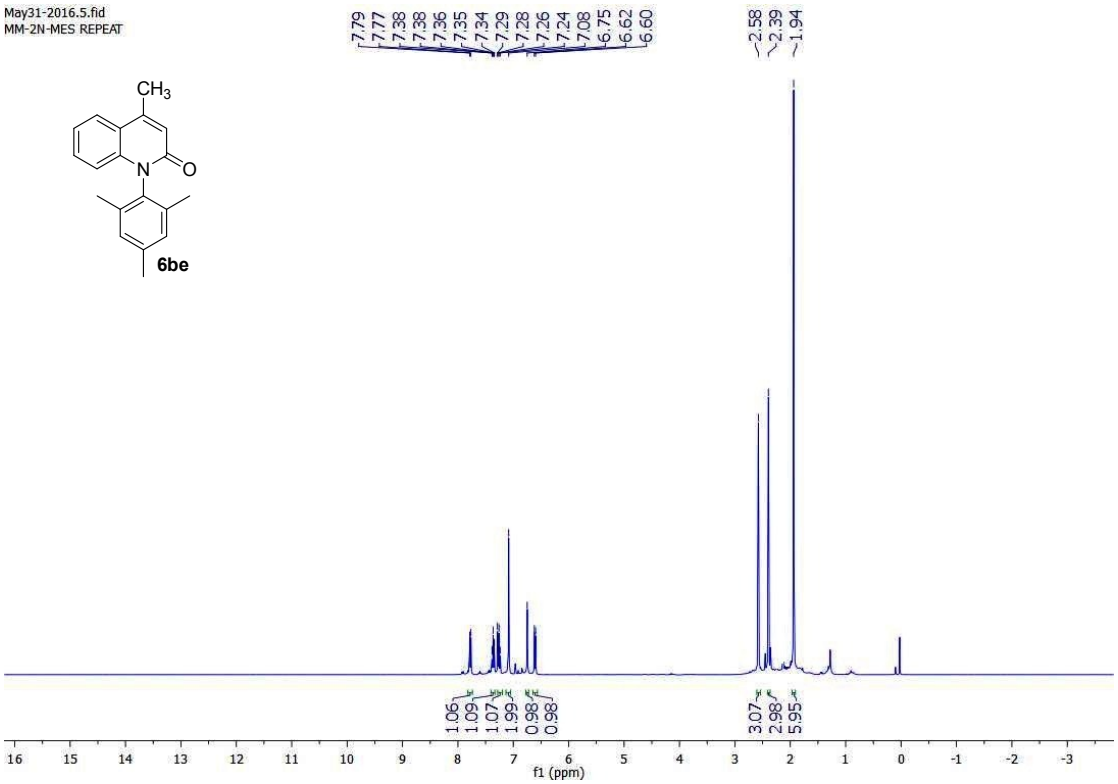


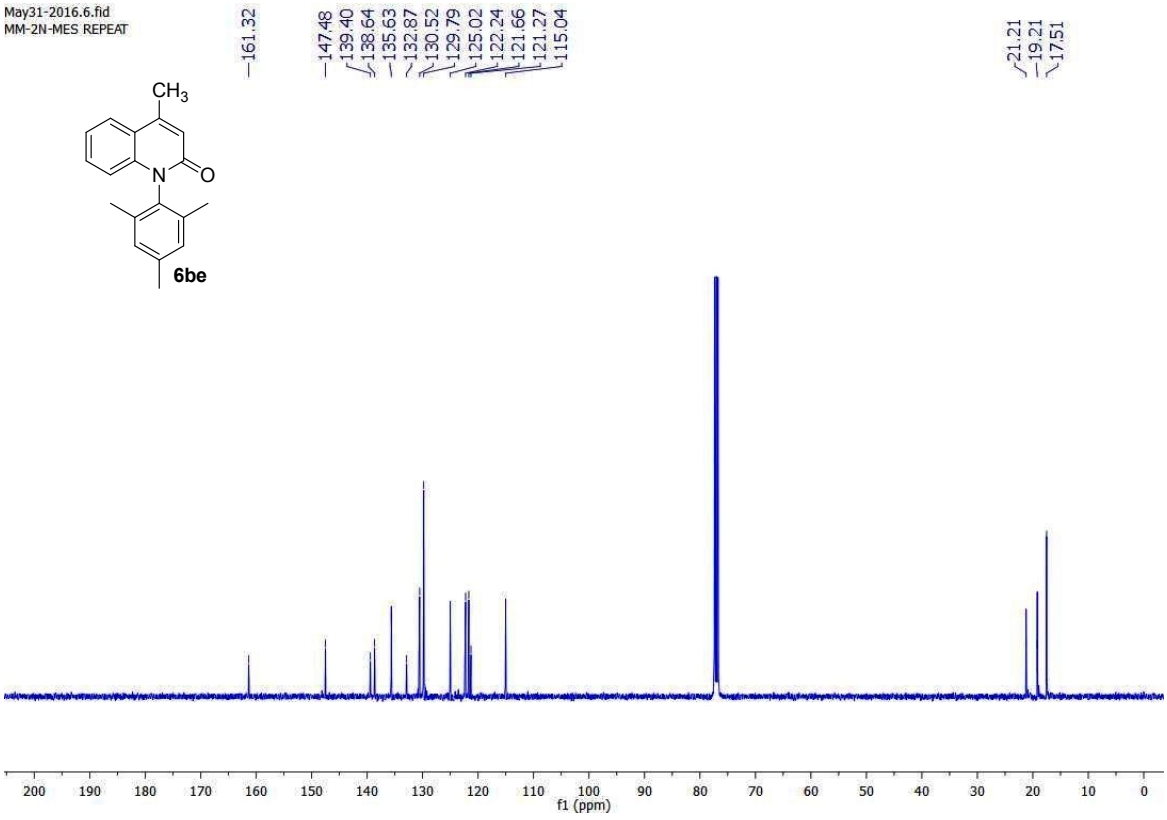
^{1}H & ^{13}C NMR spectra of 1-(4-(tert-butyl)phenyl)-4-methylquinolin-2(1*H*)-one (6bd)


May24-2016.4.fid
MM-2N-tBuPh
CH3
N
O
6bd
7.77
7.75
7.62
7.60
7.56
7.54
7.38
7.36
7.34
7.27
7.25
7.22
7.20
7.12
7.10
6.73
6.71
6.68
6.66
2.56
1.42
1.37
1.04
0.98
1.12
1.17
3.15
2.00
3.04
9.07
f1 (ppm)

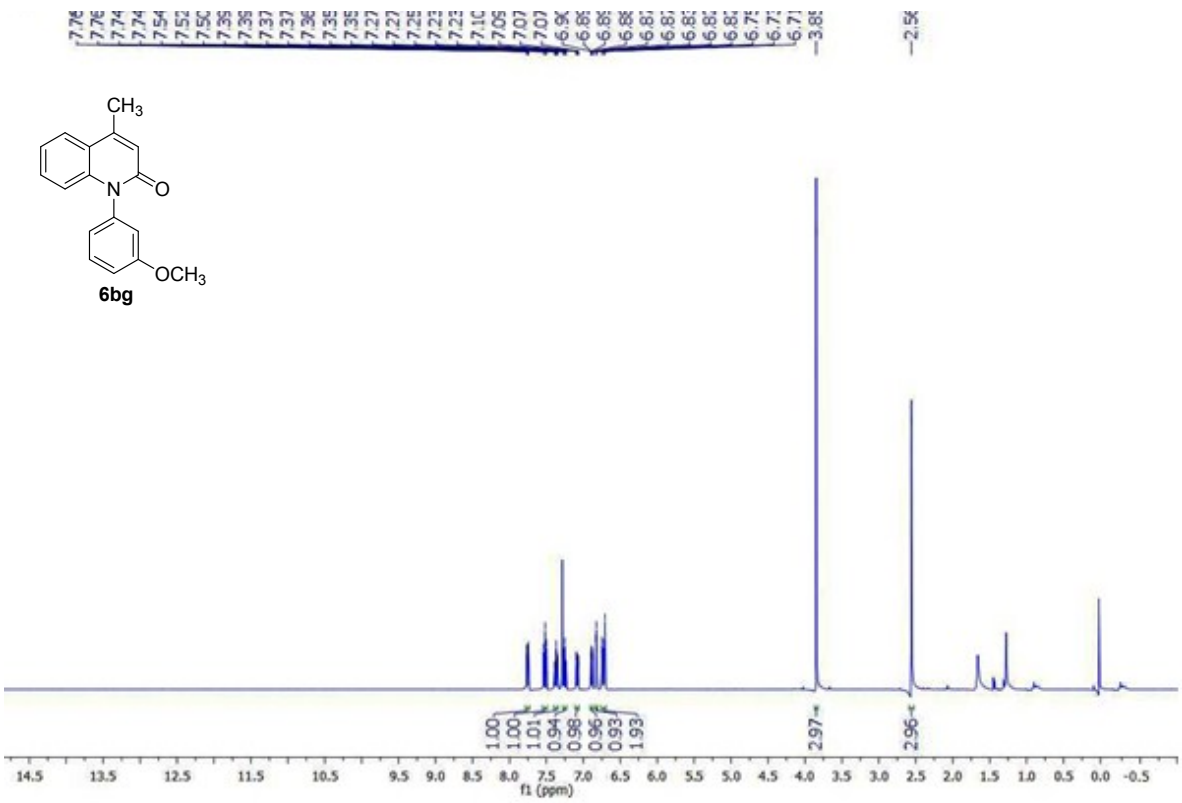

May24-2016.6.fid
MM-2N-tBuPh
CH3
N
O
6bd
162.22
153.49
147.25
141.09
137.45
129.97
128.27
127.15
125.82
124.77
121.59
121.09
116.47
34.92
31.30
19.18
f1 (ppm)

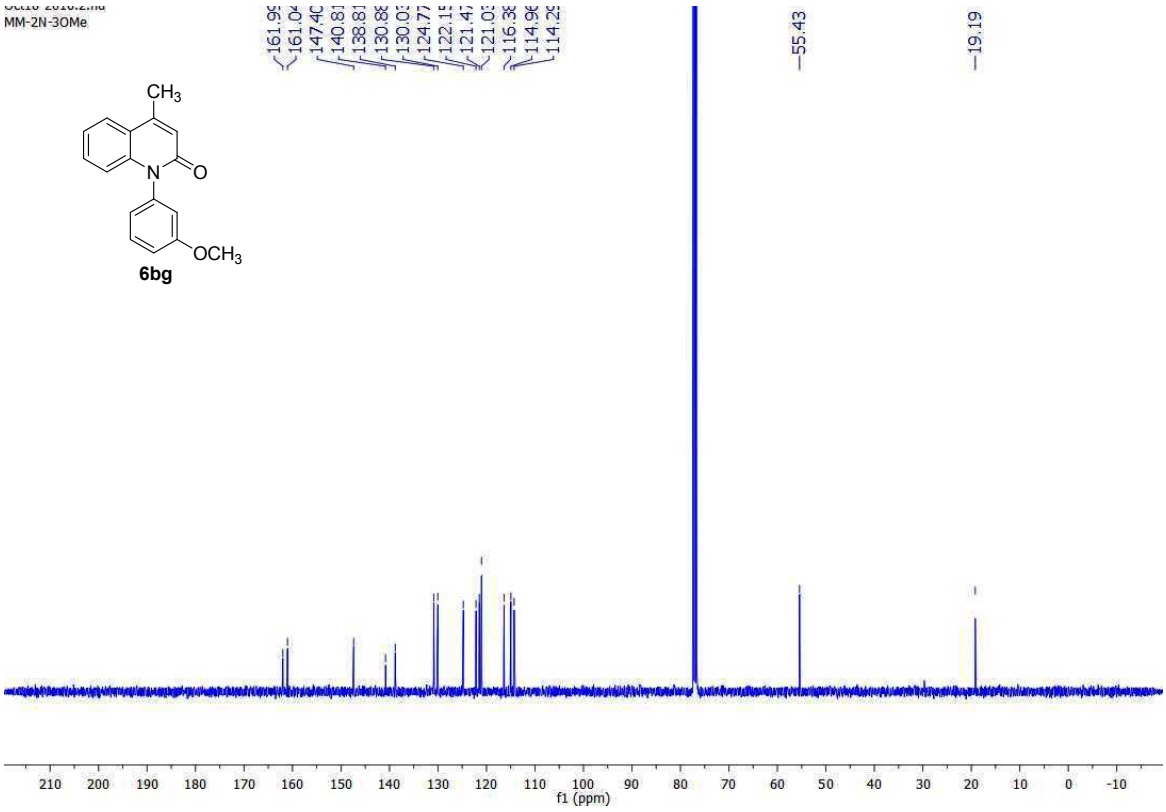
^{1}H & ^{13}C NMR spectra of 1-mesityl-4-methylquinolin-2(1*H*)-one (6be)



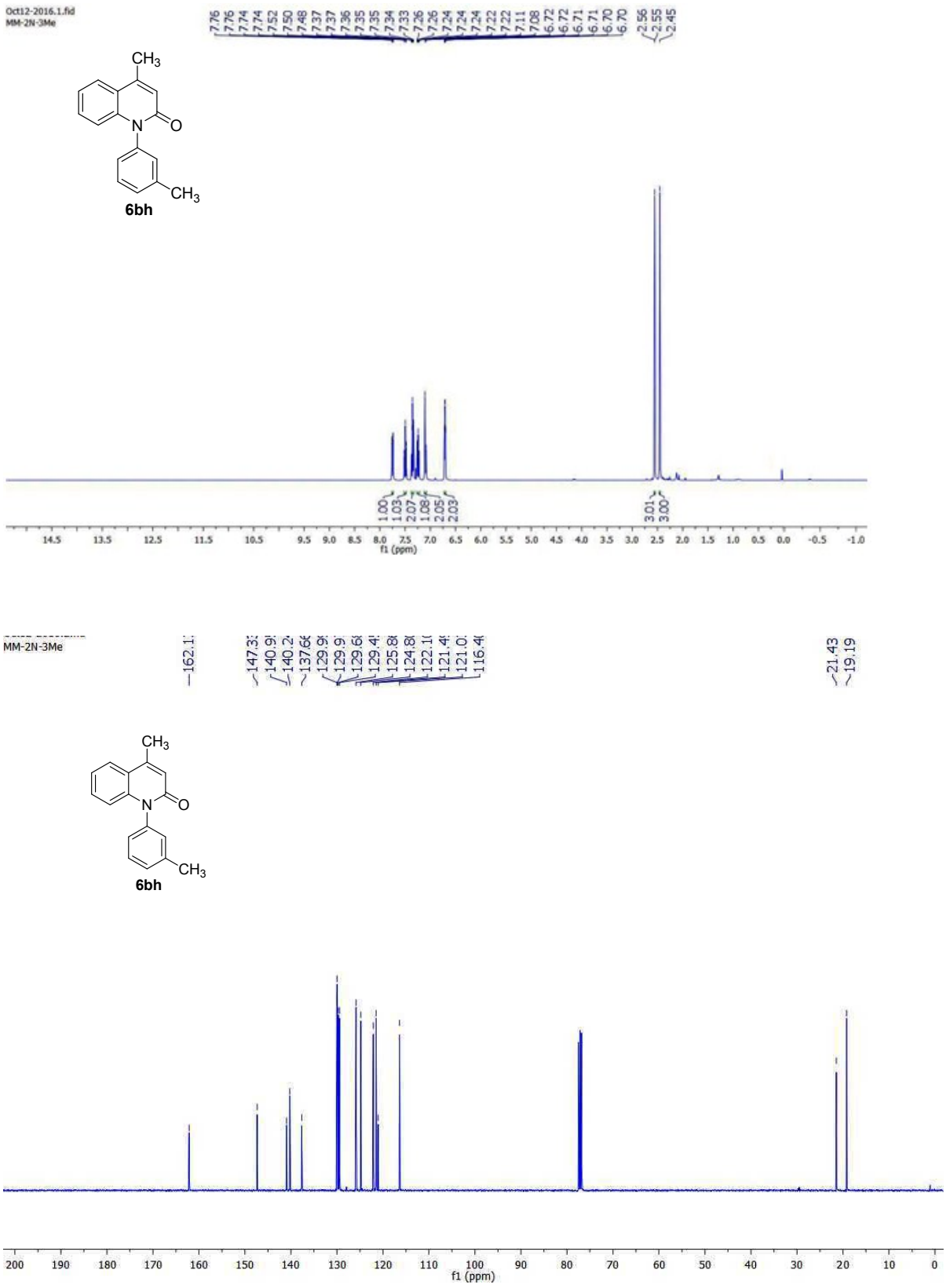


^{1}H & ^{13}C NMR spectra of 1-(3-methoxyphenyl)-4-methylquinolin-2(1*H*)-one (6bg)

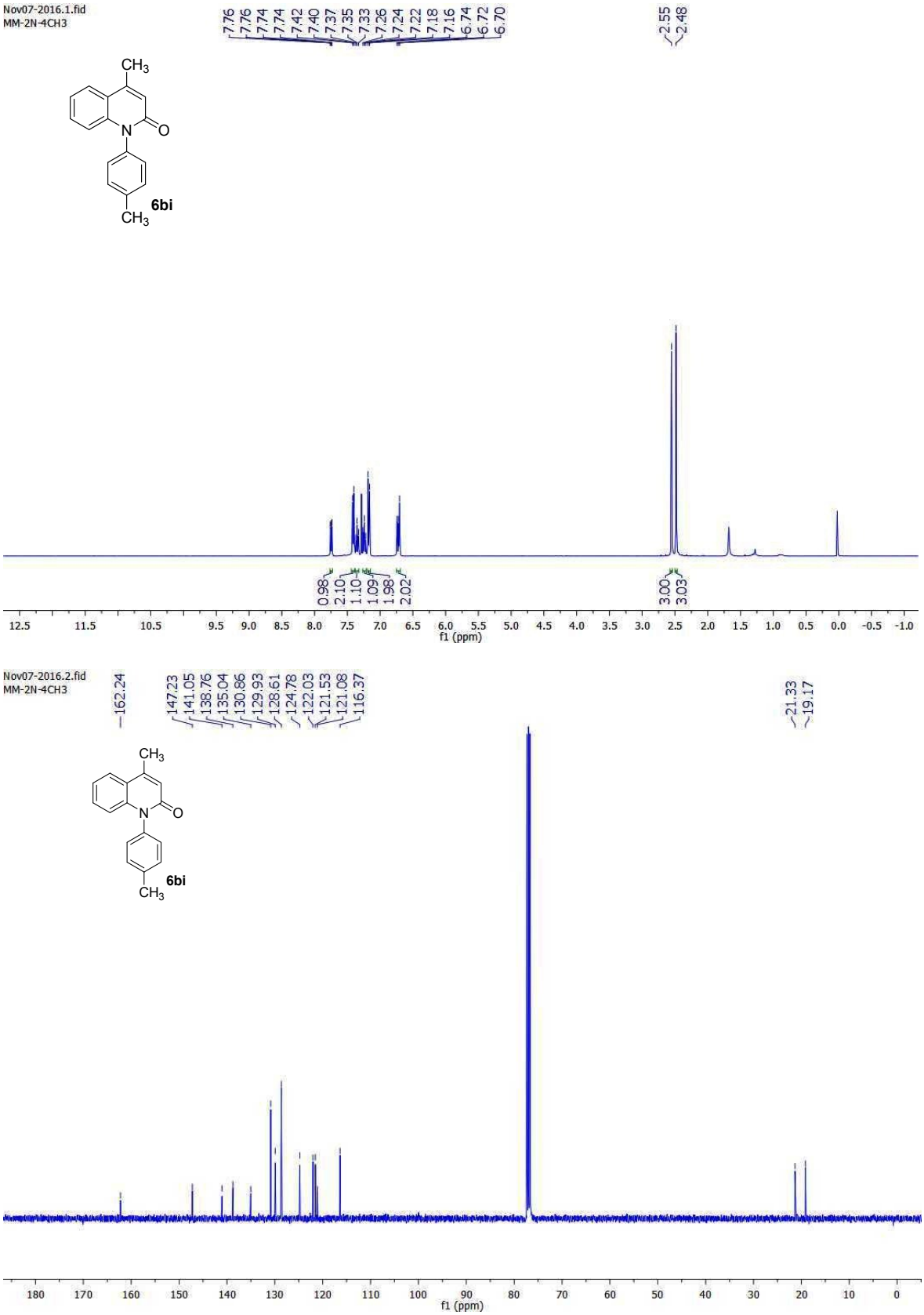




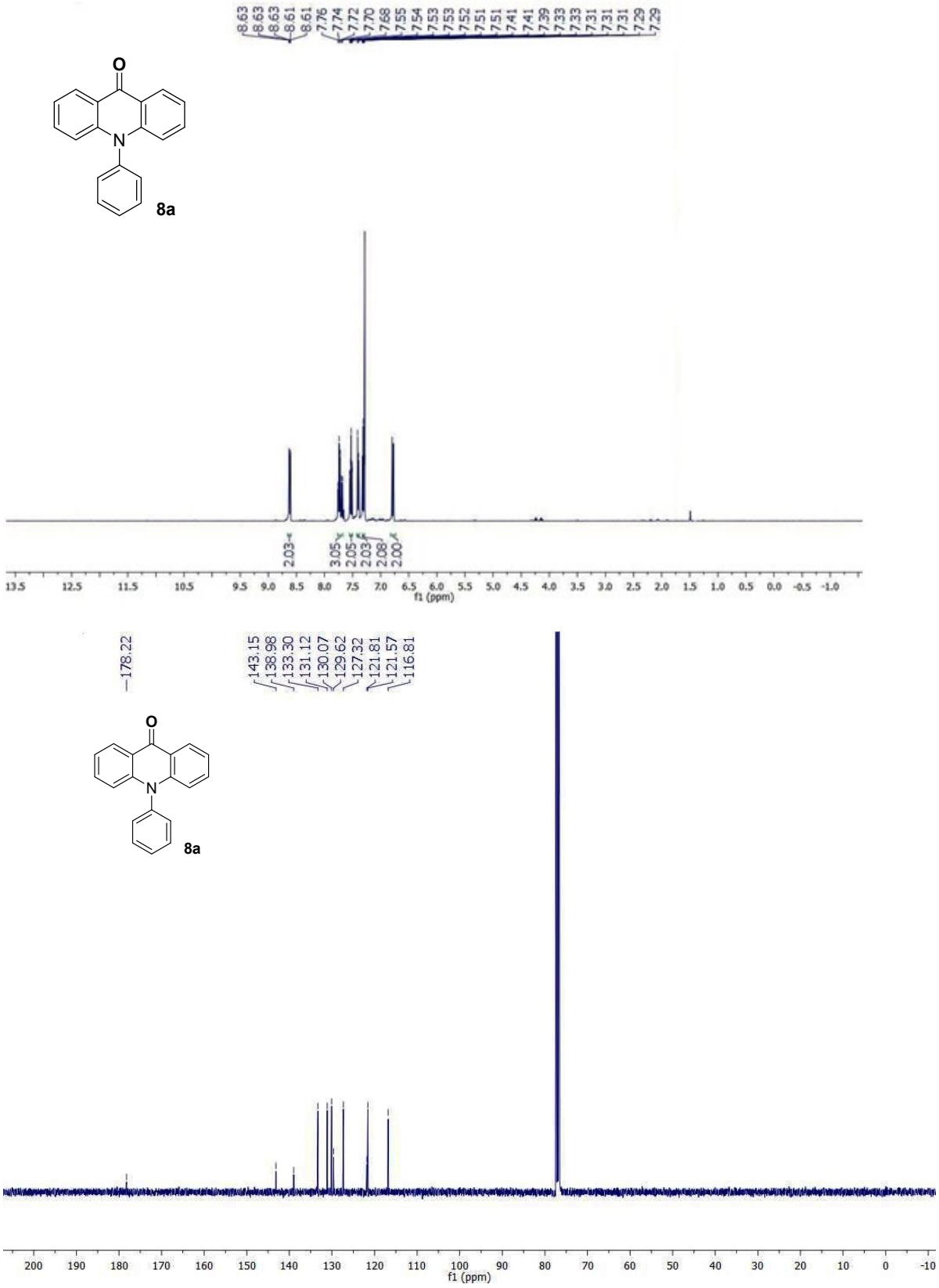
^{1}H & ^{13}C NMR spectra of 4-methyl-1-(*m*-tolyl)quinolin-2(1*H*)-one (6bh)



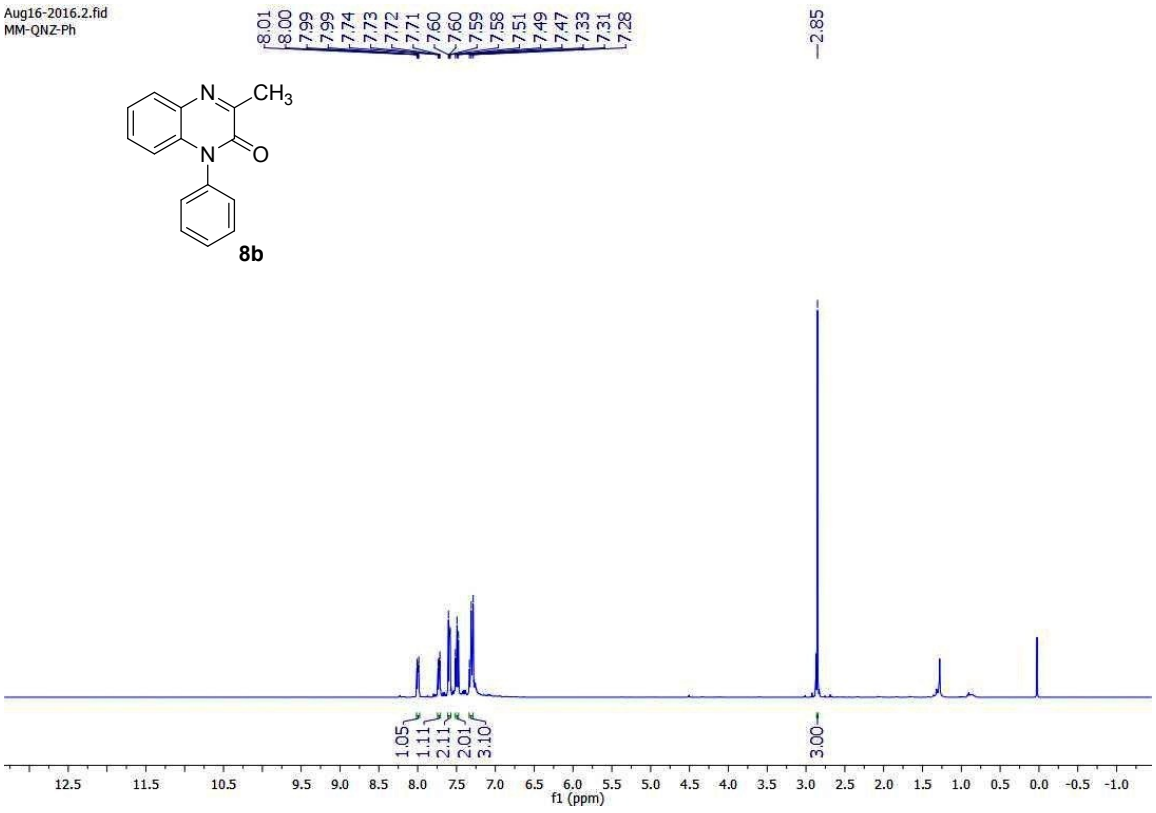
^{1}H & ^{13}C NMR spectra of 4-methyl-1-(*p*-tolyl)quinolin-2(1*H*)-one (6bi)

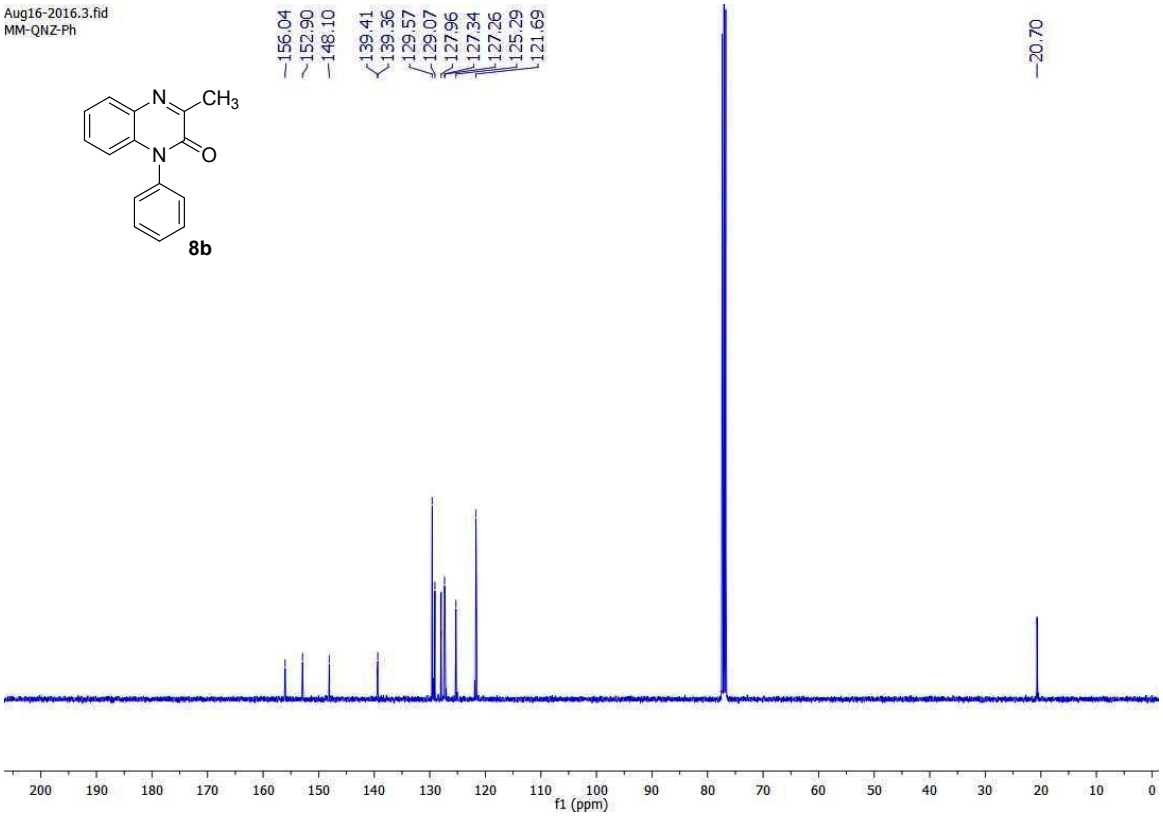


^{1}H & ^{13}C NMR spectra of 10-phenylacridin-9(10*H*)-one (8a)

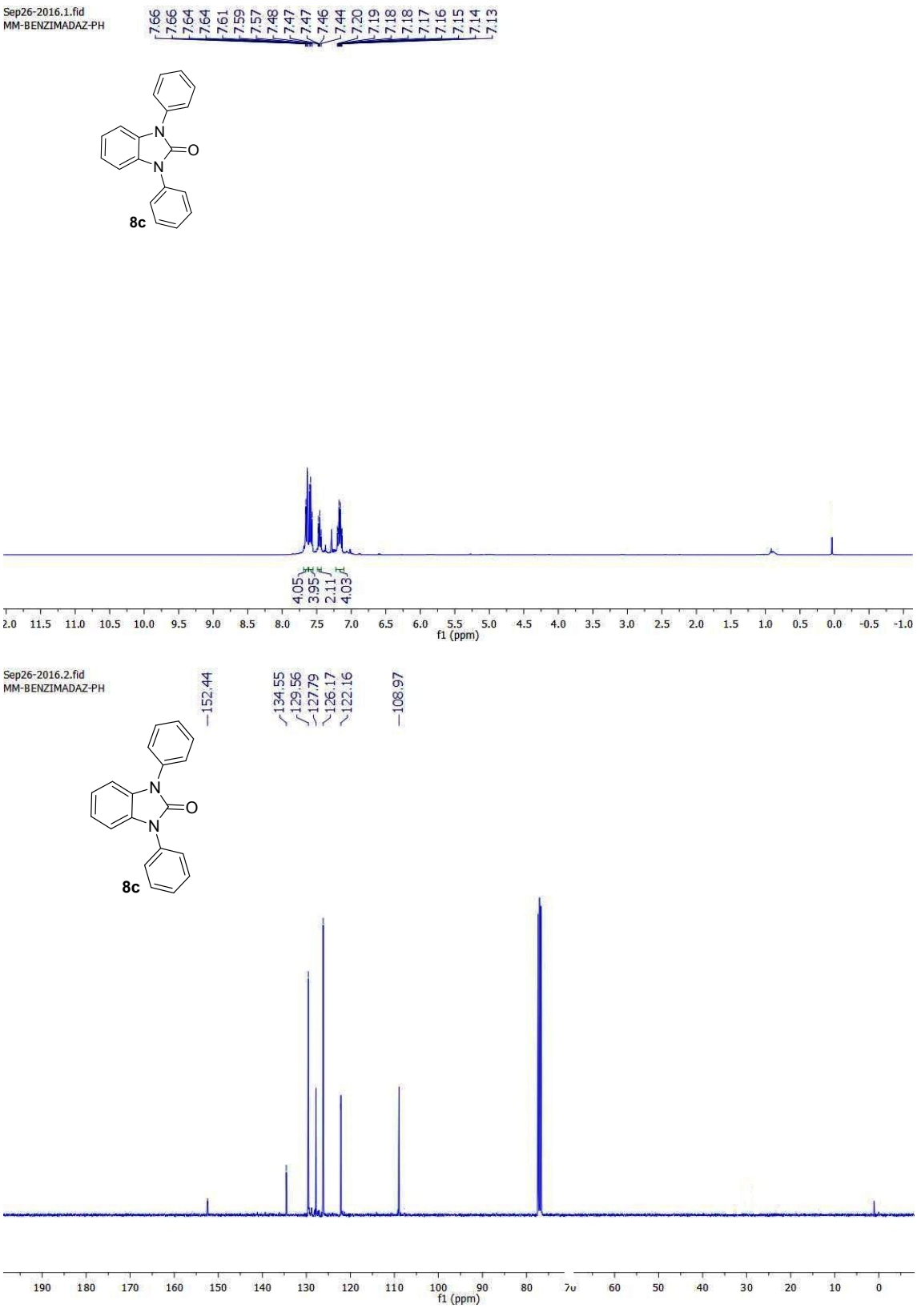


^{1}H & ^{13}C NMR spectra of 3-methyl-1-phenylquinoxalin-2(1*H*)-one (8b)

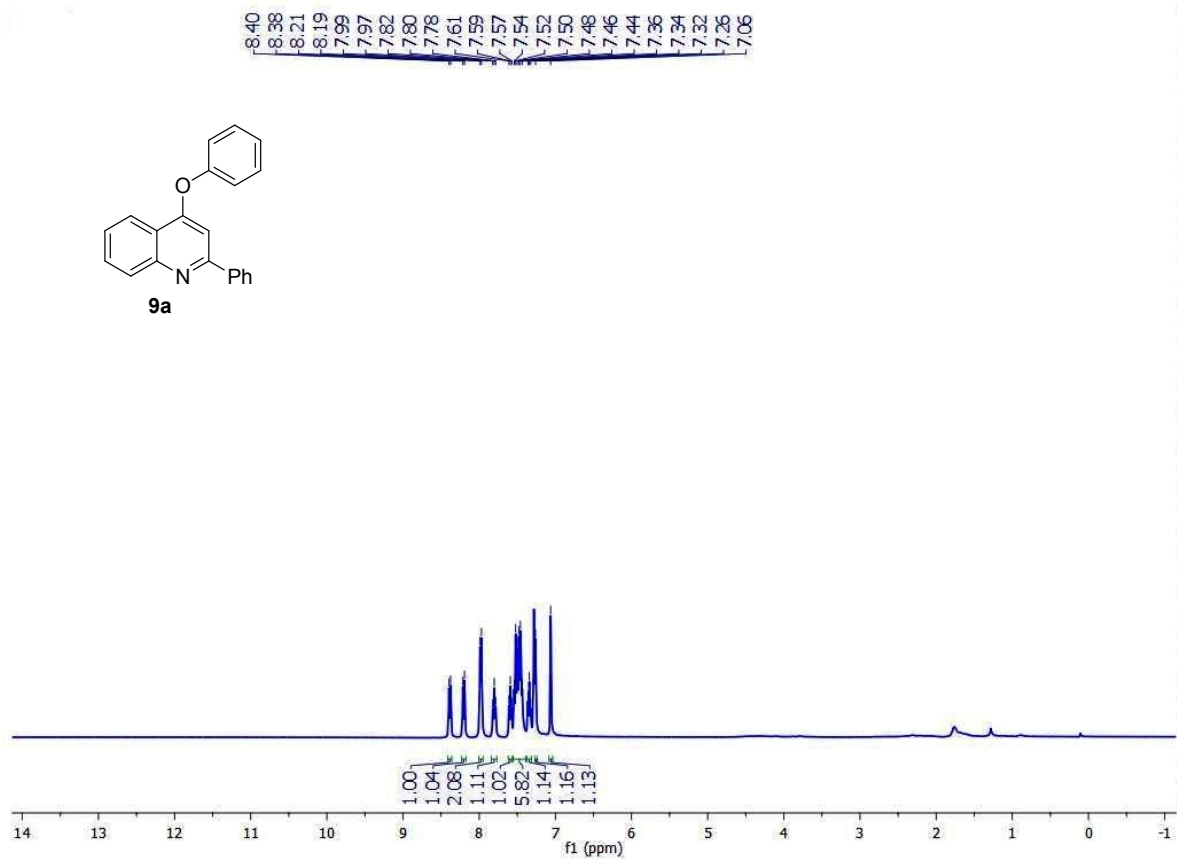


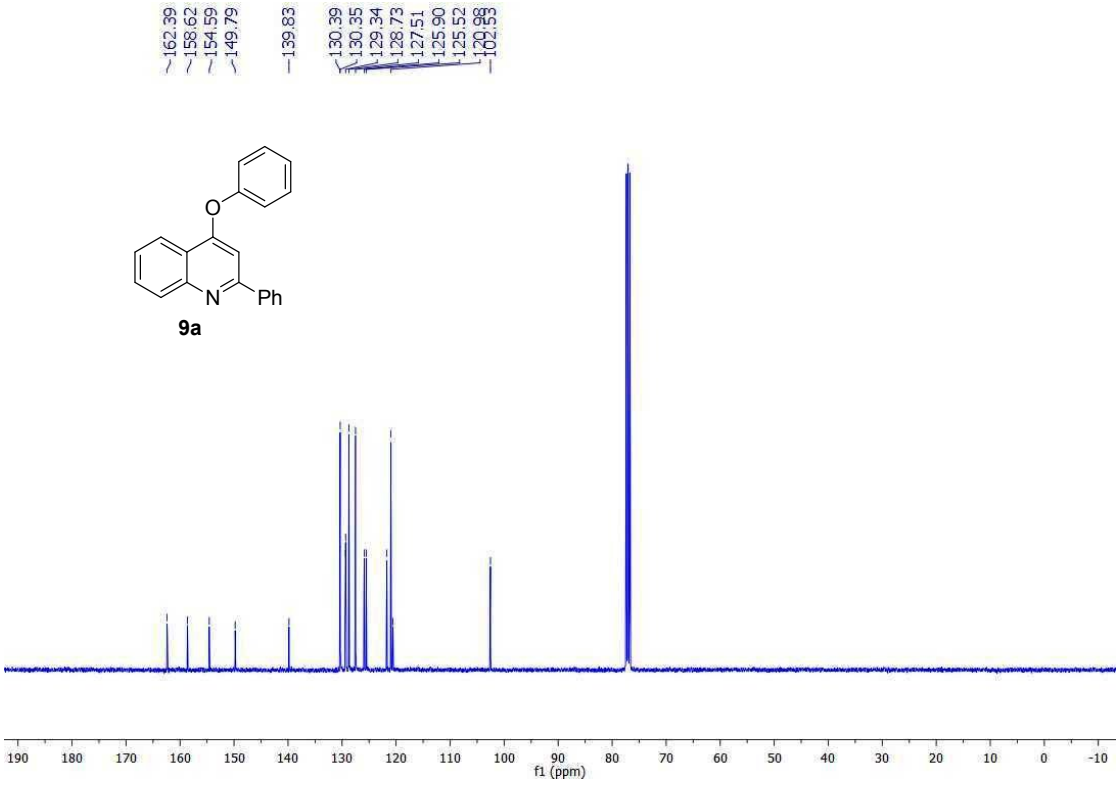


^{1}H & ^{13}C NMR spectra of 1,3-diphenyl-1*H*-benzo[*d*]imidazol-2(3*H*)-one (8c)

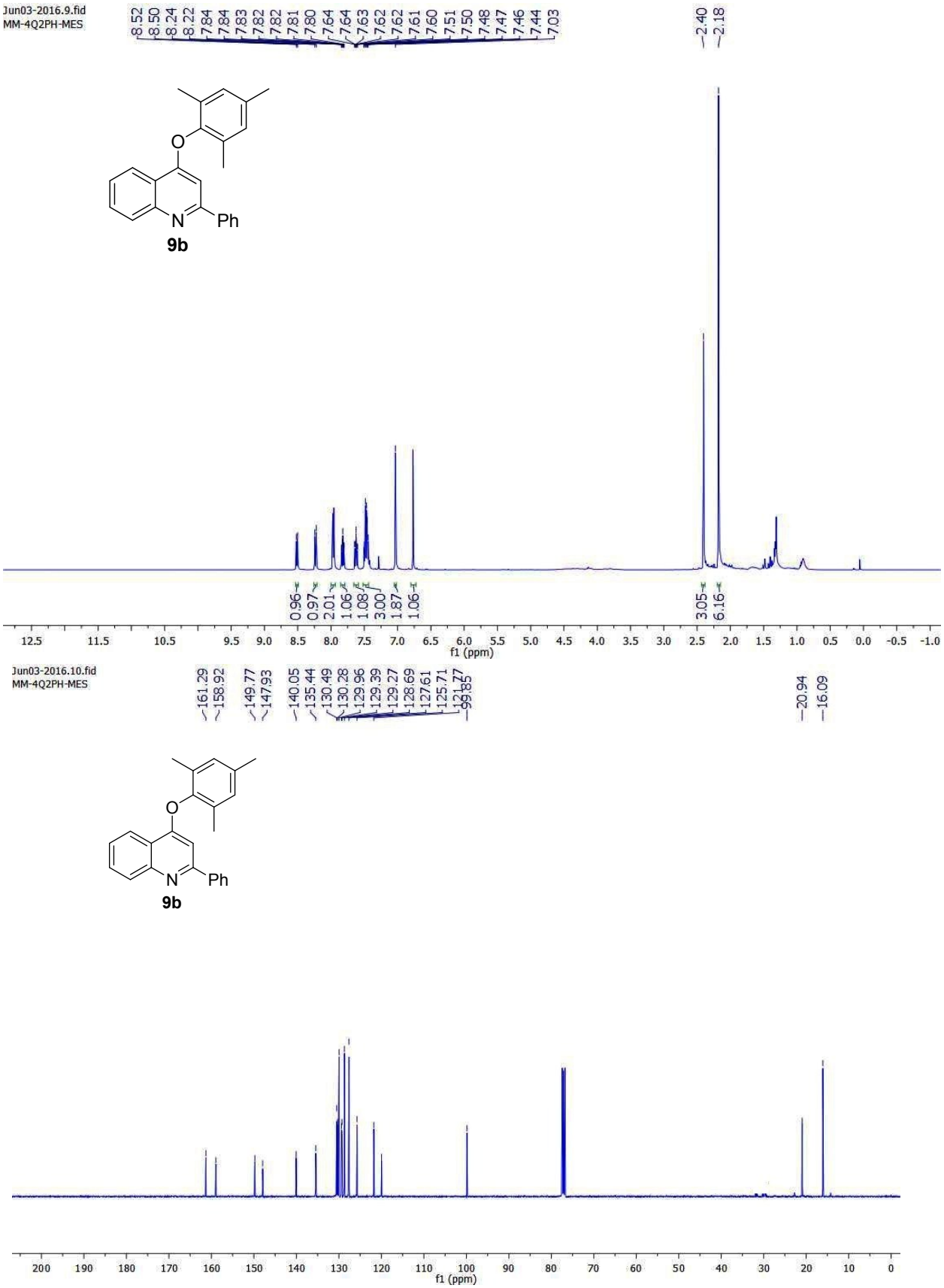


^{1}H & ^{13}C NMR spectra of 4-phenoxy-2-phenylquinoline (9a)

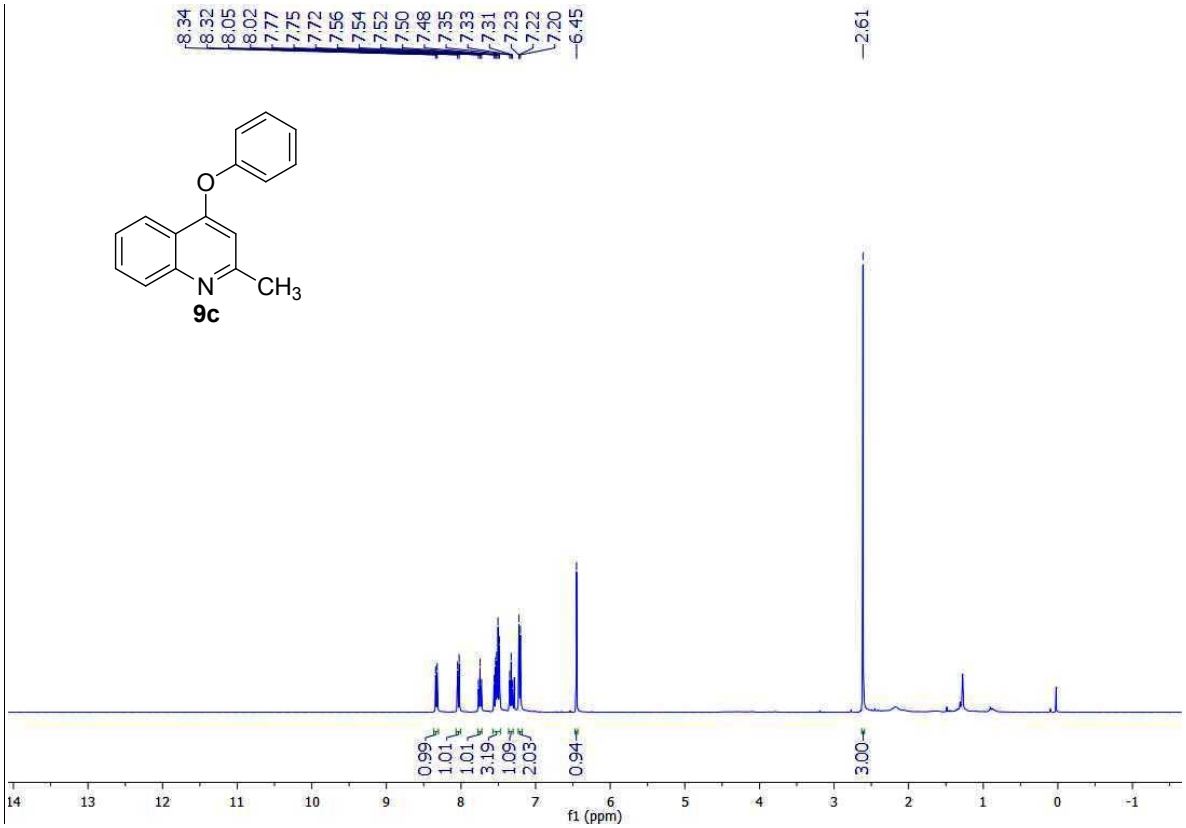


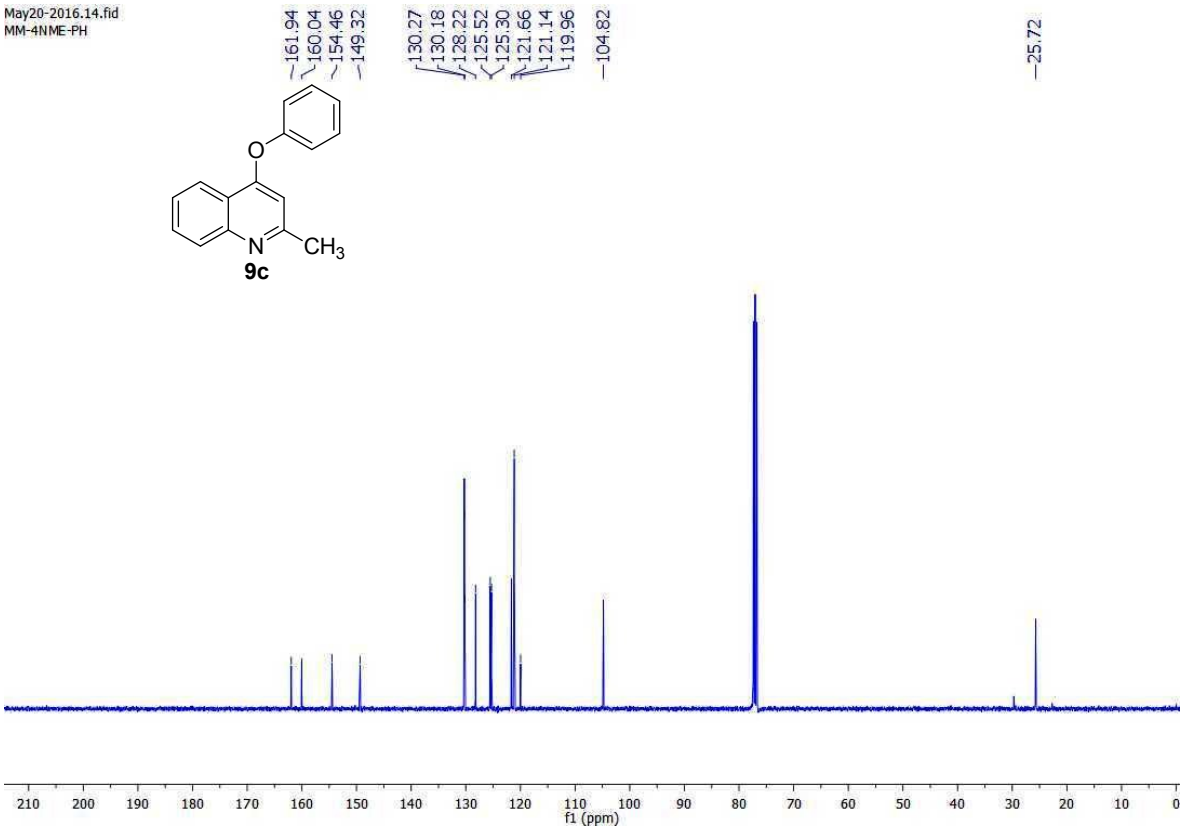


^{1}H & ^{13}C NMR spectra of 4-(mesityloxy)-2-phenylquinoline (9b)

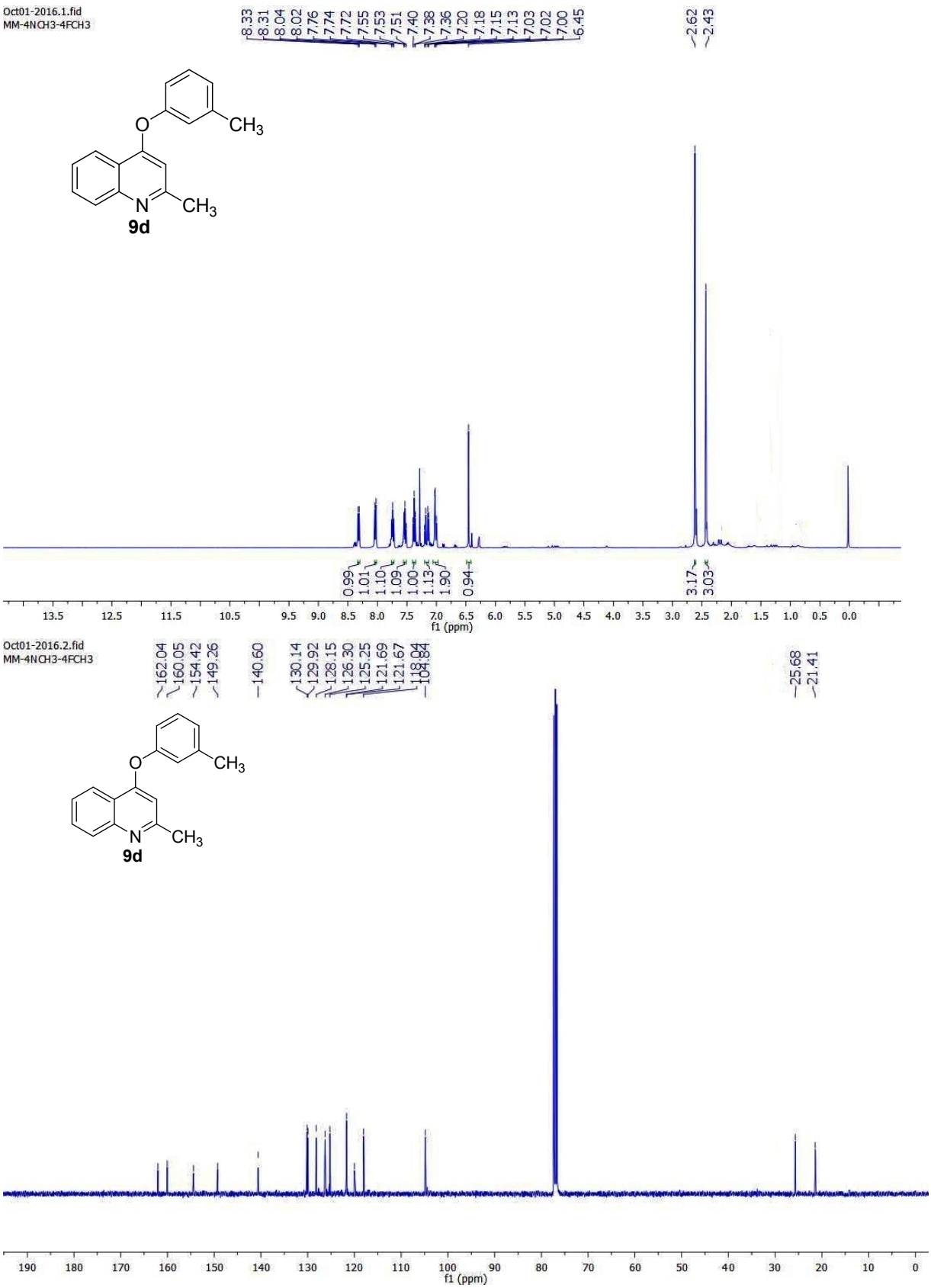


^{1}H & ^{13}C NMR spectra of 2-methyl-4-phenoxyquinoline (9c)

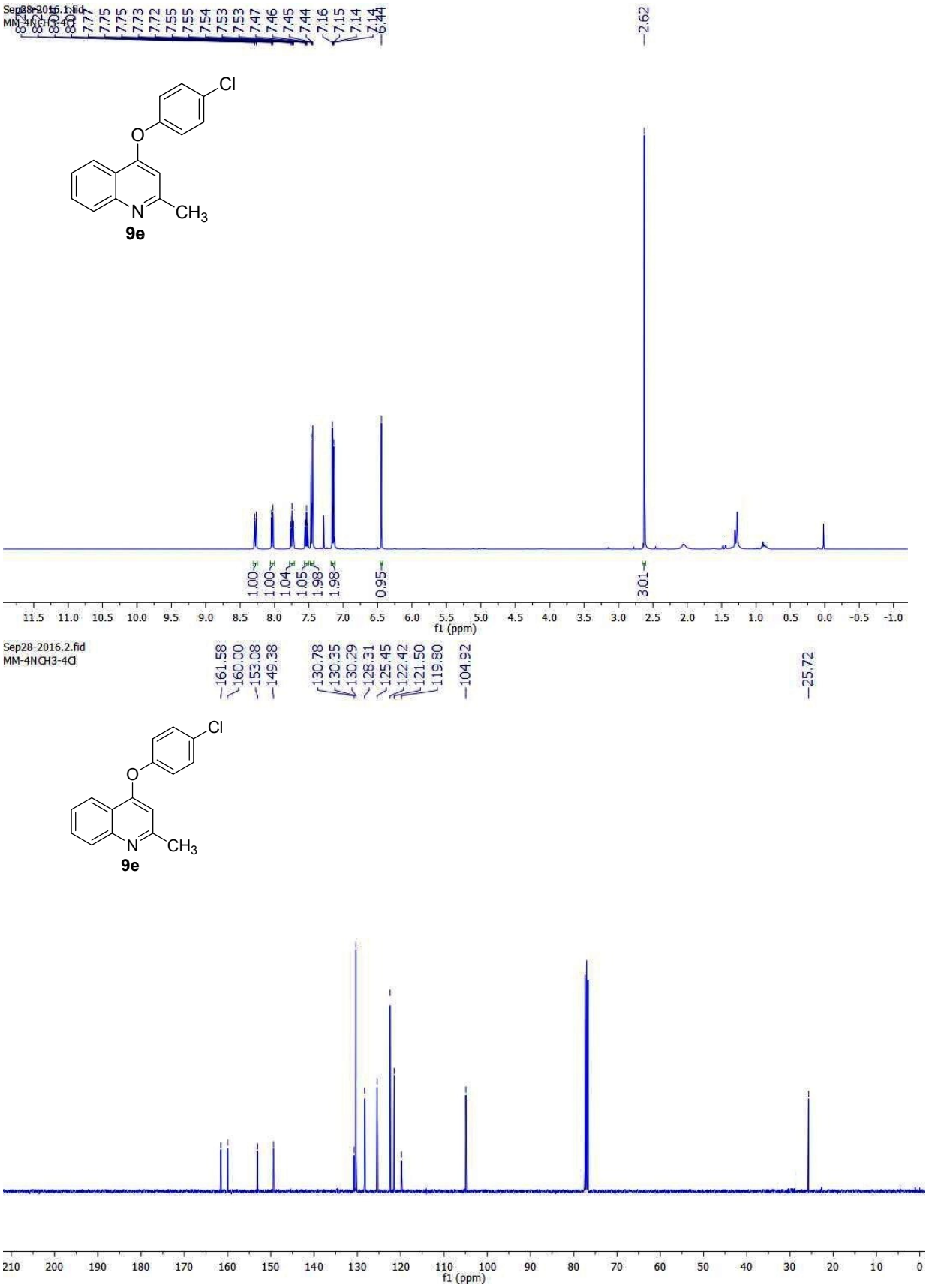




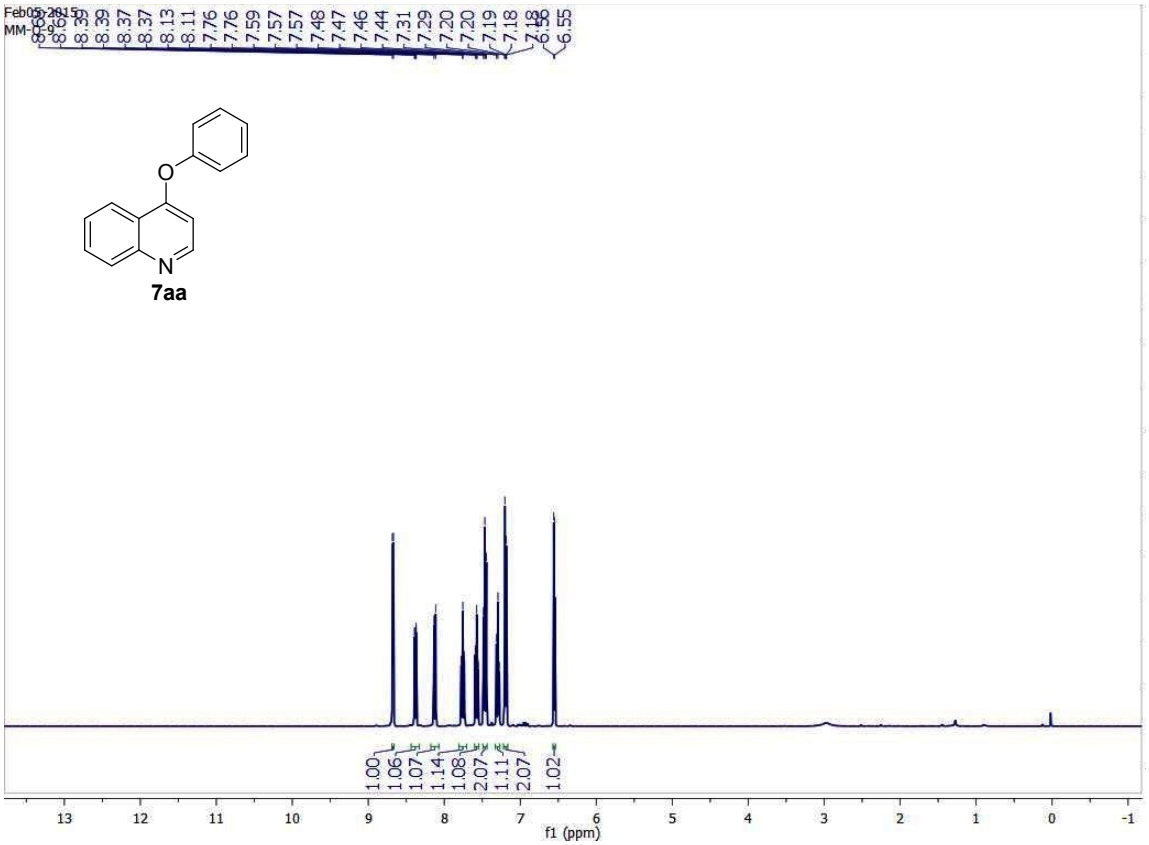
^{1}H & ^{13}C NMR spectra of 2-methyl-4-(*m*-tolyloxy)quinoline (9d)

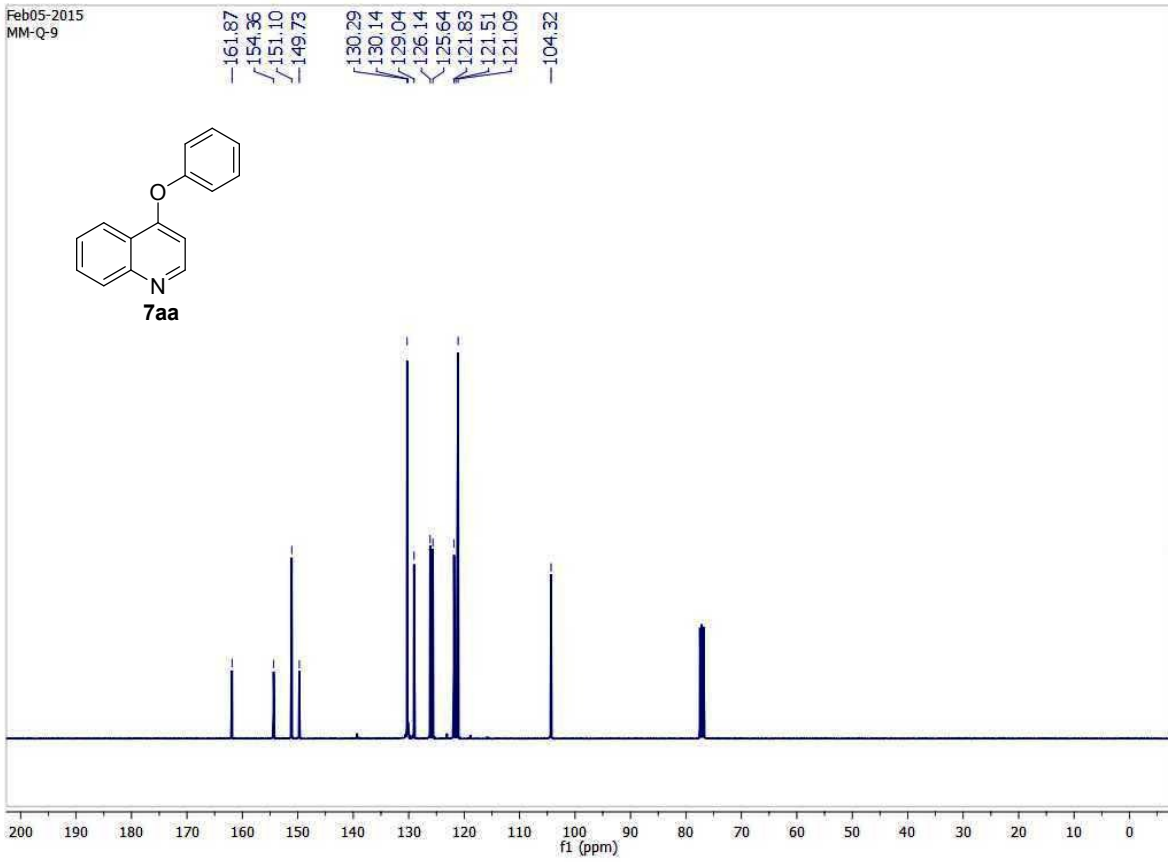


^{1}H & ^{13}C NMR spectra of 4-(4-chlorophenoxy)-2-methylquinoline (9e)



^{1}H & ^{13}C NMR spectra of 4-phenoxyquinoline (7aa)


8.65
8.39
8.37
8.13
8.11
7.76
7.59
7.57
7.48
7.47
7.46
7.44
7.31
7.29
7.20
7.19
7.18
6.55
O
N
7aa
1.00
1.06
1.07
1.14
1.08
2.07
1.11
2.07
1.02
f1 (ppm)


Feb05-2015
MM-Q-9
161.87
154.36
151.10
149.73
130.29
130.14
129.04
126.14
125.64
121.83
121.51
121.09
104.32
O
N
7aa
f1 (ppm)

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