Supplementary Information

Triflic Anhydride Mediated Synthesis of 3,4-Dihydroquinazolines: A Three-Component One-Pot Tandem Procedure

Christina L. Magyar, Tyler J. Wall, Steven B. Davies, Molly V. Campbell,
Haven A. Barna, Sydney R. Smith, Christopher J. Savich, and R. Adam Mosey*

Department of Chemistry, Lake Superior State University, Sault Sainte Marie, MI 49783
*rmosey@lssu.edu

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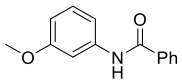
General Experimental Information.

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 SiliaFlash P60 (230 – 400 mesh) silica gel supplied by SiliCycle. 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. High resolution mass spectra were recorded at the Lumigen Instrument Center of Wayne State University on a Waters LCT Premium XE TOF mass spectrometer. Elemental analyses were performed by Robertson Microlit Laboratories using a Perkin-Elmer Model 2400 CHN Analyzer. Melting points were obtained using a Mel-Temp capillary melting point apparatus and are uncorrected. CH_2Cl_2 was distilled under N_2 from CaH_2 and 2-chloropyridine was dried over 4 Å molecular sieves; all other solvents and chemicals were purchased from commercial vendors and were used without additional purification.

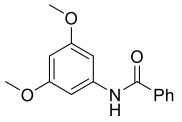
General procedure A for amide synthesis. To a mixture of an amine and triethylamine (TEA) in anhydrous CH_2Cl_2, cooled to 0 °C in an ice bath, was added dropwise an appropriate acid chloride followed by 4-DMAP. The ice bath was removed, and the reaction stirred at rt under N_2 atmosphere until complete, as determined by TLC. The reaction mixture was washed with saturated $NaHCO_3$ solution (x3) and brine before being dried (Na_2SO_4) and concentrated. The crude product was then purified either by crystallization or silica gel chromatography. This general procedure was used for the synthesis of compounds **1**, **3a**, **3c**, **3e-3h**, **3j-3k**, and **3m-3n**.

General procedure B for amide synthesis. To a mixture of an amine in pyridine, cooled to 0 °C in an ice bath, was dropwise added a solution of acid chloride in THF. The ice bath was removed, and the reaction stirred under N_2 atmosphere until complete, as determined by TLC. The reaction was poured over ice water and the resultant precipitate was collected by vacuum filtration and washed with ice water. The filtered solid was then purified by crystallization. This general procedure was used for the synthesis of compounds **3b**, **3d**, **3l**, and **3o-3q**.

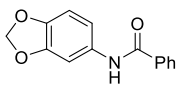
General procedure for 3,4-dihydroquinazoline synthesis: A mixture of amide (1.0 mmol), amine (1.1 mmol), aldehyde (1.1 mmol), and 4 Å molecular sieves (~1 g) in CH_2Cl_2 (10.0 mL) was prepared and stirred for 18 h at room temperature under N_2 atmosphere. The reaction mixture was cooled to -41 °C and was treated successively with 2-chloropyridine (1.2 mmol) followed by Tf_2O (1.1 mmol). The reaction was then allowed to warm to room temperature and was stirred for the indicated time. The molecular sieves were then 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 flash chromatography.



***N*-(3-methoxyphenyl)benzamide (1)**. Prepared according to general procedure A for amide synthesis using *m*-anisidine (5.60 mL, 49.8 mmol), TEA (8.40 mL, 60.3 mmol), benzoyl chloride (7.75 mL, 66.8 mmol), 4-DMAP (0.063 g, 0.51 mmol), and CH_2Cl_2 (250 mL). The reaction stirred for 18 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (10.766 g, 99% yield) of the title compound as a solid (m.p. = 112 - 113 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.87 – 7.83 (m, 2H), 7.56 – 7.51 (m, 1H), 7.50 – 7.39 (m, 3H), 7.24 (t, *J* = 8.1 Hz, 1H), 7.10 (ddd, *J* = 7.9, 2.0, 0.9 Hz, 1H), 6.70 (ddd, *J* = 8.3, 2.5, 0.9 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 160.2, 139.2, 135.0, 131.8, 129.7, 128.8, 127.0, 112.3, 110.6, 105.8, 55.3. The NMR spectral data are consistent with those reported in the literature.[1]

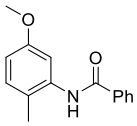


***N*-(3,5-dimethoxyphenyl)benzamide (3a)**. Prepared according to general procedure A for amide synthesis using 3,5-dimethoxyaniline (1.560 g, 9.90 mmol), TEA (1.50 mL, 10.6 mmol), benzoyl chloride (1.25 mL, 10.7 mmol), 4-DMAP (0.012 g, 0.10 mmol), and EtOAc (50 mL) instead of CH_2Cl_2. The reaction stirred for 18 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (2.107 g, 83% yield) as a solid (m.p. = 142 - 145 °C). ^{1}H NMR (400 MHz, DMSO-d6) δ 10.17 (s, 1H), 7.99 – 7.92 (m, 2H), 7.63 – 7.50 (m, 3H), 7.11 (d, *J* = 2.3 Hz, 2H), 6.28 (t, *J* = 2.3 Hz, 1H), 3.75 (s, 6H). ^{13}C NMR (101 MHz, DMSO-d6) δ 165.6, 160.4, 140.9, 134.9, 131.6, 128.4, 127.6, 98.5, 95.7, 55.1. The NMR spectral data are consistent with those reported in the literature.[2]

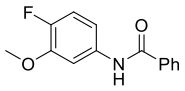


***N*-1,3-benzodioxol-5-ylbenzamide (3b)**. Prepared according to general procedure B for amide synthesis using 3,4-methylenedioxyaniline (2.740 g, 20.0 mmol), pyridine (25 mL, 310 mmol), benzoyl chloride (2.32 mL, 20.0 mmol), and THF (4.0 mL). The reaction stirred for 1 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (2.842 g, 59% yield) as a brown solid (m.p. = 137 - 140 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.82 (d, *J* = 7.4 Hz, 2H), 7.50

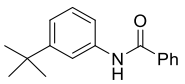
(t, J = 7.4 Hz, 1H), 7.42 (t, J = 7.5 Hz, 2H), 7.31 (d, J = 2.1 Hz, 1H), 6.90 (dd, J = 8.4, 2.1 Hz, 1H), 6.73 (d, J = 8.3 Hz, 1H), 5.94 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 147.8, 144.5, 134.8, 132.2, 131.7, 128.7, 127.0, 113.8, 108.1, 103.3, 101.3. The NMR spectral data are consistent with those reported in the literature.[3]



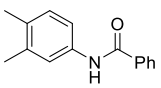
***N*-(5-methoxy-2-methylphenyl)benzamide (3c)**. Prepared according to general procedure A for amide synthesis using 5-methoxy-2-methylaniline (0.954 g, 6.95 mmol), TEA (1.20 mL, 8.6 mmol), benzoyl chloride (0.89 mL, 7.7 mmol), 4-DMAP (0.012 g, 0.10 mmol), and CH_2Cl_2 (30 mL). The reaction stirred for 18 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (1.158 g, 69% yield) as a solid (m.p. = 126 – 129 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.85 – 7.78 (m, 2H), 7.55 – 7.44 (m, 2H), 7.38 (t, J = 7.5 Hz, 2H), 7.03 (d, J = 8.8 Hz, 1H), 6.63 (dd, J = 8.4, 2.7 Hz, 1H), 3.70 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7, 158.2, 136.5, 134.8, 131.7, 130.9, 128.7, 127.1, 121.5, 111.4, 108.6, 55.3, 16.9. The NMR spectral data are consistent with those reported in the literature.[4]



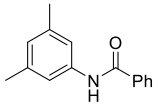
***N*-(4-fluoro-3-methoxyphenyl)benzamide (3d)**. Prepared according to general procedure B for amide synthesis using *m*-anisidine (1.413 g, 10.0 mmol), pyridine (25 mL), benzoyl chloride (1.16 mL, 9.99 mmol), and THF (4 mL). The reaction stirred for 1.5 h before being worked up as described. The residual solid was was purified by recrystallization in EtOAc and hexanes to afford the desired product (1.897 g, 77% yield) as a solid (m.p. = 133 - 135 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.85 (d, J = 7.2 Hz, 2H), 7.64 (dd, J = 7.7, 2.5 Hz, 1H), 7.55 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.4 Hz, 2H), 7.03 (dd, J = 10.9, 8.7 Hz, 1H), 6.90 (ddd, J = 8.7, 3.8, 2.6 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 149.3 (d, $^1J_{C\text{-}F}$ = 243 Hz), 147.8 (d, $^2J_{C\text{-}F}$ = 11 Hz), 134.7, 134.4 (d, $^4J_{C\text{-}F}$ = 3 Hz), 132.0, 128.8, 127.0, 115.9 (d, $^2J_{C\text{-}F}$ = 19 Hz), 112.0 (d, $^3J_{C\text{-}F}$ = 7 Hz), 106.5 (d, $^3J_{C\text{-}F}$ = 2 Hz), 56.3; IR (neat): 3297, 3048, 2985, 1649, 1620, 1515, 1280, 1215 cm^{-1}; Anal. Calcd for $C_{14}H_{12}FNO_2$: C, 68.56%; H, 4.93%; N, 5.71%; Found: C, 68.36%; H, 4.92%; N, 5.73%.



***N*-(3-tert-butylphenyl)benzamide (3e)**. Prepared according to general procedure A for amide synthesis using 3-tert-butylaniline (0.749 g, 5.02 mmol), TEA (0.84 mL, 6.0 mmol), benzoyl chloride (0.64 mL, 5.5 mmol), 4-DMAP (0.012 g, 0.10 mmol), and CH_2Cl_2 (25 mL). The reaction stirred for 18 h before being worked up as described. The residual solid was purified by recrystallization from benzene and pentane to afford the desired product (0.879 g, 65% yield) as a solid (m.p. = 115 – 118 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.88 – 7.80 (m, 2H), 7.64 (t, J = 2.0 Hz, 1H), 7.55 – 7.44 (m, 2H), 7.39 (t, J = 7.5 Hz, 2H), 7.25 (t, J = 8.0 Hz, 1H), 7.16 (ddd, J = 7.9, 1.9, 1.1 Hz, 1H), 1.30 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 152.3, 137.7, 135.1, 131.7, 128.7, 127.0, 121.7, 117.6, 117.5, 34.8, 31.3. The NMR spectral data are consistent with those reported in the literature.[5]

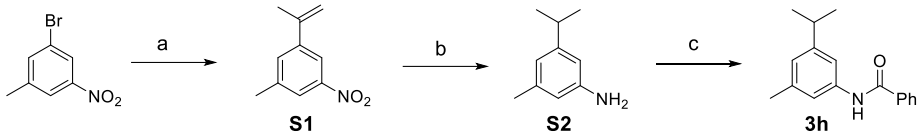


***N*-(3,4-dimethylphenyl)benzamide (3f)**. Prepared according to general procedure A for amide synthesis using 3,4-dimethylaniline (0.617 g, 5.09 mmol), TEA (0.83 mL, 6.0 mmol), benzoyl chloride (0.64 mL, 5.5 mmol), 4-DMAP (0.012 g, 0.10 mmol), and CH_2Cl_2 (25 mL). The reaction stirred for 18 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (0.952 g, 83% yield) as a solid (m.p. = 142 - 144 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.82 (m, 2H), 7.72 (s, 1H), 7.58 – 7.42 (m, 4H), 7.35 (dd, J = 8.1, 2.4 Hz, 1H), 7.12 (d, J = 8.1 Hz, 1H), 2.27 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7, 137.2, 135.7, 135.1, 132.9, 131.6, 130.0, 128.7, 127.0, 121.7, 117.9, 19.9, 19.2. The NMR spectral data are consistent with those reported in the literature.[6]

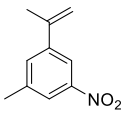


***N*-(3,5-dimethylphenyl)benzamide (3g)**. Prepared according to general procedure A for amide synthesis using 3,5-dimethylaniline (2.50 mL, 20.1 mmol), TEA (3.35 mL, 24.0 mmol), benzoyl chloride (2.55 mL, 21.9 mmol), 4-DMAP (0.024 g, 0.20 mmol), and CH_2Cl_2 (100 mL). The reaction stirred for 18 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired

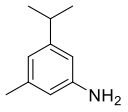
product (3.751 g, 83% yield) as a white solid (m.p. = 142 - 144 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.83 (d, *J* = 7.2 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.27 (s, 2H), 6.76 (s, 1H), 2.27 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 138.7, 137.8, 135.1, 131.6, 128.7, 127.0, 126.3, 118.1, 21.3. The NMR spectral data are consistent with those reported in the literature.[7]



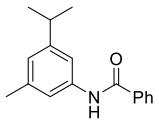
Reagents and conditions
a) 4,4,5,5-tetramethyl-2-(prop-1-en-2-yl)-1,3,2-dioxaborolane, $Pd(PPh_3)_4$, $NaHCO_3$, water, dioxane, 100 °C. b) H_2, 10% Pd/C, MeOH. c) benzoyl chloride, TEA, DMAP, CH_2Cl_2.



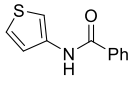
1-methyl-3-(1-methylethenyl)-5-nitrobenzene (S1). To a degassed mixture of 2 M aqueous $NaHCO_3$ solution (4.0 mL, 8.0 mmol) and 1,4-dioxane (13.5 mL) were added 3-bromo-5-nitrotoluene (0.574 g, 2.66 mmol), 4,4,5,5-tetramethyl-2-(prop-1-en-2-yl)-1,3,2-dioxaborolane (0.998 g, 5.94 mmol), and $Pd(PPh_3)_4$ (0.157 g, 0.14 mmol), and the mixture was heated at 100 °C for 5 hours. The reaction was cooled to room temperature before being diluted in CH_2Cl_2 and saturated $NaHCO_3$ solution. The organic layer was collected and washed with brine before being dried (Na_2SO_4) and concentrated. The reaction was then passed through a silica plug (5% EtOAc in hexanes), and the filtrate was concentrated to afford the desired product (0.440 g, 93% yield) as a light tan solid (m.p. = 45 – 48 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.86 (s, 1H), 7.55 (s, 1H), 5.45 (s, 1H), 5.20 (s, 1H), 2.43 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.4, 142.6, 141.4, 139.6, 132.2, 122.5, 117.6, 114.8, 21.6, 21.3; IR (neat): 3088, 2924, 1530, 1351 cm^{-1}; Anal. Calcd for $C_{10}H_{11}NO_2$: C, 67.78%; H, 6.26%; N, 7.90%; Found: C, 67.65%; H, 6.27%; N, 7.63%.



3-isopropyl-5-methylaniline (S2). To a stirring solution of **S1** (0.416 g, 2.35 mmol) in MeOH (10 mL) was added 10% Pd/C (0.121 g). The reaction was fitted with a H_2 balloon and stirred at room temperature for 24 h. The mixture was passed through a celite plug with additional MeOH, and the filtrate was concentrated to afford the desired product (0.336 g, 96% yield) as a brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.46 (s, 1H), 6.35 (s, 1H), 6.31 (s, 1H), 3.90 (s, 2H), 2.74 (hept, *J* = 6.9 Hz, 1H), 2.21 (s, 3H), 1.19 (d, *J* = 7.0 Hz, 6H), ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.3, 145.9, 139.0, 118.2, 114.0, 110.9, 34.1, 24.1, 21.6; IR (neat): 3448, 3366, 3017, 2958, 1601, 1461 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{10}H_{16}N$ [M+H], 150.1283; found,150.1274.

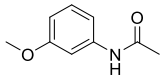


***N*-(3-isopropyl-5-methylphenyl)benzamide (3h)**. Prepared according to general procedure A for amide synthesis using **S2** (0.298 g, 1.99 mmol), TEA (0.33 mL, 2.4 mmol), benzoyl chloride (0.25 mL, 2.2 mmol), 4-DMAP (0.004 g, 0.03 mmol), and CH_2Cl_2 (10 mL). The reaction stirred for 18 h before being worked up as described. The residual solid was purified by flash chromatography (7% - 15% EtOAc in hexanes as eluent) to afford the desired product (0.441 g, 87% yield) as a solid (m.p. = 100 – 102 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (s, 1H), 7.82 (d, *J* = 7.1 Hz, 2H), 7.41 – 7.31 (m, 3H), 7.27 (dd, *J* = 8.4, 7.0 Hz, 2H), 6.77 (s, 1H), 2.74 (hept, *J* = 6.9 Hz, 1H), 2.20 (s, 3H), 1.16 (d, *J* = 7.0 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.3, 149.7, 138.6, 138.2, 135.1, 131.6, 128.5, 127.3, 123.5, 119.1, 116.1, 34.1, 24.0, 21.5; IR (neat): 3316, 2961, 1651, 1614, 1551, 1450, 1284 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{17}H_{20}NO$ [M+H], 254.1545; found, 254.1538.

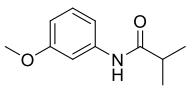


***N*-thiophen-3-yl-benzamide (3i)**. A mixture of 3-bromothiophene (1.90 mL, 20.3 mmol), benzamide (2.906 g, 24.0 mmol), K_3PO_4 (8.548 g, 40.3 mmol), *trans*-1,2-diaminocyclohexane (0.35 mL, 2.9 mmol), and CuI (0.803 g, 4.2 mmol) in degassed dioxane (20 mL) was stirred at 110 °C in a sealed vial for 18 h. The reaction was filtered through a silica plug with EtOAc and the concentrated filtrate was recrystallized from EtOAc and hexanes to afford the desired product (1.479 g, 36% yield) of the title compound as a solid (m.p. = 156 - 160 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (s, 1H), 7.89 – 7.81 (m, 2H), 7.72 (dd, *J* = 3.3, 1.4 Hz, 1H), 7.57 – 7.42 (m, 3H), 7.27 (dd, *J* = 5.0, 3.1 Hz, 1H), 7.13 (dd, *J* = 5.2, 1.4 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$)

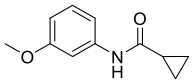
δ 165.1, 135.6, 134.4, 131.8, 128.8, 127.0, 124.7, 121.3, 110.8. The NMR spectral data are consistent with those reported in the literature.[8]



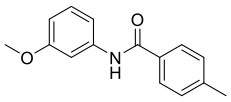
***N*-(3-methoxyphenyl)acetamide (3j)**. Prepared according to general procedure A for amide synthesis using *m*-anisidine (5.60 mL, 49.8 mmol), TEA (8.35 mL, 59.9 mmol), acetyl chloride (3.90 mL, 54.8 mmol), 4-DMAP (0.061 g, 0.50 mmol), and CH_2Cl_2 (250 mL). The reaction stirred for 3 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (6.554 g, 80% yield) of the title compound as a solid (m.p. = 84 - 86 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.27 (t, *J* = 2.1 Hz, 1H), 7.17 (t, *J* = 8.2 Hz, 1H), 7.00 (dd, *J* = 8.0, 0.9 Hz, 1H), 6.64 (dd, *J* = 8.2, 1.9 Hz, 1H), 3.74 (s, 3H), 2.13 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0, 160.1, 139.3, 129.6, 112.3, 110.0, 105.9, 55.2, 24.5. The NMR spectral data are consistent with those reported in the literature.[9]



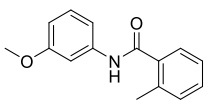
***N*-(3-methoxyphenyl)-2-methylpropanamide (3k)**. Prepared according to general procedure A for amide synthesis using *m*-anisidine (1.13 mL, 10.1 mmol), TEA (1.47 mL, 10.5 mmol), isobutyryl chloride (1.11 mL, 10.6 mmol), 4-DMAP (0.012 g, 0.11 mmol), and EtOAc (50 mL) instead of CH_2Cl_2. The reaction stirred for 18 h before being worked up as described. The residue was purified by flash chromatography (20% EtOAc in hexanes as eluent) to afford the desired product (1.766 g, 91% yield) as a solid (m.p. = 63 - 65 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.36 (t, *J* = 2.3 Hz, 1H), 7.16 (t, *J* = 8.1 Hz, 1H), 7.00 (dd, *J* = 7.8, 1.0 Hz, 1H), 6.63 (dd, *J* = 8.2, 1.8 Hz, 1H), 3.74 (s, 3H), 2.52 (hept, *J* = 6.9 Hz, 1H), 1.21 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.9, 160.1, 139.5, 129.5, 112.1, 110.1, 105.6, 55.2, 36.6, 19.6. The NMR spectral data are consistent with those reported in the literature.[10]



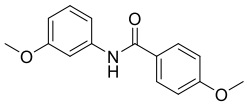
***N*-(3-methoxyphenyl)cyclopropanecarboxamide (3l)**. Prepared according to general procedure B for amide synthesis using *m*-anisidine (2.25 mL, 20.0 mmol), pyridine (25 mL, 310 mmol), cyclopropane carbonyl chloride (1.82 mL, 20.0 mmol), and THF (4.0 mL). The reaction stirred for 1 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (2.239 g, 59% yield) as a light peach solid (m.p. = 108 - 110 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (s, 1H), 7.32 (s, 1H), 7.18 (t, *J* = 8.1 Hz, 1H), 6.95 (dd, *J* = 8.0, 1.1 Hz, 1H), 6.64 (dd, *J* = 8.2, 1.8 Hz, 1H), 3.77 (s, 3H), 1.55 – 1.45 (m, 1H), 1.10 – 1.05 (m, 2H), 0.85 – 0.79 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.1, 160.2, 139.4, 129.6, 111.7, 110.1, 105.3, 55.3, 15.8, 8.0. The NMR spectral data and melting point data are consistent with those reported in the literature.[11]



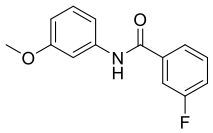
***N*-(3-methoxyphenyl)-4-methylbenzamide (3m)**. Prepared according to general procedure A for amide synthesis using *m*-anisidine (1.13 mL, 10 mmol), TEA (1.47 mL, 10.6 mmol), p-toluoyl chloride (1.45 mL, 11 mmol), 4-DMAP (0.013 g, 0.11 mmol), and CH_2Cl_2 (50 mL). The reaction stirred for 18 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (1.829 g, 79% yield) as a solid (m.p. = 117 – 120 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.74 (d, *J* = 8.2 Hz, 2H), 7.44 (t, *J* = 2.3 Hz, 1H), 7.27 – 7.19 (m, 3H), 7.09 (ddd, *J* = 8.0, 2.0, 0.9 Hz, 1H), 6.68 (ddd, *J* = 8.3, 2.5, 1.0 Hz, 1H), 3.80 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7, 160.2, 142.4, 139.3, 132.1, 129.7, 129.4, 127.0, 112.3, 110.4, 105.8, 55.3, 21.5. The NMR spectral data and melting point data are consistent with those reported in the literature.[12]



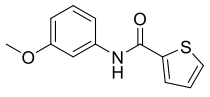
***N*-(3-methoxyphenyl)-2-methylbenzamide (3n)**. Prepared according to general procedure A for amide synthesis using *m*-anisidine (1.12 mL, 10 mmol), TEA (1.7 mL, 12 mmol), o-toluoyl chloride (1.45 mL, 11 mmol), 4-DMAP (0.012 g, 0.098 mmol), and CH_2Cl_2 (50 mL). The reaction stirred for 18 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (2.402 g, 99% yield) as a solid (m.p. = 144 – 146 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.46 – 7.37 (m, 2H), 7.33 (td, *J* = 7.5, 1.5 Hz, 1H), 7.28 – 7.18 (m, 3H), 7.06 (d, *J* = 8.1 Hz, 1H), 6.69 (ddd, *J* = 8.2, 2.5, 0.9 Hz, 1H), 3.80 (s, 3H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 160.2, 139.3, 136.42, 136.36, 131.2, 130.2, 129.7, 126.6, 125.9, 112.0, 110.4, 105.6, 55.3, 19.8. The NMR spectral data are consistent with those reported in the literature.[13]



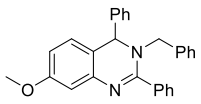
4-methoxy-*N*-(3-methoxyphenyl)benzamide (3o). Prepared according to general procedure B for amide synthesis using *m*-anisidine (2.30 mL, 20.5 mmol), pyridine (25 mL), 4-methoxybenzoyl chloride (2.79 mL, 20.6 mmol), and THF (4 mL). The reaction stirred for 1 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (4.059 g, 77% yield) as a solid (m.p. = 144 - 145 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.77 (m, 3H), 7.43 (t, *J* = 2.3 Hz, 1H), 7.23 (t, *J* = 8.2 Hz, 1H), 7.08 (ddd, *J* = 8.0, 2.1, 1.0 Hz, 1H), 6.95 (d, *J* = 8.9 Hz, 2H), 6.69 (ddd, *J* = 8.3, 2.5, 0.9 Hz, 1H), 3.86 (s, 3H), 3.81 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 162.5, 160.2, 139.4, 129.7, 128.9, 127.1, 114.0, 112.2, 110.4, 105.7, 55.5, 55.3; IR (neat): 3306, 3002, 2935, 1646, 1605, 1508, 1249, 1176, 1031 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{15}H_{16}NO_3$ [M+H], 258.1130; found, 258.1130. The melting point data is consistent with that reported in the literature.[14]



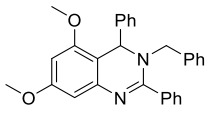
3-fluoro-*N*-(3-methoxyphenyl)-benzamide (3p). Prepared according to general procedure B for amide synthesis using *m*-anisidine (1.12 mL, 10 mmol), pyridine (25 mL), 3-fluorobenzoyl chloride (1.22 mL, 10 mmol), and THF (4 mL). The reaction stirred for 1.5 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (1.861 g, 76% yield) as a solid (m.p. = 95 - 97 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.57 (ddd, *J* = 7.7, 1.7, 1.0 Hz, 1H), 7.52 (ddd, *J* = 9.3, 2.6, 1.7 Hz, 1H), 7.39 – 7.32 (m, 2H), 7.26 – 7.14 (m, 2H), 7.10 (ddd, *J* = 7.9, 2.0, 1.0 Hz, 1H), 6.68 (ddd, *J* = 8.2, 2.5, 1.0 Hz, 1H), 3.76 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.8 (d, $^4J_{C\text{-}F}$ = 3 Hz), 162.7 (d, $^1J_{C\text{-}F}$ = 248 Hz), 160.2, 138.9, 137.2 (d, $^3J_{C\text{-}F}$ = 7 Hz), 130.4 (d, $^3J_{C\text{-}F}$ = 8 Hz), 129.7, 122.5 (d, $^4J_{C\text{-}F}$ = 3 Hz), 118.8 (d, $^2J_{C\text{-}F}$ = 21 Hz), 114.5 (d, $^2J_{C\text{-}F}$ = 23 Hz), 112.7, 110.7, 106.2, 55.3. The ^{1}H NMR spectral data are consistent with those reported in the literature.[15]



***N*-(3-methoxyphenyl)-2-thiophenecarboxamide (3q)**. Prepared according to general procedure B for amide synthesis using *m*-anisidine (2.25 mL, 20.0 mmol), pyridine (25 mL, 310 mmol), 2-thiophenecarbonyl chloride (2.14 mL, 20.0 mmol), and THF (4.0 mL). The reaction stirred for 1.5 h before being worked up as described. The residual solid was purified by recrystallization from EtOAc and hexanes to afford the desired product (3.146 g, 67% yield) as a light purple solid (m.p. = 143 - 146 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.63 (dd, *J* = 3.8, 1.2 Hz, 1H), 7.53 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.41 (t, *J* = 2.2 Hz, 1H), 7.22 (t, *J* = 8.1 Hz, 1H), 7.09 (dd, *J* = 5.0, 3.7 Hz, 1H), 7.06 (ddd, *J* = 8.0, 2.0, 0.9 Hz, 1H), 6.69 (ddd, *J* = 8.3, 2.5, 0.9 Hz, 1H), 3.80 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.2, 160.0, 139.3, 138.9, 130.8, 129.7, 128.4, 127.8, 112.3, 110.7, 105.8, 55.3. The NMR spectral data are consistent with those reported in the literature.[16]

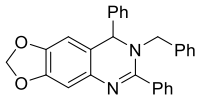


3-Benzyl-7-methoxy-2,4-diphenyl-3,4-dihydroquinazoline (2). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.226 g, 0.99 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (0% - 2% MeOH in 100:5 CH_2Cl_2:ether mixture as eluent) to afford the desired product (0.337 g, 84% yield) as a solid (m.p. = 172 – 174 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.48 (m, 2H), 7.41 – 7.23 (m, 11H), 7.19 (d, *J* = 6.8 Hz, 1H), 6.89 (d, *J* = 2.6 Hz, 1H), 6.62 (d, *J* = 8.4 Hz, 1H), 6.52 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.37 (s, 1H), 4.69 (d, *J* = 15.7 Hz, 1H), 3.98 (d, *J* = 15.7 Hz, 1H), 3.76 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 158.2, 144.0, 142.4, 136.6, 136.5, 129.3, 129.0, 128.9, 128.7, 128.1, 128.0, 127.7, 127.3, 127.2, 126.9, 117.1, 112.2, 108.7, 60.5, 55.2, 53.3. IR (neat): 3027, 2933, 1585, 1545, 1489, 1422, 1262, 1124, 1031 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{28}H_{25}N_2O$ [M+H], 405.1967; found, 405.1967.

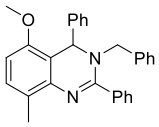


3-Benzyl-5,7-dimethoxy-2,4-diphenyl-3,4-dihydroquinazoline (4a). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3a** (0.255 g, 0.99 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18

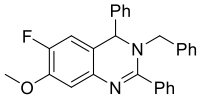
mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was purified by flash chromatography (5% - 10% ether in CH_2Cl_2 as eluent) to afford the desired product (0.260 g, 60% yield) as a solid (m.p. = 168 - 169 °C). ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.55 – 7.50 (m, 2H), 7.49 – 7.42 (m, 5H), 7.42 – 7.22 (m, 8H), 6.41 (d, *J* = 2.3 Hz, 1H), 6.21 (d, *J* = 2.3 Hz, 1H), 5.54 (s, 1H), 4.73 (d, *J* = 15.8 Hz, 1H), 4.19 (d, *J* = 15.8 Hz, 1H), 3.79 (s, 3H), 3.59 (s, 3H); ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 161.4, 158.9, 156.7, 144.9, 138.5, 138.0, 130.1, 129.6, 129.3, 129.2, 129.2, 128.58, 128.5, 128.1, 128.0, 107.5, 101.9, 96.2, 56.9, 55.8, 55.5, 54.3; IR (neat): 3027, 2935, 1597, 1541, 1487, 1422, 1128, 1107 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{29}H_{27}N_2O_2$ [M+H], 435.2073; found, 435.2074.



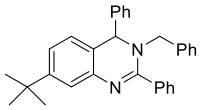
7-benzyl-7,8-dihydro-6,8-diphenyl-1,3-Dioxolo[4,5-g]quinazoline (4b). Prepared according to the general 3,4-dihydroquinazoline protocol with **3b** (0.243 g, 1.01 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (40% - 50% EtOAc in hexanes as eluent) to afford the desired product (0.289 g, 69% yield) as a solid (m.p. = 197 – 199 °C). ^{1}H NMR (400 MHz, $CDCl_3$) 7.53 – 7.46 (m, 2H), 7.41 – 7.21 (m, 11H), 7.19 (d, *J* = 6.7 Hz, 2H), 6.85 (s, 1H), 6.17 (s, 1H), 5.84 (d, *J* = 1.4 Hz, 1H), 5.79 (d, *J* = 1.4 Hz, 1H), 5.28 (s, 1H), 4.68 (d, *J* = 15.7 Hz, 1H), 3.98 (d, *J* = 15.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.5, 147.4, 144.9, 143.7, 136.7, 136.4, 136.3, 129.3, 129.1, 128.9, 128.6, 128.2, 128.1, 127.8, 127.3, 126.9, 117.4, 105.8, 100.9, 60.9, 53.3; IR (neat): 3027, 2889, 1556, 1474, 1424, 1241, 1135, 1036 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{28}H_{23}N_2O_2$ [M+H], 419.1760; found, 419.1754.



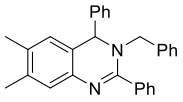
3-Benzyl-5-methoxy-8-methyl-2,4-diphenyl-3,4-dihydroquinazoline (4c). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3c** (0.245 g, 1.02 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 48 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (2% - 5% ether in CH_2Cl_2 as eluent) to afford the desired product (0.335 g, 79% yield) as a solid (m.p. = 173 - 176 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.50 (m, 2H), 7.44 (d, *J* = 6.9 Hz, 2H), 7.38 – 7.11 (m, 11H), 7.02 (d, *J* = 8.3 Hz, 1H), 6.41 (d, *J* = 8.3 Hz, 1H), 5.55 (s, 1H), 4.75 (d, *J* = 15.6 Hz, 1H), 4.16 (d, *J* = 15.6 Hz, 1H), 3.48 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.4, 153.1, 143.3, 140.9, 137.2, 136.7, 129.5, 129.2, 128.8, 128.6, 128.5, 128.4, 127.6, 127.5, 127.28, 127.25, 125.0, 114.1, 106.8, 56.0, 55.4, 53.8, 17.0; IR (neat): 3027, 2922, 1607, 1545, 1489, 1452, 1264, 1096 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{29}H_{27}N_2O$ [M+H], 419.2123; found, 419.2102.



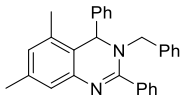
3-Benzyl-6-fluoro-7-methoxy-2,4-diphenyl-3,4-dihydroquinazoline (4d). Prepared according to the general 3,4-dihydroquinazoline protocol with **3d** (0.246 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 48 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (3% ether in CH_2Cl_2 as eluent) to afford the desired product (0.164 g, 39% yield) as a solid (m.p. = 151 – 155 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.46 (m, 2H), 7.44 – 7.25 (m, 11H), 7.18 (d, *J* = 6.7 Hz, 2H), 6.96 (d, *J* = 8.2 Hz, 1H), 6.43 (d, *J* = 11.2 Hz, 1H), 5.32 (s, 1H), 4.70 (d, *J* = 15.7 Hz, 1H), 3.96 (d, *J* = 15.7 Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.7, 149.8 (d, $^1J_{C\text{-}F}$ = 244 Hz), 147.4 (d, $^2J_{C\text{-}F}$ = 12 Hz), 143.4, 137.8 (d, $^3J_{C\text{-}F}$ = 3 Hz), 136.39, 136.36, 129.4, 129.2, 128.9, 128.7, 128.4, 127.94, 127.86, 127.3, 126.9, 116.4 (d, $^3J_{C\text{-}F}$ = 6 Hz), 113.3 (d, $^2J_{C\text{-}F}$ = 20 Hz), 109.7 (d, $^4J_{C\text{-}F}$ = 2 Hz), 60.2 (d, $^4J_{C\text{-}F}$ = 1 Hz), 56.0, 53.3; IR (neat): 3029, 2932, 1552, 1495, 1446, 1274, 1146, 1105, 1076 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{28}H_{24}FN_2O$ [M+H], 423.1873; found, 423.1873.



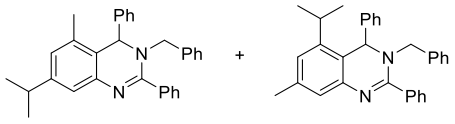
3-Benzyl-2,4-diphenyl-7-(tert-butyl)-3,4-dihydroquinazoline (4e). Prepared according to the general 3,4-dihydroquinazoline protocol with **3e** (0.254 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 48 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (5% ether in CH_2Cl_2 as eluent) to afford the desired product (0.191 g, 44% yield) as a solid (m.p. = 64 – 65 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.50 (m, 2H), 7.42 – 7.23 (m, 12H), 7.19 (d, *J* = 6.7 Hz, 2H), 6.97 (dd, *J* = 8.0, 2.1 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 5.42 (s, 1H), 4.69 (d, *J* = 15.6 Hz, 1H), 3.95 (d, *J* = 15.6 Hz, 1H), 1.28 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.8, 151.4, 143.8, 140.2, 136.3, 129.3, 129.0, 128.8, 128.7, 128.1, 128.0, 127.8, 127.5, 127.0, 126.0, 122.2, 121.9, 121.6, 60.6, 53.1, 34.6, 31.3; IR (neat): 3029, 2961, 1582, 1549, 1493, 1420, 1089 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{31}H_{31}N_2$ [M+H], 431.2487; found, 431.2468.



3-Benzyl-6,7-dimethyl-2,4-diphenyl-3,4-dihydroquinazoline (4f). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3f** (0.226 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 48 h at rt after addition of Tf_2O and was worked up as described above. The residue was purified by flash chromatography (2% MeOH, 20% EtOAc, 78% hexanes as eluent) to afford the desired product (0.279 g, 69% yield) as a solid (m.p. = 63 - 66 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.45 (m, 2H), 7.41 – 7.12 (m, 14H), 6.47 (s, 1H), 5.33 (s, 1H), 4.67 (d, *J* = 15.7 Hz, 1H), 3.96 (d, *J* = 15.7 Hz, 1H), 2.17 (s, 3H), 2.04 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.3, 144.1, 139.1, 136.8, 136.7, 136.4, 133.3, 129.1, 129.0, 128.8, 128.6, 128.5, 128.04, 128.00, 127.6, 127.28, 127.27, 126.9, 126.0, 122.1, 60.5, 53.2, 19.5, 19.2; IR (neat): 3027, 2920, 1582, 1551, 1493, 1452, 1422, 1318, 1154 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{29}H_{27}N_2$ [M+H], 403.2174; found, 403.2170.

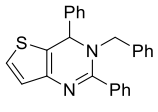


3-Benzyl-5,7-dimethyl-2,4-diphenyl-3,4-dihydroquinazoline (4g). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3g** (0.238 g, 1.06 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 48 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (0% - 2% methanol in 96:4 CH_2Cl_2:ether mixture as eluent) to afford the desired product (0.258 g, 61% yield) as a solid (m.p. = 90 - 92 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.19 (m, 15H), 7.09 (s, 1H), 6.68 – 6.62 (m, 1H), 5.32 (s, 1H), 4.64 (d, *J* = 15.7 Hz, 1H), 4.13 (d, *J* = 15.6 Hz, 1H), 2.28 (s, 3H), 1.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.5, 141.9, 137.7, 136.9, 136.6, 133.6, 129.2, 128.8, 128.6, 128.5, 128.4, 128.1, 128.0, 127.9, 127.8, 127.7, 127.2, 123.3, 120.9, 58.0, 53.2, 21.1, 18.2; IR (neat): 3027, 2915, 1588, 1543, 1446, 1325, 1157, 1047 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{29}H_{27}N_2$ [M+H], 403.2174; found, 403.2183.

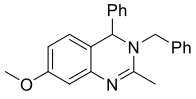


3-Benzyl-7-isopropyl-5-methyl-2,4-diphenyl-3,4-dihydroquinazoline (4ha) and 3-Benzyl-5-isopropyl-7-methyl-2,4-diphenyl-3,4-dihydroquinazoline (4hb). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3h** (0.253 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 48 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (20% to 25% EtOAc in cyclohexane as eluent) to afford the desired product (0.257 g, 60% yield) as a 2.7:1 mixture of regioisomers. **Major regioisomer 4ha** (solid, m.p. = 171 – 174 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.21 (m, 15H), 7.14 (s, 1H), 6.69 (s, 1H), 5.32 (s, 1H), 4.61 (d, *J* = 15.6 Hz, 1H), 4.08 (d, *J* = 15.7 Hz, 1H), 2.83 (hept, *J* = 6.9 Hz, 1H), 1.85 (s, 3H), 1.24 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.4, 148.7, 142.0, 141.9, 136.8, 136.8, 133.6, 129.1, 128.82, 128.80, 128.5, 128.0, 127.9, 127.7, 127.4, 125.5, 121.1,

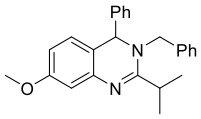
120.7, 58.2, 53.0, 33.7, 24.1, 23.7, 18.4; IR (neat): 3025, 2958, 1590, 1545, 1446, 1323, 1157, 1075 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{31}H_{31}N_2$ [M+H], 431.2487; found, 431.2477. **Minor regioisomer 4hb** (solid, m.p. = 64 – 69 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.12 (m, 16H), 6.80 (s, 1H), 5.50 (s, 1H), 4.69 (d, *J* = 15.5 Hz, 1H), 4.23 (d, *J* = 15.4 Hz, 1H), 2.61 (hept, *J* = 6.8 Hz, 1H), 2.34 (s, 3H), 0.86 (d, *J* = 6.8 Hz, 3H), 0.71 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.3, 144.3, 142.1, 138.2, 136.7, 135.8, 129.7, 128.9, 128.8, 128.6, 128.4, 128. 1, 127.9, 127.6, 127.5, 123.4, 122. 8, 118.8, 57.2, 53.6, 27.9, 24.0, 22.5, 21.4; IR (neat): 3029, 2961, 1579, 1545, 1456, 1325, 1156, 1027 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{31}H_{31}N_2$ [M+H], 431.2487; found, 431.2483.



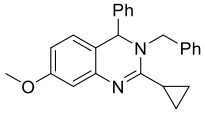
6-Benzyl-5,7-diphenyl-1-thia-4,6-diaza-3a,6,7,7a-tetrahydroindene (4i). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3i** (0.204 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was purified by flash chromatography (25% EtOAc in hexanes as eluent) to afford the desired product (0.151 g, 40% yield) as a solid (m.p. = 171 – 174 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, *J* = 7.6, 2.1 Hz, 2H), 7.43 – 7.26 (m, 11H), 7.19 (d, *J* = 6.7 Hz, 2H), 7.05 (d, *J* = 5.2 Hz, 1H), 7.01 (d, *J* = 5.2 Hz, 1H), 5.72 (s, 1H), 4.72 (d, *J* = 15.7 Hz, 1H), 3.92 (d, *J* = 15.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7, 142.7, 142.5, 136.5, 136.1, 129.2, 129.0, 128.9, 128.6, 128.4, 128.0, 127.8, 127.3, 126.8, 124.7, 123.3, 118.9, 60.0, 53.3; IR (neat): 3027, 2920, 1152, 1534, 1409, 1308, 1157 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{21}N_2S$ [M+H], 381.1425; found, 381.1424.



3-Benzyl-7-methoxy-2-methyl-4-phenyl-3,4-dihydroquinazoline (4j). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3j** (0.165 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was purified by flash chromatography (0% - 1% MeOH in EtOAc as eluent) to afford the desired product (0.218 g, 64% yield) as an oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.17 (m, 10H), 6.74 (d, *J* = 2.6 Hz, 1H), 6.59 (d, *J* = 8.4 Hz, 1H), 6.47 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.36 (s, 1H), 4.73 (d, *J* = 16.6 Hz, 1H), 4.09 (d, *J* = 16.6 Hz, 1H), 3.75 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 156.4, 144.0, 142.0, 136.1, 129.0, 129.0, 128.0, 127.7, 127.2, 126.9, 126.6, 117.1, 111.6, 107.8, 62.0, 55.2, 51.8, 22.8. IR (neat) 3025, 2952, 1588, 1556, 1493, 1442, 1150, 1029 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{23}H_{23}N_2O$ [M+H], 343.1810; found, 343.1826.

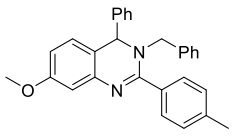


3-Benzyl-2-isopropyl-7-methoxy-4-phenyl-3,4-dihydroquinazoline (4k). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3k** (0.194 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was purified by flash chromatography (10% - 20% EtOAc in 100:2 hexanes:TEA mixture as eluent) to afford the desired product (0.329 g, 88% yield) as a solid (m.p. = 131 – 134 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.17 (m, 10H), 6.79 (s, 1H), 6.58 (d, *J* = 8.3 Hz, 1H), 6.46 (dd, *J* = 8.3, 2.6 Hz, 1H), 5.30 (s, 1H), 4.81 (d, *J* = 16.8 Hz, 1H), 4.10 (d, *J* = 16.8 Hz, 1H), 3.77 (s, 3H), 2.81 (hept, *J* = 6.6 Hz, 1H), 1.29 (d, *J* = 6.8 Hz, 3H), 1.25 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 159.6, 144.4, 142.5, 136.9, 128.9, 128.8, 127.9, 127.6, 126.9, 126.7, 126.5, 117.1, 111.6, 108.2, 62.4, 55.2, 51.0, 30.6, 20.9, 20.2; IR (neat): 3027, 2963, 1588, 1554, 1493, 1426, 1148, 1031 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{27}N_2O$ [M+H], 371.2123; found, 371.2110.

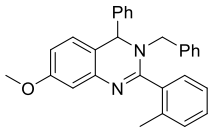


3-Benzyl-2-cyclopropyl-7-methoxy-4-phenyl-3,4-dihydroquinazoline (4l). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3l** (0.191 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as

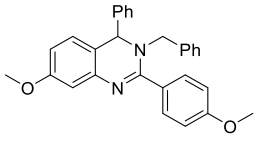
eluent) and the concentrated filtrate was further purified by flash chromatography (20% EtOAc in hexanes as eluent) to afford the desired product (0.234 g, 64% yield) as a solid (m.p. = 126 - 130 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.17 (m, 10H), 6.71 (d, *J* = 2.7 Hz, 1H), 6.58 (d, *J* = 8.4 Hz, 1H), 6.44 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.34 (s, 1H), 5.21 (d, *J* = 16.4 Hz, 1H), 4.14 (d, *J* = 16.4 Hz, 1H), 3.73 (s, 3H), 1.66 (tt, *J* = 8.3, 5.0 Hz, 1H), 1.30 – 1.24 (m, 1H), 1.04 – 0.94 (m, 1H), 0.89 – 0.75 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 158.9, 144.1, 142.5, 136.8, 128.9, 127.9, 127.5, 126.94, 126.91, 126.8, 117.2, 111.4, 108.1, 62.0, 55.2, 51.2, 14.1, 7.5, 6.0; IR (neat): 3004, 2932, 1591, 1549, 1493, 1428, 1150, 1029 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{25}N_2O$ [M+H], 369.1967; found, 369.1968.



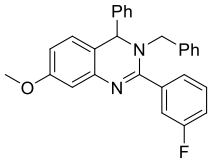
3-Benzyl-7-methoxy-4-phenyl-2-(p-tolyl)-3,4-dihydroquinazoline (4m). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3m** (0.242 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (30% EtOAc in hexanes as eluent) to afford the desired product (0.355 g, 85% yield) as a solid (m.p. = 152 – 155 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.1 Hz, 2H), 7.38 – 7.21 (m, 8H), 7.18 (d, *J* = 7.8 Hz, 4H), 6.89 (d, *J* = 2.6 Hz, 1H), 6.60 (d, *J* = 8.5 Hz, 1H), 6.50 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.36 (s, 1H), 4.74 (d, *J* = 15.7 Hz, 1H), 3.98 (d, *J* = 15.7 Hz, 1H), 3.75 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 158.4, 144.1, 142.5, 139.3, 136.7, 133.7, 129.3, 129.0, 128.9, 128.1, 128.0, 127.7, 127.3, 127.2, 126.9, 117.2, 112.1, 108.7, 60.5, 55.3, 53.4, 21.4; IR (neat): 3025, 2922, 1586, 1545, 1493, 1420, 1262, 1124, 1034 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{29}H_{27}N_2O$ [M+H], 419.2123; found, 419.2104.



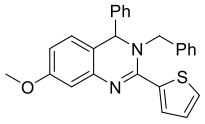
3-Benzyl-7-methoxy-4-phenyl-2-(o-tolyl)-3,4-dihydroquinazoline (4n). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3n** (0.245 g, 1.02 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (30% EtOAc in hexanes as eluent) to afford the desired product (0.205 g, 48% yield) as a solid (m.p. = 137 – 139 °C). ^{1}H NMR (400 MHz, DMSO-d6, heated to 330 K) δ 7.45 – 7.20 (m, 12H), 7.17 (d, *J* = 7.1 Hz, 2H), 6.74 (d, *J* = 8.4 Hz, 1H), 6.68 (d, *J* = 2.6 Hz, 1H), 6.56 (dd, *J* = 8.3, 2.6 Hz, 1H), 5.50 (s, 1H), 4.28 (d, *J* = 16.0 Hz, 1H), 4.04 (d, *J* = 15.9 Hz, 1H), 3.74 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (101 MHz, DMSO-d6, heated to 330 K) δ 159.1, 156.7, 143.2, 142.5, 136.2, 135.5, 135.3, 130.0, 128.54, 128.52, 128.45, 127.7, 127.3, 127.0, 126.9, 126.8, 125.5, 116.8, 110.9, 108.5, 59.9, 54.8, 51.6, 18.4; IR (neat): 3029, 2932, 1589, 1552, 1489, 1454, 1258, 1135, 1034 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{29}H_{27}N_2O$ [M+H], 419.2123; found, 419.2104.



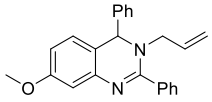
3-Benzyl-7-methoxy-2-(p-methoxyphenyl)-4-phenyl-3,4-dihydroquinazoline (4o). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3o** (0.257 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (30% EtOAc in hexanes as eluent) to afford the desired product (0.297 g, 68% yield) as solid (m.p. = 78 - 81 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.7 Hz, 2H), 7.39 – 7.21 (m, 8H), 7.18 (d, *J* = 6.7 Hz, 2H), 6.93 – 6.87 (m, 3H), 6.61 (d, *J* = 8.4 Hz, 1H), 6.50 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.35 (s, 1H), 4.79 (d, *J* = 15.7 Hz, 1H), 4.02 (d, *J* = 15.6 Hz, 1H), 3.76 (s, 3H), 3.75 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.5, 159.6, 158.0, 144.0, 142.6, 136.7, 129.6, 129.0, 128.8, 128.0, 127.7, 127.2, 127.0, 126.8, 117.3, 114.0, 112.0, 108.5, 60.5, 55.3, 55.2, 53.5; IR (neat): 3027, 2935, 1608, 1543, 1493, 1422, 1251, 1172, 1123, 1031 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{29}H_{27}N_2O_2$ [M+H], 435.2073; found, 435.2084.



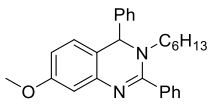
3-Benzyl-2-(m-fluorophenyl)-7-methoxy-4-phenyl-3,4-dihydroquinazoline (4p). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3p** (0.243 g, 0.99 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (20% EtOAc in hexanes as eluent) to afford the desired product (0.270 g, 65% yield) of the title compound as a solid (m.p. = 142 - 145 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.15 (m, 13H), 7.07 (tdd, *J* = 8.4, 2.7, 1.2 Hz, 1H), 6.88 (d, *J* = 2.6 Hz, 1H), 6.62 (d, *J* = 8.4 Hz, 1H), 6.53 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.37 (s, 1H), 4.65 (d, *J* = 15.7 Hz, 1H), 4.01 (d, *J* = 15.7 Hz, 1H), 3.76 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7 (d, $^1J_{C\text{-}F}$ = 248 Hz), 159.7, 156.8 (d, $^4J_{C\text{-}F}$ = 3 Hz), 143.8, 142.1, 138.7 (d, $^3J_{C\text{-}F}$ = 7 Hz), 136.3, 130.4 (d, $^3J_{C\text{-}F}$ = 8 Hz), 129.1, 128.9, 128.2, 127.9, 127.24, 127.22, 126.9, 123.7 (d, $^4J_{C\text{-}F}$ = 3 Hz), 117.1, 116.4 (d, $^2J_{C\text{-}F}$ = 21 Hz), 115.4 (d, $^2J_{C\text{-}F}$ = 23 Hz), 112.5, 108.8, 60.5, 55.2, 53.3; IR (neat): 3029, 2937, 1586, 1549, 1487, 1457, 1271, 1150, 1049 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{28}H_{24}FN_2O$ [M+H], 423.1873; found, 423.1873.



3-Benzyl-7-methoxy-4-phenyl-2-(2-thienyl)-3,4-dihydroquinazoline (4q). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **3q** (0.233 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (30% EtOAc in hexanes as eluent) to afford the desired product (0.213 g, 52% yield) as a solid (m.p. = 143 - 148 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.35 – 7.20 (m, 11H), 7.02 (dd, *J* = 5.1, 3.6 Hz, 1H), 6.87 (d, *J* = 2.6 Hz, 1H), 6.64 (d, *J* = 8.4 Hz, 1H), 6.54 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.35 (s, 1H), 5.15 (d, *J* = 15.6 Hz, 1H), 4.19 (d, *J* = 15.6 Hz, 1H), 3.77 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 152.4, 143.6, 142.3, 138.4, 136.6, 129.0, 128.9, 128.4, 128.0, 127.9, 127.8, 127.4, 127.0, 126.9, 126.7, 117.4, 112.5, 108.5, 60.8, 55.3, 53.9; IR (neat): 3027, 2928, 1584, 1541, 1491, 1275, 1150, 1030 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{26}H_{23}N_2OS$ [M+H], 411.1531; found, 411.1513.

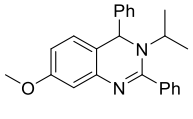


3-Allyl-7-methoxy-2,4-diphenyl-3,4-dihydroquinazoline (5a). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.227 g, 1.00 mmol), allylamine (0.080 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (35% EtOAc in hexanes as eluent) to afford the desired product (0.213 g, 61% yield) as an oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.43 (m, 2H), 7.41 – 7.36 (m, 5H), 7.38 – 7.29 (m, 2H), 7.29 – 7.24 (m, 1H), 6.86 (d, *J* = 2.6 Hz, 1H), 6.76 (d, *J* = 8.4 Hz, 1H), 6.58 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.64 (dddd, *J* = 17.2, 9.9, 7.2, 4.1 Hz, 1H), 5.55 (s, 1H), 5.24 – 5.20 (m, 1H), 5.19 (t, *J* = 1.5 Hz, 1H), 3.99 (ddt, *J* = 16.1, 4.0, 1.9 Hz, 1H), 3.76 (s, 3H), 3.52 (ddt, *J* = 16.1, 7.3, 1.3 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 158.1, 144.3, 142.5, 136.5, 133.0, 129.3, 129.0, 128.5, 128.0, 127.9, 127.1, 126.8, 118.2, 117.3, 112.3, 108.6, 60.6, 55.3, 52.8; IR (neat): 3062, 2954, 1586, 1547, 1491, 1265, 1139, 1034 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{23}N_2O$ [M+H], 355.1810; found, 355.1802.

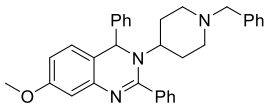


3-Hexyl-7-methoxy-2,4-diphenyl-3,4-dihydroquinazoline (5b). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.229 g, 1.01 mmol), hexylamine (0.14 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (30% EtOAc in hexanes as eluent) to

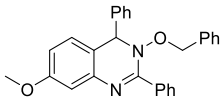
afford the desired product (0.171 g, 43% yield) as an oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.43 (m, 2H), 7.43 – 7.37 (m, 5H), 7.36 – 7.31 (m, 2H), 7.29 – 7.24 (m, 1H), 6.84 (d, *J* = 2.6 Hz, 1H), 6.79 (d, *J* = 8.5 Hz, 1H), 6.58 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.55 (s, 1H), 3.77 (s, 3H), 3.32 (ddd, *J* = 14.3, 8.9, 7.2 Hz, 1H), 2.98 (ddd, *J* = 14.0, 8.8, 4.9 Hz, 1H), 1.60 – 1.40 (m, 2H), 1.21 – 1.00 (m, 6H), 0.78 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 158.4, 144.8, 142.7, 136.9, 129.2, 129.0, 128.5, 128.0, 127.9, 126.9, 126.5, 117.4, 112.1, 108.4, 61.4, 55.3, 50.3, 31.2, 27.9, 26.0, 22.4, 13.9; IR (neat): 2930, 1586, 1545, 1491, 1273, 1142 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{27}H_{31}N_2O$ [M+H], 399.2436; found, 399.2437.



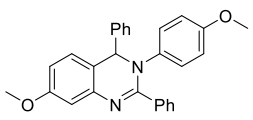
3-Isopropyl-7-methoxy-2,4-diphenyl-3,4-dihydroquinazoline (5c). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.228 g, 1.00 mmol), isopropylamine (0.095 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 48 h at rt after addition of Tf_2O and was worked up as described above. The residue was purified by flash chromatography (0% - 1% methanol in 96:4 CH_2Cl_2:ether mixture as eluent) to afford the desired product (0.141 g, 39% yield) as an oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.66 (m, 2H), 7.48 – 7.38 (m, 5H), 7.27 (t, *J* = 7.8 Hz, 2H), 7.19 (t, *J* = 7.3 Hz, 1H), 6.97 (d, *J* = 8.3 Hz, 1H), 6.87 (d, *J* = 2.6 Hz, 1H), 6.63 (dd, *J* = 8.3, 2.6 Hz, 1H), 5.56 (s, 1H), 4.09 (hept, *J* = 6.7 Hz, 1H), 3.77 (s, 3H), 1.13 (dd, *J* = 9.4, 6.7 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 159.2, 146.7, 143.1, 137.3, 129.9, 128.9, 128.6, 128.4, 127.3, 126.1, 125.4, 119.1, 112.3, 108.5, 55.7, 55.3, 52.3, 22.2, 21.5; IR (neat): 3058, 2930, 1584, 1536, 1489, 1273, 1165, 1109, 1031 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{25}N_2O$ [M+H], 357.1967; found, 357.1982.



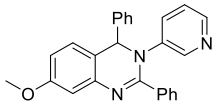
3-(1-Benzyl-4-piperidyl)-7-methoxy-2,4-diphenyl-3,4-dihydroquinazoline (5d). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.230 g, 1.01 mmol), 4-amino-1-benzylpiperidine (0.22 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (25% EtOAc in hexanes as eluent) to afford the desired product (0.422 g, 85% yield) as a solid (m.p. = 84 - 86 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.66 (m, 2H), 7.52 – 7.34 (m, 5H), 7.32 – 7.11 (m, 8H), 6.95 (d, *J* = 8.3 Hz, 1H), 6.87 (d, *J* = 2.6 Hz, 1H), 6.64 (dd, *J* = 8.3, 2.6 Hz, 1H), 5.63 (s, 1H), 3.75 (s, 3H), 3.67 – 3.55 (m, 1H), 3.36 (d, *J* = 2.6 Hz, 2H), 2.80 (ddd, *J* = 11.5, 5.6, 3.0 Hz, 2H), 2.00 (qd, *J* = 12.1, 4.1 Hz, 1H), 1.86 (qd, *J* = 12.2, 3.9 Hz, 1H), 1.78 – 1.62 (m, 3H), 1.42 (ddd, *J* = 12.6, 4.3, 2.3 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 159.1, 146.2, 143.0, 137.9, 136.9, 130.0, 129.1, 128.8, 128.6, 128.3, 128.2, 127.3, 127.1, 126.0, 125.4, 119.1, 112.3, 108.5, 62.8, 59.1, 56.5, 55.2, 52.82, 52.79, 32.0, 30.9; IR (neat): 3027, 2943, 1584, 1539, 1489, 1446, 1269, 1133, 1031 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{33}H_{34}N_3O$ [M+H], 488.2702; found, 488.2675.



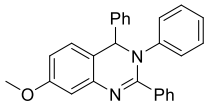
3-(Benzyloxy)-7-methoxy-2,4-diphenyl-3,4-dihydroquinazoline (5f). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.228 g, 1.00 mmol), O-benzyl hydroxylamine (0.175 g, 1.10 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (3% ether in CH_2Cl_2 as eluent) to afford the desired product (0.234 g, 56% yield) as an oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 8.2, 1.5 Hz, 2H), 7.41 – 7.23 (m, 8H), 7.23 – 7.10 (m, 3H), 6.91 (d, *J* = 2.6 Hz, 1H), 6.78 (d, *J* = 6.9 Hz, 2H), 6.68 (d, *J* = 8.5 Hz, 1H), 6.57 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.72 (s, 1H), 4.50 (d, *J* = 9.9 Hz, 1H), 4.26 (d, *J* = 9.9 Hz, 1H), 3.75 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 158.0, 142.2, 141.8, 134.3, 134.2, 129.5, 129.4, 128.8, 128.6, 128.6, 128.3, 128.1, 127.8, 127.3, 120.1, 112.3, 109.4, 76.7, 64.2, 55.3; IR (neat): 3062, 2935, 1672, 1586, 1541, 1493, 1456, 1271, 1031 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{28}H_{25}N_2O_2$ [M+H], 421.1916; found, 421.1900.



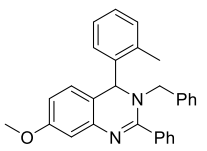
7-Methoxy-3-(p-methoxyphenyl)-2,4-diphenyl-3,4-dihydroquinazoline (5g). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.228 g, 1.00 mmol), *p*-anisidine (0.137 g, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was purified by flash chromatography (20% EtOAc in hexanes as eluent) to afford the desired product (0.372 g, 88% yield) as a solid (m.p. = 154 - 157 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 7.5, 2.2 Hz, 2H), 7.46 (d, *J* = 7.2 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 2H), 7.27 – 7.17 (m, 4H), 6.99 (d, *J* = 2.6 Hz, 1H), 6.90 (d, *J* = 8.4 Hz, 1H), 6.81 (d, *J* = 9.0 Hz, 2H), 6.66 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.59 (d, *J* = 9.0 Hz, 2H), 5.71 (s, 1H), 3.79 (s, 3H), 3.63 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 156.8, 155.6, 145.4, 142.2, 139.4, 136.7, 129.5, 129.3, 129.2, 128.0, 127.8, 126.4, 126.2, 125.7, 118.7, 113.8, 112.7, 108.9, 66.2, 55.3, 55.3; IR (neat): 3058, 2954, 1588, 1543, 1508, 1491, 1247, 1034 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{28}H_{25}N_2O_2$ [M+H], 421.1916; found, 421.1913.



7-Methoxy-2,4-diphenyl-3-(3-pyridyl)-3,4-dihydroquinazoline (5h). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.232 g, 1.02 mmol), 3-aminopyridine (0.107 g, 1.14 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was purified by flash chromatography (30% EtOAc in hexanes as eluent) to afford the desired product (0.230 g, 56% yield) as a solid (m.p. = 148 – 152 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 2.8 Hz, 1H), 8.21 (dd, *J* = 4.7, 1.4 Hz, 1H), 7.60 (dd, *J* = 6.6, 1.7 Hz, 2H), 7.49 (d, *J* = 7.1 Hz, 2H), 7.35 (t, *J* = 7.3 Hz, 2H), 7.31 – 7.22 (m, 4H), 7.19 (ddd, *J* = 8.2, 2.7, 1.5 Hz, 1H), 7.05 – 7.00 (m, 2H), 6.97 (d, *J* = 8.4 Hz, 1H), 6.72 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.79 (s, 1H), 3.83 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 154.6, 145.5, 145.4, 144.5, 142.6, 141.7, 135.7, 130.9, 130.1, 129.7, 129.4, 128.5, 128.2, 126.5, 125.6, 123.1, 118.7, 113.4, 109.4, 65.7, 55.4; IR (neat): 3030, 1590, 1549, 1491, 1325, 1273, 1046 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{26}H_{22}N_3O$ [M+H], 392.1763; found, 392.1754.

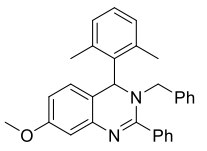


7-Methoxy-2,3,4-triphenyl-3,4-dihydroquinazoline (5i). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.227 g, 1.00 mmol), aniline (0.10 mL, 1.1 mmol), benzaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-fluoropyridine (0.10 mL, 1.2 mmol) instead of 2-chloropyridine, and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 48 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (1% ether in CH_2Cl_2 as eluent) to afford the desired product (0.208 g, 53% yield) as a solid (m.p. = 131 – 134 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (dt, *J* = 7.8, 1.3 Hz, 2H), 7.49 (dd, *J* = 8.2, 1.3 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.30 – 7.20 (m, 4H), 7.09 (t, *J* = 7.8 Hz, 2H), 7.02 (d, *J* = 2.6 Hz, 1H), 6.98 (t, *J* = 8.4 Hz, 2H), 6.92 (d, *J* = 7.6 Hz, 2H), 6.70 (dd, *J* = 8.3, 2.6 Hz, 1H), 5.81 (s, 1H), 3.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 155.5, 146.2, 145.1, 142.0, 136.4, 130.9, 129.6, 129.2, 128.7, 128.1, 127.9, 126.4, 125.6, 124.7, 124.4, 119.0, 112.9, 109.0, 65.8, 55.4; IR (neat): 3058, 2956, 1586, 1541, 1489, 1273, 1126, 1031 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{27}H_{23}N_2O$ [M+H], 391.1810; found, 391.1791.

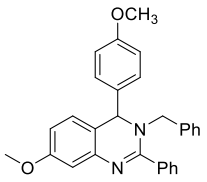


3-Benzyl-7-methoxy-2-phenyl-4-(o-tolyl)-3,4-dihydroquinazoline (5j). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.227 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), o-tolualdehyde (0.13 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (30% EtOAc in hexanes as eluent) to afford the desired product (0.262 g, 63% yield) as a solid (m.p. = 65 – 69 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.52 (m, 2H), 7.45 – 7.34 (m, 4H), 7.34 – 7.13 (m, 8H), 6.85 (d, *J* = 2.5 Hz, 1H), 6.53 (d, *J* = 8.4 Hz, 1H), 6.47 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.80 (s, 1H), 4.70 (d, *J* = 16.0 Hz, 1H), 3.83 (d, *J* = 16.0 Hz, 1H), 3.75 (s, 3H), 2.30 (s, 3H); ^{13}C NMR

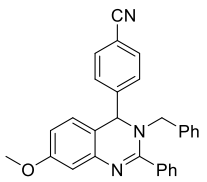
(101 MHz, $CDCl_3$) δ 159.5, 158.5, 142.4, 142.3, 136.7, 136.6, 134.9, 131.1, 129.2, 129.1, 128.8, 128.7, 127.9, 127.8, 127.7, 127.1, 126.9, 126.8, 117.0, 112.1, 108.7, 57.8, 55.2, 53.0, 19.3; IR (neat): 3023, 2924, 1586, 1547, 1491, 1444, 1424, 1258, 1154, 1129, 1032 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{29}H_{27}N_2O$ [M+H], 419.2123; found, 419.2098.



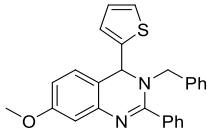
3-Benzyl-7-methoxy-2-phenyl-4-(2,6-xylyl)-3,4-dihydroquinazoline (5k). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.227 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), 2,6-dimethylbenzaldehyde (0.15 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 48 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (40% EtOAc in hexanes as eluent) to afford the desired product (0.167 g, 39% yield) as a solid (m.p. = 63 - 66 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.51 (m, 2H), 7.40 – 7.22 (m, 6H), 7.17 – 7.06 (m, 4H), 6.96 (d, *J* = 6.8 Hz, 1H), 6.78 (d, *J* = 2.6 Hz, 1H), 6.43 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.40 – 6.32 (m, 2H), 4.68 (d, *J* = 16.5 Hz, 1H), 3.76 (s, 3H), 3.67 (d, *J* = 16.5 Hz, 1H), 2.45 (s, 3H), 1.87 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 158.9, 142.7, 138.6, 138.3, 136.9, 136.7, 136.3, 131.0, 129.1, 128.9, 128.7, 128.3, 127.9, 127.6, 127.4, 126.8, 126.3, 115.4, 111.9, 108.5, 56.0, 55.3, 52.3, 20.1, 19.9; IR (neat): 2922, 1588, 1551, 1493, 1154 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{30}H_{29}N_2O$ [M+H], 433.2280; found, 433.2275.



3-Benzyl-7-methoxy-4-(p-methoxyphenyl)-2-phenyl-3,4-dihydroquinazoline (5l). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.229 g, 1.01 mmol), benzylamine (0.12 mL, 1.1 mmol), p-anisaldehyde (0.13 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was purified by flash chromatography (5% - 10% ether in CH_2Cl_2 as eluent) to afford the desired product (0.214 g, 49% yield) as a solid (m.p. = 133 – 137 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.45 (m, 2H), 7.41 – 7.34 (m, 3H), 7.33 – 7.24 (m, 5H), 7.19 (d, *J* = 6.8 Hz, 2H), 6.88 (dd, *J* = 5.7, 3.0 Hz, 3H), 6.60 (d, *J* = 8.4 Hz, 1H), 6.52 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.33 (s, 1H), 4.67 (d, *J* = 15.7 Hz, 1H), 4.01 (d, *J* = 15.7 Hz, 1H), 3.78 (s, 3H), 3.77 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 159.4, 158.1, 142.3, 136.6, 136.6, 136.5, 129.3, 128.9, 128.6, 128.2, 127.9, 127.7, 127.3, 127.2, 117.4, 114.3, 112.2, 108.5, 59.8, 55.3, 53.1; IR (neat): 3006, 2963, 1586, 1547, 1493, 1251, 1174, 1034 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{29}H_{27}N_2O_2$ [M+H], 435.2073; found, 435.2092.

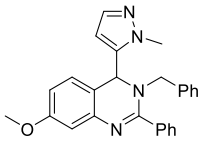


p-(3-Benzyl-7-methoxy-2-phenyl-3,4-dihydroquinazolin-4-yl)benzonitrile (5m). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.229 g, 1.01 mmol), benzylamine (0.12 mL, 1.1 mmol), 4-cyanobenzaldehyde (0.151 g, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was purified by flash chromatography (2% - 10% ether in CH_2Cl_2 as eluent) to afford the desired product (0.388 g, 90% yield) as a solid (m.p. = 65 – 67 °C). ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.80 (d, *J* = 8.4 Hz, 2H), 7.70 – 7.61 (m, 4H), 7.48 – 7.43 (m, 3H), 7.33 – 7.20 (m, 5H), 6.85 – 6.79 (m, 2H), 6.59 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.64 (s, 1H), 4.83 (d, *J* = 15.9 Hz, 1H), 4.20 (d, *J* = 15.9 Hz, 1H), 3.76 (s, 3H); ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 160.9, 158.5, 150.1, 143.9, 137.9, 137.4, 133.7, 130.3, 129.5, 129.2, 129.2, 128.5, 128.3, 128.0, 127.8, 119.1, 117.6, 112.5, 112.3, 110.0, 60.9, 55.5, 54.8; IR (neat): 3064, 2935, 2229, 1586, 1547, 1489, 1446, 1264, 1126, 1025 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{29}H_{24}N_3O$ [M+H], 430.1919; found, 430.1920.

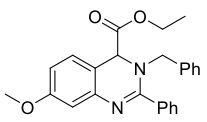


3-Benzyl-7-methoxy-2-phenyl-4-(2-thienyl)-3,4-dihydroquinazoline (5n). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.227 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), 2-thiophenecarboxaldehyde (0.10 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-

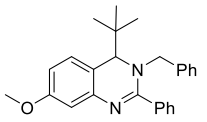
chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (0% - 2% MeOH in 100:3 CH_2Cl_2:ether mixture as eluent) to afford the desired product (0.281 g, 68% yield) as a solid (m.p. = 73 – 75 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.50 (m, 2H), 7.42 – 7.36 (m, 3H), 7.34 – 7.23 (m, 4H), 7.20 (d, *J* = 6.5 Hz, 2H), 6.98 – 6.87 (m, 3H), 6.74 (d, *J* = 8.4 Hz, 1H), 6.59 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.66 (s, 1H), 4.75 (d, *J* = 15.6 Hz, 1H), 4.23 (d, *J* = 15.6 Hz, 1H), 3.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 157.5, 147.3, 142.4, 136.6, 136.4, 129.4, 128.9, 128.6, 128.2, 127.9, 127.4, 126.9, 126.6, 125.7, 124.5, 116. 9, 112.4, 108.7, 55.6, 55.3, 53.6; IR (neat): 3027, 2926, 1584, 1545, 1489, 1325, 1128, 1031 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{26}H_{23}N_2OS$ [M+H], 411.1531; found, 411.1523.



5-(3-Benzyl-7-methoxy-2-phenyl-3,4-dihydroquinazolin-4-yl)-1-methyl-1H-pyrazole (5o). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.227 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), 1-methyl-1H-pyrazole-5-carboxaldehyde (0.11 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 48 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (80% EtOAc in hexanes as eluent) to afford the desired product (0.304 g, 75% yield) as a solid (m.p. = 133 - 134 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.52 (m, 2H), 7.47 – 7.38 (m, 4H), 7.35 – 7.24 (m, 3H), 7.18 (d, *J* = 6.8 Hz, 2H), 6.86 (d, *J* = 1.8 Hz, 1H), 6.58 – 6.55 (m, 2H), 6.23 (d, *J* = 1.8 Hz, 1H), 5.80 (s, 1H), 4.77 (d, *J* = 15.8 Hz, 1H), 3.93 (d, *J* = 15.7 Hz, 1H), 3.78 (s, 3H), 3.77 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1, 158.0, 142.4, 142.3, 138.2, 136.2, 135.7, 129.6, 129.0, 128.8, 128.0, 127.9, 127.3, 127.0, 113.3, 112.6, 108.9, 107.0, 55.3, 53.2, 52.2, 37.1; IR (neat): 3029, 2943, 1586, 1547, 1491, 1420, 1258, 1129 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{26}H_{25}N_4O$ [M+H], 409.2028; found, 409.2023.

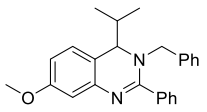


Ethyl 3-benzyl-7-methoxy-2-phenyl-3,4-dihydroquinazoline-4-carboxylate (5p). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.227 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), 50% ethyl glyoxylate in toluene solution (0.225 g, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was purified by flash chromatography (5% - 15% ether in CH_2Cl_2 as eluent) to afford the desired product (0.282 g, 70% yield) as an oil. ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.79 – 7.72 (m, 2H), 7.52 – 7.43 (m, 3H), 7.30 – 7.21 (m, 3H), 7.20 – 7.13 (m, 2H), 7.03 (d, *J* = 8.4 Hz, 1H), 6.69 (d, *J* = 2.6 Hz, 1H), 6.64 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.05 (s, 1H), 4.85 (d, *J* = 15.7 Hz, 1H), 4.31 (d, *J* = 15.7 Hz, 1H), 4.17 (qd, *J* = 7.1, 1.2 Hz, 2H), 3.78 (s, 3H), 1.23 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 171.3, 161.4, 158.9, 144.8, 138.0, 137.7, 130.3, 129.6, 129.5, 129.1, 128.5, 128.3, 128.2, 113.8, 112.1, 109.6, 62.1, 60.0, 55.7, 55.5, 14.5; IR (neat): 3062, 2978, 1735, 1586, 1552, 1491, 1128, 1029 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{25}N_2O_3$ [M+H], 401.1865; found, 401.1868.

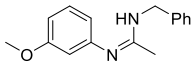


3-Benzyl-4-(tert-butyl)-7-methoxy-2-phenyl-3,4-dihydroquinazoline (5q). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.227 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), trimethylacetaldehyde (0.12 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 24 h at rt after addition of Tf_2O and was worked up as described above. The residue was passed through a silica plug (90:10:0.5 EtOAc:hexanes:TEA as eluent) and the concentrated filtrate was further purified by flash chromatography (3% ether in CH_2Cl_2 as eluent) to afford the desired product (0.234 g, 61% yield) as a solid (m.p. = 45 - 47 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.71 (m, 2H), 7.45 – 7.37 (m, 3H), 7.13 – 7.04 (m, 3H), 6.93 – 6.81 (m, 3H), 6.65 – 6.59 (m, 2H), 4.97 (d, *J* = 15.8 Hz, 1H), 4.28 (d, *J* = 15.9 Hz, 1H), 3.96 (s, 1H), 3.81 (s, 3H), 0.99 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 159.4, 145.1, 138.3, 136. 6, 130.0, 129.1, 128.5, 128.4, 127.9, 127.3, 126.7, 115.3, 111.3, 107.9, 66.6, 58.9, 55.2, 40.9, 26.0; IR (neat): 3029, 2954, 1586,

1541, 1487, 1465, 1333, 1124, 1036 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{26}H_{29}N_2O$ [M+H], 385.2280; found, 385.2277.

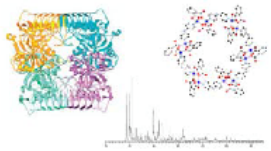


3-Benzyl-4-isopropyl-7-methoxy-2-phenyl-3,4-dihydroquinazoline (5r). Prepared according to the general 3,4-dihydroquinazoline synthesis protocol with **1** (0.227 g, 1.00 mmol), benzylamine (0.12 mL, 1.1 mmol), isobutyraldehyde (0.10 mL, 1.1 mmol), CH_2Cl_2 (10.0 mL), 2-chloropyridine (0.11 mL, 1.2 mmol), and Tf_2O (0.18 mL, 1.1 mmol). The reaction proceeded for 48 h at rt after addition of Tf_2O and was worked up as described above. The residue was purified by flash chromatography (45% EtOAc in cyclohexane as eluent) to afford the desired product (0.014 g, 4% yield) as an oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.62 (m, 2H), 7.41 (ddd, *J* = 4.5, 2.6, 1.4 Hz, 3H), 7.22 – 7.15 (m, 3H), 7.03 – 6.98 (m, 2H), 6.88 (d, *J* = 2.4 Hz, 1H), 6.67 – 6.59 (m, 2H), 4.89 (d, *J* = 15.8 Hz, 1H), 4.31 (d, *J* = 15.8 Hz, 1H), 4.12 (d, *J* = 5.0 Hz, 1H), 3.81 (s, 3H), 2.12 – 2.02 (m, 1H), 1.01 (d, *J* = 6.9 Hz, 3H), 0.96 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.5, 159.4, 144.4, 137.8, 136.4, 129.8, 128.8, 128.60, 128.56, 127.4, 126.80, 126.77, 115.7, 111.4, 107.9, 62.7, 56.4, 55.3, 35.7, 18.5, 18.0; IR (neat): 2957, 1584, 1541, 1489, 1271, 1128, 1034 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{26}H_{25}N_4O$ [M+H], 371.2123; found, 371.2122.



1-Benzylamino-1-(m-methoxyphenylimino)ethane (6). A mixture of **3j** (0.168 g, 1.02 mmol) and 2,6-lutidine (0.26 mL, 2.2 mmol) in CH_2Cl_2 (3.5 mL), cooled to 0 °C in an ice bath, was treated with Tf_2O (0.18 mL, 1.1 mmol). The ice bath was removed and the reaction stirred at rt under N_2 atmosphere for one hour. The reaction was again cooled to 0 °C and benzylamine was added (0.16 mL, 1.5 mmol). The ice bath was removed and the reaction stirred at rt overnight under N_2 atmosphere. The reaction was then diluted with saturated aqueous $NaHCO_3$ solution and the mixture was extracted with CH_2Cl_2 (x3). The pooled organic extracts were dried (Na_2SO_4) and concentrated. The residue was purified by flash chromatography (10% - 30% EtOAc in hexanes as eluent) to afford the desired product (0.217 g, 84% yield) as an oil. ^{1}H NMR (400 MHz, DMSO-d6) δ 7.39 – 7.31 (m, 4H), 7.25 (ddt, *J* = 8.6, 6.0, 2.1 Hz, 1H), 7.14 – 7.04 (m, 2H), 6.46 (ddd, *J* = 8.2, 2.5, 1.0 Hz, 1H), 6.27 – 6.19 (m, 2H), 4.42 (d, *J* = 5.1 Hz, 2H), 3.70 (s, 3H), 1.78 (s, 3H); ^{13}C NMR (101 MHz, DMSO-d6) δ 159.7, 155.0, 153.5, 140.0, 129.1, 128.1, 127.5, 126.5, 114.6, 107.5, 106.6, 54.8, 43.9, 16.7; IR (neat): 3420, 3029, 2937, 1634, 1592, 1482, 1258, 1150 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{16}H_{18}N_2O$ [M+H], 225.1497; found, 225.1487.

X-Ray Crystal Data for Compound **2** (RAM717A)

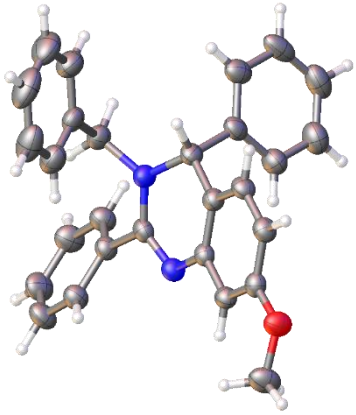


Submitted by: **R. Adam Mosey**
Lake Superior State University
Solved by: **Richard J Staples**
Sample ID: **RAM717A**

Center Crystallographic for Research
Michigan State University
Department of Chemistry
East Lansing, MI 48824
Dr. Richard J. Staples
staples@chemistry.msu.edu

Crystal structure from block-shaped crystals grown by slow evaporation from benzene and pentane (1:1).

Crystal Data and Experimental



Experimental. Single colourless block-shaped crystals of **RAM717A** were used as received. A suitable crystal 0.34×0.32×0.22 mm^3 was selected and mounted on a nylon loop with paratone oil on an Bruker APEX-II CCD diffractometer. The crystal was kept at a steady T = 173(2) K during data collection. The structure was solved with the ShelXT[17] structure solution program using the Intrinsic Phasing solution method and by using **Olex2**[18] as the graphical interface. The model was refined with version 2018/3 of ShelXL[19] using Least Squares minimisation.

Crystal Data. $C_{28}H_{24}N_2O$, M_r = 404.49, orthorhombic, $Pna2_1$ (No. 33), a = 13.3870(8) Å, b = 12.8591(8) Å, c = 12.5553(8) Å, $\alpha = \beta = \gamma = 90^\circ$, V = 2161.3(2) Å^3, T = 173(2) K, Z = 4, Z' = 1, μ(MoK$_\alpha$) = 0.076, 16762 reflections measured, 3954 unique (R_{int} = 0.0381) which were used in all calculations. The final wR_2 was 0.1035 (all data) and R_1 was 0.0400 (I > 2(I)).

Compound	**RAM717A**
Formula	$C_{28}H_{24}N_2O$
$D_{calc.}$/ g cm^{-3}	1.243
μ/mm^{-1}	0.076
Formula Weight	404.49
Colour	colourless
Shape	block
Size/mm^3	0.34×0.32×0.22
T/K	173(2)
Crystal System	orthorhombic
Flack Parameter	0.3(9)
Hooft Parameter	0.2(8)
Space Group	$Pna2_1$
a/Å	13.3870(8)
b/Å	12.8591(8)
c/Å	12.5553(8)
α/°	90
β/°	90
γ/°	90
V/Å^3	2161.3(2)
Z	4
Z'	1
Wavelength/Å	0.710730
Radiation type	MoK$_\alpha$
Θ_{min}/°	2.196
Θ_{max}/°	25.371
Measured Refl.	16762
Independent Refl.	3954
Reflections with I > 2(I)	3442
R_{int}	0.0381
Parameters	281
Restraints	1
Largest Peak	0.119
Deepest Hole	-0.166
GooF	1.055
wR_2 (all data)	0.1035
wR_2	0.0967
R_1 (all data)	0.0478
R_1	0.0400

Structure Quality Indicators

Reflections:	d min (Mo) 0.83	I/σ 30.8	Rint 3.81%	complete 100%
Refinement:	Shift 0.000	Max Peak 0.1	Min Peak -0.2	GooF 1.055	Flack .3(9)

A colourless block-shaped crystal with dimensions 0.34×0.32×0.22 mm^3 was mounted on a nylon loop with paratone oil. Data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford Cryosystems low-temperature device, operating at T = 173(2) K.

Data were measured using ω of -0.50° per frame for 100.84 s using MoK$_\alpha$ radiation (sealed tube, 50 kV, 40 mA). The total number of runs and images was based on the strategy calculation from the program **COSMO**.[20] The actually achieved resolution was Θ = 25.371.

Cell parameters were retrieved using the **SAINT**[21] software and refined using **SAINT** on 7459 reflections, 44% of the observed reflections. Data reduction was performed using the **SAINT** software which corrects for Lorentz polarisation. The final completeness is 100.00 out to 25.371 in Θ. A multi-scan absorption correction was performed using **SADABS**-2014/5 was used for absorption correction. wR_2(int) was 0.0583 before and 0.0549 after correction. The Ratio of minimum to maximum transmission is 0.9049. The λ/2 correction factor is 0.00150. The absorption coefficient μ of this material is 0.076 mm^{-1} at this wavelength (λ = 0.711Å) and the minimum and maximum transmissions are 0.674 and 0.745. **SADABS**-2014/5 was used for absorption correction. wR_2(int) was 0.0583 before and 0.0549 after correction. The Ratio of minimum to maximum transmission is 0.9049. The λ/2 correction factor is 0.00150.

The structure was solved in the space group $Pna2_1$ (# 33) by Intrinsic Phasing using the ShelXT[17] structure solution program. The structure was refined by Least Squares using version 2014/6 of **XL**[3] incorporated in **Olex2**.[18] All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 4 and Z' is 1.

The Flack parameter was refined to 0.3(9). Determination of absolute structure using Bayesian statistics on Bijvoet differences using the Olex2 results in 0.2(8). Note: The Flack parameter is used to determine chirality of the crystal studied, the value should be near 0, a value of 1 means that the stereochemistry is wrong and the model should be inverted. A value of 0.5 means that the crystal consists of a racemic mixture of the two enantiomers.

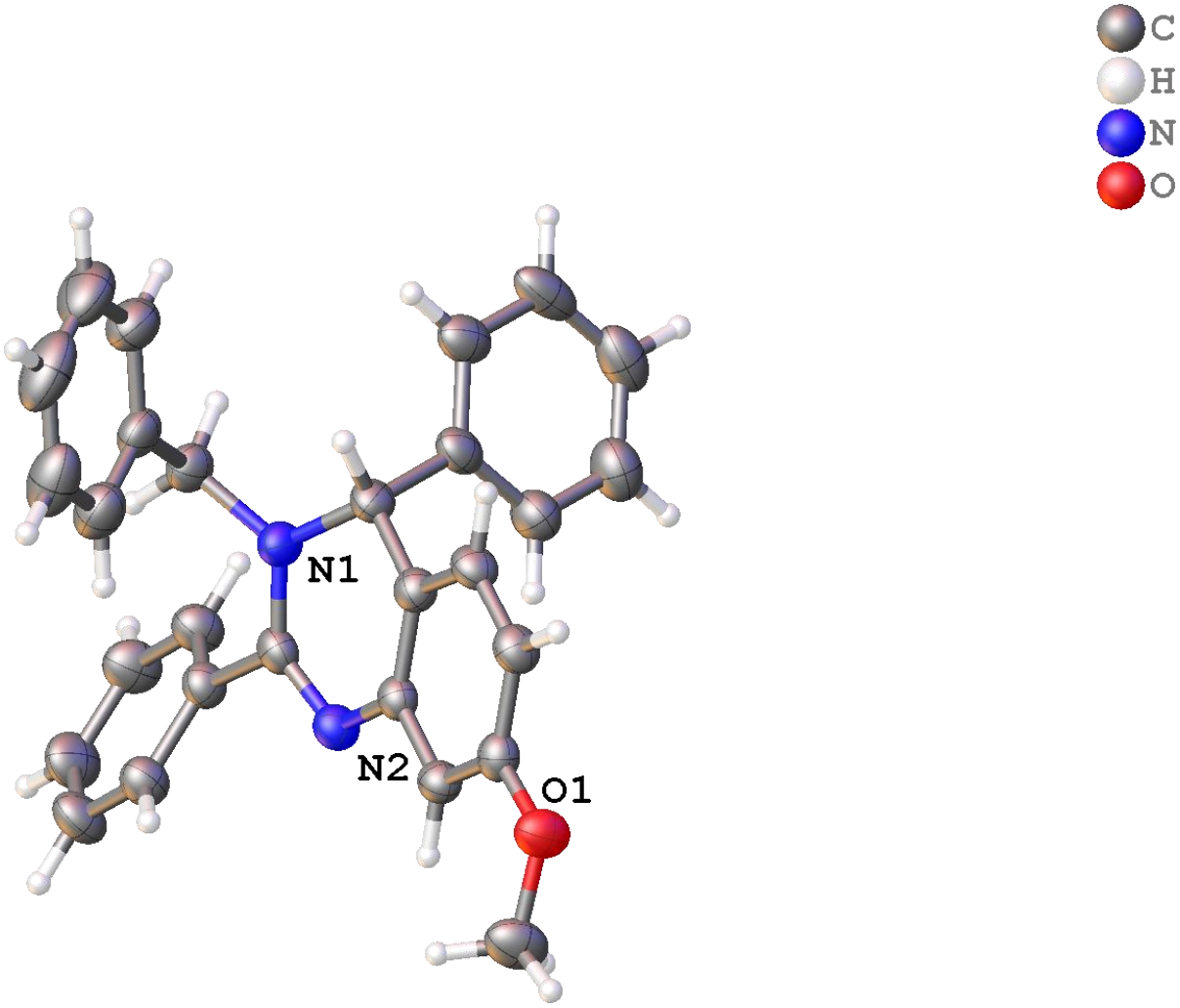


Figure S1. ORTEP representation of compound **2**. Thermal ellipsoids are drawn with 50% probability.

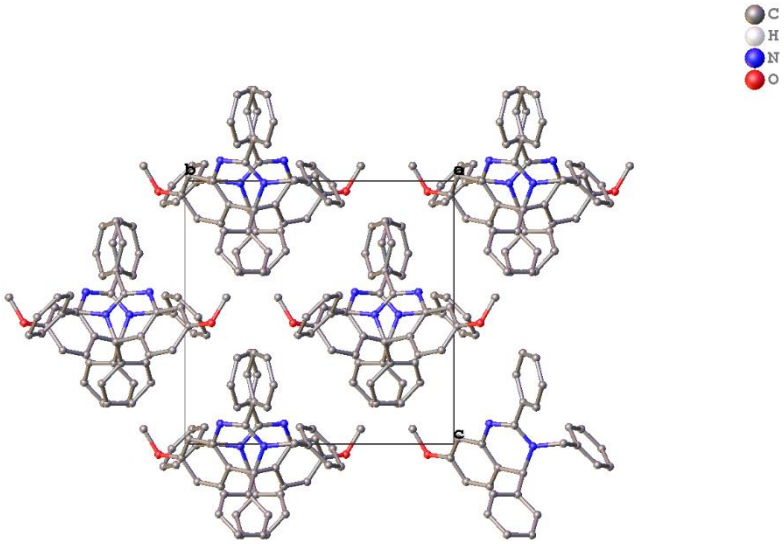
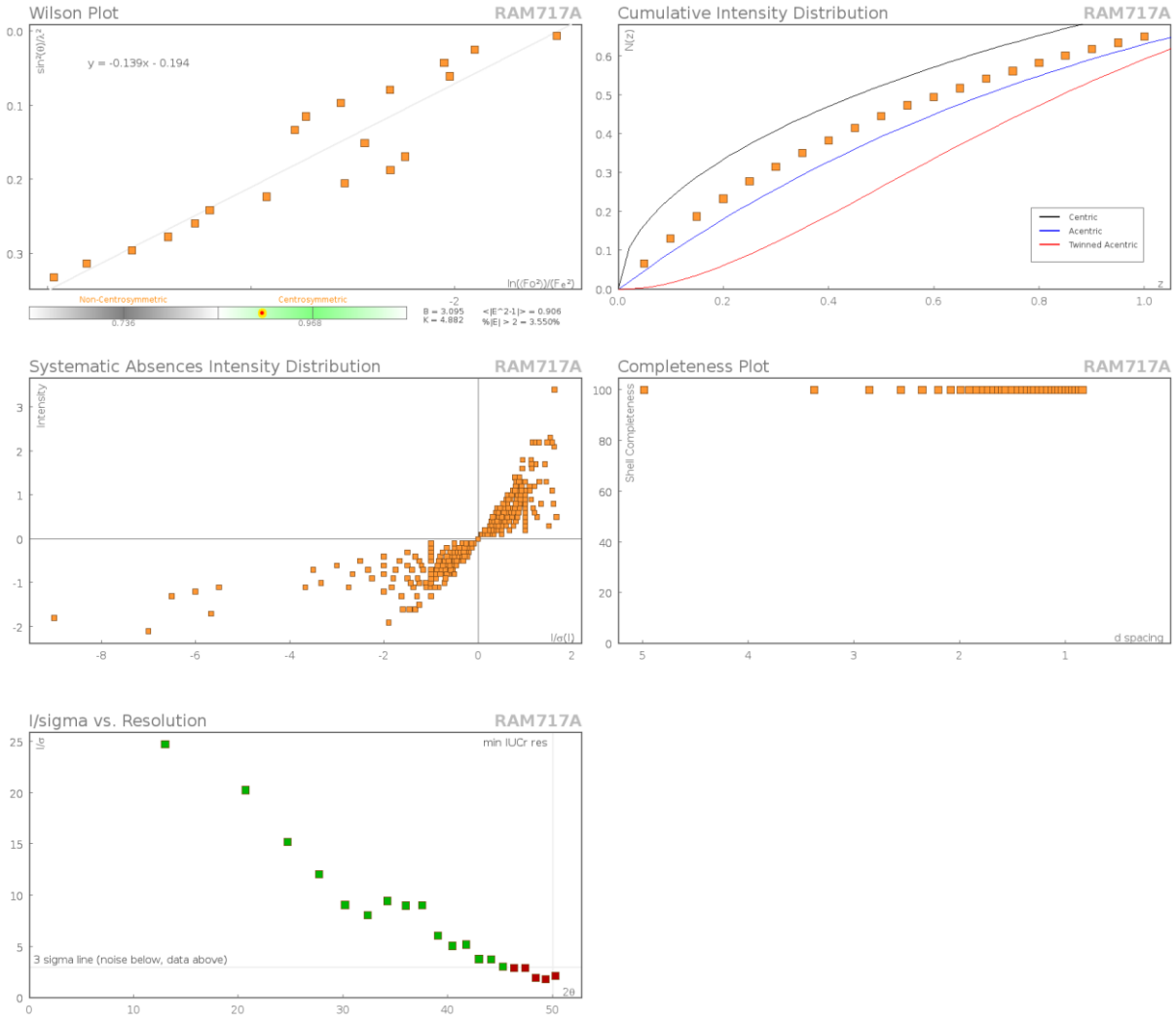
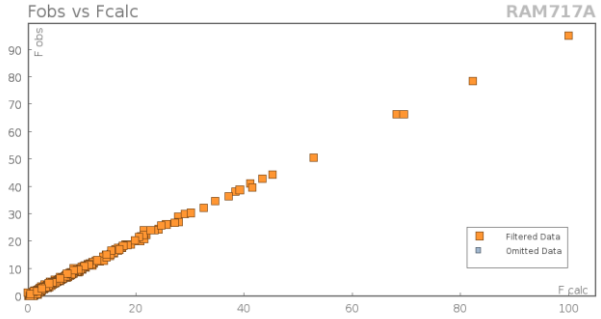


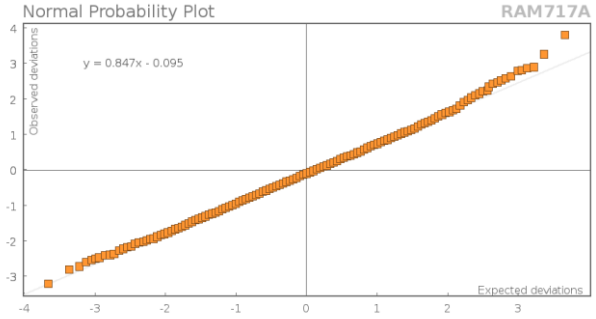
Figure S2: Packing diagram of RAM717A.

Data Plots: Diffraction Data



Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	17607	Unique reflections	3954
Completeness	0.999	Mean I/σ	17.24
hkl_{max} collected	(16, 15, 15)	hkl_{min} collected	(-16, -15, -15)
hkl_{max} used	(16, 15, 15)	hkl_{min} used	(0, 0, -15)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.36
d_{max} used	13.39	d_{min} used	0.83
Friedel pairs	7030	Friedel pairs merged	0
Inconsistent equivalents	0	R_{int}	0.0381
R_{sigma}	0.0325	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	0
Multiplicity	(12302, 2540, 75)	Maximum multiplicity	9
Removed systematic absences	845	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

Table S1: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **RAM717A**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
O1	6094.5(14)	5980.8(17)	5398.8(17)	43.2(5)
N1	3288.5(17)	2059.4(18)	5086.6(19)	35.9(5)
N2	3465.8(17)	3682.6(18)	4228.4(18)	34.5(5)
C1	3098(2)	2747(2)	4290(2)	32.8(6)
C2	3696(2)	2431(2)	6110(2)	35.0(6)
C3	4344(2)	3366(2)	5905(2)	32.7(6)
C4	5087(2)	3667(2)	6610(2)	36.4(7)
C5	5656(2)	4541(2)	6434(2)	36.5(7)
C6	5491(2)	5128(2)	5522(2)	34.0(6)
C7	4757(2)	4844(2)	4804(2)	32.3(6)
C8	4179.6(19)	3958(2)	4992(2)	29.7(6)
C9	3223(2)	929(2)	4977(3)	39.6(7)
C10	4238(2)	421(2)	5049(2)	40.0(7)
C11	5000(3)	724(2)	4363(3)	52.1(8)
C12	5937(3)	269(3)	4428(4)	65.7(11)
C13	6113(3)	-490(3)	5177(4)	73.4(13)

Atom	x	y	z	U_{eq}
C14	5372(3)	-793(3)	5855(4)	69.1(11)
C15	4438(3)	-334(3)	5800(3)	53.2(9)
C16	2419(2)	2427(2)	3412(3)	34.3(6)
C17	2682(2)	2680(2)	2366(2)	39.5(7)
C18	2043(3)	2435(3)	1542(3)	47.4(8)
C19	1151(3)	1947(3)	1733(3)	51.6(9)
C20	878(2)	1705(2)	2761(3)	48.0(8)
C21	1510(2)	1942(2)	3600(3)	41.7(7)
C22	2867(2)	2631(2)	6925(2)	38.2(7)
C23	2328(2)	3552(3)	6908(3)	46.3(8)
C24	1600(3)	3742(3)	7663(3)	56.7(9)
C25	1401(3)	3026(3)	8445(3)	56.8(9)
C26	1913(3)	2098(3)	8456(3)	54.3(9)
C27	2647(2)	1902(2)	7700(3)	43.7(8)
C28	6006(2)	6537(3)	4429(3)	51.6(8)

Table S2: Anisotropic Displacement Parameters ($\times 10^4$) **RAM717A**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	42.5(11)	45.4(13)	41.7(12)	3.1(9)	-6.1(10)	-12.6(9)
N1	42.4(13)	32.7(12)	32.7(13)	-0.8(10)	-4.9(11)	-2.5(10)
N2	34.7(12)	38.0(13)	30.7(13)	-0.4(10)	-4.0(10)	-2.8(10)
C1	32.0(14)	38.7(16)	27.6(15)	-3.5(12)	1.8(11)	2.4(11)
C2	41.2(16)	35.1(15)	28.6(14)	0.3(12)	-5.6(12)	0.9(12)
C3	33.5(14)	32.6(15)	32.1(15)	-0.7(11)	-1.0(12)	2.0(12)
C4	39.2(16)	41.4(16)	28.7(15)	1.7(12)	-4.9(13)	2.0(13)
C5	34.3(15)	42.5(17)	32.8(16)	-2.5(13)	-5.4(12)	-0.1(13)
C6	31.0(14)	35.3(15)	35.8(15)	-4.9(12)	1.0(12)	0.4(12)
C7	33.5(14)	33.5(15)	29.9(14)	1.0(11)	-1.1(12)	2.3(11)
C8	28.3(12)	32.4(15)	28.3(14)	-2.8(12)	-0.7(12)	2.5(11)
C9	44.0(16)	34.1(15)	40.8(17)	-2.0(14)	-3.1(14)	-6.0(13)
C10	48.7(17)	27.6(15)	43.8(17)	-4.6(13)	-3.3(14)	-2.3(13)
C11	55.1(19)	40.5(17)	61(2)	-4.1(17)	6.0(17)	-2.0(15)
C12	53(2)	52(2)	92(3)	-20(2)	15(2)	-4.5(17)
C13	61(2)	51(2)	108(4)	-24(2)	-15(3)	15.0(18)
C14	85(3)	48(2)	75(3)	-5(2)	-17(2)	19(2)
C15	65(2)	40.7(18)	54(2)	0.9(16)	-4.9(17)	4.0(16)
C16	35.3(15)	36.6(15)	30.8(14)	-2.5(13)	-3.5(12)	-1.8(12)
C17	38.2(16)	44.1(17)	36.2(16)	-1.6(13)	-0.9(13)	-6.3(13)
C18	52(2)	60(2)	29.5(15)	-0.8(15)	-2.5(14)	-10.1(16)
C19	58(2)	58(2)	39.5(19)	-4.8(16)	-14.9(16)	-12.3(17)
C20	42.0(18)	54.2(19)	47.8(19)	3.0(17)	-5.2(15)	-14.4(15)
C21	41.7(16)	46.5(17)	36.9(17)	1.5(14)	-1.1(14)	-8.1(13)
C22	43.5(17)	44.4(17)	26.7(14)	-2.0(13)	-3.7(13)	-8.0(14)
C23	50.4(19)	48.6(19)	40.0(17)	-0.2(14)	4.6(15)	1.9(15)
C24	56(2)	65(2)	49(2)	-10.1(19)	6.5(18)	0.2(17)
C25	51(2)	77(3)	42(2)	-16.3(19)	8.2(17)	-17.0(18)
C26	55(2)	78(3)	29.9(17)	2.3(17)	-1.7(16)	-32.8(19)
C27	48.8(19)	48.3(18)	34.2(16)	1.1(15)	-8.6(14)	-13.4(15)
C28	48.5(19)	59(2)	47.2(19)	9.1(17)	-1.6(16)	-19.6(16)

Table S3: Bond Lengths in Å for **RAM717A**.

Atom	Atom	Length/Å
O1	C6	1.371(3)
O1	C28	1.417(4)
N1	C1	1.360(4)
N1	C2	1.476(4)
N1	C9	1.463(4)
N2	C1	1.302(3)
N2	C8	1.400(3)
C1	C16	1.486(4)
C2	C3	1.505(4)
C2	C22	1.531(4)

Atom	Atom	Length/Å
C3	C4	1.386(4)
C3	C8	1.393(4)
C4	C5	1.375(4)
C5	C6	1.390(4)
C6	C7	1.383(4)
C7	C8	1.396(4)
C9	C10	1.509(4)
C10	C11	1.391(5)
C10	C15	1.380(5)
C11	C12	1.387(5)
C12	C13	1.376(7)
C13	C14	1.365(6)
C14	C15	1.385(6)

Atom	Atom	Length/Å
C16	C17	1.398(4)
C16	C21	1.388(4)
C17	C18	1.378(4)
C18	C19	1.370(5)
C19	C20	1.378(5)
C20	C21	1.384(4)
C22	C23	1.386(4)
C22	C27	1.383(4)
C23	C24	1.382(5)
C24	C25	1.372(5)
C25	C26	1.377(5)
C26	C27	1.389(5)

Table S4: Bond Angles in ° for **RAM717A**.

Atom	Atom	Atom	Angle/°
C6	O1	C28	116.8(2)
C1	N1	C2	120.0(2)
C1	N1	C9	124.5(2)
C9	N1	C2	115.2(2)
C1	N2	C8	116.9(2)
N1	C1	C16	118.7(2)
N2	C1	N1	125.0(3)
N2	C1	C16	116.3(2)
N1	C2	C3	108.8(2)
N1	C2	C22	111.6(2)
C3	C2	C22	113.5(2)
C4	C3	C2	121.8(3)
C4	C3	C8	119.1(3)
C8	C3	C2	119.1(2)
C5	C4	C3	121.5(3)
C4	C5	C6	119.3(3)
O1	C6	C5	115.7(2)
O1	C6	C7	123.9(3)
C7	C6	C5	120.4(3)
C6	C7	C8	119.9(2)
C3	C8	N2	122.2(2)
C3	C8	C7	119.8(2)
C7	C8	N2	117.9(2)
N1	C9	C10	111.7(2)
C11	C10	C9	120.1(3)
C15	C10	C9	121.3(3)
C15	C10	C11	118.5(3)
C12	C11	C10	120.6(4)
C13	C12	C11	119.6(4)
C14	C13	C12	120.3(4)
C13	C14	C15	120.3(4)
C10	C15	C14	120.6(4)
C17	C16	C1	118.5(3)
C21	C16	C1	122.4(3)
C21	C16	C17	119.0(3)
C18	C17	C16	119.7(3)
C19	C18	C17	120.9(3)
C18	C19	C20	119.9(3)
C19	C20	C21	120.1(3)
C20	C21	C16	120.4(3)
C23	C22	C2	120.7(3)
C27	C22	C2	120.7(3)
C27	C22	C23	118.6(3)

Atom	Atom	Atom	Angle/°
C24	C23	C22	120.5(3)
C25	C24	C23	120.6(4)
C24	C25	C26	119.5(3)
C25	C26	C27	120.2(3)
C22	C27	C26	120.6(3)

Table S5: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **RAM717A**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H2	4134.41	1869.33	6402.06	42
H4	5206.13	3259.77	7228.65	44
H5	6155.54	4740.53	6930.37	44
H7	4644.74	5250.54	4183.44	39
H9A	2915.85	756.58	4282.13	48
H9B	2786.93	648.16	5545.17	48
H11	4877.38	1247.59	3845.58	63
H12	6454.41	479.96	3957.24	79
H13	6754.12	-804.6	5222.45	88
H14	5496.77	-1321.53	6367.16	83
H15	3929.58	-540.88	6284.28	64
H17	3297.62	3019.86	2224.1	47
H18	2224.75	2607.15	832.21	57
H19	721.77	1776.32	1156.49	62
H20	255.76	1375.32	2894.79	58
H21	1319.48	1771.04	4307.44	50
H23	2460.63	4055.99	6373.06	56
H24	1233.55	4374.37	7641.09	68
H25	912.75	3169.41	8974.45	68
H26	1764.47	1589.8	8981.72	65
H27	3000.82	1262.28	7715.1	52
H28A	6151.87	6071.3	3831.07	77
H28B	6481.14	7117.05	4426.27	77
H28C	5325.01	6807.34	4359.39	77

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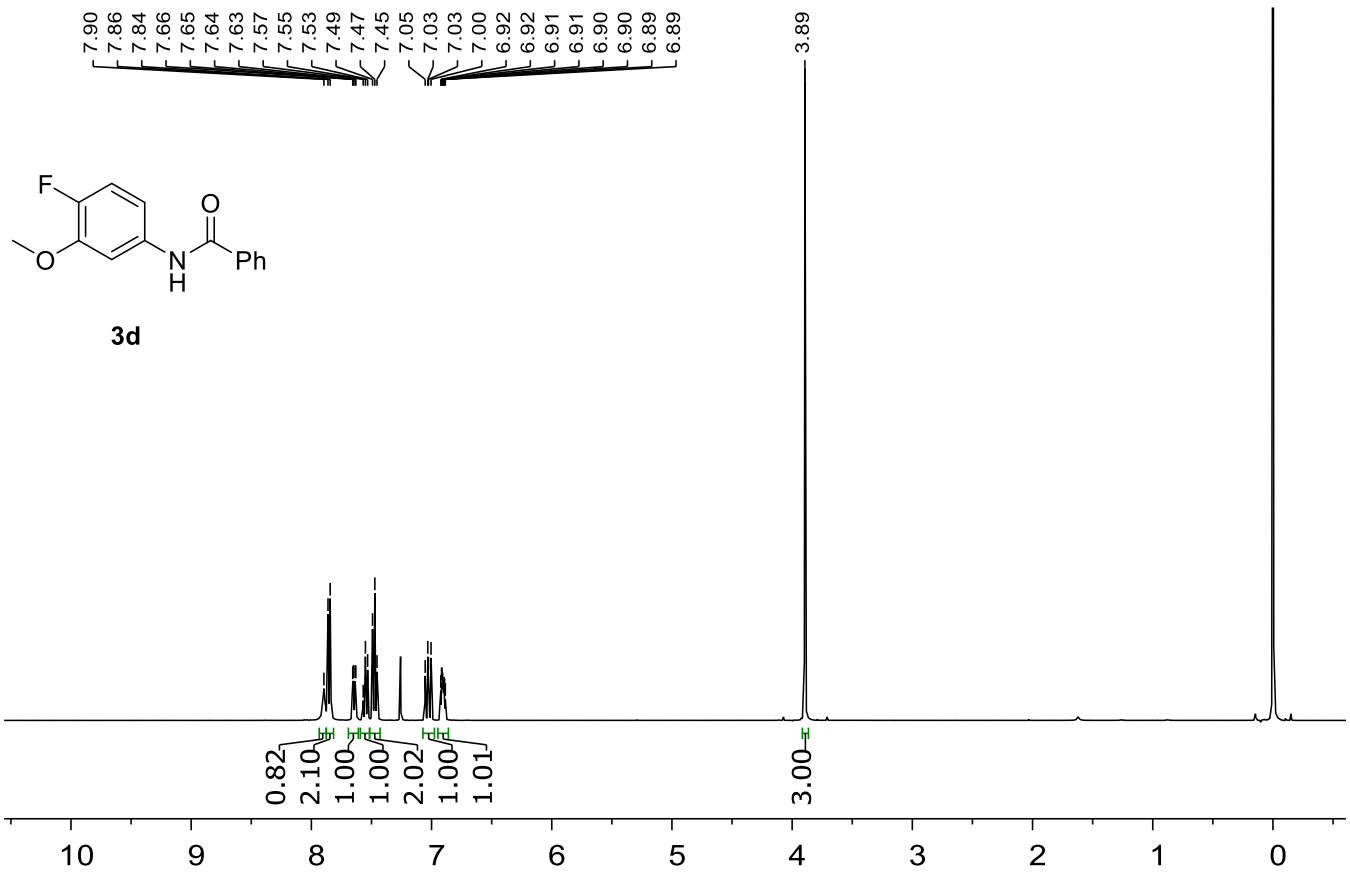
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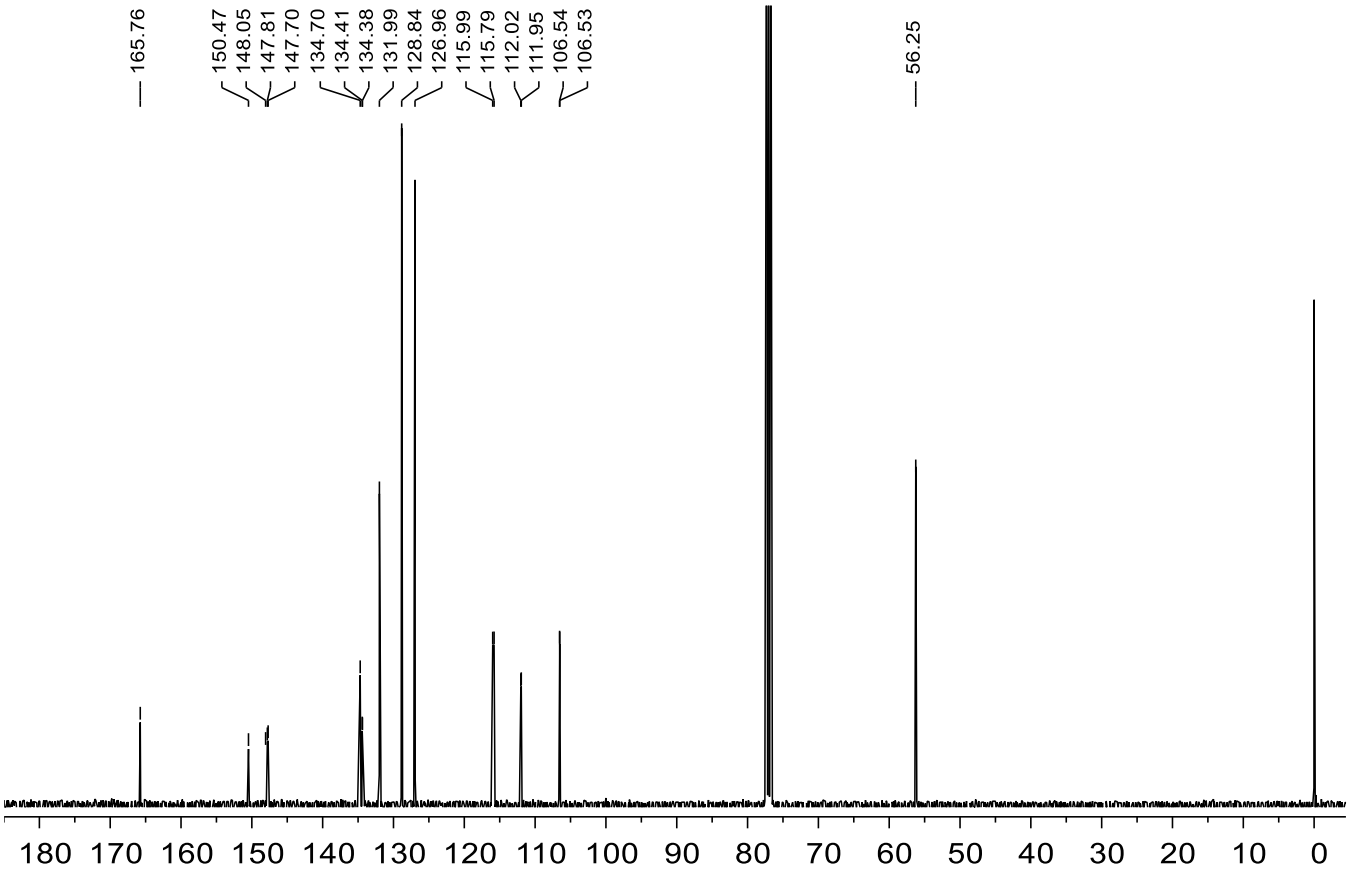
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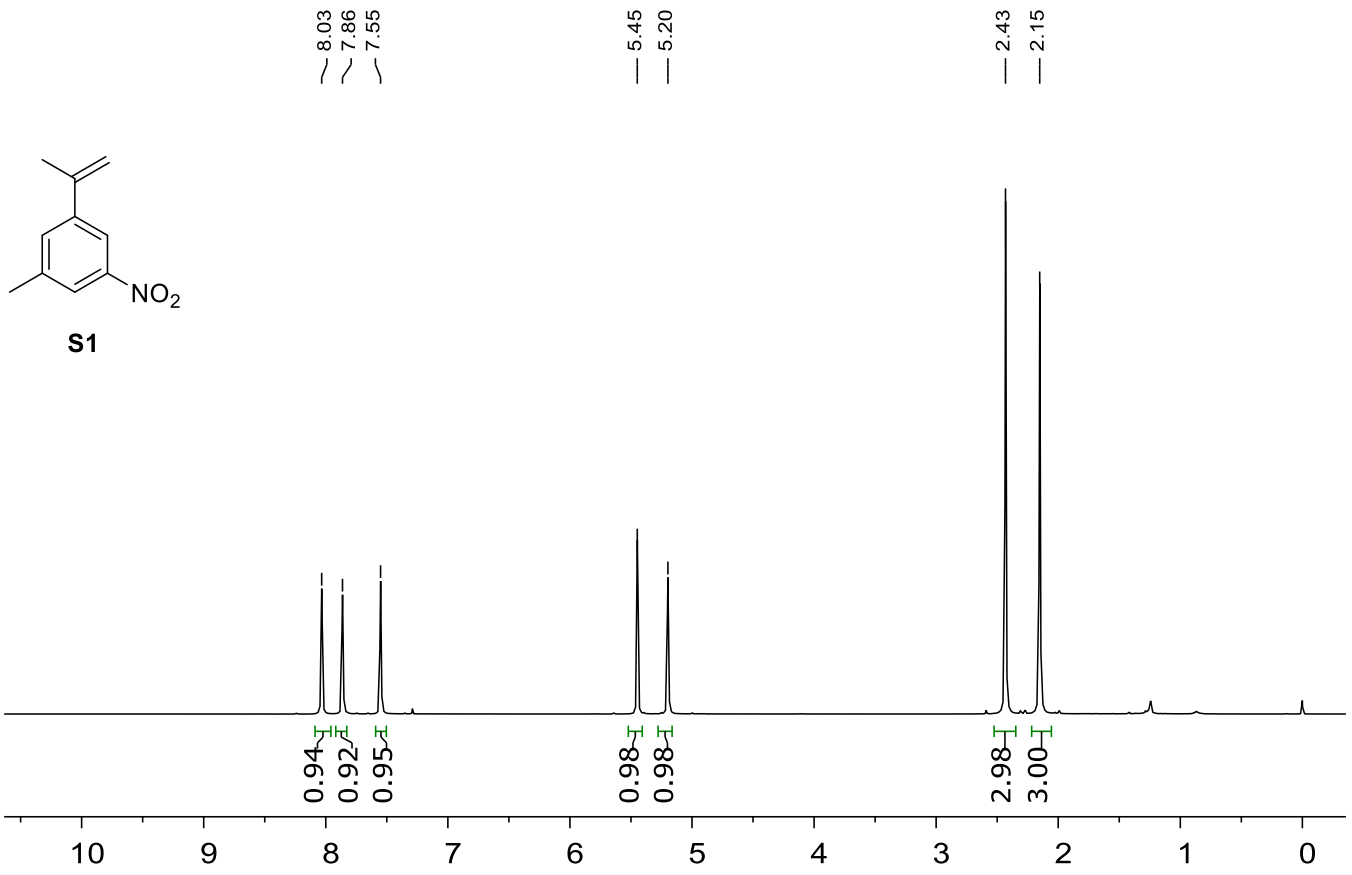
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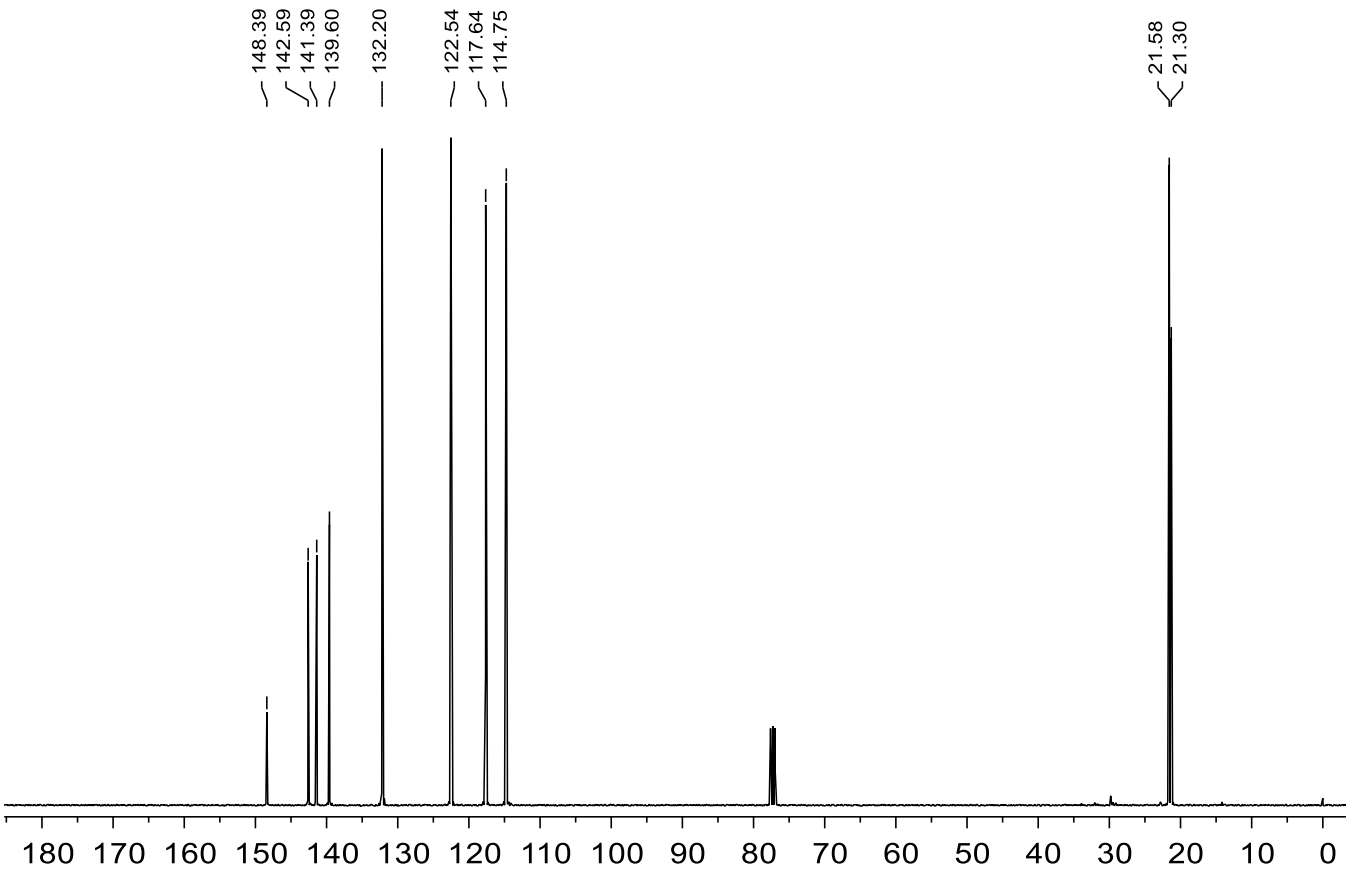
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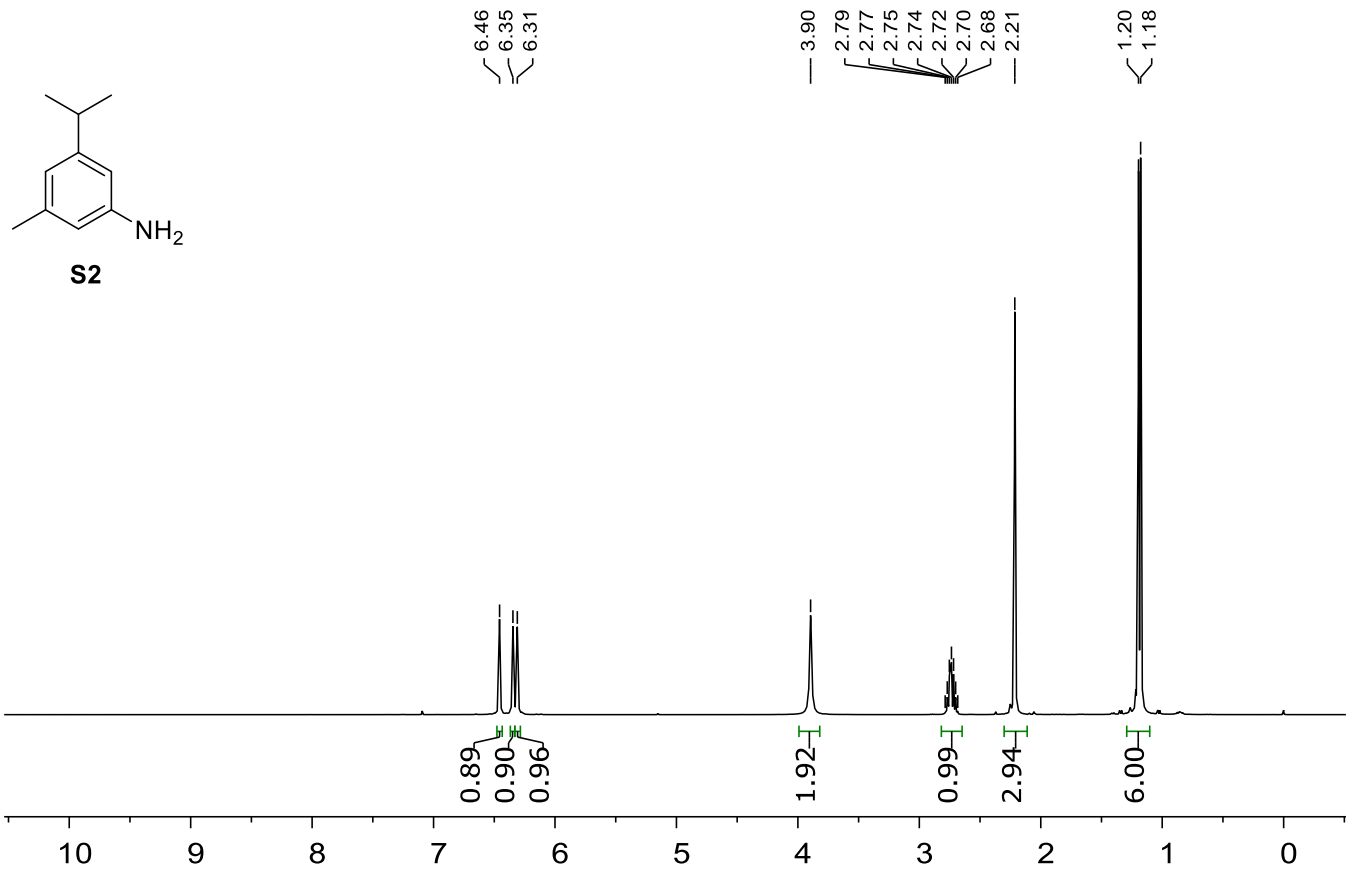
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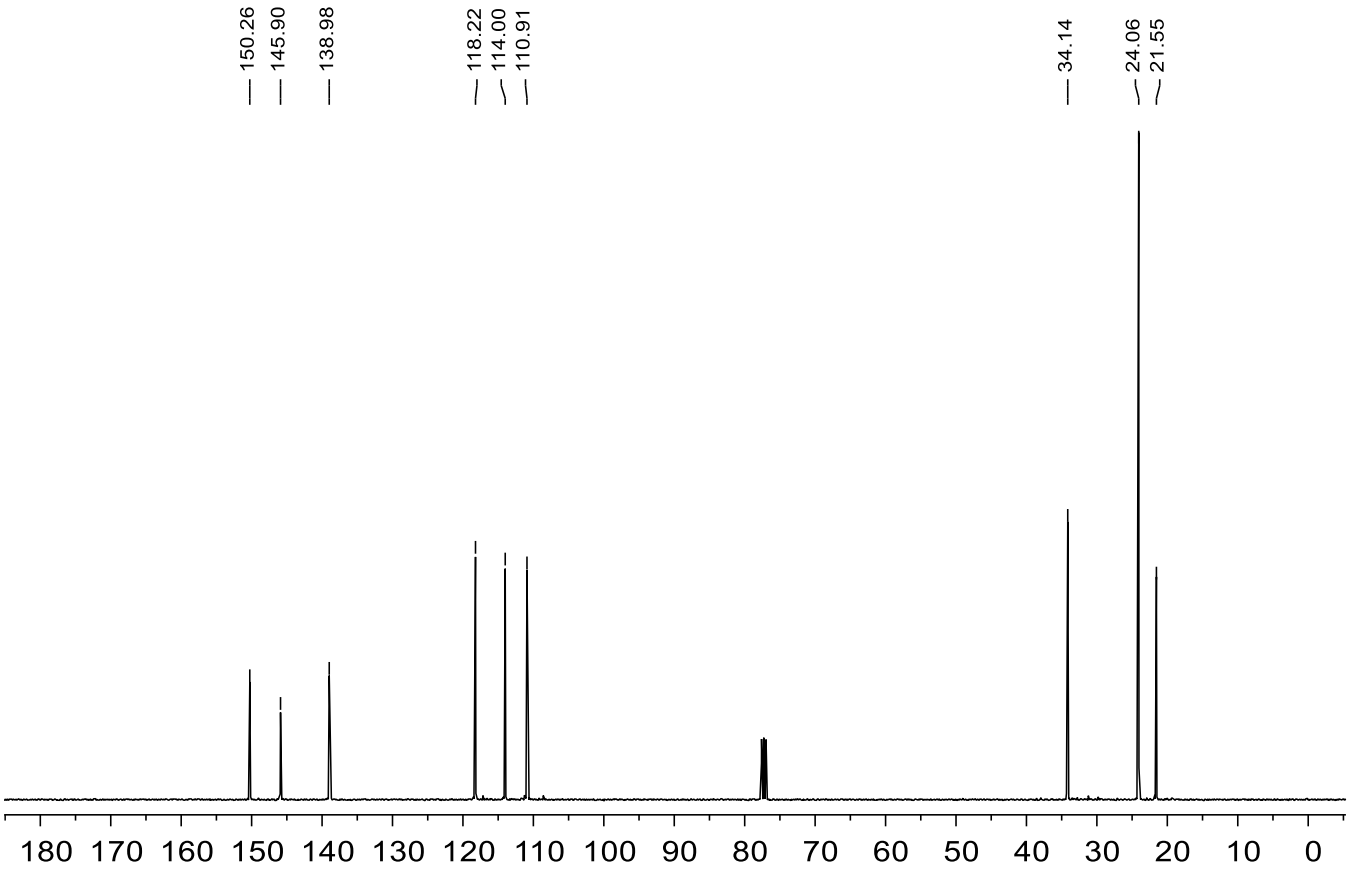
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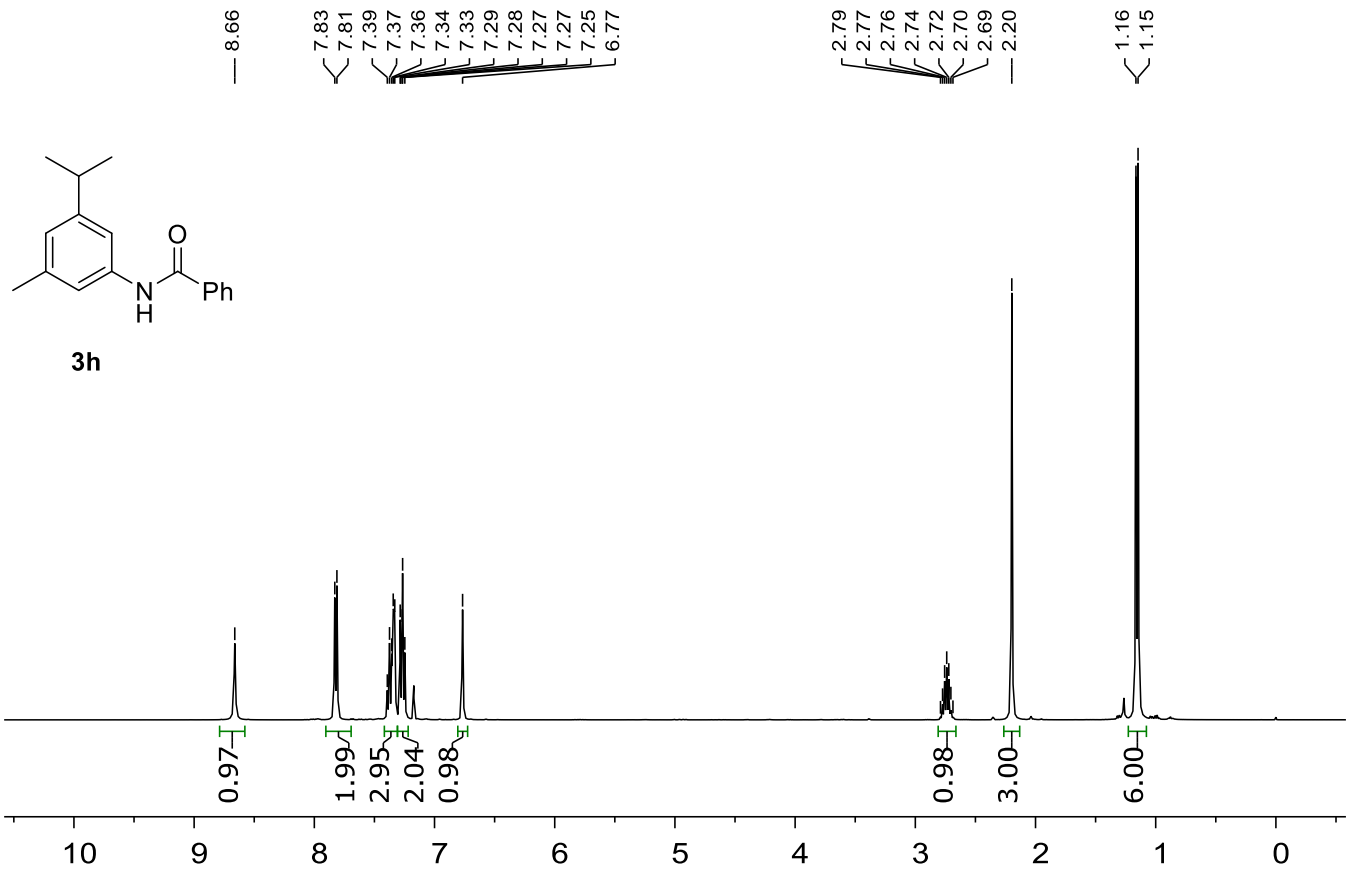
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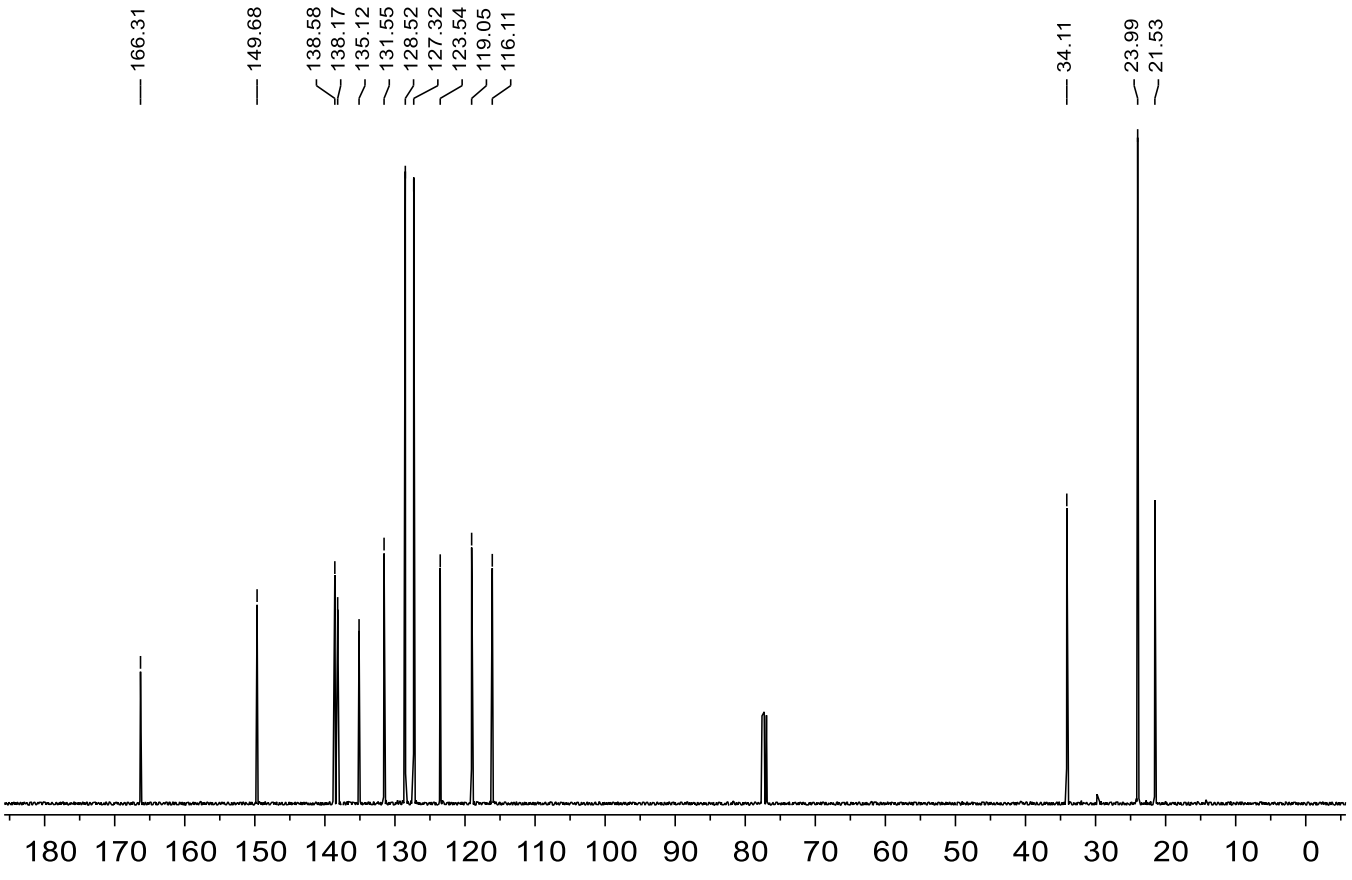
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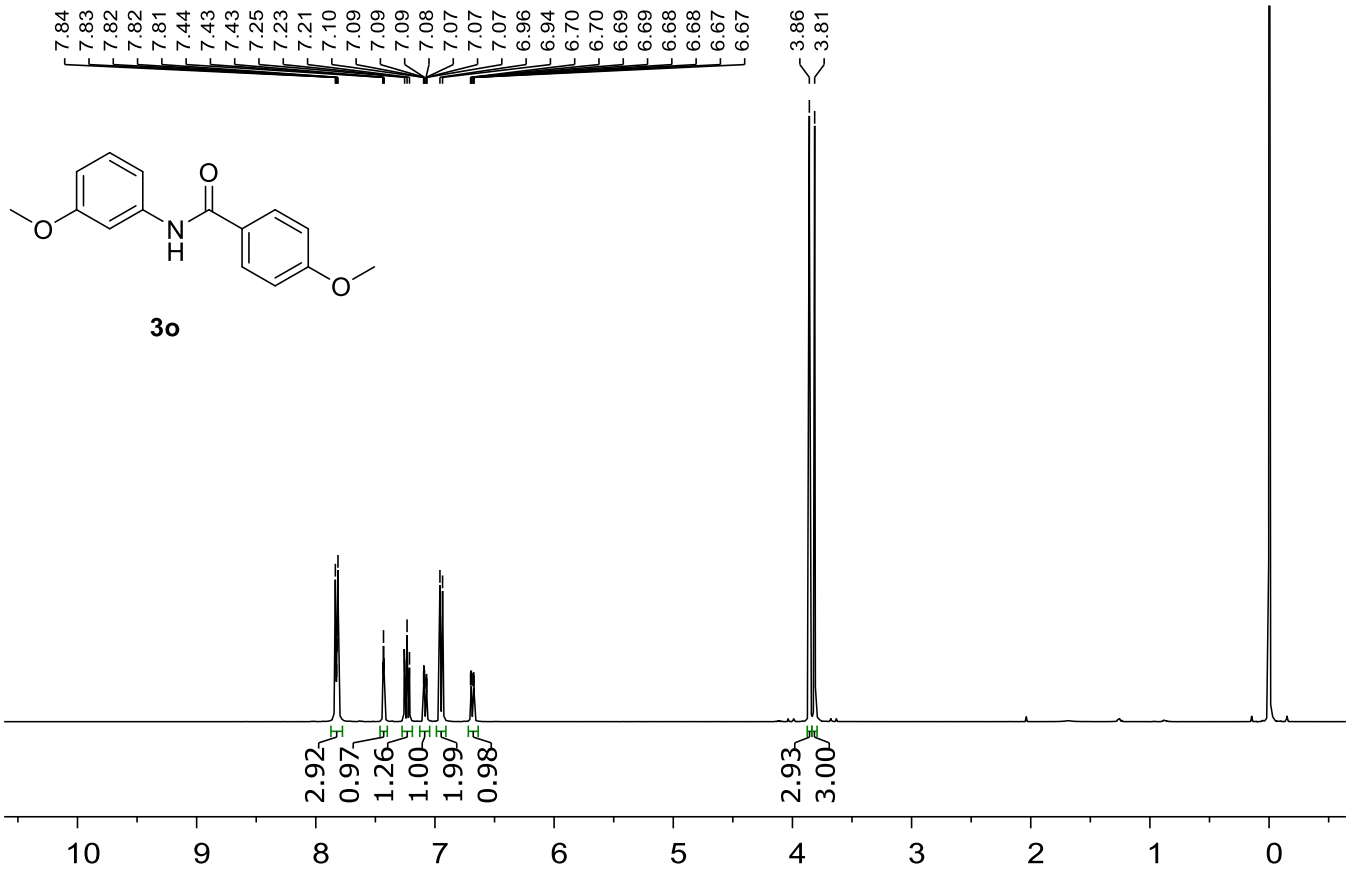
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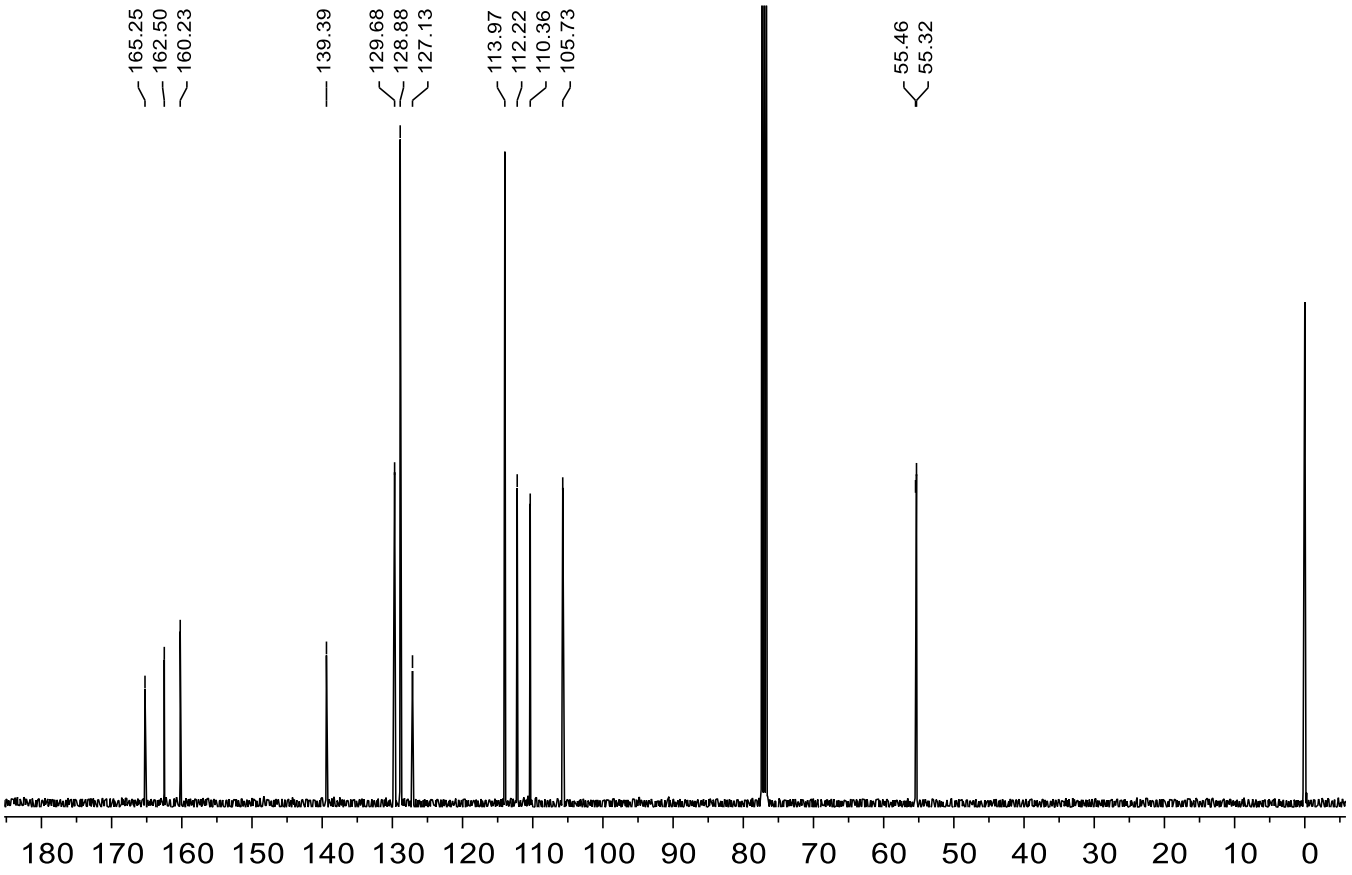
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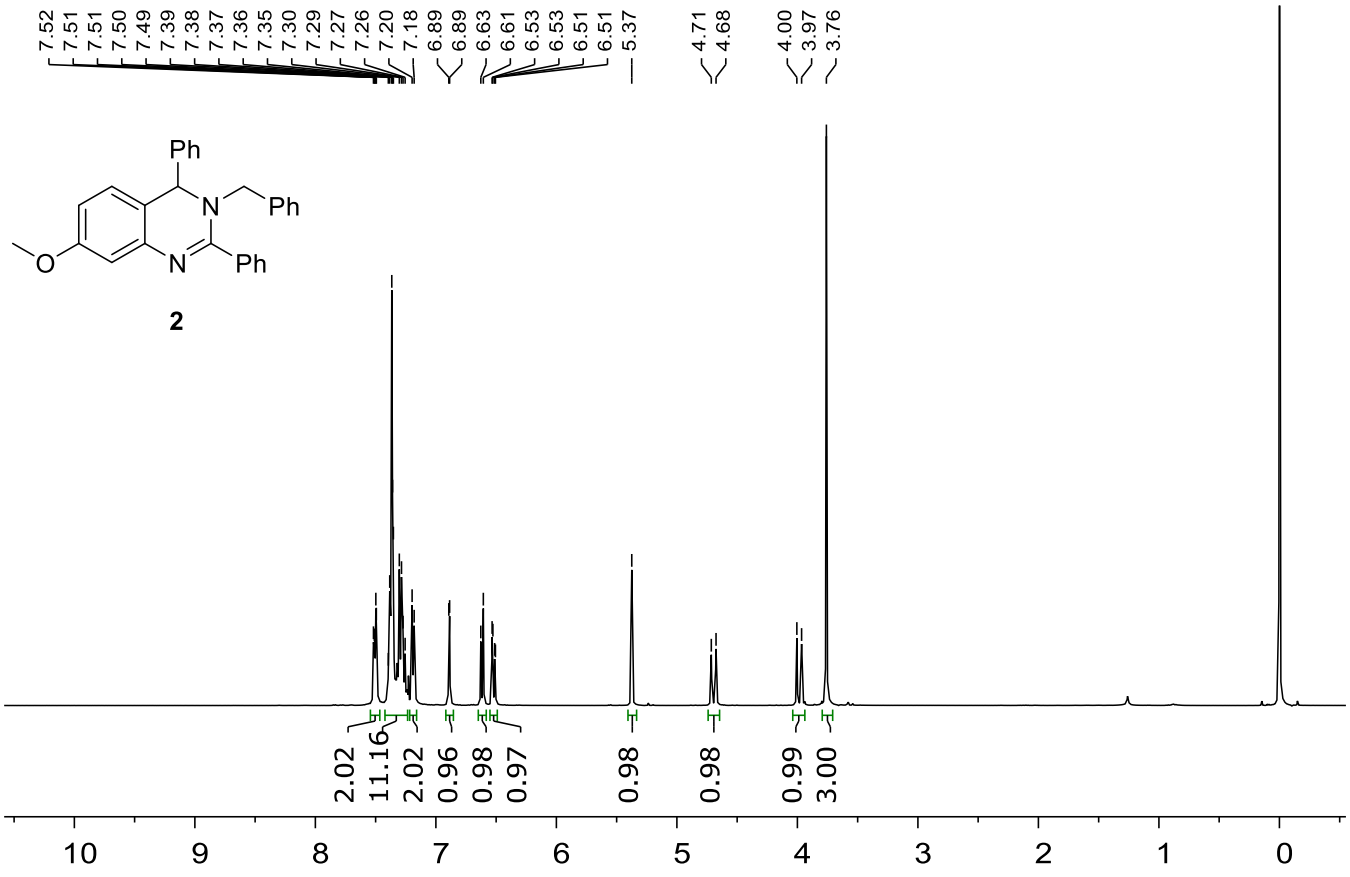
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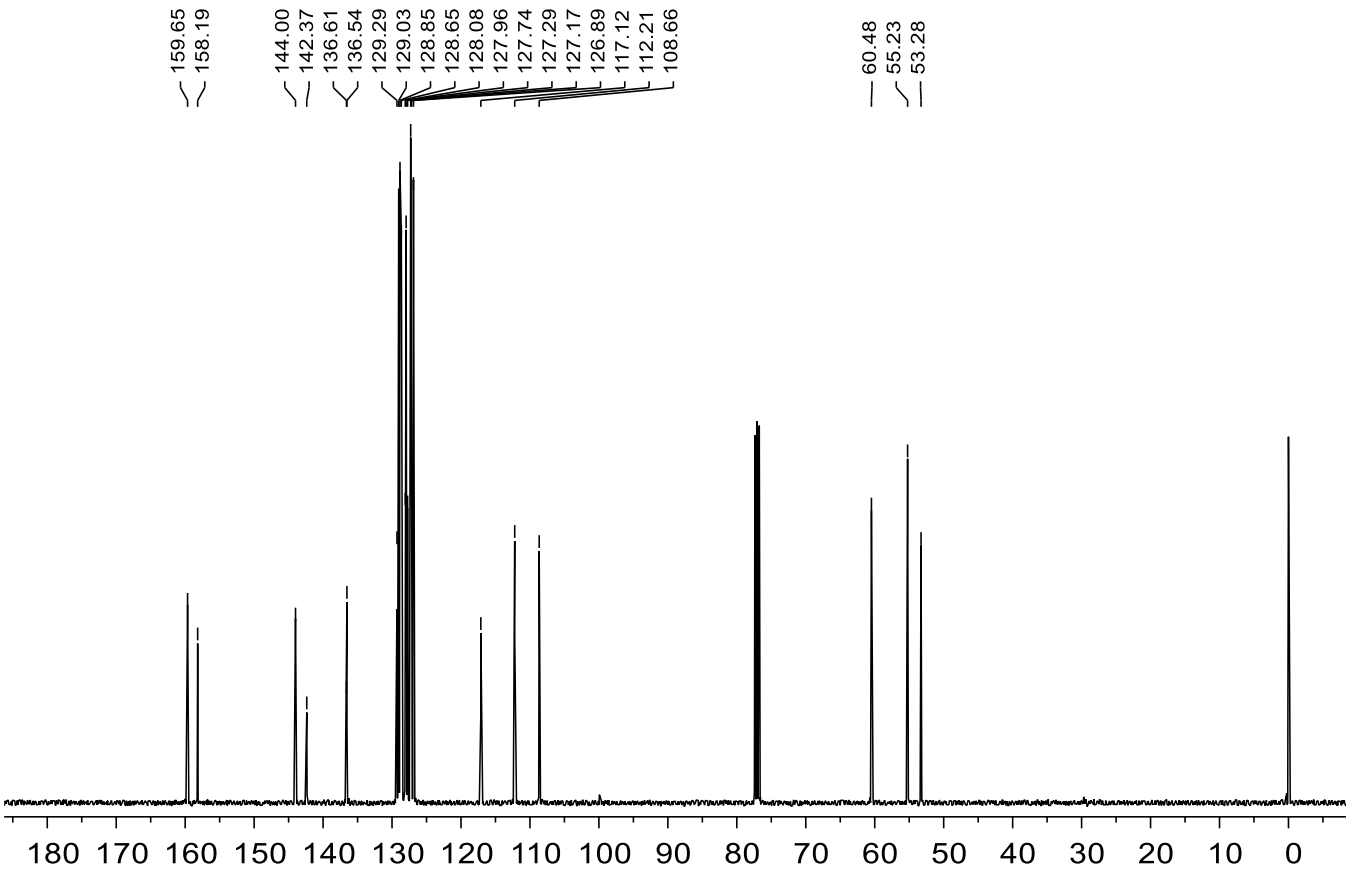
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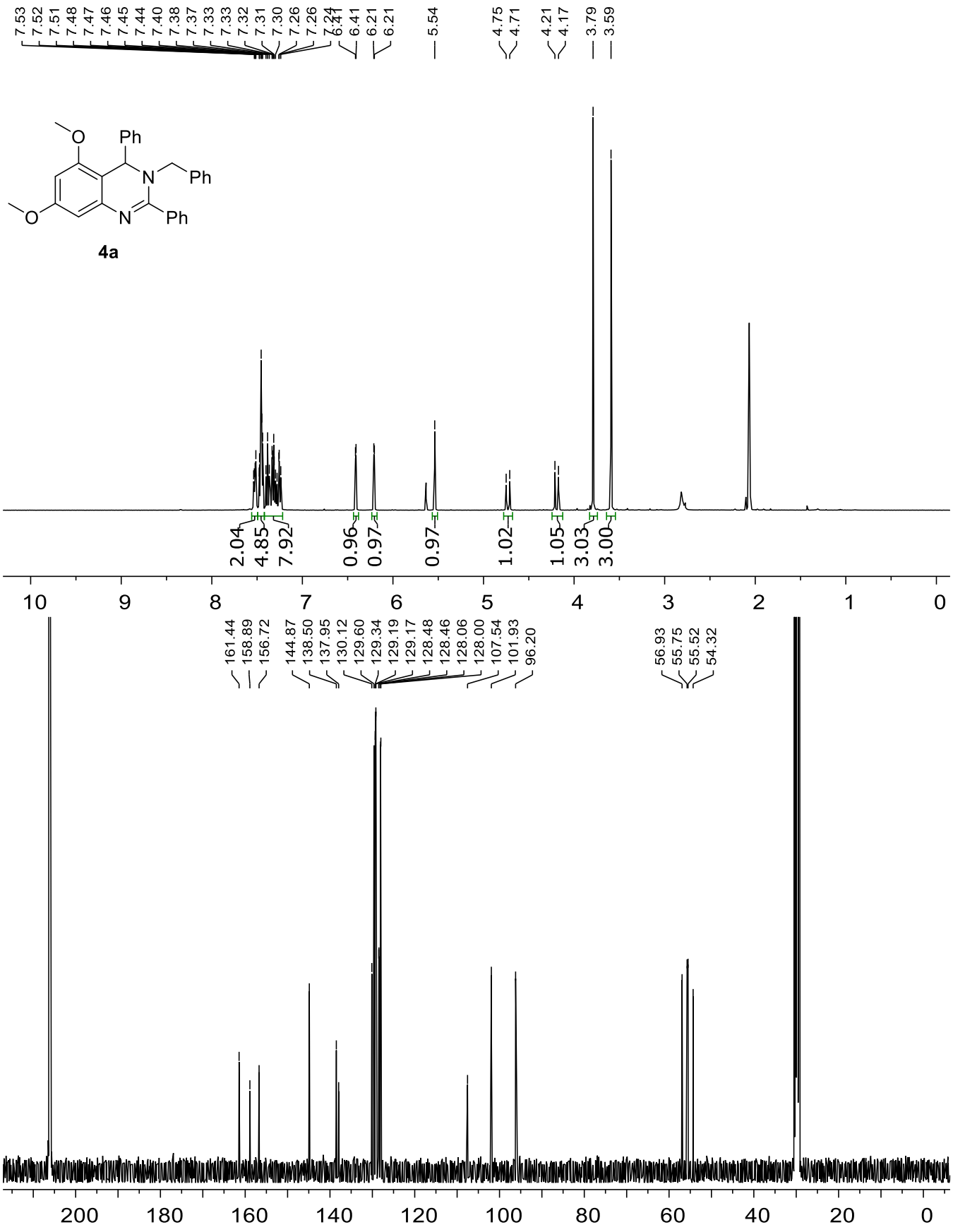
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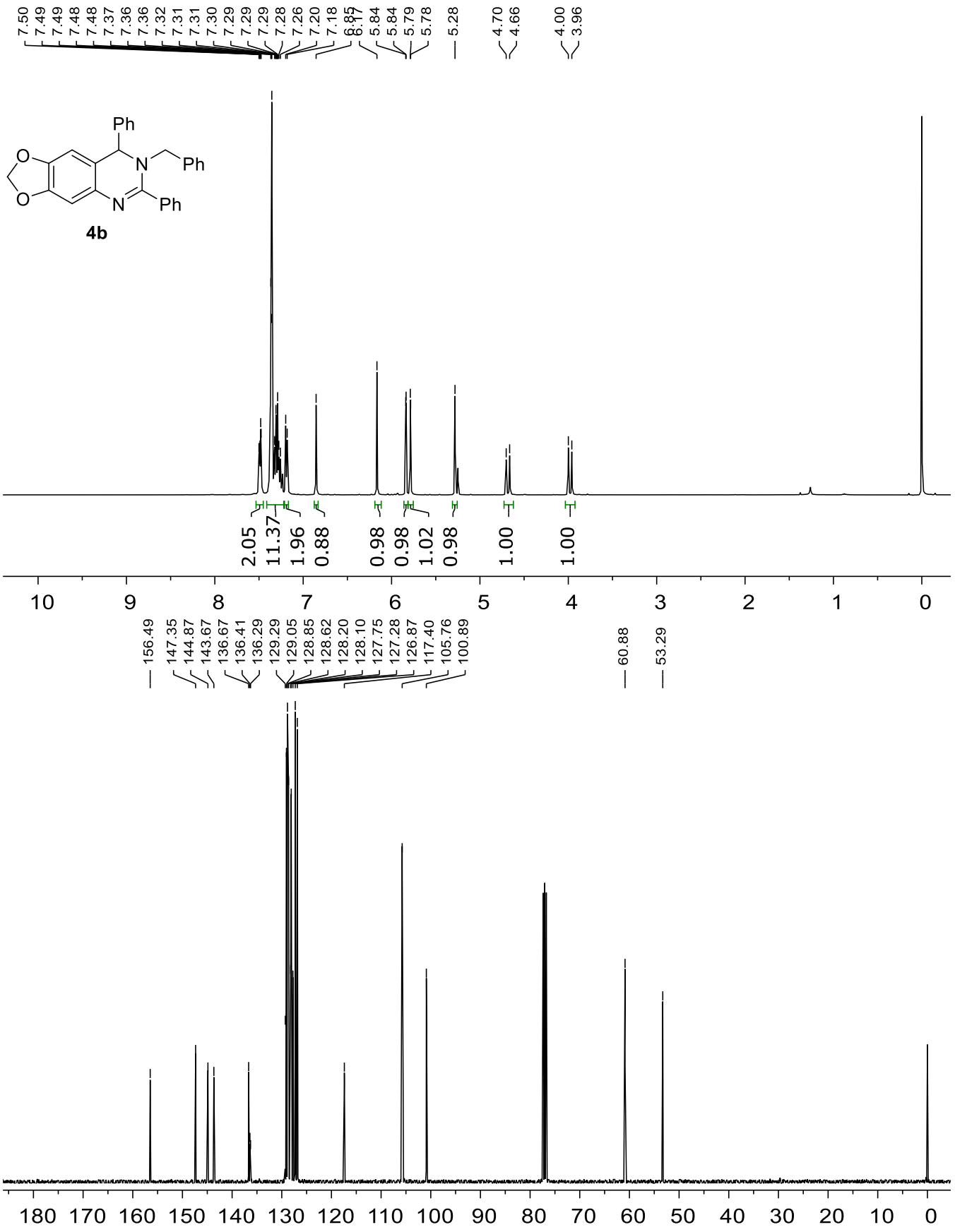
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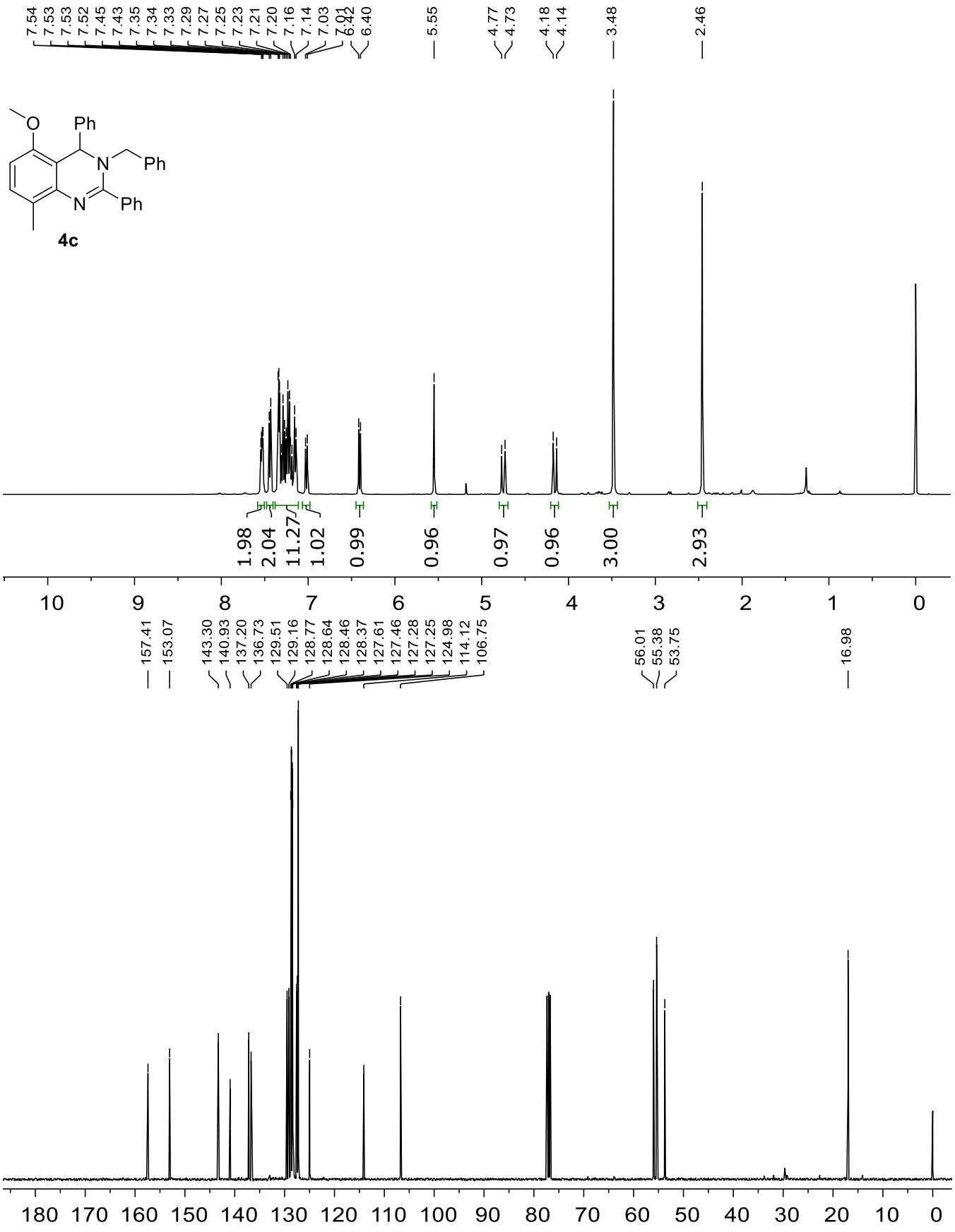
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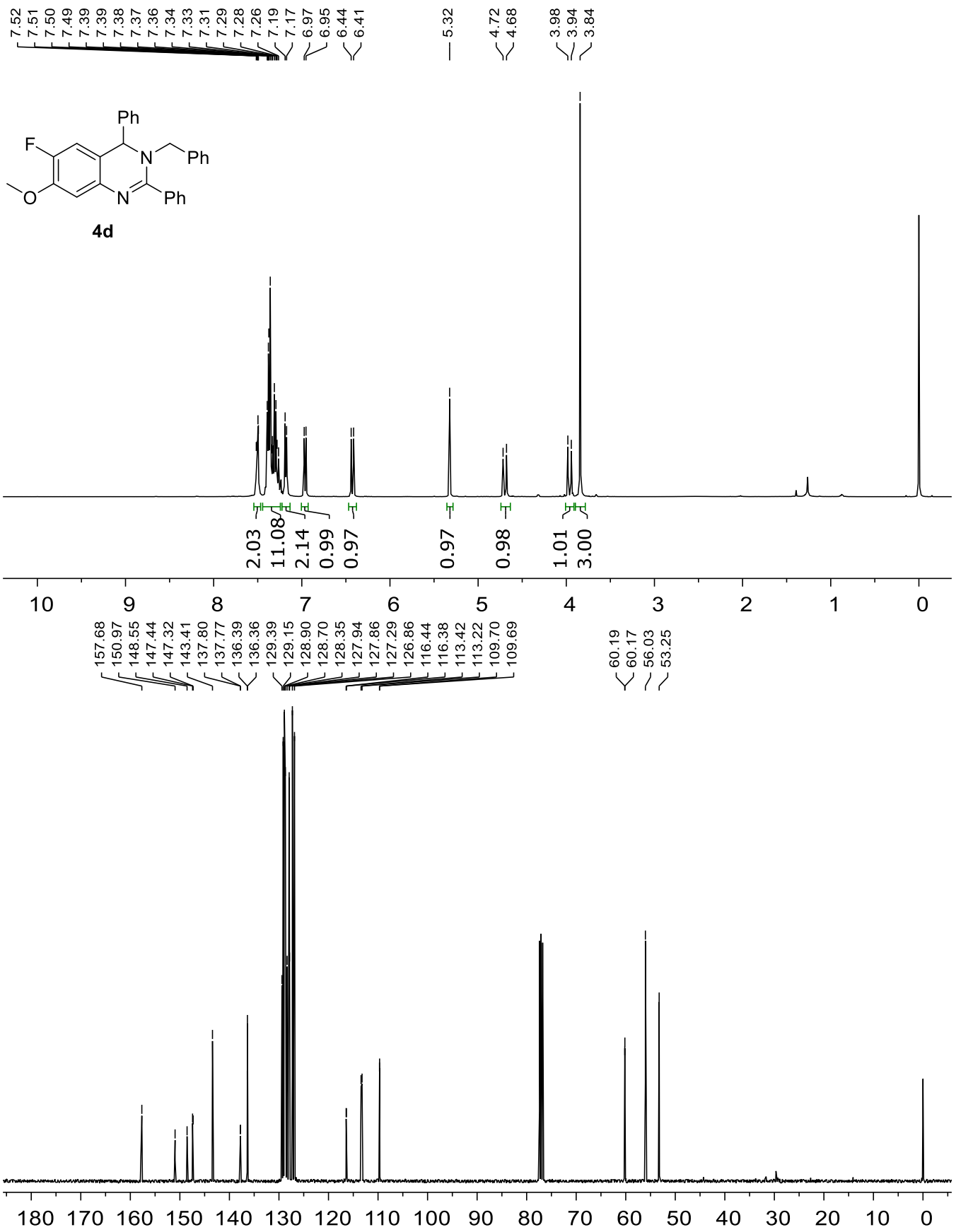
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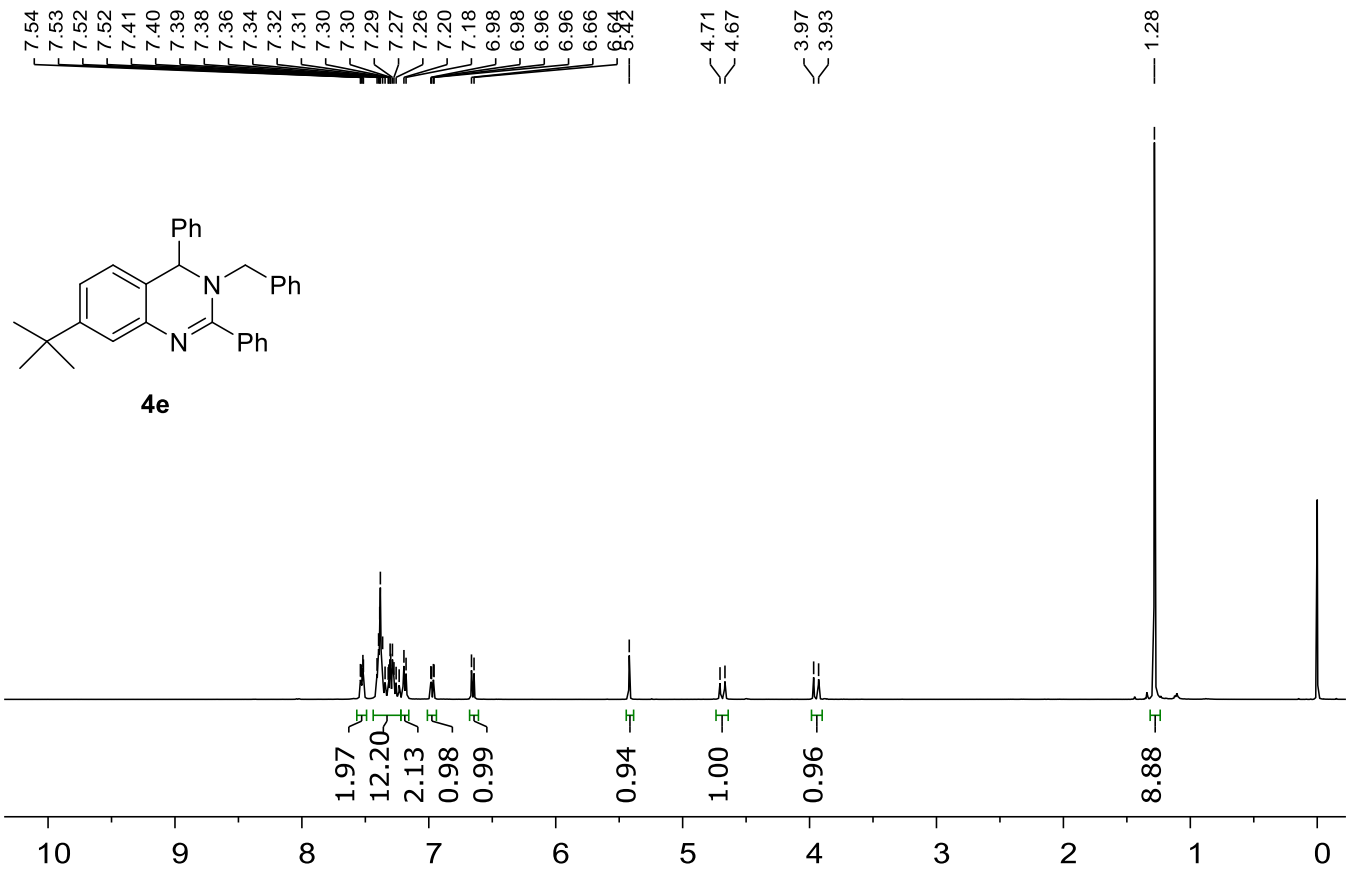
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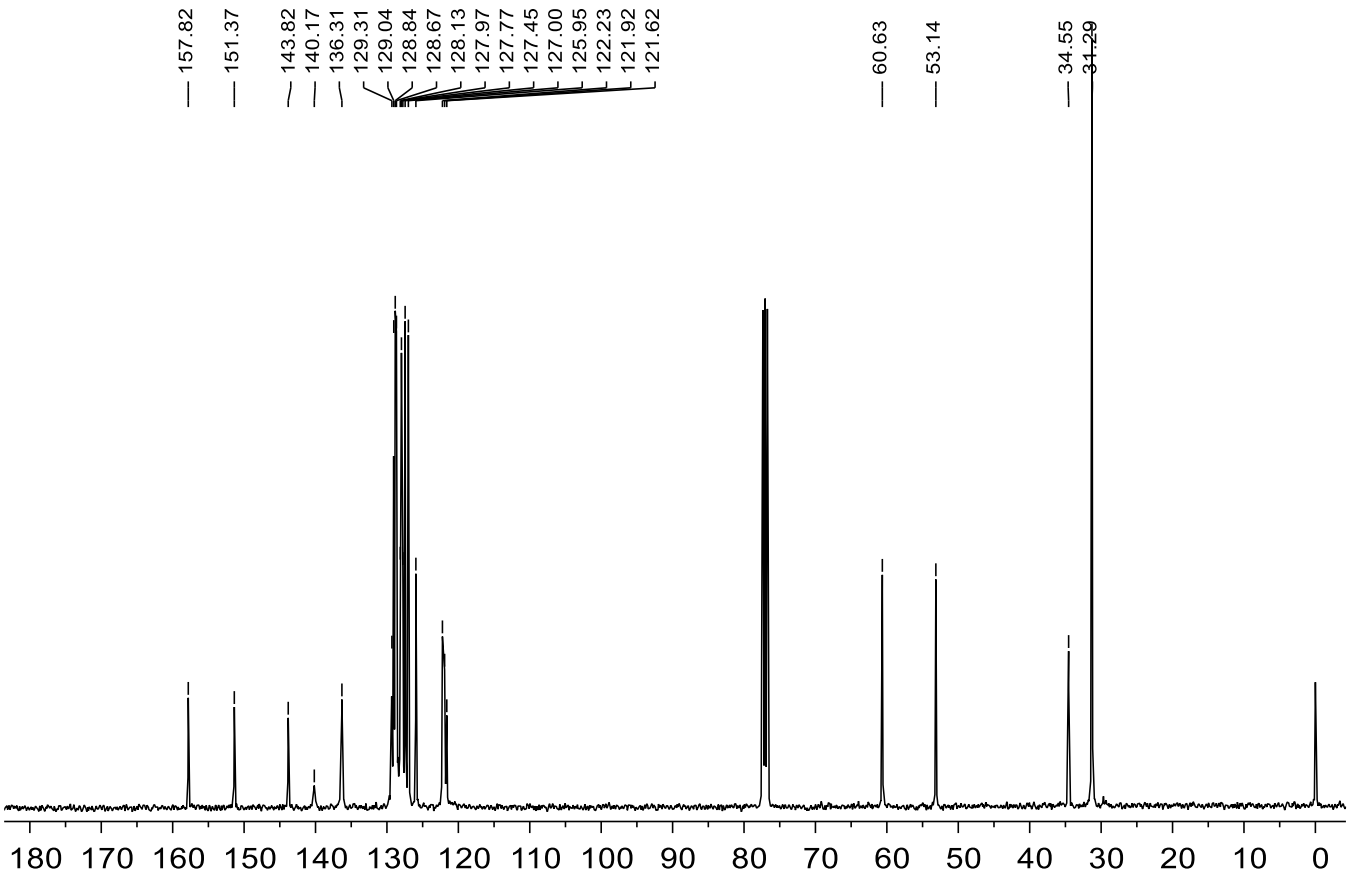
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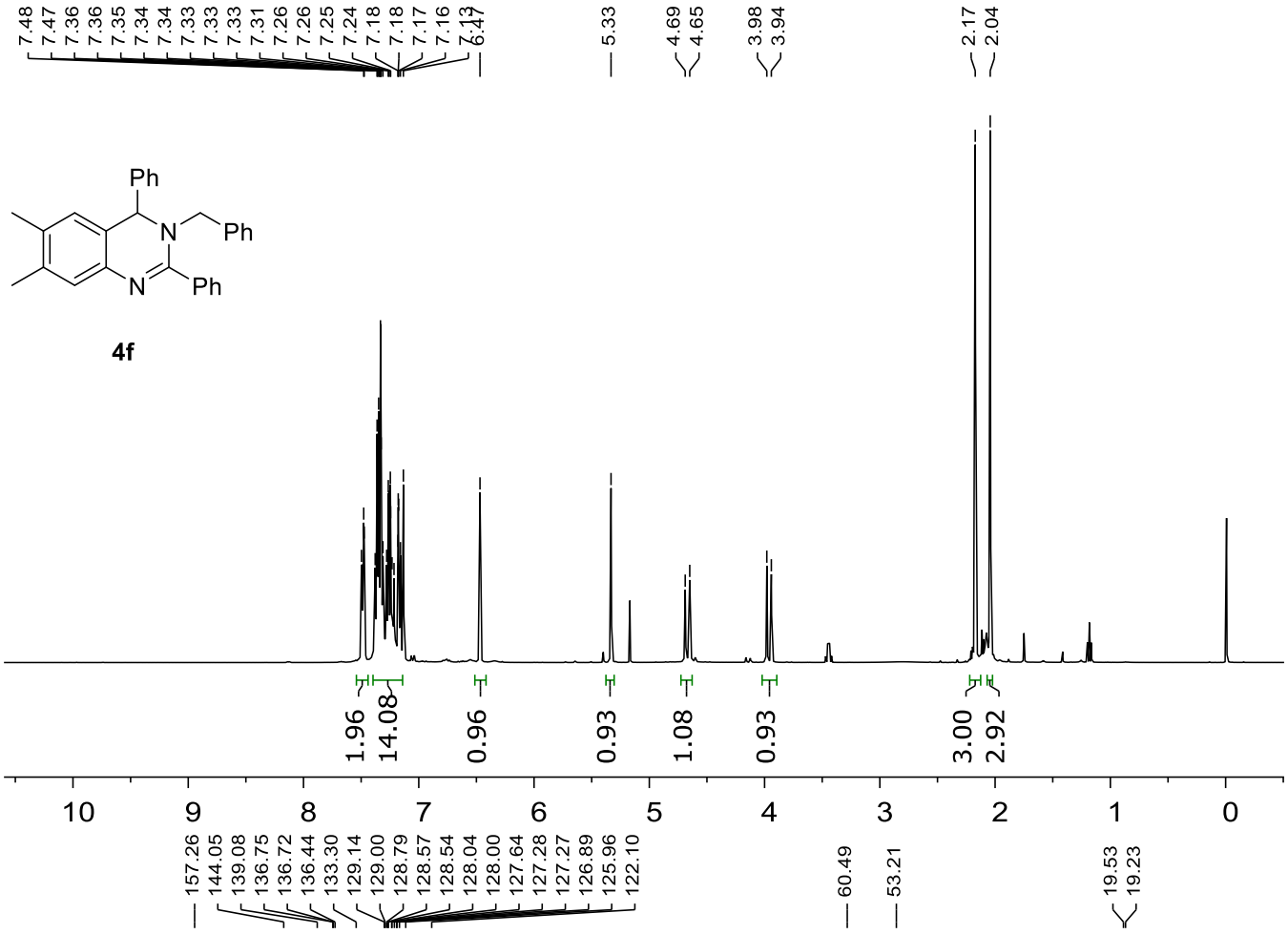
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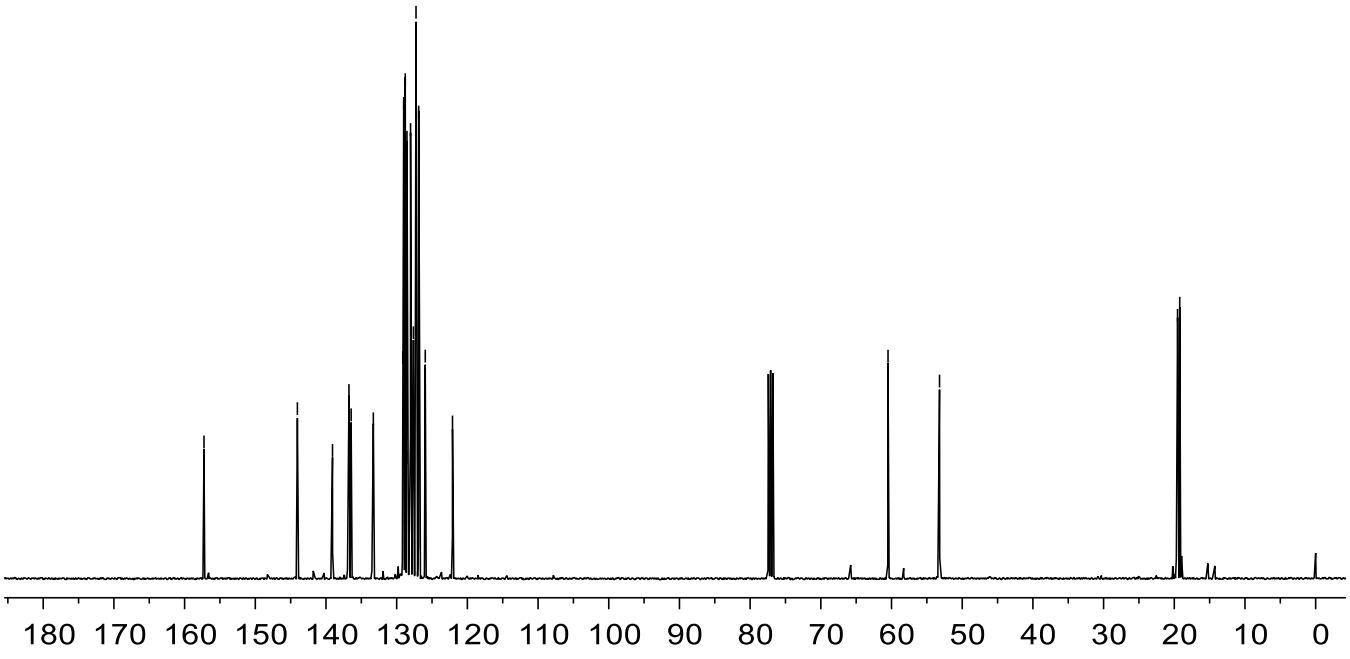
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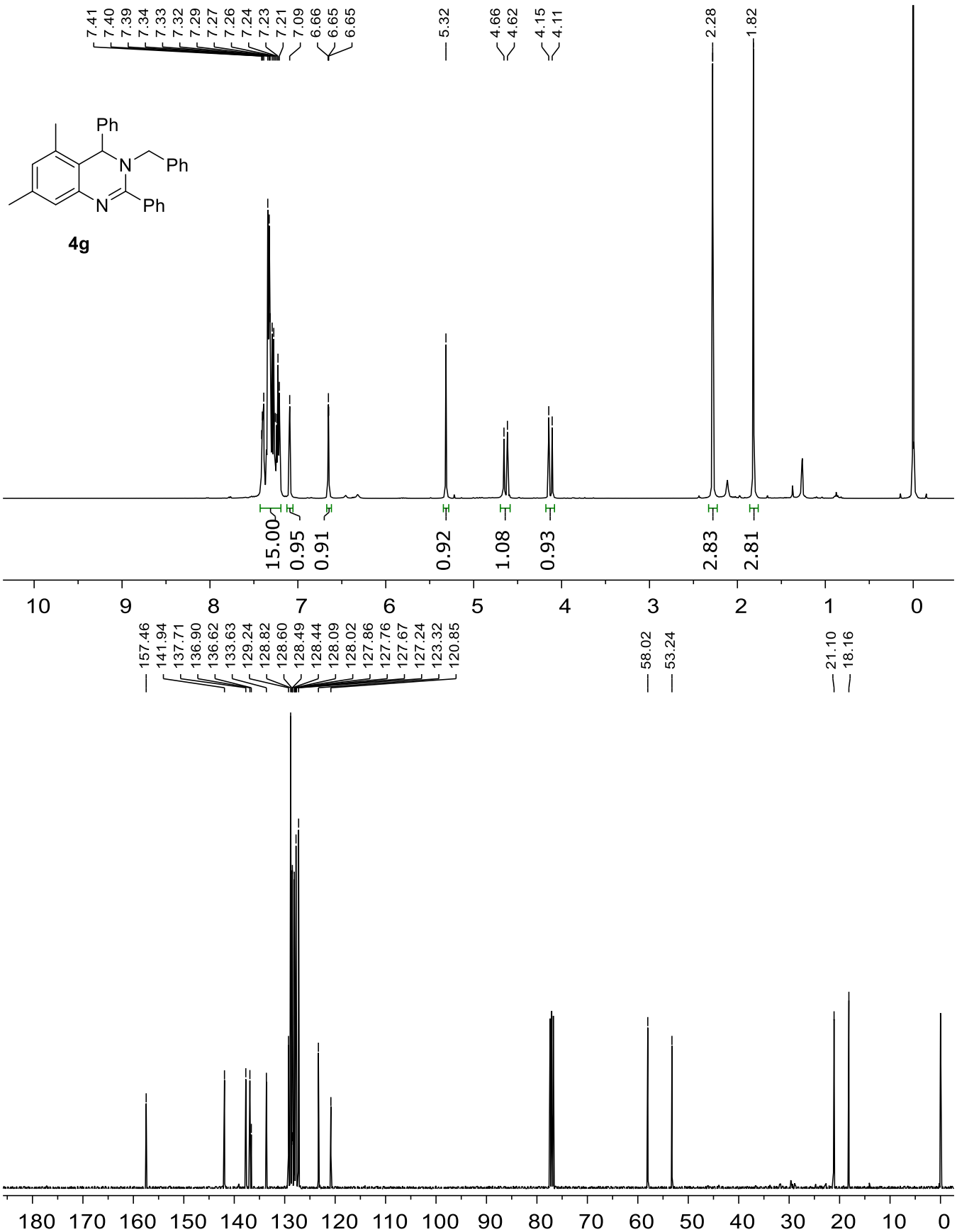
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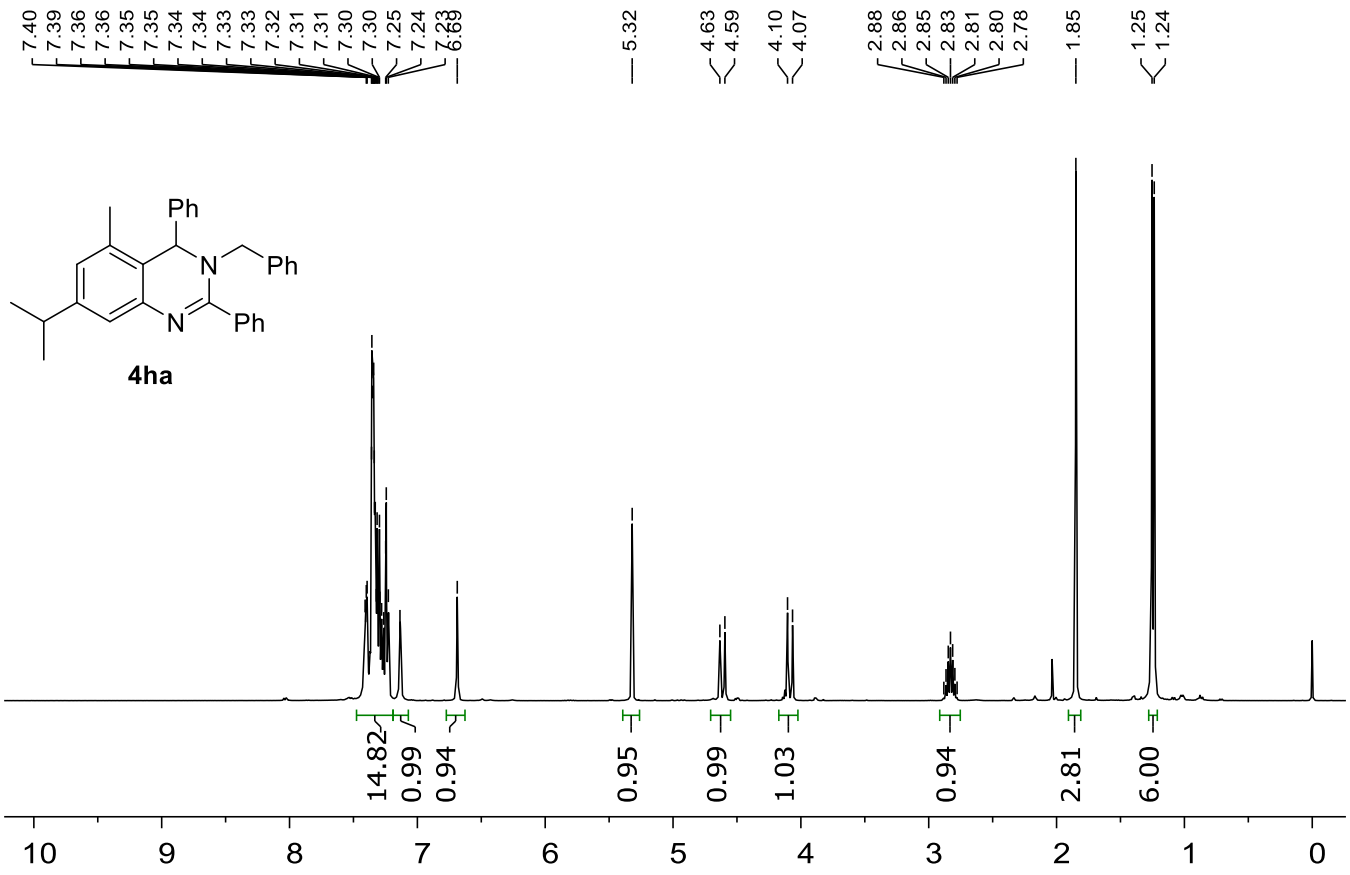
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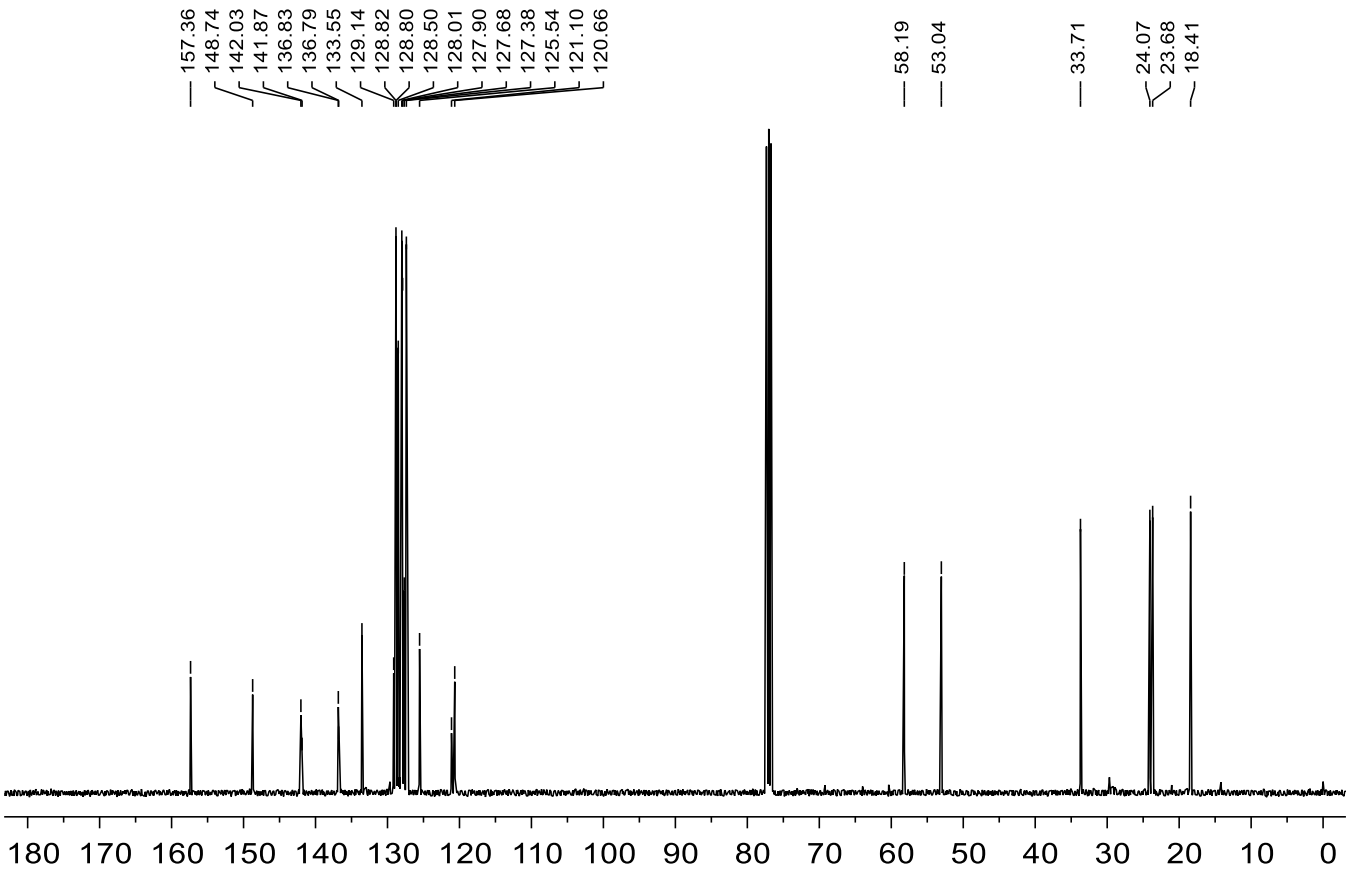
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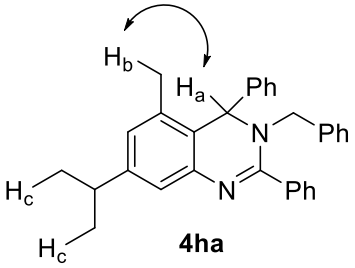
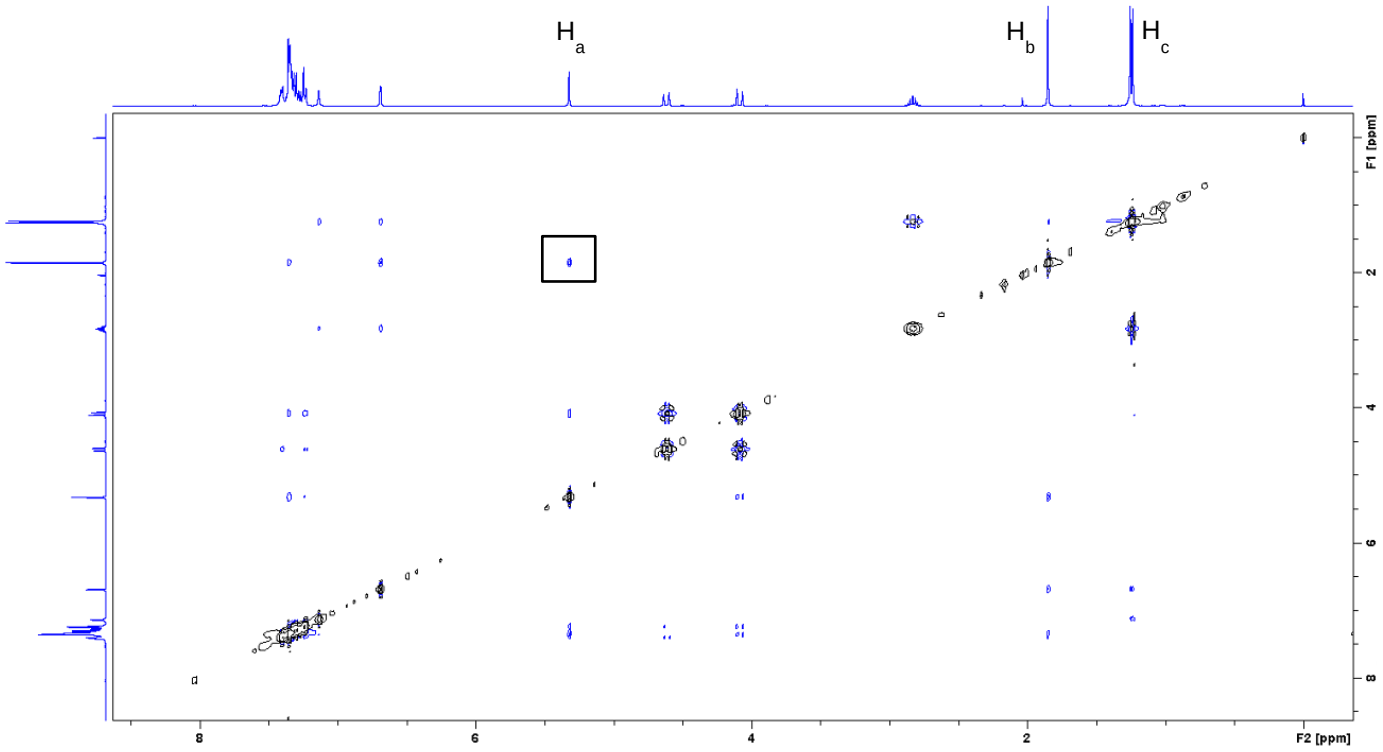
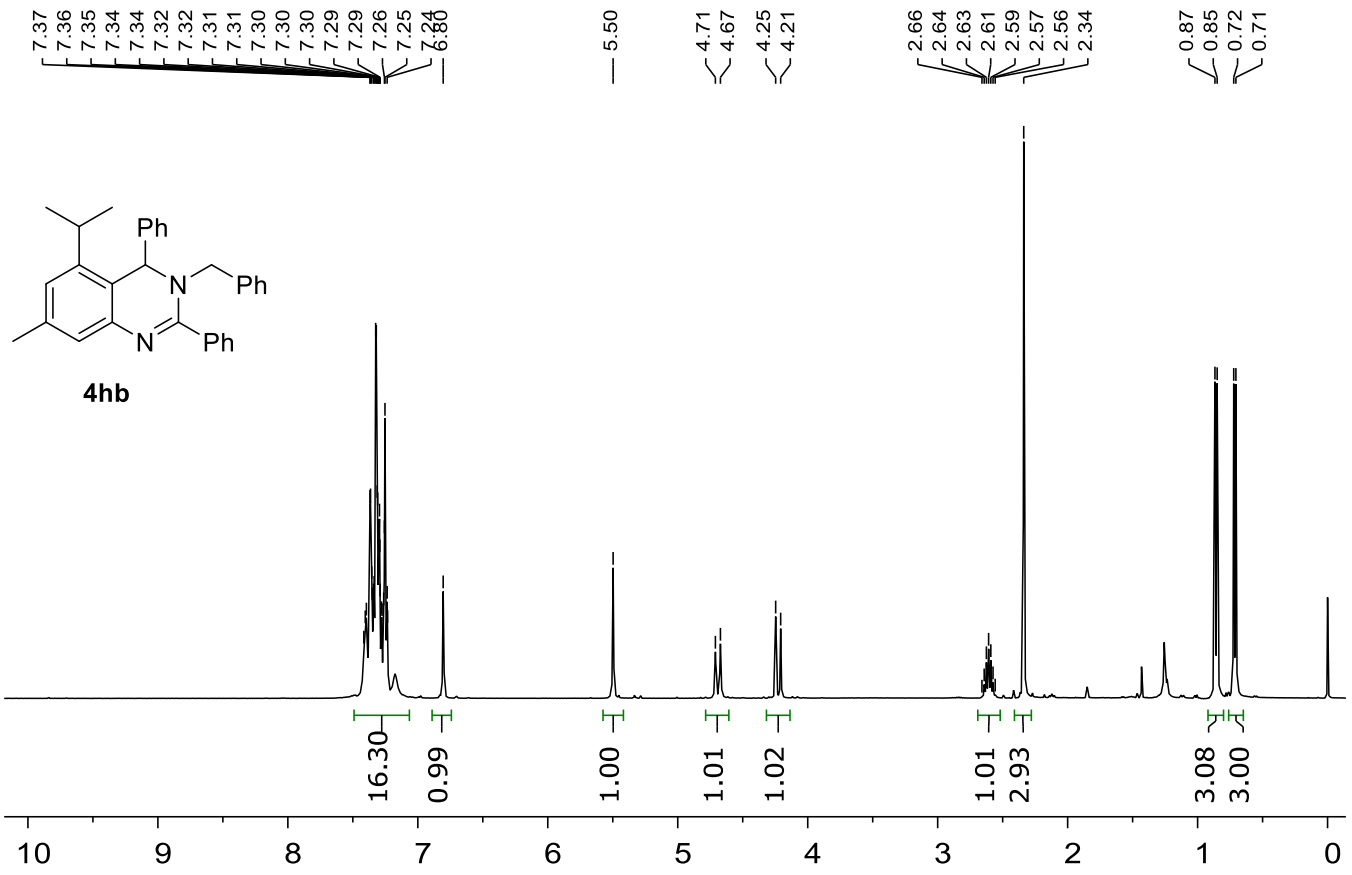
NOESY Spectrum of **4ha**



4ha

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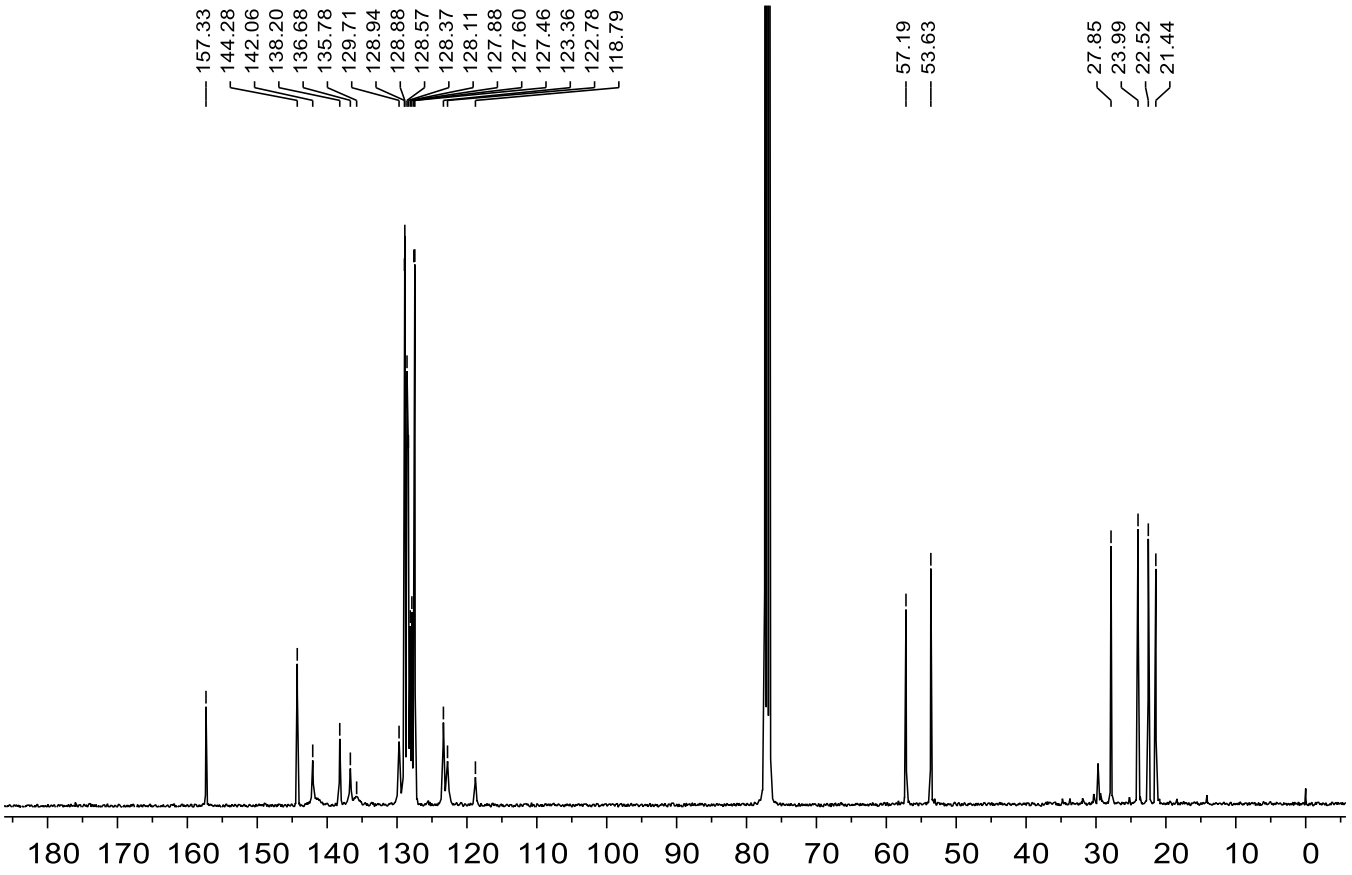
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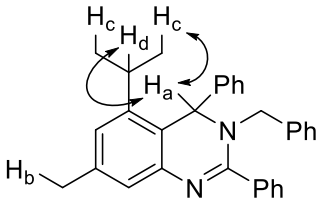
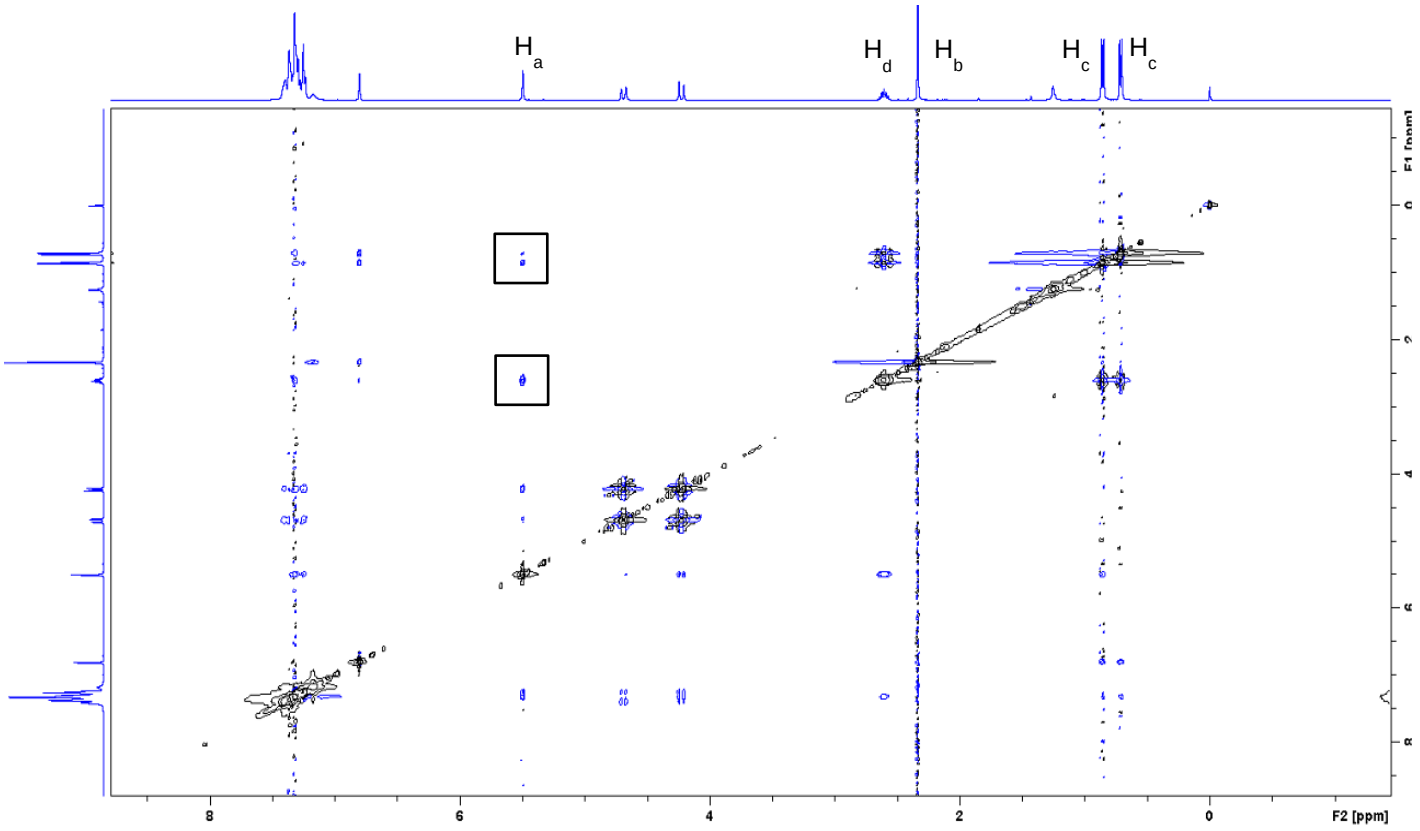
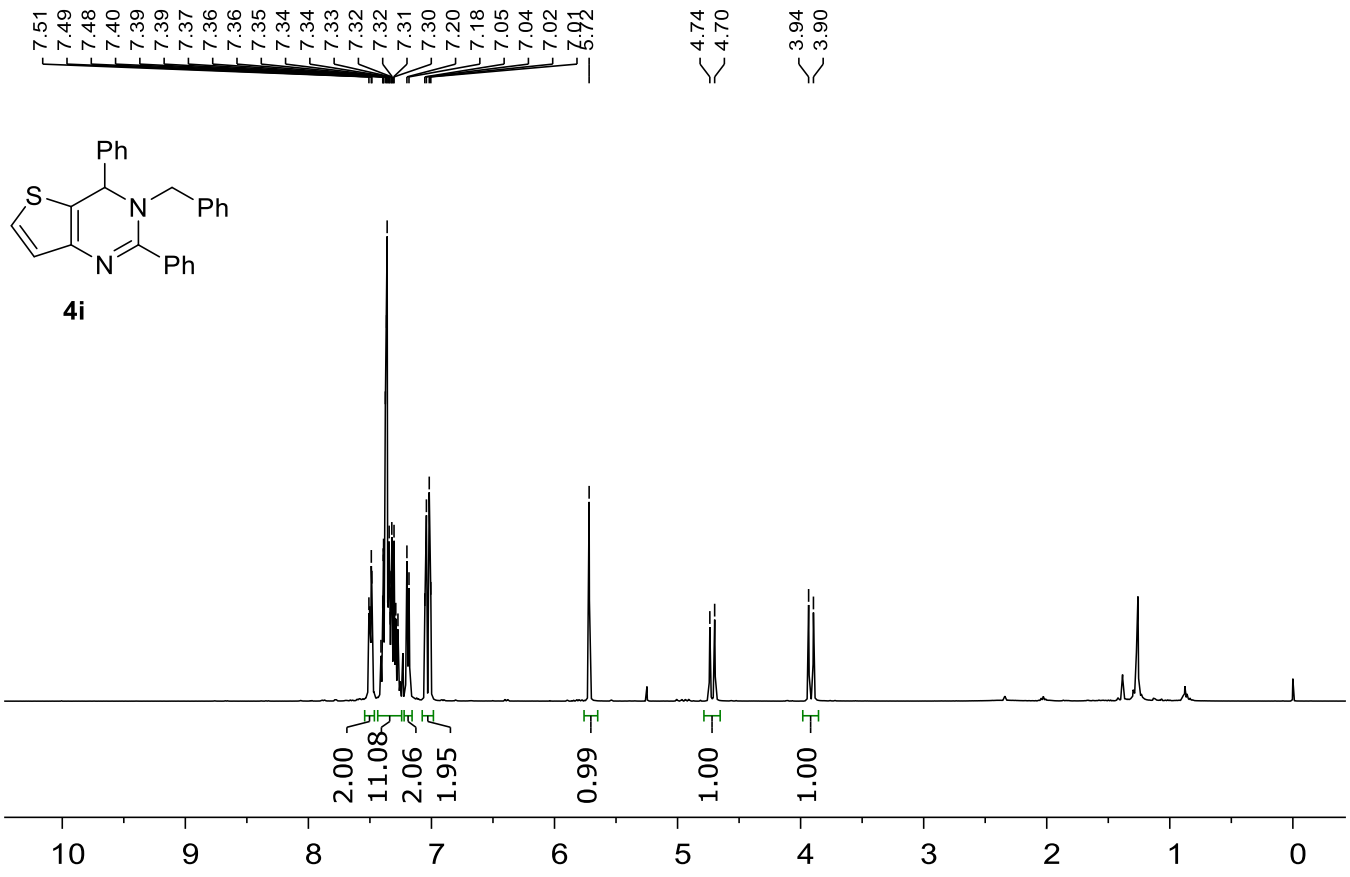
NOESY Spectrum of **4hb**



4hb

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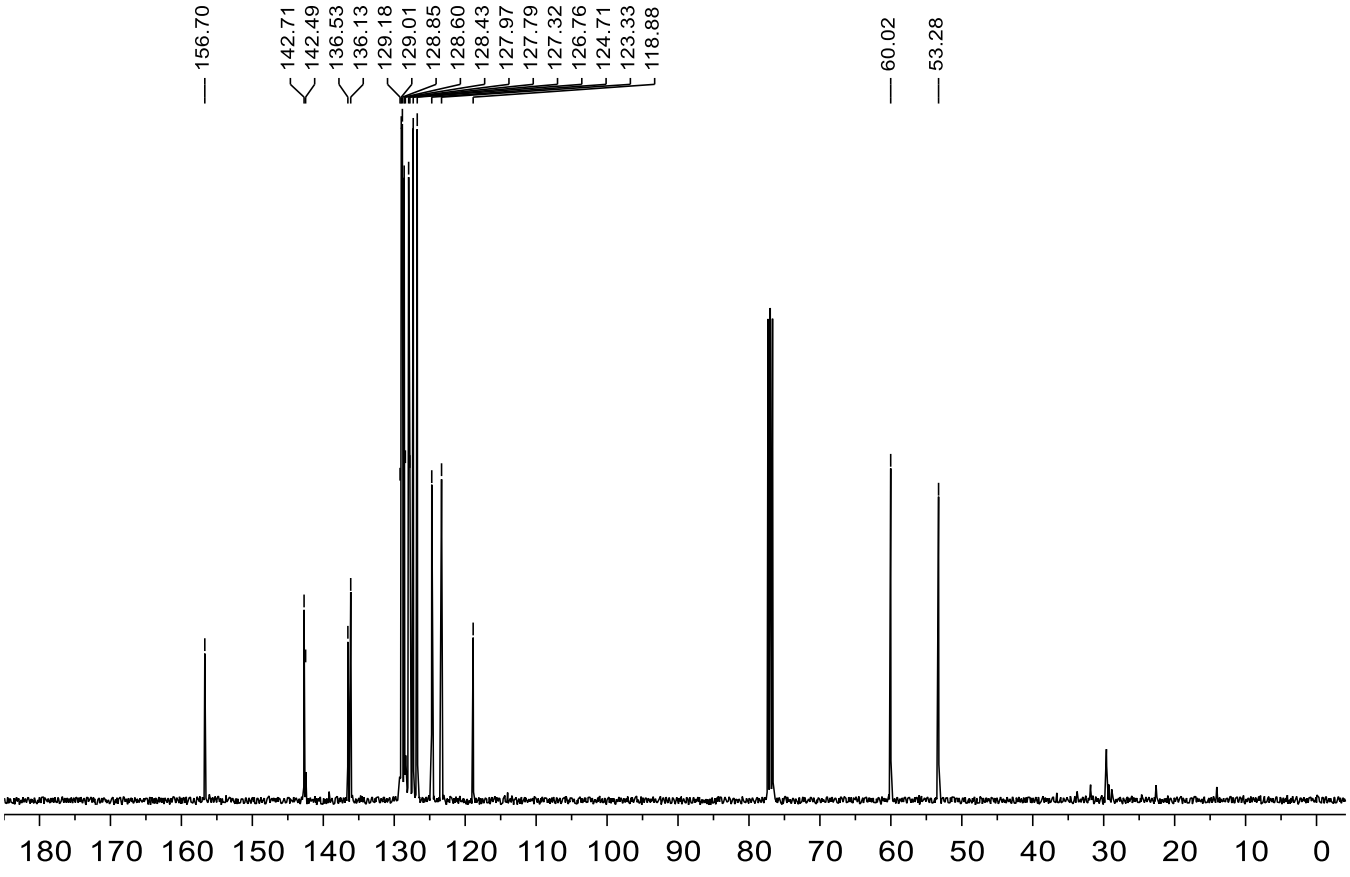
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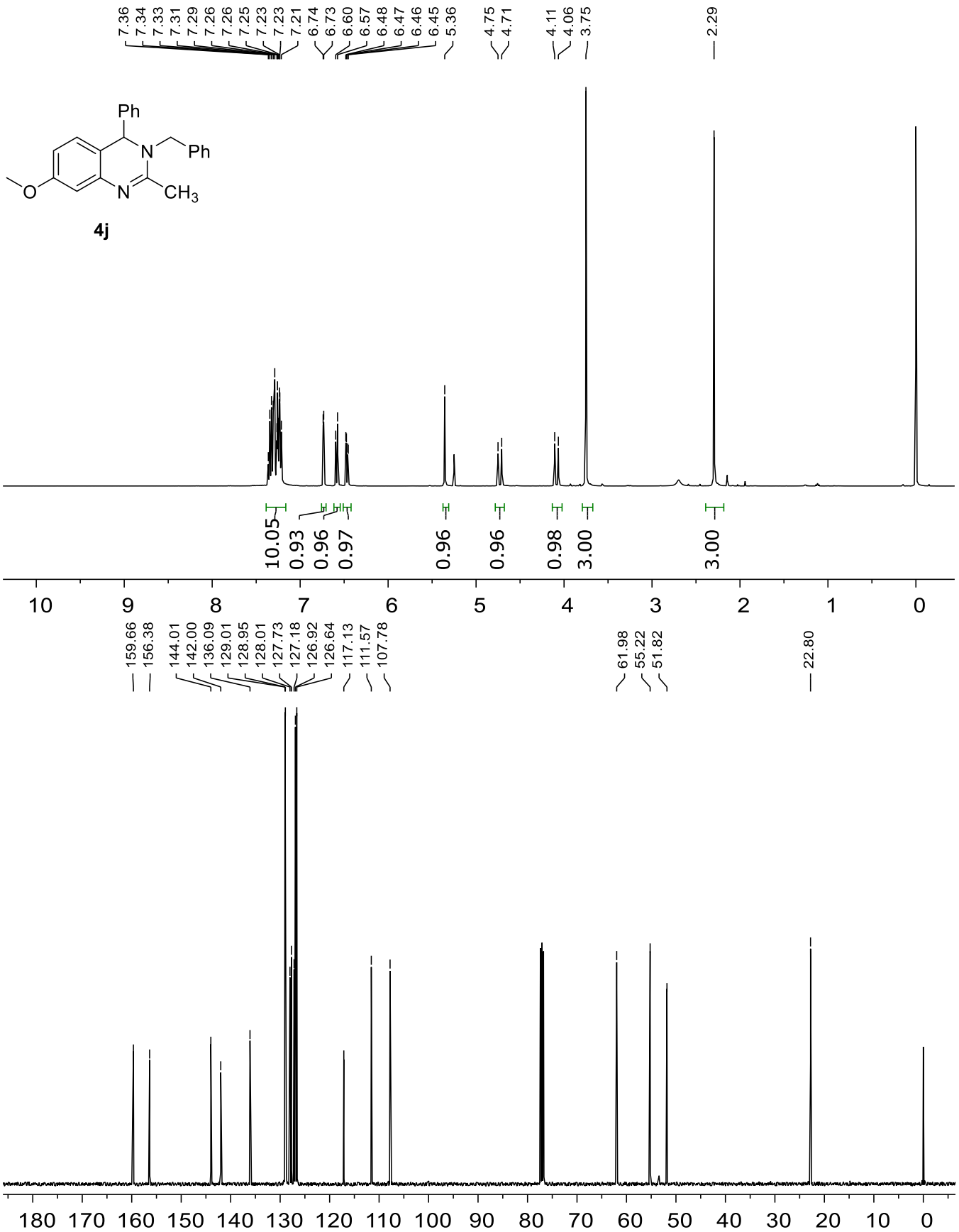
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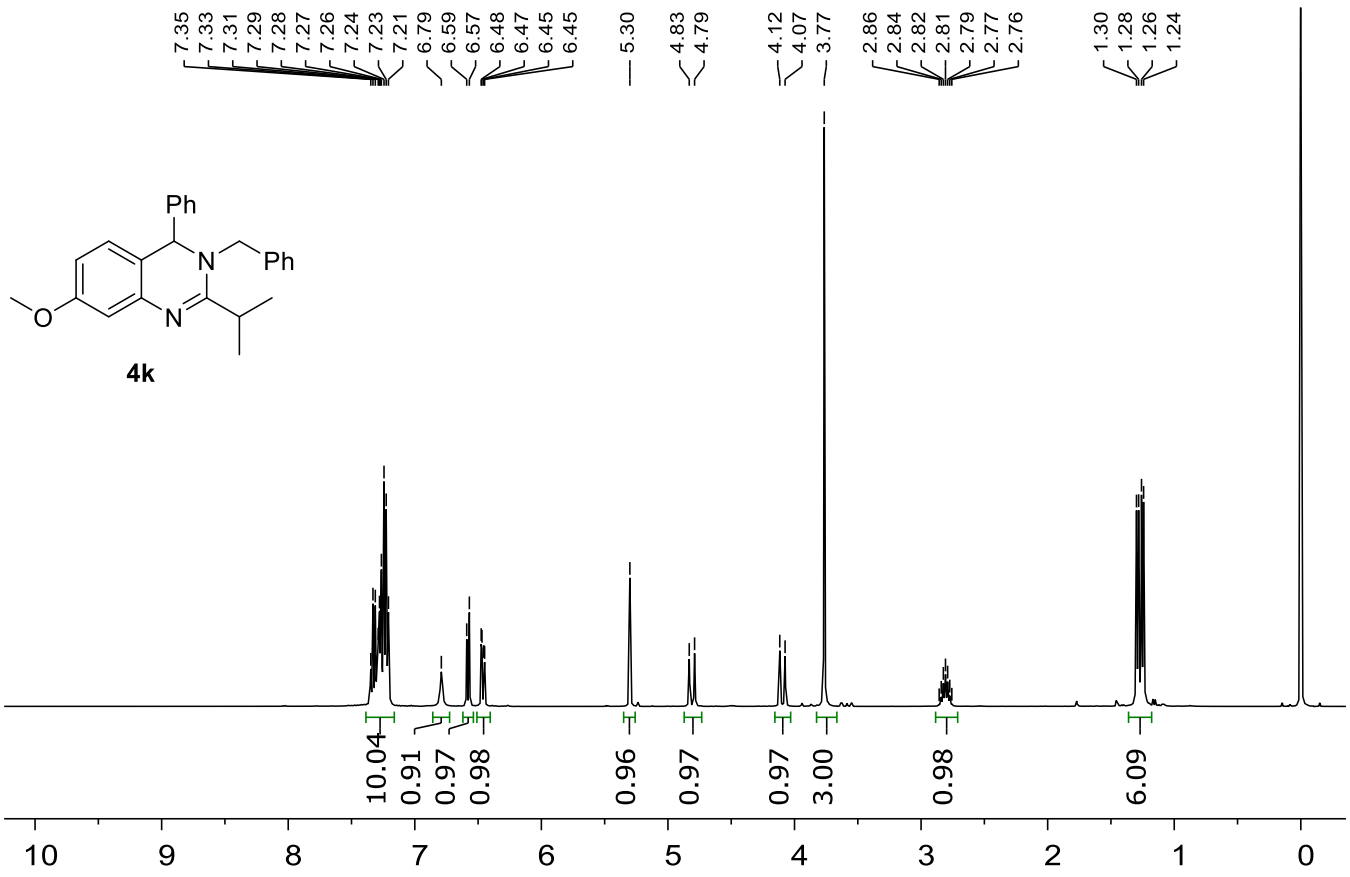
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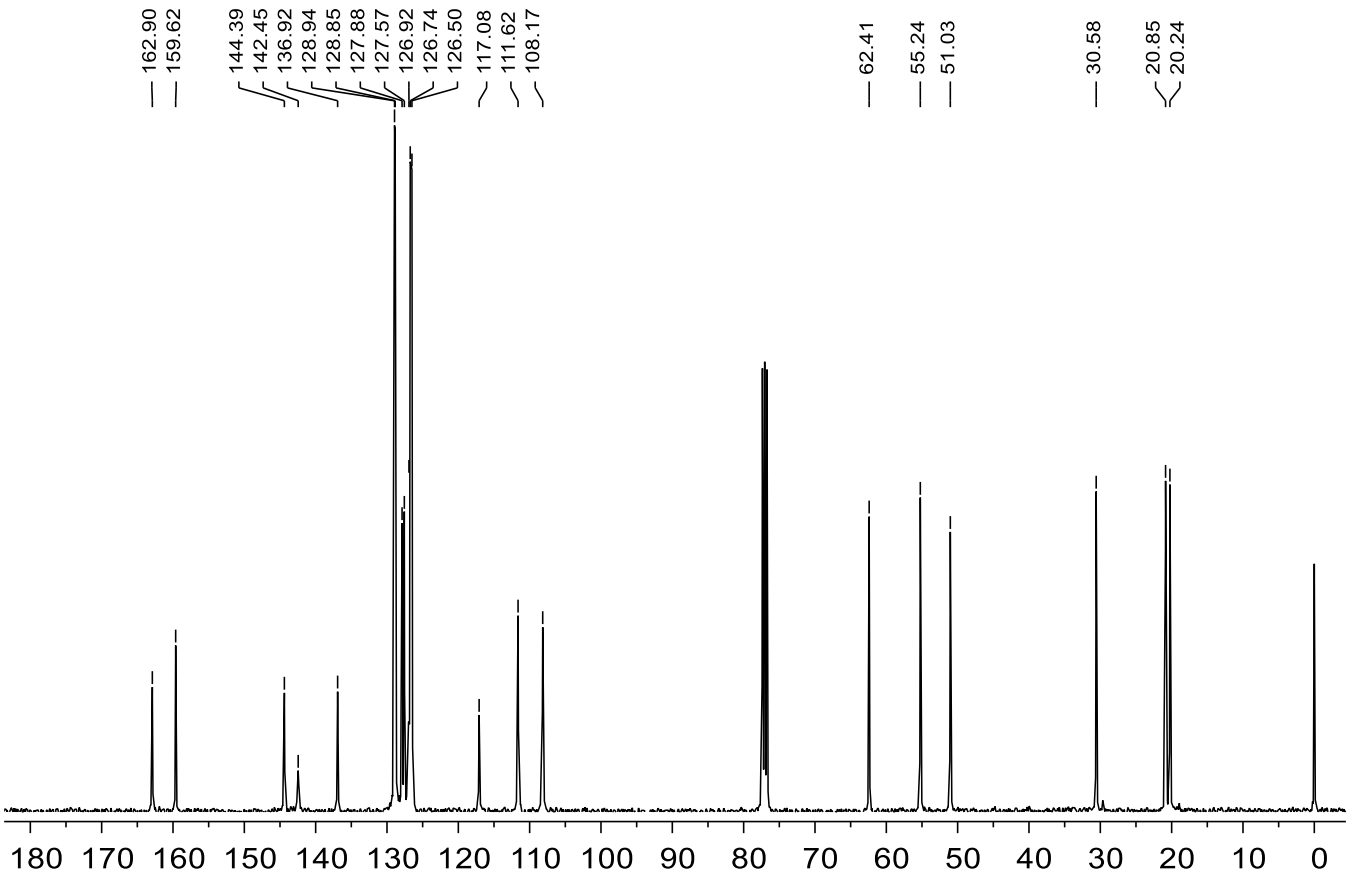
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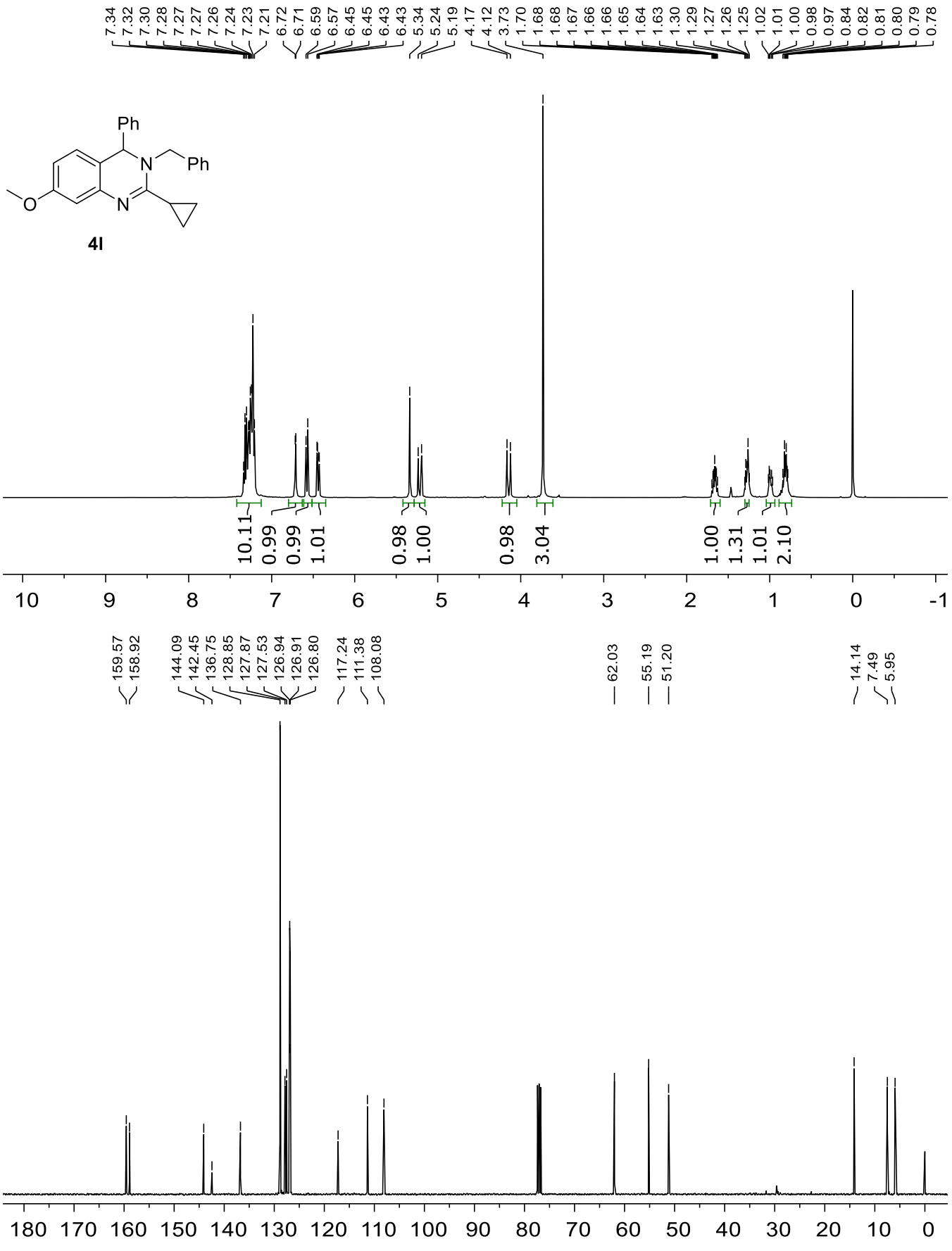
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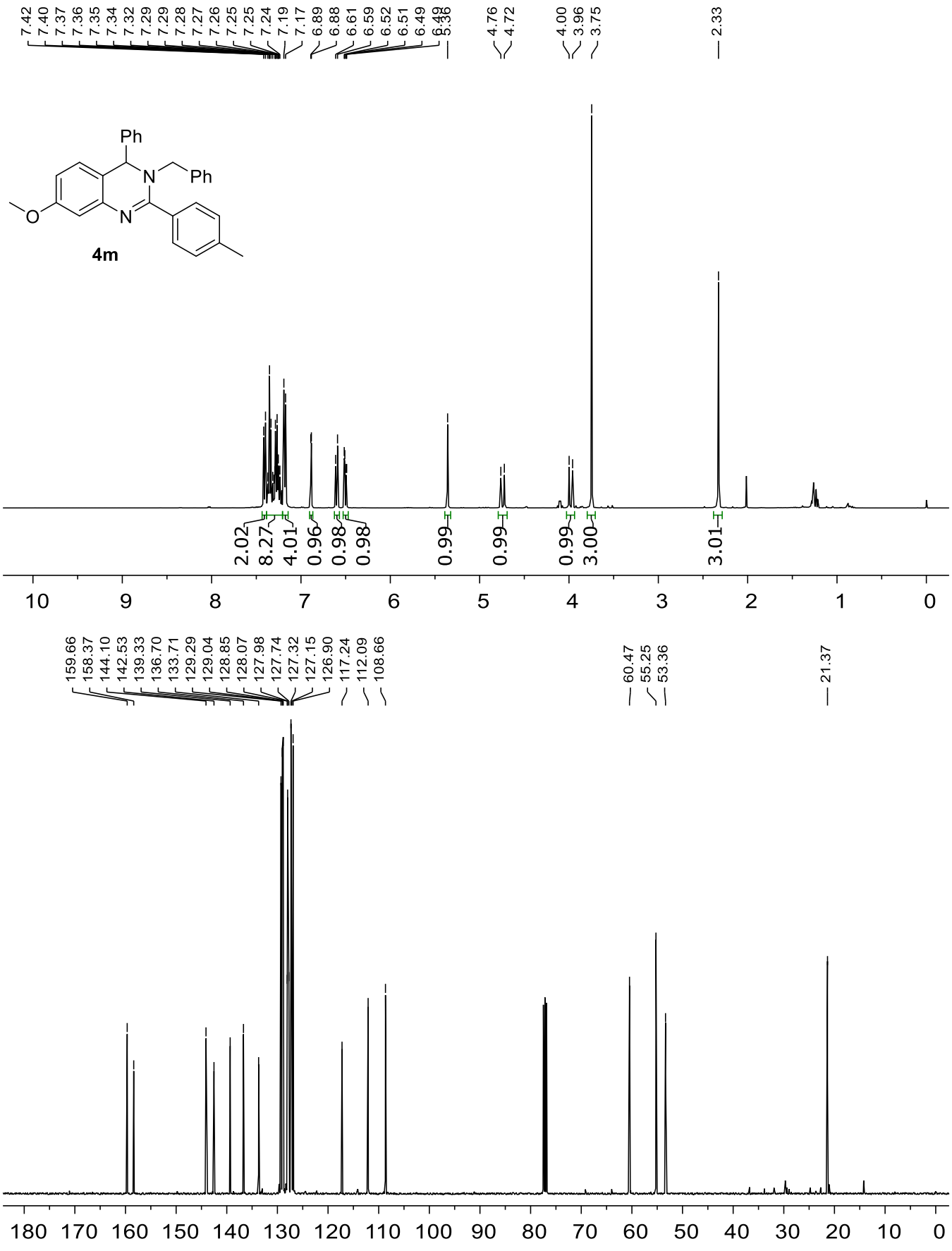
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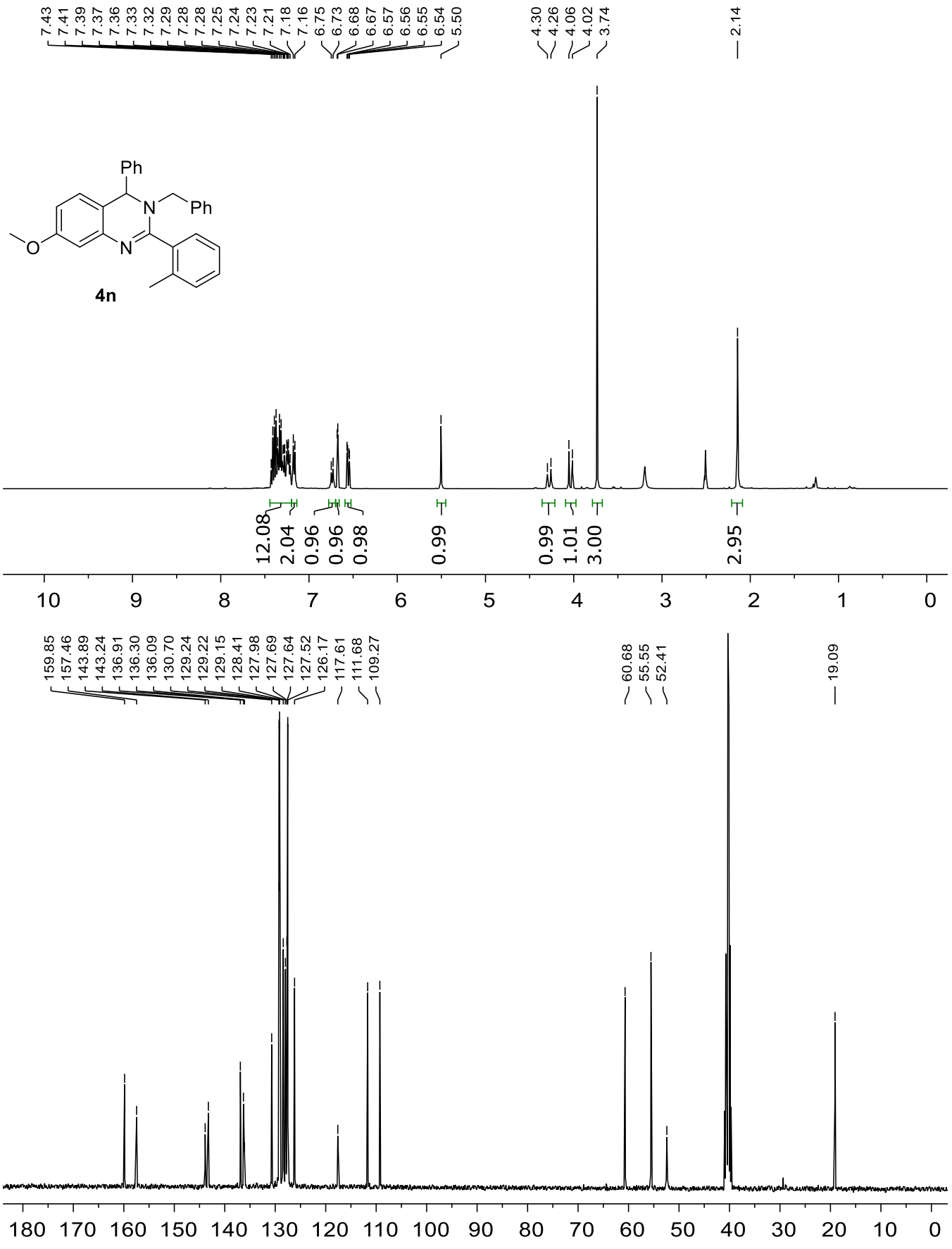
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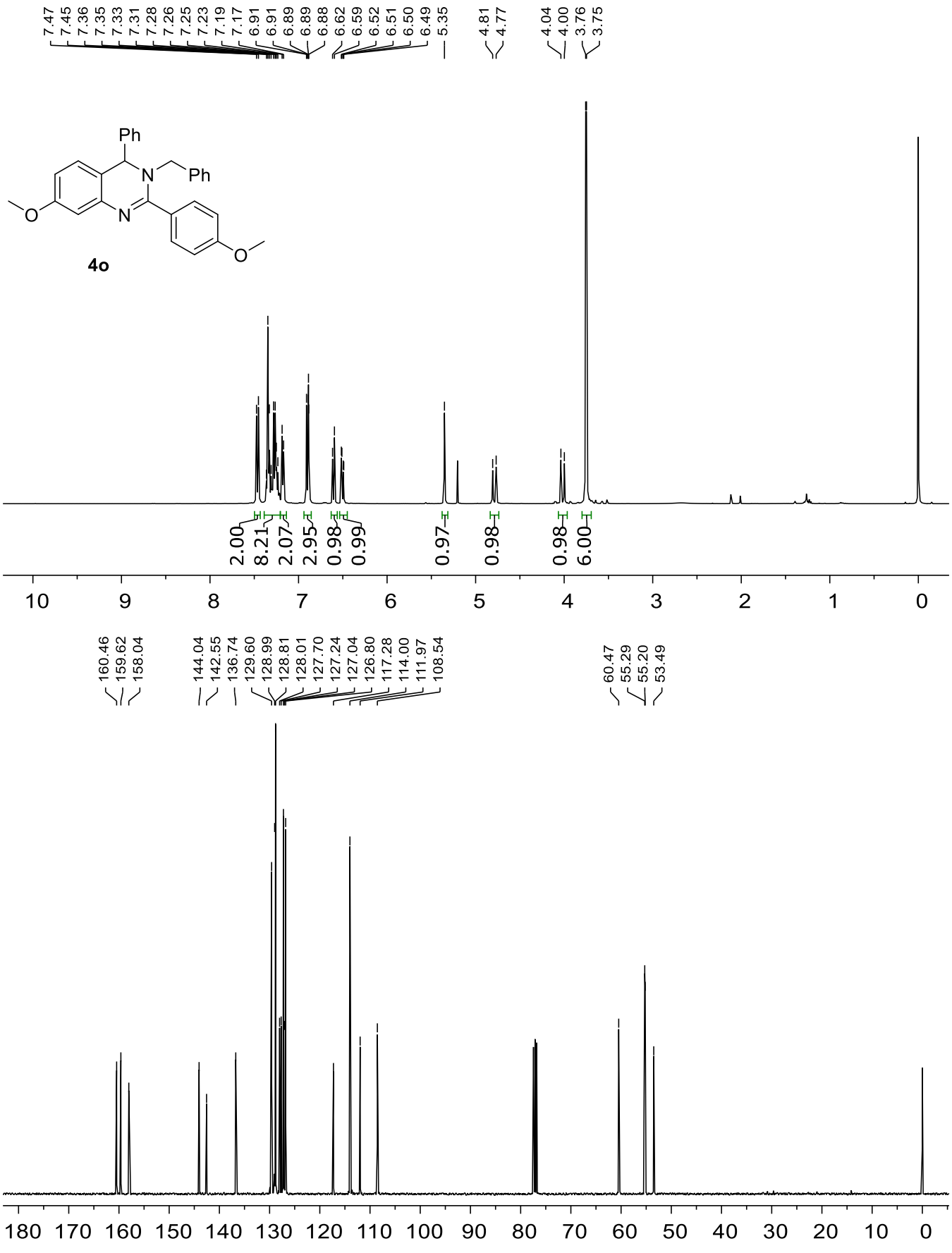
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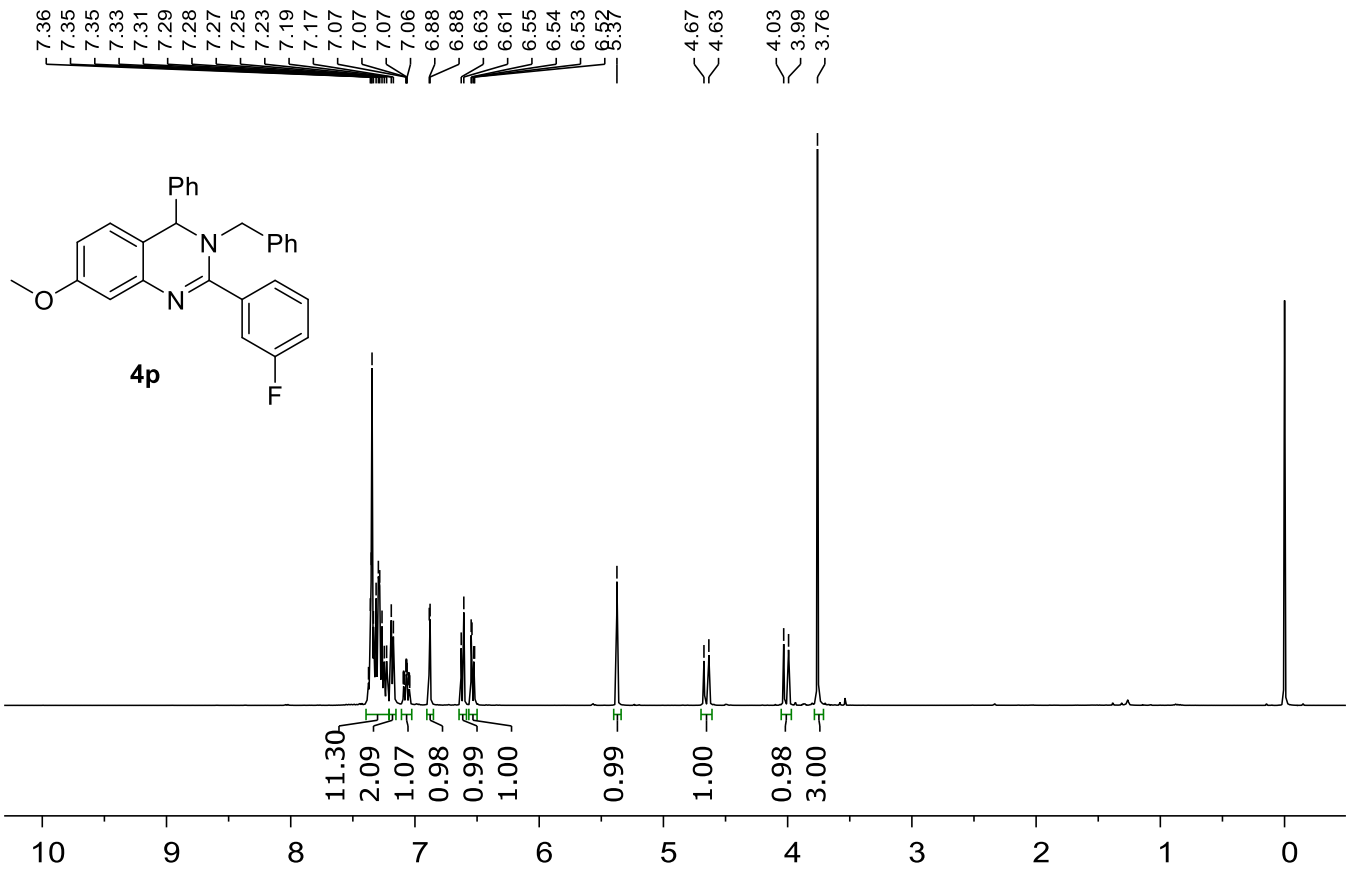
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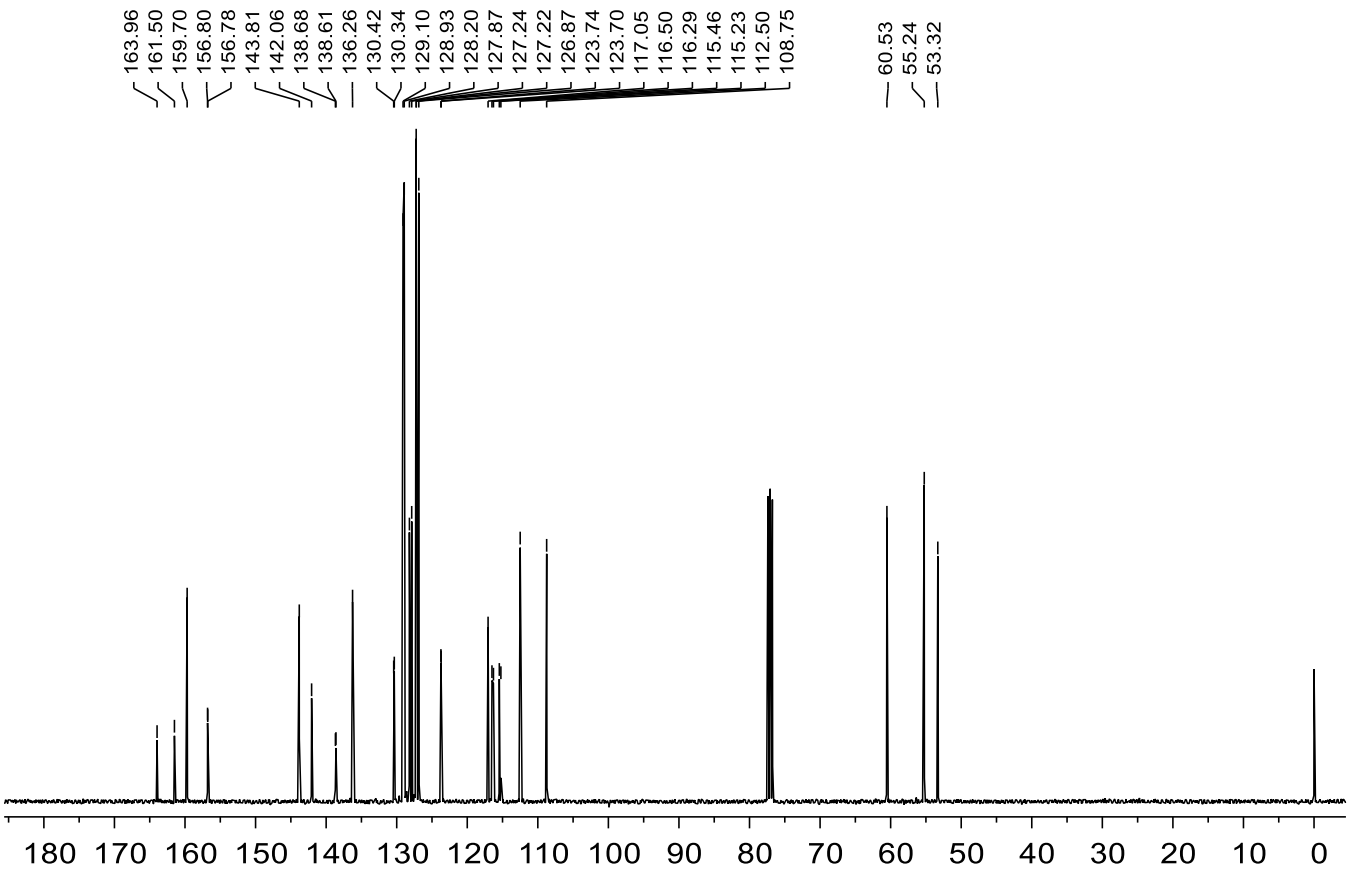
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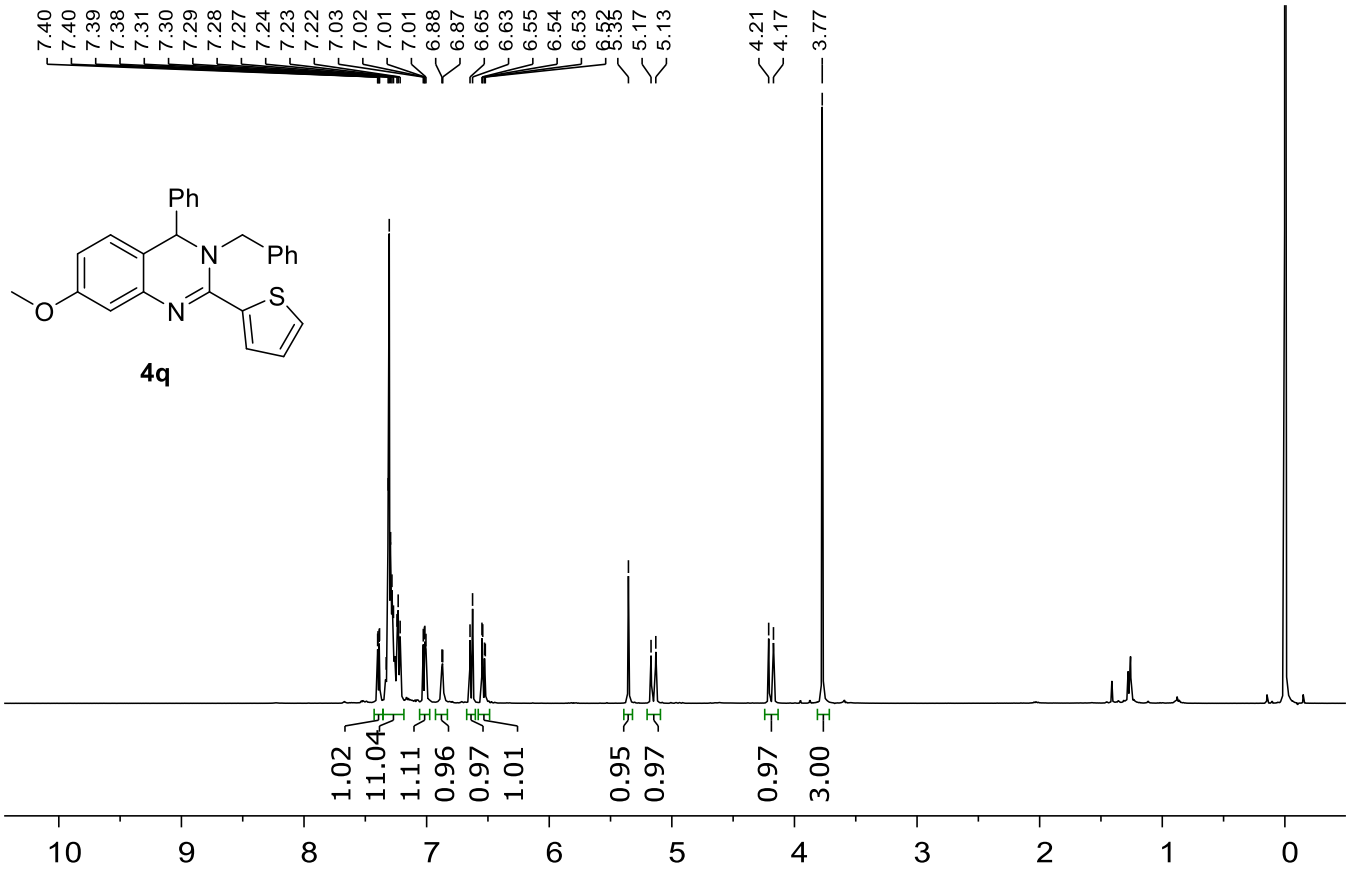
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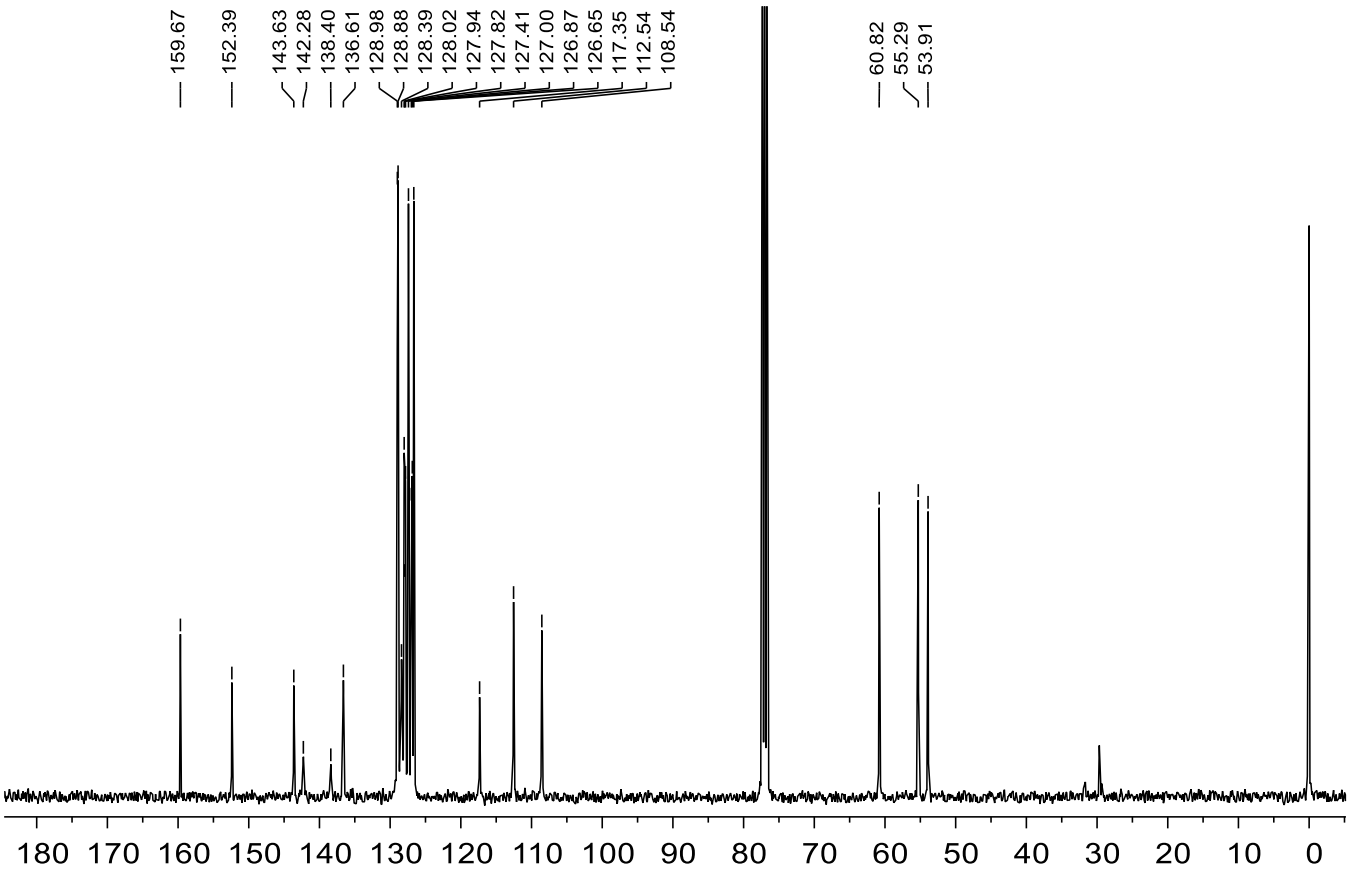
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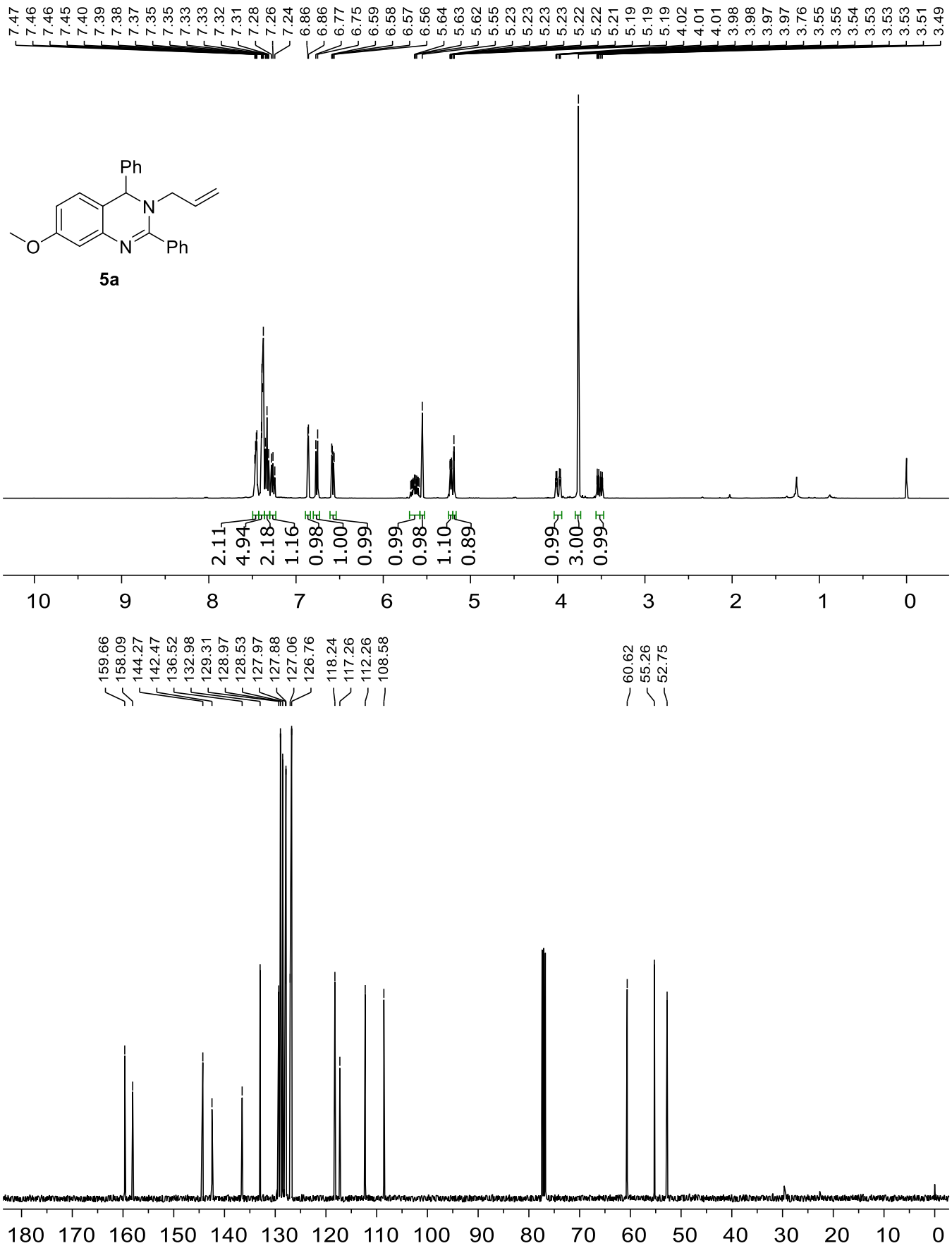
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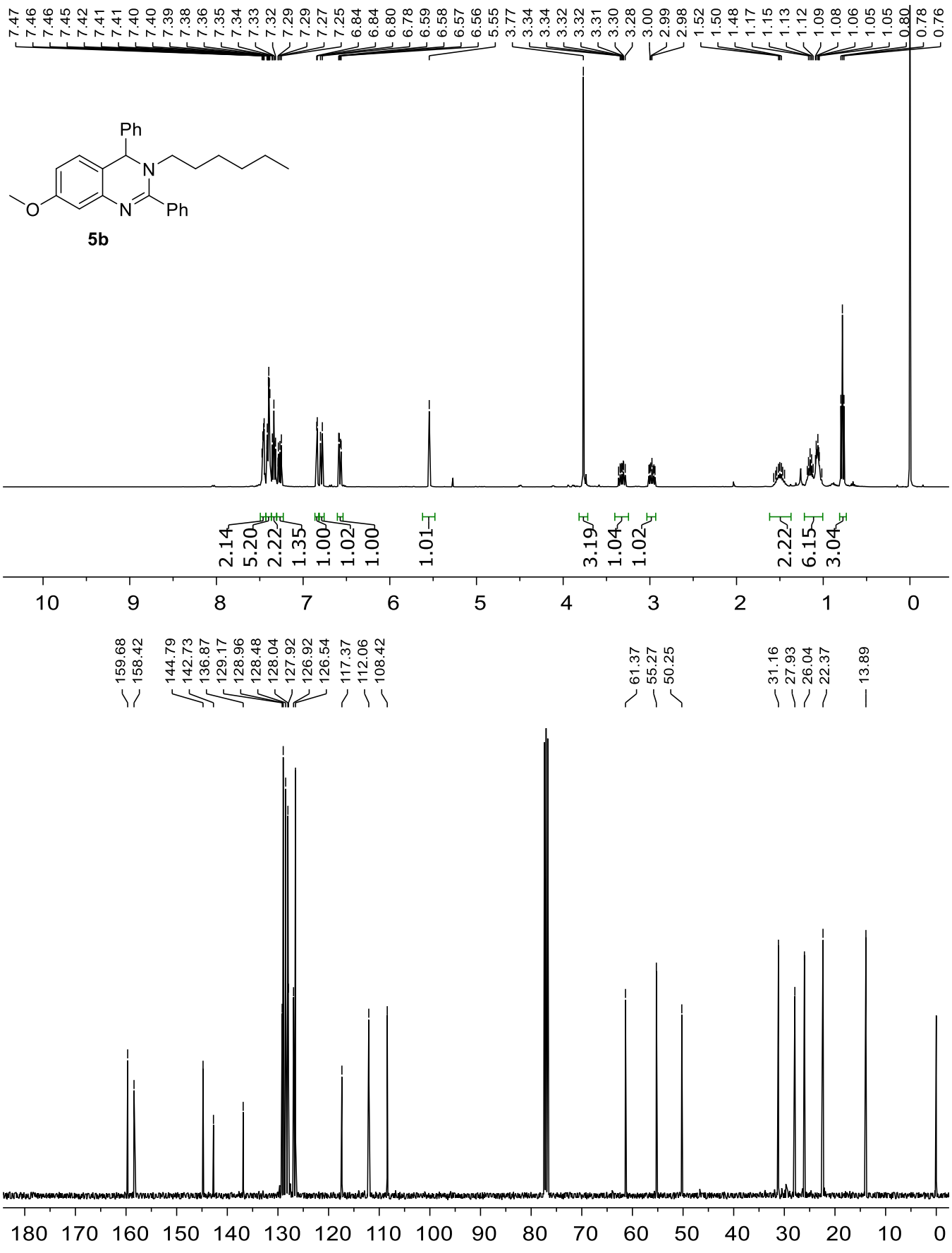
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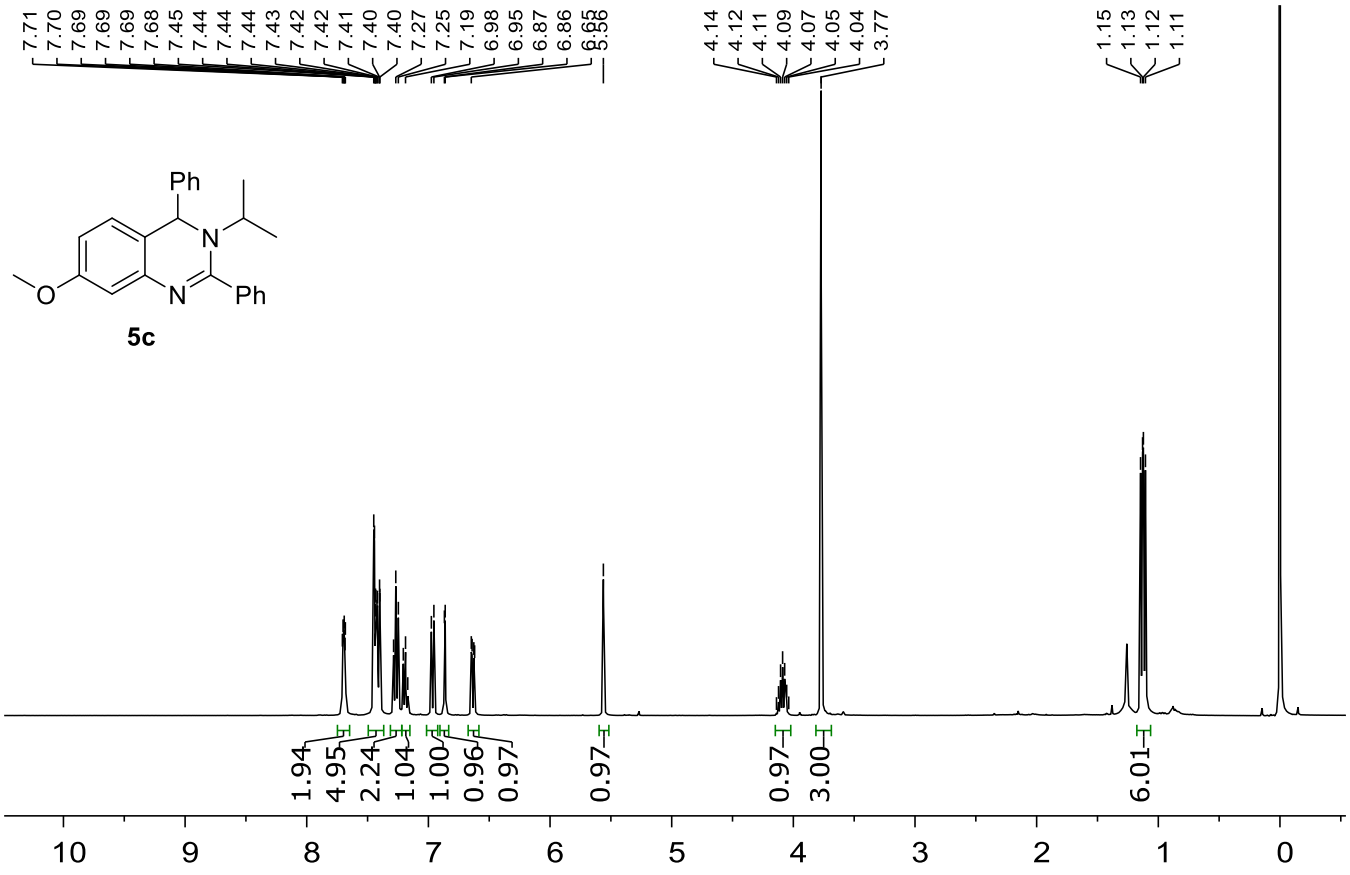
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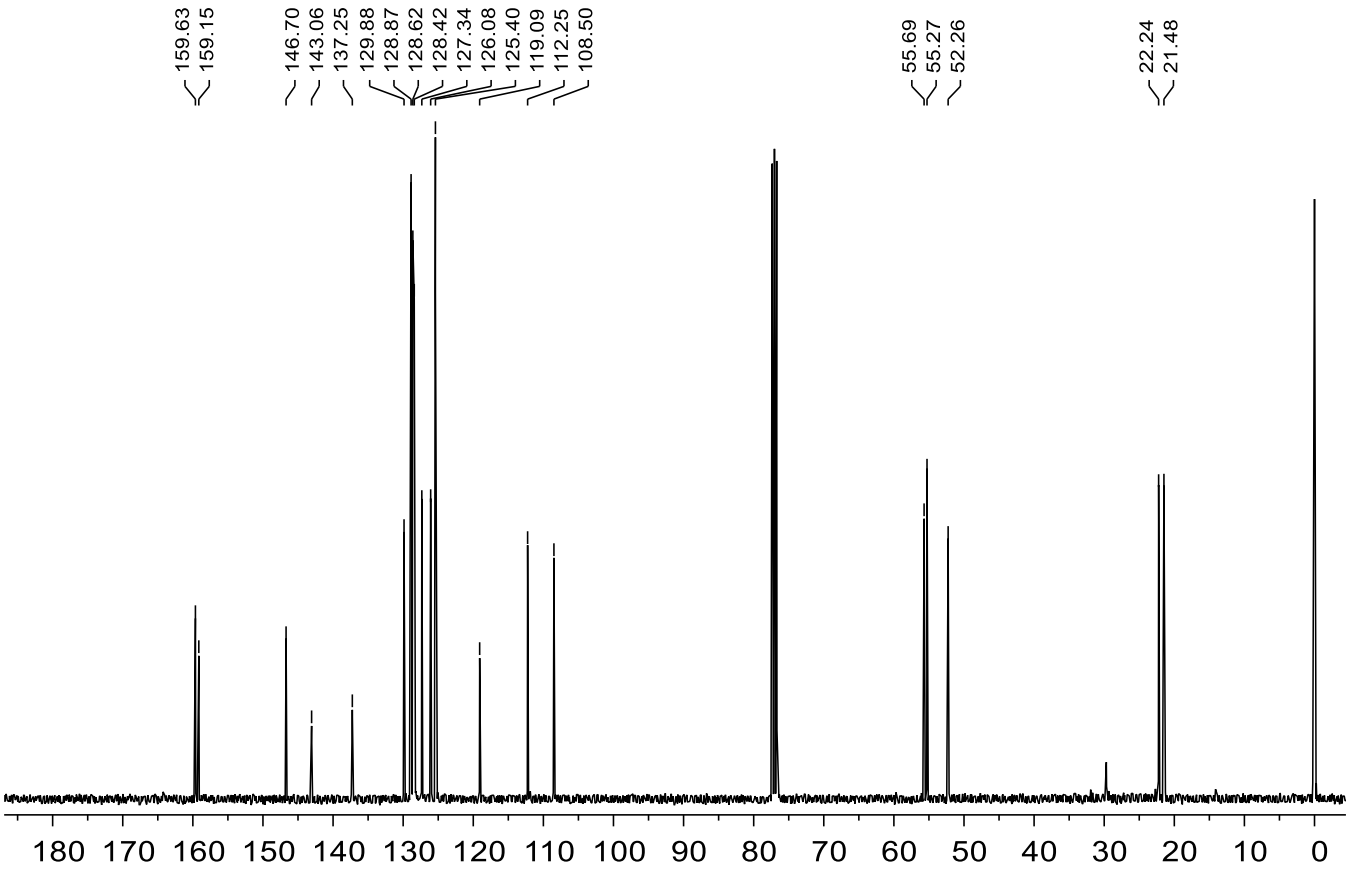
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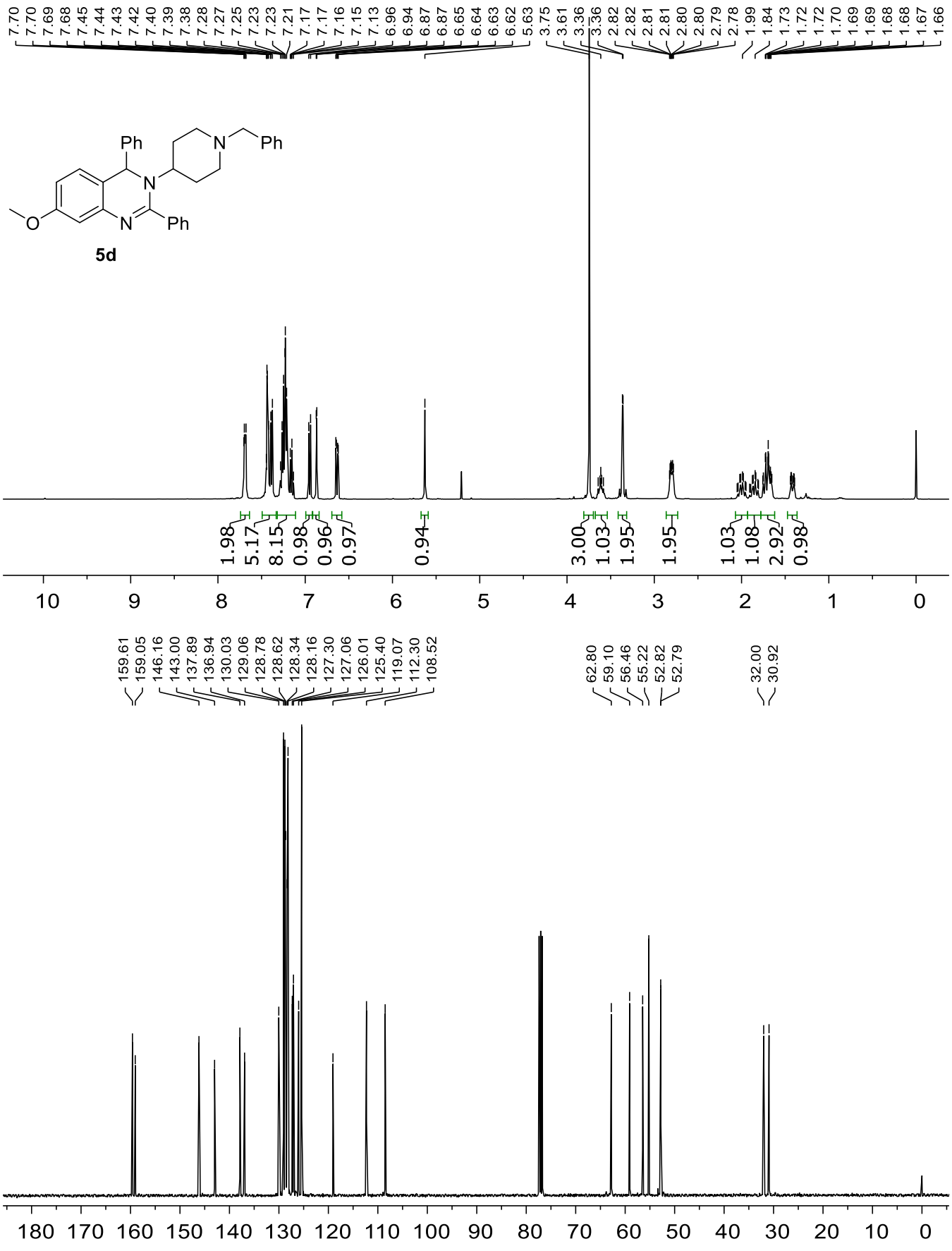
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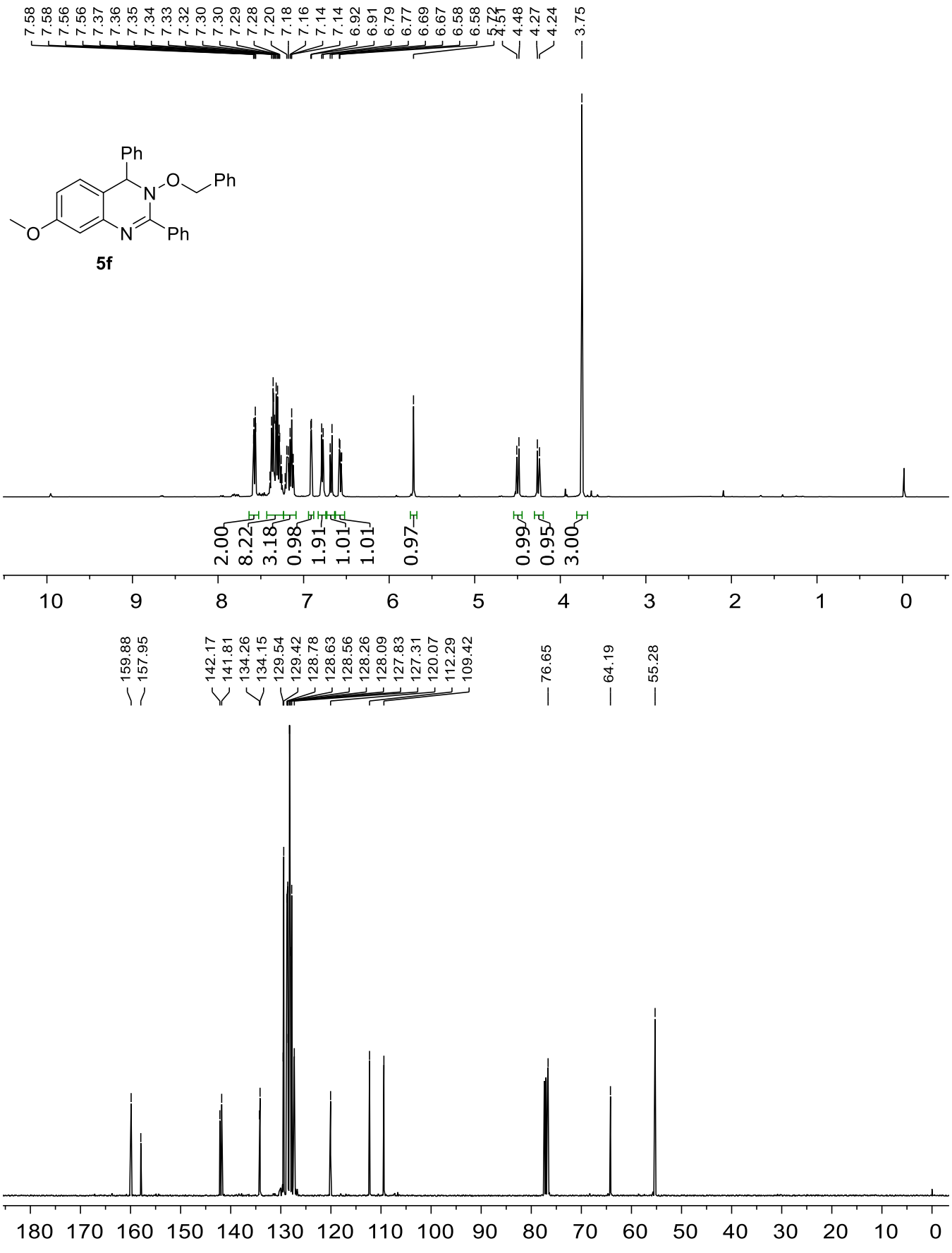
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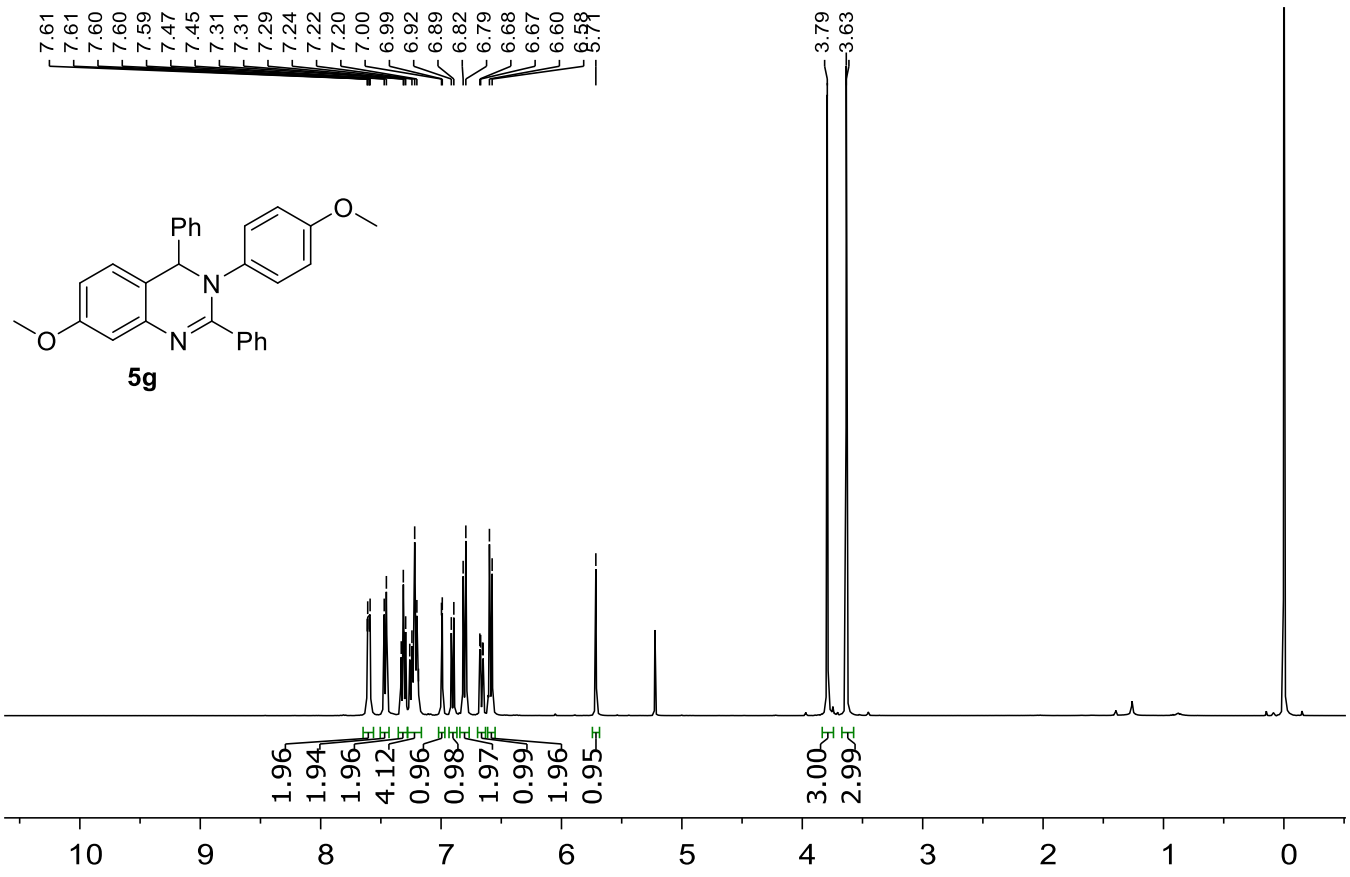
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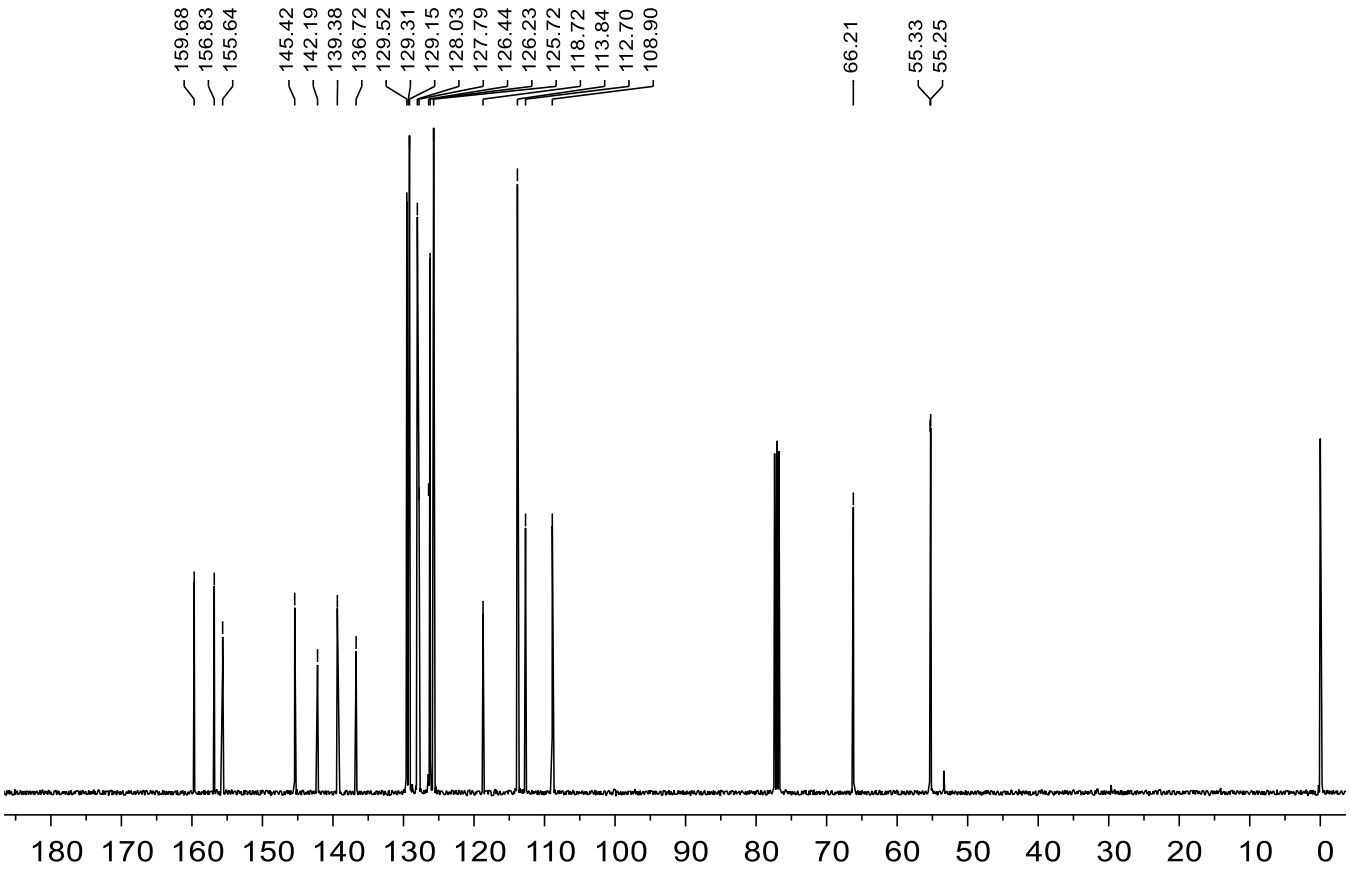
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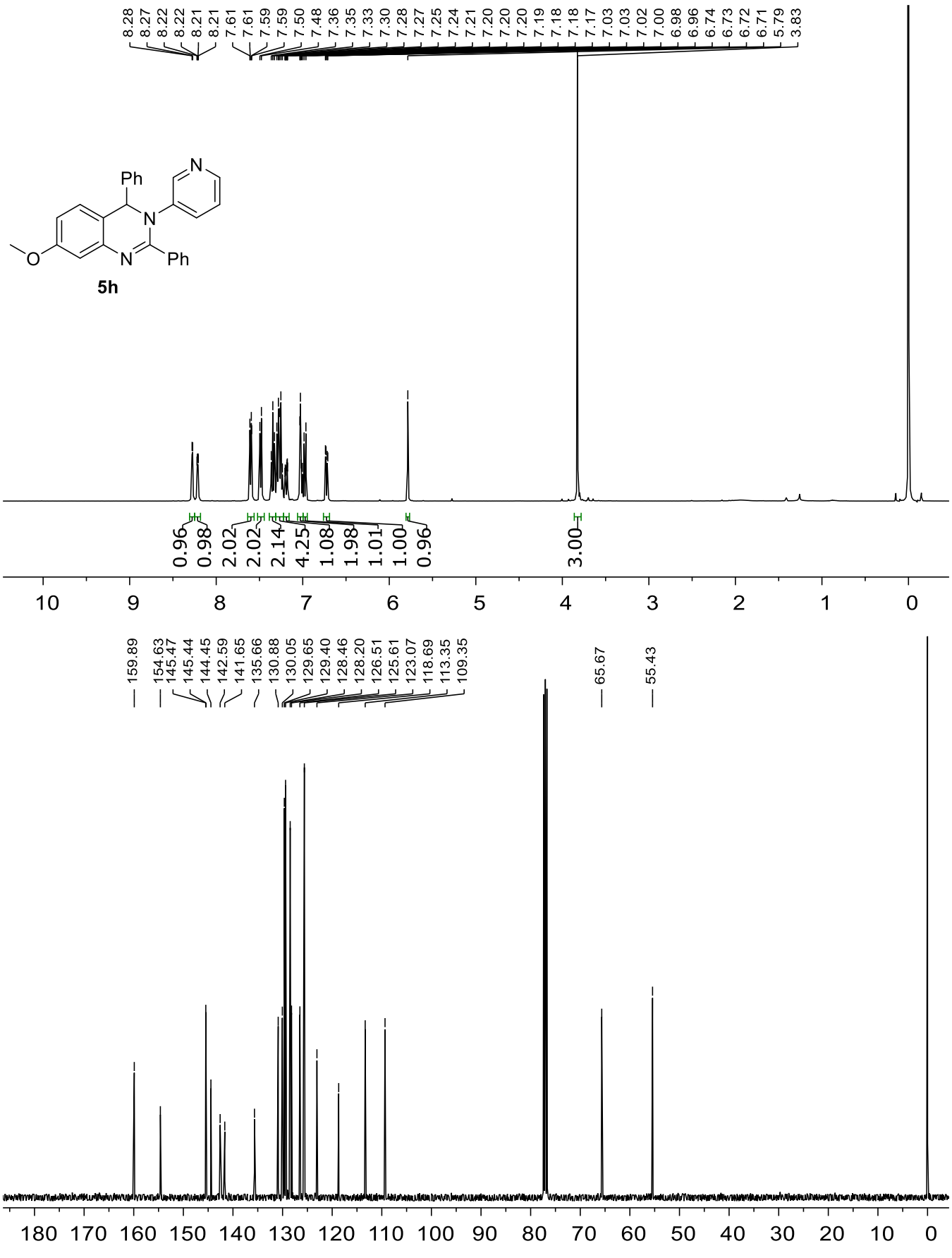
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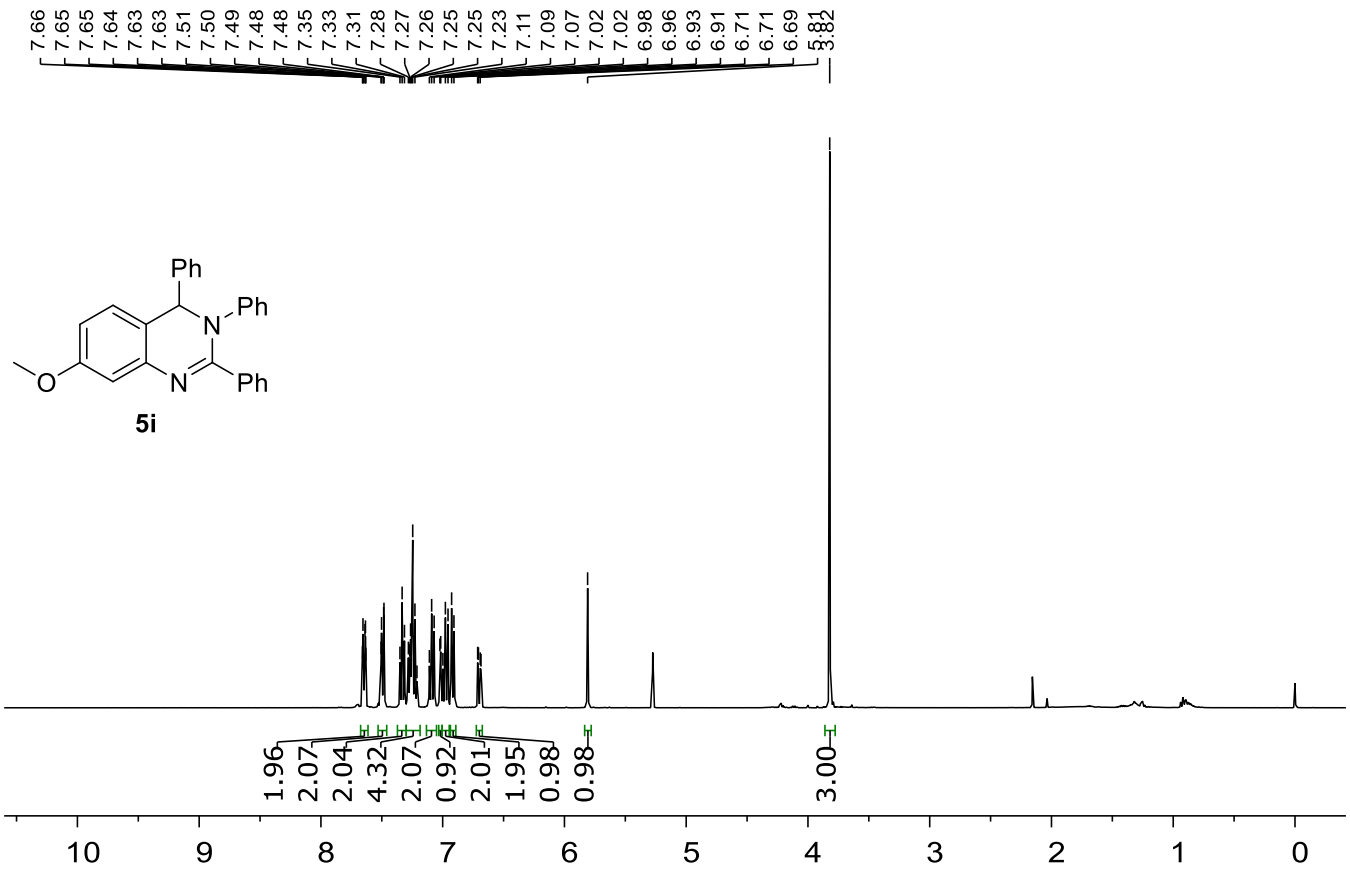
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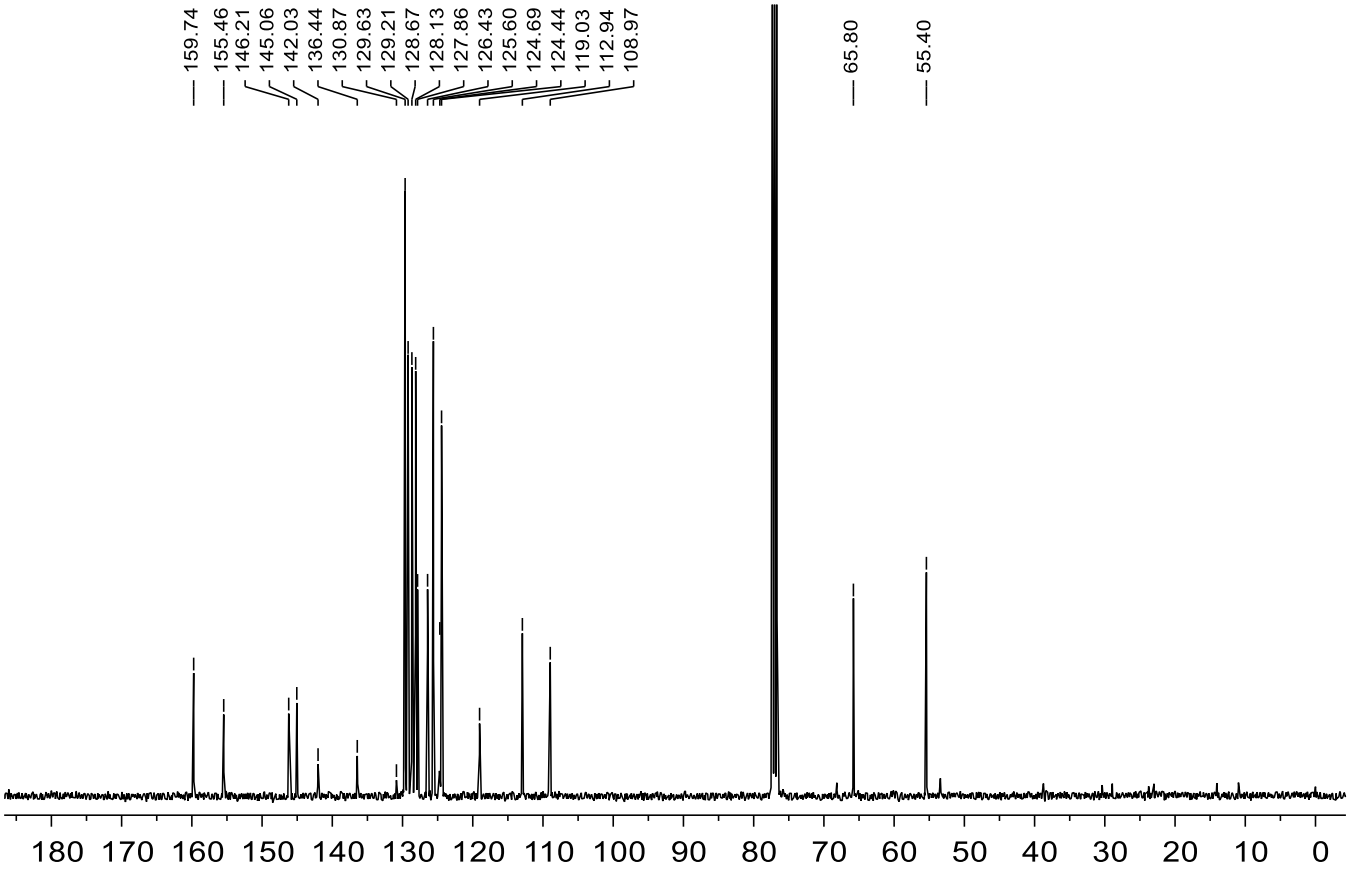
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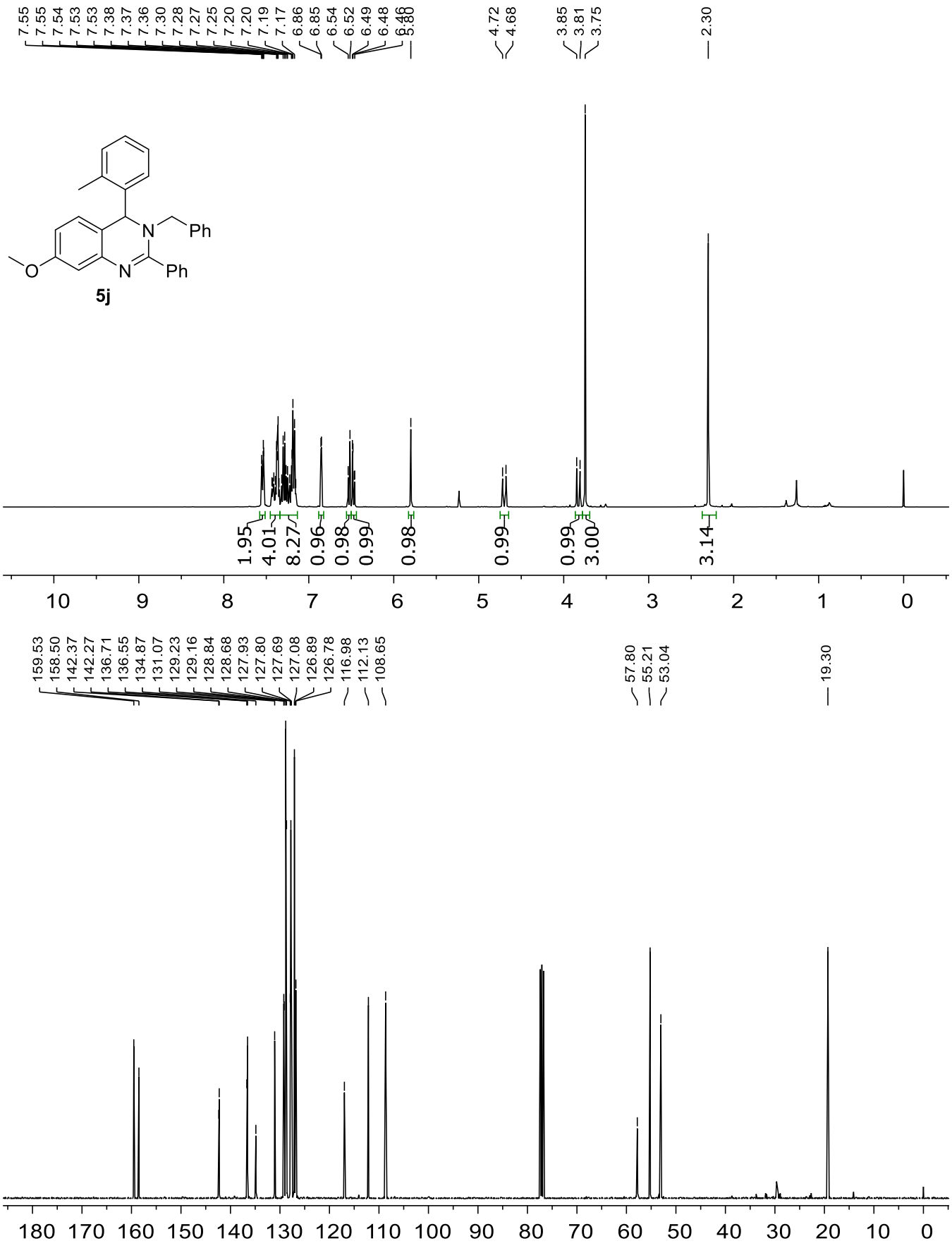
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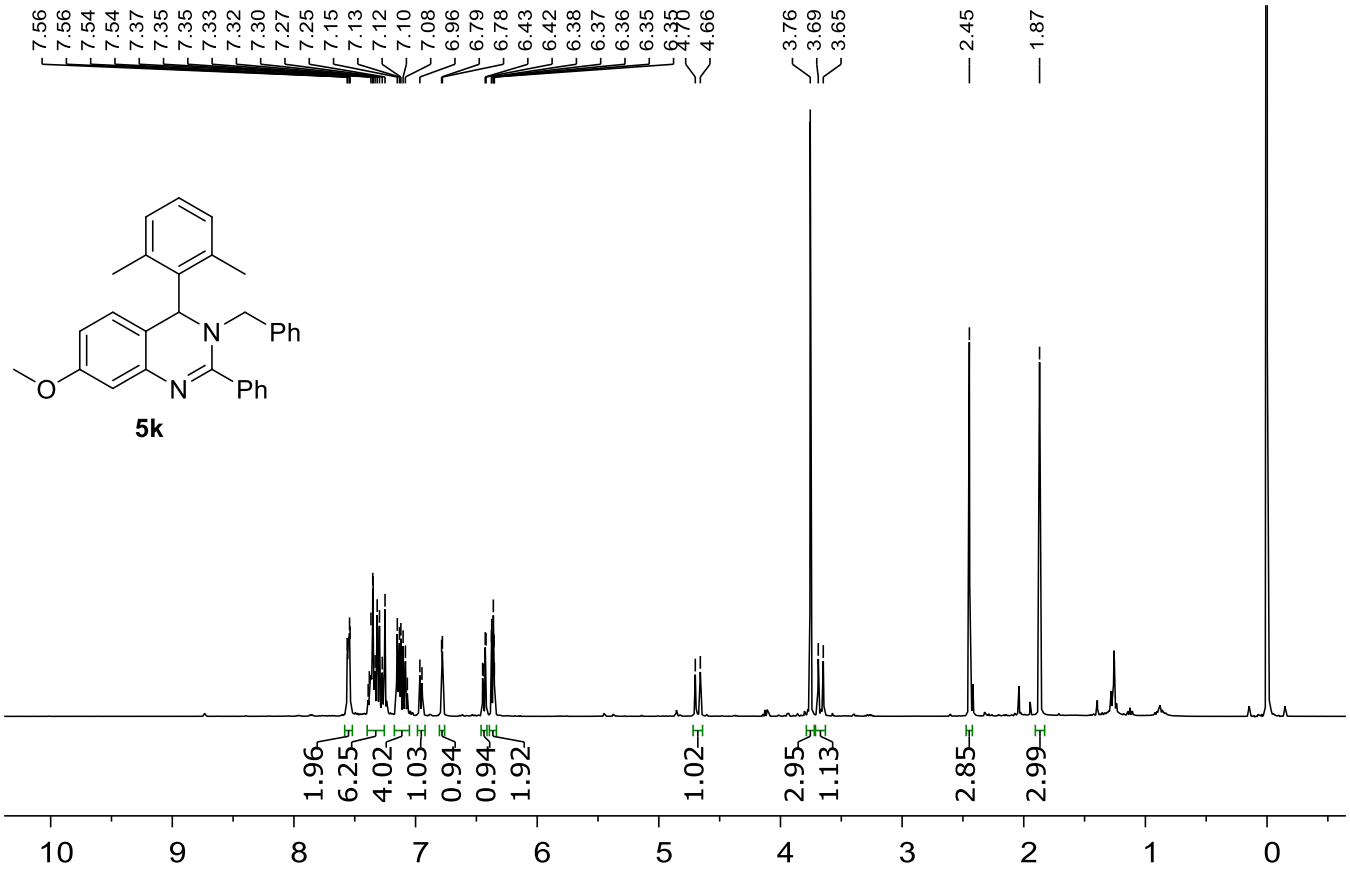
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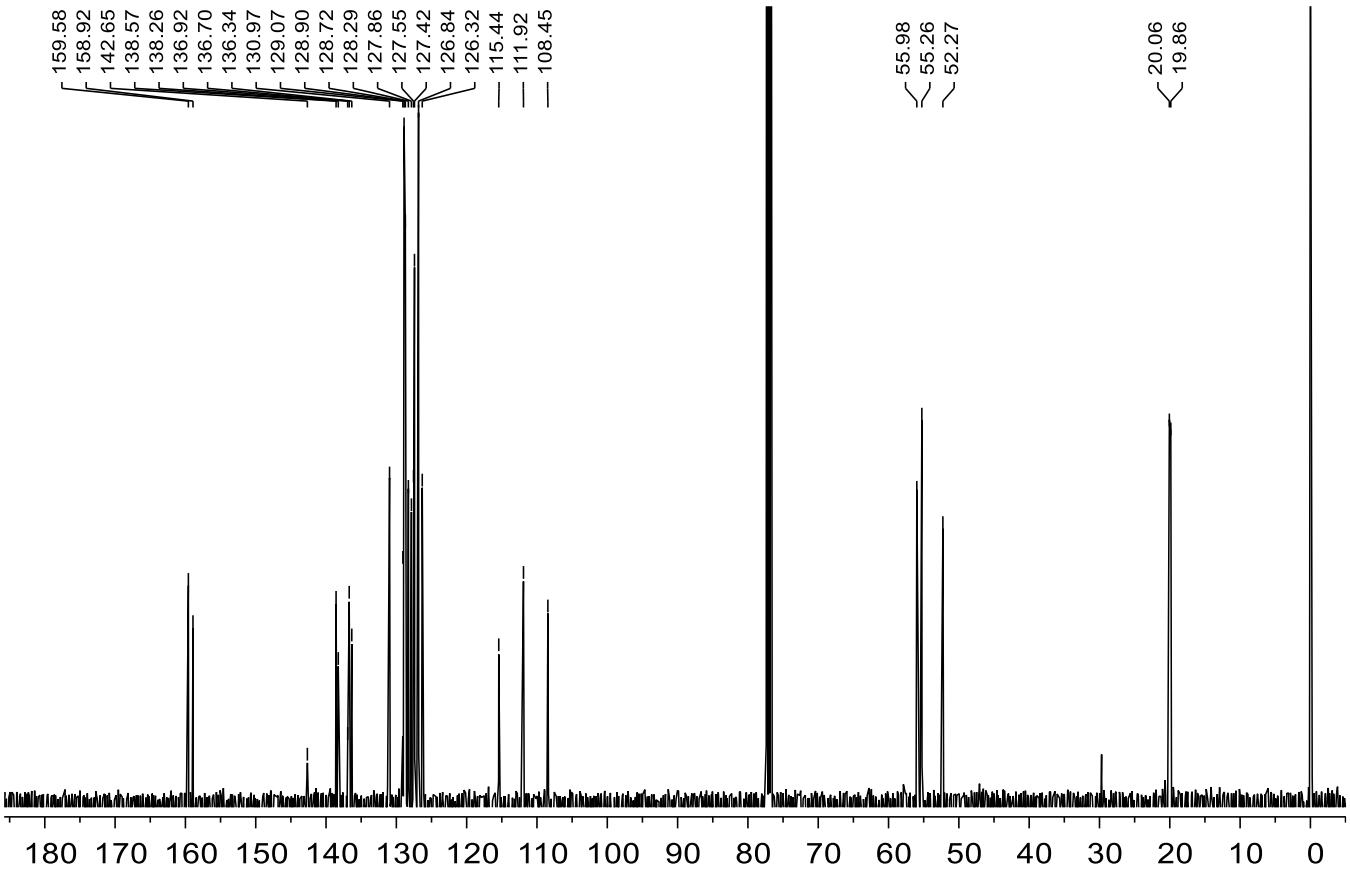
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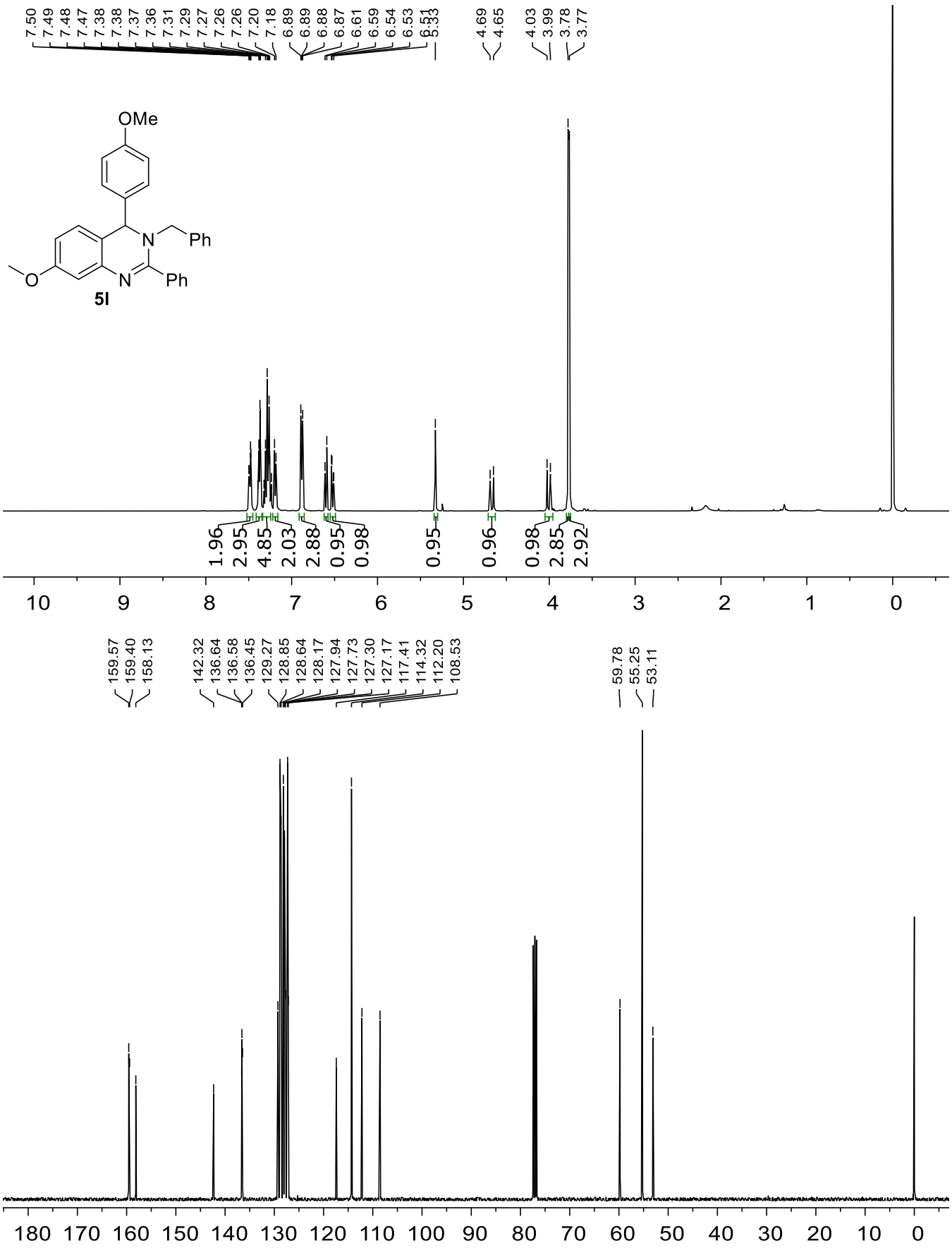
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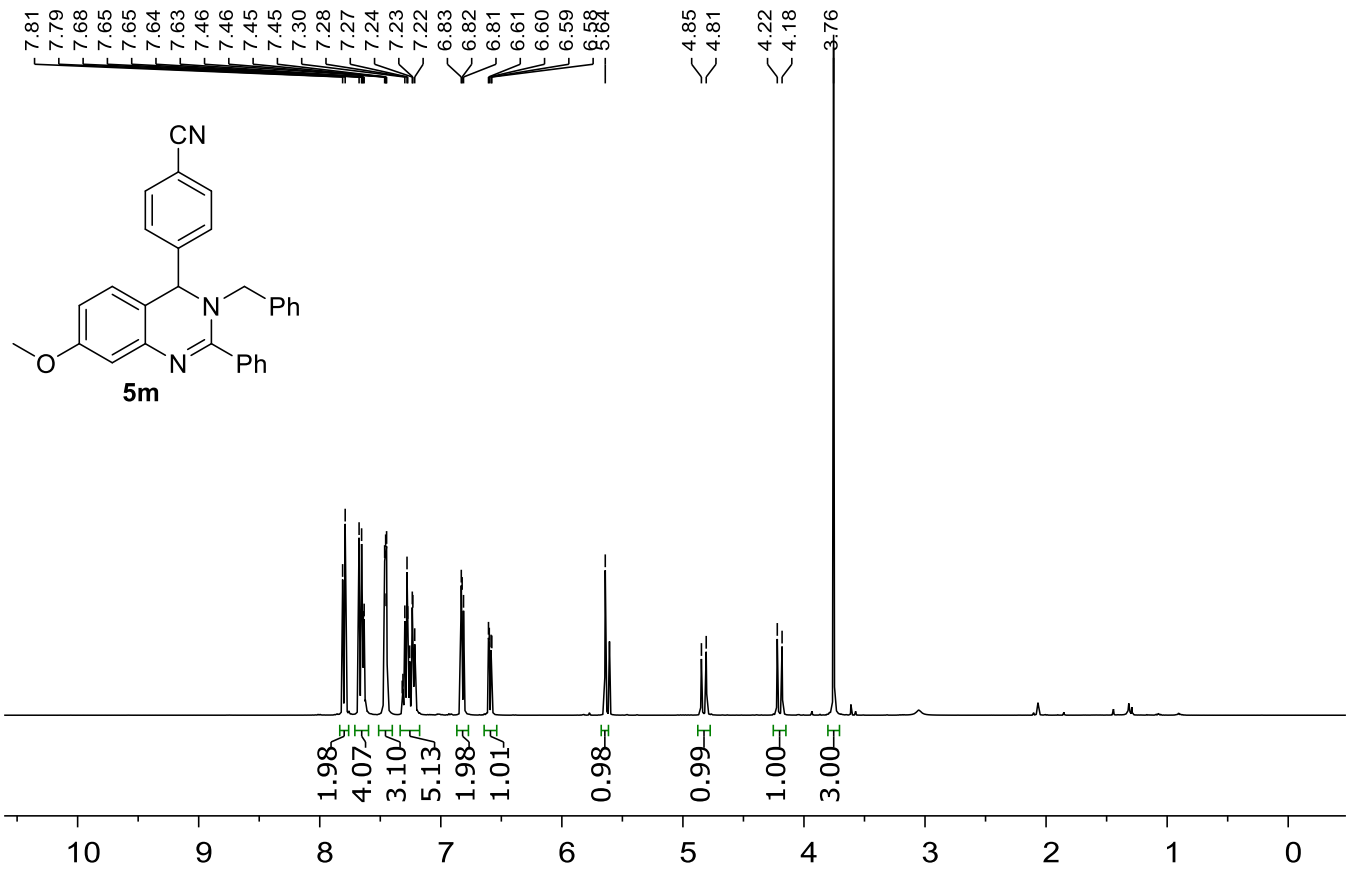
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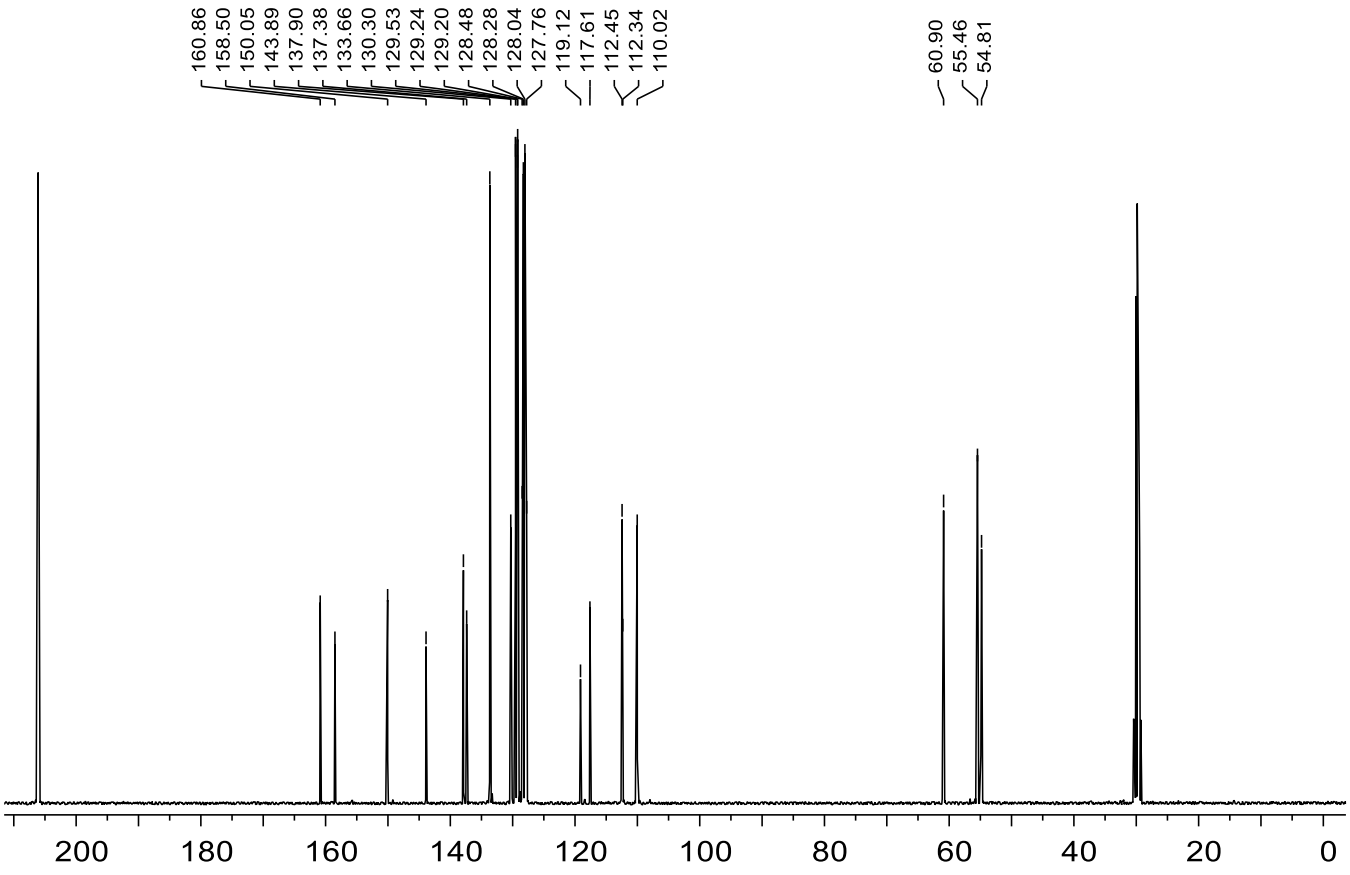
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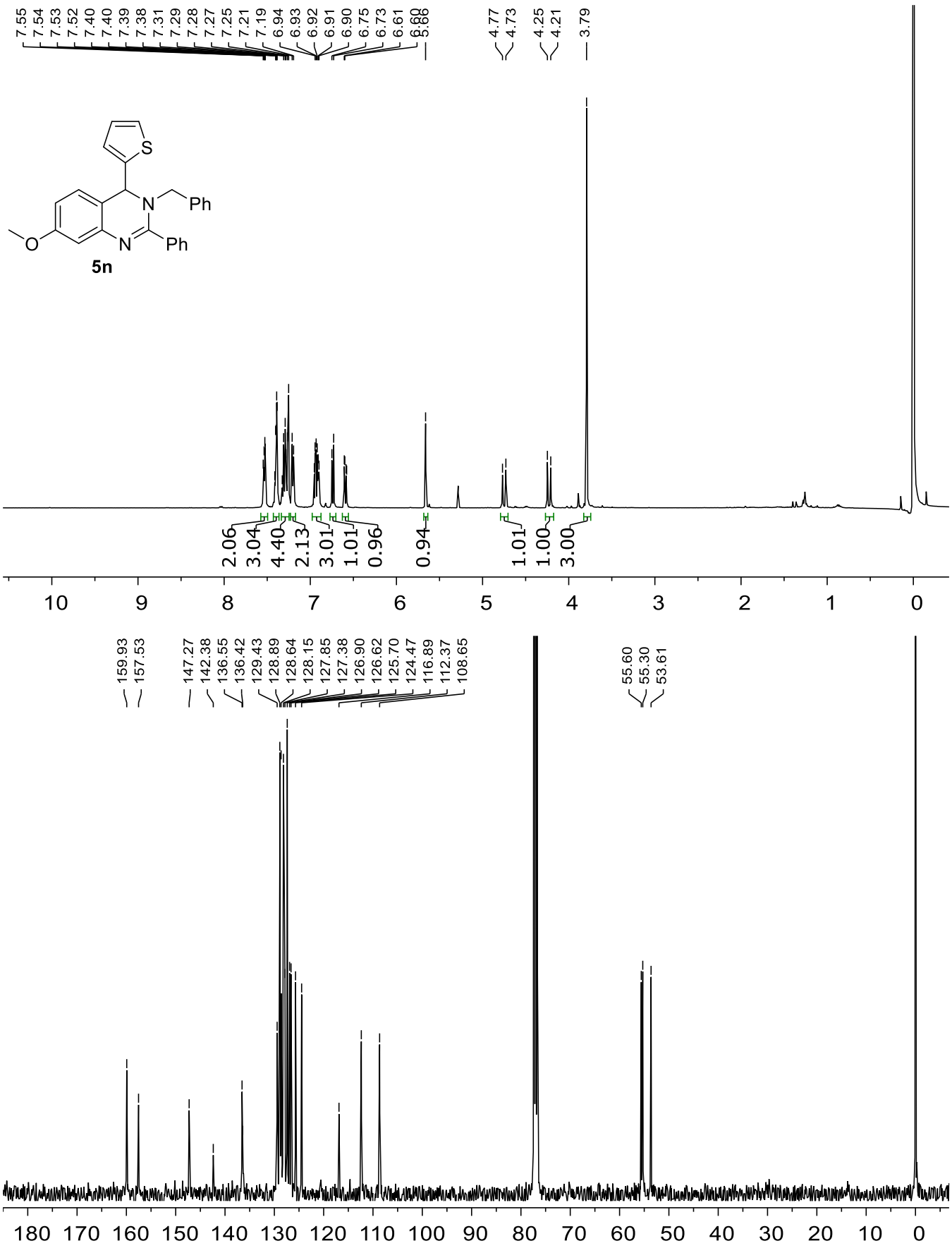
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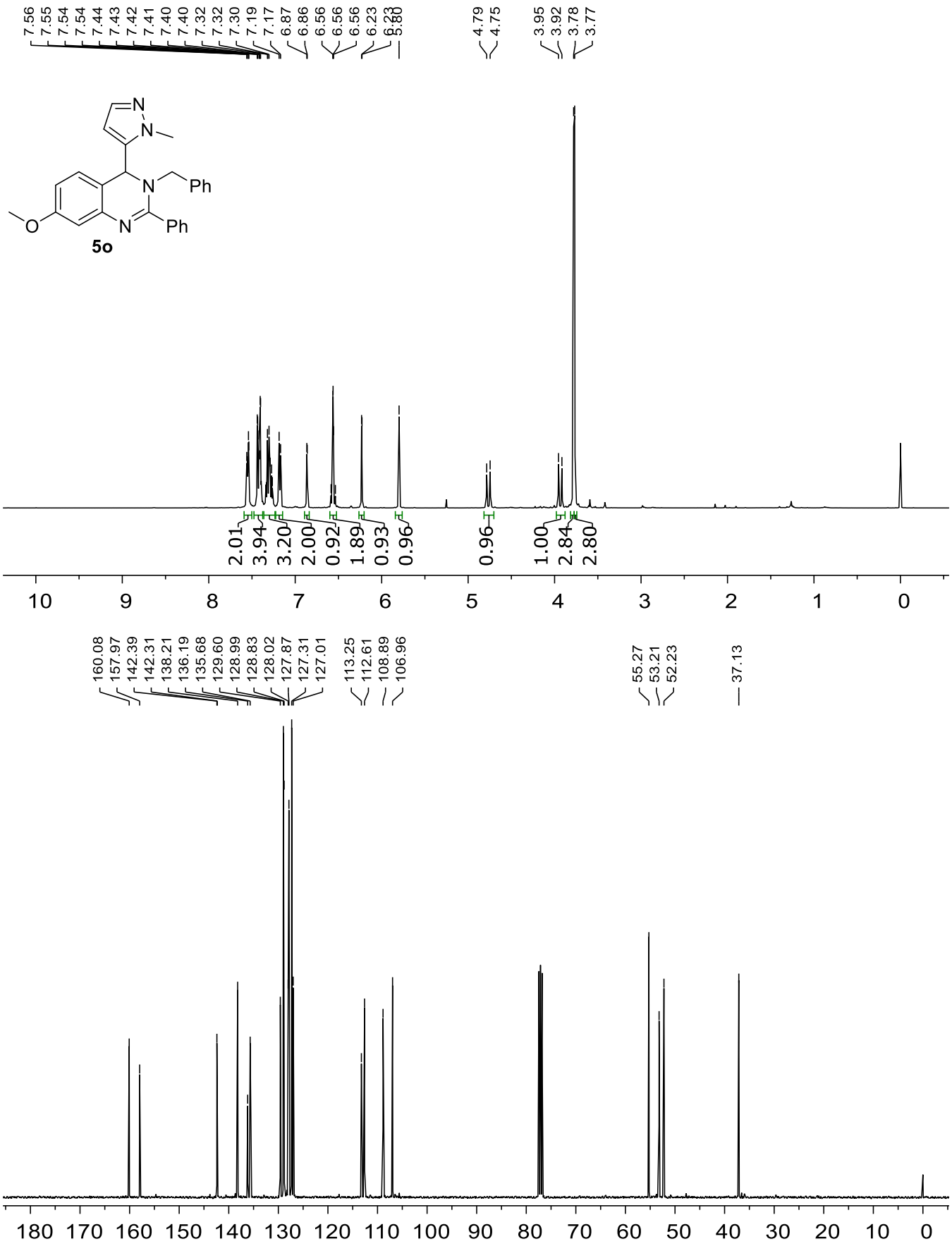
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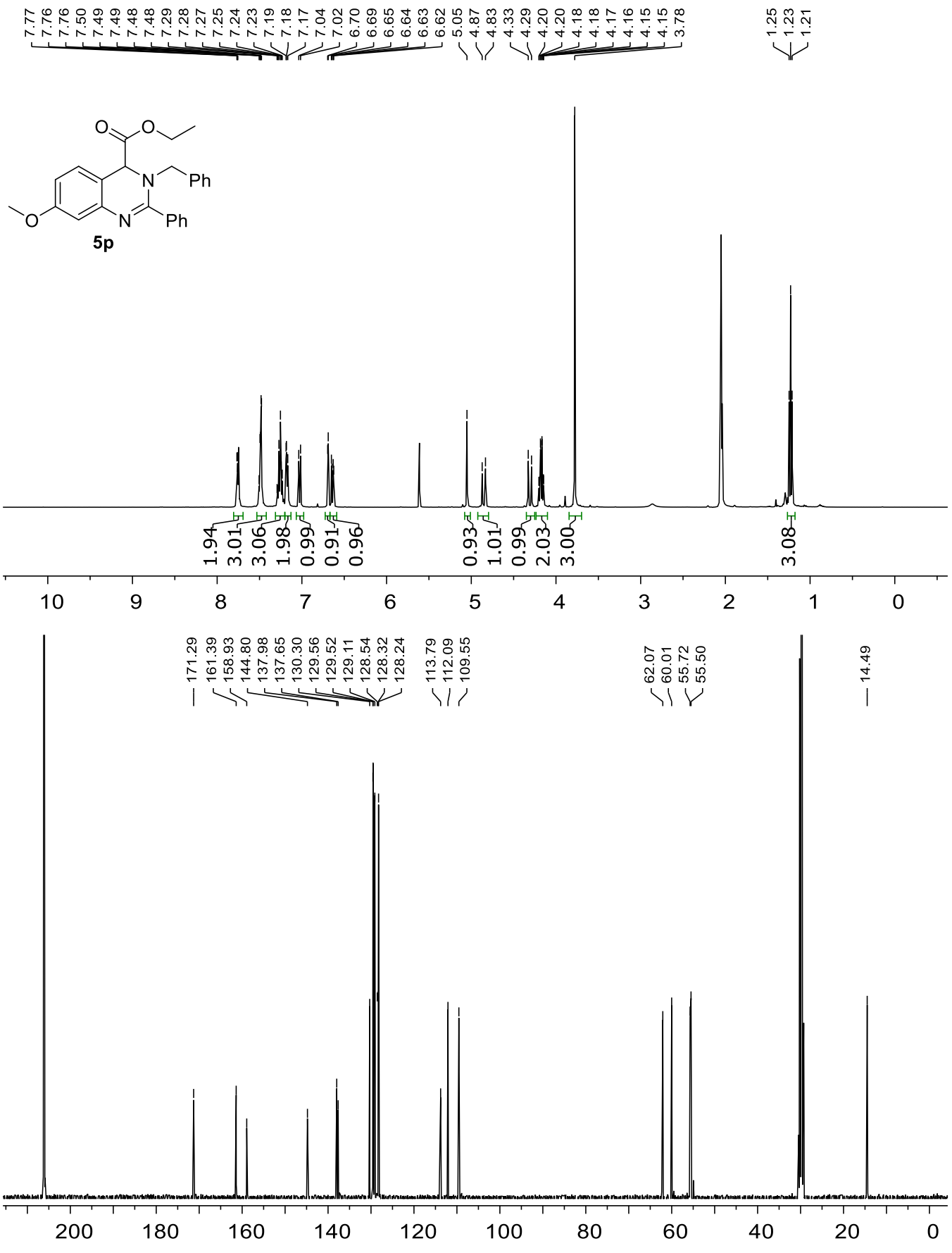
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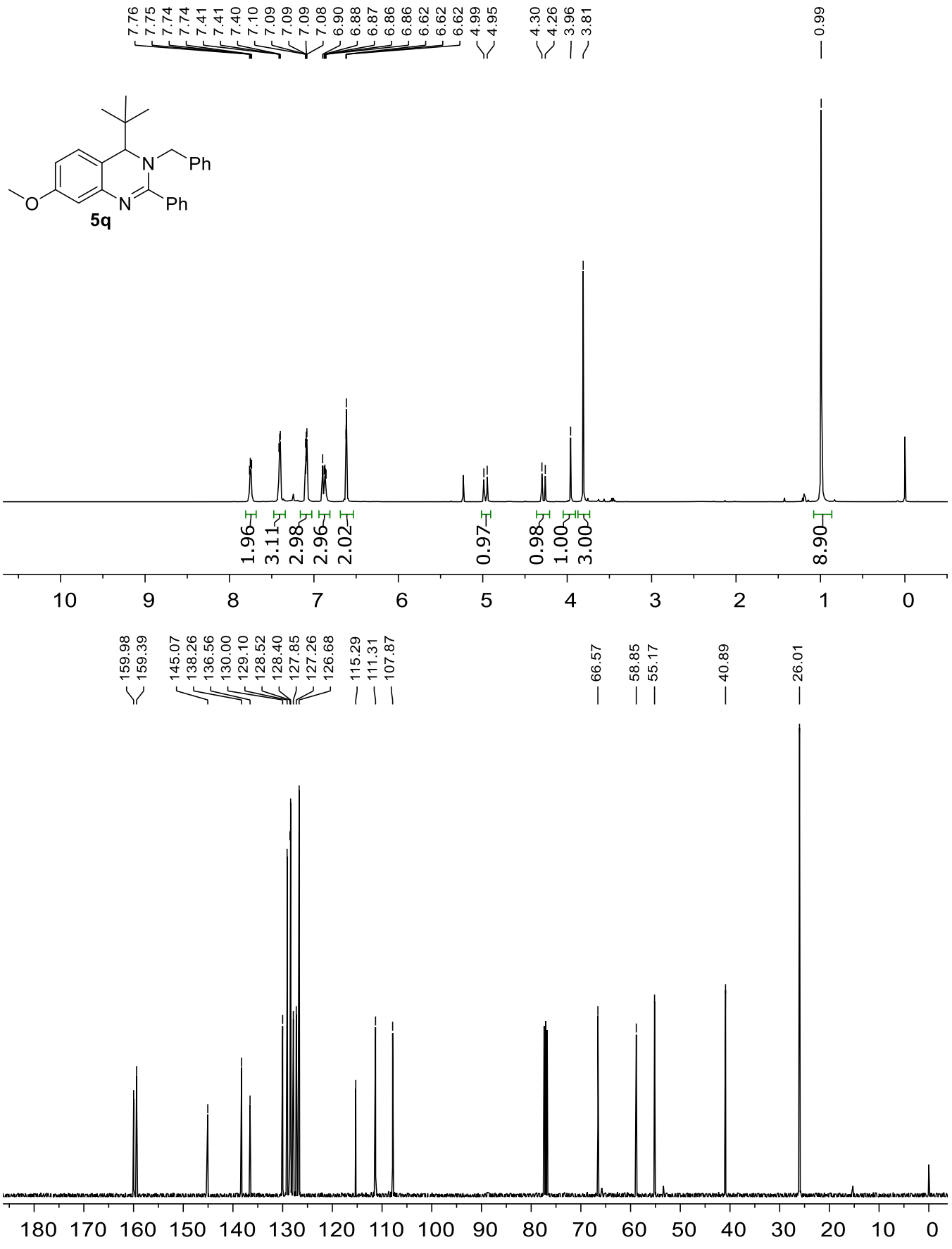
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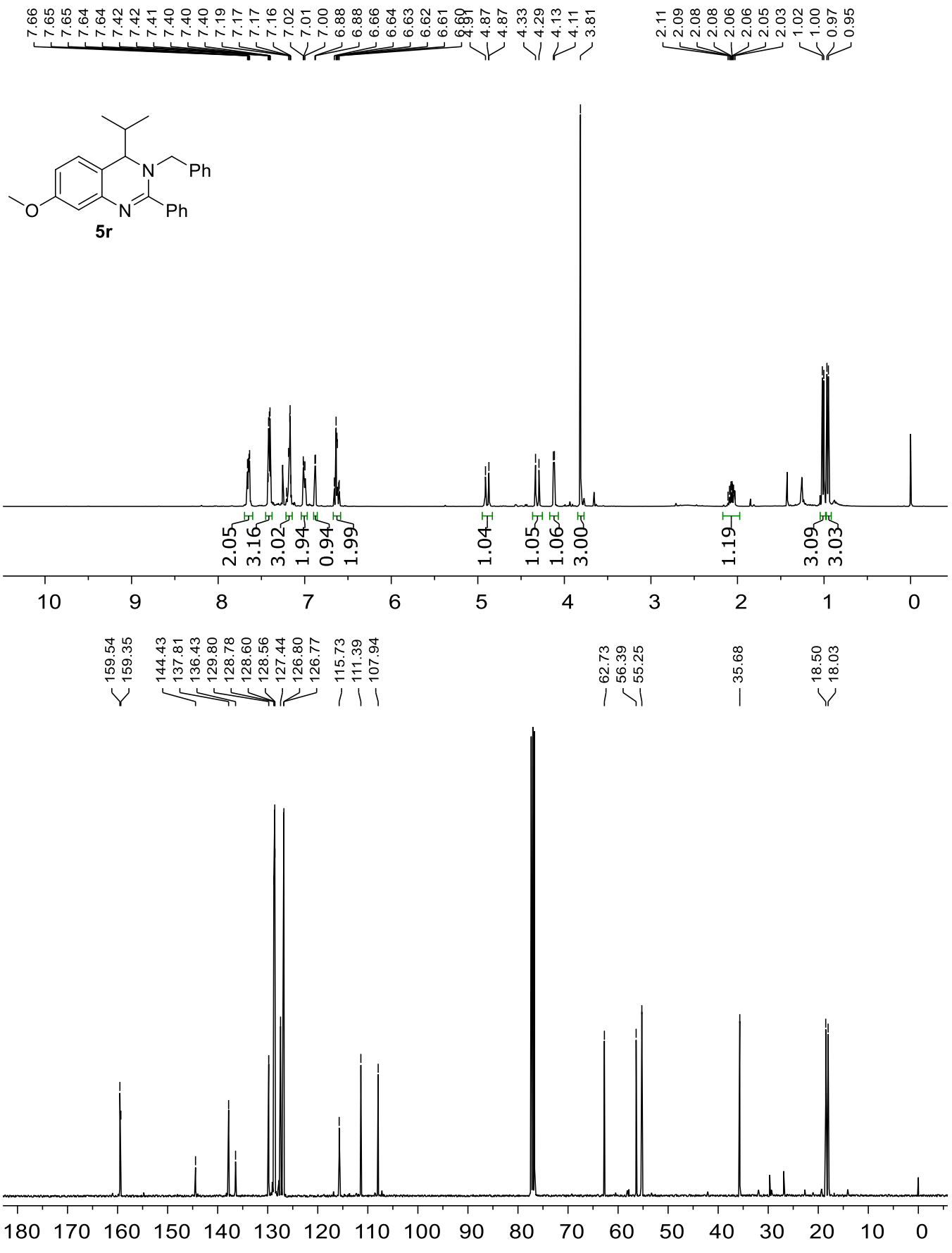
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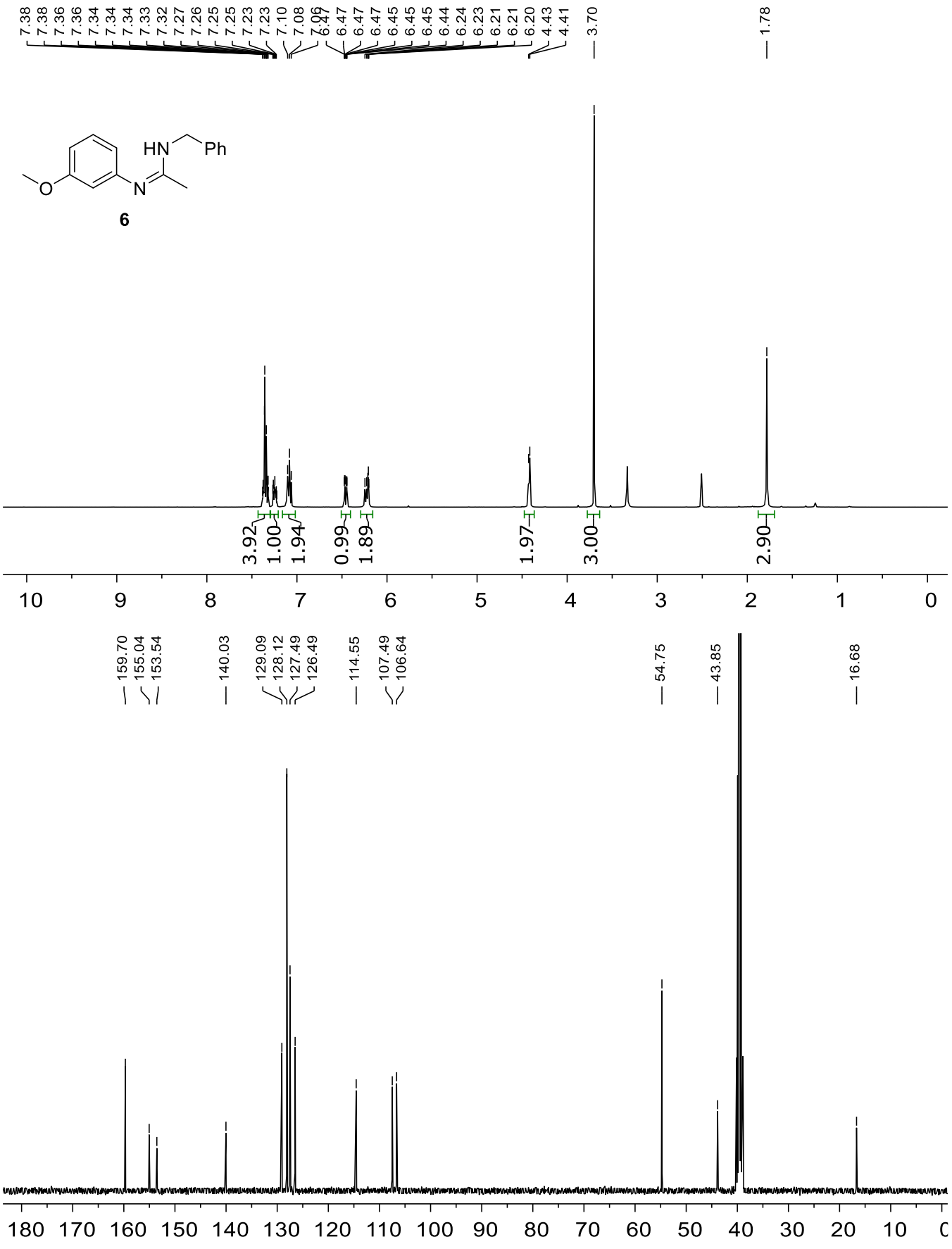
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