Supporting Information

Constructing New Bonds to Carbon in Dihydroquinazolines via Hypervalent Iodine(III)-Mediated C(sp^3)-C(sp^3) Bond Functionalization

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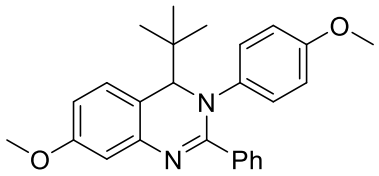
General Experimental Information. Reactions were carried out in flame-dried glassware under nitrogen atmosphere. All reactions were magnetically stirred and monitored by TLC on EMD Millipore silica gel $60F_{254}$ pre-coated glass plates using UV light (254 nm) to visualize the compounds. Column chromatography was carried out on a Yamazen AKROS MPLC system using silica gel columns supplied by Yamazen Corporation. Infrared spectra were recorded on an Agilent Technologies Cary 630 FT-IR spectrometer. Proton (^{1}H NMR) and carbon (^{13}C NMR) nuclear magnetic resonance spectra were recorded on a Bruker Avance III 400 MHz spectrometer. The chemical shifts are given in parts per million (ppm) on the delta (δ) scale. Tetramethylsilane (TMS) or the residual solvent peak was used as a reference value. NMR spectra were obtained at 300 K unless otherwise noted. High resolution mass spectra were recorded at the LSSU Cannabis Center of Excellence on an Agilent 1290 Ultra-High Pressure Liquid Chromatograph with a Time of Flight Mass Spectrometer (UHPLC-TOF). Melting points were obtained using a Mel-Temp capillary melting point apparatus and are uncorrected. 2-Chloropyridine, MeCN, DCE, HFIP, and toluene were dried over 4 Å molecular sieves; all other solvents and chemicals were purchased from commercial vendors and were used without additional purification. DHQ compound **3i** and all amides except *N*-(4-chloro-3-methoxyphenyl)benzamide (**S1**) and *N*-(4-cyano-3-methoxyphenyl)benzamide (**S2**) were prepared as previously reported.[1]

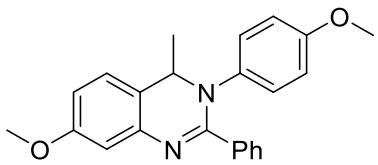
General Procedure for C4-^{t}Bu DHQ Synthesis (General Procedure A): A mixture of amide (1.0 equiv), amine (1.1 equiv), pivaldehyde (1.1 equiv), and 4 Å molecular sieves (~1 g/mmol of amide) in CH_2Cl_2 (10 mL/mmol amide) was prepared and stirred for 18 h at room temperature under N_2 atmosphere. The reaction mixture was cooled to -41 °C in an acetonitrile/dry ice bath and was treated successively with 2-chloropyridine (1.2 equiv) followed by Tf_2O (1.1 equiv). The reaction was then allowed to warm to room temperature and was stirred for 24 h. The molecular sieves were filtered from the reaction, and the filtrate was washed with saturated aqueous $NaHCO_3$ solution before being dried (Na_2SO_4) and concentrated. The crude mixture was then purified via chromatography or crystallization.

General Procedure for sp^3 C-C Bond Functionalization with Grignard Nucleophiles (General Procedure B): A mixture of DHQ (0.25 mmol) and PIFA (0.50 mmol) in a suitable solvent (MeCN, DCE, or toluene, 1.0 mL) was heated to 95 °C in a sealed vial set in an aluminum block for 2 h. The reaction was then cooled to -41 °C in an acetonitrile/dry ice bath and a Grignard solution (0.75 mmol) was added. The reaction stirred at -41 °C for 10 min, after which time the reaction was quenched by the addition of saturated aqueous NH_4Cl solution (1 mL) followed by the addition of saturated aqueous $NaHCO_3$ solution (10 mL). The mixture was extracted with CH_2Cl_2 (3 x 30 mL), and the pooled organic extracts were dried (Na_2SO_4) and concentrated. The crude mixture was then purified via chromatography.

General Procedure for sp^3 C-C Bond Functionalization with non-Grignard Nucleophiles (General Procedure C): A mixture of DHQ (0.25 mmol) and PIFA (0.50 mmol) in HFIP (1.0 mL) was heated to 95 °C in a sealed vial set in an aluminum block for 2 h. The reaction was then cooled to 0 °C in an ice bath, and a nucleophile (0.75 mmol) and a base (0.75 mmol) were successively added. The ice bath was removed and the reaction stirred for 30 min, after which time the reaction was quenched by the addition of saturated aqueous NH_4Cl solution (1 mL) followed by the addition of saturated aqueous $NaHCO_3$ solution (10 mL). The mixture was extracted with CH_2Cl_2 (3 x 30 mL), and the pooled organic extracts were dried (Na_2SO_4) and concentrated. The crude mixture was then purified via chromatography.



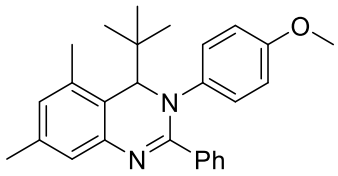
7-Methoxy-3-(*p*-methoxyphenyl)-2-phenyl-4-(*tert*-butyl)-3,4-dihydroquinazoline (1). Prepared according to general procedure A with *N*-(3-methoxyphenyl)benzamide (2.351 g, 10.3 mmol), p-anisidine (1.360 g, 11.0 mmol), pivaldehyde (1.20 mL, 11.0 mmol), CH_2Cl_2 (100 mL), 2-chloropyridine (1.17 mL, 12.4 mmol), and Tf_2O (1.93 mL, 11.4 mmol). Following workup, the residue was passed through a silica plug with 10% EtOAc in CH_2Cl_2 as eluent, and the resultant concentrated filtrate was purified by crystallization from EtOAc and hexanes to afford the desired product (3.049 g, 74%) as a light yellow solid (m.p. = 144 - 146 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.85 (m, 2H), 7.34 – 7.26 (m, 3H), 7.05 (d, *J* = 2.6 Hz, 1H), 6.92 (d, *J* = 9.0 Hz, 2H), 6.85 (d, *J* = 8.3 Hz, 1H), 6.75 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.64 (d, *J* = 9.0 Hz, 2H), 4.25 (s, 1H), 3.87 (s, 3H), 3.66 (s, 3H), 1.04 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.6, 158.0, 156.4, 144.3, 141.1, 136.7, 130.1, 129.8, 128.8, 128.4, 125.7, 116.1, 114.3, 112.4, 108.4, 72.1, 55.51, 55.46, 39.1, 27.0, IR (neat): 3056, 2952, 1545, 1506, 1487, 1247, 1230, 1034 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{26}H_{29}N_2O_2$ 401.2229; Found 401.2226.



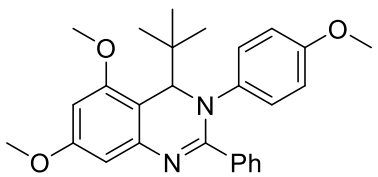
7-Methoxy-3-(*p*-methoxyphenyl)-4-methyl-2-phenyl-3,4-dihydroquinazoline (2). Prepared according to general procedure B with **1** (0.100 g, 0.25 mmol), PIFA (0.217 g, 0.50 mmol), MeCN (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (21% - 42% EtOAc in hexanes as eluent) to afford the desired product (0.059 g, 66%) as a yellow solid (m.p. = 108 - 110 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.57 (m, 2H), 7.25 – 7.16 (m, 3H), 7.00 (d, *J* = 2.6 Hz, 1H), 6.91 – 6.82 (m, 3H), 6.70 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.63 (d, *J* = 9.0 Hz, 2H), 4.84 (q, *J* = 6.6 Hz, 1H), 3.80 (s, 3H), 3.62 (s, 3H), 1.53 (d, *J* = 6.6 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.5, 156.4, 154.7, 142.8, 138.8, 136.7, 129.6, 129.4, 128.0, 125.1, 120.6, 114.0, 112.3, 108.5, 58.0, 55.3, 55.2, 23.5; IR (neat): 3062, 2963, 1541, 1508, 1489, 1245, 1128, 1034 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{23}N_2O_2$ 359.1760; Found 359.1753.

Synthesis of Compound 2 on 1.0 g Scale. Prepared according to general procedure B with **1** (1.001 g, 2.50 mmol), PIFA (2.150 g, 5.00 mmol), MeCN (10.0 mL), and MeMgBr (3.0 M in ether, 2.50 mL, 7.5 mmol). Following workup, the residue was purified by MPLC (21% - 42% EtOAc in hexanes as eluent) to afford the desired product (0.574 g, 64%) as a dark yellow solid.

Synthesis of Compound 2 from 4n. Prepared according to general procedure B with **4n** (0.038 g, 0.087 mmol), PIFA (0.078 g, 0.18 mmol), MeCN (0.40 mL), and MeMgBr (3.0 M in ether, 0.09 mL, 0.3 mmol). Following workup, the residue was purified by MPLC (21% - 42% EtOAc in hexanes as eluent) to afford the desired product (0.009 g, 29%) as a light yellow oil.

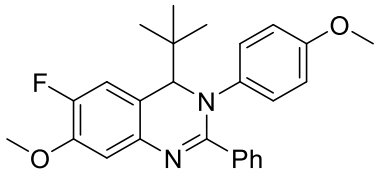


3-(*p*-Methoxyphenyl)-5,7-dimethyl-2-phenyl-4-(*tert*-butyl)-3,4-dihydroquinazoline (3a). Prepared according to general procedure A with *N*-(3,5-dimethylphenyl)benzamide (0.452 g, 2.01 mmol), p-anisidine (0.272 g, 2.21 mmol), pivaldehyde (0.24 mL, 2.2 mmol), CH_2Cl_2 (20 mL), 2-chloropyridine (0.23 mL, 2.4 mmol), and Tf_2O (0.37 mL, 2.2 mmol). Following workup, the residue was purified by MPLC (0% - 19% EtOAc in hexanes as eluent) to afford the desired product (0.385 g, 48%) as a light tan solid (m.p. = 117 - 120 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.83 (m, 2H), 7.29 – 7.24 (m, 3H), 7.19 (d, *J* = 2.2 Hz, 1H), 6.88 (d, *J* = 9.0 Hz, 3H), 6.60 (d, *J* = 9.0 Hz, 2H), 4.57 (s, 1H), 3.60 (s, 3H), 2.35 (s, 3H), 2.16 (s, 3H), 1.06 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 156.8, 156.2, 143.7, 140.6, 136.8, 136.5, 134.4, 129.9, 129.8, 129.4, 128.3, 125.3, 122.7, 119.5, 114.1, 68.6, 55.3, 40.4, 27.3, 21.2, 19.5; IR (neat): 3055, 2954, 1543, 1506, 1243, 1036 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{27}H_{31}N_2O$ 399.2436; Found 399.2436.

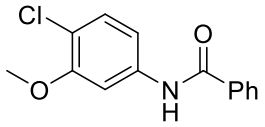


5,7-Dimethoxy-3-(p-methoxyphenyl)-2-phenyl-4-(tert-butyl)-3,4-dihydroquinazoline (3b). Prepared according to general procedure A with *N*-(3,5-dimethoxyphenyl)benzamide (0.515 g, 2.00 mmol), p-anisidine (0.272 g, 2.21 mmol), pivaldehyde (0.24 mL, 2.2 mmol), CH_2Cl_2 (20 mL), 2-chloropyridine (0.23

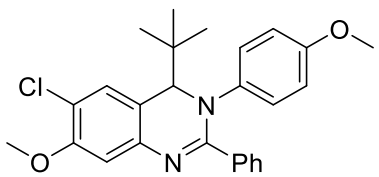
mL, 2.4 mmol), and Tf_2O (0.37 mL, 2.2 mmol). Following workup, the residue was purified by MPLC (0% - 5% EtOAc in CH_2Cl_2 as eluent) to afford the desired product (0.362 g, 42%) as a light yellow solid (m.p. = 170 - 173 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.86 (m, 2H), 7.31 – 7.22 (m, 3H), 6.91 (d, *J* = 8.9 Hz, 2H), 6.70 (d, *J* = 2.3 Hz, 1H), 6.61 (d, *J* = 9.0 Hz, 2H), 6.36 (d, *J* = 2.3 Hz, 1H), 4.72 (s, 1H), 3.85 (s, 3H), 3.66 (s, 3H), 3.61 (s, 3H), 1.04 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.8, 158.1, 156.22, 156.15, 144.9, 140.8, 136.6, 130.0, 129.8, 128.3, 125.5, 114.1, 105.1, 100.0, 96.9, 65.7, 55.4, 55.3, 55.1, 40.0, 26.9; IR (neat): 3059, 2952, 1541, 1506, 1241, 1100, 1034 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{27}H_{31}N_2O_3$ 431.2335; Found 431.2339.



6-Fluoro-7-methoxy-3-(*p*-methoxyphenyl)-2-phenyl-4-(*tert*-butyl)-3,4-dihydroquinazoline (3c). Prepared according to general procedure A with *N*-(4-fluoro-3-methoxyphenyl)benzamide (0.492 g, 2.01 mmol), p-anisidine (0.272 g, 2.21 mmol), pivaldehyde (0.24 mL, 2.2 mmol), CH_2Cl_2 (20 mL), 2-chloropyridine (0.23 mL, 2.4 mmol), and Tf_2O (0.37 mL, 2.2 mmol). Following workup, the residue was purified by MPLC (8% - 28% EtOAc in hexanes as eluent) to afford the desired product (0.601 g, 72%) as a white solid (m.p. = 170 - 173 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.89 (m, 2H), 7.31 – 7.24 (m, 3H), 7.13 (d, *J* = 8.2 Hz, 1H), 6.90 (d, *J* = 9.0 Hz, 2H), 6.68 (d, *J* = 11.1 Hz, 1H), 6.62 (d, *J* = 9.0 Hz, 2H), 4.20 (s, 1H), 3.91 (s, 3H), 3.59 (s, 3H), 1.04 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 157.4 (d, $^6J_{C\text{-}F}$ = 2 Hz), 156.4, 150.2 (d, $^1J_{C\text{-}F}$ = 244 Hz), 147.2 (d, $^2J_{C\text{-}F}$ =12 Hz), 140.6, 139.6 (d, $^3J_{C\text{-}F}$ = 3 Hz), 136.3, 130.1, 129.5, 128.3, 125.5, 115.3 (d, $^3J_{C\text{-}F}$ = 6 Hz), 114.9 (d, $^2J_{C\text{-}F}$ = 19 Hz), 114.2, 109.0 (d, $^4J_{C\text{-}F}$ = 2 Hz), 71.6, 56.1, 55.2, 38.9, 26.7; IR (neat): 3060, 2954, 1497, 1243, 1101, 1038 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{26}H_{28}FN_2O_2$ 419.2135; Found 419.2141.

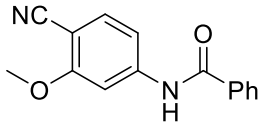


***N*-(4-fluoro-3-methoxyphenyl)benzamide (S1).** To a mixture of 4-chloro-3-methoxyaniline (1.571 g, 9.97 mmol) and TEA (1.70 mL, 12.2 mmol) in CH_2Cl_2 (50 mL), cooled to 0 °C in an ice bath, were successively added benzoyl chloride (1.30 mL, 11.2 mmol) and DMAP (0.012 g, 0.10 mmol). The ice bath was removed, and the reaction stirred at room temperature under N_2 atmosphere for 18 hours. The reaction was then washed with saturated $NaHCO_3$ solution (x3) before being dried (Na_2SO_4) and concentrated. The crude reaction was passed through a silica plug with 40:60 EtOAc:hexanes (200 mL). The filtrate was concentrated and the residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (1.799 g, 69%) as a white solid (m.p. = 127 - 129 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.88 – 7.81 (m, 2H), 7.66 (d, *J* = 2.4 Hz, 1H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.28 (d, *J* = 8.5 Hz, 1H), 6.94 (dd, *J* = 8.5, 2.4 Hz, 1H), 3.88 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 166.0, 155.4, 137.9, 134.7, 132.2, 130.1, 129.0, 127.1, 117.8, 112.6, 104.9, 56.3. The NMR spectral data are consistent with those reported in the literature.[2]

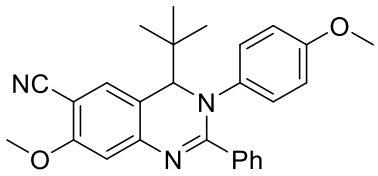


6-Chloro-7-methoxy-3-(*p*-methoxyphenyl)-2-phenyl-4-(*tert*-butyl)-3,4-dihydroquinazoline (3d). Prepared according to general procedure A with **S1** (0.522 g, 1.99 mmol), p-anisidine (0.270 g, 2.19 mmol),

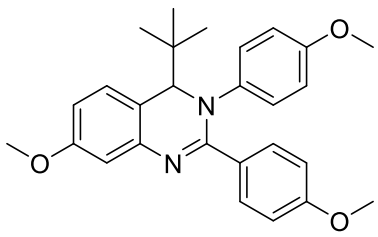
pivaldehyde (0.24 mL, 2.2 mmol), CH_2Cl_2 (20 mL), 2-chloropyridine (0.23 mL, 2.4 mmol), and Tf_2O (0.37 mL, 2.2 mmol). Following workup, the residue was purified by MPLC (5% - 30% EtOAc in hexanes as eluent) to afford the desired product (0.770 g, 89%) as a tan solid (m.p. = 203 - 205 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.81 (m, 2H), 7.30 (dt, *J* = 5.3, 1.5 Hz, 3H), 7.10 (s, 1H), 6.94 (s, 1H), 6.90 (dd, *J* = 9.0, 1.2 Hz, 2H), 6.63 (dd, *J* = 9.0, 1.3 Hz, 2H), 4.22 (s, 1H), 3.96 (s, 3H), 3.63 (s, 2H), 1.05 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 158.5, 156.5, 154.6, 142.7, 140.5, 136.1, 130.3, 129.7, 128.8, 128.3, 125.7, 118.8, 116.3, 114.2, 107.6, 71.6, 56.2, 55.3, 38.9, 26.7; IR (neat): 3061, 2958, 1541, 1508, 1485, 1245, 1230, 1038 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{26}H_{28}ClN_2O_2$ 435.1839; Found 435.1840.



***N*-(4-cyano-3-methoxyphenyl)benzamide (S2).** To a mixture of 4-amino-2-methoxybenzonitrile (0.889 g, 6.00 mmol) and TEA (1.00 mL, 7.2 mmol) in CH_2Cl_2 (30 mL), cooled to 0 °C in an ice bath, were successively added benzoyl chloride (0.77 mL, 6.6 mmol) and DMAP (0.007 g, 0.06 mmol). The ice bath was removed, and the reaction stirred at room temperature under N_2 atmosphere for 18 hours. The reaction was then washed with saturated $NaHCO_3$ solution (x3) before being dried (Na_2SO_4) and concentrated. The residue was purified by MPLC (25% - 50% EtOAc in hexanes as eluent) to afford the desired product (0.889 g, 59%) as a yellow solid (m.p. = 156 - 157 °C). ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 9.85 (s, 1H), 8.05 – 7.98 (m, 2H), 7.90 (d, *J* = 1.8 Hz, 1H), 7.65 – 7.59 (m, 2H), 7.57 – 7.50 (m, 3H), 3.96 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $(CD_3)_2CO$) δ 166.9, 162.7, 146.0, 135.5, 134.8, 132.8, 129.4, 128.4, 117.1, 112.9, 103.6, 96.6, 56.4; IR (neat): 3327, 3060, 2939, 1662, 1590, 1523, 1508, 1400, 1254, 1027 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{13}N_2O_2$ 253.0977; Found 253.0976.

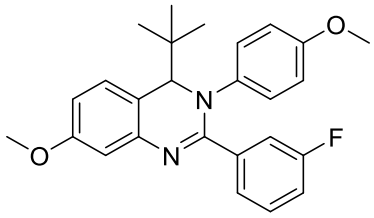


7-Methoxy-3-(*p*-methoxyphenyl)-2-phenyl-4-(*tert*-butyl)-3,4-dihydroquinazoline-6-carbonitrile (3e). Prepared according to general procedure A with **S2** (0.505 g, 2.00 mmol), p-anisidine (0.271 g, 2.20 mmol), pivaldehyde (0.24 mL, 2.2 mmol), CH_2Cl_2 (20 mL), 2-chloropyridine (0.23 mL, 2.4 mmol), and Tf_2O (0.37 mL, 2.2 mmol). Following workup, the residue was purified by MPLC (0% - 11% EtOAc in CH_2Cl_2 as eluent) to afford the desired product (0.180 g, 21%) as a light yellow solid (m.p. = 235 - 239 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.37 – 7.28 (m, 3H), 7.13 (s, 1H), 7.06 (s, 1H), 6.92 (d, *J* = 9.0 Hz, 2H), 6.65 (d, *J* = 9.0 Hz, 2H), 4.25 (s, 1H), 3.99 (s, 3H), 3.67 (s, 3H), 1.04 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 161.4, 160.4, 157.0, 148.5, 140.3, 135.9, 132.8, 130.8, 130.0, 128.5, 126.0, 117.1, 116.4, 114.4, 106.8, 97.9, 71.8, 56.2, 55.4, 39.0, 26.7; IR (neat): 3060, 2965, 2220, 1508, 1487, 1249, 1100 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{27}H_{28}N_3O_2$ 426.2182; Found 426.2178.

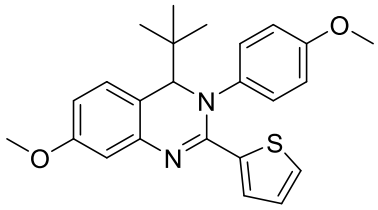


7-Methoxy-2-(*p*-methoxyphenyl)-3-(*p*-methoxyphenyl)-4-(*tert*-butyl)-3,4-dihydroquinazoline (3f). Prepared according to general procedure A with 4-methoxy-*N*-(3-methoxyphenyl)benzamide (0.515 g, 2.00

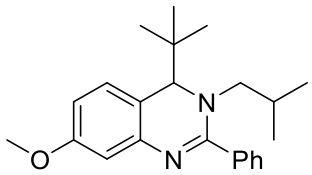
mmol), p-anisidine (0.271 g, 2.20 mmol), pivaldehyde (0.24 mL, 2.2 mmol), CH_2Cl_2 (20 mL), 2-chloropyridine (0.23 mL, 2.4 mmol), and Tf_2O (0.37 mL, 2.2 mmol). Following workup, the residue was purified by MPLC (17% - 38% EtOAc in hexanes as eluent) to afford the desired product (0.726 g, 84%) as a white solid (m.p. = 90 - 94 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.9 Hz, 2H), 7.06 (d, *J* = 2.6 Hz, 1H), 6.89 (d, *J* = 9.0 Hz, 2H), 6.81 (d, *J* = 8.3 Hz, 1H), 6.76 (d, *J* = 8.9 Hz, 2H), 6.70 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.57 (d, *J* = 9.0 Hz, 2H), 4.22 (s, 1H), 3.78 (s, 3H), 3.61 (s, 3H), 3.52 (s, 3H), 1.03 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 161.0, 159.3, 157.4, 156.0, 144.1, 141.0, 131.1, 128.7, 128.4, 125.2, 115.8, 113.9, 113.5, 111.7, 108.0, 71.8, 55.03, 54.96, 54.90, 38.6, 26.7 IR (neat): 3034, 2952, 1605, 1506, 1485, 1245, 1230, 1109, 1032 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{27}H_{31}N_2O_3$ 431.2335; Found 431.2336.



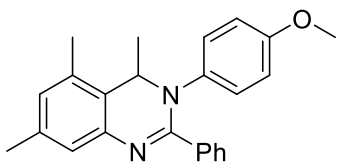
2-(*m*-Fluorophenyl)-7-methoxy-3-(*p*-methoxyphenyl)-4-(*tert*-butyl)-3,4-dihydroquinazoline (3g). Prepared according to general procedure A with 3-fluoro-*N*-(3-methoxyphenyl)benzamide (0.491 g, 2.00 mmol), p-anisidine (0.271 g, 2.20 mmol), pivaldehyde (0.24 mL, 2.2 mmol), CH_2Cl_2 (20 mL), 2-chloropyridine (0.23 mL, 2.4 mmol), and Tf_2O (0.37 mL, 2.2 mmol). Following workup, the residue was purified by MPLC (0% - 19% EtOAc in hexanes as eluent) to afford the desired product (0.635 g, 76%) as a yellow solid (m.p. = 78 - 83 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.2 Hz, 2H), 7.24 – 7.14 (m, 1H), 7.07 (d, *J* = 2.6 Hz, 1H), 6.98 – 6.88 (m, 3H), 6.83 (d, *J* = 8.4 Hz, 1H), 6.75 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.62 (d, *J* = 9.1 Hz, 2H), 4.24 (s, 1H), 3.80 (s, 3H), 3.57 (s, 3H), 1.02 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 162.6 (d, $^1J_{C\text{-}F}$ = 246 Hz), 159.5, 156.6, 156.6, 156.4, 143.7, 140.4, 139.0 (d, $^3J_{C\text{-}F}$ = 8 Hz), 129.7 (d, $^3J_{C\text{-}F}$ = 8 Hz), 128.6, 125.4, 125.2 (d, $^4J_{C\text{-}F}$ = 3 Hz), 116.9 (d, $^2J_{C\text{-}F}$ = 21 Hz), 116.3 (d, $^2J_{C\text{-}F}$ = 23 Hz), 115.6, 114.2, 112.5, 108.3, 72.0, 55.2, 55.1, 38.7, 26.7; IR (neat): 3061, 2956, 1549, 1508, 1485, 1249, 1036 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{26}H_{28}FN_2O_2$ 419.2135; Found 419.2132.



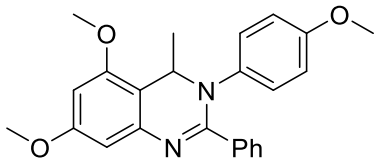
7-Methoxy-3-(*p*-methoxyphenyl)-4-(*tert*-butyl)-2-(2-thienyl)-3,4-dihydroquinazoline (3h). Prepared according to general procedure A with *N*-(3-Methoxyphenyl)-2-thiophenecarboxamide (0.467 g, 2.00 mmol), p-anisidine (0.271 g, 2.20 mmol), pivaldehyde (0.24 mL, 2.2 mmol), CH_2Cl_2 (20 mL), 2-chloropyridine (0.23 mL, 2.4 mmol), and Tf_2O (0.37 mL, 2.2 mmol). Following workup, the residue was purified by MPLC (17% - 38% EtOAc in hexanes as eluent) to afford the desired product (0.199 g, 24%) as a yellow solid (m.p. = 80 - 84 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (dd, *J* = 3.7, 1.3 Hz, 1H), 7.27 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.01 – 6.95 (m, 3H), 6.88 (dd, *J* = 5.0, 3.7 Hz, 1H), 6.81 (d, *J* = 8.3 Hz, 1H), 6.72 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.67 (d, *J* = 9.0 Hz, 2H), 4.16 (s, 1H), 3.83 (s, 3H), 3.65 (s, 3H), 1.02 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.6, 156.6, 153.0, 143.9, 141.6, 141.3, 130.1, 128.9, 128.7, 127.5, 125.5, 115.9, 114.2, 112.4, 108.1, 72.3, 55.37, 55.35, 38.7, 26.7; IR (neat): 3070, 2954, 1548, 1506, 1247, 1230, 1036 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{24}H_{27}N_2O_2S$ 407.1793; Found 407.1792.



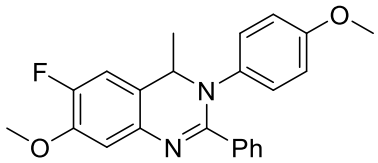
3-Isobutyl-7-methoxy-2-phenyl-4-(*tert*-butyl)-3,4-dihydroquinazoline (3j) Prepared according to general procedure A with *N*-(3-methoxyphenyl)benzamide (0.681 g, 3.00 mmol), isobutylamine (0.33 mL g, 3.3 mmol), pivaldehyde (0.34 mL, 3.1 mmol), CH_2Cl_2 (30 mL), 2-chloropyridine (0.34 mL, 3.6 mmol), and Tf_2O (0.56 mL, 3.3 mmol). Following workup, the residue was purified by MPLC (23% - 44% EtOAc in hexanes as eluent) to afford the desired product (0.418 g, 42%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.66 (m, 2H), 7.49 – 7.37 (m, 3H), 6.88 (d, *J* = 2.6 Hz, 1H), 6.84 (d, *J* = 8.3 Hz, 1H), 6.70 (dd, *J* = 8.3, 2.6 Hz, 1H), 3.97 (s, 1H), 3.82 (s, 3H), 3.46 (dd, *J* = 14.2, 9.1 Hz, 1H), 2.97 (dd, *J* = 14.2, 5.5 Hz, 1H), 1.82 – 1.64 (m, 1H), 0.96 (s, 9H), 0.66 (d, *J* = 6.7 Hz, 3H), 0.47 (d, *J* = 6.6 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 160.2, 159.5, 145.5, 136.8, 129.9, 129.4, 128.5, 127.8, 115.5, 111.2, 107.8, 67.2, 62.7, 55.2, 40.8, 29.3, 25.8, 20.1, 19.5; IR (neat): 3067, 2958, 1541, 1489, 1267, 1142, 1088 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{31}N_2O$ 351.2436; Found 351.2436.



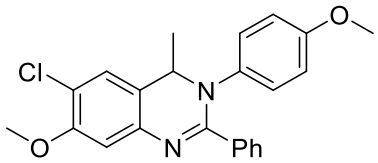
3-(*p*-Methoxyphenyl)-4,5,7-trimethyl-2-phenyl-3,4-dihydroquinazoline (4a). Prepared according to general procedure B with **3a** (0.099 g, 0.25 mmol), PIFA (0.215 g, 0.50 mmol), MeCN (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (10% - 31% EtOAc in hexanes as eluent) to afford the desired product (0.036 g, 40%) as a tan solid (m.p. = 139 - 141 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.60 (m, 2H), 7.28 – 7.21 (m, 3H), 7.13 (d, *J* = 1.7 Hz, 1H), 6.90 (d, *J* = 9.0 Hz, 2H), 6.84 (s, 1H), 6.67 (d, *J* = 9.0 Hz, 2H), 4.98 (q, *J* = 6.6 Hz, 1H), 3.70 (s, 3H), 2.34 (s, 3H), 2.23 (s, 3H), 1.53 (d, *J* = 6.6 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 156.4, 154.2, 141.9, 139.4, 137.2, 136.9, 131.9, 129.8, 129.5, 128.3, 128.2, 124.9, 124.4, 123.0, 114.1, 55.6, 55.5, 21.3, 21.2, 17.9; IR (neat): 3060, 2965, 1543, 1508, 1247, 1034 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{24}H_{25}N_2O$ 357.1967; Found 357.1969.



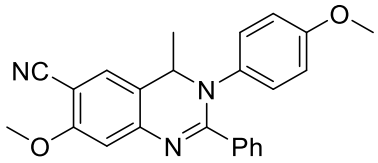
5,7-Dimethoxy-3-(p-methoxyphenyl)-4-methyl-2-phenyl-3,4-dihydroquinazoline (4b). Prepared according to general procedure B with **3b** (0.107 g, 0.25 mmol), PIFA (0.215 g, 0.50 mmol), MeCN (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (4% - 60% EtOAc in hexanes as eluent) to afford the desired product (0.061 g, 63%) as a light brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (dd, *J* = 7.5, 2.0 Hz, 2H), 7.32 – 7.18 (m, 3H), 6.92 (d, *J* = 9.0 Hz, 2H), 6.73 – 6.60 (m, 3H), 6.31 (d, *J* = 2.3 Hz, 1H), 5.12 (q, *J* = 6.5 Hz, 1H), 3.84 (s, 3H), 3.77 (s, 3H), 3.70 (s, 3H), 1.52 (d, *J* = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 160.1, 156.5, 155.3, 154.8, 143.4, 139.3, 137.0, 129.8, 129.6, 128.2, 125.2, 114.1, 109.4, 100.2, 96.3, 55.6, 55.53, 55.49, 53.2, 21.8; IR (neat): 3056, 2960, 1596, 1508, 1245, 1135 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{24}H_{25}N_2O_3$ 389.1865; Found 389.1866.



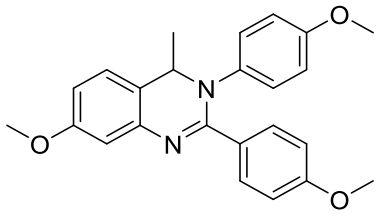
6-Fluoro-7-methoxy-3-(*p*-methoxyphenyl)-4-methyl-2-phenyl-3,4-dihydroquinazoline (4c). Prepared according to general procedure B with **3c** (0.105 g, 0.25 mmol), PIFA (0.216 g, 0.50 mmol), MeCN (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (20% - 41% EtOAc in hexanes as eluent) to afford the desired product (0.079 g, 84%) as a light tan solid (m.p. = 184 - 188 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.57 (m, 2H), 7.30 – 7.20 (m, 3H), 7.06 (d, J = 8.1 Hz, 1H), 6.89 (d, J = 8.9 Hz, 2H), 6.71 (d, J = 10.9 Hz, 1H), 6.67 (d, J = 9.0 Hz, 2H), 4.82 (q, J = 6.6 Hz, 1H), 3.92 (s, 3H), 3.70 (s, 3H), 1.55 (d, J = 6.6 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 156.6, 154.3 (d, $^{6}J_{C\text{-}F}$ = 2 Hz), 150.4 (d, $^{1}J_{C\text{-}F}$ = 244 Hz), 147.2 (d, $^{2}J_{C\text{-}F}$ = 12 Hz), 138.8, 138.3 (d, $^{3}J_{C\text{-}F}$ = 3 Hz), 136.6, 129.52, 129.49, 128.1, 125.2, 119.8 (d, $^{3}J_{C\text{-}F}$ = 6 Hz), 114.1, 111.6 (d, $^{2}J_{C\text{-}F}$ = 20 Hz), 109.5 (d, $^{4}J_{C\text{-}F}$ = 2 Hz), 57.7, 56.3, 55.4, 23.3; IR (neat): 3060, 2965, 1500, 1245, 1115, 1034 cm^{-1}; HRMS (ESI-TOF) m/z: [M+H]$^{+}$ Calcd for $C_{23}H_{22}FN_2O_2$ 377.1665; Found 377.1661.



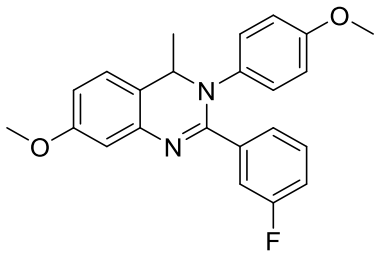
6-Chloro-7-methoxy-3-(*p*-methoxyphenyl)-4-methyl-2-phenyl-3,4-dihydroquinazoline (4d). Prepared according to general procedure B with **3d** (0.109 g, 0.25 mmol), PIFA (0.216 g, 0.50 mmol), MeCN (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (0% - 30% EtOAc in CH_2Cl_2 as elent) to afford the desired product (0.069 g, 70%) as an light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.56 (m, 2H), 7.32 – 7.20 (m, 3H), 7.04 (s, 1H), 6.98 (s, 1H), 6.89 (d, J = 8.9 Hz, 2H), 6.68 (d, J = 9.0 Hz, 2H), 4.83 (q, J = 6.7 Hz, 1H), 3.94 (s, 3H), 3.70 (s, 3H), 1.55 (d, J = 6.7 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 156.8, 155.2, 154.7, 141.7, 138.8, 136.6, 129.8, 129.7, 128.2, 125.7, 125.4, 121.0, 118.6, 114.2, 108.3, 57.9, 56.4, 55.5, 23.6; IR (neat): 3058, 2965, 1580, 1485, 1245, 1128 cm^{-1}; HRMS (ESI-TOF) m/z: [M+H]$^{+}$ Calcd for $C_{23}H_{22}ClN_2O_2$ 393.1370; Found 393.1376.



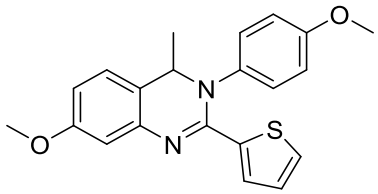
7-Methoxy-3-(*p*-methoxyphenyl)-4-methyl-2-phenyl-3,4-dihydroquinazoline-6-carbonitrile (4e). Prepared according to general procedure B with **3e** (0.107 g, 0.25 mmol), PIFA (0.215 g, 0.50 mmol), MeCN (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (0% - 6% EtOAc in CH_2Cl_2 as eluent) to afford the desired product (0.041 g, 42%) as a yellow solid (m.p. = 189 - 192 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.55 (m, 2H), 7.34 – 7.22 (m, 3H), 7.17 (s, 1H), 6.98 (s, 1H), 6.92 (d, J = 9.0 Hz, 2H), 6.70 (d, J = 9.1 Hz, 2H), 4.86 (q, J = 6.6 Hz, 1H), 3.96 (s, 3H), 3.72 (s, 3H), 1.57 (d, J = 6.6 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 161.6, 157.3, 157.2, 147.5, 138.2, 136.2, 130.2, 129.8, 129.6, 128.3, 125.8, 120.9, 117.2, 114.4, 107.0, 97.5, 58.0, 56.3, 55.5, 23.7; IR (neat): 3062, 2956, 2220, 1536, 1489, 1251, 1109 cm^{-1}; HRMS (ESI-TOF) m/z: [M+H]$^{+}$ Calcd for $C_{24}H_{22}N_3O_2$ 384.1712; Found 384.1710.



7-Methoxy-2-(*p*-methoxyphenyl)-3-(*p*-methoxyphenyl)-4-methyl-3,4-dihydroquinazoline (4f). Prepared according to general procedure B with **3f** (0.108 g, 0.25 mmol), PIFA (0.216 g, 0.50 mmol), MeCN (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (0% - 2% MeOH in CH_2Cl_2) to afford the desired product (0.039 g, 40%) as a peach colored oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.8 Hz, 2H), 6.97 (d, *J* = 2.6 Hz, 1H), 6.88 (t, *J* = 8.8 Hz, 3H), 6.76 (d, *J* = 8.9 Hz, 2H), 6.73 – 6.64 (m, 3H), 4.84 (q, *J* = 6.6 Hz, 1H), 3.84 (s, 3H), 3.76 (s, 3H), 3.71 (s, 3H), 1.54 (d, *J* = 6.7 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 160.7, 159.7, 156.4, 154.5, 143.2, 139.5, 131.4, 129.2, 125.2, 125.1, 121.0, 114.1, 113.6, 112.2, 108.4, 58.3, 55.53, 55.50, 55.4, 23.6; IR (neat): 3043, 2961, 1607, 1508, 1489, 1249, 1172, 1034 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{24}H_{25}N_2O_3$ 389.1865; Found 389.1865.

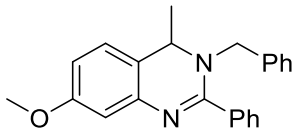


2-(*m*-Fluorophenyl)-7-methoxy-3-(*p*-methoxyphenyl)-4-methyl-3,4-dihydroquinazoline (4g). Prepared according to general procedure B with **3g** (0.105 g, 0.25 mmol), PIFA (0.215 g, 0.50 mmol), MeCN (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (14% - 35% EtOAc in hexanes) to afford the desired product (0.046 g, 49%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.31 (m, 2H), 7.23 – 7.12 (m, 1H), 7.00 – 6.86 (m, 5H), 6.73 (dd, *J* = 8.2, 2.6 Hz, 1H), 6.69 (d, *J* = 9.0 Hz, 2H), 4.86 (q, *J* = 6.6 Hz, 1H), 3.84 (s, 3H), 3.71 (s, 3H), 1.54 (d, *J* = 6.7 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 162.6 (d, $^1J_{C\text{-}F}$ = 246 Hz), 159.7, 156.8, 153.6 (d, $^4J_{C\text{-}F}$ = 3 Hz), 142.7, 139.3 (d, $^3J_{C\text{-}F}$ = 8 Hz), 138.7, 129.7 (d, $^3J_{C\text{-}F}$ = 8 Hz), 125.5 (d, $^4J_{C\text{-}F}$ = 3 Hz), 125.3, 120.6, 116.7 (d, $^2J_{C\text{-}F}$ = 23 Hz), 116.6 (d, $^2J_{C\text{-}F}$ = 21 Hz), 114.3, 112.8, 108.7, 58.3, 55.6, 55.5, 23.8; IR (neat): 3070, 2963, 1582, 1508, 1485, 1247, 1034 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{22}FN_2O_2$ 377.1665; Found 377.1662.

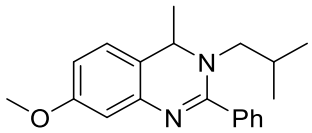


7-Methoxy-3-(*p*-methoxyphenyl)-4-methyl-2-(2-thienyl)-3,4-dihydroquinazoline (4h). Prepared according to general procedure B with **3h** (0.102 g, 0.25 mmol), PIFA (0.216 g, 0.50 mmol), MeCN (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (14% - 35% EtOAc in hexanes) to afford the desired product (0.043 g, 47%) as a yellow solid (m.p. = 157 - 160 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.04 (d, *J* = 8.9 Hz, 2H), 6.94 (d, *J* = 2.6 Hz, 2H), 6.87 – 6.82 (m, 2H), 6.76 (d, *J* = 9.0 Hz, 2H), 6.70 (dd, *J* = 8.2, 2.6 Hz, 1H), 4.77 (q, *J* = 6.6 Hz, 1H), 3.84 (s, 3H), 3.76 (s, 3H), 1.51 (d, *J* = 6.6 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.7, 157.3, 149.4, 142.8, 140.8, 139.3, 130.4, 128.7, 127.3, 125.9, 125.2, 120.7, 114.3, 112.6, 108.3,

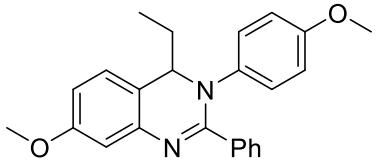
58.8, 55.57, 55.56, 23.7; IR (neat): 3073, 2961, 1541, 1508, 1487, 1247, 1131, 1031 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{21}H_{21}N_2O_2S$ 365.1324; Found 365.1324.



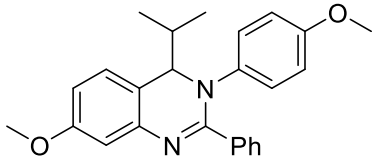
3-Benzyl-7-methoxy-4-methyl-2-phenyl-3,4-dihydroquinazoline (4i). Prepared according to general procedure B with **3i** (0.096 g, 0.25 mmol), PIFA (0.216 g, 0.50 mmol), MeCN (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (17% - 75% EtOAc in hexanes) to afford the desired product (0.045 g, 53%) as a light orange oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.49 (m, 2H), 7.40 (dd, *J* = 5.0, 2.0 Hz, 3H), 7.28 – 7.21 (m, 3H), 7.14 (dd, *J* = 8.0, 1.7 Hz, 1H), 6.85 (d, *J* = 2.6 Hz, 1H), 6.71 (d, *J* = 8.3 Hz, 1H), 6.61 (dd, *J* = 8.3, 2.6 Hz, 1H), 4.73 (d, *J* = 15.8 Hz, 1H), 4.46 (q, *J* = 6.4 Hz, 1H), 4.28 (d, *J* = 15.8 Hz, 1H), 3.79 (s, 3H), 1.41 (d, *J* = 6.4 Hz, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 159.7, 158.3, 143.3, 137.4, 136.7, 129.6, 128.8, 128.7, 128.4, 127.7, 127.1, 125.6, 119.2, 111.9, 108.3, 55.4, 53.8, 52.6, 22.0; IR (neat): 3058, 2961, 1543, 1489, 1333, 1128, 1034 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{23}N_2O$ 343.1810; Found 343.1809.



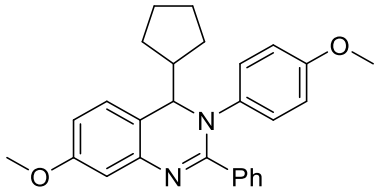
3-Isobutyl-7-methoxy-4-methyl-2-phenyl-3,4-dihydroquinazoline (4j). Prepared according to general procedure B with **3j** (0.084 g, 0.25 mmol), PIFA (0.215 g, 0.50 mmol), MeCN (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (85% - 100% EtOAc in hexanes as eluent) to afford the desired product (0.027 g, 43%) as a tan oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.45 (m, 2H), 7.45 – 7.35 (m, 3H), 6.85 (d, *J* = 8.2 Hz, 1H), 6.82 (d, *J* = 2.6 Hz, 1H), 6.66 (dd, *J* = 8.2, 2.6 Hz, 1H), 4.50 (q, *J* = 6.4 Hz, 1H), 3.80 (s, 3H), 3.20 (dd, *J* = 14.0, 9.3 Hz, 1H), 3.02 (dd, *J* = 14.1, 5.3 Hz, 1H), 1.91 – 1.75 (m, 1H), 1.36 (d, *J* = 6.5 Hz, 3H), 0.76 (d, *J* = 6.7 Hz, 3H), 0.62 (d, *J* = 6.6 Hz, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 159.7, 158.5, 143.7, 136.8, 129.5, 128.9, 128.5, 125.3, 119.7, 111.7, 108.1, 58.0, 55.4, 53.6, 28.3, 22.0, 20.1, 19.7; IR (neat): 3061, 2963, 1541, 1489, 1148 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{20}H_{25}N_2O$ 309.1967; Found 309.1968.



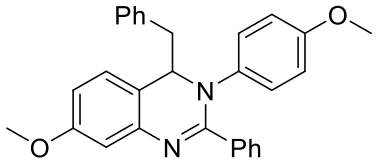
4-Ethyl-7-methoxy-3-(*p*-methoxyphenyl)-2-phenyl-3,4-dihydroquinazoline (4k). Prepared according to general procedure B with **1** (0.101 g, 0.25 mmol), PIFA (0.216 g, 0.50 mmol), DCE (1.0 mL), and EtMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (13% - 33% EtOAc in hexanes as eluent) to afford the desired product (0.072 g, 77%) as a light orange oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.63 (m, 2H), 7.28 – 7.21 (m, 3H), 7.01 (d, *J* = 2.6 Hz, 1H), 6.92 – 6.82 (m, 3H), 6.72 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.66 (d, *J* = 9.0 Hz, 2H), 4.59 (dd, *J* = 7.4, 6.0 Hz, 1H), 3.84 (s, 3H), 3.69 (s, 3H), 1.95 – 1.81 (m, 2H), 1.04 (t, *J* = 7.4 Hz, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 159.7, 156.5, 155.6, 143.4, 139.4, 136.8, 129.8, 129.7, 128.2, 126.3, 125.4, 118.9, 114.1, 112.2, 108.6, 63.9, 55.50, 55.46, 30.0, 9.9; IR (neat): 3058, 2960, 1508, 1489, 1245, 1036 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{24}H_{25}N_2O_2$ 373.1916; Found 373.1921.



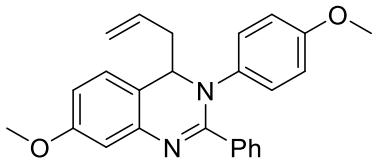
4-Isopropyl-7-methoxy-3-(*p*-methoxyphenyl)-2-phenyl-3,4-dihydroquinazoline (4l). Prepared according to general procedure B with **1** (0.101 g, 0.25 mmol), PIFA (0.217 g, 0.50 mmol), DCE (1.0 mL), and iPrMgBr (2.9 M 2-methylTHF, 0.26 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (5% - 26% EtOAc in hexanes as eluent) to afford the desired product (0.064 g, 66%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.73 (m, 2H), 7.30 – 7.22 (m, 3H), 7.02 (d, *J* = 2.6 Hz, 1H), 6.89 (d, *J* = 9.0 Hz, 2H), 6.83 (d, *J* = 8.3 Hz, 1H), 6.72 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.65 (d, *J* = 9.0 Hz, 2H), 4.36 (d, *J* = 6.8 Hz, 1H), 3.85 (s, 3H), 3.68 (s, 3H), 2.18 – 2.01 (m, *J* = 6.6 Hz, 1H), 1.17 (d, *J* = 6.9 Hz, 3H), 0.88 (d, *J* = 6.7 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.7, 156.5, 156.3, 143.9, 140.0, 136.6, 129.83, 129.81, 128.3, 127.4, 125.6, 117.0, 114.2, 112.1, 108.4, 68.7, 55.48, 55.46, 34.8, 19.9, 18.2; IR (neat): 3059, 2956, 1508, 1489, 1247, 1036 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{25}H_{27}N_2O_2$ 387.2073; Found 387.2070.



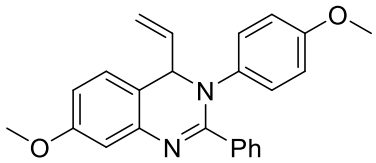
4-Cyclopentyl-7-methoxy-3-(p-methoxyphenyl)-2-phenyl-3,4-dihydroquinazoline (4m). Prepared according to general procedure B with **1** (0.102 g, 0.25 mmol), PIFA (0.215 g, 0.50 mmol), DCE (1.0 mL), and cyclopropylmagnesium bromide (2.0 M in ether, 0.38 mL, 0.76 mmol). Following workup, the residue was purified by MPLC (0% - 27% EtOAc in CH_2Cl_2 as eluent) to afford the desired product (0.074 g, 71%) as a tan oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.71 (m, 2H), 7.31 – 7.23 (m, 3H), 7.03 (d, *J* = 2.6 Hz, 1H), 6.92 – 6.83 (m, 3H), 6.72 (dd, *J* = 8.2, 2.6 Hz, 1H), 6.65 (d, *J* = 9.0 Hz, 2H), 4.48 (d, *J* = 8.1 Hz, 1H), 3.85 (s, 3H), 3.68 (s, 3H), 2.34 – 2.19 (m, 1H), 2.08 – 1.94 (m, 1H), 1.77 – 1.43 (m, 6H), 1.37 – 1.24 (m, 1H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.7, 156.4, 156.1, 143.7, 139.7, 136.6, 129.9, 128.3, 126.8, 125.4, 118.7, 114.2, 112.2, 108.5, 66.5, 55.5, 55.5, 46.6, 30.3, 28.9, 24.7, 24.7; IR (neat): 3060, 2952, 1508, 1487, 1245, 1032 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{27}H_{29}N_2O_2$ 413.2229; Found 413.2229.



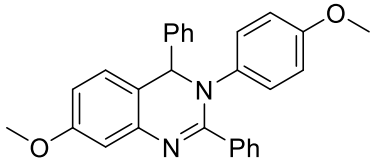
4-Benzyl-7-methoxy-3-(*p*-methoxyphenyl)-2-phenyl-3,4-dihydroquinazoline (4n). Prepared according to general procedure B with **1** (0.100 g, 0.25 mmol), PIFA (0.217 g, 0.50 mmol), DCE (1.0 mL), and benzylmagnesium chloride (1.4 M in THF, 0.54 mL, 0.76 mmol). Following workup, the residue was purified by MPLC (0% - 36% EtOAc in hexanes as eluent) to afford the desired product (0.021 g, 19%) as a light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.70 (m, 2H), 7.41 – 7.26 (m, 6H), 7.23 – 7.18 (m, 2H), 7.06 (s, 1H), 6.65 (dd, *J* = 8.3, 2.4 Hz, 1H), 6.61 (d, *J* = 8.3 Hz, 1H), 6.54 (d, *J* = 9.0 Hz, 2H), 6.44 (d, *J* = 9.0 Hz, 2H), 4.80 (dd, *J* = 8.3, 6.3 Hz, 1H), 3.86 (s, 3H), 3.65 (s, 3H), 3.12 (dd, *J* = 13.4, 8.3 Hz, 1H), 2.94 (dd, *J* = 13.4, 6.3 Hz, 1H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.9, 156.7, 155.2, 143.4, 139.4, 137.8, 136.2, 130.4, 130.2, 130.0, 128.7, 128.2, 127.0, 126.1, 125.7, 119.1, 114.1, 112.3, 108.6, 65.6, 55.6, 55.5, 43.1; IR (neat): 3029, 2933, 1508, 1489, 1247, 1034 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{29}H_{27}N_2O_2$ 435.2073; Found 435.2080.



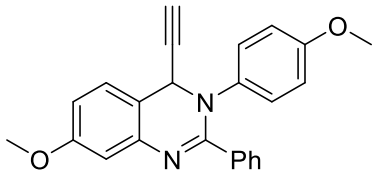
4-Allyl-7-methoxy-3-(*p*-methoxyphenyl)-2-phenyl-3,4-dihydroquinazoline (4o). Prepared according to general procedure B with **1** (0.100 g, 0.25 mmol), PIFA (0.215 g, 0.50 mmol), DCE (1.0 mL), and allylmagnesium bromide (1.0 M in ether, 0.75 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (19% - 40% EtOAc in hexanes as eluent) to afford the desired product (0.026 g, 27%) as an light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.28 – 7.21 (m, 3H), 7.01 (d, *J* = 2.6 Hz, 1H), 6.91 (d, *J* = 8.9 Hz, 2H), 6.87 (d, *J* = 8.3 Hz, 1H), 6.72 (dd, *J* = 8.2, 2.6 Hz, 1H), 6.66 (d, *J* = 9.0 Hz, 2H), 5.95 (ddt, *J* = 16.8, 10.3, 7.3 Hz, 1H), 5.23 – 5.09 (m, 2H), 4.75 (t, *J* = 6.6 Hz, 1H), 3.85 (s, 3H), 3.69 (s, 4H), 2.68 – 2.46 (m, 2H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.8, 156.6, 155.5, 143.4, 139.3, 136.7, 134.1, 129.9, 129.8, 128.2, 126.0, 125.7, 119.0, 118.9, 114.2, 112.4, 108.6, 62.8, 55.54, 55.50, 42.0; IR (neat): 3064, 2924, 1610, 1588, 1508, 1247, 1036 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{25}H_{25}N_2O_2$ 385.1916; Found 385.1918.



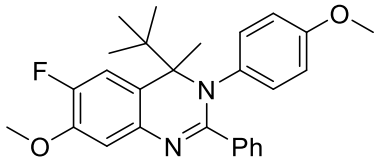
7-Methoxy-3-(*p*-methoxyphenyl)-2-phenyl-4-vinyl-3,4-dihydroquinazoline (4p). Prepared according to general procedure B with **1** (0.099 g, 0.25 mmol), PIFA (0.216 g, 0.50 mmol), CH_3CN (1.0 mL), and vinylmagnesium bromide (0.7 M in THF, 1.10 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (22% - 43% EtOAc in hexanes as eluent) to afford the desired product (0.048 g, 52%) as a light orange oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.30 – 7.20 (m, 3H), 7.00 – 6.89 (m, 4H), 6.73 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.67 (d, *J* = 9.1 Hz, 2H), 6.15 (ddd, *J* = 17.1, 10.2, 5.9 Hz, 1H), 5.31 (dt, *J* = 17.0, 1.2 Hz, 1H), 5.23 (d, *J* = 5.9 Hz, 1H), 5.15 (dt, *J* = 10.1, 1.1 Hz, 1H), 3.84 (s, 3H), 3.70 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 160.0, 156.8, 154.9, 143.1, 139.4, 138.4, 136.5, 129.9, 129.6, 128.2, 126.1, 125.7, 117.4, 114.4, 114.1, 112.7, 108.8, 64.7, 55.6, 55.5; IR (neat): 3058, 2928, 1592, 1508, 1245, 1128, 1034 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{24}H_{23}N_2O_2$ 371.1760; Found 371.1756.



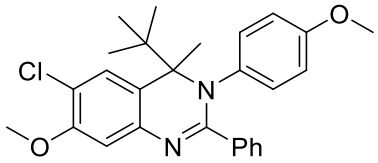
7-Methoxy-3-(p-methoxyphenyl)-2,4-diphenyl-3,4-dihydroquinazoline (4q). Prepared according to general procedure B with **1** (0.100 g, 0.25 mmol), PIFA (0.216 g, 0.50 mmol), DCE (1.0 mL), and phenyl magnesium bromide (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (16% - 37% EtOAc in hexanes as eluent) to afford the desired product (0.068 g, 64%) as a light yellow solid (m.p. = 150 - 154 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 7.7, 1.8 Hz, 2H), 7.47 (d, *J* = 7.0 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 2H), 7.30 – 7.18 (m, 4H), 6.99 (d, *J* = 2.6 Hz, 1H), 6.91 (d, *J* = 8.4 Hz, 1H), 6.81 (d, *J* = 9.0 Hz, 2H), 6.67 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.60 (d, *J* = 9.0 Hz, 2H), 5.72 (s, 1H), 3.81 (s, 3H), 3.66 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.8, 157.0, 115.8, 145.5, 142.3, 139.5, 136.8, 129.7, 129.5, 129.3, 128.2, 127.9, 126.6, 126.4, 125.9, 118.8, 114.0, 112.9, 109.0, 66.4, 55.5, 55.4. The NMR spectral data are consistent with those reported in the literature.[1]



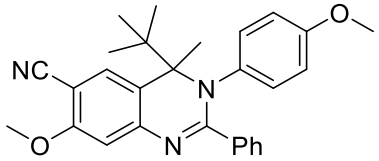
4-Ethynyl-7-methoxy-3-(*p*-methoxyphenyl)-2-phenyl-3,4-dihydroquinazoline (4r). Prepared according to general procedure B with **1** (0.101 g, 0.25 mmol), PIFA (0.217 g, 0.50 mmol), DCE (1.0 mL), and ethynyl magnesium bromide (0.5 M in THF, 1.5 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (22% - 43% EtOAc in hexanes as eluent) to afford the desired product (0.057 g, 61%) as a light orange oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.52 (m, 2H), 7.29 – 7.19 (m, 3H), 7.07 (d, *J* = 8.9 Hz, 2H), 7.03 (d, *J* = 8.4 Hz, 1H), 7.00 (d, *J* = 2.6 Hz, 1H), 6.76 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.69 (d, *J* = 9.0 Hz, 2H), 5.58 (d, *J* = 2.3 Hz, 1H), 3.84 (s, 3H), 3.71 (s, 3H), 2.61 (d, *J* = 2.3 Hz, 1H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 160.5, 157.0, 154.7, 142.8, 138.3, 136.4, 129.8, 129.6, 128.2, 125.7, 125.5, 115.4, 114.1, 113.1, 109.1, 83.1, 74.2, 55.6, 55.5, 52.7; IR (neat): 3282, 3066, 2957, 1510, 1489, 1247, 1036 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{24}H_{21}N_2O_2$ 369.1603; Found 369.1606.



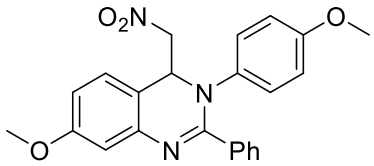
6-Fluoro-7-methoxy-3-(p-methoxyphenyl)-4-methyl-2-phenyl-4-(tert-butyl)-3,4-dihydroquinazoline (5c). Prepared according to general procedure B with **3c** (0.105 g, 0.25 mmol), PIFA (0.215 g, 0.50 mmol), DCE (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (20% - 41% EtOAc in hexanes) to afford the desired product (0.031 g, 28%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.71 (m, 2H), 7.46 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.29 – 7.19 (m, 3H), 7.06 (d, *J* = 8.4 Hz, 1H), 6.85 (d, *J* = 12.6 Hz, 1H), 6.78 – 6.72 (m, 1H), 6.52 – 6.43 (m, 2H), 3.96 (s, 3H), 3.67 (s, 3H), 1.31 (s, 3H), 1.09 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, 330 K) δ 160.0, 158.0, 150.7 (d, $^1J_{C\text{-}F}$ = 243 Hz), 147.1 (d, $^2J_{C\text{-}F}$ = 12 Hz), 140.2, 138.0, 136.3, 132.5, 131.5, 129.7, 129.4, 127.9, 120.6 (d, $^3J_{C\text{-}F}$ = 5 Hz), 113.66 (d, $^3J_{C\text{-}F}$ = 12 Hz), 113.72 (d, $^2J_{C\text{-}F}$ = 19 Hz), 110.0, 66.2, 56.3, 55.3, 42.8, 26.1, 21.3; IR (neat): 3055, 2956, 1500, 1247, 1202, 1109 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{27}H_{30}FN_2O_2$ 433.2291; Found 433.2282.



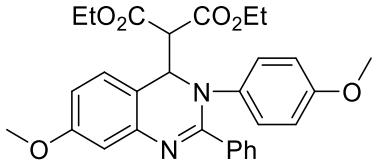
6-Chloro-7-methoxy-3-(p-methoxyphenyl)-4-methyl-2-phenyl-4-(tert-butyl)-3,4-dihydroquinazoline (5d). Prepared according to general procedure B with **3d** (0.109 g, 0.25 mmol), PIFA (0.215 g, 0.50 mmol), DCE (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (0% - 30% EtOAc in CH_2Cl_2 as eluent) to afford the desired product (0.010 g, 9%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.73 (m, 2H), 7.46 (ddd, *J* = 8.9, 2.4, 0.7 Hz, 1H), 7.25 – 7.20 (m, 3H), 7.10 (s, 1H), 7.03 (s, 1H), 6.75 (ddd, *J* = 8.9, 2.6, 0.8 Hz, 1H), 6.52 – 6.43 (m, 2H), 3.98 (s, 3H), 3.67 (s, 3H), 1.33 (s, 3H), 1.09 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 160.9, 158.0, 154.4, 143.5, 137.9, 136.2, 132.6, 131.4, 129.8, 129.7, 128.1, 127.8, 121.4, 118.6, 113.8, 113.6, 108.4, 66.3, 56.3, 55.4, 42.8, 26.1, 21.3; IR (neat): 3059, 2954, 1508, 1485, 1247, 1202 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{27}H_{30}ClN_2O_2$ 449.1996; Found 449.2019.



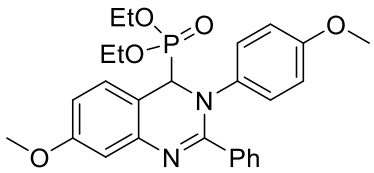
6-Cyano-7-methoxy-3-(p-methoxyphenyl)-4-methyl-2-phenyl-4-(tert-butyl)-3,4-dihydroquinazoline (5e). Prepared according to general procedure B with **3e** (0.106 g, 0.25 mmol), PIFA (0.214 g, 0.50 mmol), DCE (1.0 mL), and MeMgBr (3.0 M in ether, 0.25 mL, 0.75 mmol). Following workup, the residue was purified by MPLC (0% - 6% EtOAc in CH_2Cl_2) to afford the desired product (0.014 g, 13%) as an yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.69 (m, 2H), 7.46 (ddd, *J* = 8.8, 2.2, 0.9 Hz, 1H), 7.28 (s, 1H), 7.24 – 7.20 (m, 3H), 6.98 (s, 1H), 6.76 (ddd, *J* = 8.9, 2.4, 1.0 Hz, 1H), 6.46 (td, *J* = 1.9, 0.9 Hz, 2H), 3.99 (s, 3H), 3.67 (s, 3H), 1.34 (s, 3H), 1.08 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 162.9, 161.2, 158.2, 149.1, 137.5, 135.7, 132.7, 131.9, 131.3, 130.2, 129.9, 128.2, 121.3, 117.6, 113.9, 113.7, 107.2, 97.7, 66.7, 56.3, 55.4, 42.9, 26.0, 21.2; IR (neat): 3064, 2965, 2222, 1526, 1507, 1485, 1247, 1107, 1033 cm^{-1}; HRMS (ESI-TOF) m/z: [M+H]$^+$ Calcd for $C_{28}H_{30}N_3O_2$ 440.2338; Found 440.2339.



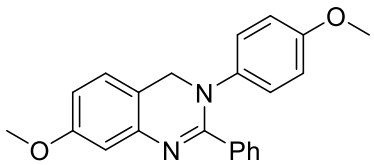
7-Methoxy-3-(*p*-methoxyphenyl)-4-(nitromethyl)-2-phenyl-3,4-dihydroquinazoline (6). Prepared according to general procedure C with **1** (0.100 g, 0.25 mmol), PIFA (0.216 g, 0.50 mmol), HFIP (1.0 mL), CH_3NO_2 (0.040 mL, 0.75 mmol), and DBU (0.11 mL, 0.74 mmol). Following workup, the residue was purified by MPLC (28% - 49% EtOAc in hexanes as eluent) to afford the desired product (0.069 g, 69%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (dd, *J* = 8.1, 1.6 Hz, 2H), 7.37 – 7.26 (m, 3H), 7.08 (d, *J* = 2.6 Hz, 1H), 7.01 (d, *J* = 8.3 Hz, 1H), 6.83 – 6.75 (m, 3H), 6.65 (d, *J* = 9.0 Hz, 2H), 5.47 (dd, *J* = 10.2, 4.2 Hz, 1H), 4.61 (dd, *J* = 11.4, 10.3 Hz, 1H), 4.41 (dd, *J* = 11.5, 4.2 Hz, 1H), 3.87 (s, 3H), 3.68 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 161.0, 157.4, 155.6, 143.8, 137.8, 135.5, 130.6, 130.1, 128.4, 126.1, 114.6, 113.8, 113.7, 109.4, 78.0, 62.0, 55.6, 55.5; IR (neat): 3056, 2958, 1545, 1508, 1487, 1247, 1030 cm^{-1}; HRMS (ESI-TOF) m/z: [M+H]$^+$ Calcd for $C_{23}H_{22}N_3O_4$ 404.1610; Found 404.1605.



Diethyl [7-methoxy-3-(p-methoxyphenyl)-2-phenyl-3,4-dihydroquinazolin-4-yl]malonate (7). Prepared according to general procedure C with **1** (0.101 g, 0.25 mmol), PIFA (0.215 g, 0.50 mmol), HFIP (1.0 mL), diethyl malonate (0.11 mL, 0.72 mmol), and DBU (0.11 mL, 0.74 mmol). Following workup, the residue was purified by MPLC (14% - 35% EtOAc in hexanes as eluent) to afford the desired product (0.093 g, 73%) as a light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 8.3, 1.5 Hz, 2H), 7.35 – 7.21 (m, 3H), 7.09 – 6.95 (m, 4H), 6.71 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.65 (d, *J* = 9.0 Hz, 2H), 5.50 (d, *J* = 10.4 Hz, 1H), 4.36 – 4.21 (m, 2H), 4.10 – 3.95 (m, 2H), 3.84 (s, 3H), 3.75 (d, *J* = 10.4 Hz, 1H), 3.66 (s, 3H), 1.21 (t, *J* = 7.1 Hz, 3H), 1.09 (t, *J* = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 168.0, 166.8, 160.4, 156.8, 155.9, 143.6, 138.4, 135.6, 130.5, 129.9, 128.2, 127.2, 125.6, 116.4, 114.3, 112.8, 108.9, 62.05, 61.98, 61.8, 56.6, 55.5, 55.4, 14.04, 13.96; IR (neat): 3058, 2982, 1750, 1731, 1508, 1485, 1245, 1033 cm^{-1}; HRMS (ESI-TOF) m/z: [M+H]$^+$ Calcd for $C_{29}H_{31}N_2O_6$ 503.2182; Found 503.2183.



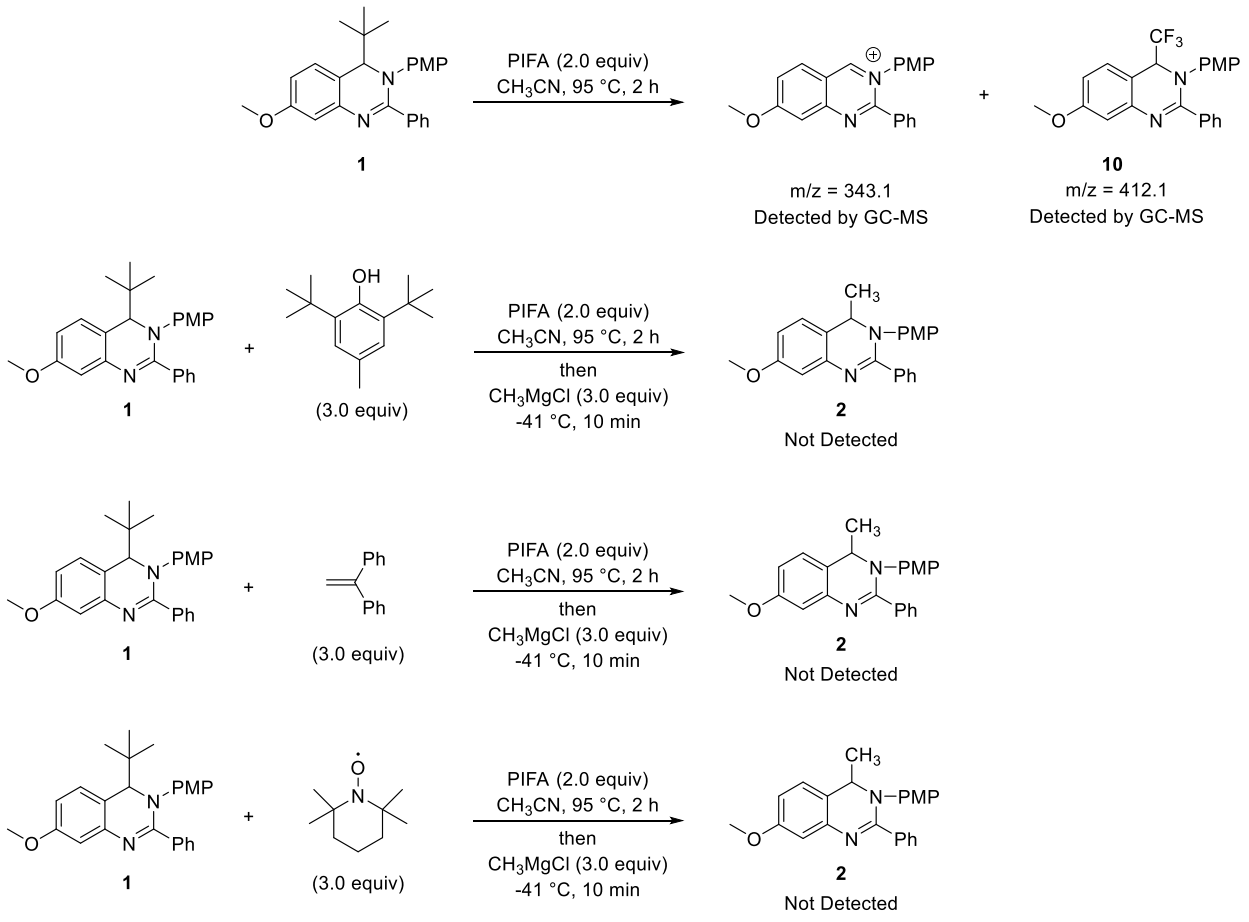
Diethyl 7-methoxy-3-(p-methoxyphenyl)-2-phenyl-3,4-dihydroquinazolin-4-ylphosphonate (8). Prepared according to general procedure C with **1** (0.100 g, 0.25 mmol), PIFA (0.216 g, 0.50 mmol), HFIP (1.0 mL), diethyl phosphite (0.10 mL, 0.78 mmol), and DBU (0.11 mL, 0.74 mmol). Following workup, the residue was purified by MPLC (70% - 95% EtOAc in hexanes as eluent) to afford the desired product (0.086 g, 72%) as a light orange oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.72 (m, 2H), 7.30 – 7.23 (m, 3H), 7.20 (d, *J* = 8.9 Hz, 2H), 7.03 – 6.95 (m, 2H), 6.75 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.66 (d, *J* = 9.2 Hz, 2H), 5.15 (d, *J* = 12.4 Hz, 1H), 4.17 – 3.91 (m, 4H), 3.85 (s, 3H), 3.69 (s, 3H), 1.22 (td, *J* = 7.1, 0.8 Hz, 6H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 160.6 (d, $^{3}J_{C\text{-}P}$ = 3 Hz), 156.9, 156.2 (d, $^{4}J_{C\text{-}P}$ = 2 Hz), 144.0, 139.7 (d, $^{3}J_{C\text{-}P}$ = 3 Hz), 136.3, 130.04, 130.02, 128.3, 127.5 (d, $^{2}J_{C\text{-}P}$ = 5 Hz), 126.3 (d, $^{3}J_{C\text{-}P}$ = 2 Hz), 114.1, 112.9, 112.2, 108.9 (d, $^{3}J_{C\text{-}P}$ = 3 Hz), 63.3 (d, $^{2}J_{C\text{-}P}$ = 8 Hz), 63.1 (d, $^{2}J_{C\text{-}P}$ = 7 Hz), 61.5 (d, $^{1}J_{C\text{-}P}$ = 165 Hz), 55.54, 55.48, 16.7 (d, $^{3}J_{C\text{-}P}$ = 5 Hz), 16.6 (d, $^{3}J_{C\text{-}P}$ = 5 Hz); ^{31}P NMR (162 MHz, $CDCl_3$) δ 19.2; IR (neat): 3065, 2963, 1508, 1489, 1251, 1232, 1033 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{26}H_{30}N_2O_5P$ 481.1892; Found 481.1889.



7-**Methoxy-3-(*p*-methoxyphenyl)-2-phenyl-3,4-dihydroquinazoline (9).** Prepared according to general procedure C with **1** (0.100 g, 0.25 mmol), PIFA (0.216 g, 0.50 mmol), HFIP (1.0 mL), and $NaBH(OAc)_3$ (0.160 g, 0.75 mmol). Following workup, the residue was purified by MPLC (11% - 62% EtOAc in hexanes as eluent) to afford the desired product (0.085 g, 99%) as a light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.27 – 7.16 (m, 3H), 6.93 (d, *J* = 2.6 Hz, 1H), 6.91 – 6.85 (m, 3H), 6.72 – 6.66 (m, 3H), 4.97 (s, 2H), 3.83 (s, 3H), 3.71 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 160.1, 157.0, 156.8, 143.9, 138.9, 136.3, 129.8, 129.5, 128.1, 125.8, 125.6, 114.4, 114.1, 112.2, 108.6, 55.6, 55.5, 52.2; IR (neat): 3058, 2957, 1508, 1491, 1247, 1034 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{21}N_2O_2$ 345.1603; Found 345.1608.

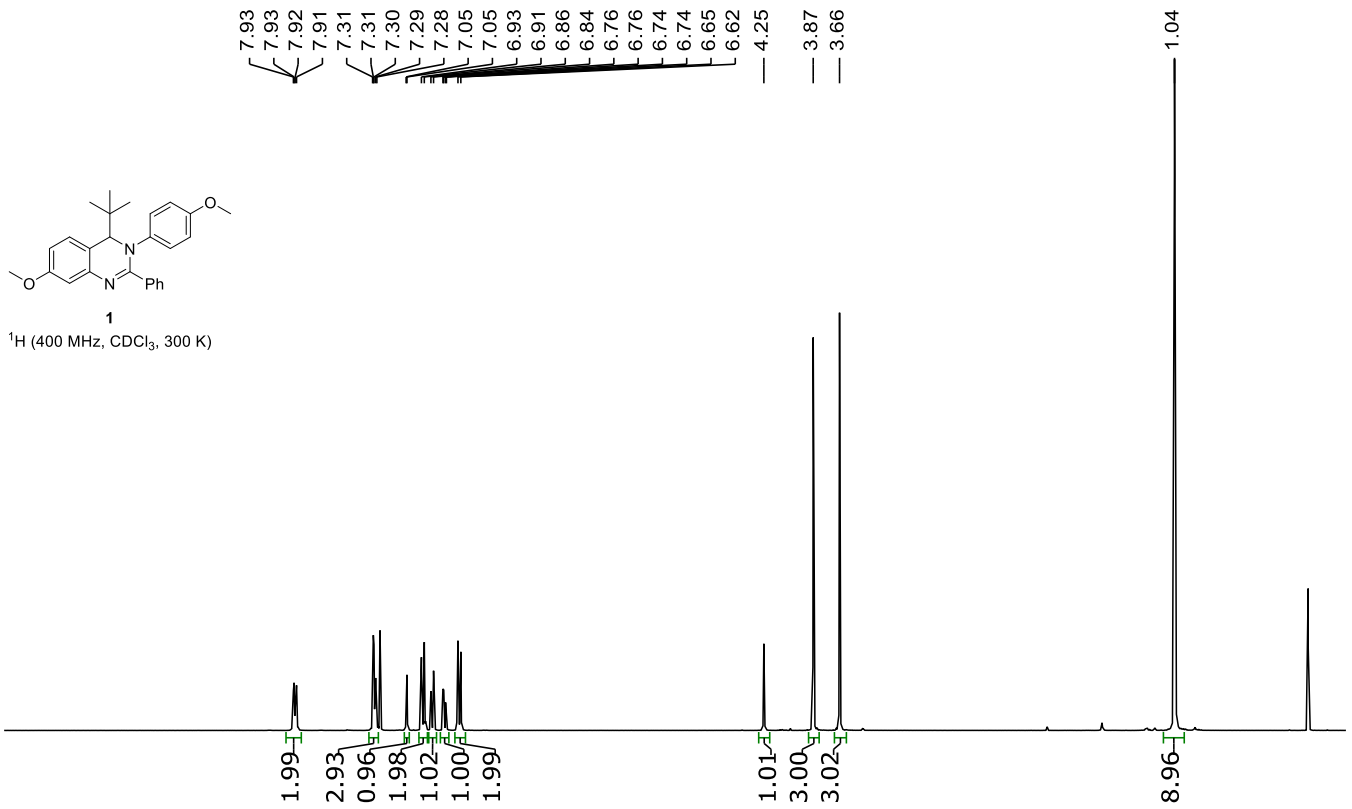
Radical Trapping Experiments

A mixture of **1** (0.100 g, 0.25 mmol) and PIFA (0.215 g, 0.50 mmol), with or without a radical scavenger (0.75 mmol, 3 equiv), in MeCN (1 mL) was heated to 95 °C in a sealed flame-dried vial set in an aluminum block for 2 hours. The reaction was removed from heat, and 5 μL of the reaction mixture was removed and transferred to a 2 mL autosampler vial containing 1 mL of MeCN. This sample was submitted for GC-MS analysis. The remaining reaction mixture was cooled to -41 °C in an acetonitrile/dry ice bath before MeMgCl (3.0 M in THF, 0.25 mL, 0.75 mmol) was added. The reaction stirred at -41 °C for 10 min, after which time the reaction was quenched by the addition of saturated aqueous NH_4Cl solution (2 mL) followed by the addition of saturated aqueous $NaHCO_3$ solution (10 mL). The mixture was extracted with CH_2Cl_2 (3x), and the pooled organic extracts were dried (Na_2SO_4) and concentrated. The crude mixture was then analyzed by ^1H NMR with 1,3,5-trimethoxybenzene as an internal standard.



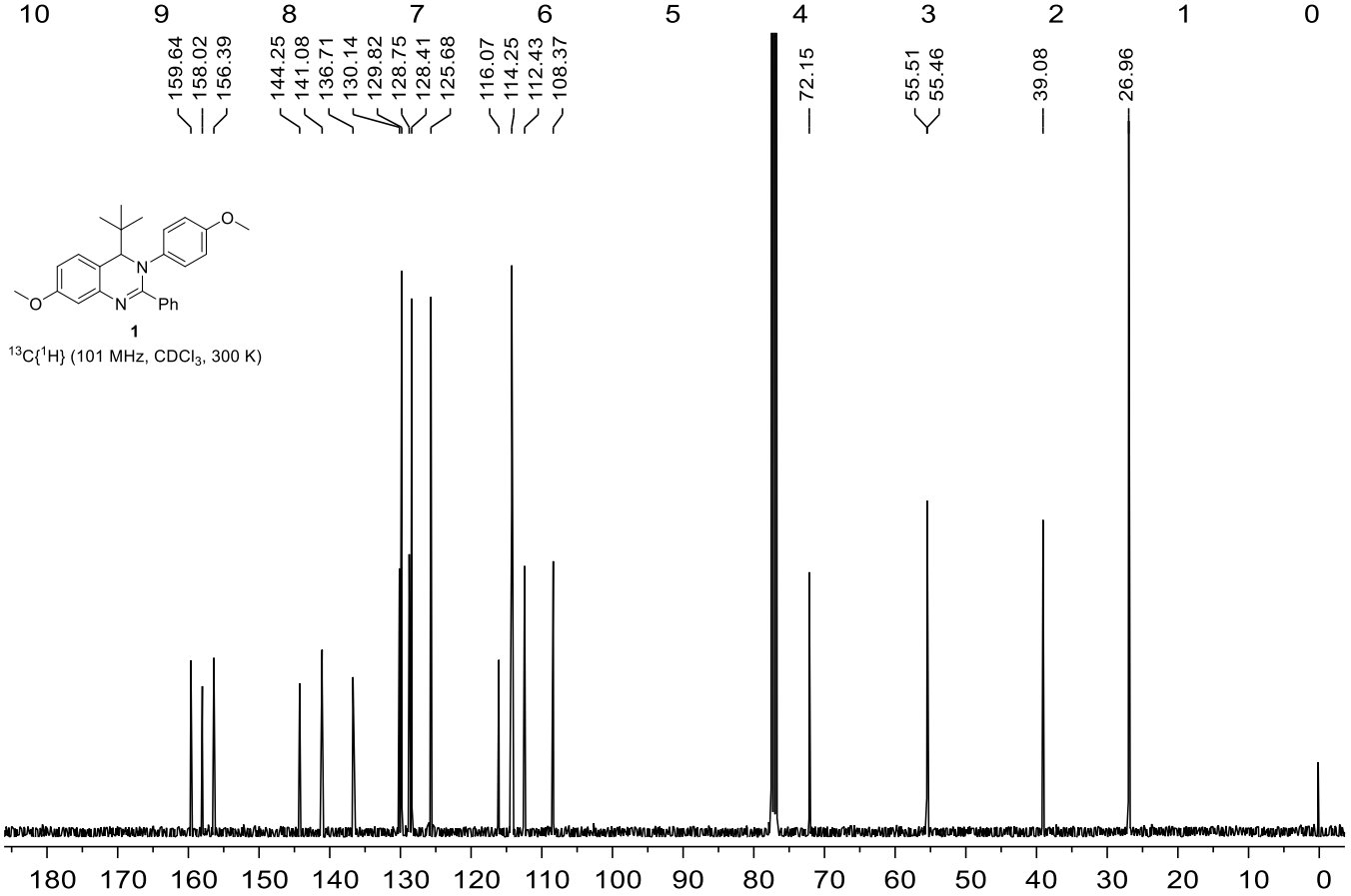
References and Notes

1. C. L. Magyar, T. J. Wall, S. B. Davies, M. V. Campbell, H. A. Barna, S. R. Smith, C. J. Savich and R. A. Mosey, *Org. Biomol. Chem.*, 2019, **17**, 7995-8000.
2. W. C. Fu and T. F. Jamison, *Org. Lett.*, 2019, **21**, 6112-6116.



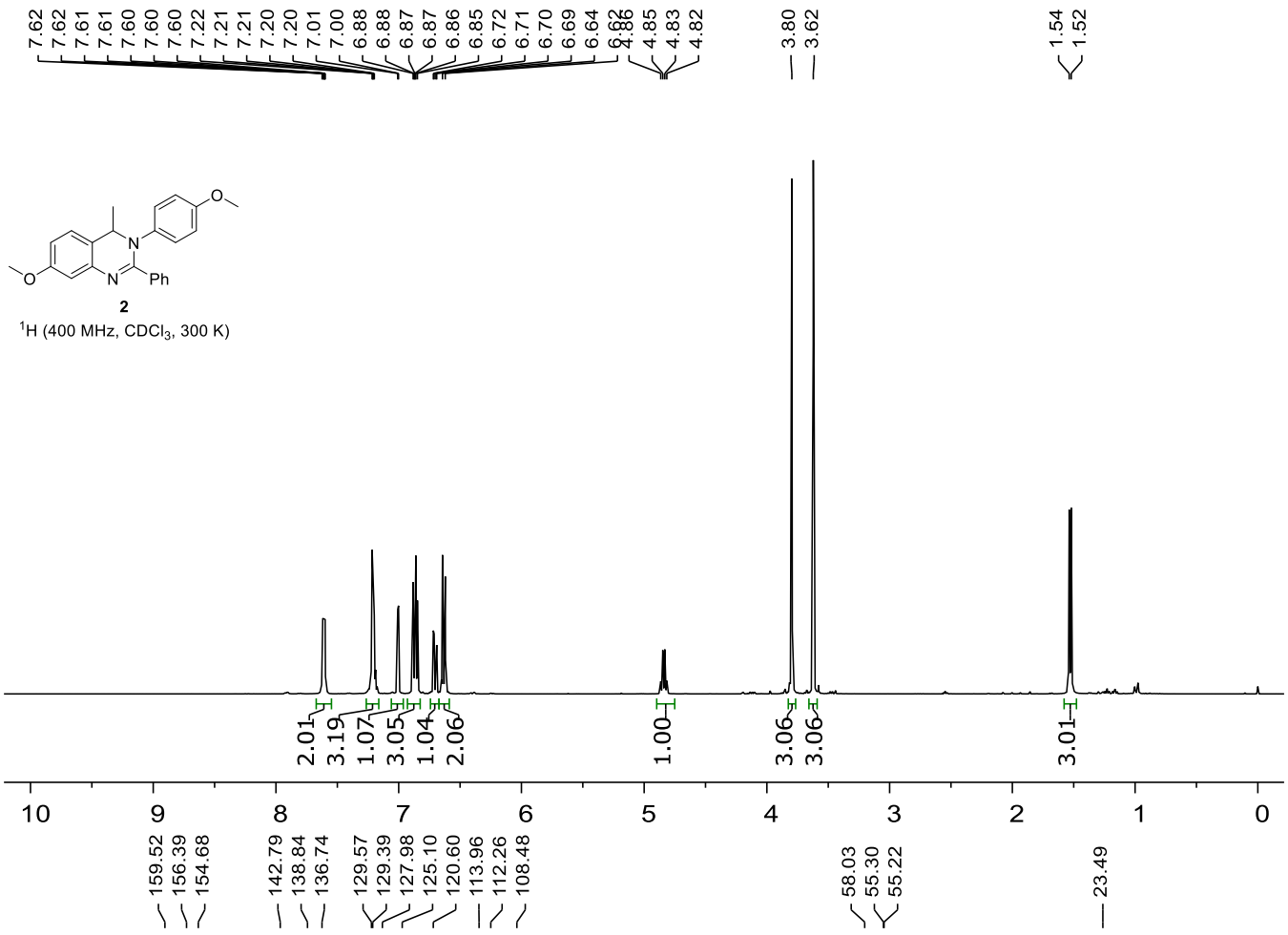
1

^{1}H (400 MHz, $CDCl_3$, 300 K)



1

$^{13}C\{^{1}H\}$ (101 MHz, $CDCl_3$, 300 K)


7.62
7.62
7.61
7.61
7.60
7.60
7.60
7.22
7.21
7.21
7.20
7.20
7.01
7.00
6.88
6.88
6.87
6.87
6.86
6.85
6.72
6.71
6.70
6.69
6.64
4.85
4.83
4.82
3.80
3.62
1.54
1.52
O
N
N
O
Ph
2
1H (400 MHz, CDCl3, 300 K)
2.01
3.19
1.07
3.05
1.04
2.06
1.00
3.06
3.06
3.01
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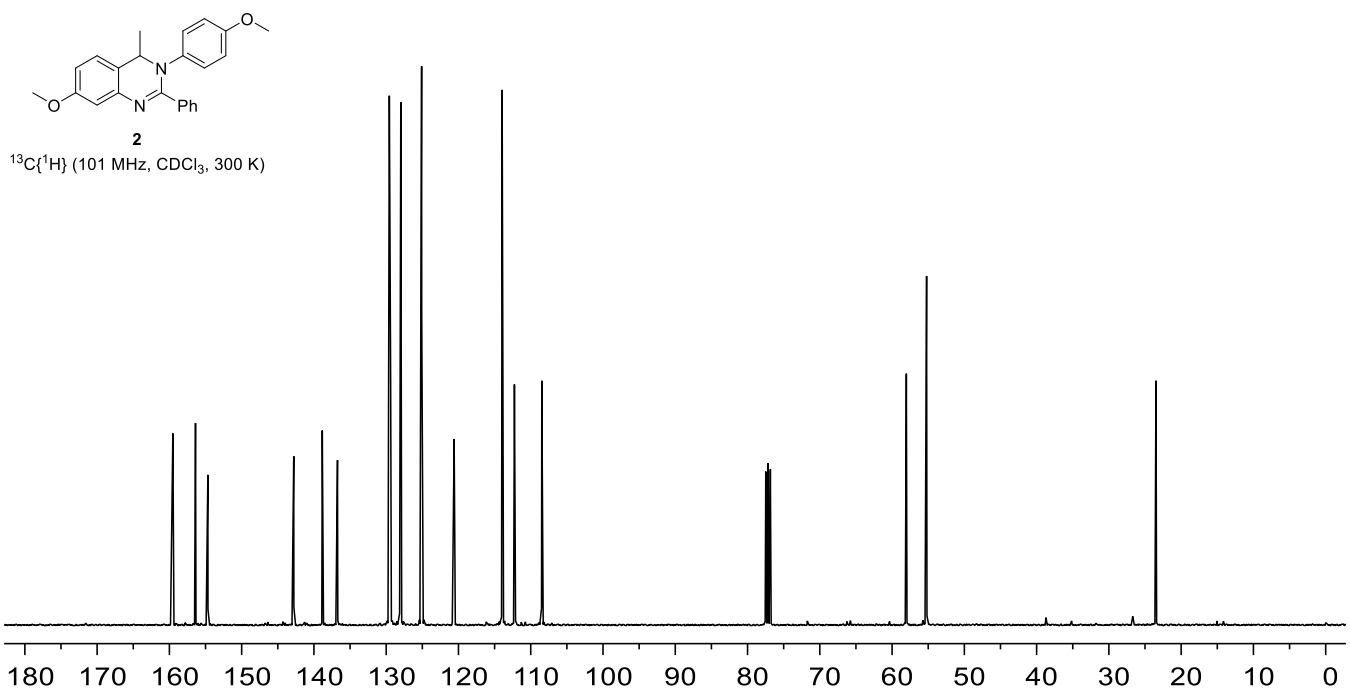
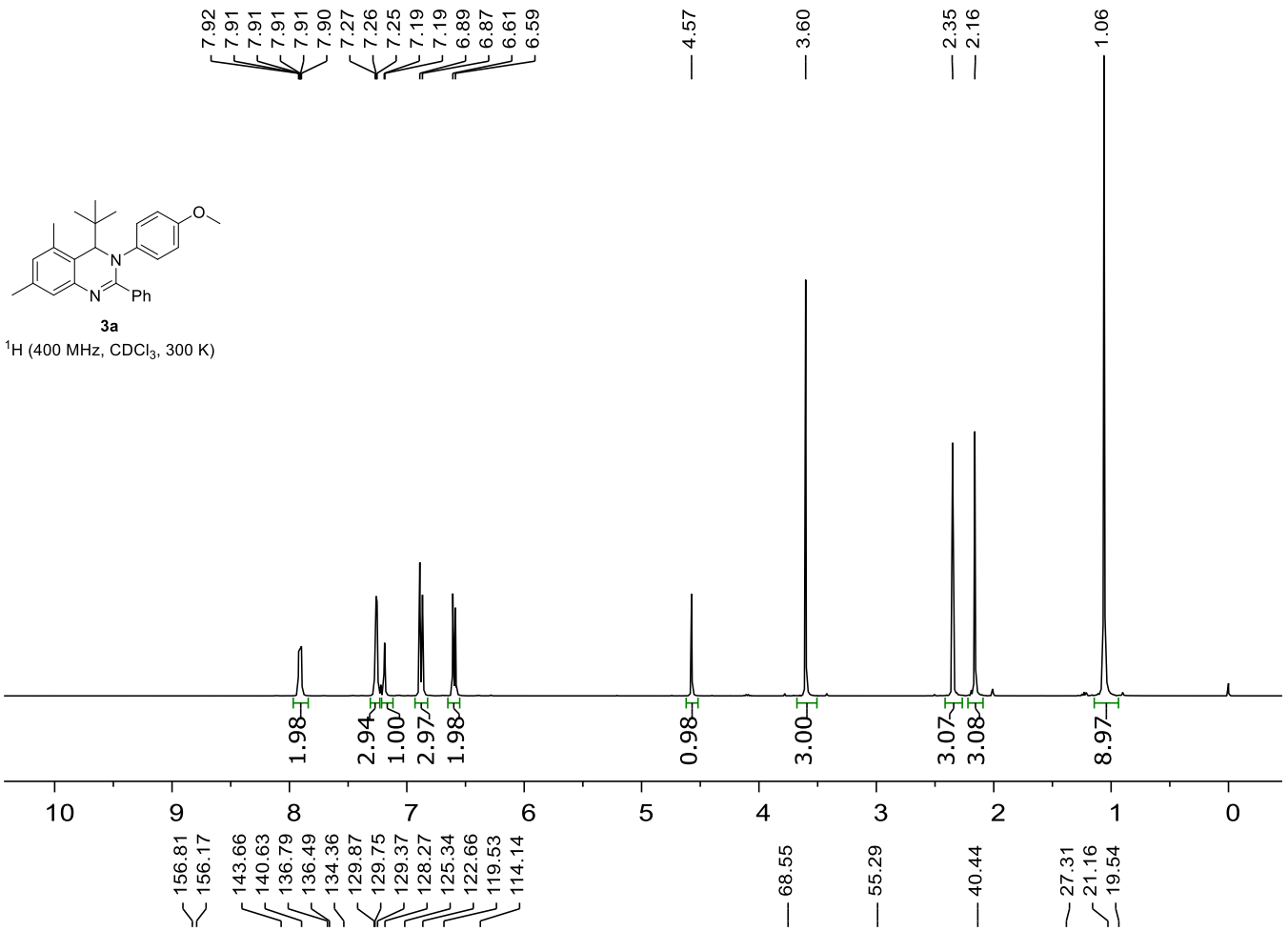
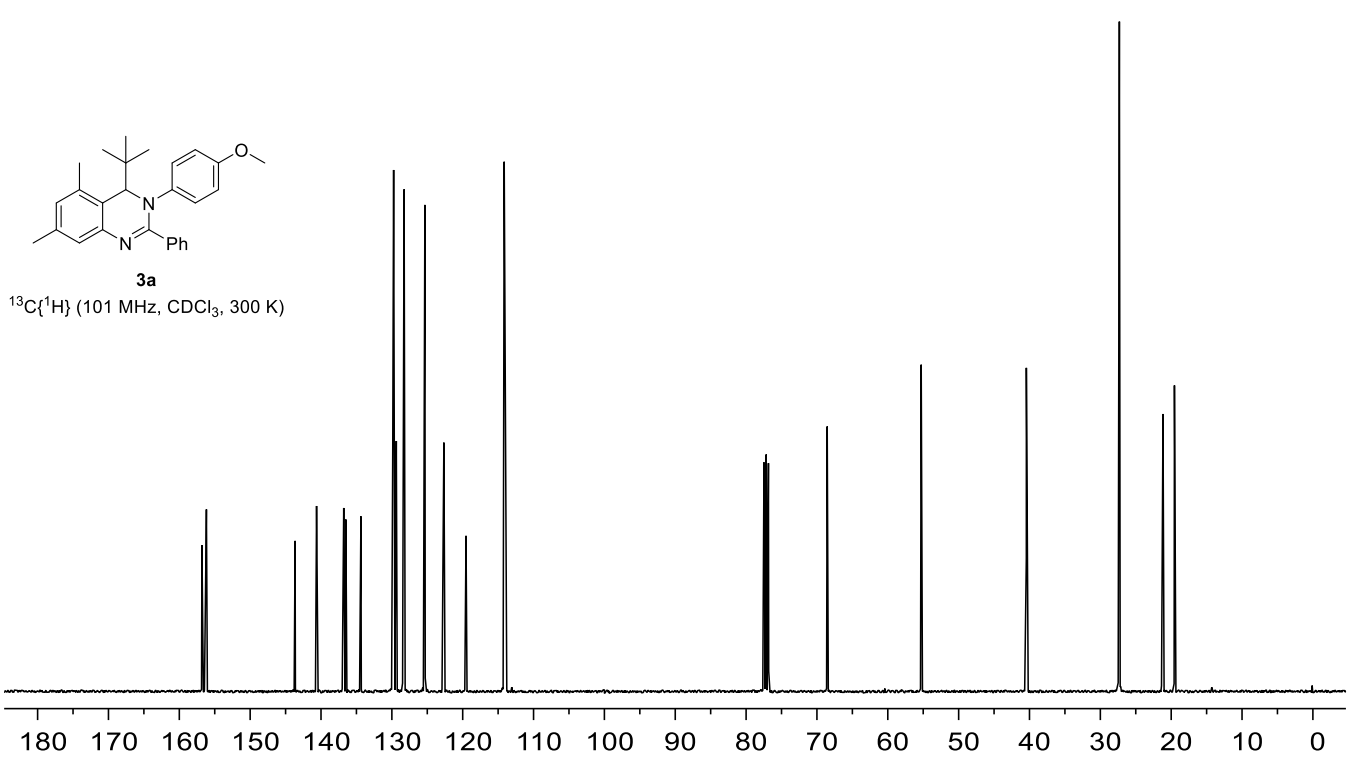
9
8
7
6
5
4
3
2
1
0


159.52
156.39
154.68
142.79
138.84
136.74
129.57
129.39
127.98
125.10
120.60
113.96
112.26
108.48
58.03
55.30
55.22
23.49
O
N
N
O
Ph
2
13C{1H} (101 MHz, CDCl3, 300 K)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



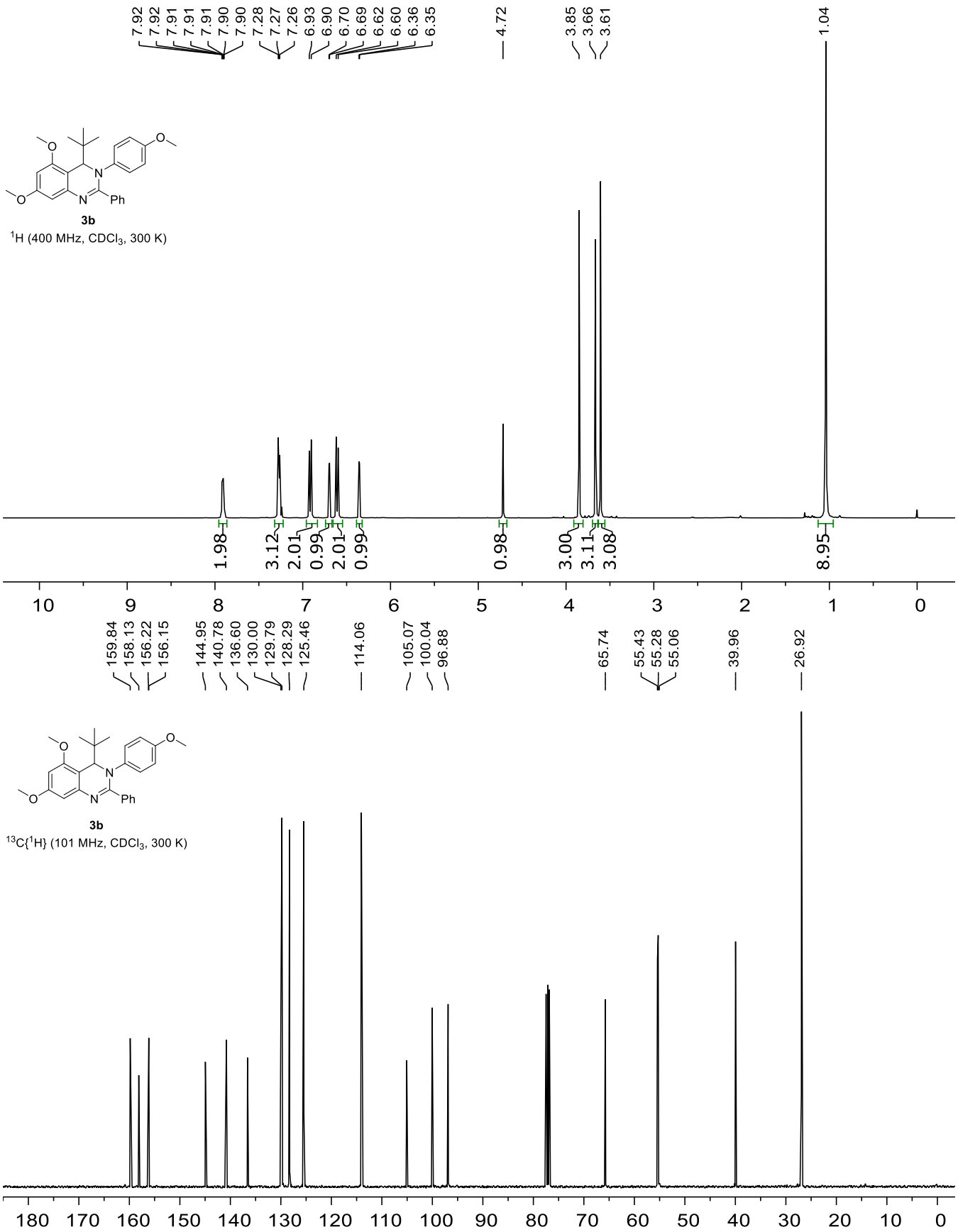
3a

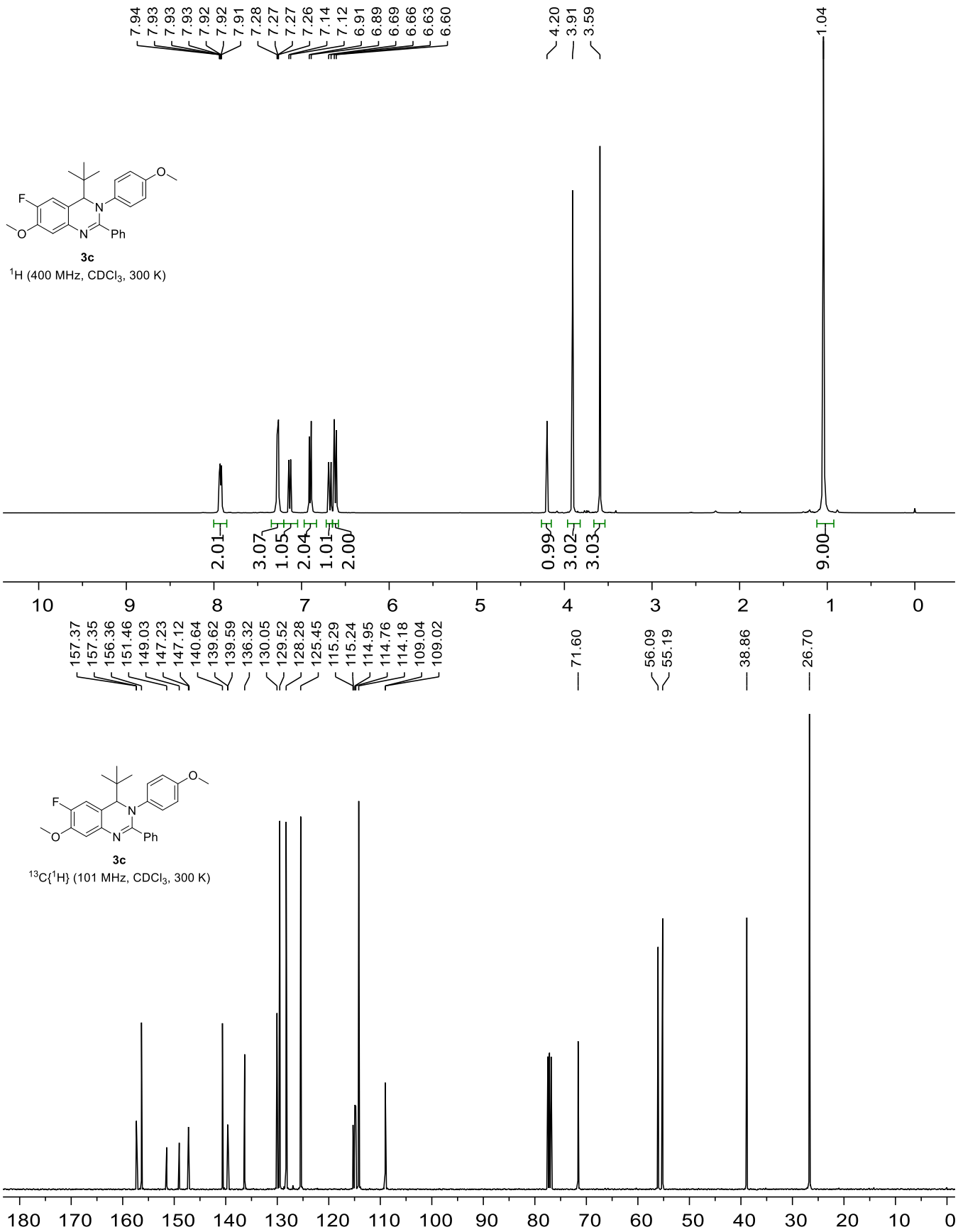
^{1}H (400 MHz, $CDCl_3$, 300 K)

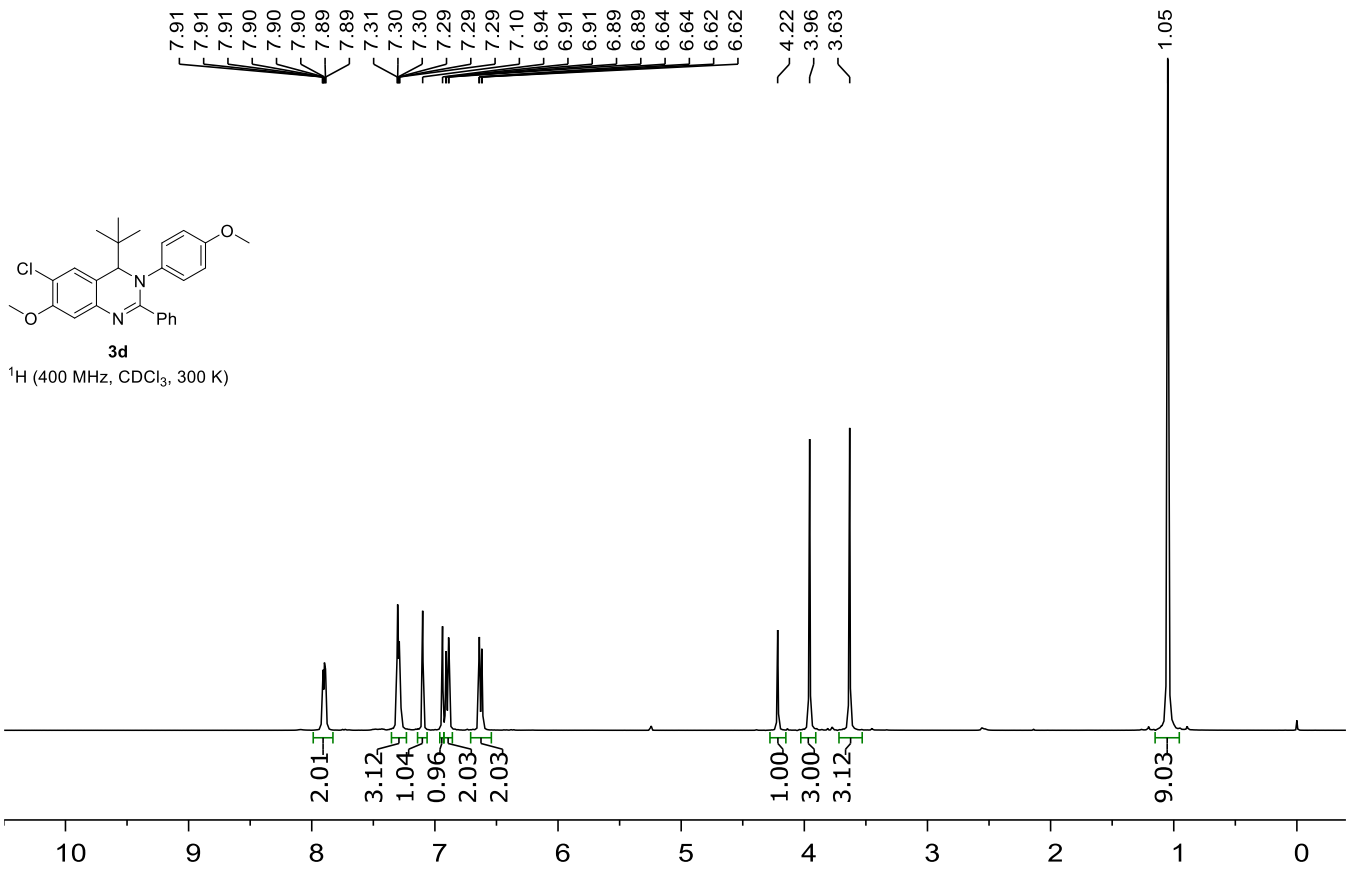


3a

$^{13}C\{^{1}H\}$ (101 MHz, $CDCl_3$, 300 K)

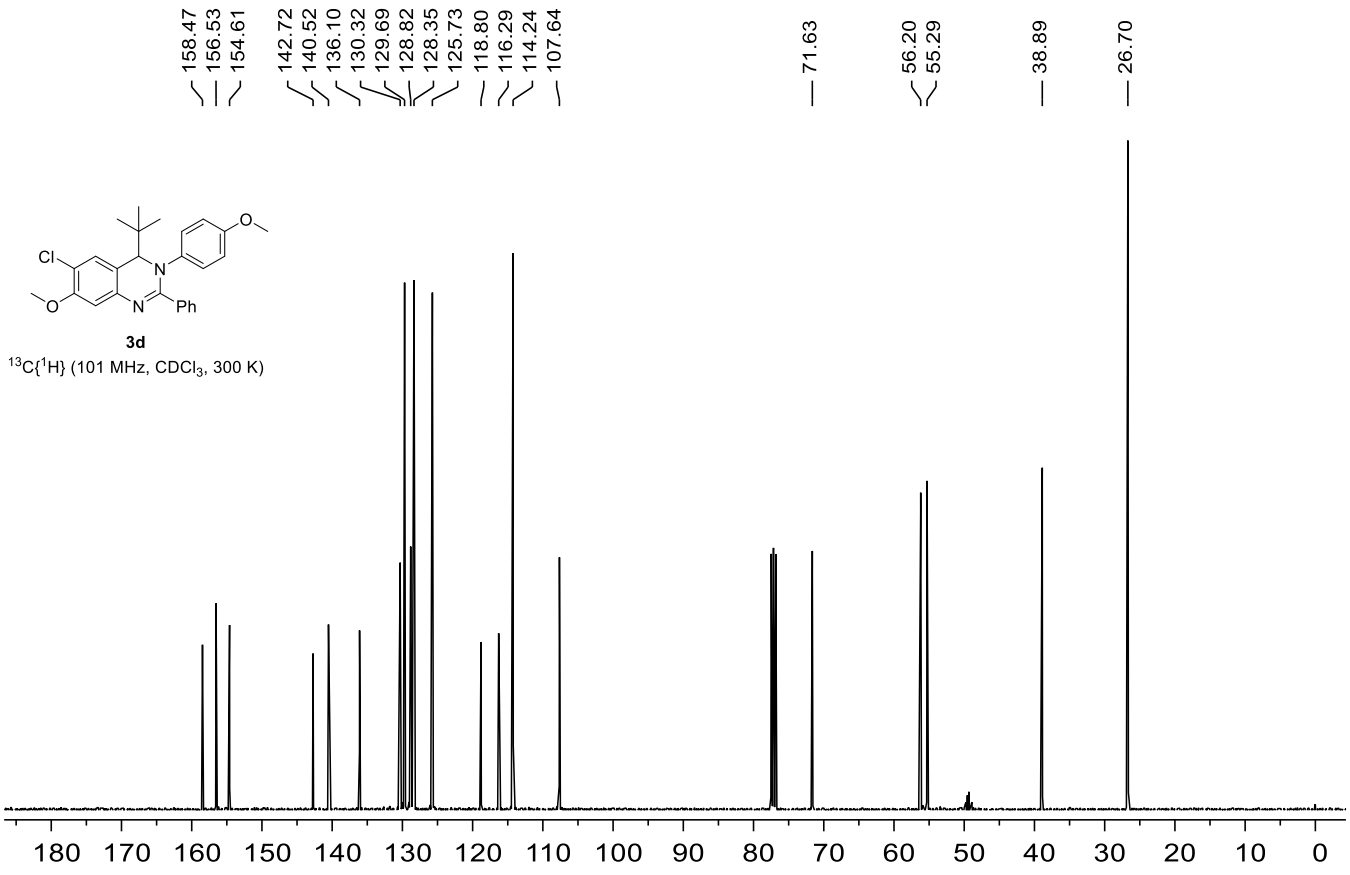

7.92
7.92
7.91
7.91
7.91
7.90
7.90
7.28
7.27
7.26
6.93
6.90
6.70
6.69
6.62
6.60
6.36
6.35
4.72
3.85
3.66
3.61
1.04
3b
1H (400 MHz, CDCl3, 300 K)
1.98
3.12
2.01
0.99
2.01
0.99
0.98
3.00
3.11
3.08
8.95
10
9
8
7
6
5
4
3
2
1
0
159.84
158.13
156.22
156.15
144.95
140.78
136.60
130.00
129.79
128.29
125.46
114.06
105.07
100.04
96.88
65.74
55.43
55.28
55.06
39.96
26.92
3b
13C{1H} (101 MHz, CDCl3, 300 K)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


7.94
7.93
7.93
7.93
7.92
7.92
7.91
7.28
7.27
7.27
7.26
7.14
7.12
6.91
6.89
6.69
6.66
6.63
6.60
4.20
3.91
3.59
1.04
F
O
N
N
O
Ph
3c
1H (400 MHz, CDCl3, 300 K)
2.01
3.07
1.05
2.04
1.01
2.00
0.99
3.02
3.03
9.00
10
9
8
7
6
5
4
3
2
1
0
157.37
157.35
156.36
151.46
149.03
147.23
147.12
140.64
139.62
139.59
136.32
130.05
129.52
128.28
125.45
115.29
115.24
114.95
114.76
114.18
109.04
109.02
71.60
56.09
55.19
38.86
26.70
F
O
N
N
O
Ph
3c
13C{1H} (101 MHz, CDCl3, 300 K)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



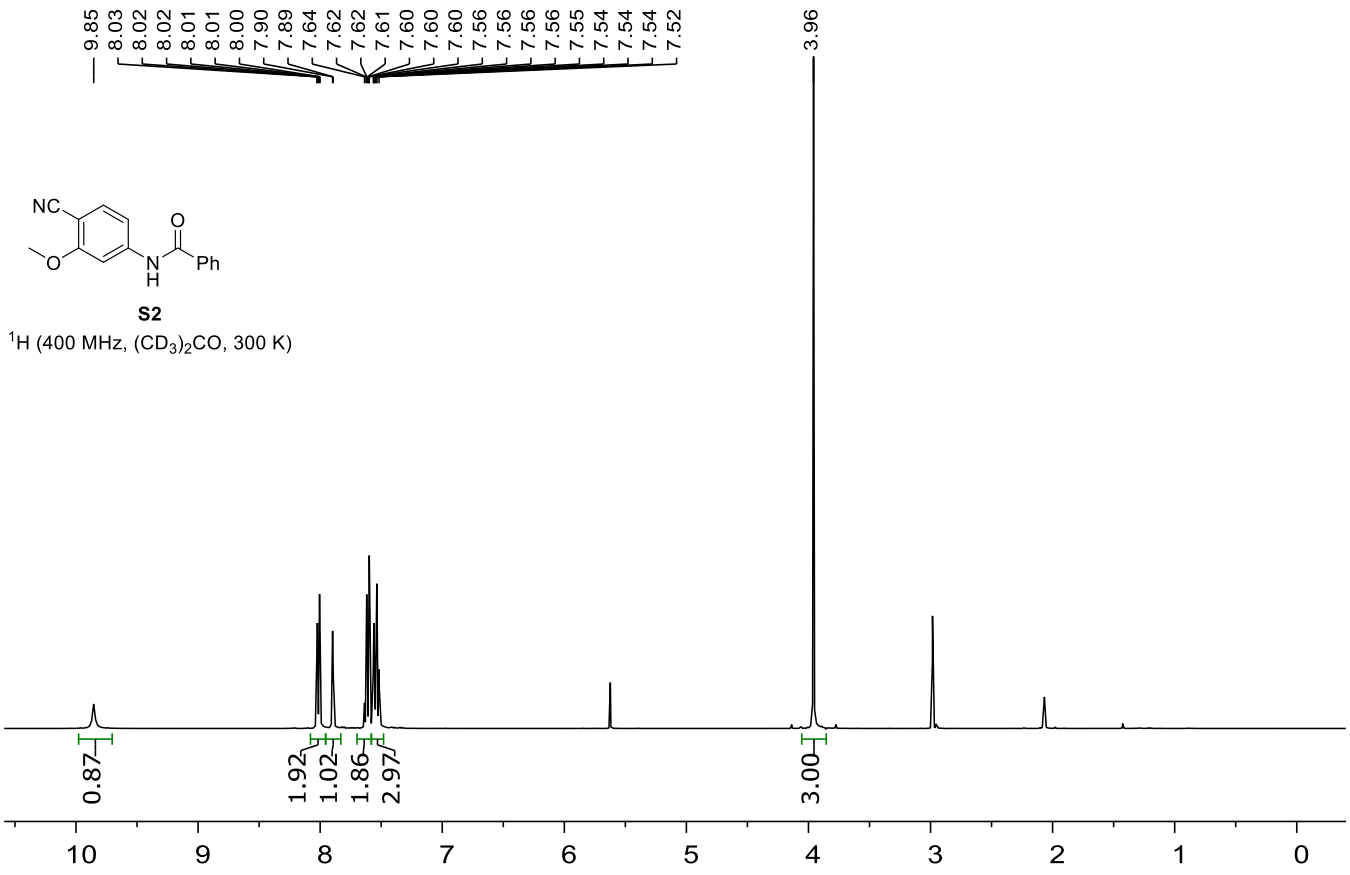
3d

^{1}H (400 MHz, $CDCl_3$, 300 K)



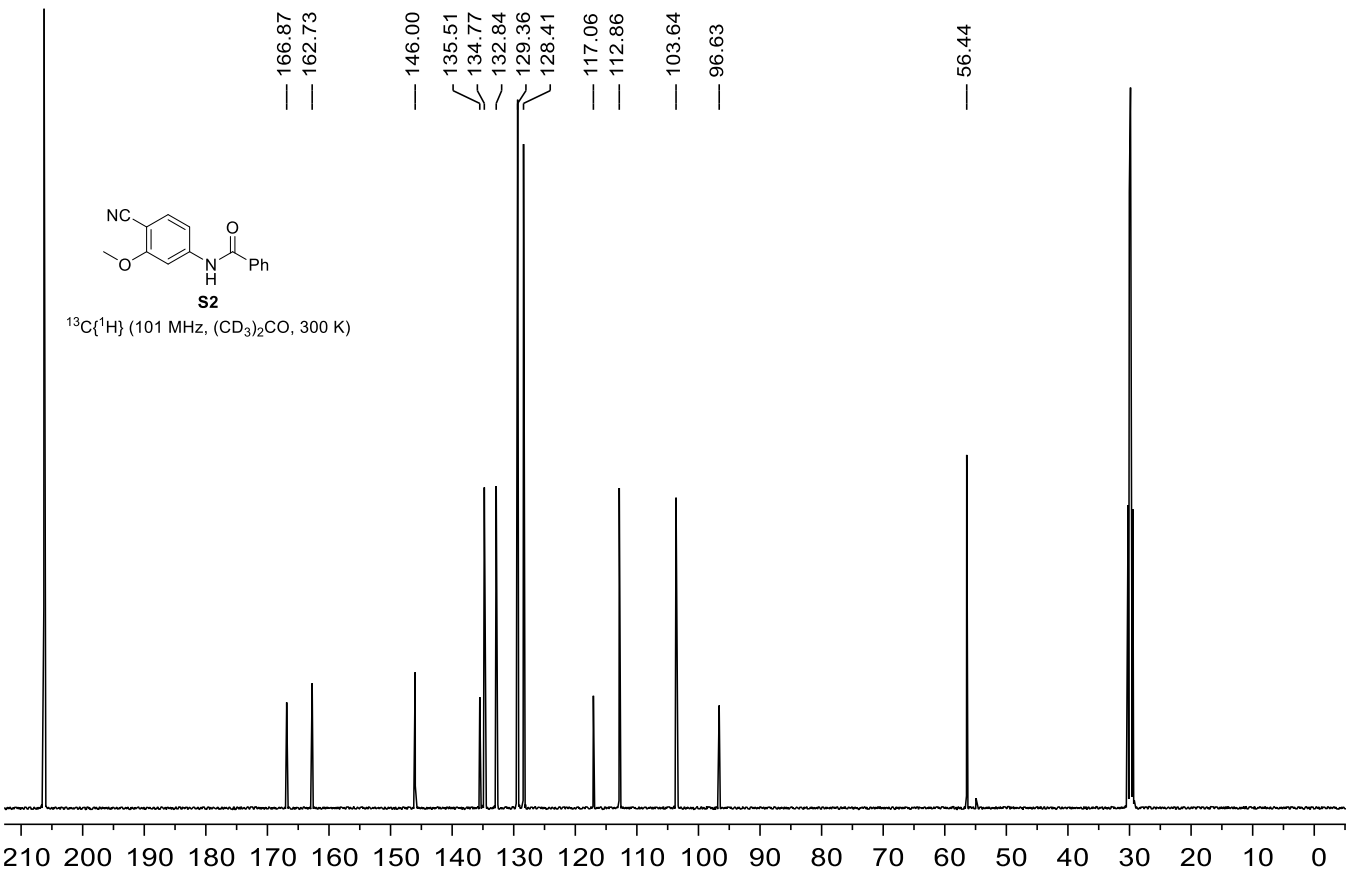
3d

$^{13}C\{^{1}H\}$ (101 MHz, $CDCl_3$, 300 K)



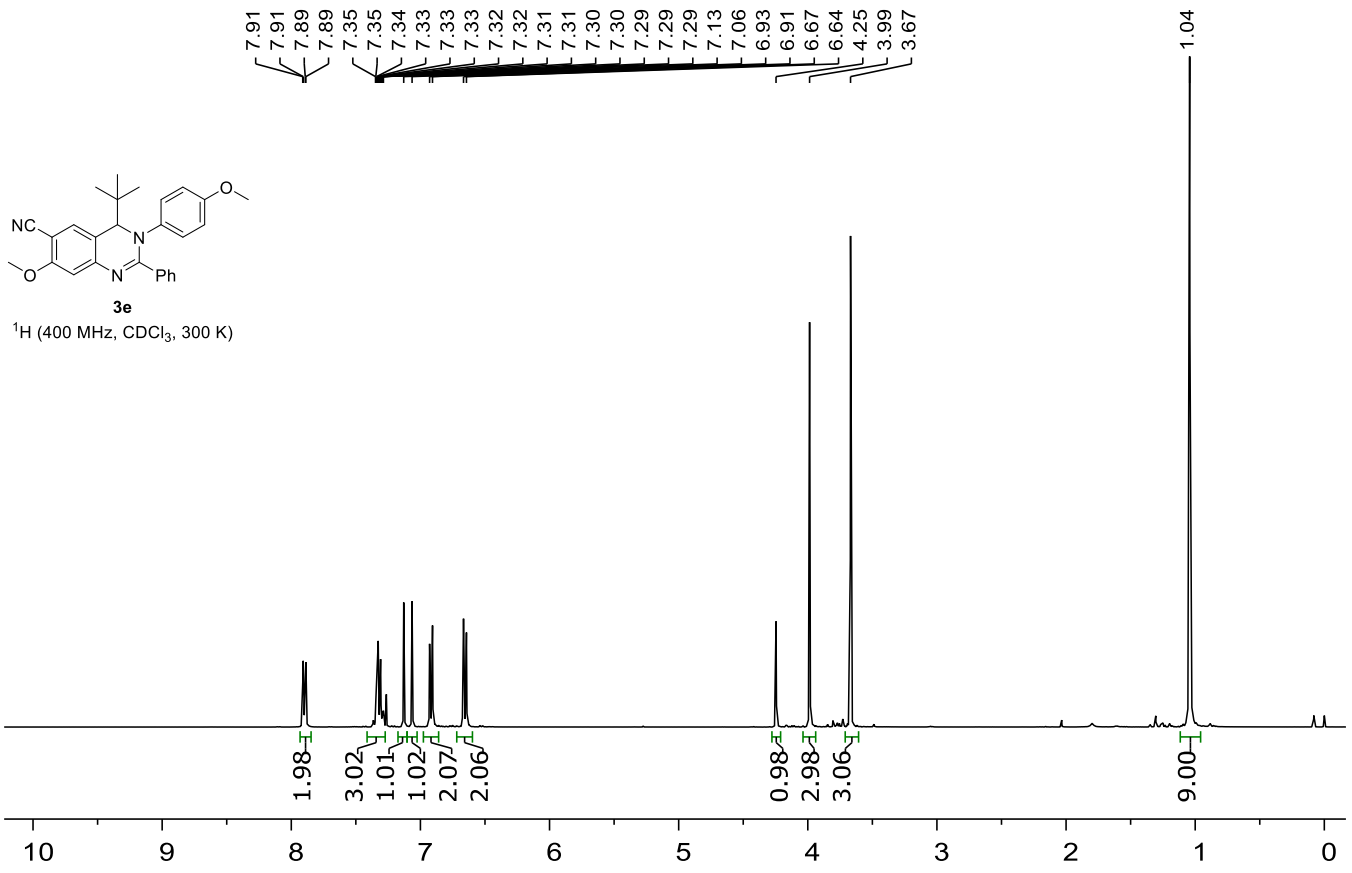
S2

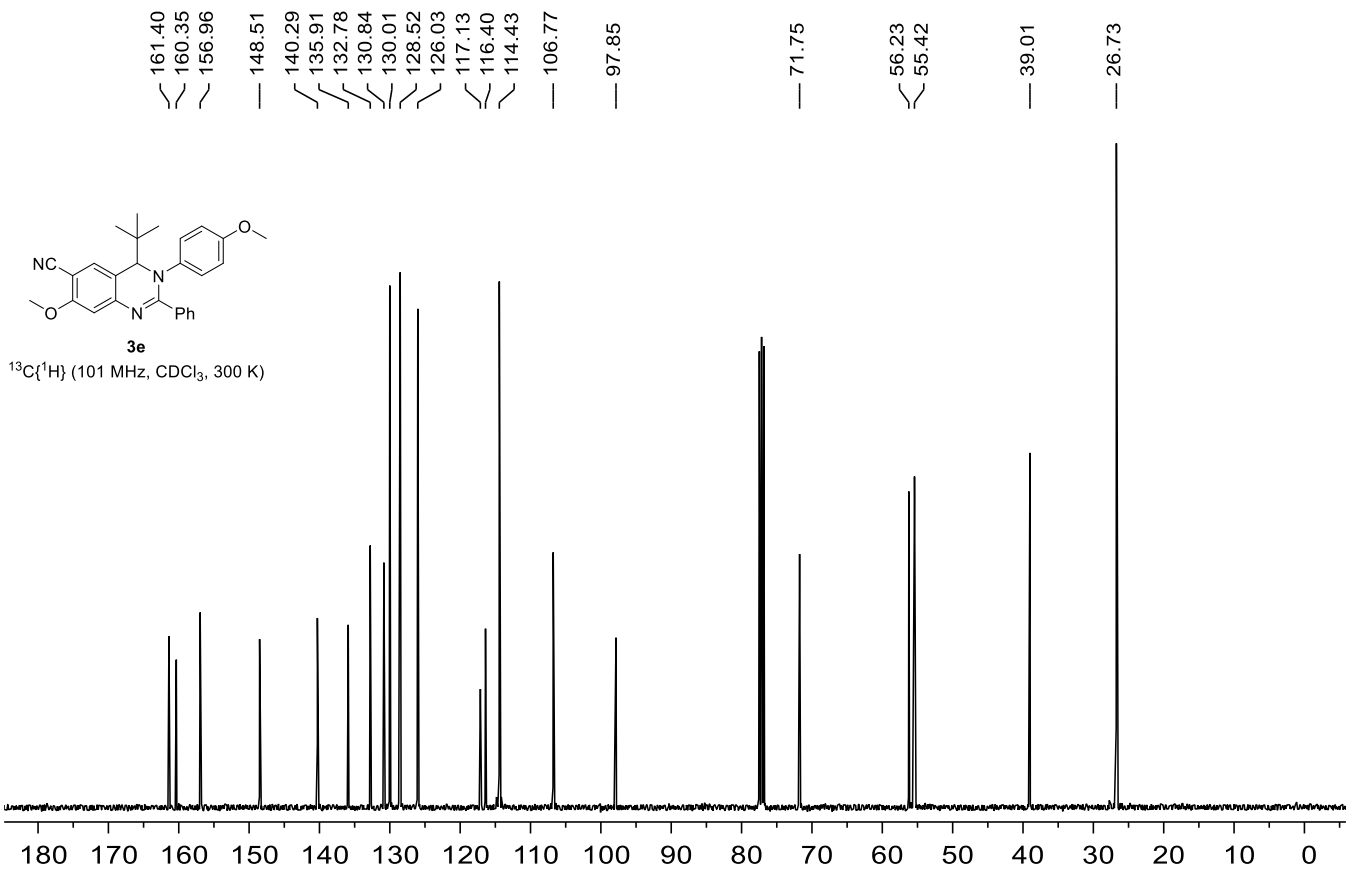
^{1}H (400 MHz, $(CD_3)_2CO$, 300 K)

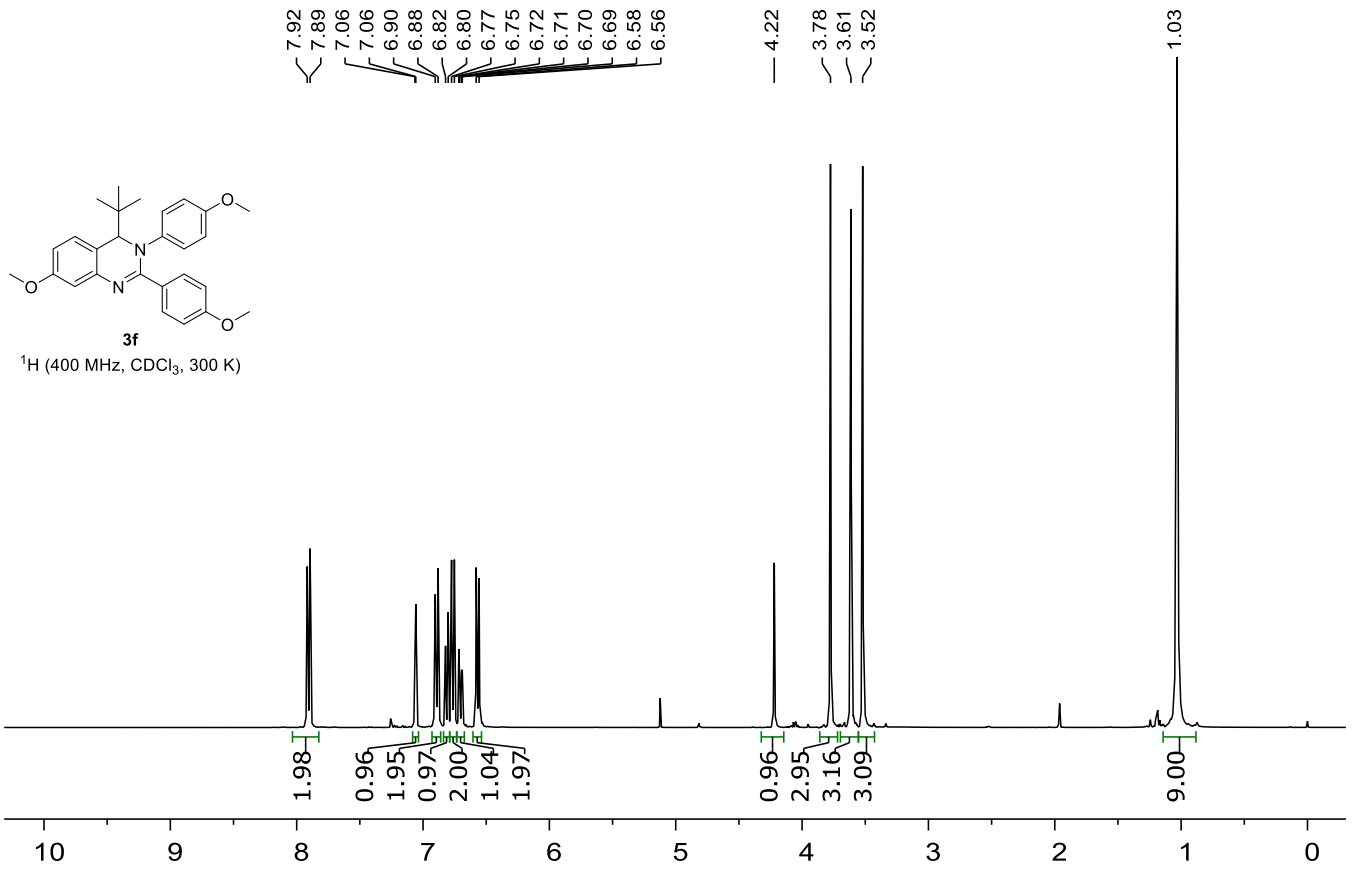


S2

$^{13}C\{^{1}H\}$ (101 MHz, $(CD_3)_2CO$, 300 K)

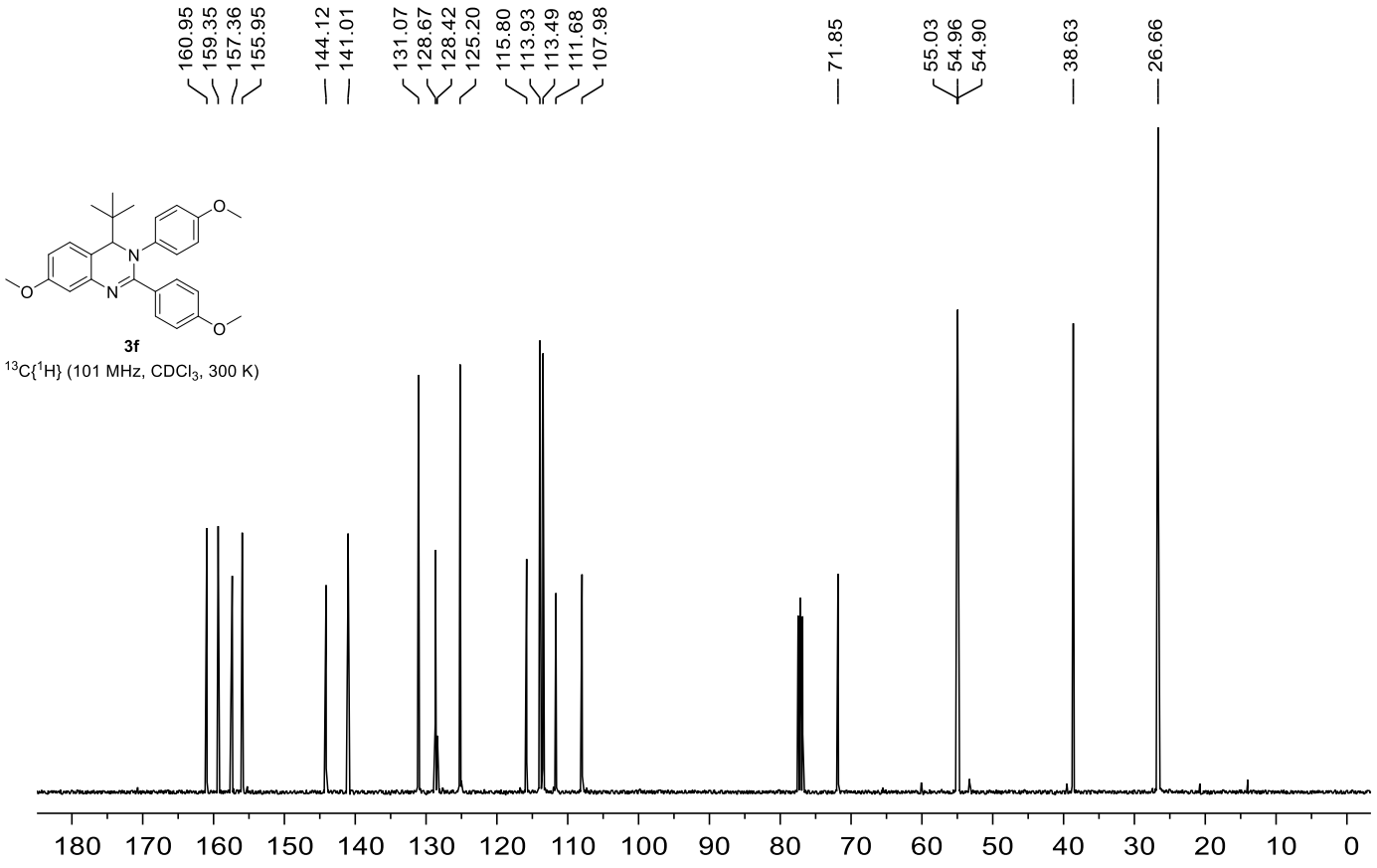

7.91
7.91
7.89
7.89
7.35
7.35
7.34
7.33
7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.30
7.29
7.29
7.29
7.13
7.06
6.93
6.91
6.67
6.64
4.25
3.99
3.67
1.04
NC
O
N
O
N
Ph
3e
1H (400 MHz, CDCl3, 300 K)
1.98
3.02
1.01
1.02
2.07
2.06
0.98
2.98
3.06
9.00
10
9
8
7
6
5
4
3
2
1
0


161.40
160.35
156.96
148.51
140.29
135.91
132.78
130.84
130.01
128.52
126.03
117.13
116.40
114.43
106.77
97.85
71.75
56.23
55.42
39.01
26.73
NC
O
N
O
N
Ph
3e
13C{1H} (101 MHz, CDCl3, 300 K)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



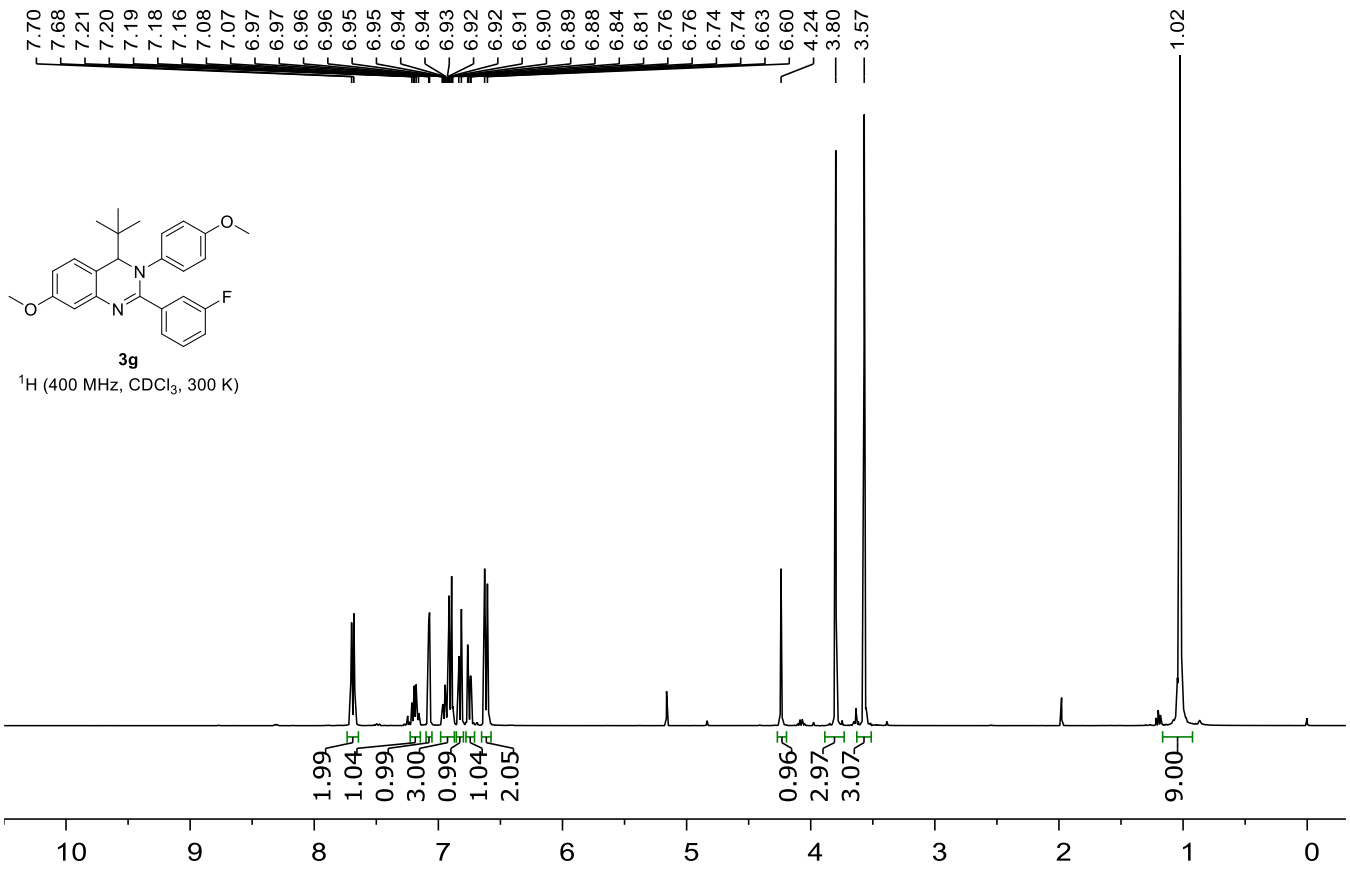
3f

^{1}H (400 MHz, $CDCl_3$, 300 K)



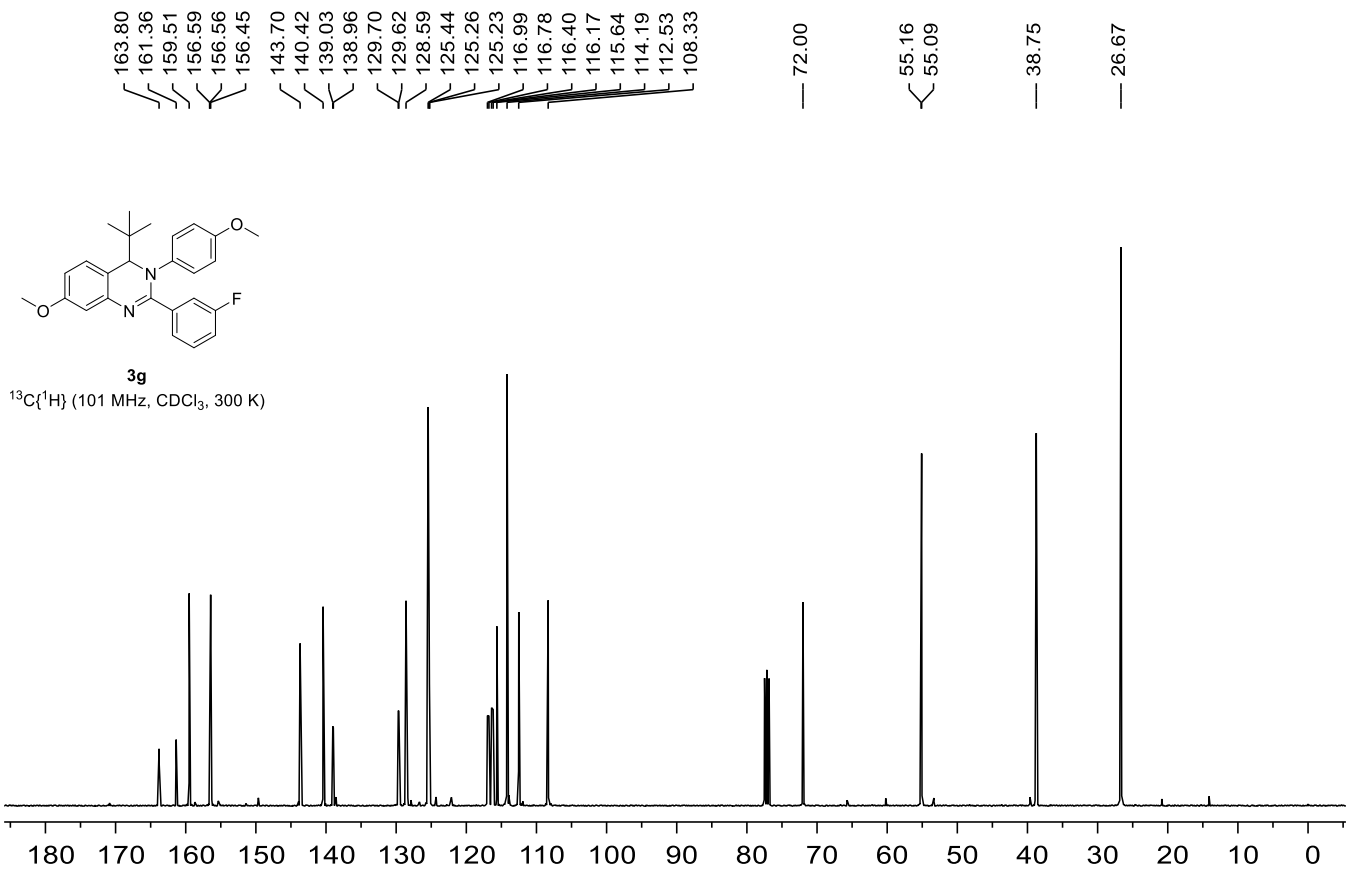
3f

$^{13}C\{^{1}H\}$ (101 MHz, $CDCl_3$, 300 K)



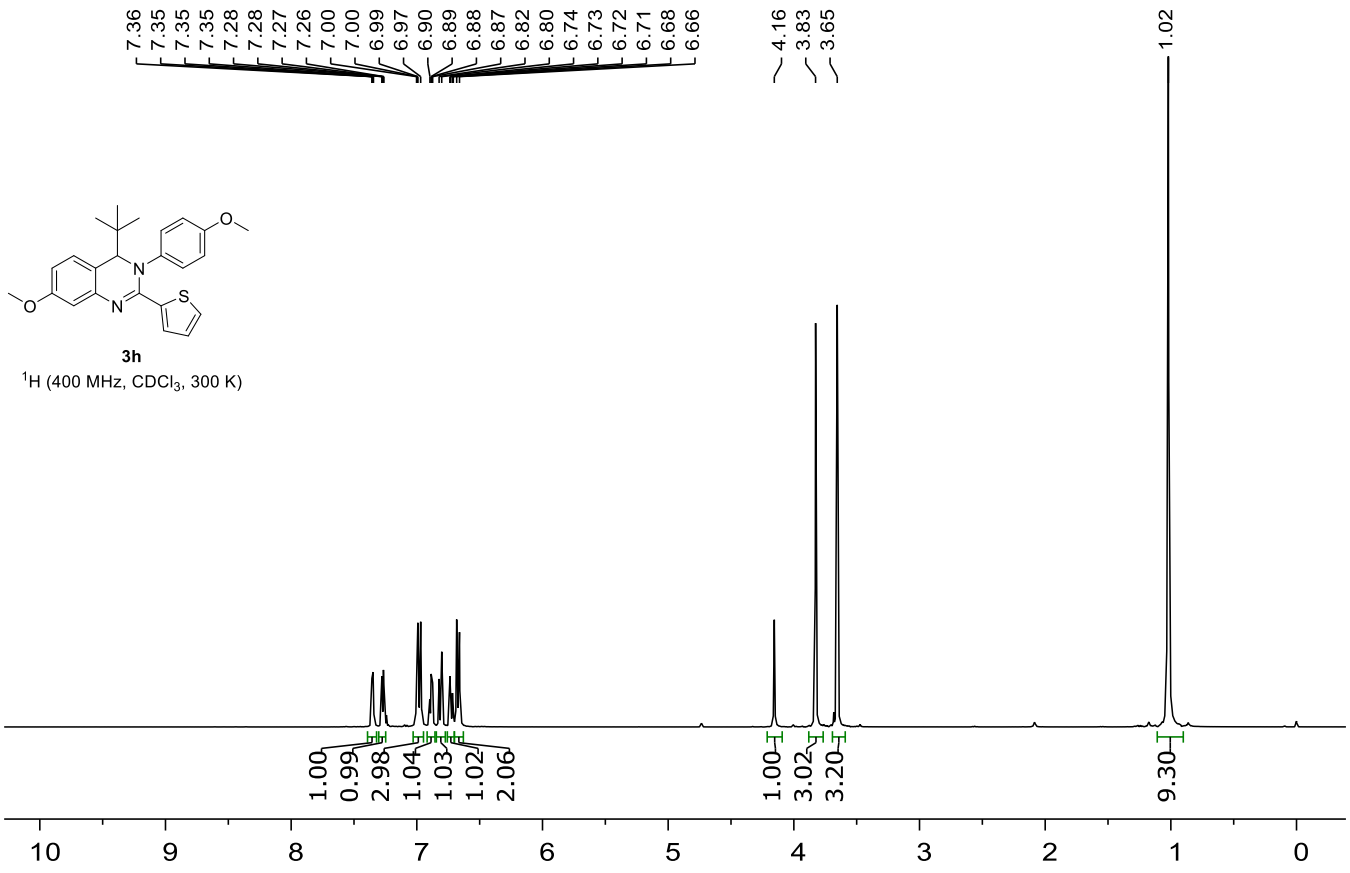
3g

^{1}H (400 MHz, $CDCl_3$, 300 K)



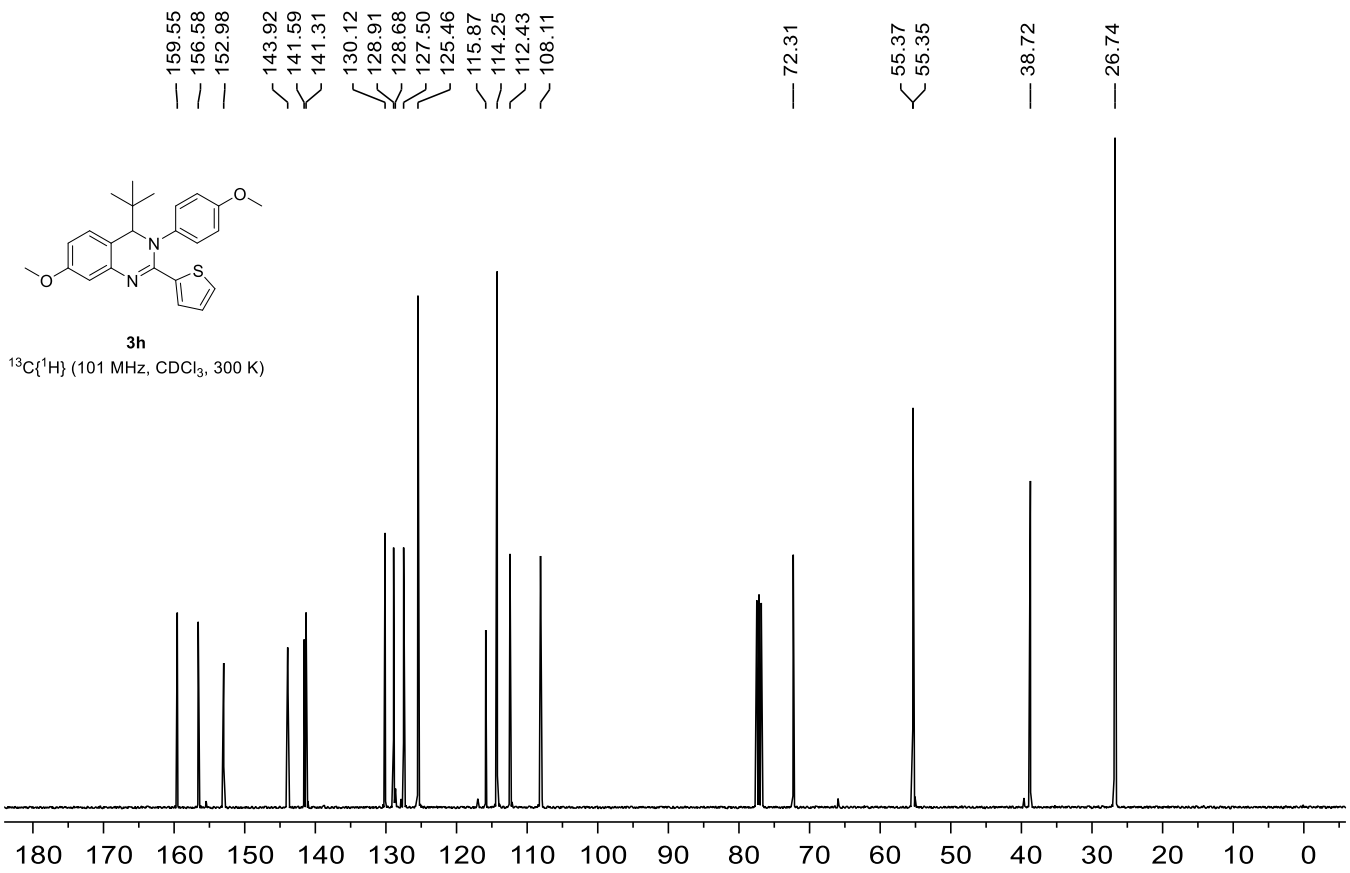
3g

^{13}C{^{1}H} (101 MHz, $CDCl_3$, 300 K)



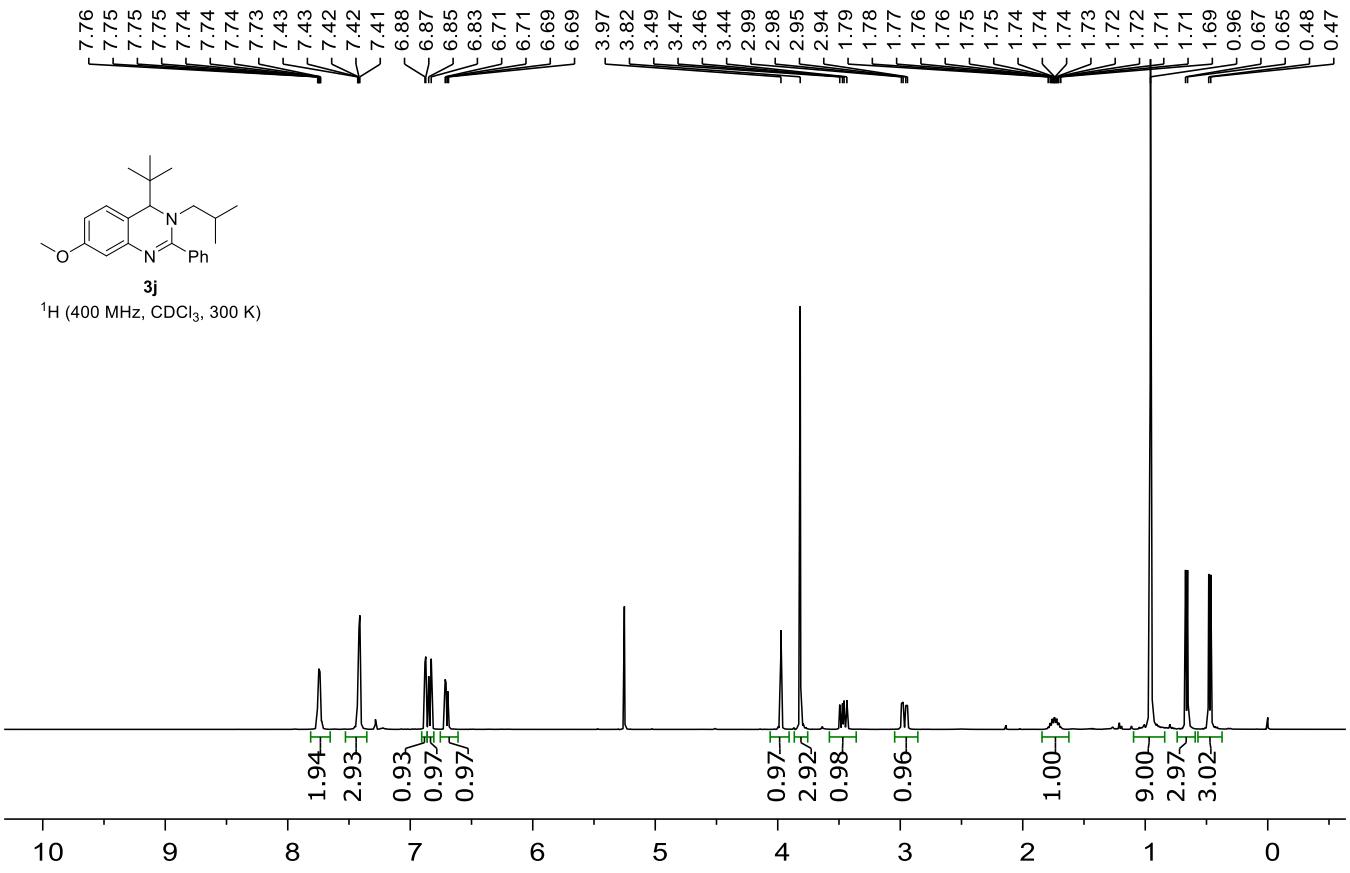
3h

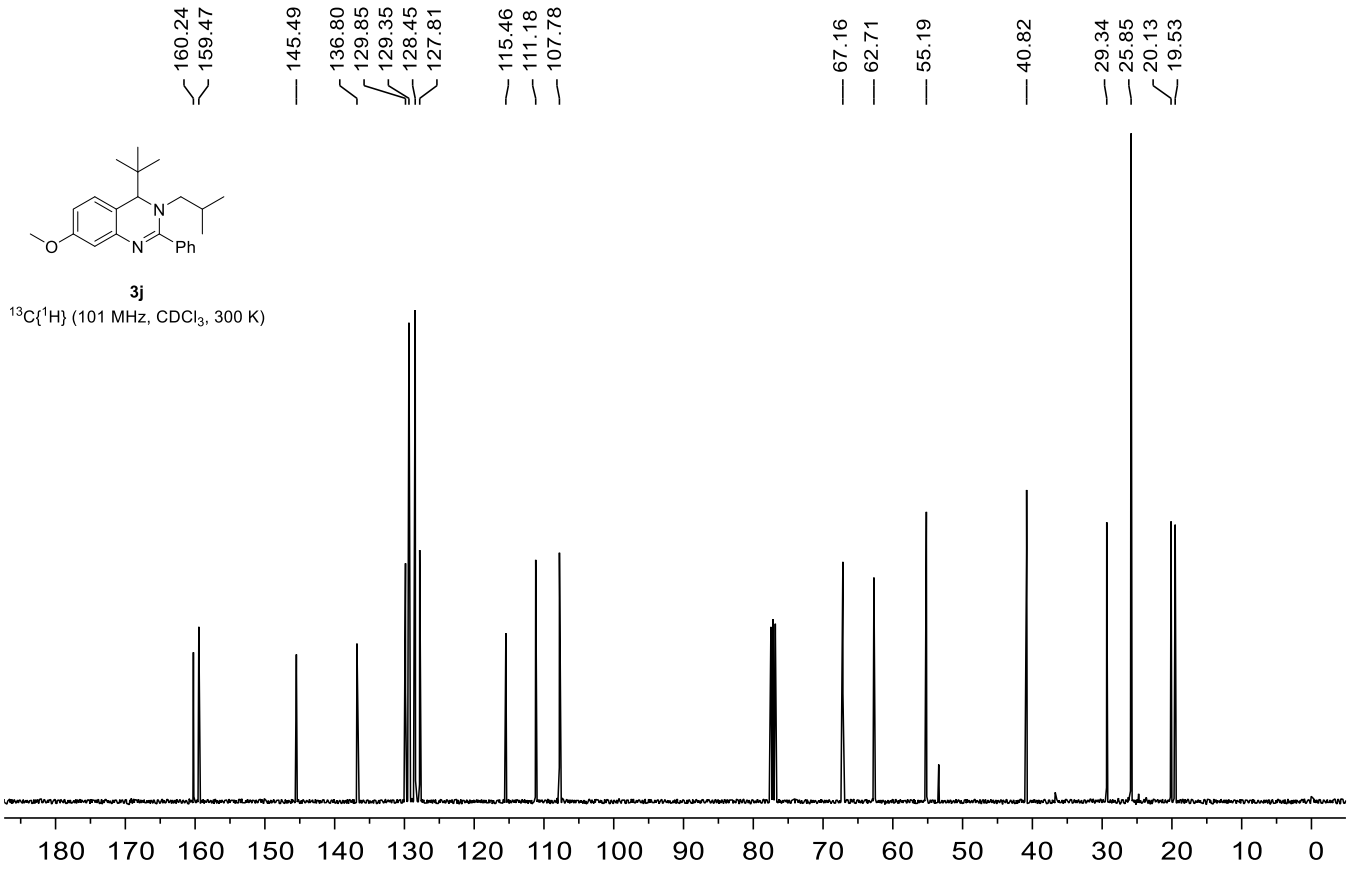
^{1}H (400 MHz, $CDCl_3$, 300 K)

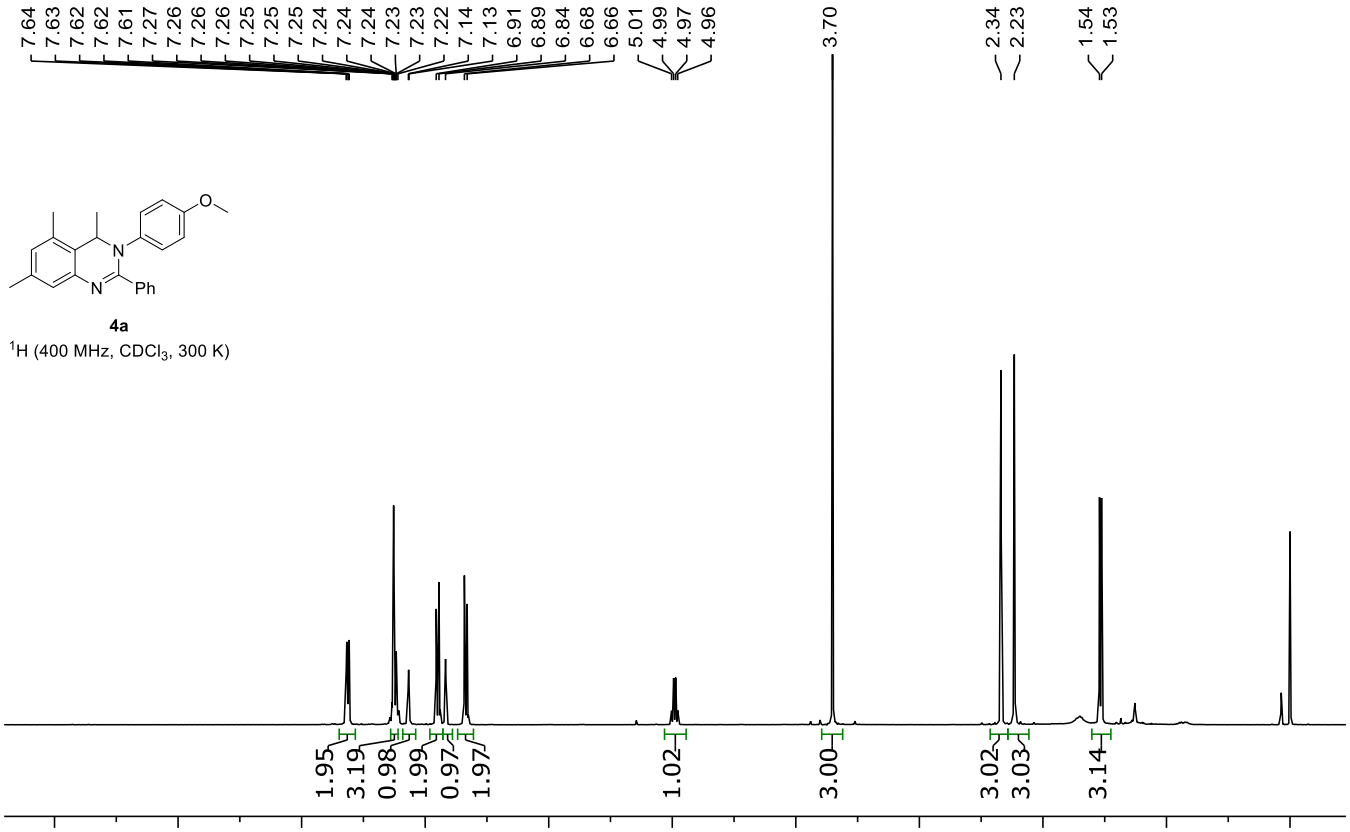


3h

$^{13}C\{^{1}H\}$ (101 MHz, $CDCl_3$, 300 K)

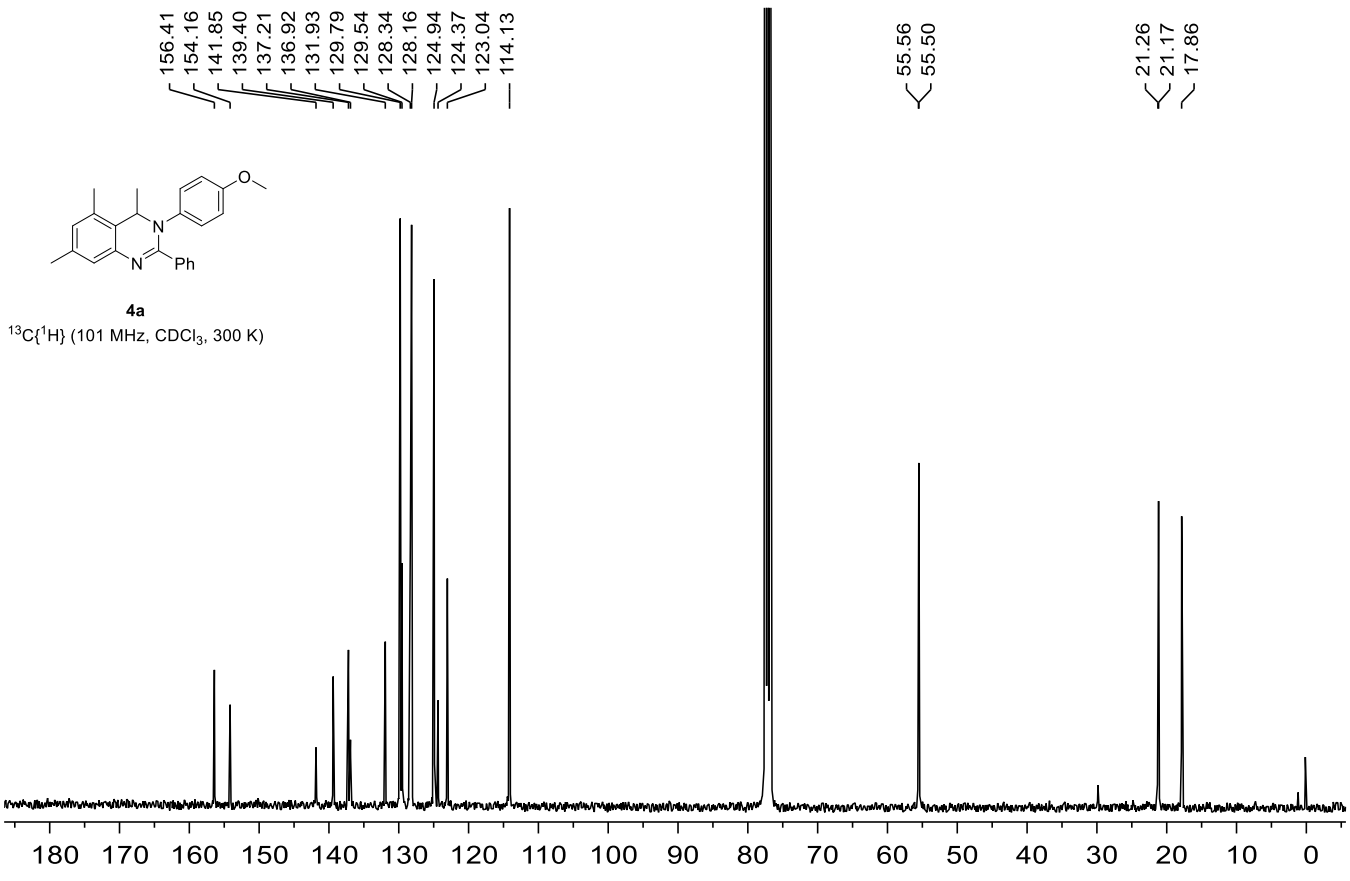

7.76 7.75 7.75 7.75 7.74 7.74 7.74 7.73 7.43 7.43 7.42 7.42 7.41 6.88 6.87 6.85 6.83 6.71 6.71 6.69 6.69 3.97 3.82 3.49 3.47 3.46 3.44 2.99 2.98 2.95 2.94 1.79 1.78 1.77 1.76 1.76 1.75 1.75 1.74 1.74 1.74 1.73 1.72 1.72 1.71 1.71 1.69 0.96 0.67 0.65 0.48 0.47
N
O
N
Ph
3j
1H (400 MHz, CDCl3, 300 K)
1.94 2.93 0.93 0.97 0.97 0.97 2.92 0.98 0.96 1.00 9.00 2.97 3.02
10 9 8 7 6 5 4 3 2 1 0


160.24 159.47 145.49 136.80 129.85 129.35 128.45 127.81 115.46 111.18 107.78 67.16 62.71 55.19 40.82 29.34 25.85 20.13 19.53
N
O
N
Ph
3j
13C{1H} (101 MHz, CDCl3, 300 K)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0



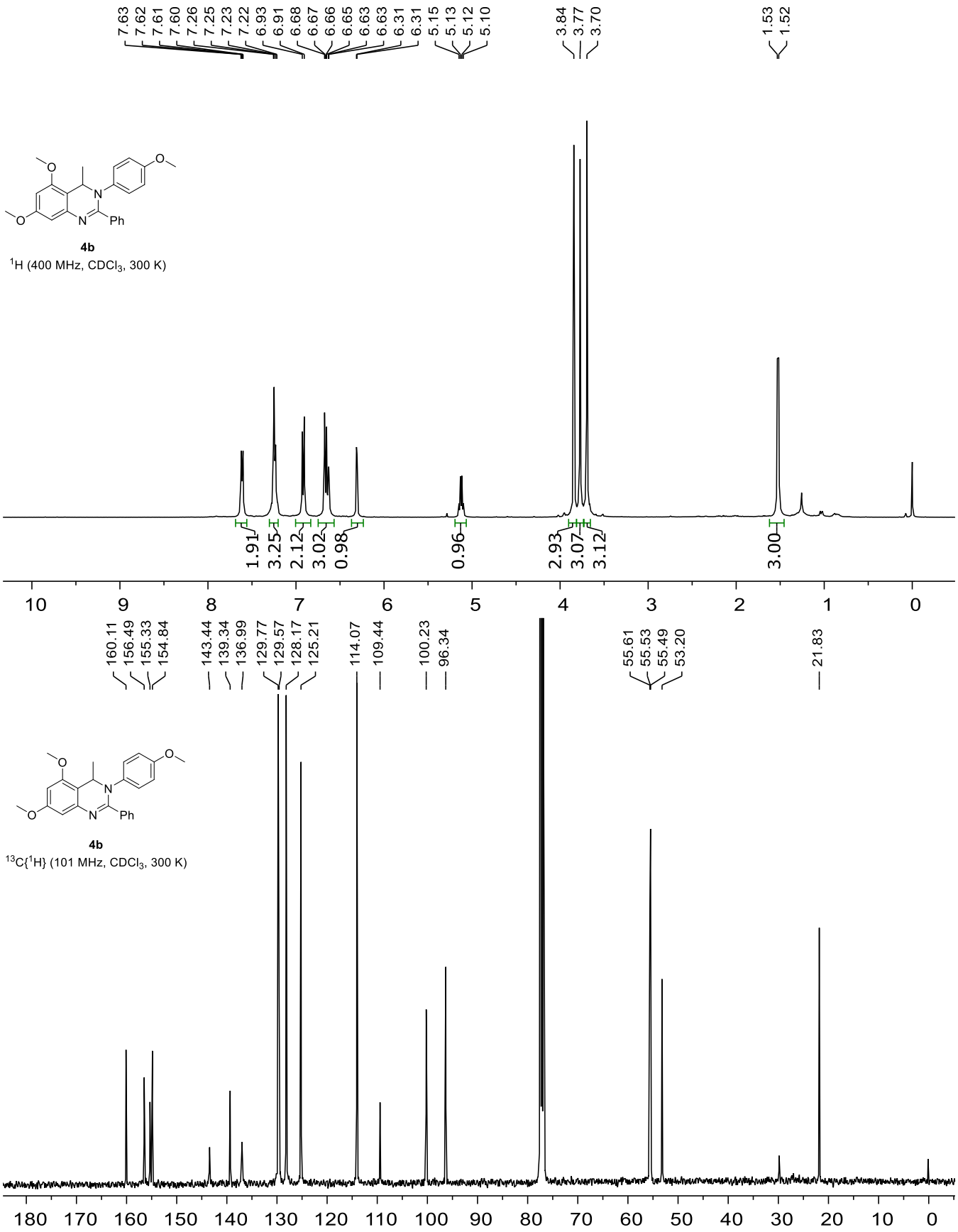
4a

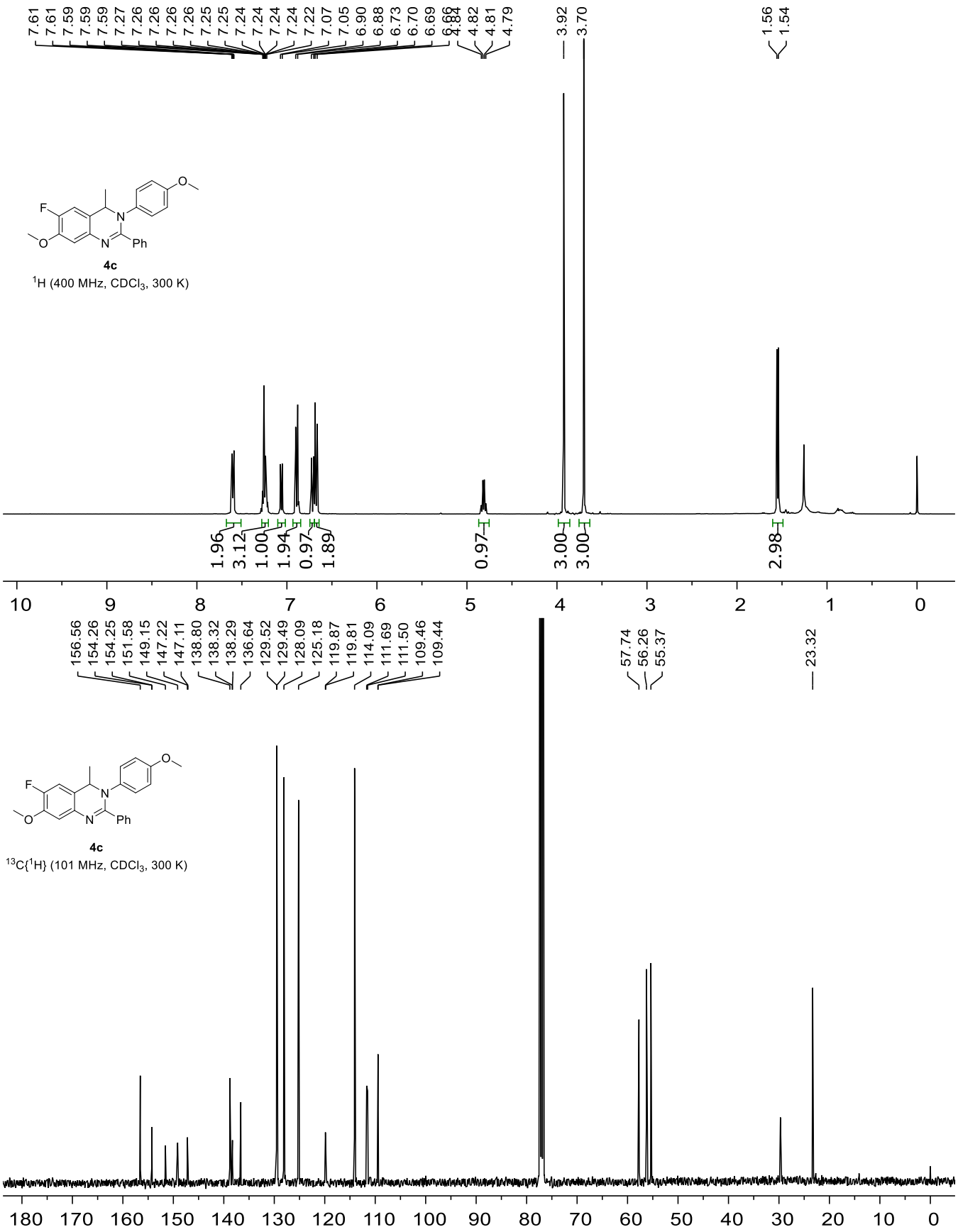
^{1}H (400 MHz, $CDCl_3$, 300 K)



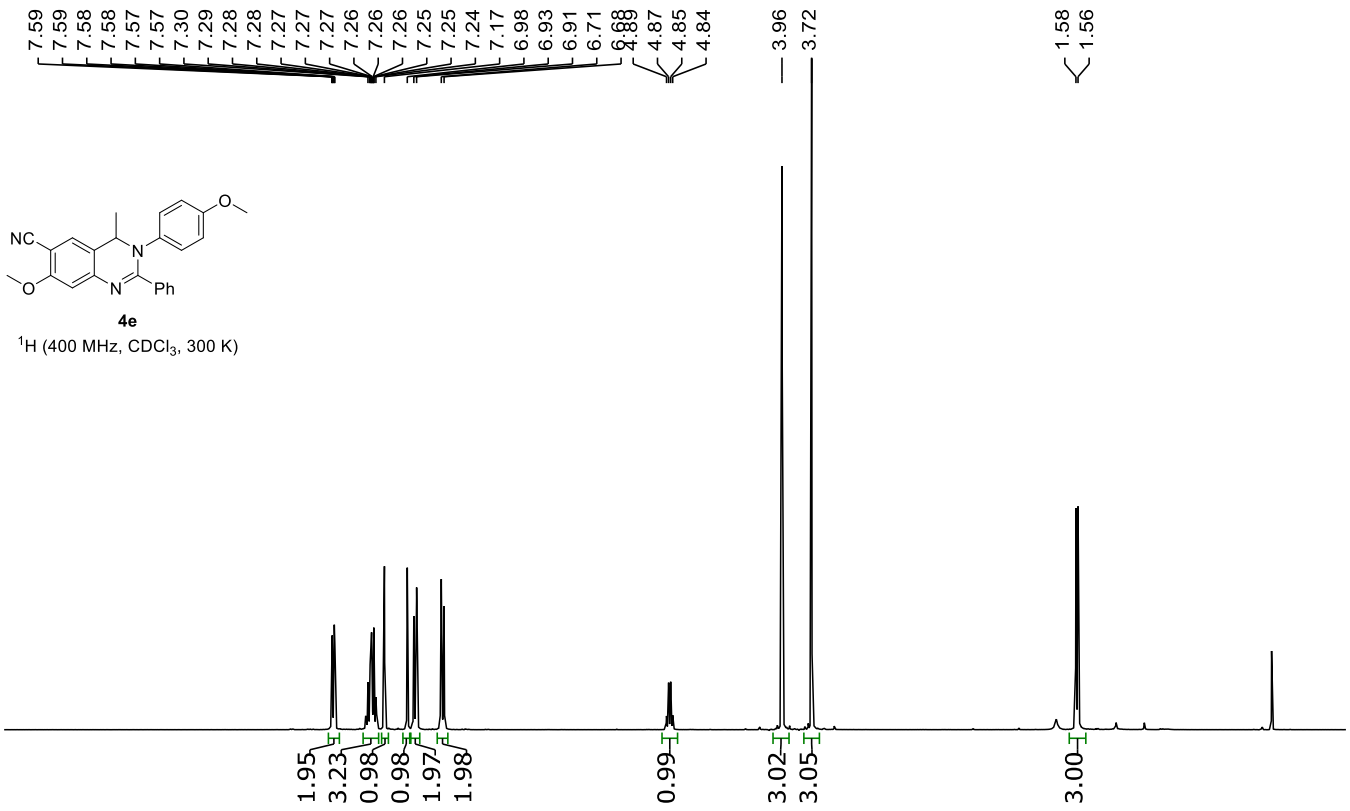
4a

$^{13}C\{^{1}H\}$ (101 MHz, $CDCl_3$, 300 K)


7.63
7.62
7.61
7.60
7.26
7.25
7.23
7.22
6.93
6.91
6.68
6.67
6.66
6.65
6.63
6.63
6.31
6.31
5.15
5.13
5.12
5.10
3.84
3.77
3.70
1.53
1.52
4b
1H (400 MHz, CDCl3, 300 K)
1.91
3.25
2.12
3.02
0.98
0.96
2.93
3.07
3.12
3.00
10
9
8
7
6
5
4
3
2
1
0
160.11
156.49
155.33
154.84
143.44
139.34
136.99
129.77
129.57
128.17
125.21
114.07
109.44
100.23
96.34
55.61
55.53
55.49
53.20
21.83
4b
13C{1H} (101 MHz, CDCl3, 300 K)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

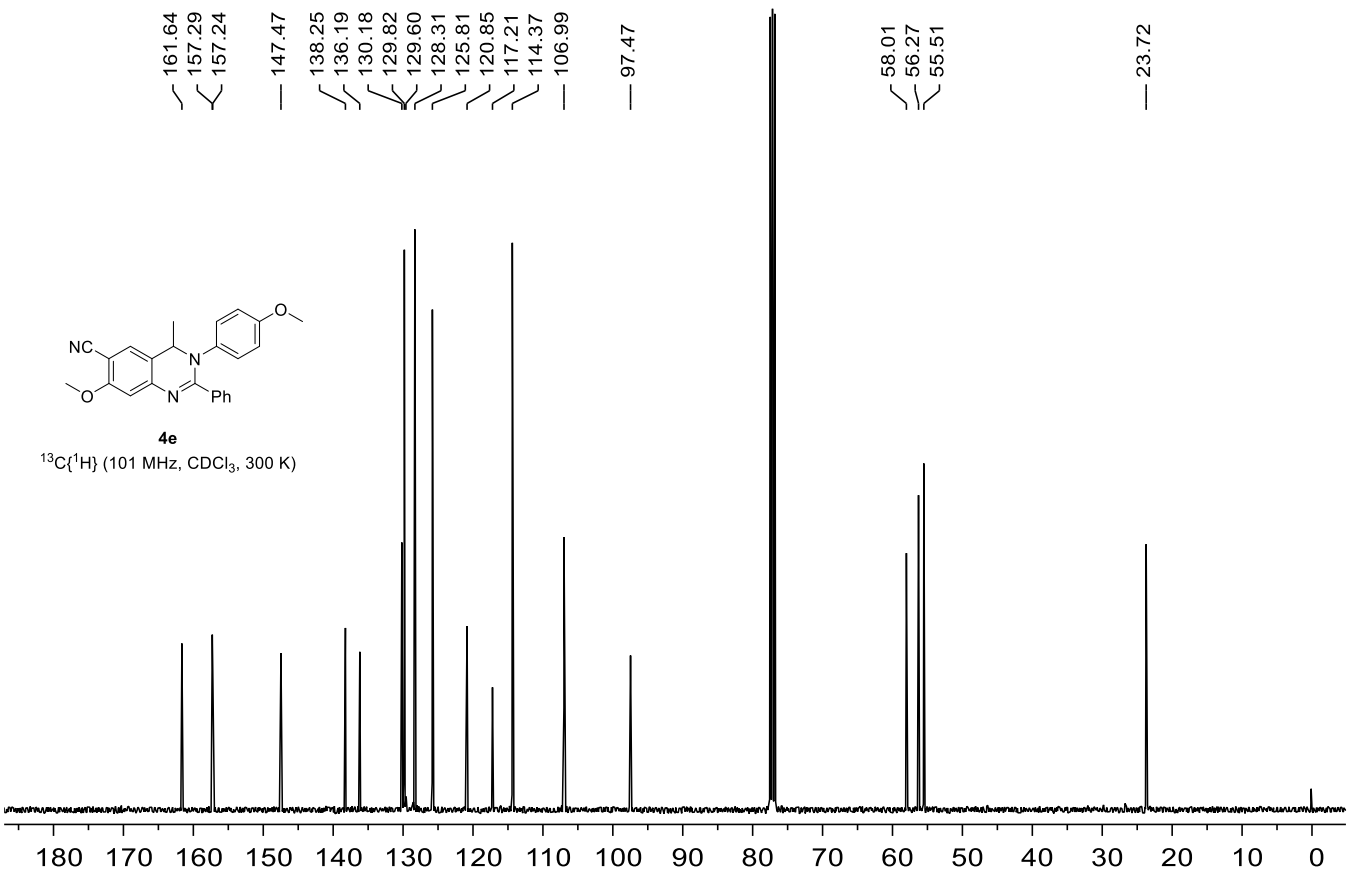

7.61 7.61 7.59 7.59 7.59 7.27 7.26 7.26 7.26 7.26 7.25 7.24 7.24 7.24 7.24 7.22 7.07 7.05 6.90 6.88 6.73 6.70 6.69 6.66 4.84 4.82 4.81 4.79
3.92 3.70
1.56 1.54
1.96 3.12 1.00 1.94 0.97 1.89 0.97 3.00 3.00 2.98
10 9 8 7 6 5 4 3 2 1 0
F O O N N Ph
4c
1H (400 MHz, CDCl3, 300 K)
156.56 154.26 154.25 151.58 149.15 147.22 147.11 138.80 138.32 138.29 136.64 129.52 129.49 128.09 125.18 119.87 119.81 114.09 111.69 111.50 109.46 109.44
57.74 56.26 55.37
23.32
F O O N N Ph
4c
13C{1H} (101 MHz, CDCl3, 300 K)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


7.61
7.61
7.59
7.59
7.59
7.28
7.27
7.27
7.26
7.26
7.25
7.25
7.24
7.24
7.24
7.23
7.23
7.23
7.22
7.22
7.04
6.98
6.90
6.88
6.69
6.66
4.85
4.84
4.82
4.80
3.94
3.70
1.56
1.54
Cl
O
N
O
N
Ph
4d
1H (400 MHz, CDCl3, 300 K)
1.93
3.28
1.00
0.98
1.93
1.94
0.98
3.09
3.10
3.00
10
9
8
7
6
5
4
3
2
1
0
156.81
155.18
154.73
141.68
138.79
136.61
129.75
129.70
128.23
125.73
125.44
120.99
118.63
114.24
108.27
57.91
56.39
55.49
23.61
Cl
O
N
O
N
Ph
4d
13C{1H} (101 MHz, CDCl3, 300 K)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



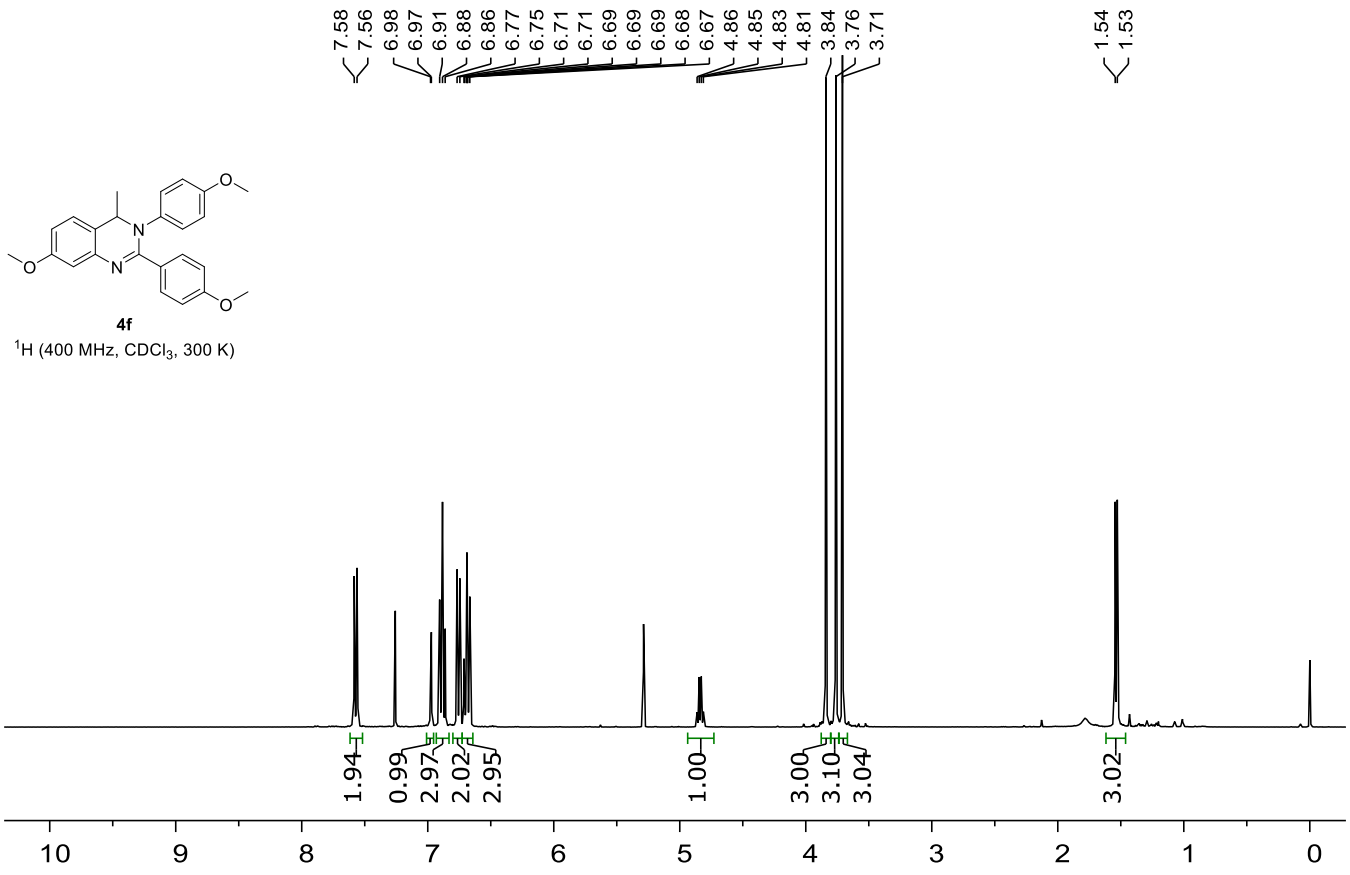
4e

^{1}H (400 MHz, $CDCl_3$, 300 K)



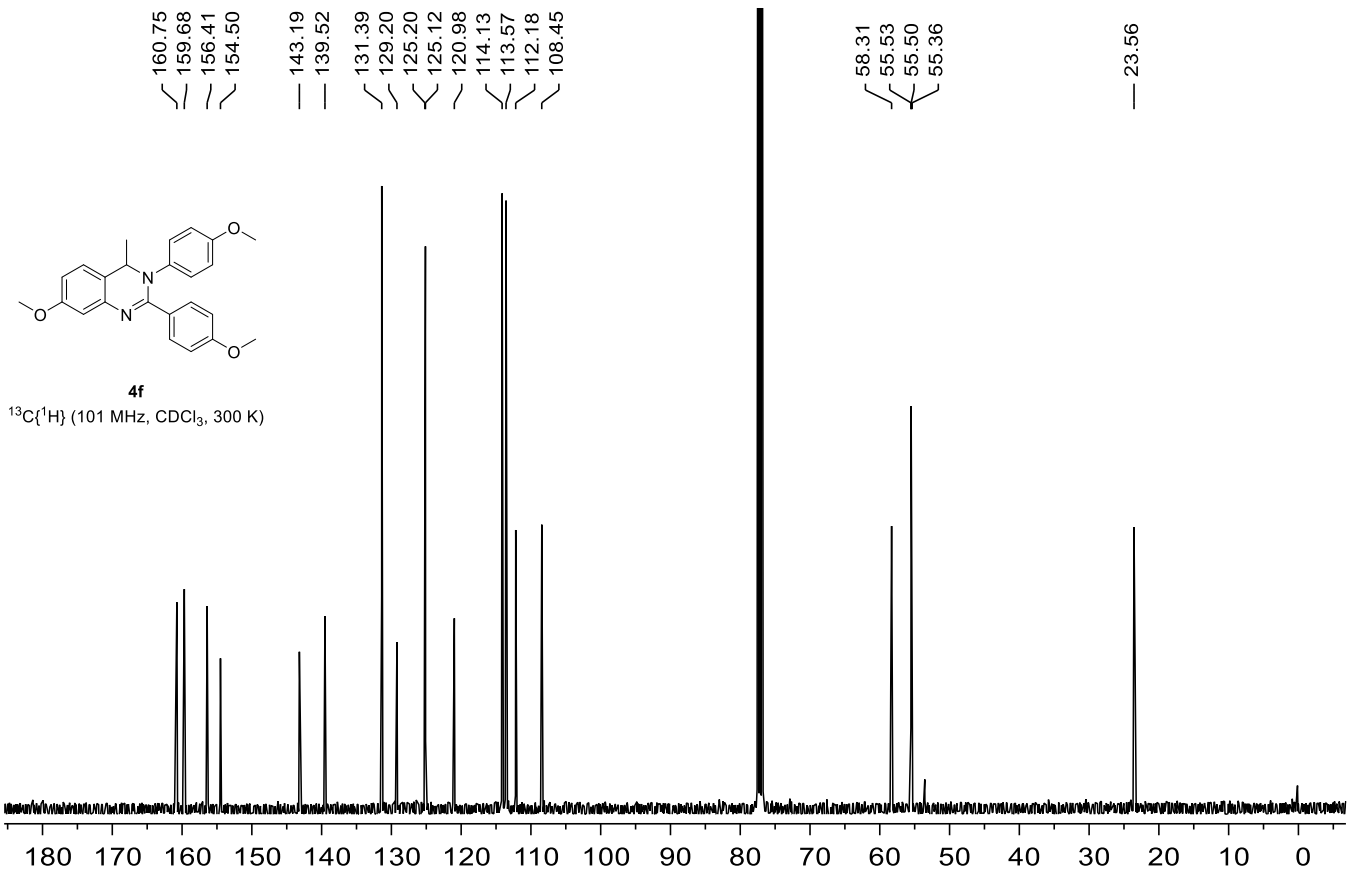
4e

$^{13}C\{^{1}H\}$ (101 MHz, $CDCl_3$, 300 K)



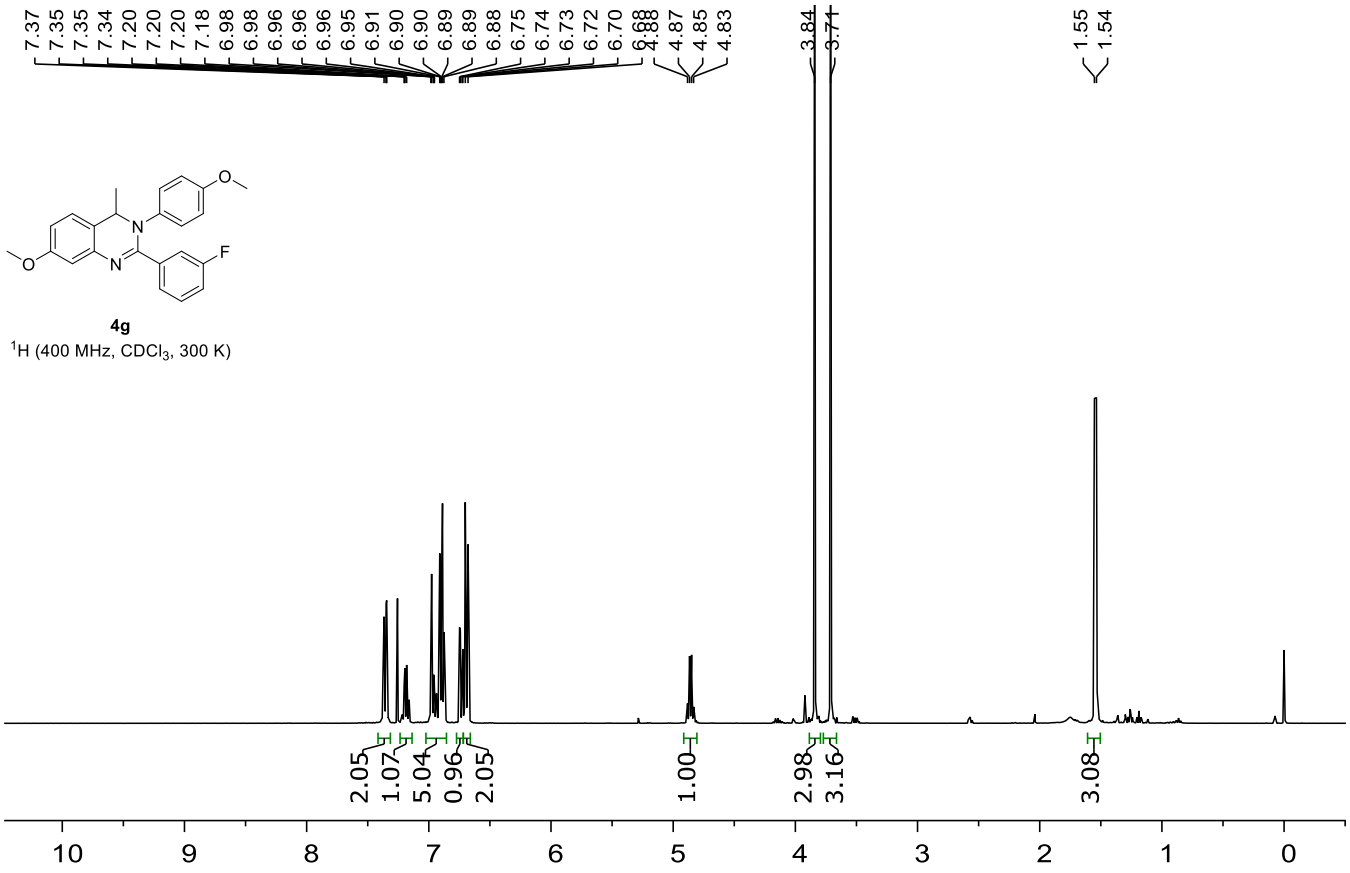
4f

^{1}H (400 MHz, $CDCl_3$, 300 K)



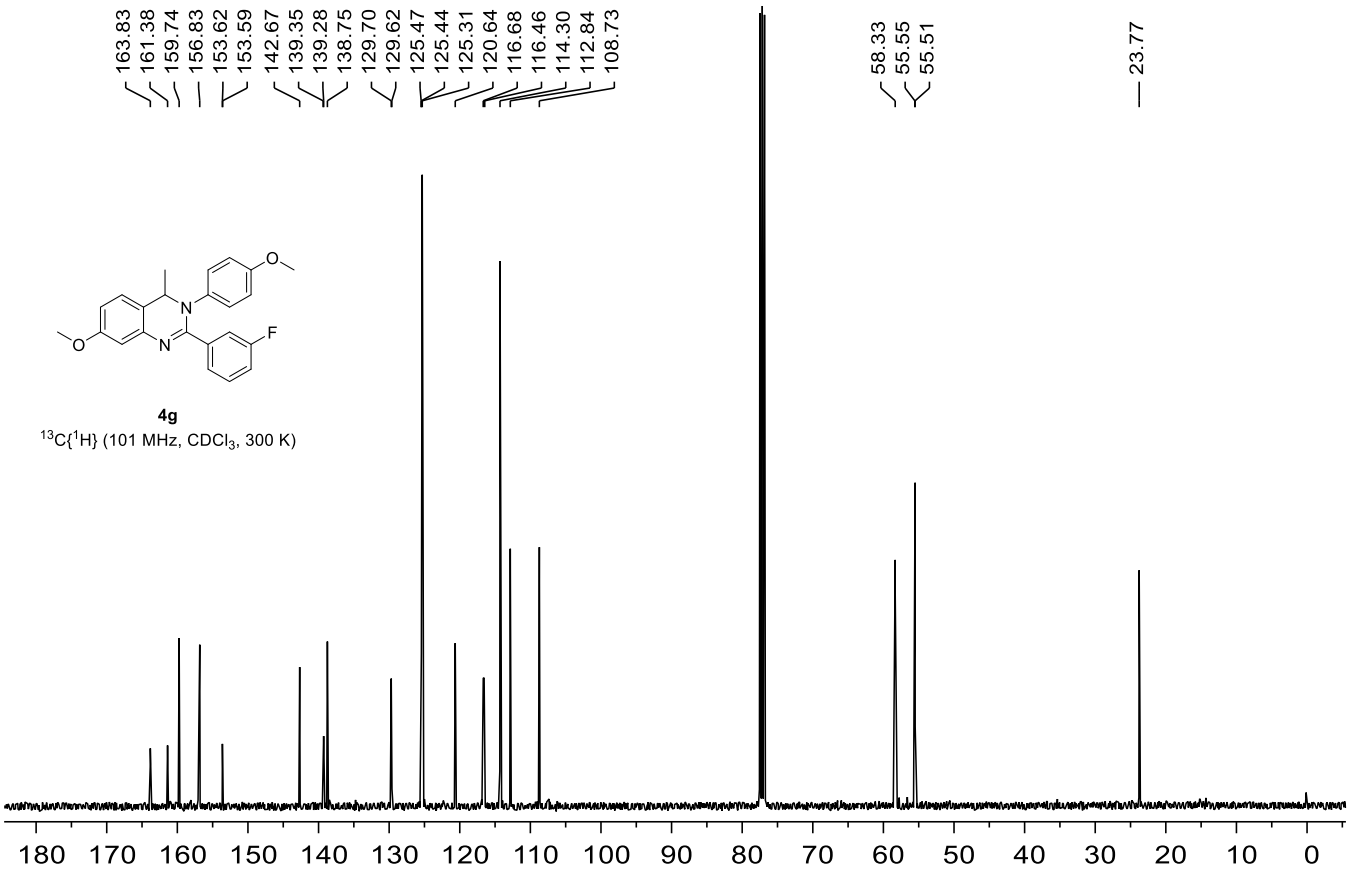
4f

$^{13}C\{^{1}H\}$ (101 MHz, $CDCl_3$, 300 K)



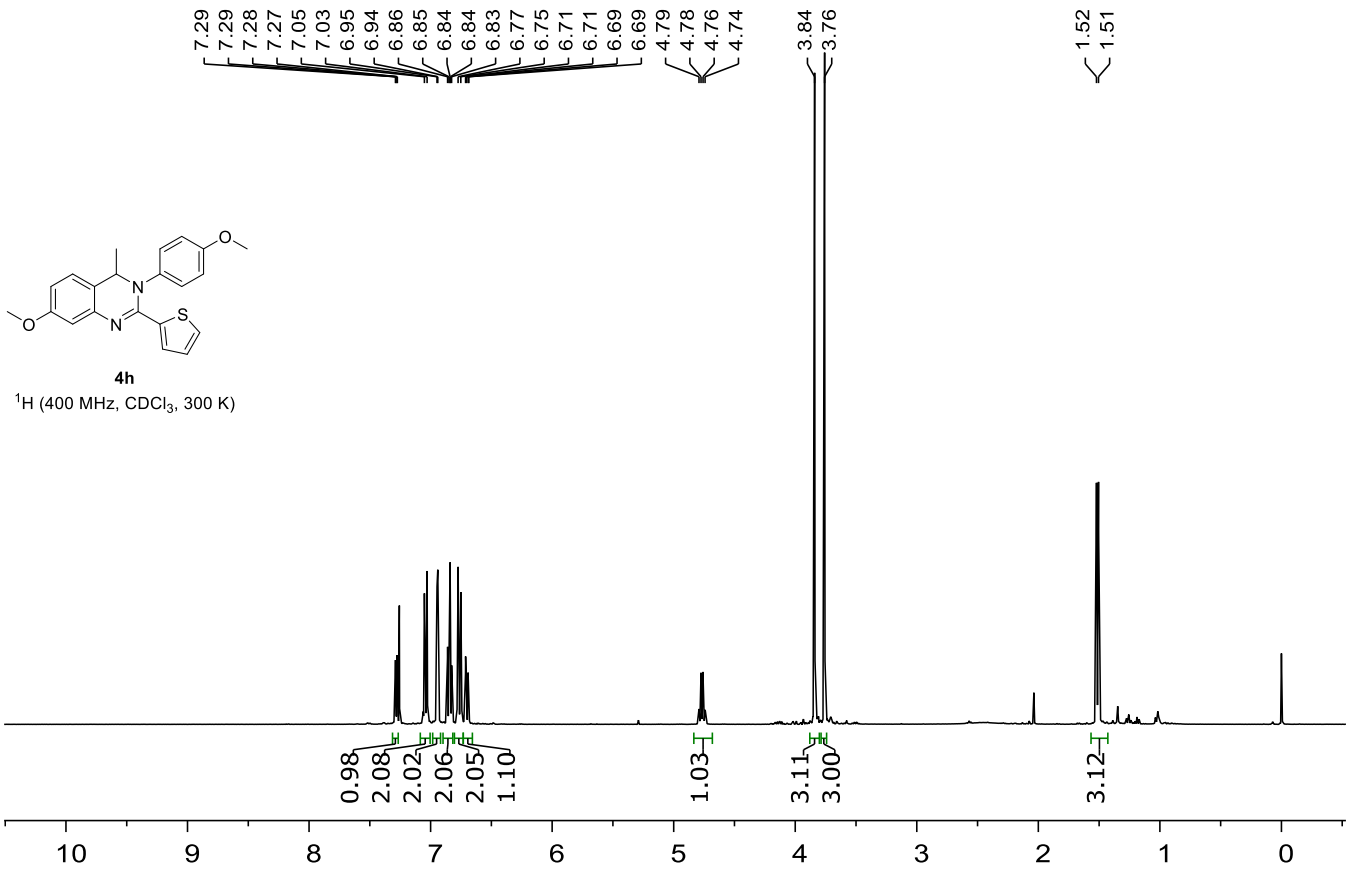
4g

^{1}H (400 MHz, $CDCl_3$, 300 K)



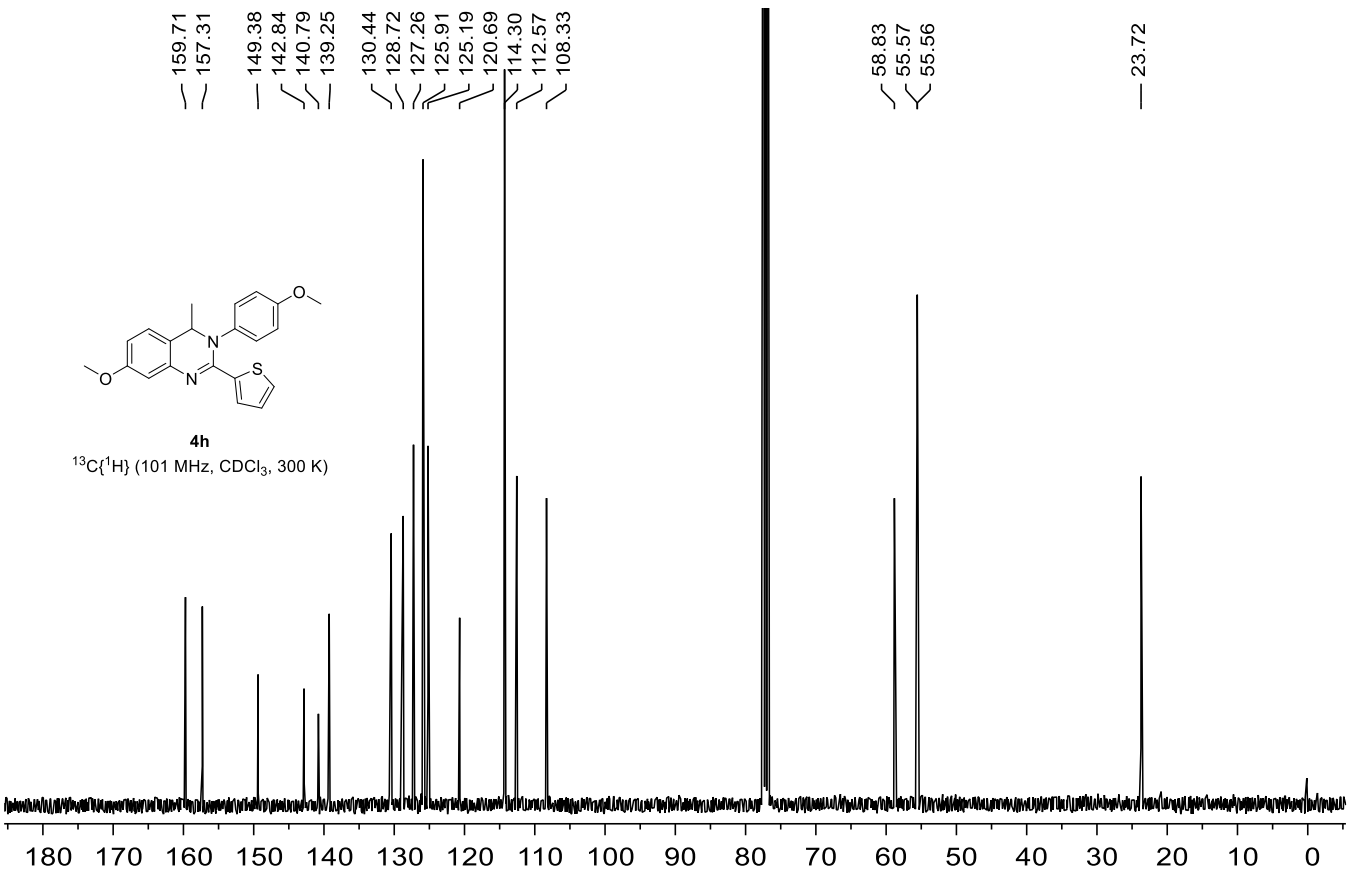
4g

$^{13}C\{^{1}H\}$ (101 MHz, $CDCl_3$, 300 K)



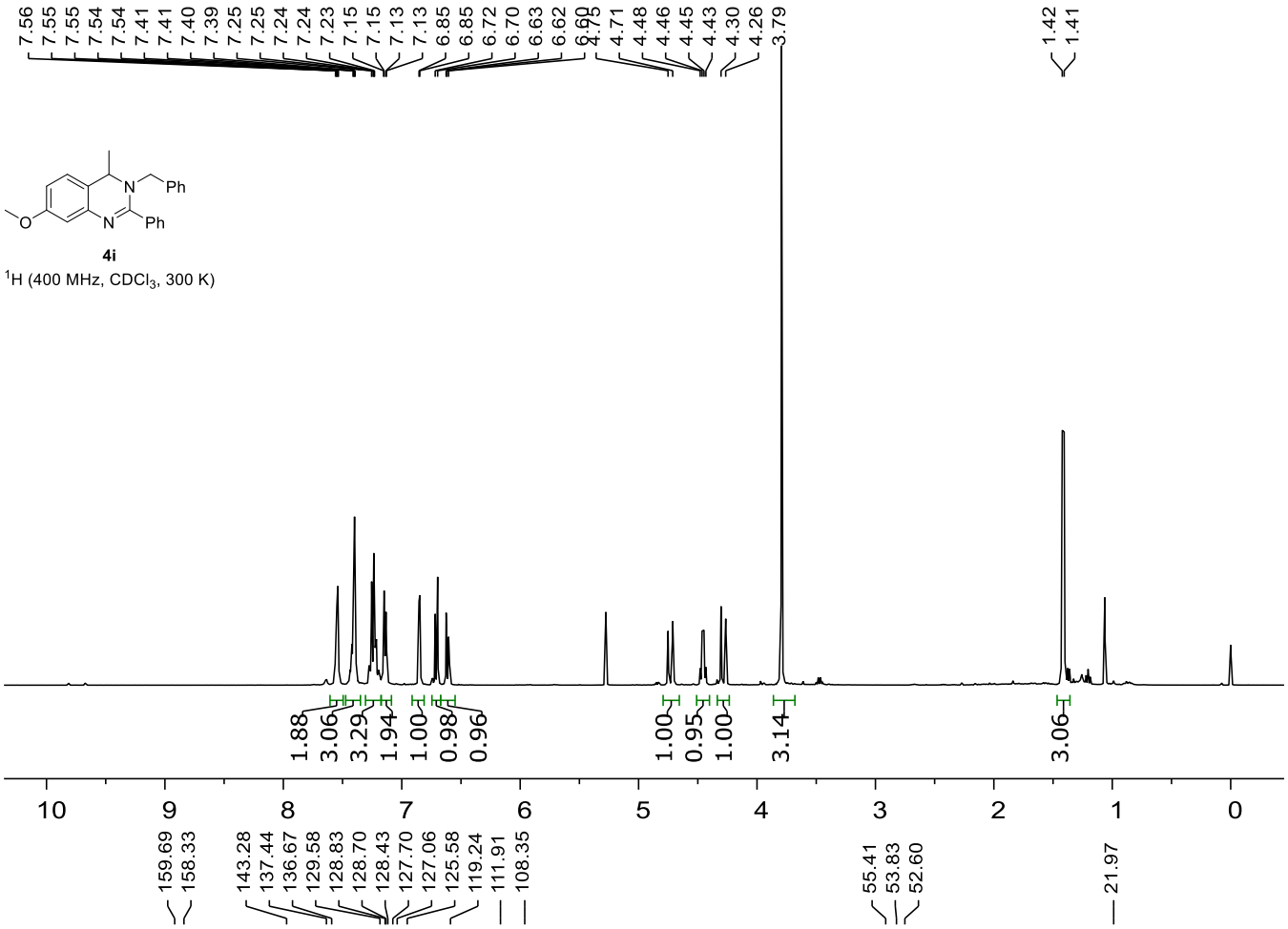
4h

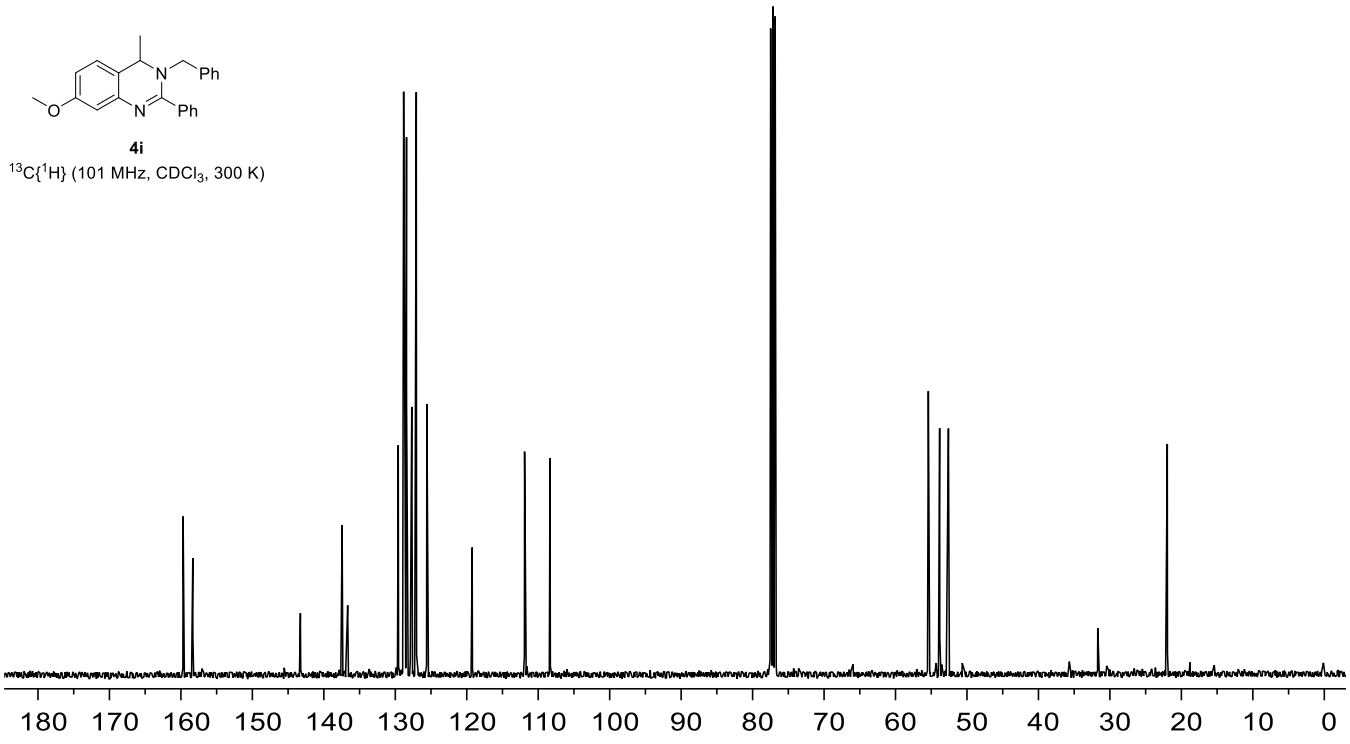
^{1}H (400 MHz, $CDCl_3$, 300 K)

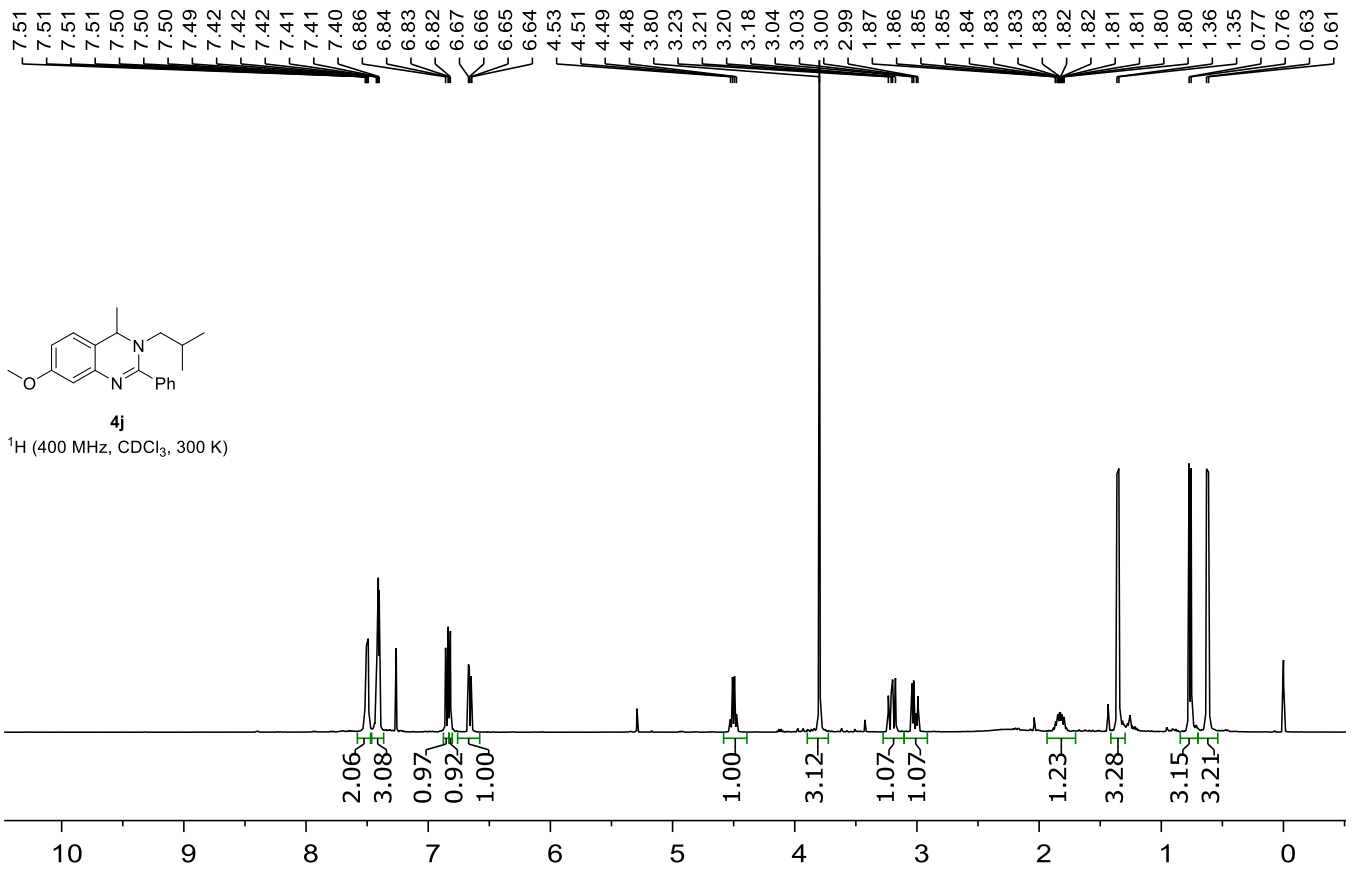


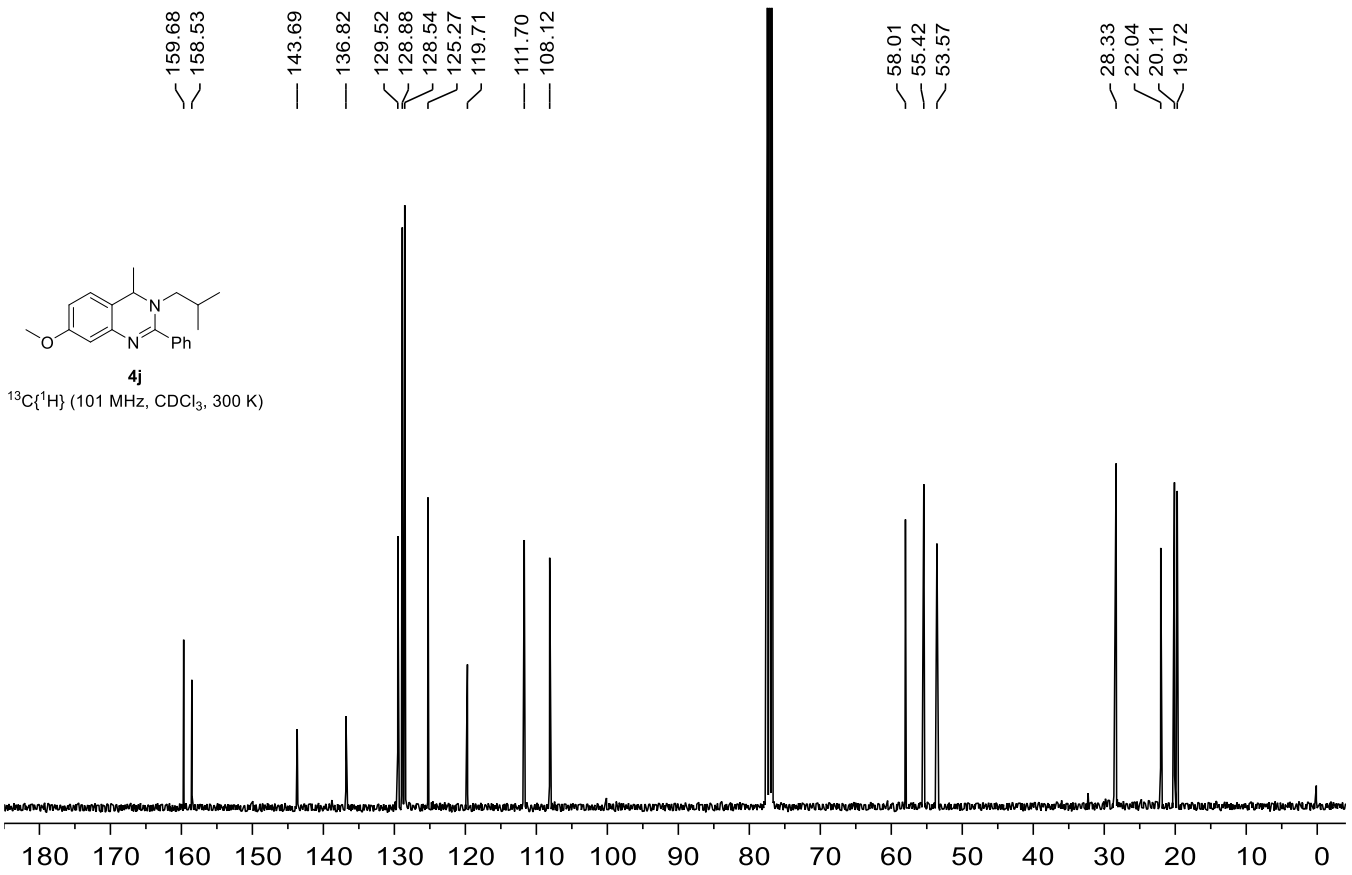
4h

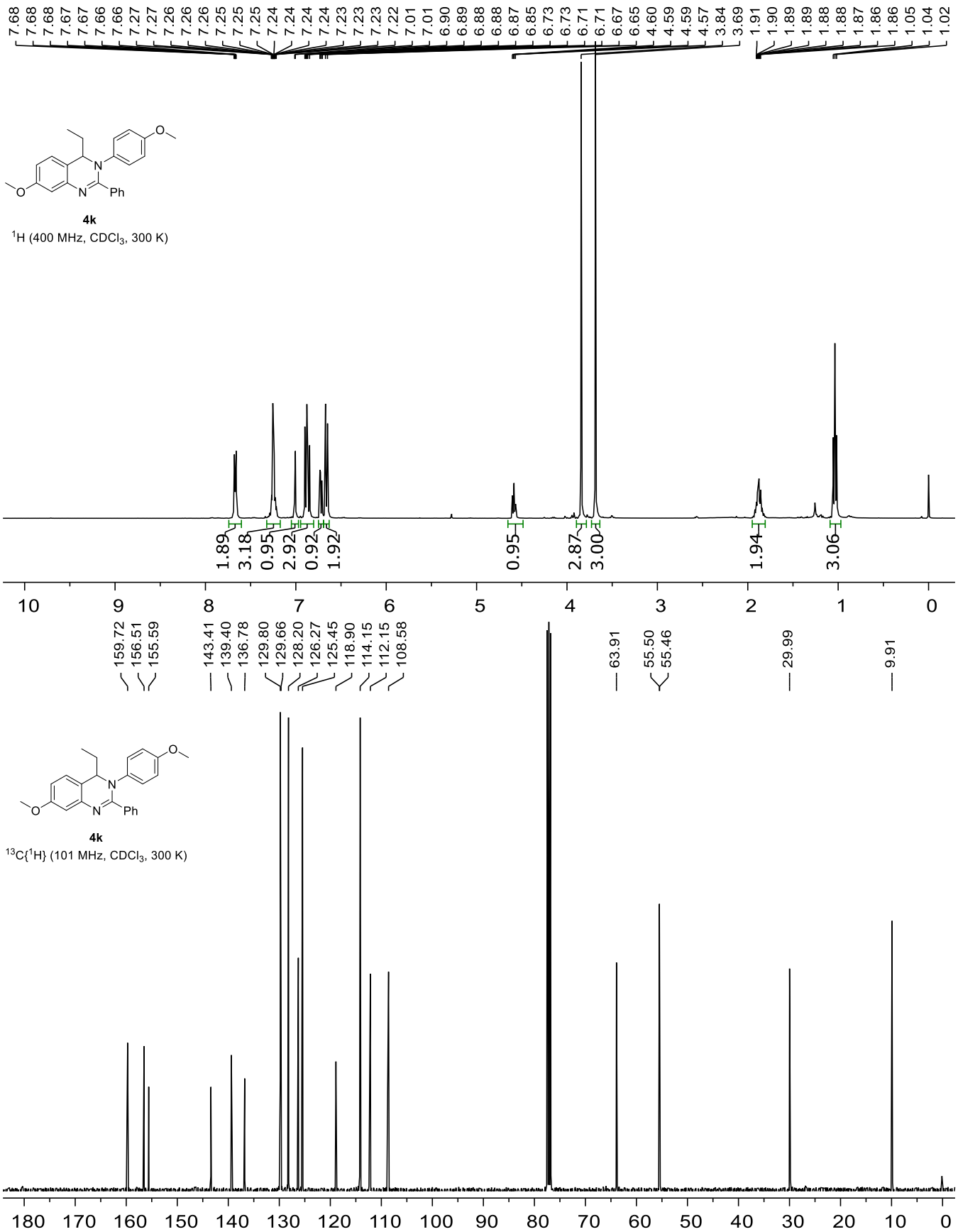
$^{13}C\{^{1}H\}$ (101 MHz, $CDCl_3$, 300 K)

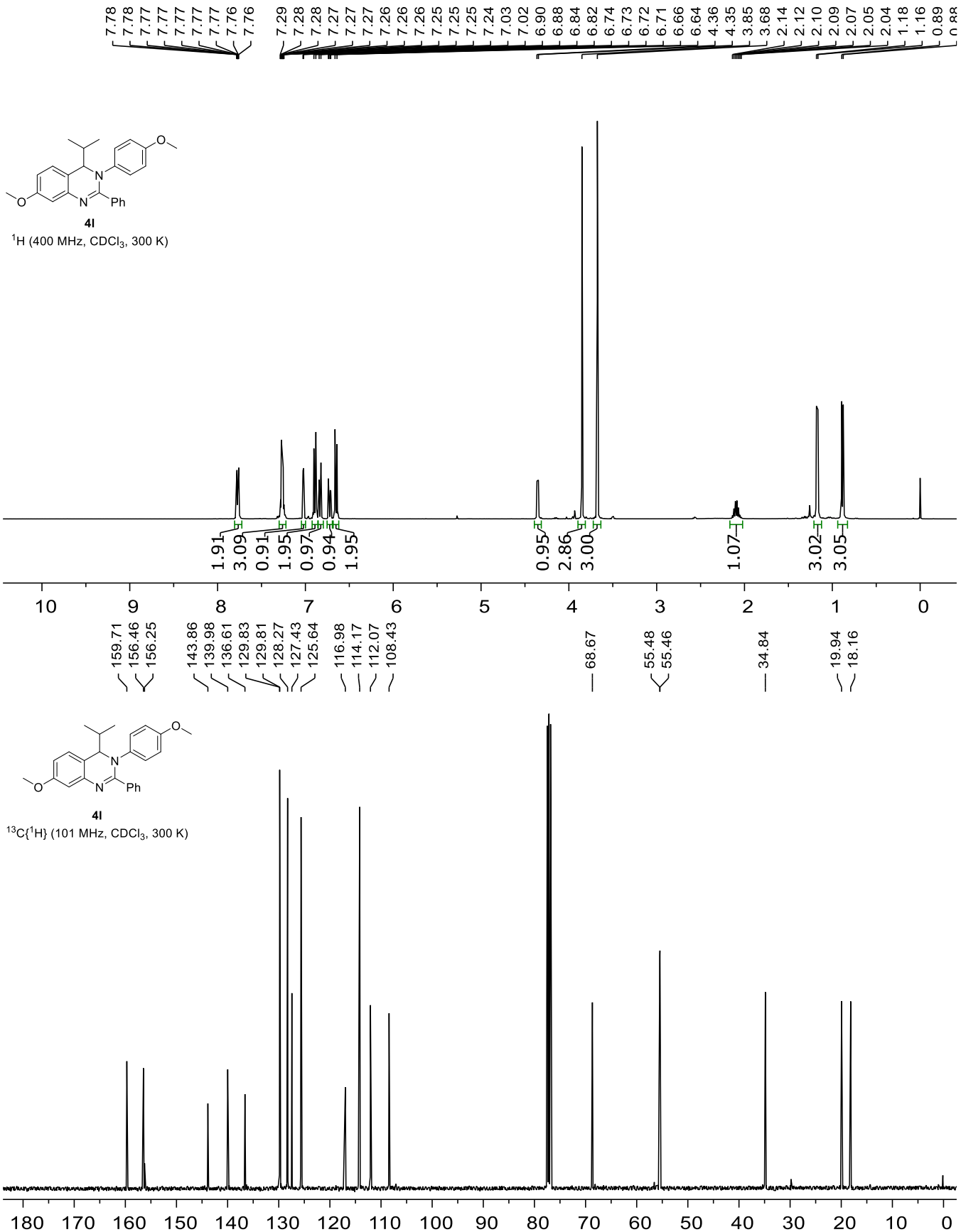

7.56
7.55
7.55
7.54
7.54
7.41
7.41
7.40
7.39
7.25
7.25
7.24
7.24
7.23
7.15
7.15
7.13
7.13
6.85
6.85
6.72
6.70
6.63
6.62
6.60
4.75
4.71
4.48
4.46
4.45
4.43
4.30
4.26
3.79
1.42
1.41
Ph
N
Ph
N
O
4i
1H (400 MHz, CDCl3, 300 K)
1.88
3.06
3.29
1.94
1.00
0.98
0.96
1.00
0.95
1.00
3.14
3.06
10
9
8
7
6
5
4
3
2
1
0

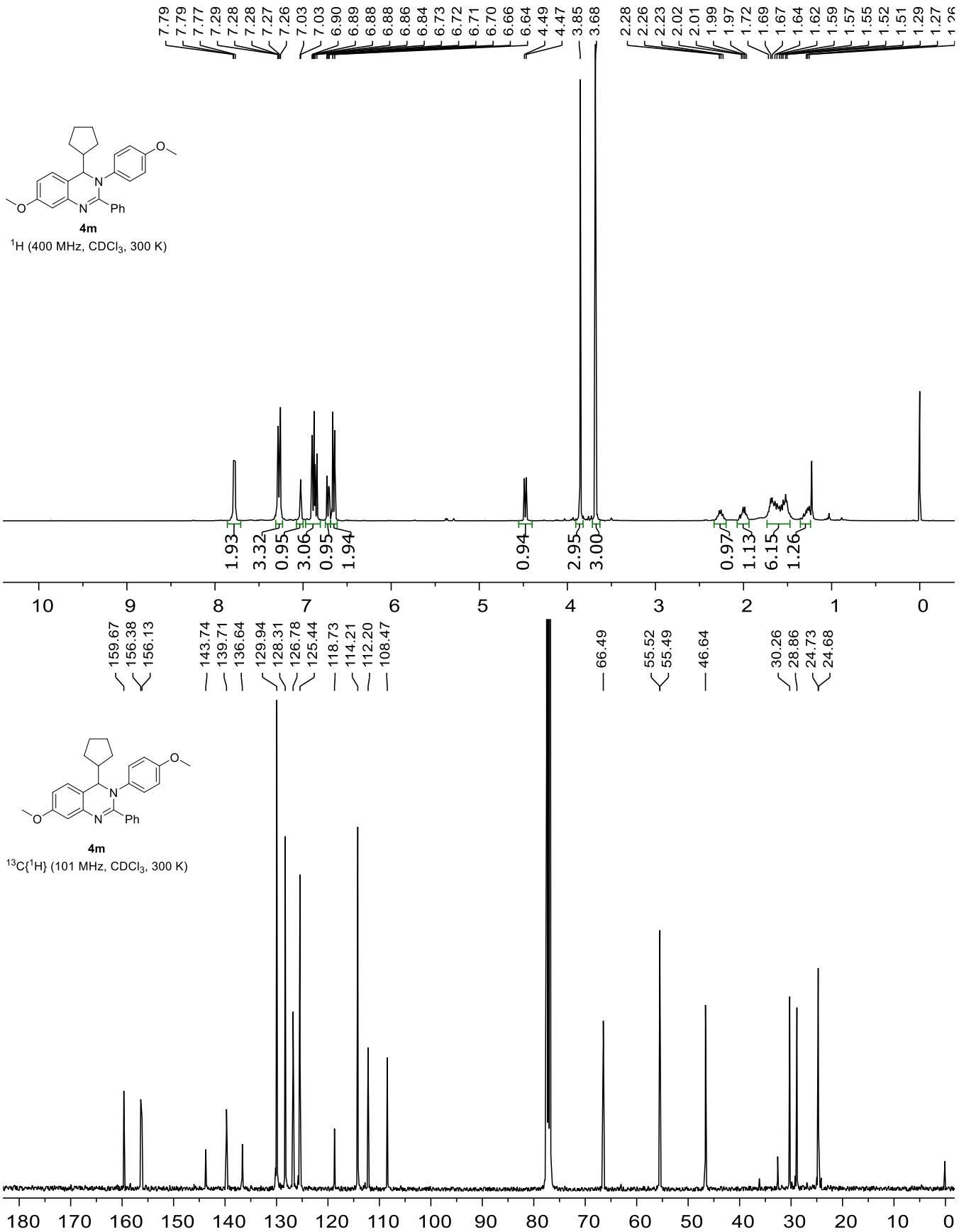

159.69
158.33
143.28
137.44
136.67
129.58
128.83
128.70
128.43
127.70
127.06
125.58
119.24
111.91
108.35
55.41
53.83
52.60
21.97
Ph
N
Ph
N
O
4i
13C{1H} (101 MHz, CDCl3, 300 K)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

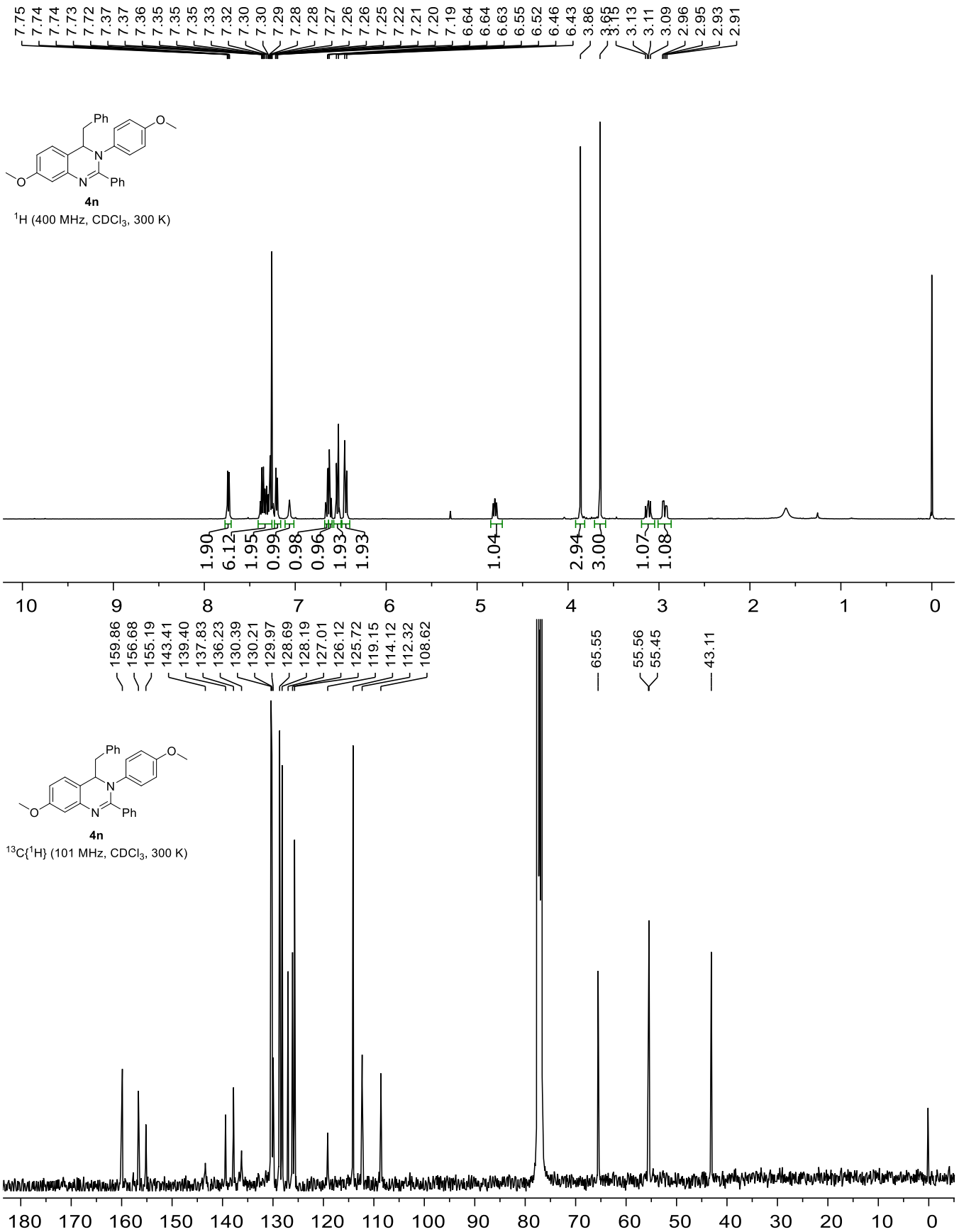

7.51 7.51 7.51 7.51 7.50 7.50 7.50 7.49 7.42 7.42 7.42 7.41 7.41 7.40 6.86 6.84 6.83 6.82 6.67 6.66 6.65 6.64 4.53 4.51 4.49 4.48 3.80 3.23 3.21 3.20 3.18 3.04 3.03 3.00 2.99 1.87 1.86 1.85 1.85 1.84 1.83 1.83 1.83 1.82 1.82 1.81 1.81 1.80 1.80 1.36 1.35 0.77 0.76 0.63 0.61
N
O
N
Ph
4j
1H (400 MHz, CDCl3, 300 K)
2.06 3.08 0.97 0.92 1.00 1.00 3.12 1.07 1.07 1.23 3.28 3.15 3.21
10 9 8 7 6 5 4 3 2 1 0

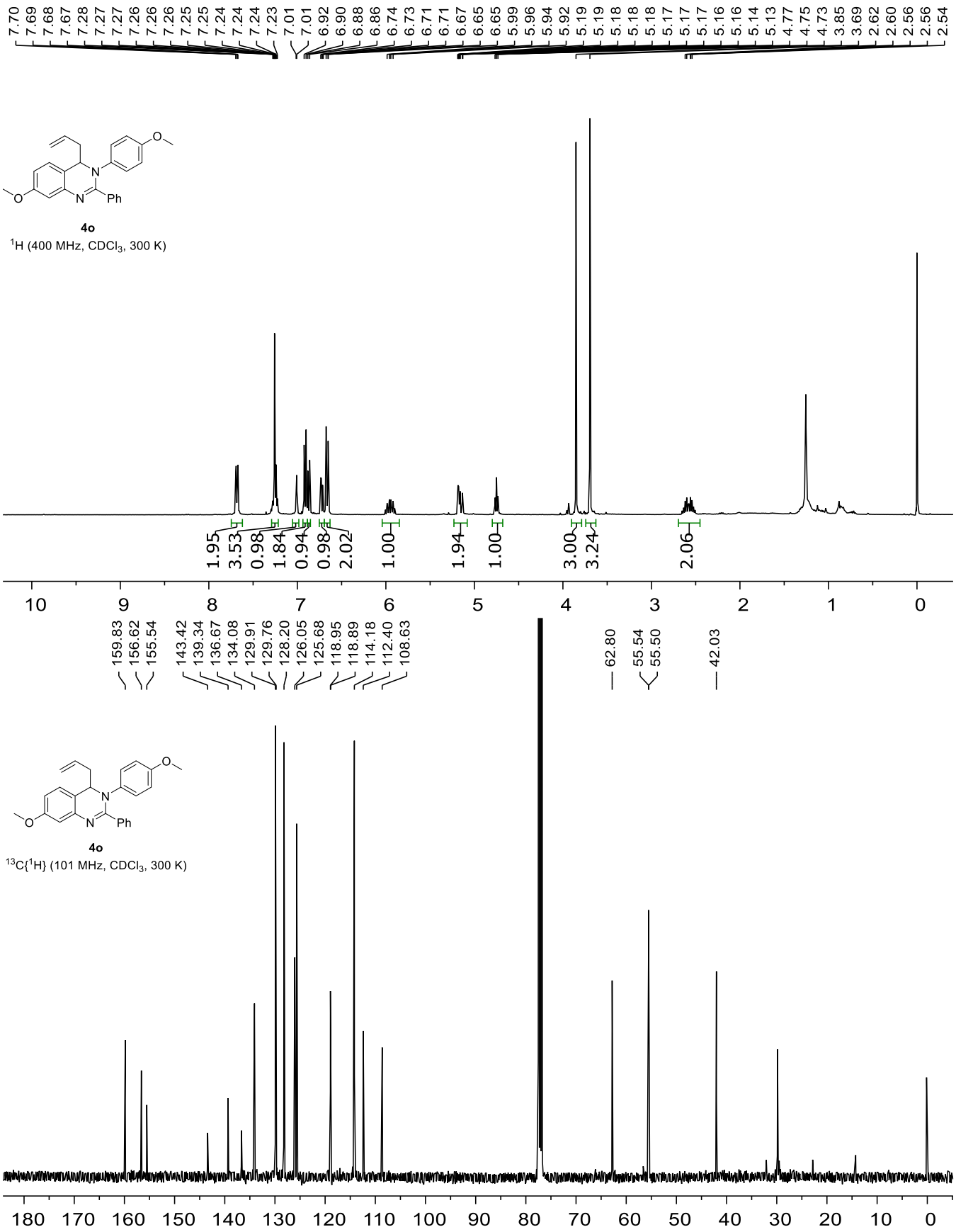

159.68 158.53 143.69 136.82 129.52 128.88 128.54 125.27 119.71 111.70 108.12 58.01 55.42 53.57 28.33 22.04 20.11 19.72
N
O
N
Ph
4j
13C{1H} (101 MHz, CDCl3, 300 K)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

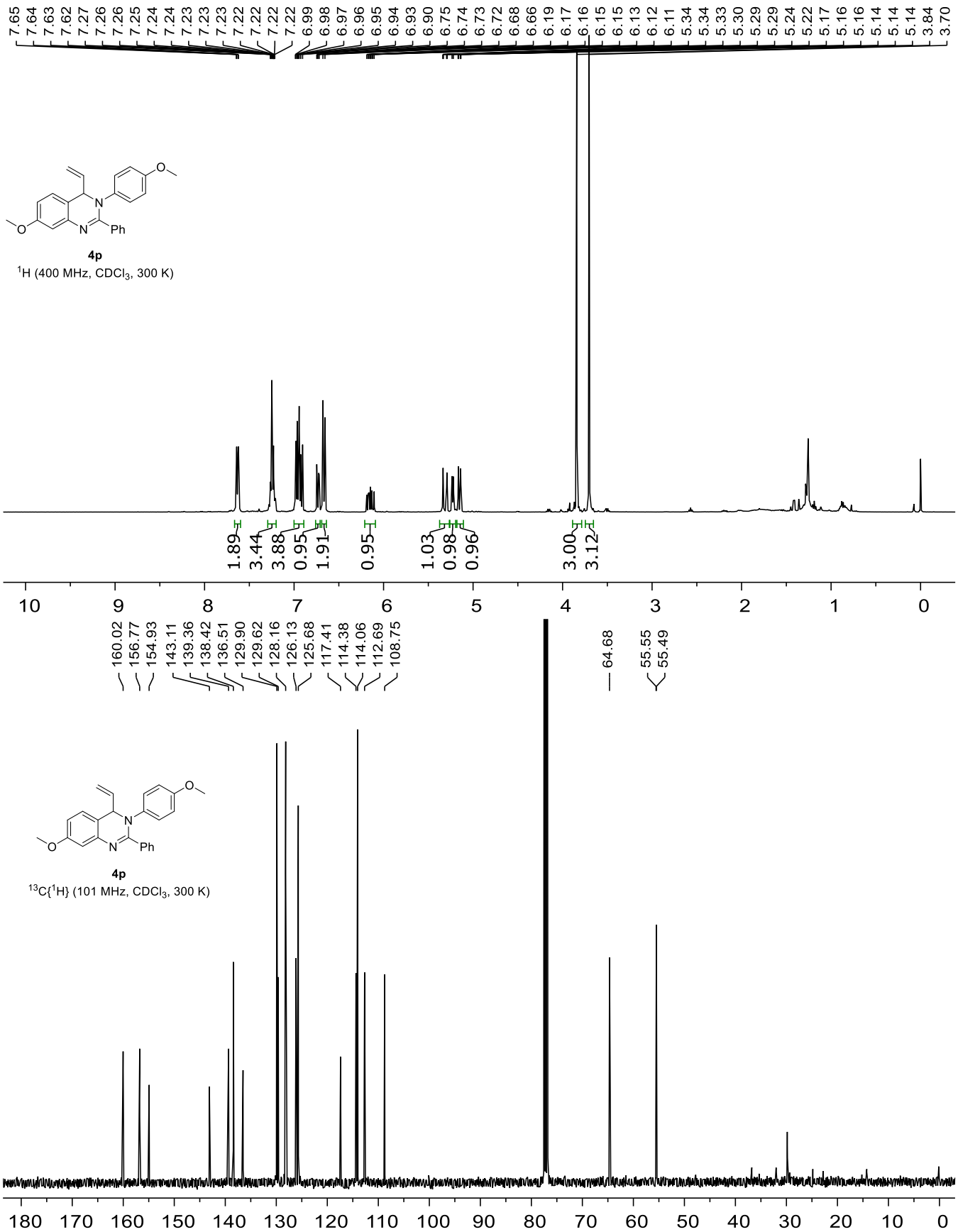

7.68 7.68 7.68 7.67 7.67 7.66 7.66 7.27 7.27 7.26 7.26 7.26 7.25 7.25 7.25 7.24 7.24 7.24 7.24 7.23 7.23 7.23 7.22 7.01 7.01 6.90 6.89 6.88 6.88 6.87 6.85 6.73 6.73 6.71 6.71 6.67 6.65 4.60 4.59 4.59 4.57 3.84 3.69 1.91 1.90 1.89 1.89 1.88 1.88 1.87 1.86 1.86 1.05 1.04 1.02
4k
1H (400 MHz, CDCl3, 300 K)
1.89 3.18 0.95 2.92 0.92 1.92 0.95 2.87 3.00 1.94 3.06
10 9 8 7 6 5 4 3 2 1 0
159.72 156.51 155.59 143.41 139.40 136.78 129.80 129.66 128.20 126.27 125.45 118.90 114.15 112.15 108.58 63.91 55.50 55.46 29.99 9.91
4k
13C{1H} (101 MHz, CDCl3, 300 K)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

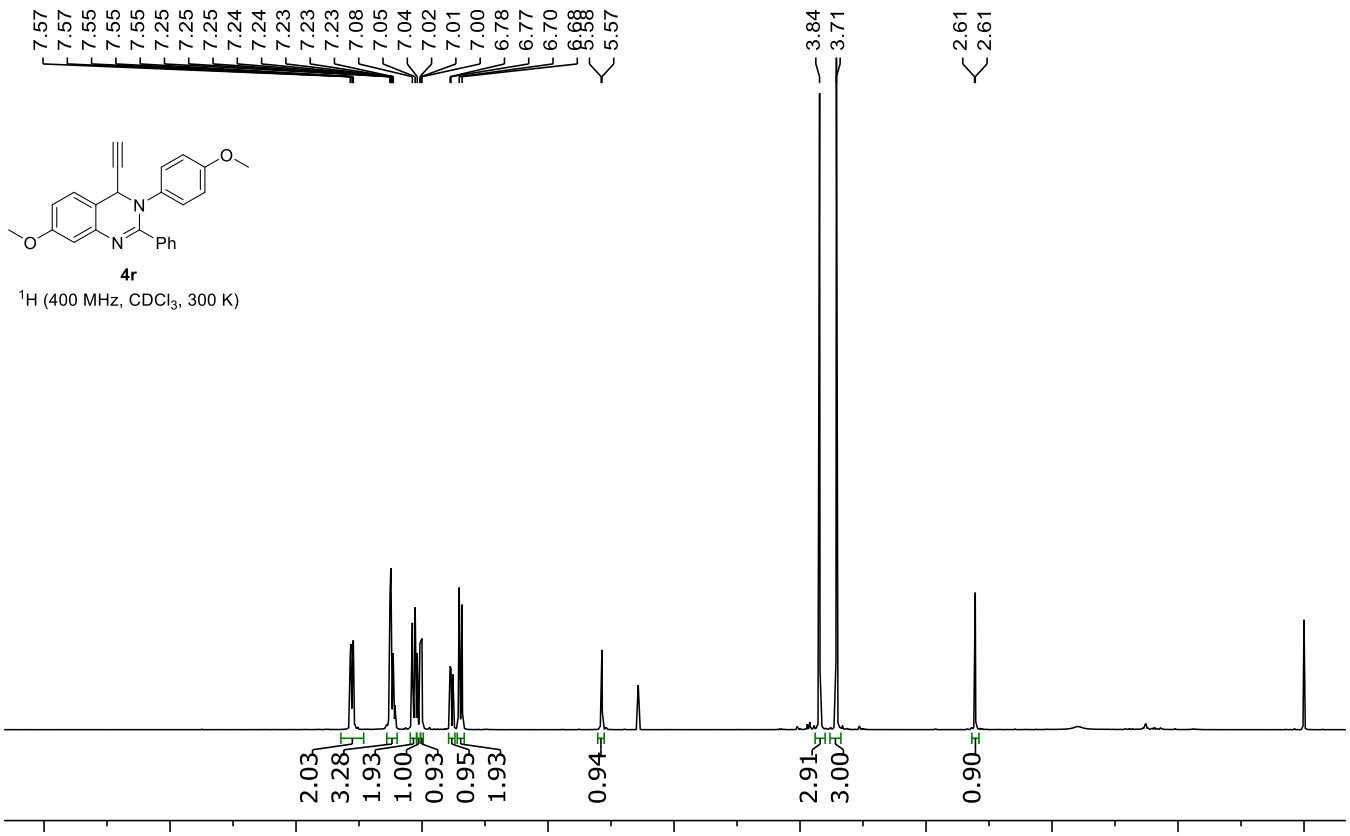

7.78 7.78 7.77 7.77 7.77 7.77 7.77 7.76 7.76
7.29 7.28 7.28 7.27 7.27 7.27 7.26 7.26 7.26 7.25 7.25 7.25 7.24 7.03 7.02 6.90 6.88 6.84 6.82 6.74 6.73 6.72 6.71 6.66 6.64 4.36 4.35 3.85 3.68 2.14 2.12 2.10 2.09 2.07 2.05 2.04 1.18 1.16 0.89
O
N
O
N
Ph
4l
1H (400 MHz, CDCl3, 300 K)
1.91 3.09 0.91 1.95 0.97 0.94 1.95
0.95 2.86 3.00
1.07
3.02 3.05
10 9 8 7 6 5 4 3 2 1 0
159.71 156.46 156.25 143.86 139.98 136.61 129.83 129.81 128.27 127.43 125.64 116.98 114.17 112.07 108.43
68.67
55.48 55.46
34.84
19.94 18.16
4l
13C{1H} (101 MHz, CDCl3, 300 K)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

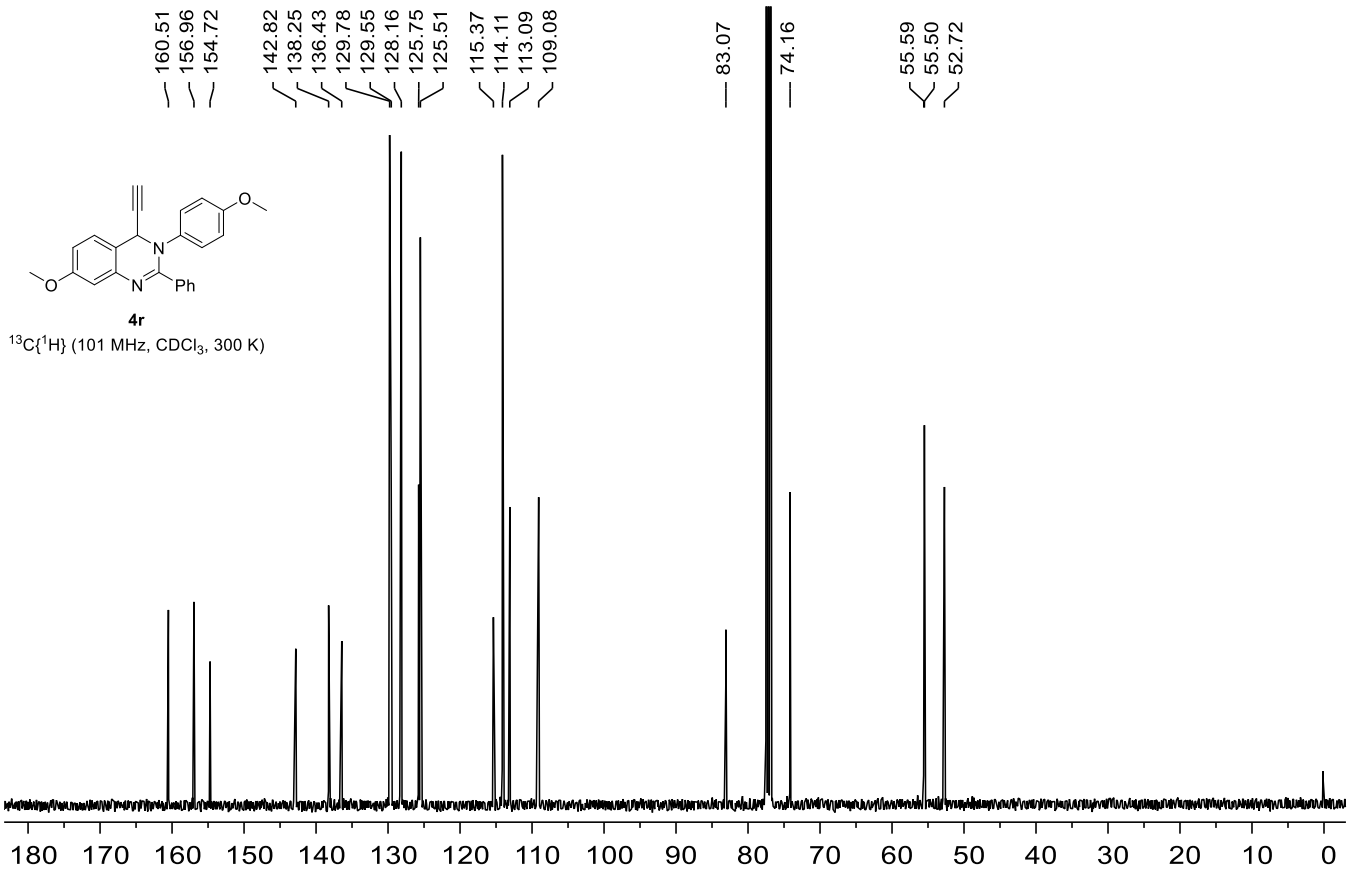

4m
1H (400 MHz, CDCl3, 300 K)
4m
13C{1H} (101 MHz, CDCl3, 300 K)

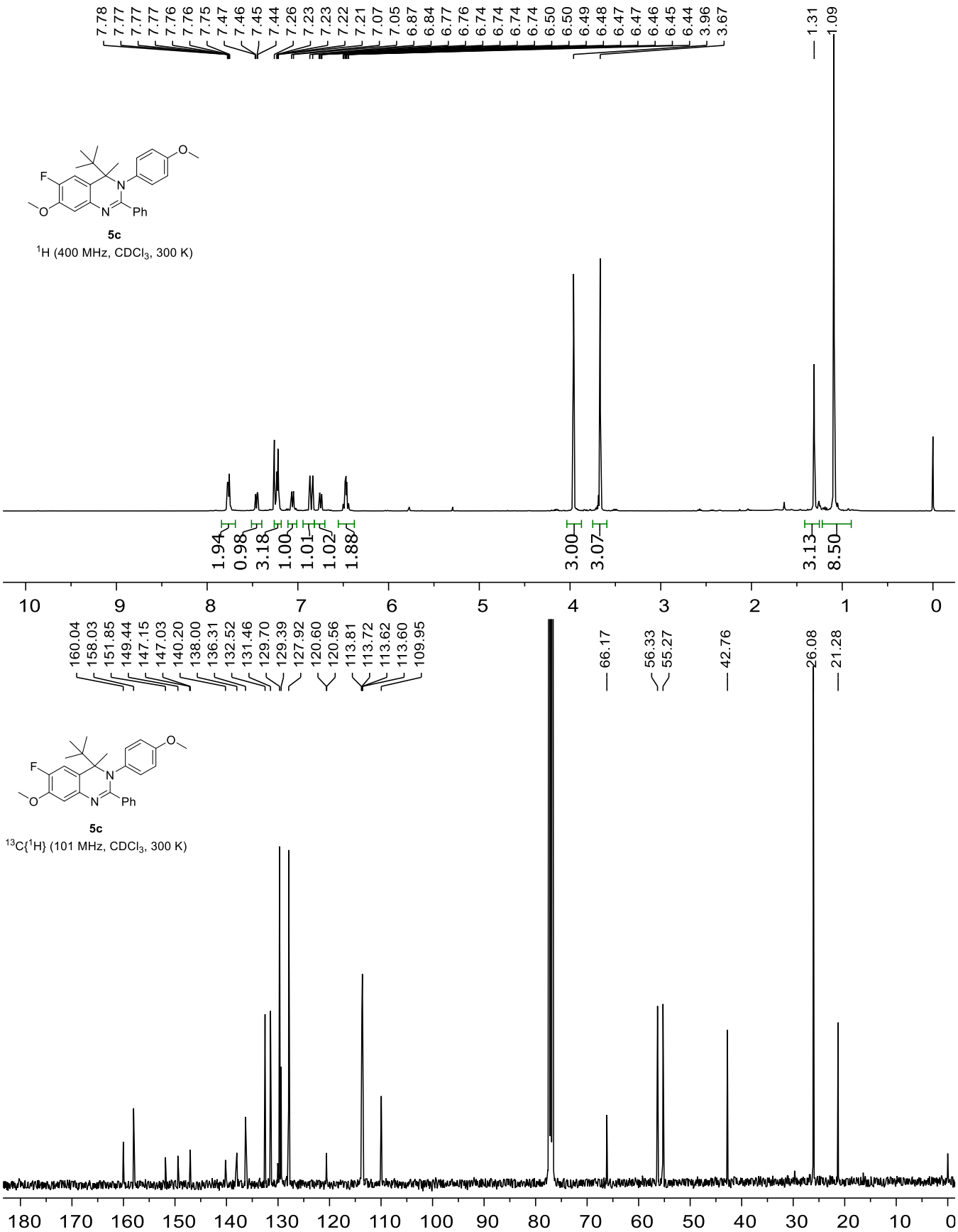

7.75 7.74 7.74 7.73 7.72 7.37 7.37 7.36 7.35 7.35 7.35 7.33 7.32 7.30 7.30 7.29 7.28 7.28 7.27 7.26 7.26 7.25 7.22 7.21 7.20 7.19 6.64 6.64 6.63 6.55 6.52 6.46 6.43 3.86 3.65 3.15 3.13 3.11 3.09 2.96 2.95 2.93 2.91
Ph
O
N
O
N
Ph
4n
1H (400 MHz, CDCl3, 300 K)
1.90 6.12 1.95 0.99 0.98 0.96 1.93 1.93 1.04 2.94 3.00 1.07 1.08
10 9 8 7 6 5 4 3 2 1 0
159.86 156.68 155.19 143.41 139.40 137.83 136.23 130.39 130.21 129.97 128.69 128.19 127.01 126.12 125.72 119.15 114.12 112.32 108.62
65.55
55.56 55.45
43.11
4n
13C{1H} (101 MHz, CDCl3, 300 K)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

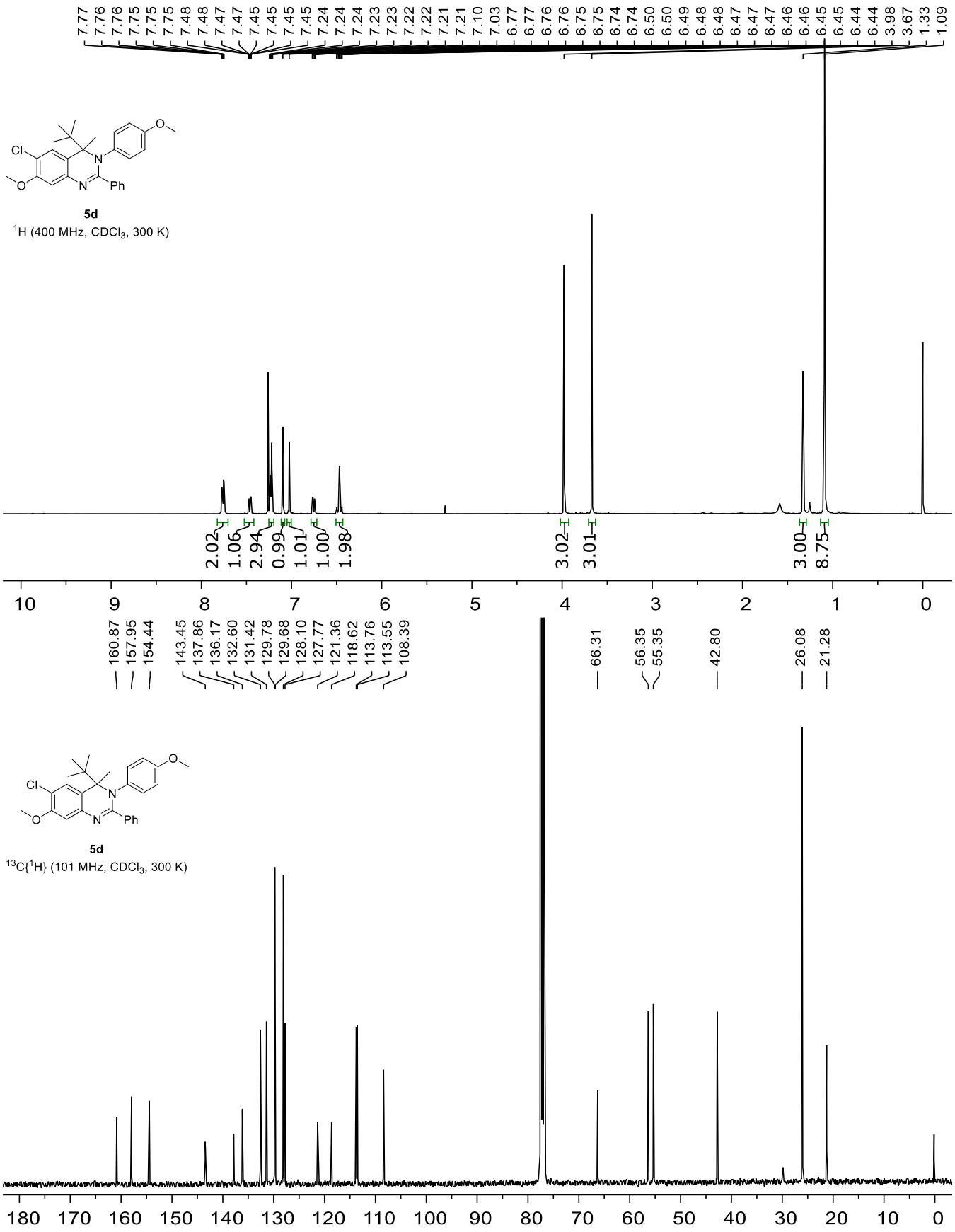

7.70 7.69 7.68 7.67 7.28 7.27 7.27 7.26 7.26 7.26 7.25 7.25 7.24 7.24 7.24 7.23 7.01 7.01 6.92 6.90 6.88 6.86 6.74 6.73 6.71 6.71 6.67 6.65 6.65 5.99 5.96 5.94 5.92 5.19 5.19 5.18 5.18 5.18 5.17 5.17 5.17 5.16 5.16 5.14 5.13 4.77 4.75 4.73 3.85 3.69 2.62 2.60 2.56 2.56 2.54
4o
1H (400 MHz, CDCl3, 300 K)
1.95 3.53 0.98 1.84 0.94 0.98 2.02 1.00 1.94 1.00 3.00 3.24 2.06
10 9 8 7 6 5 4 3 2 1 0
159.83 156.62 155.54 143.42 139.34 136.67 134.08 129.91 129.76 128.20 126.05 125.68 118.95 118.89 114.18 112.40 108.63 62.80 55.54 55.50 42.03
4o
13C{1H} (101 MHz, CDCl3, 300 K)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

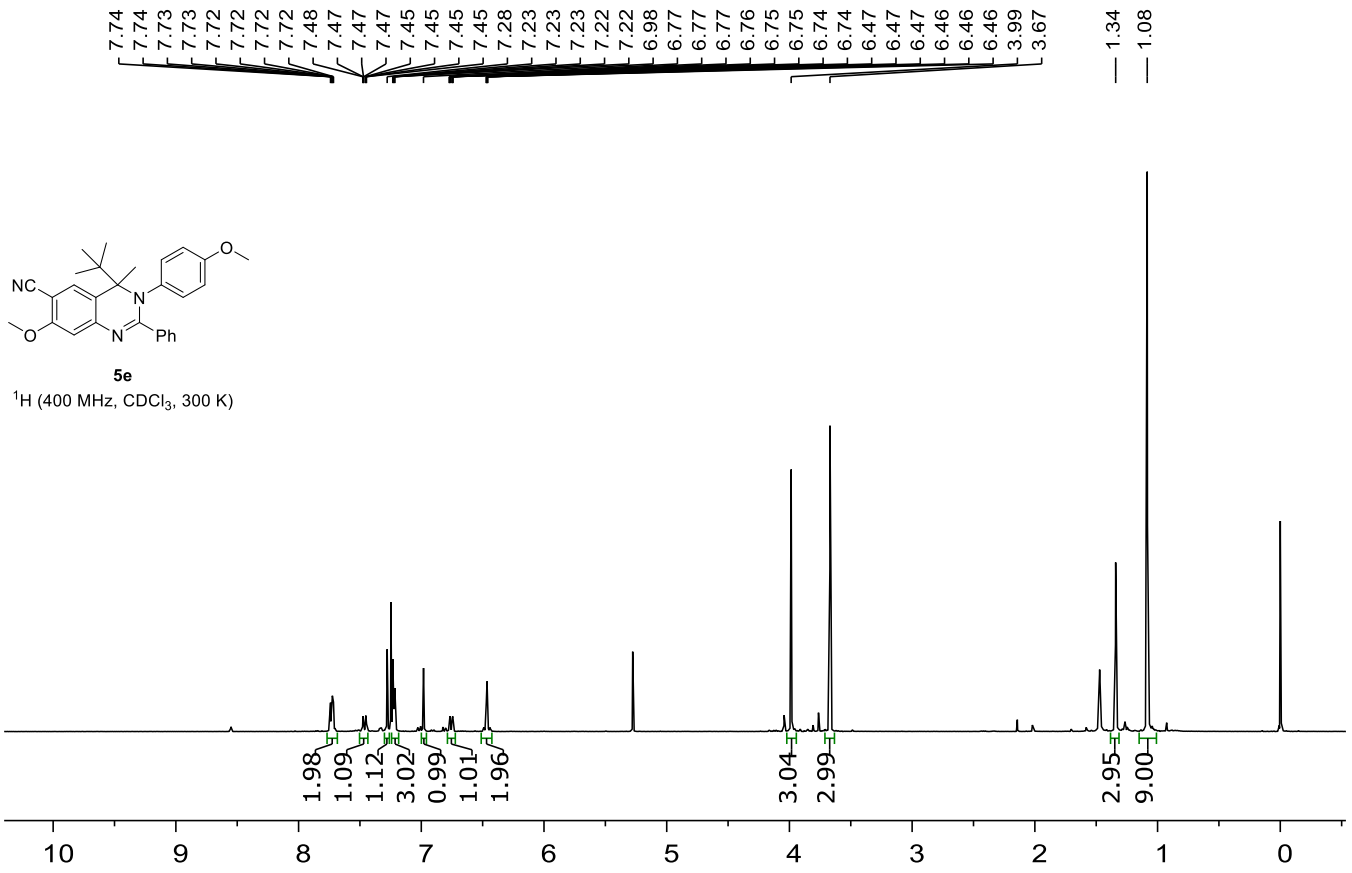

7.65 7.64 7.63 7.62 7.27 7.26 7.26 7.25 7.24 7.24 7.23 7.23 7.23 7.22 7.22 7.22 7.22 6.99 6.98 6.97 6.96 6.95 6.94 6.93 6.90 6.75 6.74 6.73 6.72 6.68 6.66 6.19 6.17 6.16 6.15 6.15 6.13 6.12 6.11 5.34 5.34 5.33 5.30 5.29 5.29 5.24 5.22 5.17 5.16 5.16 5.14 5.14 5.14 3.84 3.70
4p
1H (400 MHz, CDCl3, 300 K)
1.89 3.44 3.88 0.95 1.91 0.95 1.03 0.98 0.96 3.00 3.12
10 9 8 7 6 5 4 3 2 1 0
160.02 156.77 154.93 143.11 139.36 138.42 136.51 129.90 129.62 128.16 126.13 125.68 117.41 114.38 114.06 112.69 108.75 64.68 55.55 55.49
4p
13C{1H} (101 MHz, CDCl3, 300 K)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

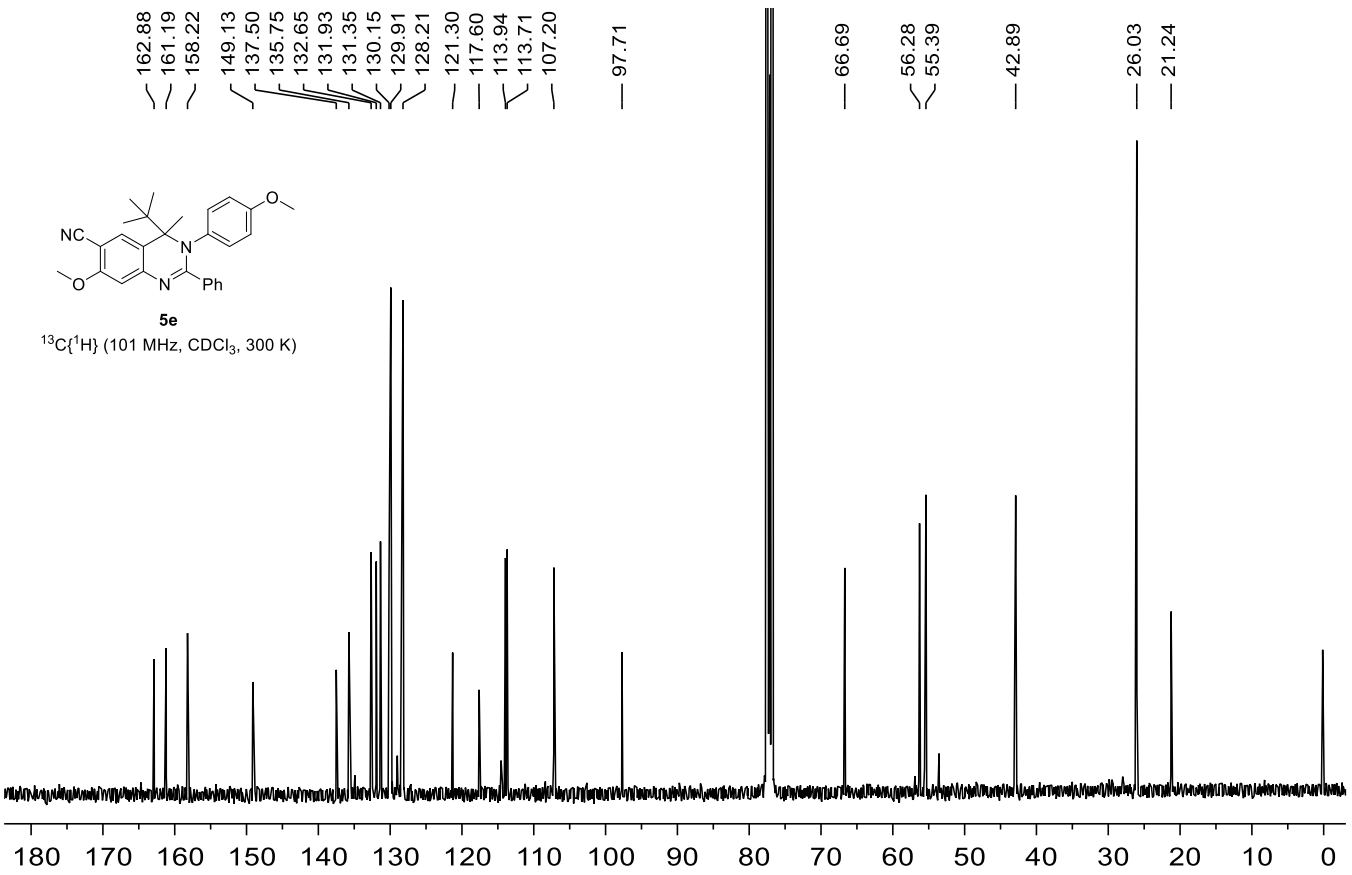

7.57
7.57
7.55
7.55
7.55
7.25
7.25
7.25
7.24
7.24
7.23
7.23
7.23
7.08
7.05
7.04
7.02
7.01
7.00
6.78
6.77
6.70
6.68
6.68
5.57
3.84
3.71
2.61
2.61
O
N
N
O
Ph
4r
1H (400 MHz, CDCl3, 300 K)
2.03
3.28
1.93
1.00
0.93
0.95
1.93
0.94
2.91
3.00
0.90
10
9
8
7
6
5
4
3
2
1
0

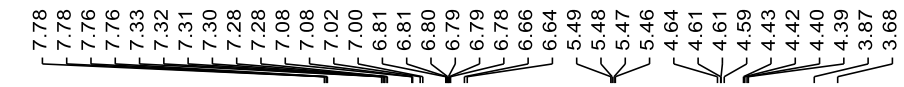

160.51
156.96
154.72
142.82
138.25
136.43
129.78
129.55
128.16
125.75
125.51
115.37
114.11
113.09
109.08
83.07
74.16
55.59
55.50
52.72
O
N
N
O
Ph
4r
13C{1H} (101 MHz, CDCl3, 300 K)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

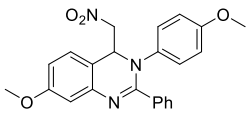

7.78
7.77
7.77
7.77
7.76
7.76
7.75
7.47
7.46
7.45
7.44
7.26
7.23
7.23
7.22
7.21
7.07
7.05
6.87
6.84
6.77
6.76
6.74
6.74
6.74
6.74
6.50
6.50
6.49
6.48
6.47
6.47
6.46
6.45
6.44
3.96
3.67
1.31
1.09
F
O
N
O
N
Ph
5c
1H (400 MHz, CDCl3, 300 K)
1.94
0.98
3.18
1.00
1.01
1.02
1.88
3.00
3.07
3.13
8.50
10
9
8
7
6
5
4
3
2
1
0
160.04
158.03
151.85
149.44
147.15
147.03
140.20
138.00
136.31
132.52
131.46
129.70
129.39
127.92
120.60
120.56
113.81
113.72
113.62
113.60
109.95
66.17
56.33
55.27
42.76
26.08
21.28
F
O
N
O
N
Ph
5c
13C{1H} (101 MHz, CDCl3, 300 K)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


7.77 7.76 7.76 7.75 7.75 7.75 7.48 7.48 7.47 7.47 7.45 7.45 7.45 7.45 7.24 7.24 7.24 7.23 7.23 7.22 7.22 7.21 7.21 7.10 7.03 6.77 6.77 6.76 6.76 6.75 6.75 6.74 6.74 6.50 6.50 6.49 6.48 6.48 6.47 6.47 6.47 6.46 6.46 6.45 6.45 6.44 6.44 3.98 3.67 1.33 1.09
Cl
N
O
O
N
Ph
5d
1H (400 MHz, CDCl3, 300 K)
2.02 1.06 2.94 0.99 1.01 1.00 1.98 3.02 3.01 3.00 8.75
10 9 8 7 6 5 4 3 2 1 0
160.87 157.95 154.44 143.45 137.86 136.17 132.60 131.42 129.78 129.68 128.10 127.77 121.36 118.62 113.76 113.55 108.39 66.31 56.35 55.35 42.80 26.08 21.28
5d
13C{1H} (101 MHz, CDCl3, 300 K)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


7.74 7.74 7.73 7.73 7.72 7.72 7.72 7.72 7.48 7.47 7.47 7.47 7.45 7.45 7.45 7.45 7.28 7.23 7.23 7.23 7.22 7.22 6.98 6.77 6.77 6.77 6.76 6.75 6.75 6.74 6.74 6.47 6.47 6.47 6.46 6.46 6.46 3.99 3.67
1.34 1.08
NC
O
N
O
N
Ph
O
5e
1H (400 MHz, CDCl3, 300 K)
1.98 1.09 1.12 3.02 0.99 1.01 1.96 3.04 2.99 2.95 9.00
10 9 8 7 6 5 4 3 2 1 0

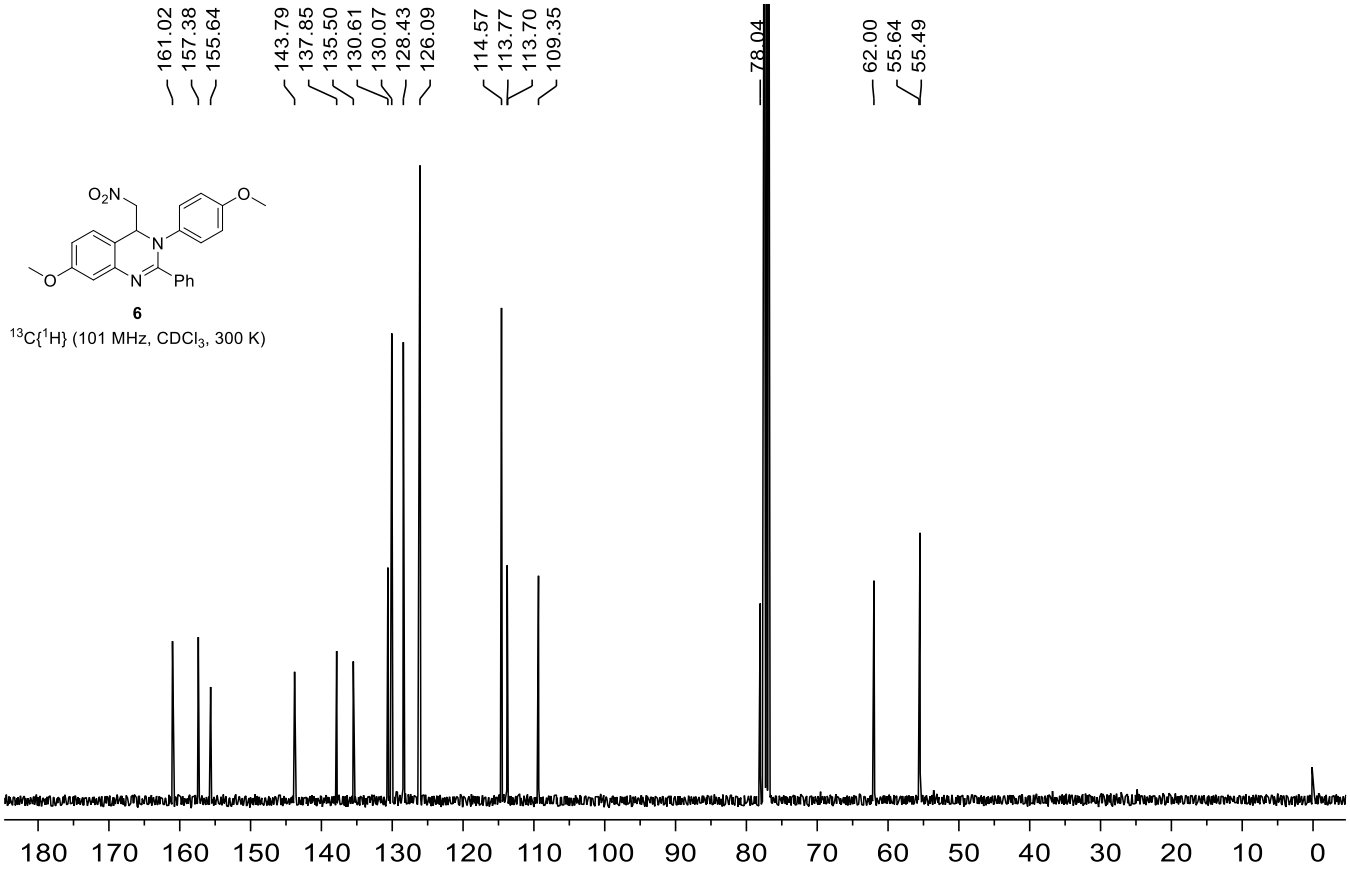

162.88 161.19 158.22 149.13 137.50 135.75 132.65 131.93 131.35 130.15 129.91 128.21 121.30 117.60 113.94 113.71 107.20 97.71 66.69 56.28 55.39 42.89 26.03 21.24
NC
O
N
O
N
Ph
O
5e
13C{1H} (101 MHz, CDCl3, 300 K)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0





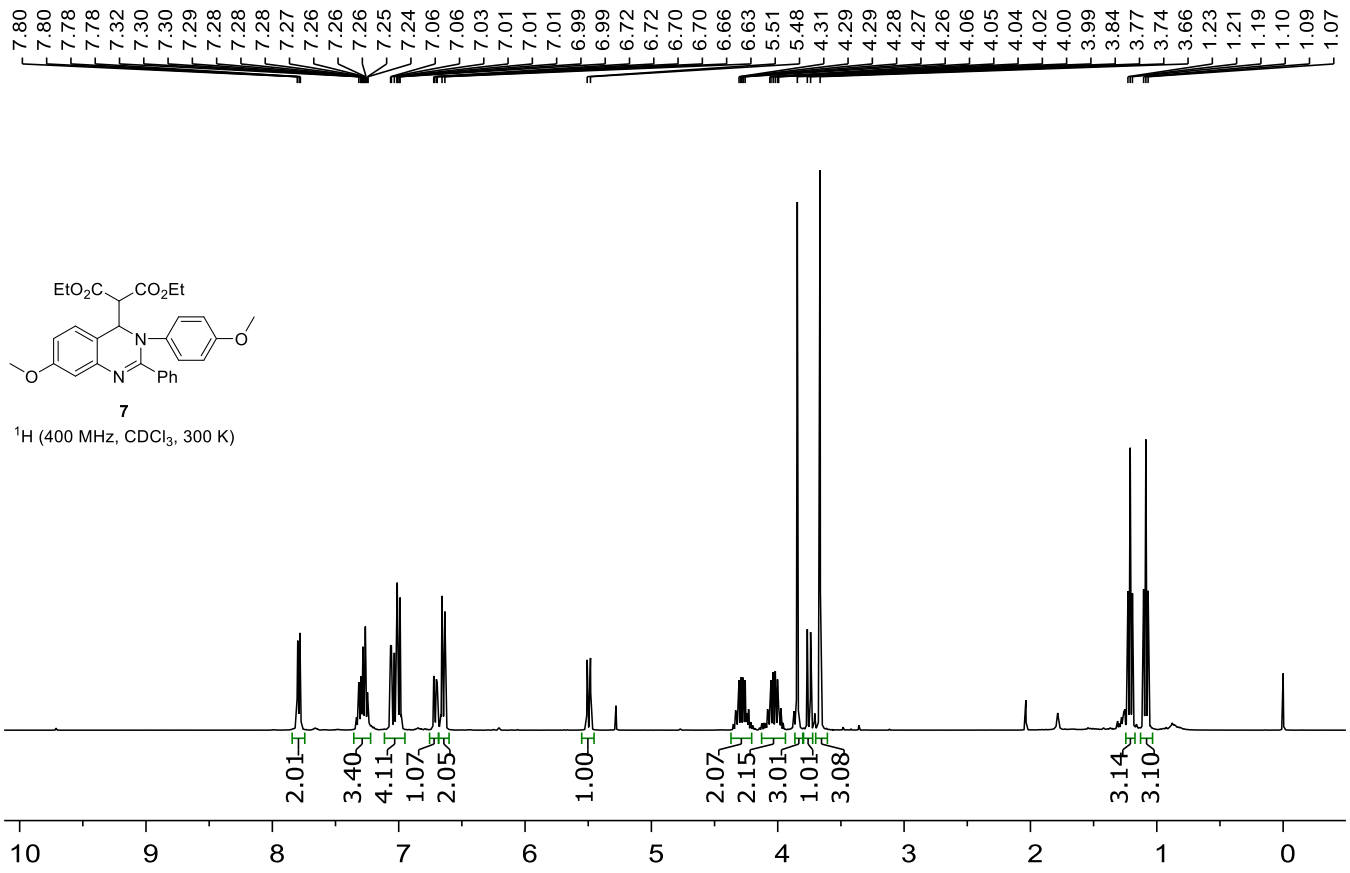
6

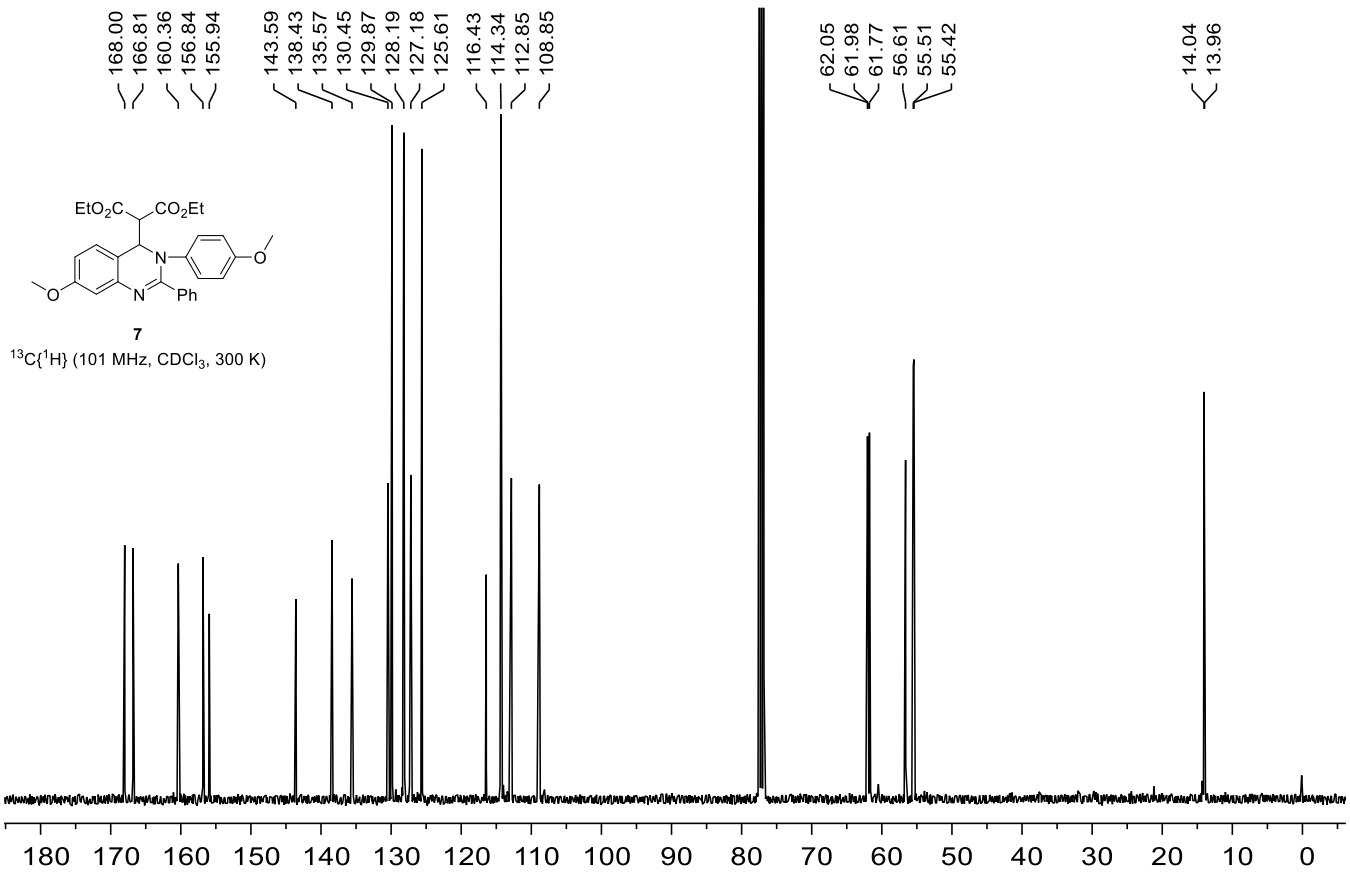
^{1}H (400 MHz, $CDCl_3$, 300 K)

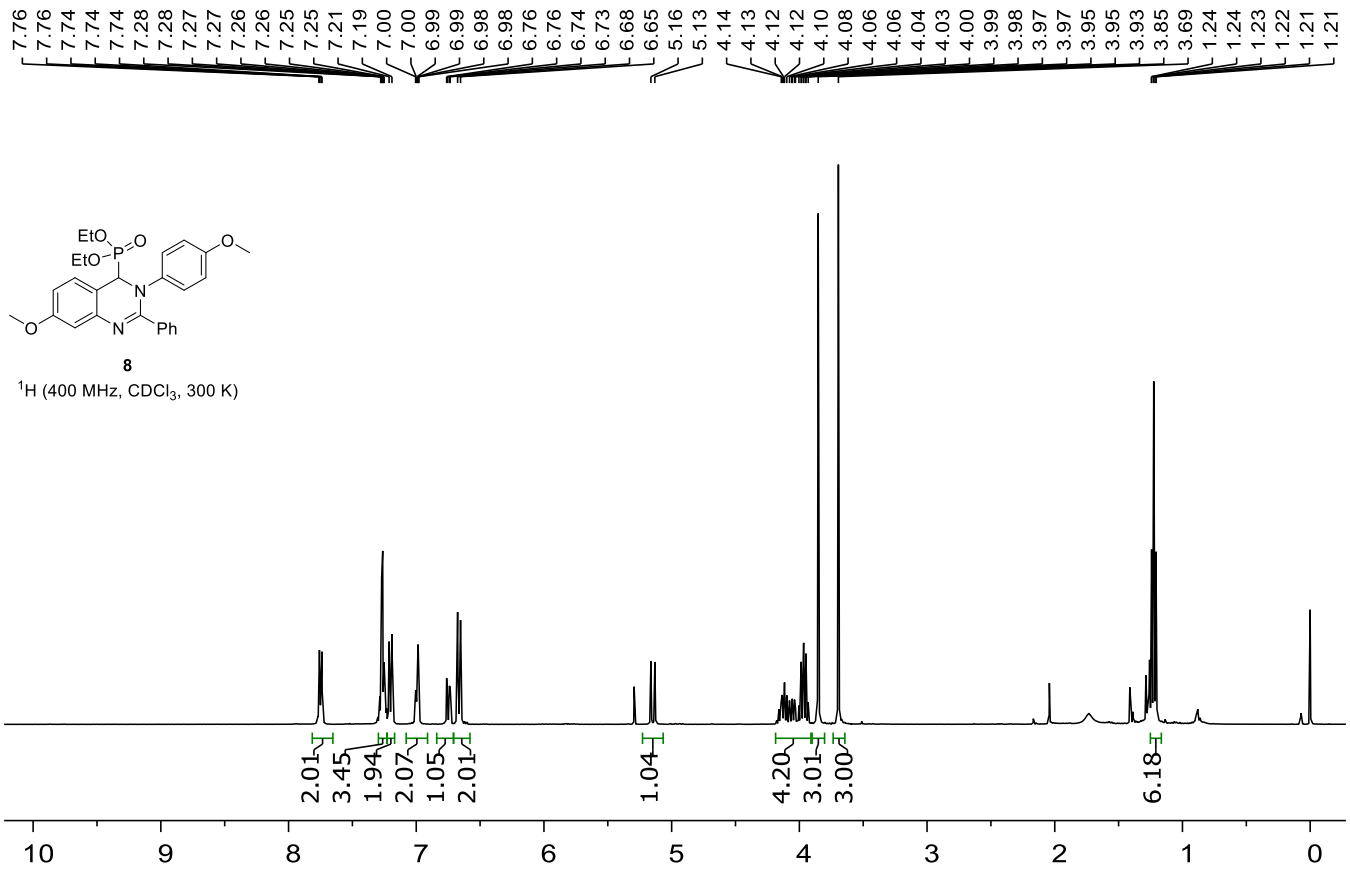


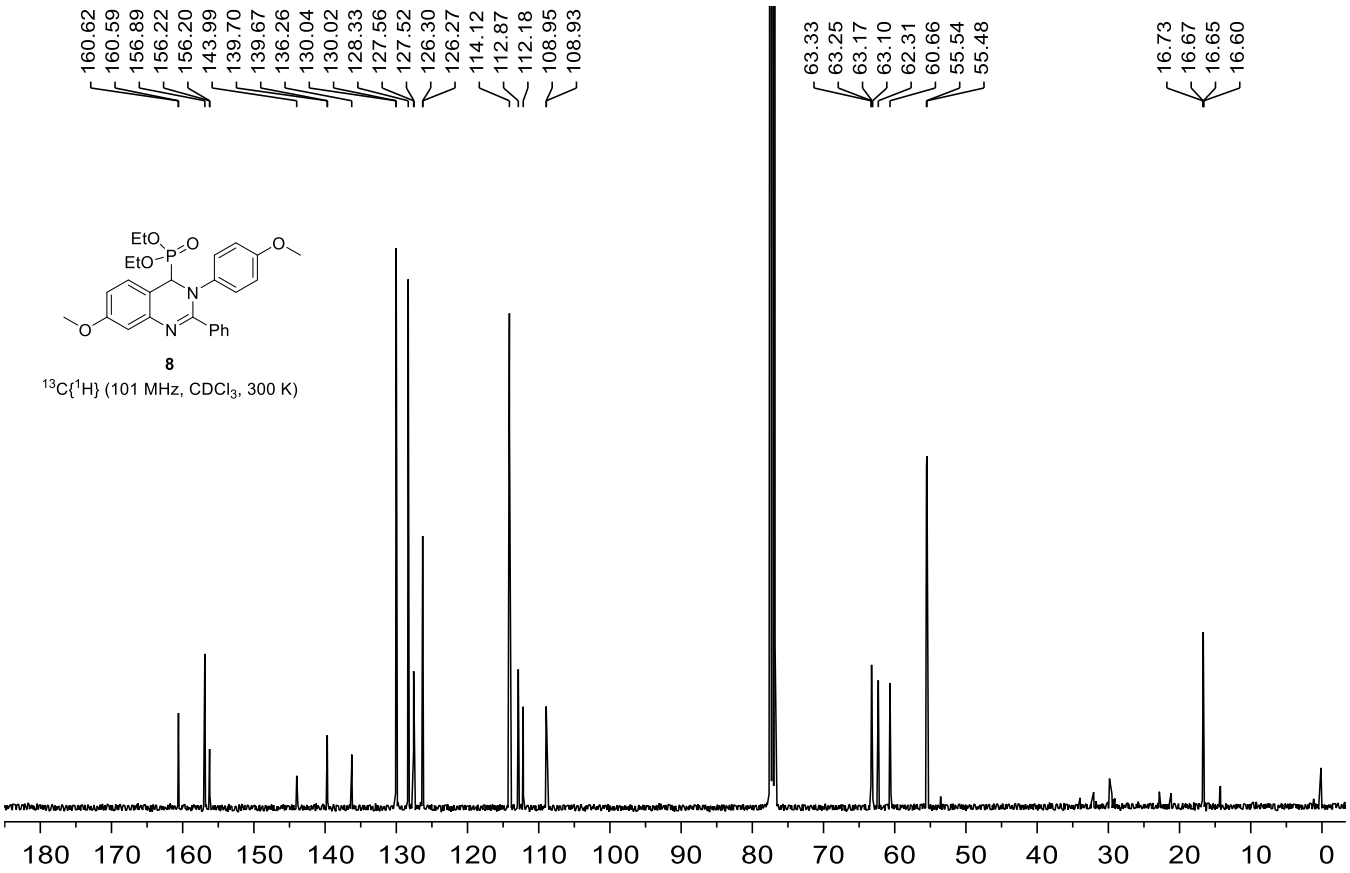
6

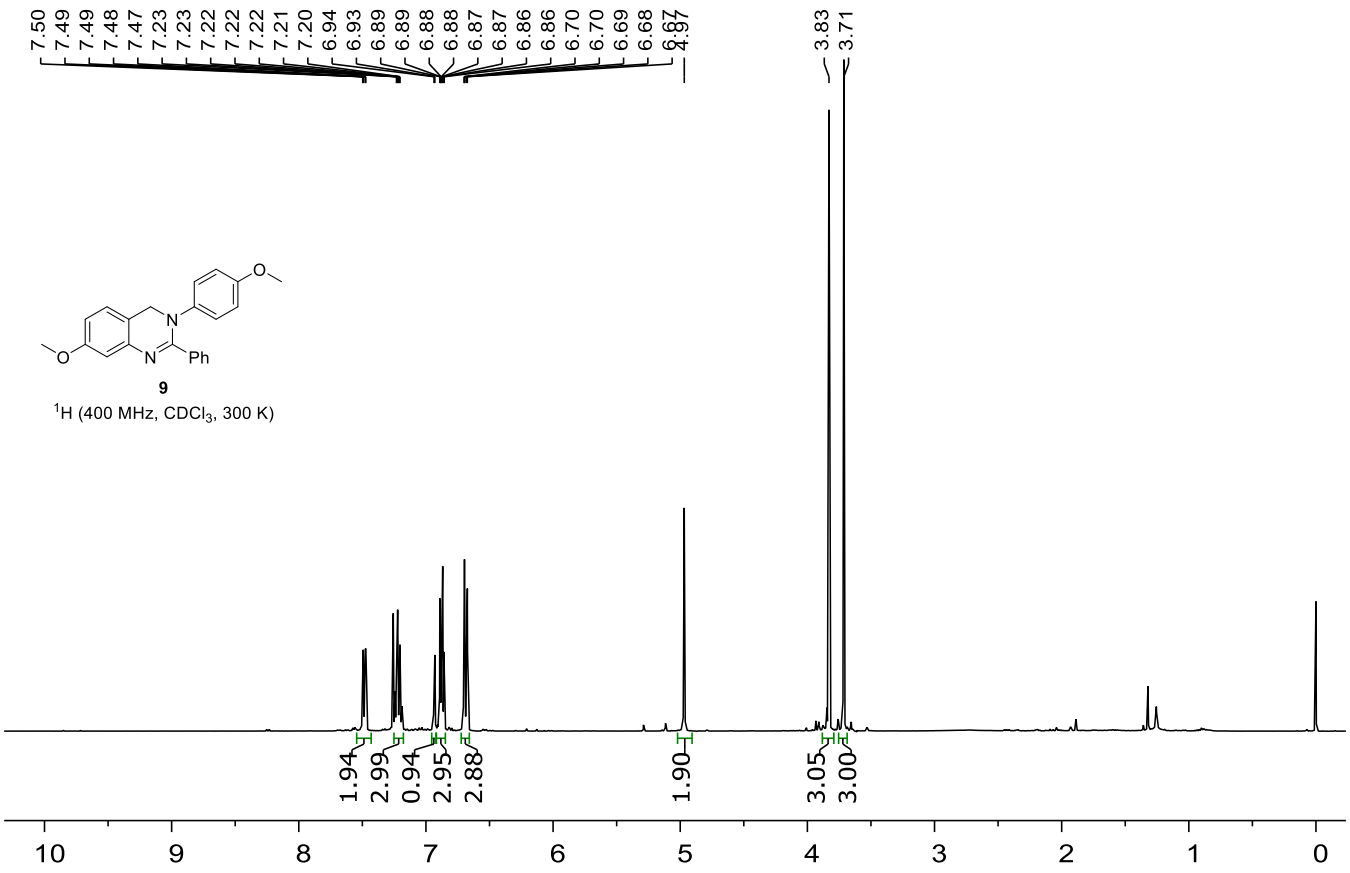
$^{13}C\{^{1}H\}$ (101 MHz, $CDCl_3$, 300 K)

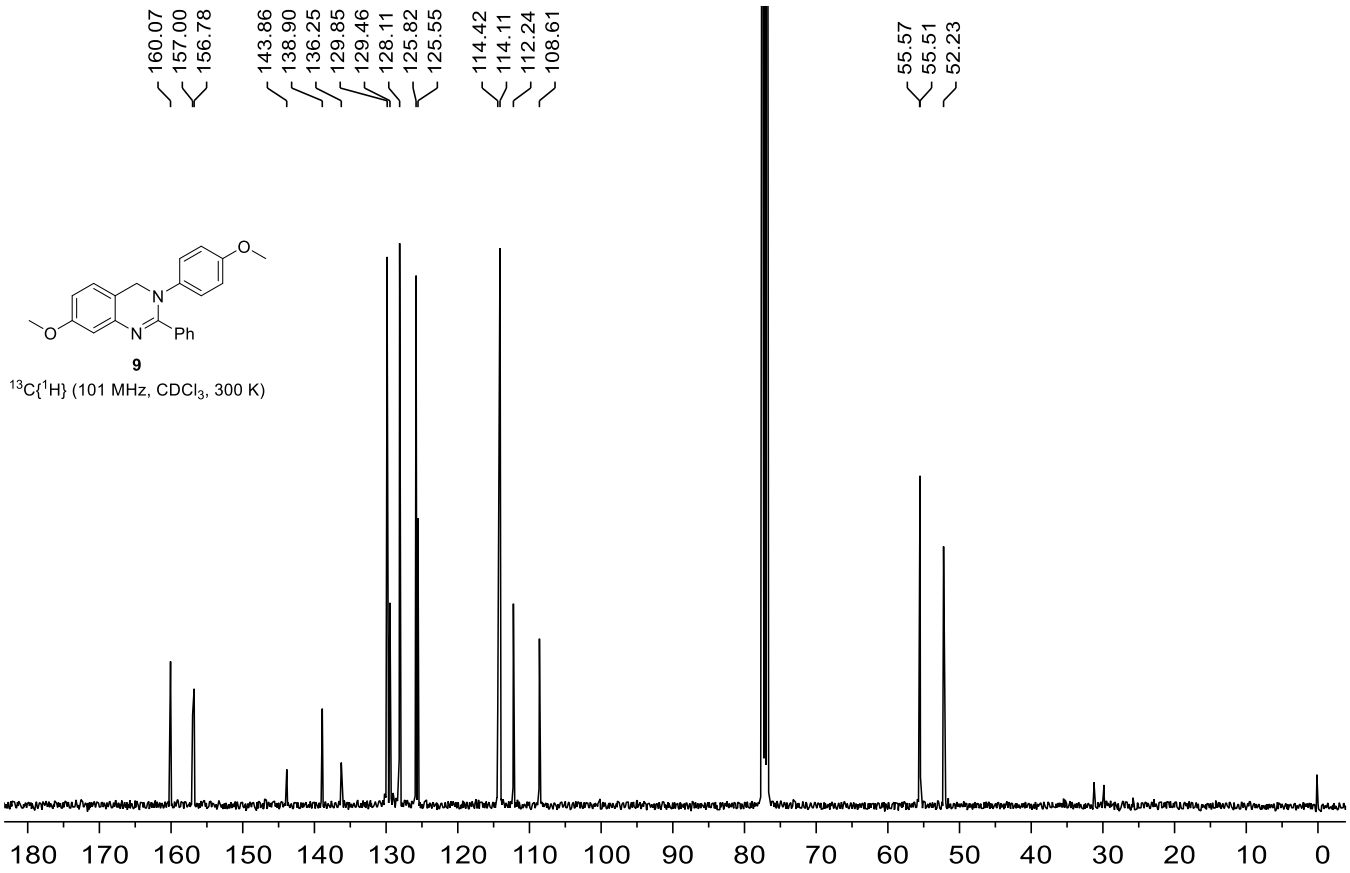

7.80 7.80 7.78 7.78 7.32 7.30 7.30 7.29 7.28 7.28 7.28 7.27 7.26 7.26 7.26 7.25 7.24 7.06 7.06 7.03 7.01 7.01 7.01 6.99 6.99 6.72 6.72 6.70 6.70 6.66 6.63 5.51 5.48 4.31 4.29 4.29 4.28 4.27 4.26 4.06 4.05 4.04 4.02 4.00 3.99 3.84 3.77 3.74 3.66 1.23 1.21 1.19 1.10 1.09 1.07
EtO2C CO2Et
N
O
O
N
Ph
7
1H (400 MHz, CDCl3, 300 K)
2.01 3.40 4.11 1.07 2.05 1.00 2.07 2.15 3.01 1.01 3.08 3.14 3.10
10 9 8 7 6 5 4 3 2 1 0


168.00 166.81 160.36 156.84 155.94 143.59 138.43 135.57 130.45 129.87 128.19 127.18 125.61 116.43 114.34 112.85 108.85 62.05 61.98 61.77 56.61 55.51 55.42 14.04 13.96
EtO2C CO2Et
N
O
O
N
Ph
7
13C{1H} (101 MHz, CDCl3, 300 K)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


7.76 7.76 7.74 7.74 7.74 7.28 7.28 7.27 7.27 7.26 7.26 7.25 7.25 7.21 7.19 7.00 7.00 6.99 6.99 6.98 6.98 6.76 6.76 6.74 6.73 6.68 6.65 5.16 5.13 4.14 4.13 4.12 4.12 4.10 4.08 4.06 4.06 4.04 4.03 4.00 3.99 3.98 3.97 3.97 3.95 3.95 3.93 3.85 3.69 1.24 1.24 1.23 1.22 1.21 1.21
EtO
EtO
P
O
N
O
O
N
Ph
8
1H (400 MHz, CDCl3, 300 K)
2.01
3.45
1.94
2.07
1.05
2.01
1.04
4.20
3.01
3.00
6.18
10 9 8 7 6 5 4 3 2 1 0


160.62 160.59 156.89 156.22 156.20 143.99 139.70 139.67 136.26 130.04 130.02 128.33 127.56 127.52 126.30 126.27 114.12 112.87 112.18 108.95 108.93
63.33 63.25 63.17 63.10 62.31 60.66 55.54 55.48
16.73 16.67 16.65 16.60
EtO
EtO
P
O
N
O
O
N
Ph
8
13C{1H} (101 MHz, CDCl3, 300 K)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


7.50
7.49
7.49
7.48
7.47
7.23
7.23
7.22
7.22
7.22
7.21
7.20
6.94
6.93
6.89
6.89
6.88
6.88
6.87
6.87
6.86
6.86
6.70
6.69
6.68
6.67
4.97
3.83
3.71
O
N
O
N
Ph
9
1H (400 MHz, CDCl3, 300 K)
1.94
2.99
0.94
2.95
2.88
1.90
3.05
3.00
10
9
8
7
6
5
4
3
2
1
0


160.07
157.00
156.78
143.86
138.90
136.25
129.85
129.46
128.11
125.82
125.55
114.42
114.11
112.24
108.61
55.57
55.51
52.23
O
N
O
N
Ph
9
13C{1H} (101 MHz, CDCl3, 300 K)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0