Supporting Information

Access to 2-Arylquinazolines via Catabolism/Reconstruction of Amino Acids with Insertion of Dimethyl Sulfoxide

Jin-Tian Ma, Li-Sheng Wang, Zhi Chai, Xin-Feng Chen, Bo-Cheng Tang, Xiang-Long Chen, Cai He, Yan-Dong Wu and An-Xin Wu**

Key Laboratory of Pesticide & Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, P. R. China.

E-mail: chwuyd@mail.ccnu.edu.cn
chwuax@mail.ccnu.edu.cn

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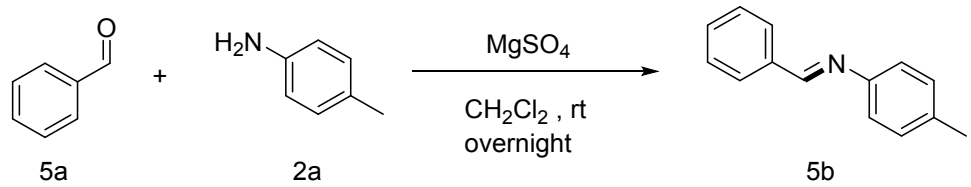
1. General

All other substrates and reagents were commercially available and used without further purification. TLC analysis was performed using pre-coated glass plates. Column chromatography was performed using silica gel (200–300 mesh). ^{1}H spectra were recorded in $CDCl_3$/DMSO-d_6 on 600/400 MHz NMR spectrometers and resonances (δ) are given in parts per million relative to tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz) and integration. ^{13}C spectra were recorded in $CDCl_3$/DMSO-d_6 on 150/100 MHz NMR spectrometers and resonances (δ) are given in ppm. HRMS were obtained on a Bruker 7-tesla FT-ICR MS equipped with an electrospray source. The X-ray crystal-structure determinations of **4ba** were obtained on a Bruker SMART APEX CCD system. Melting points were determined using XT-4 apparatus and not corrected.

2. General procedure for the synthesis of 4 (4aa as an example)

A sealed tube was charged with phenylglycine (**1a**) (151 mg, 1 mmol), p-toluidine (**2a**) (53.5 mg, 0.5 mmol), 3 ml of DMSO and HI (50 wt % solution in H_2O, 320mg, 2.5 mmol) at 140 ^{o}C (heating block) for 18 h till almost completed conversion of the substrates by TLC analysis, the mixture was quenched with saturation $Na_2S_2O_3$ solution (50 mL), extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 30:1) to afford the product **4aa** (87.1 mg, 79% yield).

3. General procedure for the synthesis of 5b

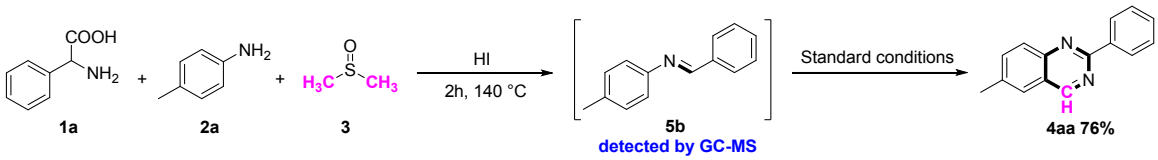


5a 2a 5b

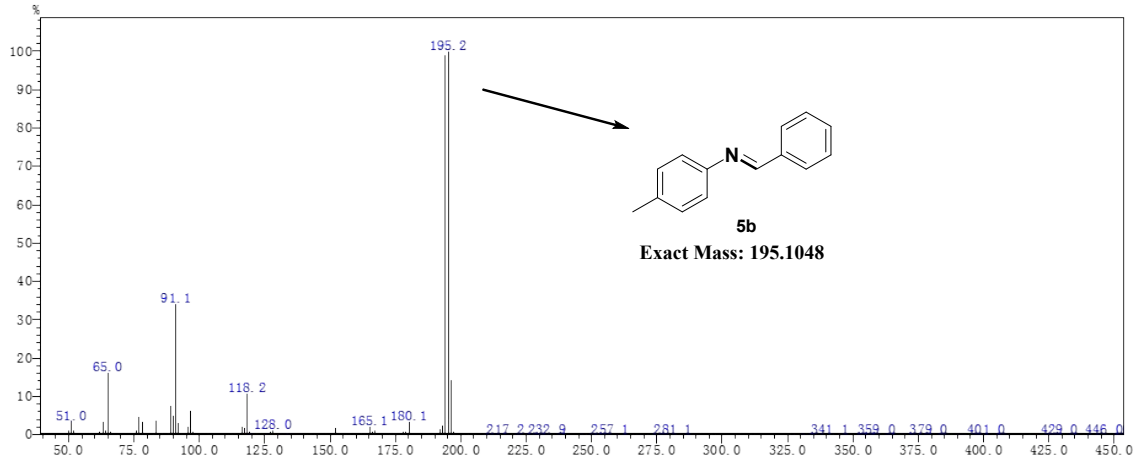
A mixture of benzaldehyde (**5a**) (254.4 mg, 2.4 mmol), p-toluidine (**2a**) (214 mg, 2.0 mmol) and $MgSO_4$ (0.5 g) in CH_2Cl_2 (5 mL) was stirred overnight at room temperature. After filtration of $MgSO_4$, CH_2Cl_2 was removed under reduced pressure and the residue was subjected to column chromatography to give product **5b** over 90% yield.[1]

4. Mechanistic studies

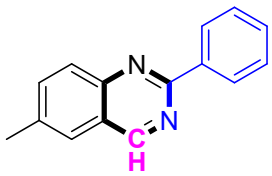
1a, **2a** reacted with **3**, and HI at 140 °C for 2 h , obtained the **intermediate 5b** (detected by GC-MS), which could converted to **4aa** after 16 h under standard conditions.



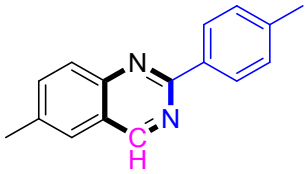
The GC-MS Spectra is listed below:



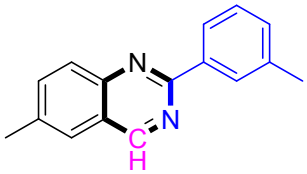
5. Characterization data for compounds 4 and 5b.



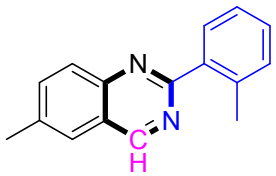
6-methyl-2-phenylquinazoline (4aa): Yield 79%; 87.1 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 105-107 ℃; ^{1}H NMR (600 MHz, CDCl3) δ 9.37 (s, 1H), 8.59 (d, J = 7.2 Hz, 2H), 7.99 (d, J = 8.4 Hz, 1H), 7.73 (d, J = 7.8 Hz, 1H), 7.67 (s, 1H), 7.55–7.49 (m, 3H), 2.56 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 160.3, 159.7, 149.3, 138.0, 137.4, 136.4, 130.4, 128.6, 128.4, 128.2, 125.8, 123.5, 21.6. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{12}N_2^+$: 221.1073, found: 221.0175.



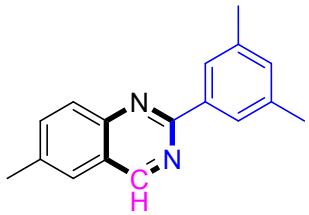
6-methyl-2-(p-tolyl)quinazoline (4ba): Yield 77%; 90.8 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 111-113 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.33 (s, 1H), 8.48 (d, J = 7.8 Hz, 2H), 7.95 (d, J = 8.4 Hz, 1H), 7.69 (d, J = 8.4 Hz, 1H), 7.63 (s, 1H), 7.33 (d, J = 7.2 Hz, 2H), 2.53 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.3, 159.6, 149.2, 140.6, 137.1, 136.3, 135.3, 129.3, 128.3, 128.1, 125.8, 123.4, 21.6, 21.5; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{15}N_2^+$: 235.1230, found: 235.1231.



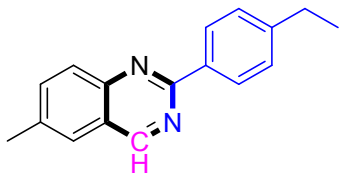
6-methyl-2-(m-tolyl)quinazoline (4ca): Yield 75%, 87.7 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 115-117 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.39 (s, 1H), 8.41 (d, J = 8.4 Hz, 2H), 8.02 (d, J = 7.8 Hz, 1H), 7.75 (d, J = 7.8 Hz, 1H), 7.70 (s, 1H), 7.44 (d, J = 7.2 Hz, 1H), 7.33 (s, 1H), 2.58 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 160.4, 159.8, 149.2, 138.3, 137.8, 137.5, 136.6, 131.3, 129.0, 128.6, 128.2, 125.8, 125.6, 123.5, 21.7, 21.5; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{15}N_2^+$; 235.1230, found: 235.1231.



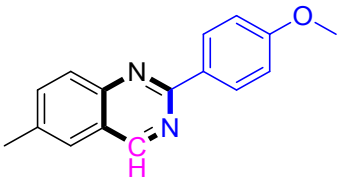
6-methyl-2-(o-tolyl)quinazoline (4da): Yield 69%; 80.7 mg; yellow oil; column chromatography, silica gel (PE/EA, 30:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.42 (s, 1H), 8.00 (d, J = 7.2 Hz, 1H), 7.88 (s, 1H), 7.78–7.71 (m, 2H), 7.34 (d, J = 7.8 Hz, 3H), 2.59 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 163.3, 159.3, 148.9, 138.6, 137.7, 137.2, 136.4, 131.2, 130.5, 129.1, 128.2, 125.9, 125.7, 122.9, 21.7, 20.9; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{15}N_2^+$: 235.1230, found: 235.1231.



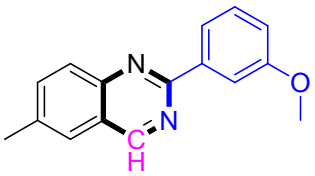
2-(3,5-dimethylphenyl)-6-methylquinazoline (4ea): Yield 73%; 86.8 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 150-152 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.37 (s, 1H), 8.21 (s, 2H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.67 (s, 1H), 7.14 (s, 1H), 2.56 (s, 3H), 2.44 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 160.6, 159.7, 149.3, 138.2, 137.9, 137.3, 136.4, 132.2, 128.1, 126.2, 125.8, 123.5, 21.6, 21.4. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{17}N_2^+$: 249.1386, found: 249.1388.



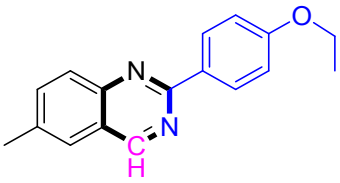
2-(4-ethylphenyl)-6-methylquinazoline (4fa): Yield 75%; 92.9 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 77-78 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.36 (s, 1H), 8.51 (d, *J* = 7.8 Hz, 2H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.66 (s, 1H), 7.36 (d, *J* = 7.8 Hz, 2H), 2.74 (d, *J* = 7.8 Hz, 2H), 2.56 (s, 3H), 1.29 (t, *J* = 7.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 160.4, 159.7, 149.3, 146.9, 137.2, 136.3, 135.6, 128.4, 128.2, 125.8, 123.5, 28.8, 21.6, 15.4; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{17}N_2^+$: 249.1386, found: 249.1389.



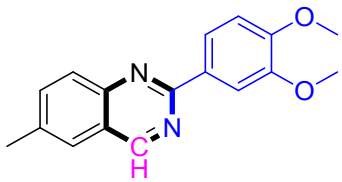
2-(4-methoxyphenyl)-6-methylquinazoline (4ga): Yield 76%; 94.8 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 113-115 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.34 (s, 1H), 8.56 (s, 2H), 7.96 (s, 1H), 7.72 (s, 1H), 7.66 (s, 1H), 7.05 (s, 2H), 3.90 (s, 3H), 2.56 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 161.6, 160.2, 159.7, 149.3, 136.9, 136.4, 130.7, 130.0, 128.0, 125.8, 123.3, 113.9, 55.4, 21.6; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{15}N_2O^+$: 251.1179, found: 251.1181.



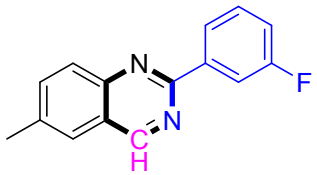
2-(3-methoxyphenyl)-6-methylquinazoline (4ha): Yield 72%; 90.1 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 111-113 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.38 (s, 1H), 8.20 (d, J = 7.8 Hz, 1H), 8.17 (s, 1H), 7.99 (d, J = 8.4 Hz, 1H), 7.74 (d, J = 8.4 Hz, 1H), 7.69 (s, 1H), 7.44 (t, J = 7.8 Hz, 1H), 7.06 (d, J = 7.8 Hz, 1H), 3.96 (s, 3H), 2.57 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 160.1, 159.9, 159.7, 149.2, 139.5, 137.5, 136.4, 129.6, 128.2, 125.8, 123.6, 120.9, 117.1, 112.7, 55.4, 21.7; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{15}N_2O^+$: 251.1179, found: 251.1181.



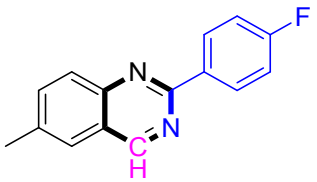
2-(4-ethoxyphenyl)-6-methylquinazoline (4ia): Yield 74%; 97.6 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 130-132 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.31 (s, 1H), 8.53 (d, J = 8.4 Hz, 2H), 7.93 (d, J = 8.4 Hz, 1H), 7.69 (d, J = 8.4 Hz, 1H), 7.62 (s, 1H), 7.02 (d, J = 8.4 Hz, 2H), 4.12 (dd, J = 13.2, 6.6 Hz, 2H), 2.53 (s, 3H), 1.45 (t, J = 6.6 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 161.0, 160.2, 159.6, 149.3, 136.8, 136.3, 130.6, 129.9, 128.0, 125.8, 123.2, 114.4, 63.5, 21.6, 14.8; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{17}N_2O^+$: 265.1335; found: 265.1337.



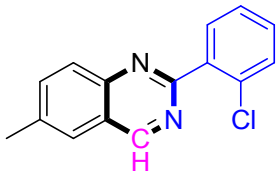
2-(3,4-dimethoxyphenyl)-6-methylquinazoline (4ja): Yield 68%; 95.1 mg; yellow solid; column chromatography, silica gel (PE/EA, 15:1); mp 113-115 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.34 (s, 1H), 8.24 (d, J = 7.8 Hz, 1H), 8.19 (s, 1H), 7.98 (d, J = 5.4 Hz, 1H), 7.73 (d, J = 8.4 Hz, 1H), 7.67 (s, 1H), 7.02 (d, J = 8.4 Hz, 1H), 4.07 (s, 3H), 3.98 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 159.9, 159.7, 151.2, 149.0, 137.1, 136.5, 127.9, 125.8, 123.3, 121.8, 111.1, 110.84, 110.76, 56.00, 55.95, 21.6; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{17}N_2O_2^+$: 281.1285; found: 281.1287.



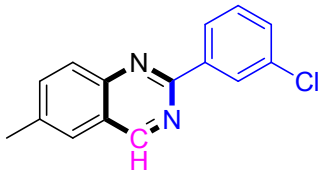
2-(3-fluorophenyl)-6-methylquinazoline (4ka): Yield 67%; 79.7 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 116-118 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.36 (s, 1H), 8.39 (dd, J = 8.0, 0.8 Hz, 1H), 8.33–8.28 (m, 1H), 7.98 (d, J = 8.8 Hz, 1H), 7.74 (dd, J = 8.8, 1.6 Hz, 1H), 7.68 (s, 1H), 7.51–7.45 (m, 1H), 7.18 (ddd, J = 8.4, 5.6, 2.0 Hz, 1H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 163.3 (d, J = 243.0 Hz, $^{1}J_{CF}$), 159.8, 159.2 (d, J = 3.0 Hz, $^{4}J_{CF}$), 149.2, 140.5 (d, J = 8.0 Hz, $^{3}J_{CF}$), 137.9, 136.6, 130.0 (d, J = 8.0 Hz, $^{3}J_{CF}$), 128.3, 125.8, 124.0 (d, J = 3.0 Hz, $^{4}J_{CF}$), 123.8, 117.2 (d, J = 21.0 Hz, $^{2}J_{CF}$), 115.2 (d, J = 23.0 Hz, $^{2}J_{CF}$), 21.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -113.28; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{12}FN_2^+$: 239.0979; found: 239.0981.



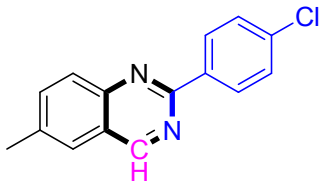
2-(4-fluorophenyl)-6-methylquinazoline (4la): Yield 68%; 80.9 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 101-103 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.37 (s, 1H), 8.63–8.59 (m, 2H), 7.99 (d, J = 8.4 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.70 (s, 1H), 7.21 (t, J = 8.4 Hz, 2H), 2.58 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 165.4, 159.8, 149.2, 141.4, 137.6, 136.7, 131.1 (d, J = 249.0 Hz, $^{1}J_{CF}$), 130.5 (d, J = 9.0 Hz, $^{3}J_{CF}$), 128.1, 125.8, 123.4, 115.6 (d, J = 21.0 Hz, $^{2}J_{CF}$), 115.5, 21.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -110.80; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{12}FN_2^+$: 239.0979; found: 239.0981.



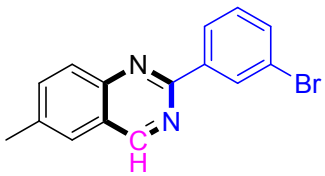
2-(2-chlorophenyl)-6-methylquinazoline (4ma): Yield 66%; 83.8 mg; white solid; column chromatography, silica gel (PE/EA, 30:1); mp 64-66 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.44 (s, 1H), 8.03 (d, *J* = 8.8 Hz, 1H), 7.81 (dd, *J* = 12.4, 7.2 Hz, 2H), 7.75 (s, 1H), 7.53 (dd, *J* = 6.8, 2.8 Hz, 1H), 7.43–7.37 (m, 2H), 2.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 161.2, 159.5, 148.9, 138.34, 138.32, 136.7, 132.9, 131.8, 130.5, 130.2, 128.3, 126.8, 125.8, 123.3, 21.7; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{12}ClN_2^+$: 255.0684; found: 255.0686.



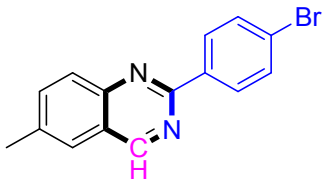
2-(3-chlorophenyl)-6-methylquinazoline (4na): Yield 69%; 87.5 mg; white solid; column chromatography, silica gel (PE/EA, 30:1); mp 131-133 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.38 (s, 1H), 8.61 (s, 1H), 8.49 (s, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.70 (s, 1H), 7.46 (s, 2H), 2.58 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 159.8, 159.0, 149.2, 139.9, 137.9, 136.6, 134.7, 130.3, 129.8, 128.4, 128.3, 126.4, 125.8, 123.7, 21.7; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{12}ClN_2^+$: 255.0684; found: 255.0685.



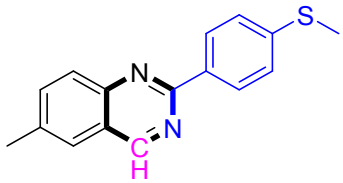
2-(4-chlorophenyl)-6-methylquinazoline (4oa): Yield 74%; 93.8 mg; white solid; column chromatography, silica gel (PE/EA, 30:1); mp 185-187℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.37 (s, 1H), 8.55 (d, *J* = 8.4 Hz, 2H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.70 (s, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 2.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.8, 159.3, 149.2, 137.9, 136.8, 136.4, 129.8, 128.8, 128.2, 125.9, 123.6, 21.7; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{12}ClN_2^+$: 255.0684; found: 255.0685.



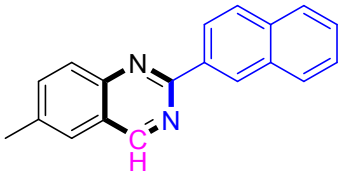
2-(3-bromophenyl)-6-methylquinazoline (4pa): Yield 70%; 104.5 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 179-182℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.36 (s, 1H), 8.76 (s, 1H), 8.53 (d, J = 7.8 Hz, 1H), 7.97 (d, J = 8.4 Hz, 1H), 7.74 (d, J = 8.4 Hz, 1H), 7.68 (s, 1H), 7.61 (d, J = 7.8 Hz, 1H), 7.39 (t, J = 7.8 Hz, 1H), 2.57 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.8, 158.8, 149.2, 140.2, 137.9, 136.6, 133.2, 131.4, 130.1, 128.3, 126.9, 125.8, 123.7, 122.9, 21.7; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{12}BrN_2^+$: 301.0158; found:301.0160.



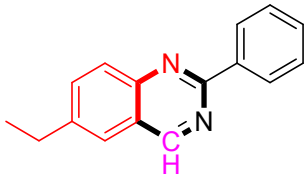
2-(4-bromophenyl)-6-methylquinazoline (4qa): Yield 71%; 106.1 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 186-188 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.36 (s, 1H), 8.48 (d, J = 8.4 Hz, 2H), 7.97 (d, J = 8.4 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.71–7.63 (m, 3H), 2.57 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 159.8, 159.3, 149.2, 137.8, 136.9, 136.6, 131.7, 130.0, 128.2, 125.8, 125.2, 123.6, 21.7; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{12}BrN_2^+$: 301.0158; found: 301.0160.



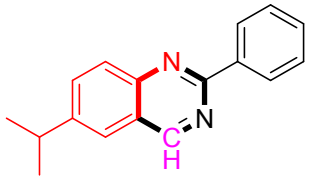
6-methyl-2-(4-(methylthio)phenyl)quinazoline (4ra): Yield 69%; 91.7 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 109-111 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.35 (s, 1H), 8.52 (d, J = 8.4 Hz, 2H), 7.96 (d, J = 8.4 Hz, 1H), 7.73–7.71 (m, 1H), 7.66 (s, 1H), 7.37 (d, J = 8.4 Hz, 2H), 2.56 (d, J = 3.0 Hz, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 159.9, 159.7, 149.2, 141.7, 137.3, 136.5, 134.6, 128.7, 128.1, 125.82, 125.77, 123.5, 21.6, 15.2; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{15}N_2S^+$: 267.0950; found:267.0953.



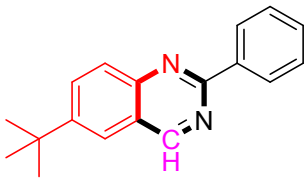
6-methyl-2-(naphthalen-2-yl)quinazoline (4sa): Yield 65%; 87.7 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 148-151 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.39 (s, 1H), 9.12 (s, 1H), 8.70 (d, J = 7.8 Hz, 1H), 8.01 (d, J = 8.4 Hz, 2H), 7.98 (d, J = 7.8 Hz, 1H), 7.88 (s, 1H), 7.73 (d, J = 7.2 Hz, 1H), 7.66 (s, 1H), 7.52 (s, 2H), 2.54 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 160.2, 159.7, 149.3, 137.5, 136.4, 135.4, 134.5, 133.4, 129.2, 128.6, 128.2, 127.7, 126.9, 126.1, 125.8, 125.3, 123.5, 21.6; HRMS (ESI): m/z [M+H]+ calcd for $C_{19}H_{15}N_2^+$: 271.1230; found:271.1229.



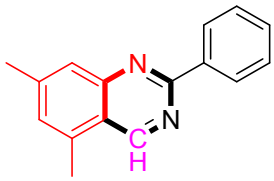
6-ethyl-2-phenylquinazoline (4ab): Yield 79%; 92.4 mg; yellow solid; column chromatography; silica gel (PE/EA, 30:1); mp 87-89 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.41 (s, 1H), 8.59 (d, J = 7.2 Hz, 2H), 8.02 (d, J = 8.4 Hz, 1H), 7.78 (d, J = 7.8 Hz, 1H), 7.70 (s, 1H), 7.55–7.50 (m, 3H), 2.87 (dd, J = 15.0, 7.2 Hz, 2H), 1.36 (t, J = 7.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 160.3, 159.9, 149.5, 143.7, 138.0, 135.5, 130.4, 128.6, 128.4, 128.3, 124.4, 123.6, 28.9, 15.2; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{15}N_2^+$: 235.1230; found:235.1231.



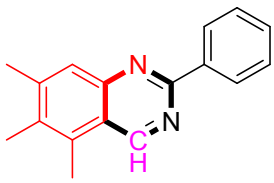
6-isopropyl-2-phenylquinazoline (4ac): Yield 73%; 90.5 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 104-106 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.42 (s, 1H), 8.59 (d, J = 7.2 Hz, 2H), 8.03 (d, J = 9.0 Hz, 1H), 7.82 (dd, J = 9.0, 1.8 Hz, 1H), 7.72 (s, 1H), 7.55–7.50 (m, 3H), 3.14 (dd, J = 13.8, 6.6 Hz, 1H), 1.37 (d, J = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.4, 160.0, 149.6, 148.2, 138.1, 134.2, 130.4, 128.6, 128.4, 123.6, 123.0, 34.1, 23.7; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{17}N_2^+$: 249.1386; found: 249.1388.



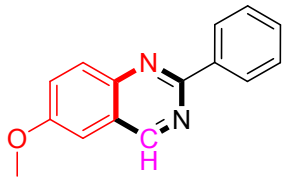
6-(tert-butyl)-2-phenylquinazoline (4ad): Yield 55%; 72.0 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 107-109 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.44 (d, J = 7.2 Hz, 1H), 8.61 (s, 2H), 8.03 (d, J = 4.8 Hz, 2H), 7.84 (d, J = 5.6 Hz, 1H), 7.59–7.50 (m, 3H), 1.46 (d, J = 7.2 Hz, 9H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 160.3, 150.5, 149.3, 138.1, 133.2, 130.4, 128.6, 128.5, 128.1, 123.4, 121.9, 35.1, 31.1; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{18}H_{19}N_2^+$: 263.1543; found: 263.1542.



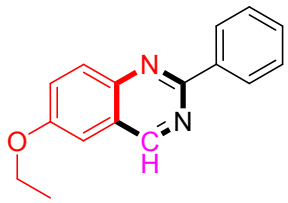
5,7-dimethyl-2-phenylquinazoline (4ae): Yield 53%; 61.9 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 85-87 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.57 (s, 1H), 8.60 (d, J = 6.0 Hz, 2H), 7.71 (s, 1H), 7.53 (d, J = 6.6 Hz, 3H), 7.22 (s, 1H), 2.74 (s, 3H), 2.54 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 160.6, 157.0, 151.5, 145.0, 138.1, 135.0, 130.4, 130.2, 128.6, 128.4, 125.7, 121.0, 22.3, 17.5; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{15}N_2^+$: 235.1230; found:235.1231.



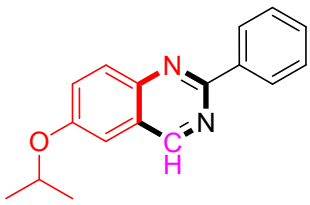
5,6,7-trimethyl-2-phenylquinazoline (4af): Yield 62%; 76.8 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 136-138 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.64 (s, 1H), 8.59 (d, J = 7.2 Hz, 2H), 7.77 (s, 1H), 7.53 (d, J = 7.8 Hz, 2H), 7.51–7.48 (m, 1H), 2.70 (s, 3H), 2.53 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 156.8, 156.6, 149.7, 145.3, 138.0, 135.2, 131.9, 130.3, 128.6, 128.3, 126.2, 121.5, 22.2, 15.9, 13.8; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{17}N_2^+$: 249.1386; found:249.1388.



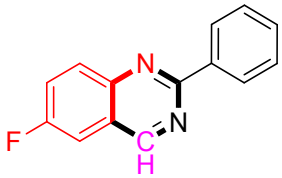
6-methoxy-2-phenylquinazoline (4ag): Yield 75%; 88.5 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 106-108 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.38 (s, 1H), 8.58 (d, *J* = 6.6 Hz, 2H), 8.02 (d, *J* = 9.0 Hz, 1H), 7.58–7.47 (m, 4H), 7.16 (s, 1H), 3.97 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 159.2, 158.8, 158.3, 146.9, 137.9, 130.3, 130.1, 128.6, 128.2, 127.3, 124.4, 103.9, 55.8; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{13}N_2O^+$: 237.1022; found 237.1024.



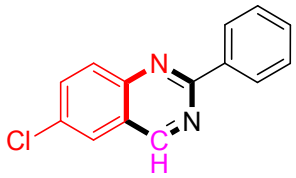
6-ethoxy-2-phenylquinazoline (4ah): Yield 73%; 91.2 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 142-144 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.36 (s, 1H), 8.57 (d, *J* = 7.8 Hz, 2H), 8.01 (d, *J* = 9.0 Hz, 1H), 7.54 (dd, *J* = 16.2, 9.0 Hz, 3H), 7.50–7.48 (m, 1H), 7.14 (s, 1H), 4.18 (dd, *J* = 13.8, 6.6 Hz, 2H), 1.52 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 159.1, 158.7, 157.6, 146.8, 137.9, 130.2, 130.0, 128.6, 128.2, 127.6, 124.5, 104.5, 64.1, 14.6; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{15}N_2O^{++}$: 251.1179; found:251.1181.



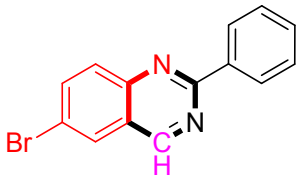
6-isopropoxy-2-phenylquinazoline (4ai): Yield 69%; 91.0 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 108-110 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.33 (s, 1H), 8.57 (d, J = 7.2 Hz, 2H), 7.99 (d, J = 9.0 Hz, 1H), 7.58–7.46 (m, 4H), 7.13 (s, 1H), 4.79–4.69 (m, 1H), 1.43 (d, J = 5.4 Hz, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 159.2, 158.7, 156.4, 146.6, 138.2, 130.1, 128.6, 128.14, 128.11, 124.5, 105.8, 103.8, 70.4, 21.8. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{17}N_2O^+$: 265.1335; found: 265.1337.



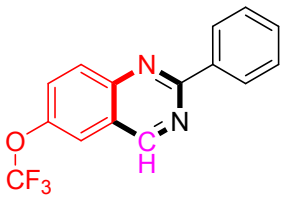
6-fluoro-2-phenylquinazoline (4aj): Yield 63%; 70.5 mg; white solid; column chromatography, silica gel (PE/EA, 30:1); mp 120-122 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.42 (s, 1H), 8.59 (d, J = 6.6 Hz, 2H), 8.12–8.07 (m, 1H), 7.67 (s, 1H), 7.53 (d, J = 7.2 Hz, 4H) ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.6, 160.4 (d, J = 250.5 Hz, $^{1}J_{CF}$), 159.8 (d, J = 4.5 Hz, $^{4}J_{CF}$), 147.9, 137.6, 131.3 (d, J = 9.0 Hz, $^{3}J_{CF}$) 130.7, 128.7, 128.4, 124.5 (d, J = 25.5 Hz, $^{2}J_{CF}$), 123.9 (d, J = 9.0 Hz, $^{3}J_{CF}$), 110.1 (d, J = 22.5 Hz, $^{2}J_{CF}$). ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -110.60 HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{10}FN_2^+$: 225.0823; found: 225.0824.



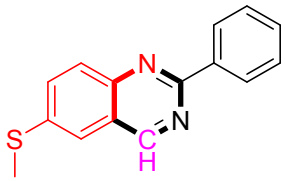
6-chloro-2-phenylquinazoline (4ak): Yield 70%; 83.9 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 137-139 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.41 (s, 1H), 8.60 (d, J = 6.6 Hz, 2H), 8.05 (d, J = 9.0 Hz, 1H), 7.92 (s, 1H), 7.84 (d, J = 9.0 Hz, 1H), 7.54 (d, J = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.2, 159.5, 149.2, 137.4, 135.2, 132.8, 130.9, 130.3, 128.7, 128.6, 125.8, 123.9. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{10}ClN_2^+$: 241.0527; found: 241.0529.



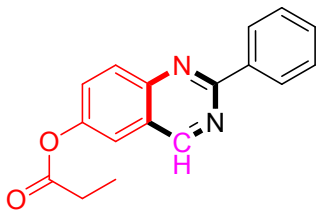
6-bromo-2-phenylquinazoline (4al): Yield 58%; 82.6 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 162-164 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.41 (s, 1H), 8.61 (d, J = 5.4 Hz, 2H), 8.10 (s, 1H), 7.98 (s, 2H), 7.54 (s, 3H) ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 161.2, 159.4, 149.4, 137.7, 137.5, 130.9, 130.4, 129.2, 128.7, 128.6, 124.4, 120.8, 77.2. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{10}BrN_2^+$: 287.0001; found: 287.0180.



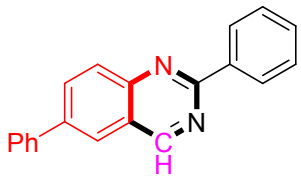
2-phenyl-6-(trifluoromethoxy)quinazoline (4am): Yield 63 %; 91.3 mg; yellow solid; column chromatography, silica gel (PE/EA, 15:1); mp 104-106 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.46 (s, 1H), 8.60 (d, J = 6.0 Hz, 2H), 8.13 (d, J = 9.6 Hz, 1H), 7.73 (s, 2H), 7.54 (d, J = 6.6 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 161.5, 160.2, 149.0, 147.0, 137.4, 131.1, 130.9, 128.7, 128.6, 128.3, 128.2, 123.4, 121.3, 120.4 (q, J = 256.5 Hz, $^{1}J_{CF}$); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -57.90; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}F_3N_2O^+$: 291.0740; found: 291.0741.



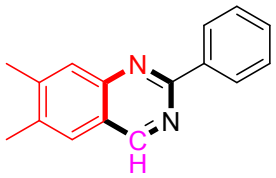
6-(methylthio)-2-phenylquinazoline (4an): Yield 69%; 86.9 mg; yellow solid; column chromatography, silica gel (PE/EA, 20:1); mp 132-134 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.36 (s, 1H), 8.58 (d, J = 7.2 Hz, 2H), 7.97 (d, J = 9.0 Hz, 1H), 7.77–7.74 (m, 1H), 7.59 (s, 1H), 7.55–7.50 (m, 3H), 2.63 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 160.3, 158.9, 149.0, 138.9, 137.9, 133.4, 130.5, 128.7, 128.6, 128.3, 124.0, 120.9, 15.5. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{13}N_2S^+$: 253.0794; found: 253.0796.



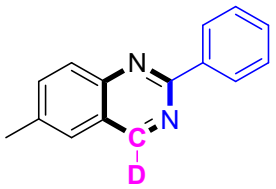
2-phenylquinazolin-6-yl propionate (4ao): Yield 52%; 72.2 mg; white solid; column chromatography, silica gel (PE/EA, 15:1); mp 180-182 ℃; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 9.91 (s, 1H), 8.85 (d, J = 1.6 Hz, 1H), 8.63–8.58 (m, 2H), 8.45 (dd, J = 8.8, 2.0 Hz, 1H), 8.14 (d, J = 8.8 Hz, 1H), 7.63–7.59 (m, 3H), 4.42 (q, J = 7.2 Hz, 2H), 1.40 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 164.9, 163.1, 161.6, 151.9, 137.1, 133.6, 131.5, 130.7, 129.0, 128.7, 128.5, 122.8, 61.5, 14.3. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{15}N_2O_2$+: 279.1128; found: 279.1130.



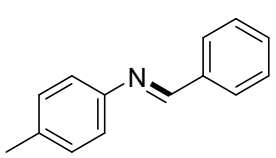
2,6-diphenylquinazoline (4ap): Yield 55%; 77.5 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 155-157 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.54 (s, 1H), 8.65 (d, J = 7.2 Hz, 2H), 8.20 (s, 2H), 8.12 (s, 1H), 7.74 (d, J = 7.6 Hz, 2H), 7.54 (dd, J = 10.8, 7.6 Hz, 5H), 7.45 (d, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.8, 160.7, 150.0, 140.3, 139.6, 137.7, 134.0, 130.8, 129.1, 129.0, 128.7, 128.6, 128.2, 127.4, 124.6, 123.8. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{20}H_{15}N_2^+$: 283.1230; found: 283.1232.



6,7-dimethyl-2-phenylquinazoline (4aq): Yield 62%; 72.5 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 118-121 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.33 (s, 1H), 8.58 (d, J = 7.6 Hz, 2H), 7.86 (s, 1H), 7.65 (s, 1H), 7.56–7.47 (m, 3H), 2.51 (s, 3H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.3, 159.1, 149.8, 145.3, 138.2, 137.6, 130.3, 128.6, 128.3, 127.8, 126.1, 122.3, 20.9, 20.1. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{15}N_2^+$: 235.1230; found: 235.1232.

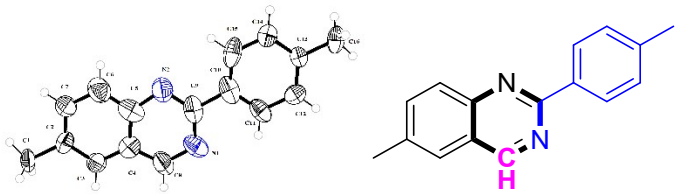


6-methyl-2-phenylquinazoline (4aa-d_1): Yield 62%; 68.5 mg; yellow solid; column chromatography, silica gel (PE/EA, 30:1); mp 107-109 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.60 (s, 2H), 8.03 (s, 1H), 7.77 (s, 1H), 7.72 (s, 1H), 7.54 (s, 3H), 2.59 (s, 3H). HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{12}DN_2^+$: 222.1136, found: 222.1135.



1-phenyl-N-(p-tolyl)methanimine (5b): Yield 90%; 351 mg; yellow oil; column chromatography, silica gel (PE/EA, 50:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.84–7.80 (m, 2H), 7.34–7.31 (m, 3H), 7.09 (s, 4H), 2.26 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.2, 148.9, 135.9, 135.4, 130.8, 129.5, 128.43, 128.37, 120.6, 20.7. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{14}N^+$: 196.1121, found: 196.1109.

6. Crystallographic data and molecular structure of 4ba



4ba

Figure S1. X-ray crystal structure of **4ba**, thermal ellipsoids shown at 50% probability level. Sample preparation: 30 mg of **4ba** was dissolved in 4 ml CH_2Cl_2 and 2 ml EtOAc at room temperature for slow evaporation about a week. The crystals were mounted on a glass fiber for diffraction experiments. Intensity data were collected on a Bruker SMART APEX CCD diffractometer with Mo Kα radiation (0.71073 Å) at room temperature. Crystal Data for Compound **4ba**: CCDC 2055069 contains the supplementary crystallographic data for this paper. These data could be obtained free of charge from The Cambridge Crystallographic.

```
Bond precision:  = 0.0000 A              Wavelength=0.71073

Cell:             a=9.856(4)     b=4.9044(18)        c=12.905(5)
                  alpha=90       beta=92.965(7)      gamma=90
Temperature:      296 K

                 Calculated                Reported
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Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C16 H14 N2                C16 H14 N2
Sum formula      C16 H14 N2                C16 H14 N2
Mr               234.29                    234.29
Dx,g cm-3        1.249                     1.249
Z                2                         2
Mu (mm-1)        0.074                     0.074
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F000'            248.08
h,k,lmax         11,5,15                   11,5,15
Nref             1097                      1058
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Tmin'            0.978

Correction method= # Reported T Limits: Tmin=0.633 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.964          Theta(max)= 24.999

R(reflections)= 0.1243( 703)      wR2(reflections)= 0.3918( 1058)

S = 1.604                 Npar= 141
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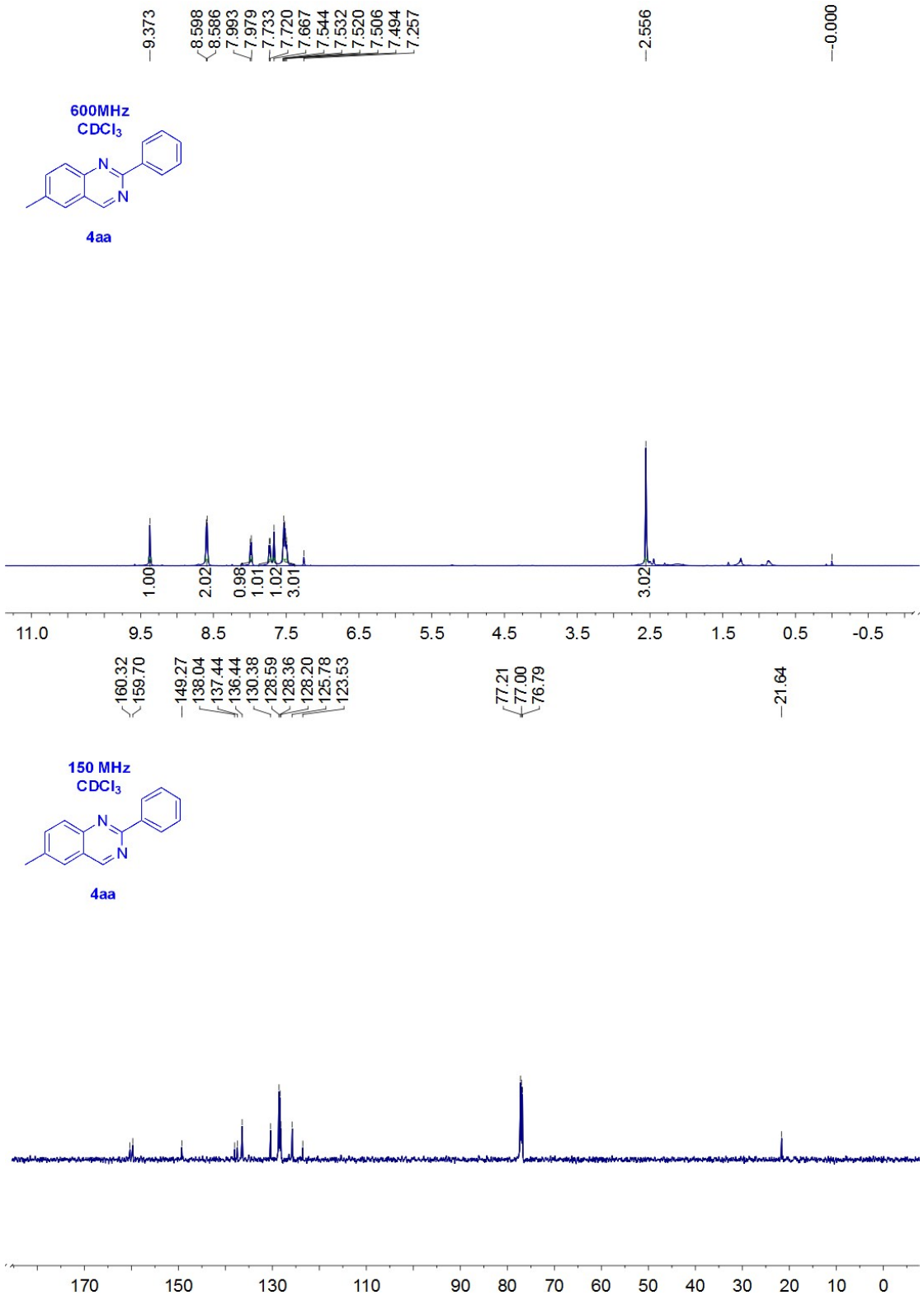
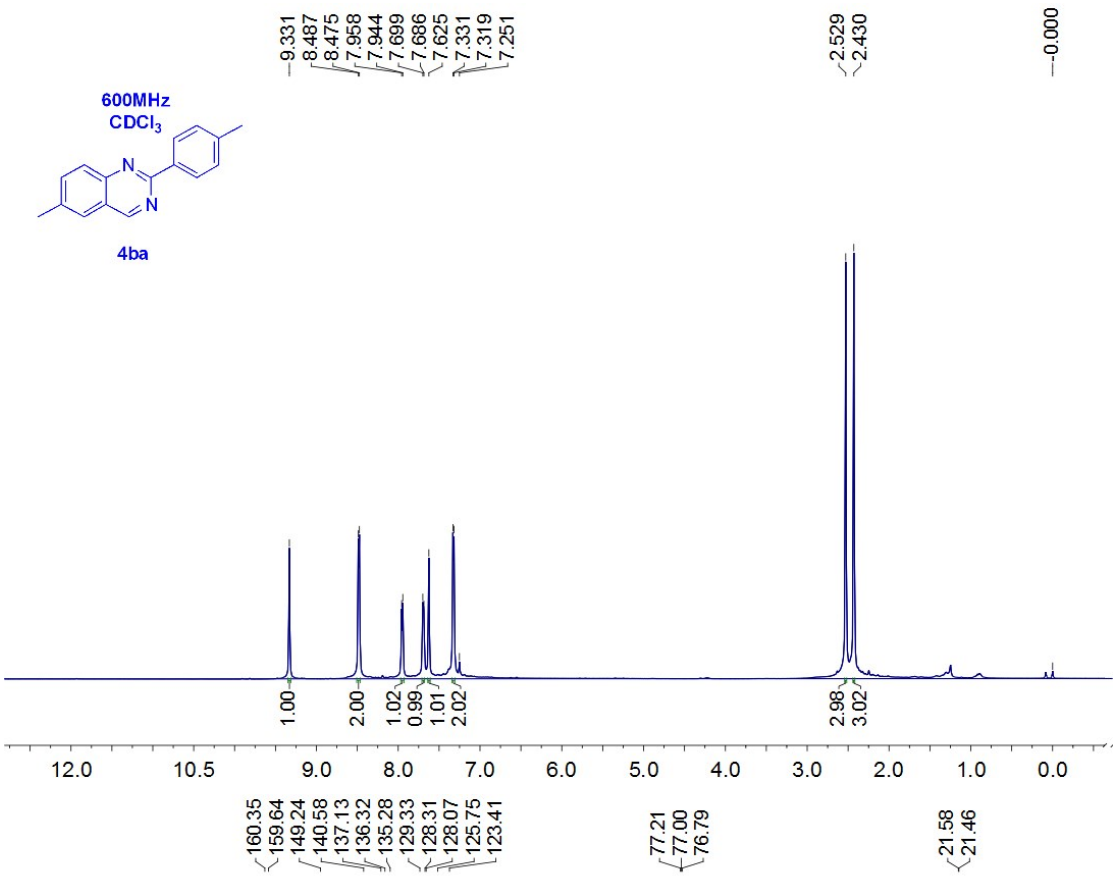
7. References

(1) A. K. Ghosh, S. Mondal, A. Hajra, *Org. Lett.* 2020, **22**, 2771–2775

8. ^{1}H and ^{13}C NMR spectra of compounds 4 and 5b

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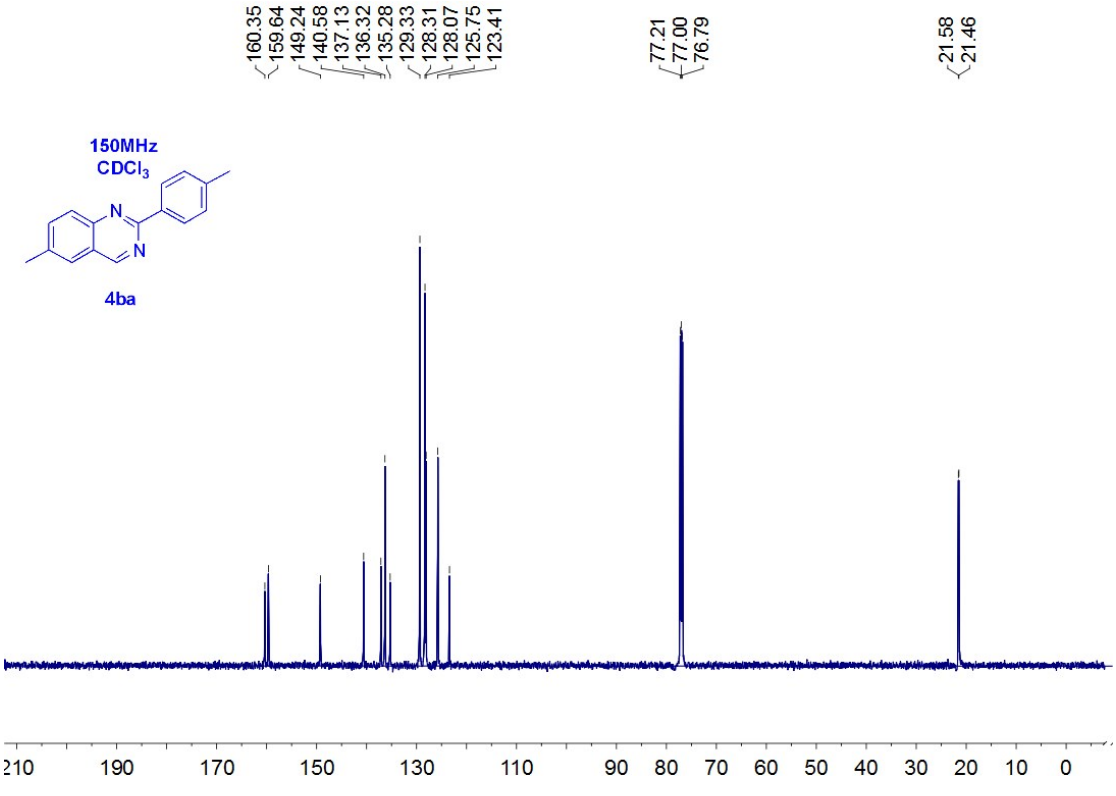
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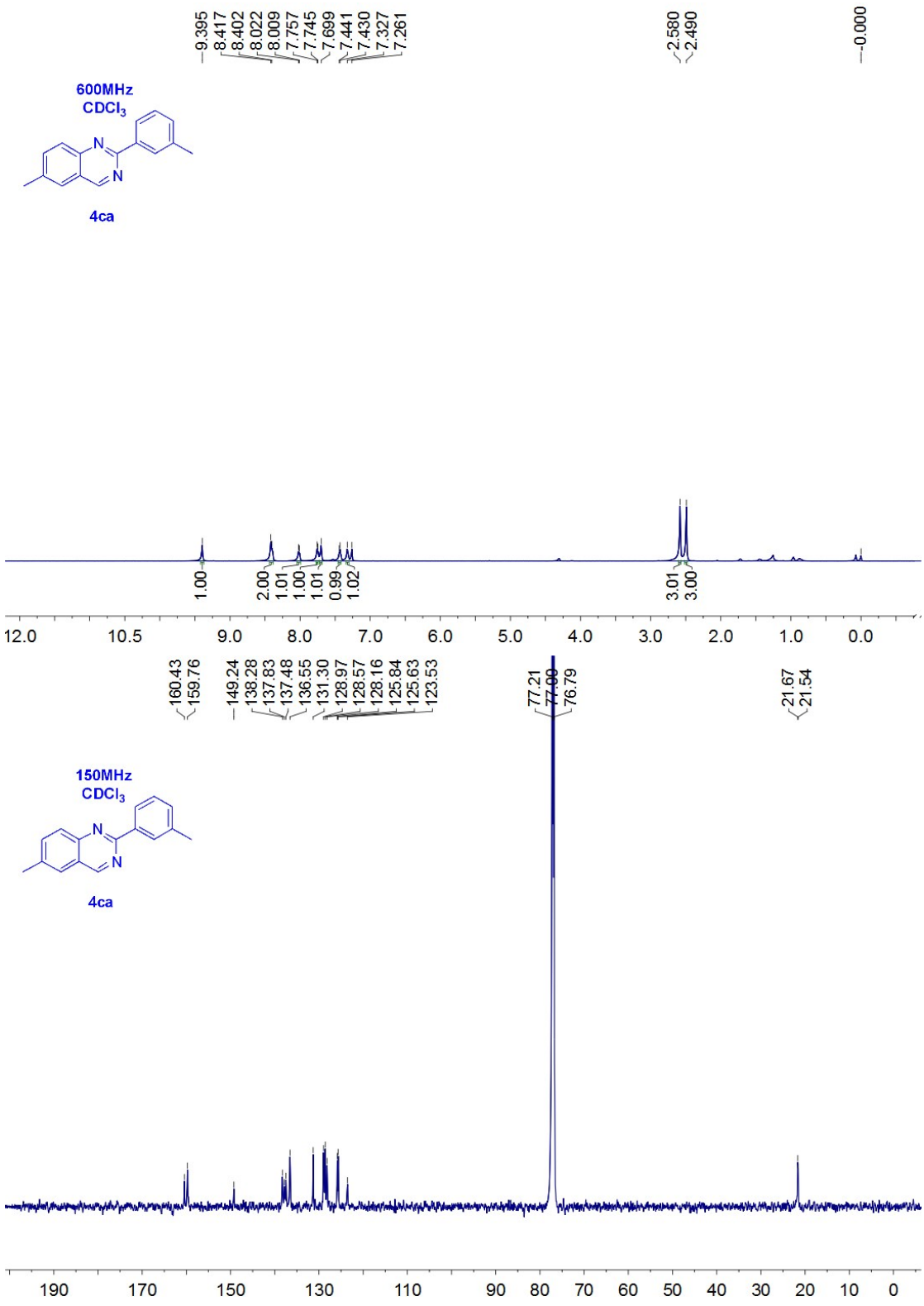
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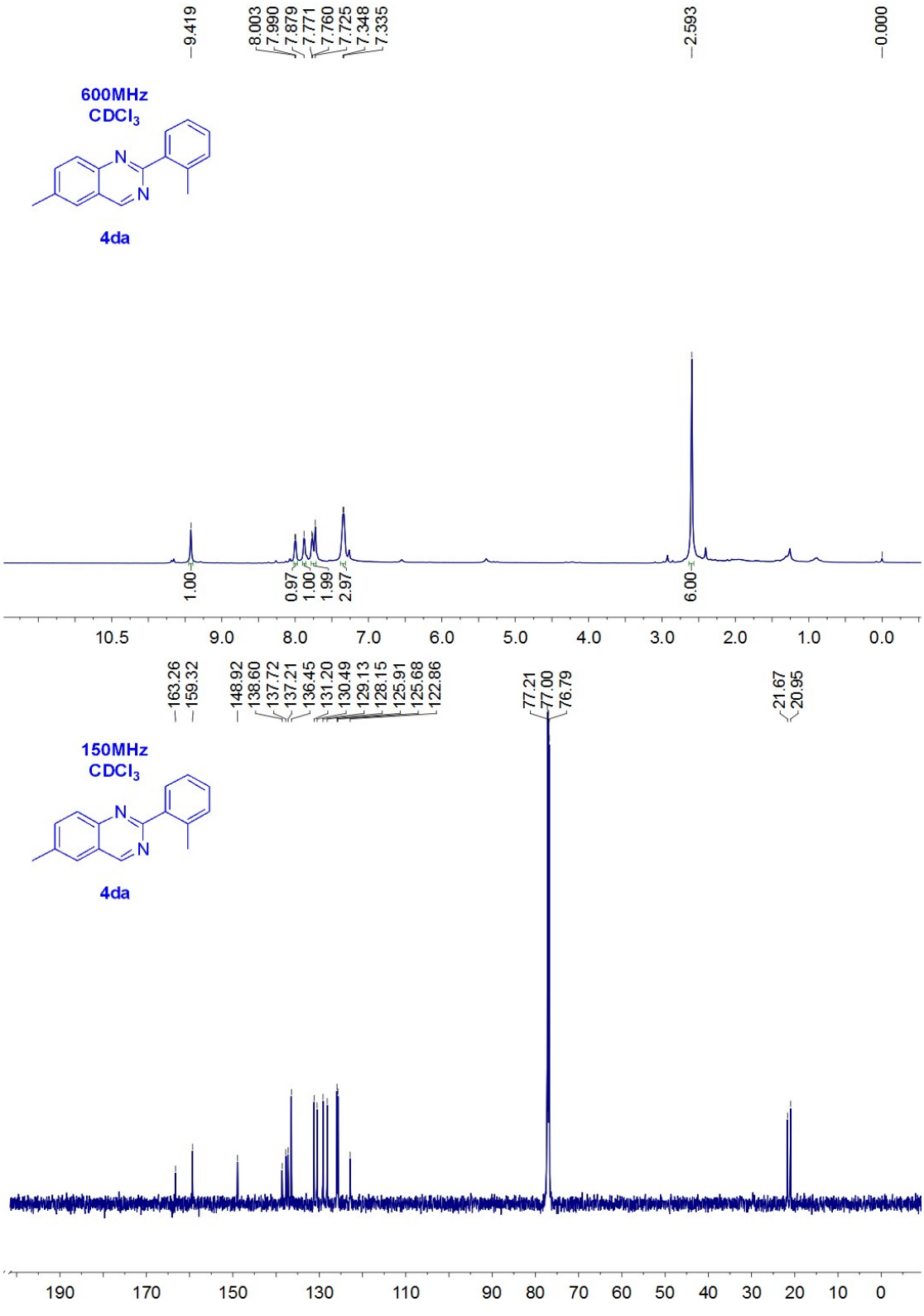
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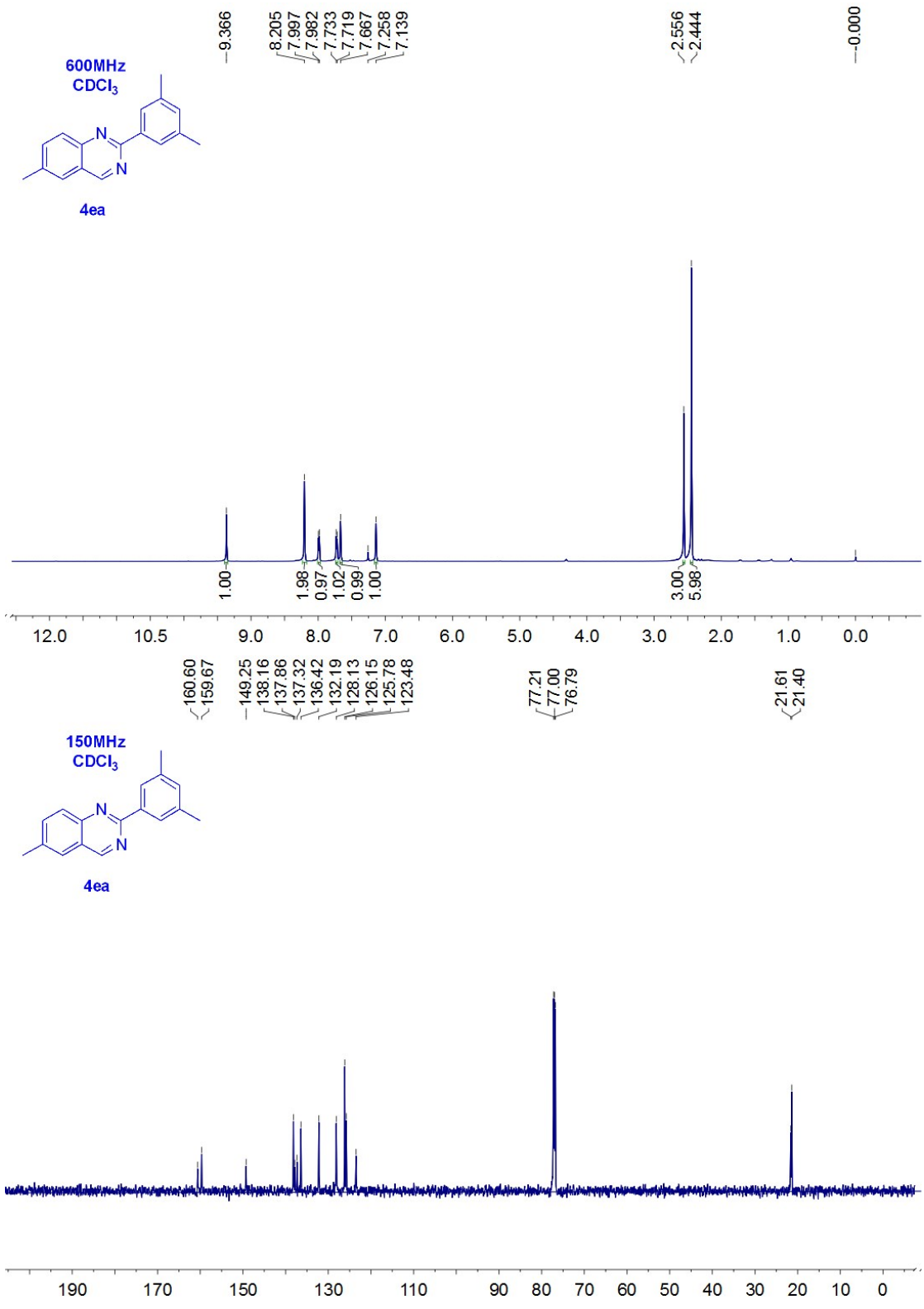
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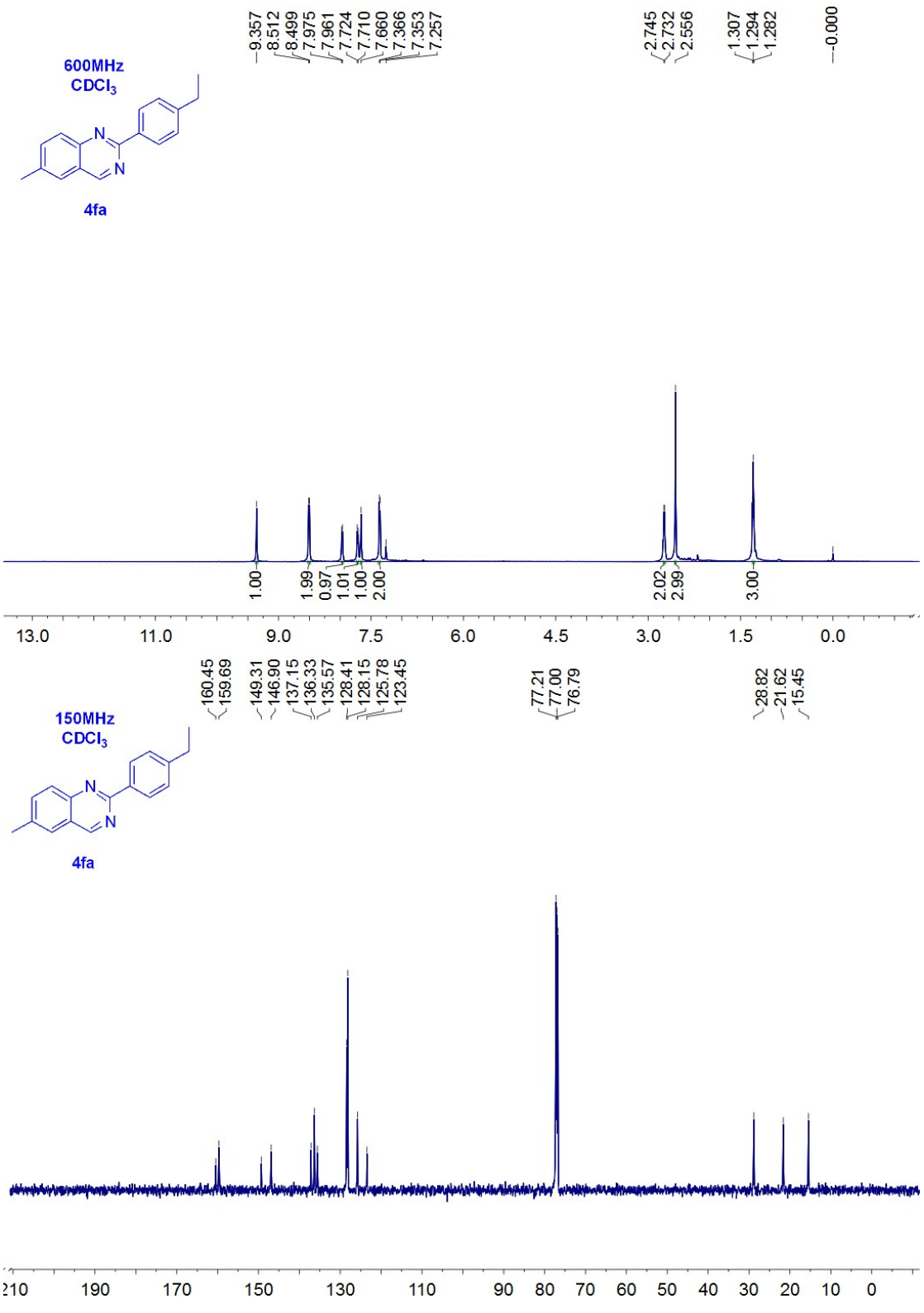
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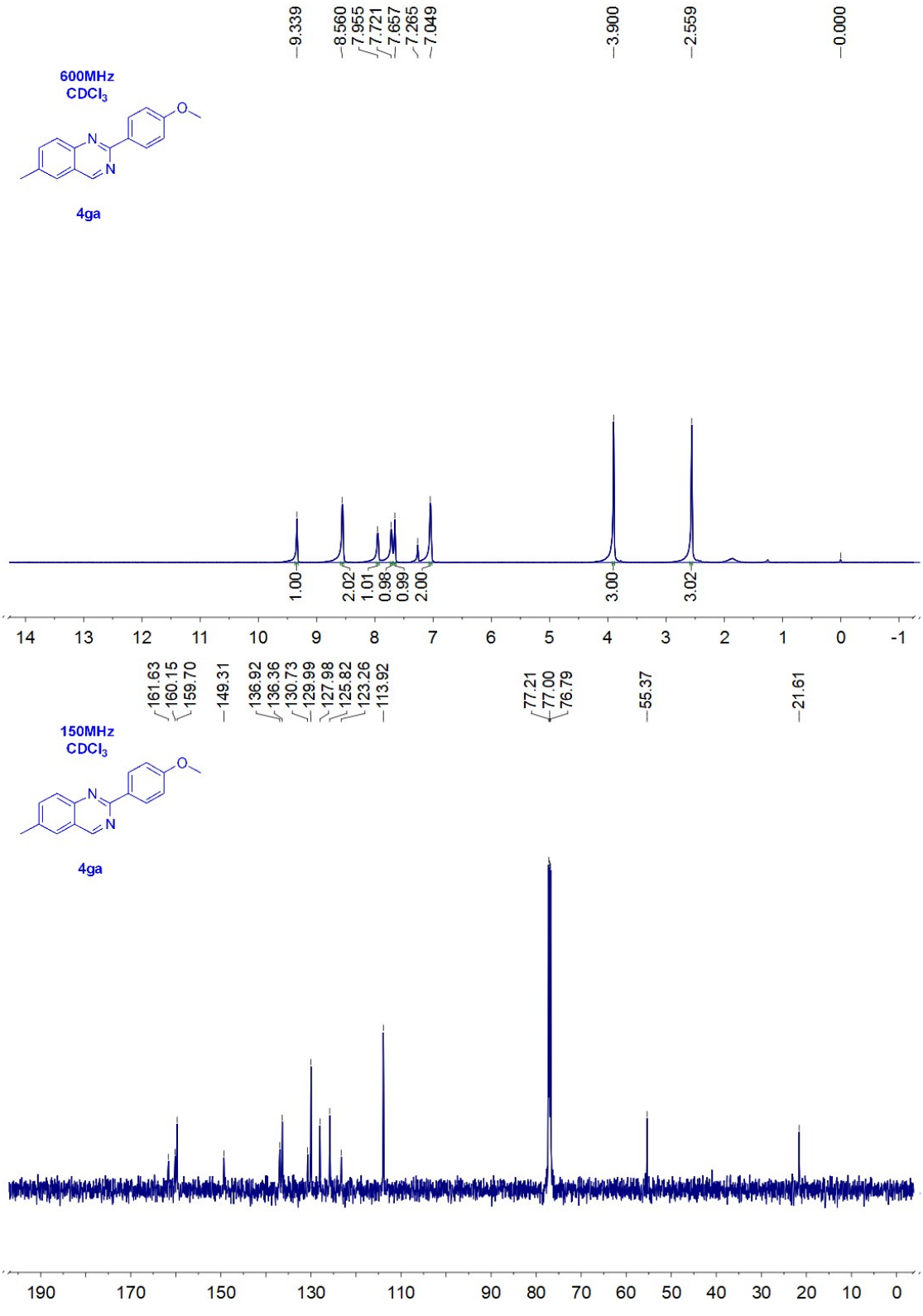
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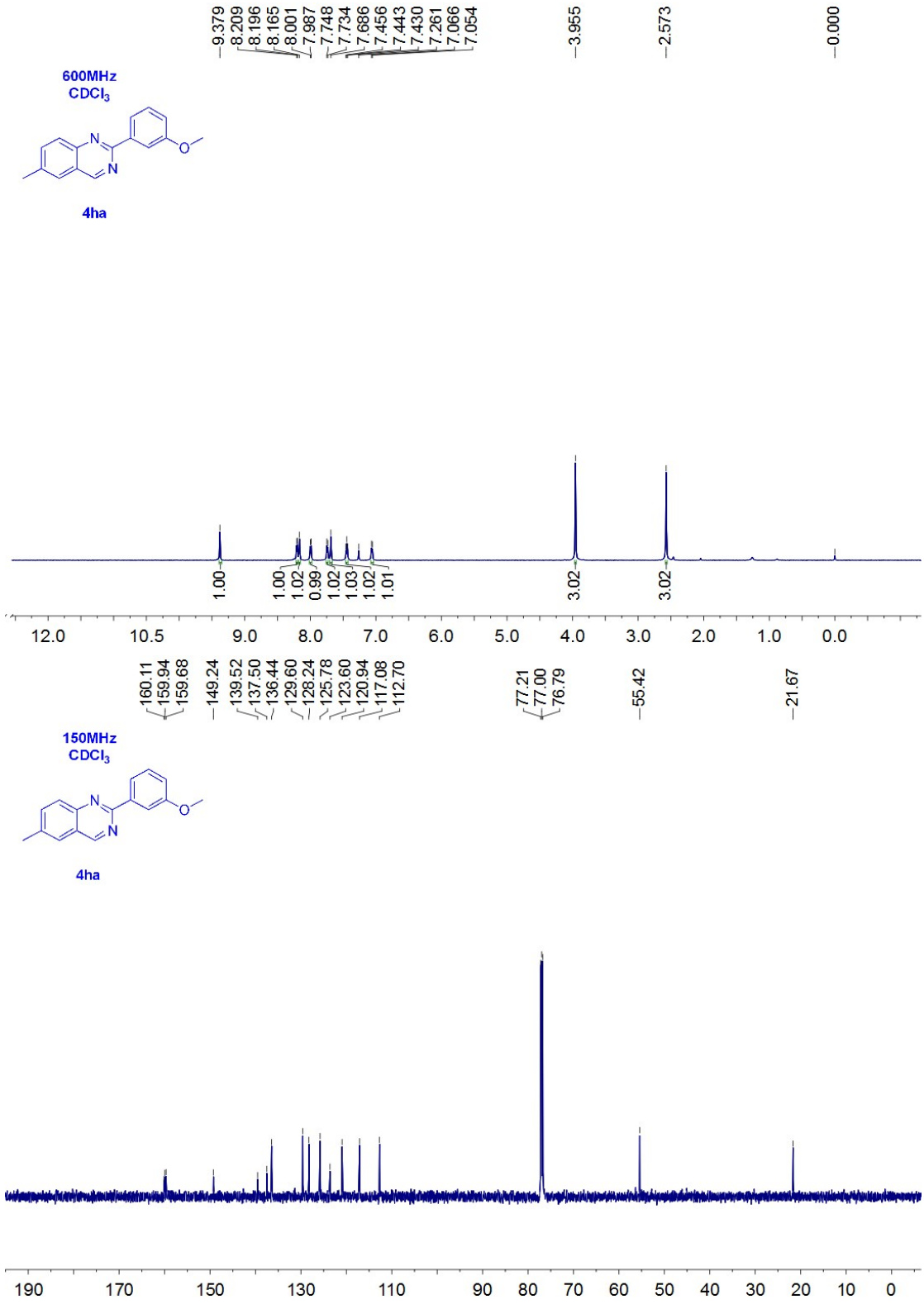
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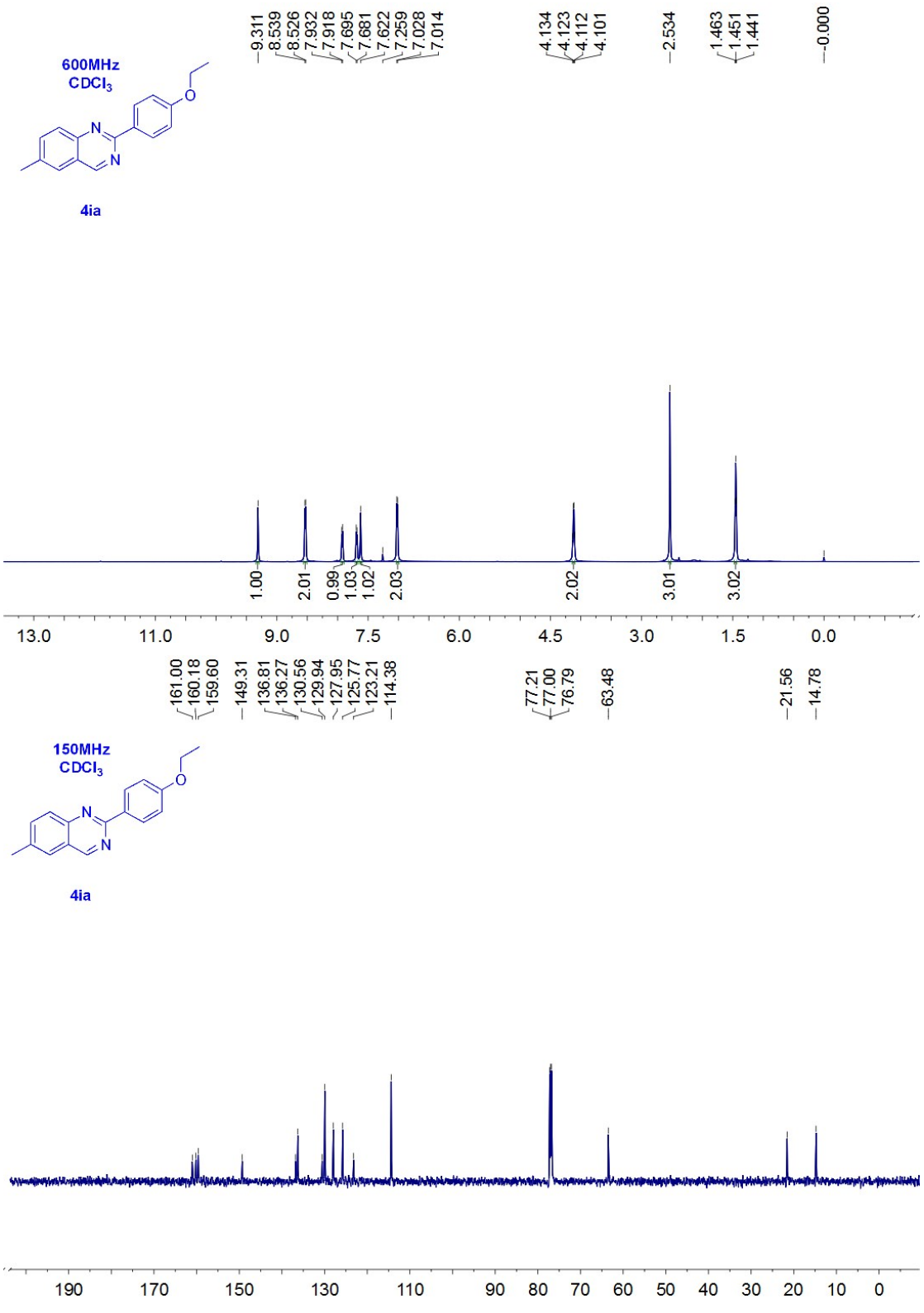
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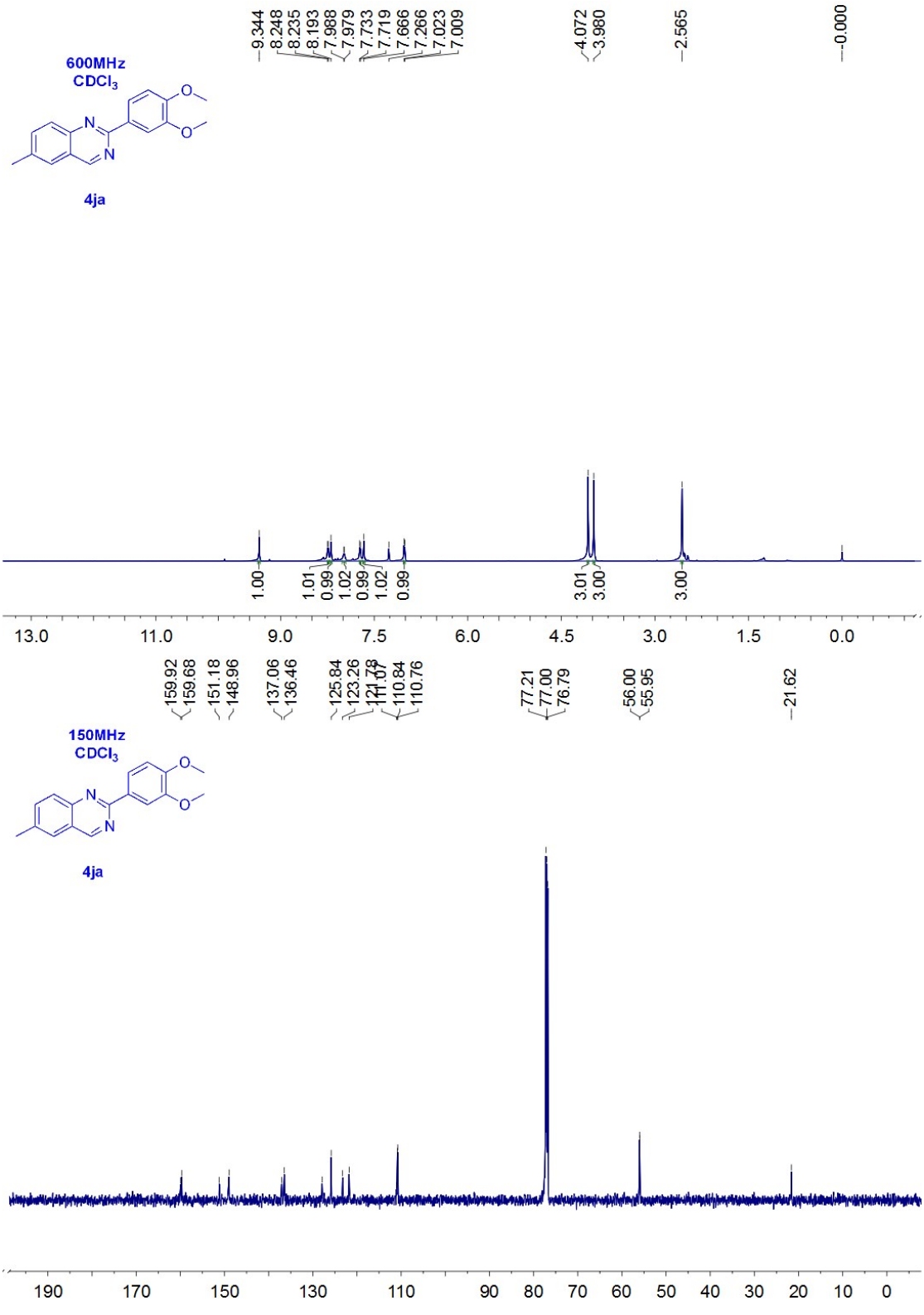
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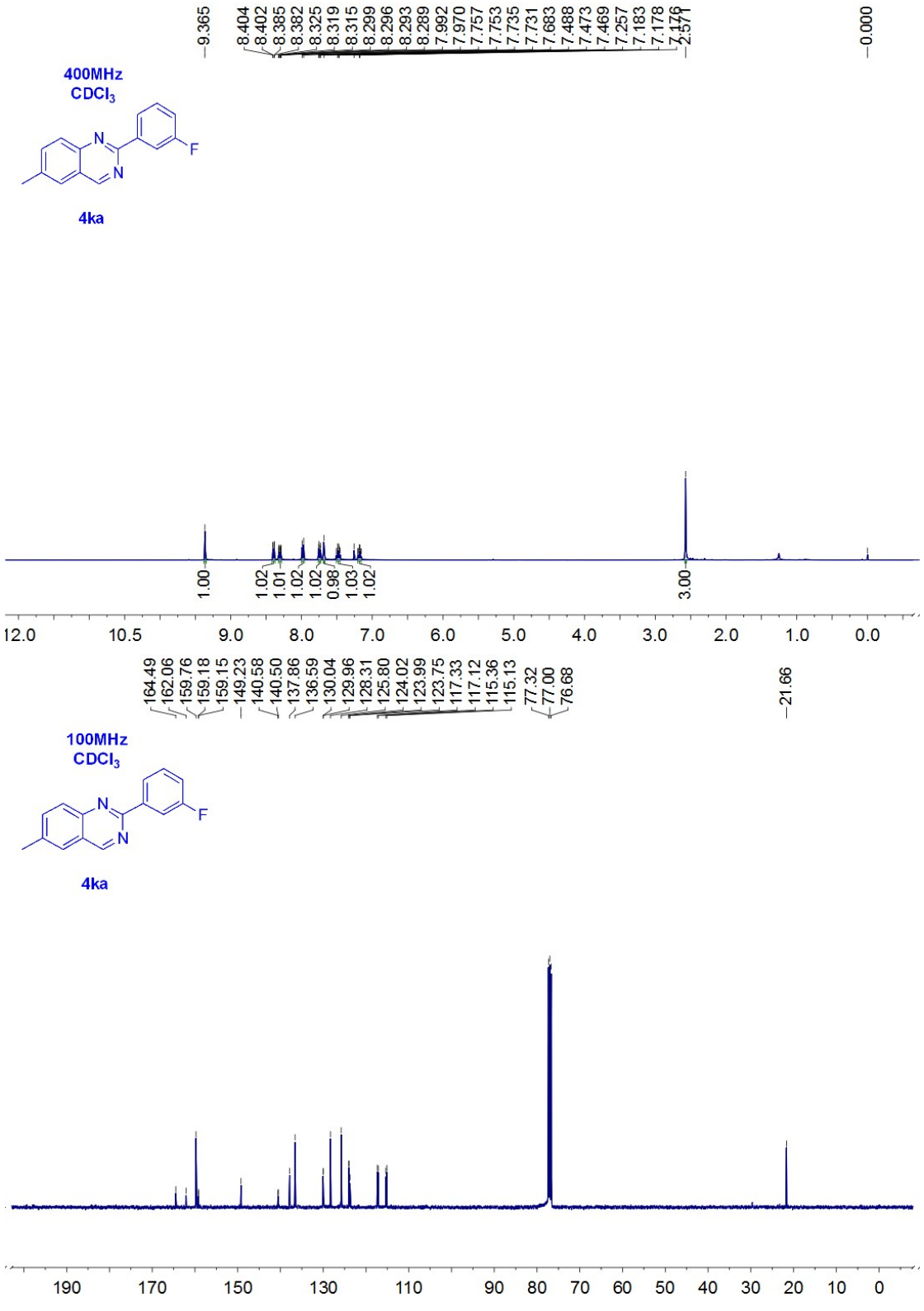
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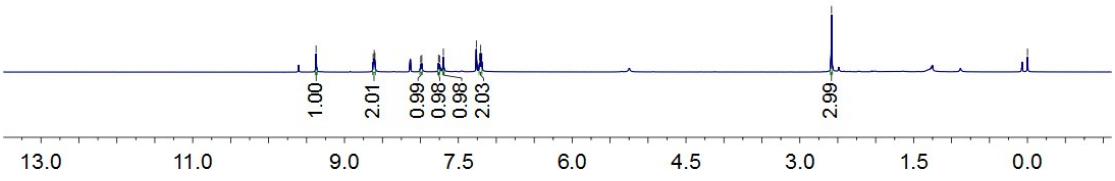

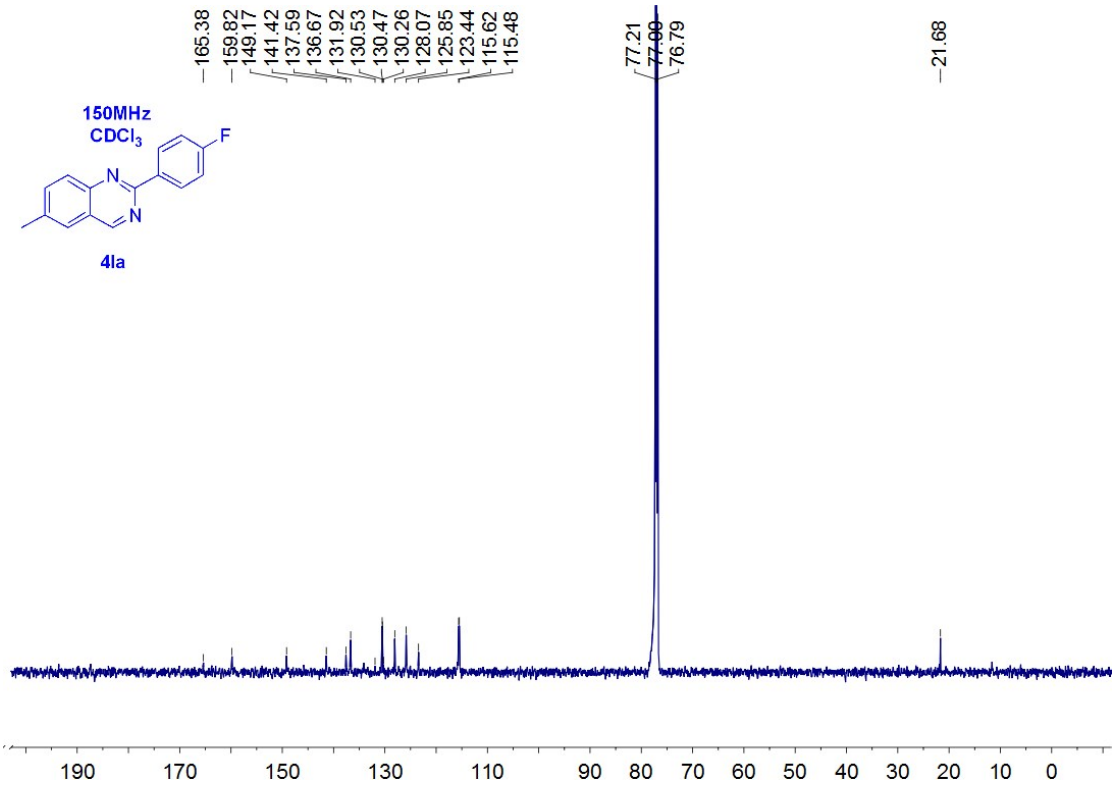
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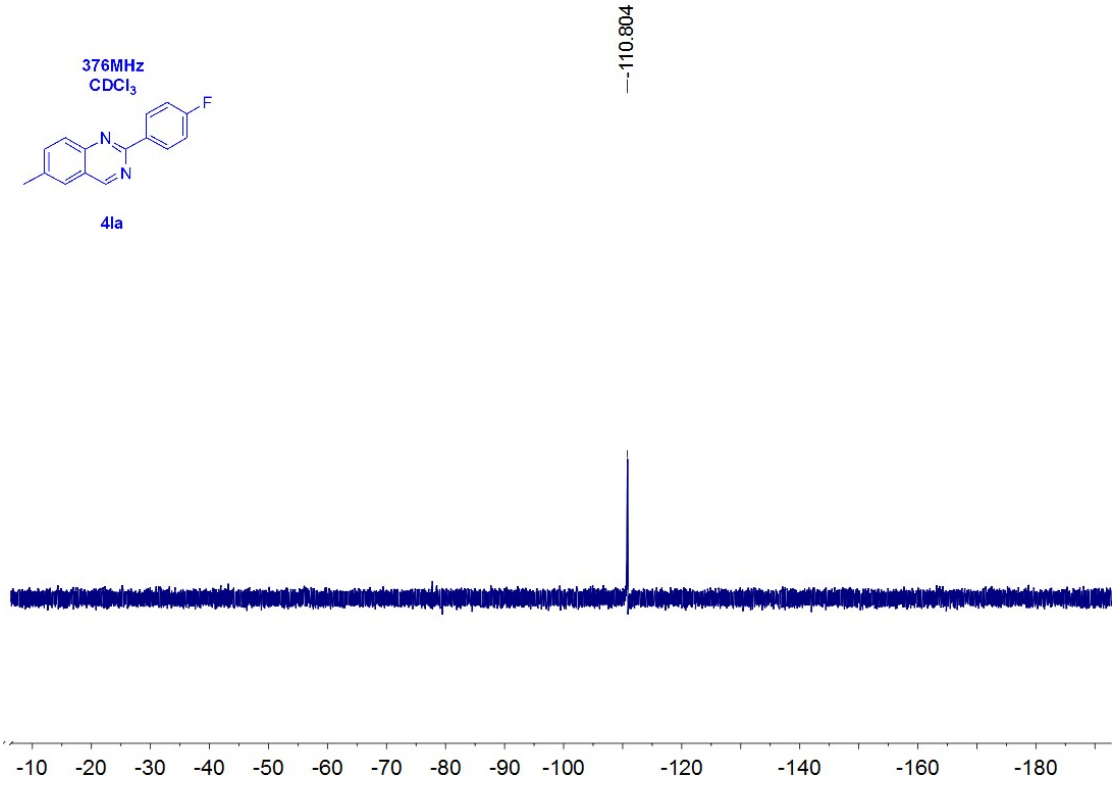
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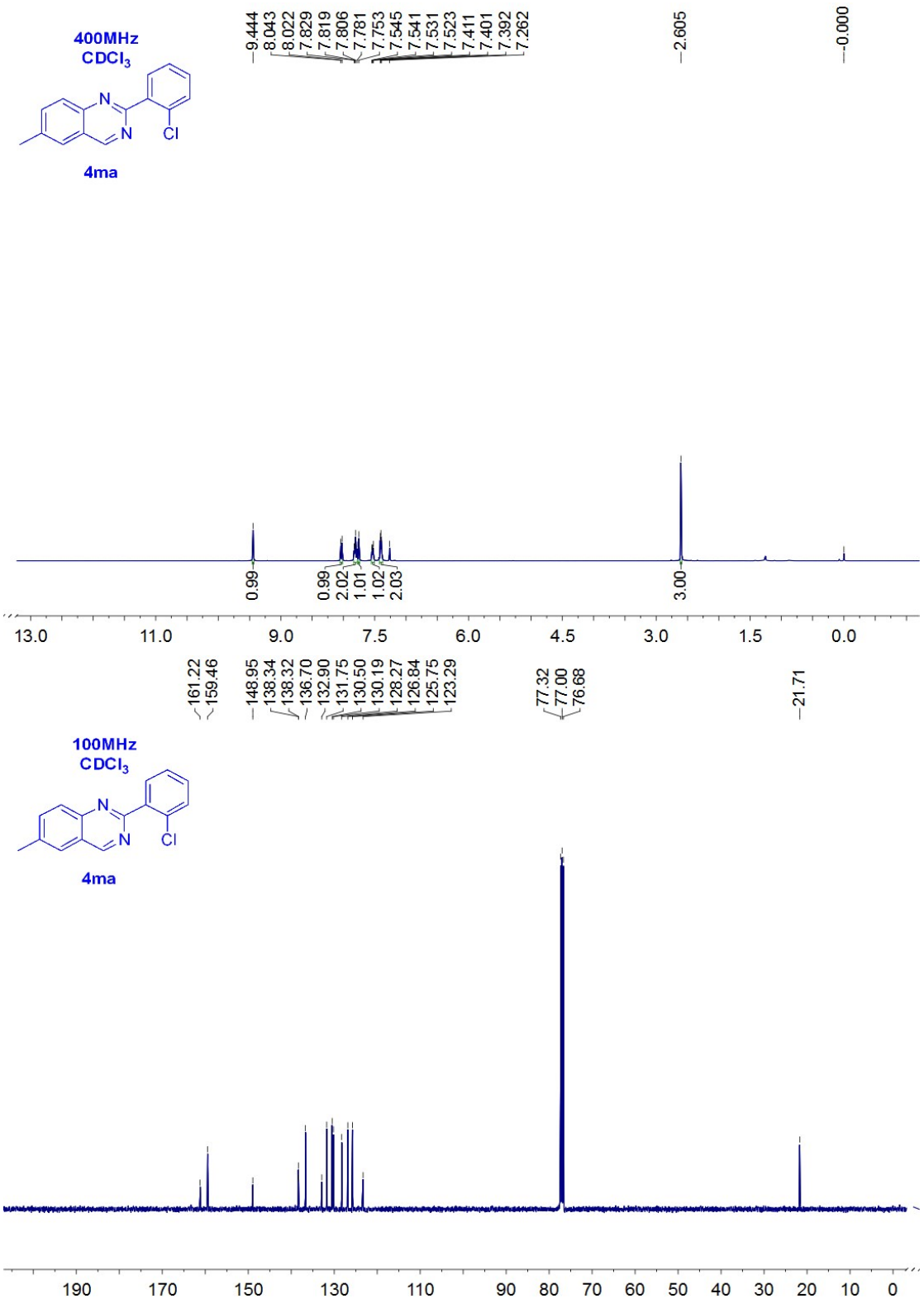
-100
-120
-140
-160
-180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7.541
7.531
7.523
7.411
7.401
7.392
7.262
2.605
0.000
0.99
0.99
2.02
1.01
1.02
2.03
3.00
13.0
11.0
9.0
7.5
6.0
4.5
3.0
1.5
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138.34
138.32
136.70
132.90
131.75
130.50
130.19
128.27
126.84
125.75
123.29
77.32
77.00
76.68
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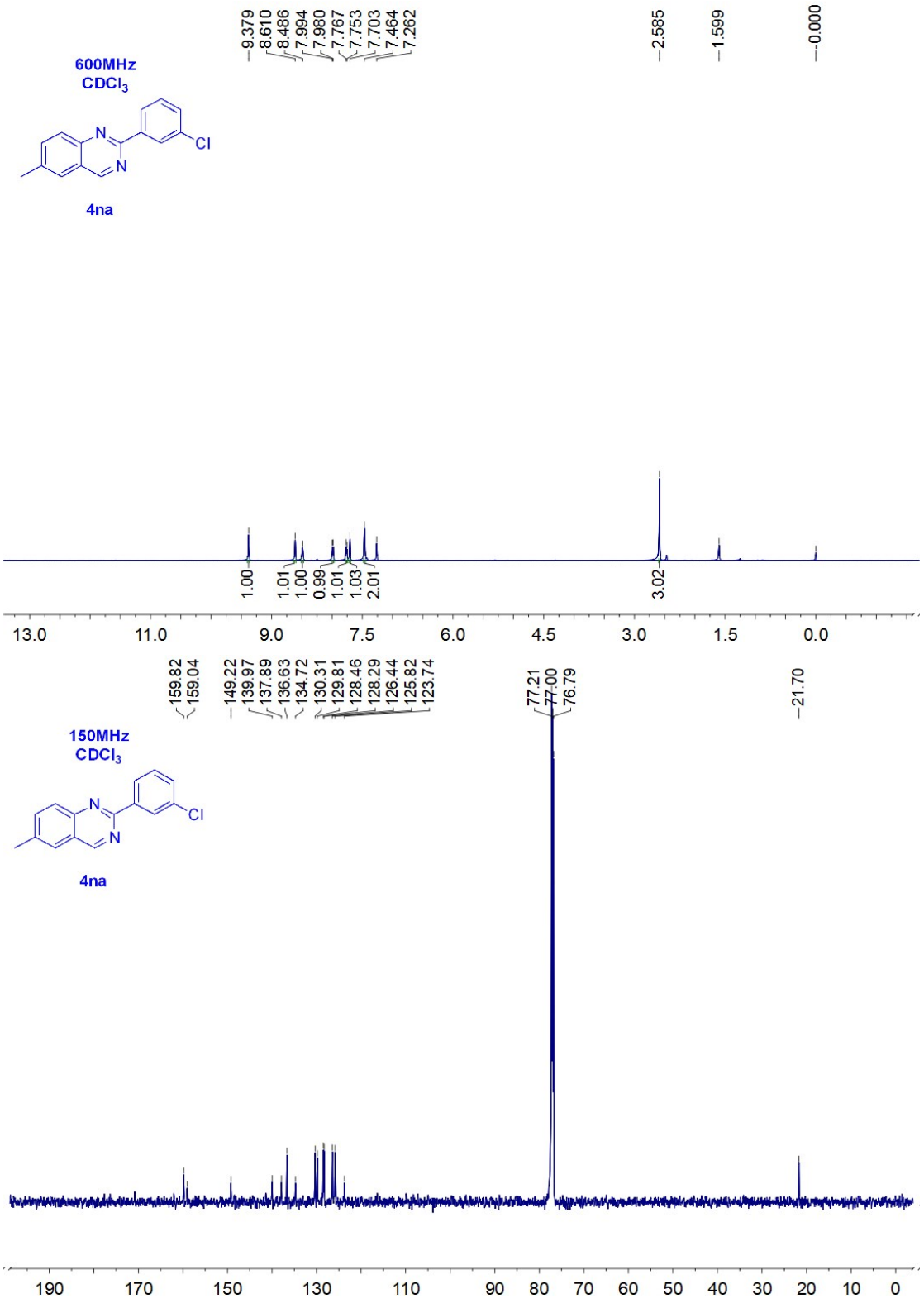
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7.262
2.585
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1.00
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1.01
1.03
2.01
3.02
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11.0
9.0
7.5
6.0
4.5
3.0
1.5
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150MHz
CDCl3
4na
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159.04
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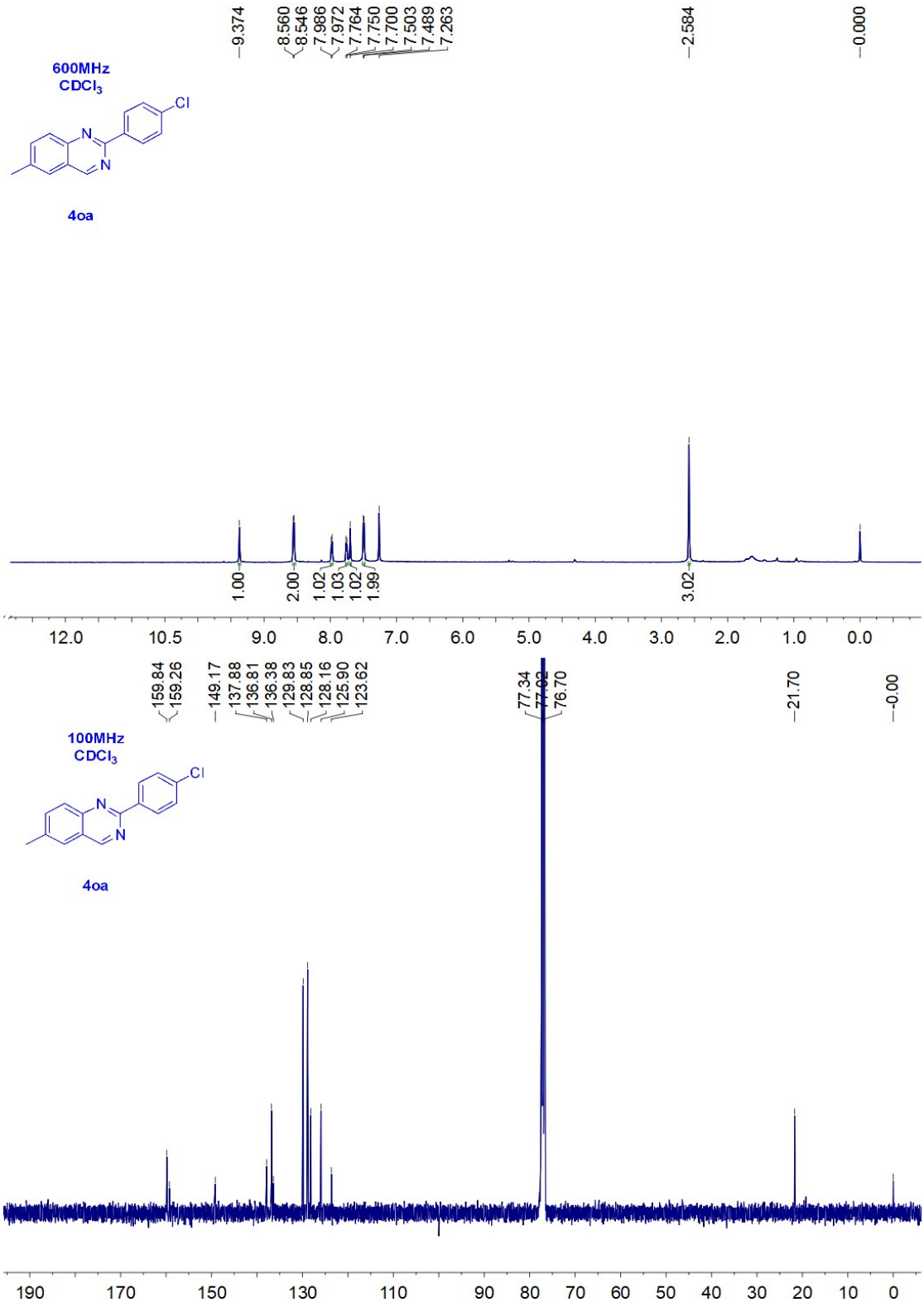
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7.489
7.263
2.584
0.000
1.00
2.00
1.02
1.03
1.02
1.99
3.02
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
100MHz
CDCl3
4oa
159.84
159.26
149.17
137.88
136.81
136.38
129.83
128.85
128.16
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77.02
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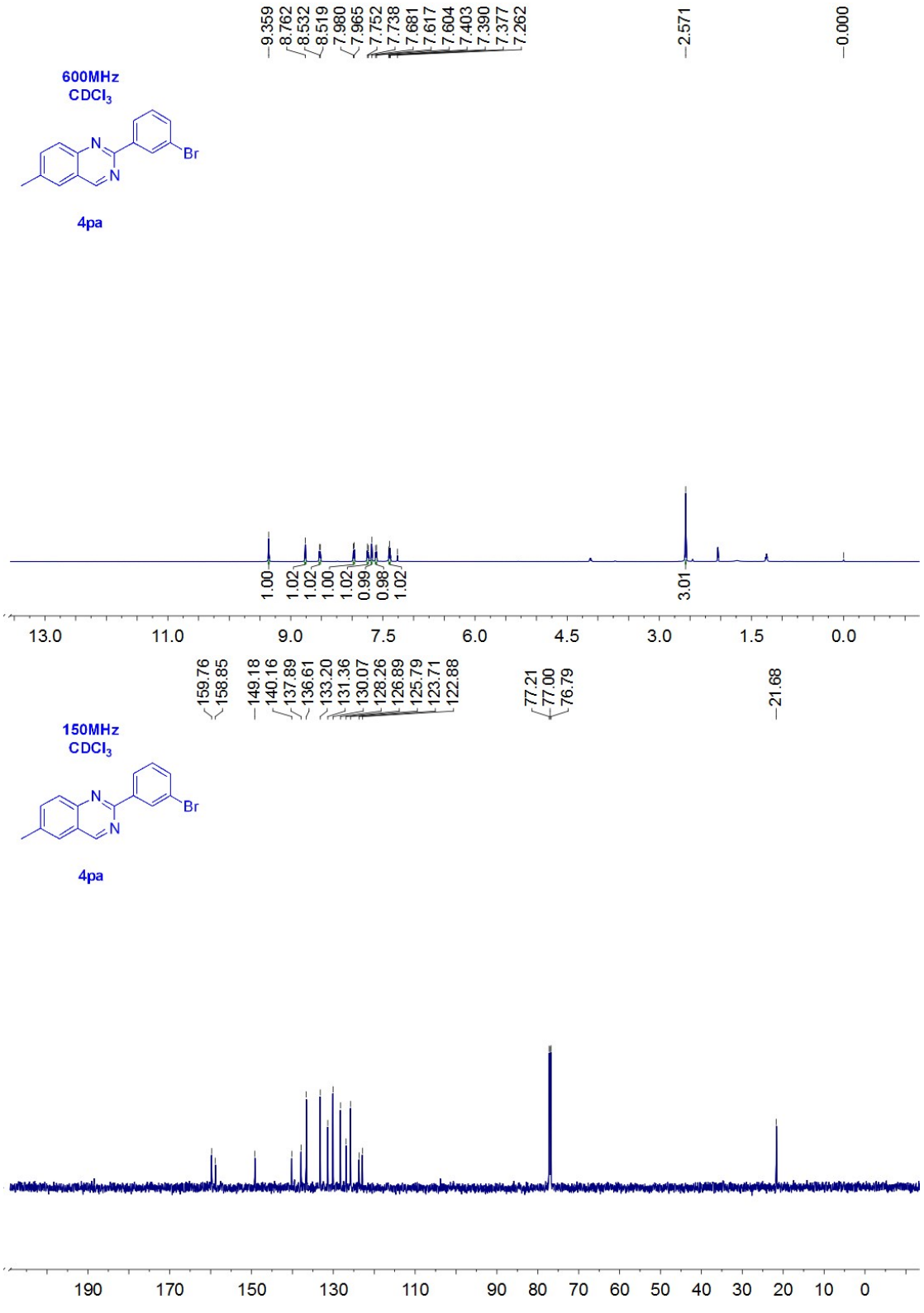
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8.762
8.532
8.519
7.980
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7.752
7.738
7.681
7.617
7.604
7.403
7.390
7.377
7.262
2.571
0.000
600MHz
CDCl3
Br
4pa
1.00
1.02
1.02
1.00
1.02
0.99
0.98
1.02
3.01
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11.0
9.0
7.5
6.0
4.5
3.0
1.5
0.0
159.76
158.85
149.18
140.16
137.89
136.61
133.20
131.36
130.07
128.26
126.89
125.79
123.71
122.88
77.21
77.00
76.79
21.68
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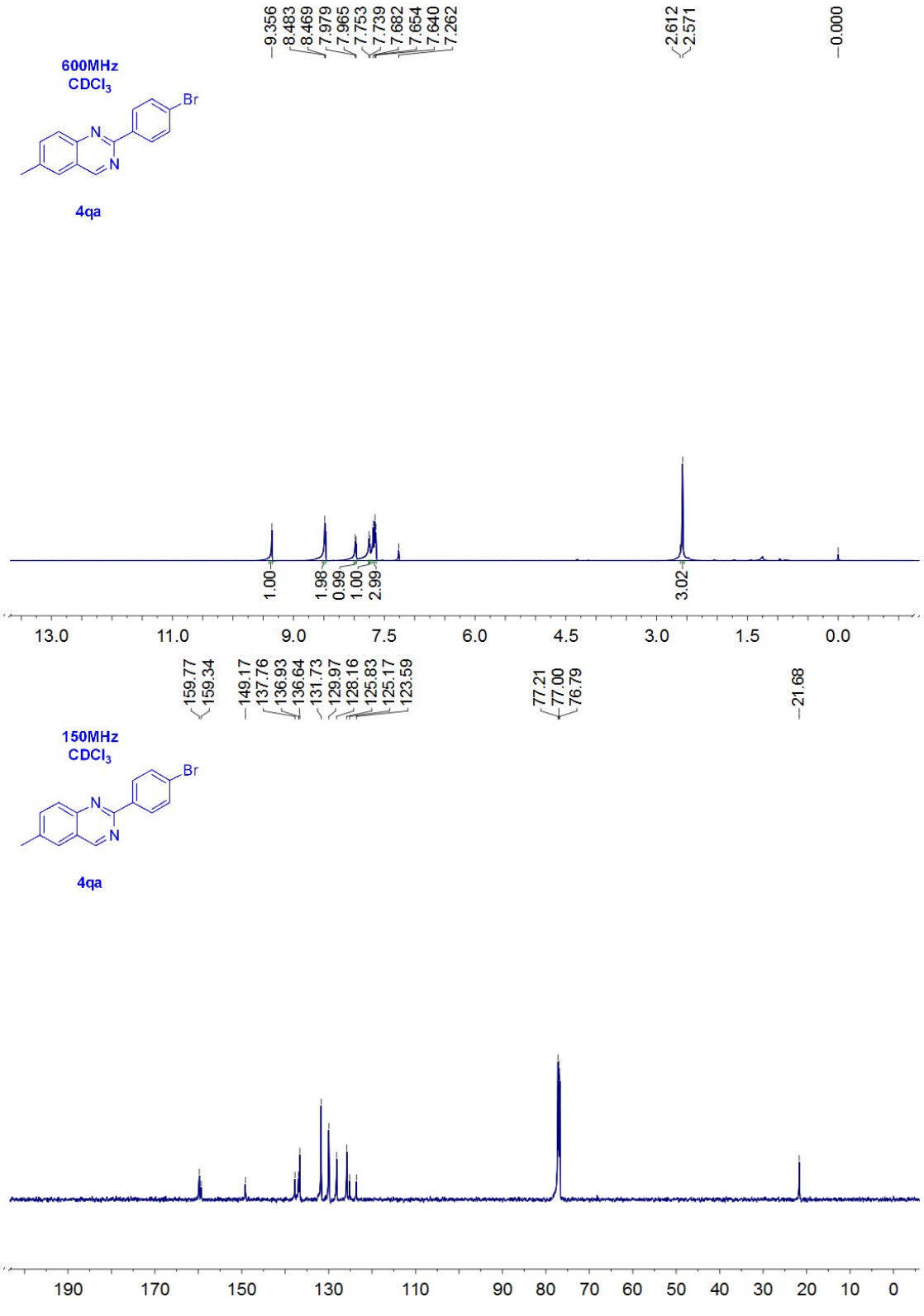
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8.469
7.979
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7.739
7.682
7.654
7.640
7.262
2.612
2.571
0.000
600MHz
CDCl3
Br
N
N
4qa
1.00
1.98
0.99
1.00
2.99
3.02
13.0
11.0
9.0
7.5
6.0
4.5
3.0
1.5
0.0
159.77
159.34
149.17
137.76
136.93
136.64
131.73
129.97
128.16
125.83
125.17
123.59
77.21
77.00
76.79
21.68
150MHz
CDCl3
Br
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N
4qa
190
170
150
130
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70
60
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40
30
20
10
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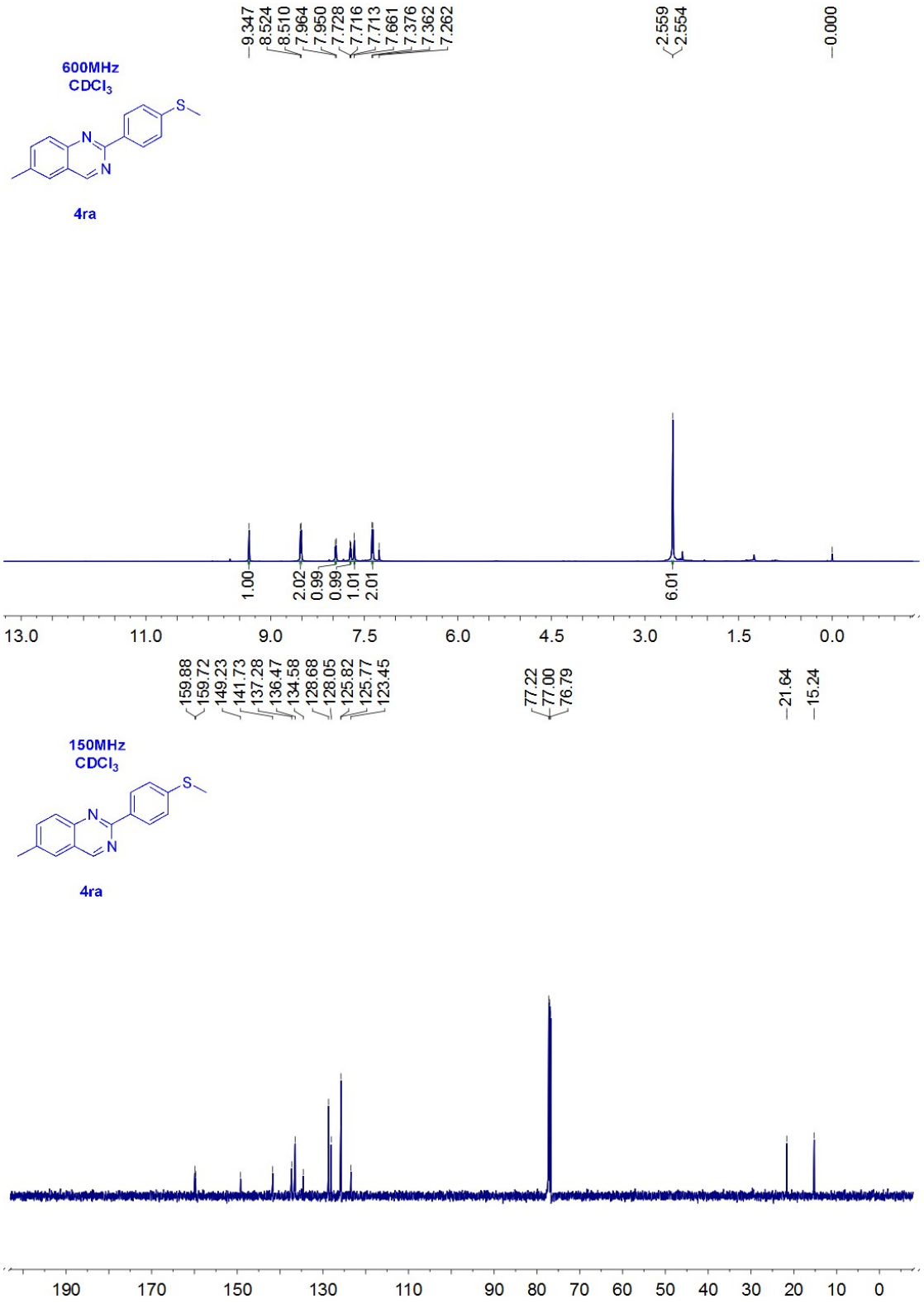
9.347
8.524
8.510
7.964
7.950
7.728
7.716
7.713
7.661
7.376
7.362
7.262
2.559
2.554
0.000
600MHz
CDCl3
4ra
1.00
2.02
0.99
0.99
1.01
2.01
6.01
13.0
11.0
9.0
7.5
6.0
4.5
3.0
1.5
0.0
159.88
159.72
149.23
141.73
137.28
136.47
134.58
128.68
128.05
125.82
125.77
123.45
77.22
77.00
76.79
21.64
15.24
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4ra
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170
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130
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70
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40
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20
10
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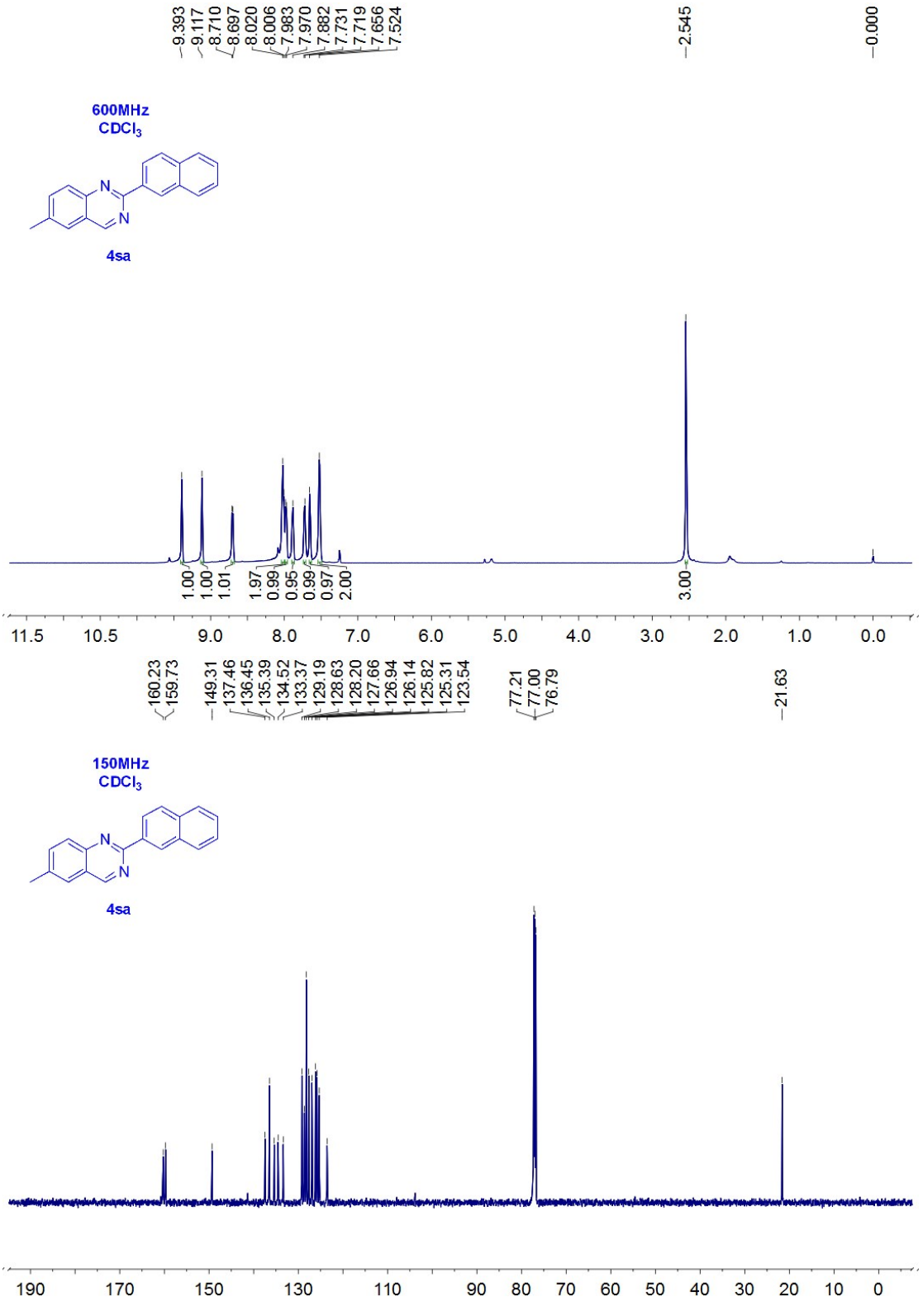
9.393
9.117
8.710
8.697
8.020
8.006
7.983
7.970
7.882
7.731
7.719
7.656
7.524
2.545
0.000
600MHz
CDCl3
4sa
1.00
1.00
1.01
1.97
0.99
0.95
0.99
0.97
2.00
3.00
11.5
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
160.23
159.73
149.31
137.46
136.45
135.39
134.52
133.37
129.19
128.63
128.20
127.66
126.94
126.14
125.82
125.31
123.54
77.21
77.00
76.79
21.63
150MHz
CDCl3
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190
170
150
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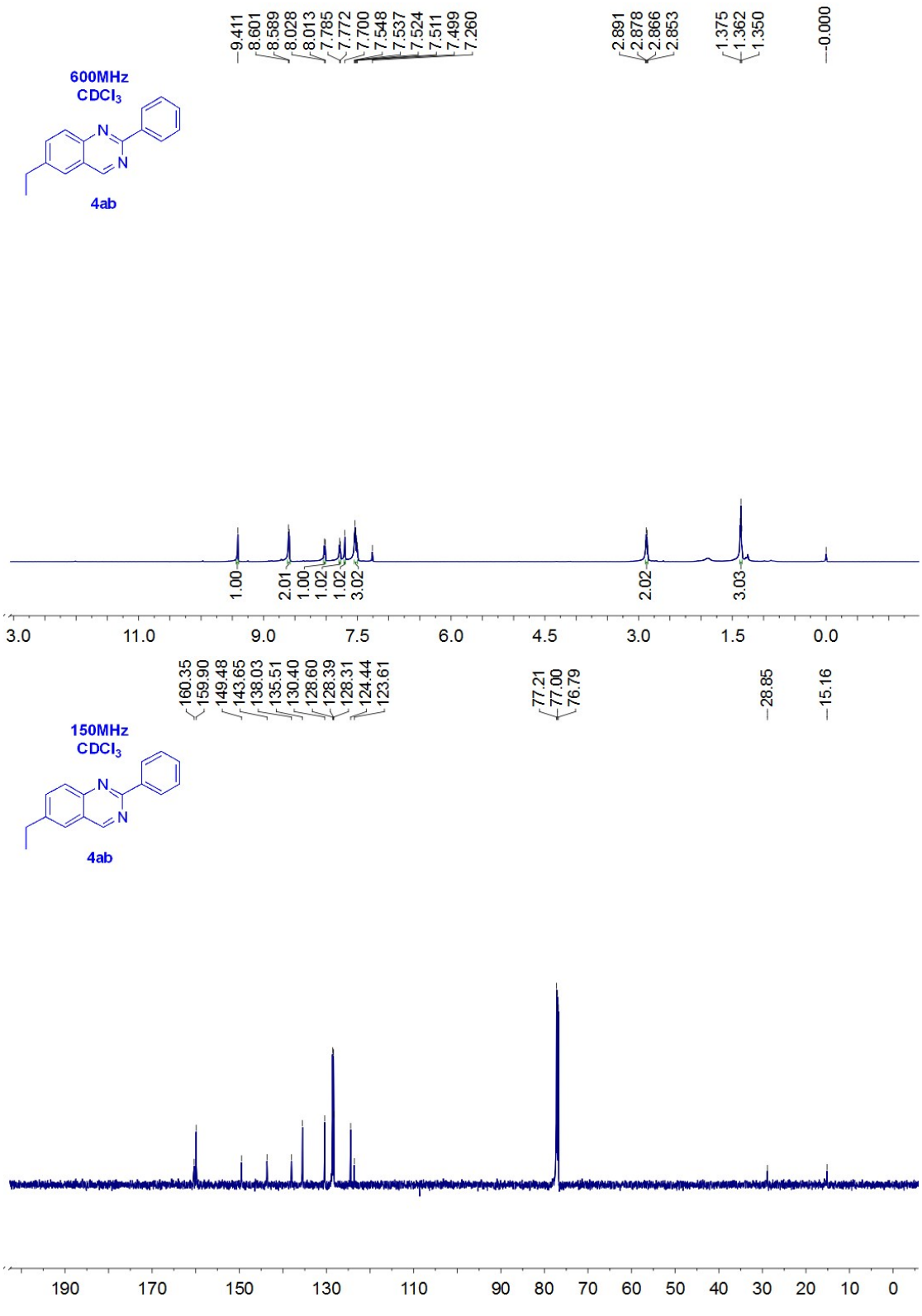
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8.013
7.785
7.772
7.700
7.548
7.537
7.524
7.511
7.499
7.260
2.891
2.878
2.866
2.853
1.375
1.362
1.350
0.000
600MHz
CDCl3
4ab
1.00
2.01
1.00
1.02
1.02
3.02
2.02
3.03
3.0
11.0
9.0
7.5
6.0
4.5
3.0
1.5
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159.90
149.48
143.65
138.03
135.51
130.40
128.60
128.39
128.31
124.44
123.61
77.21
77.00
76.79
28.85
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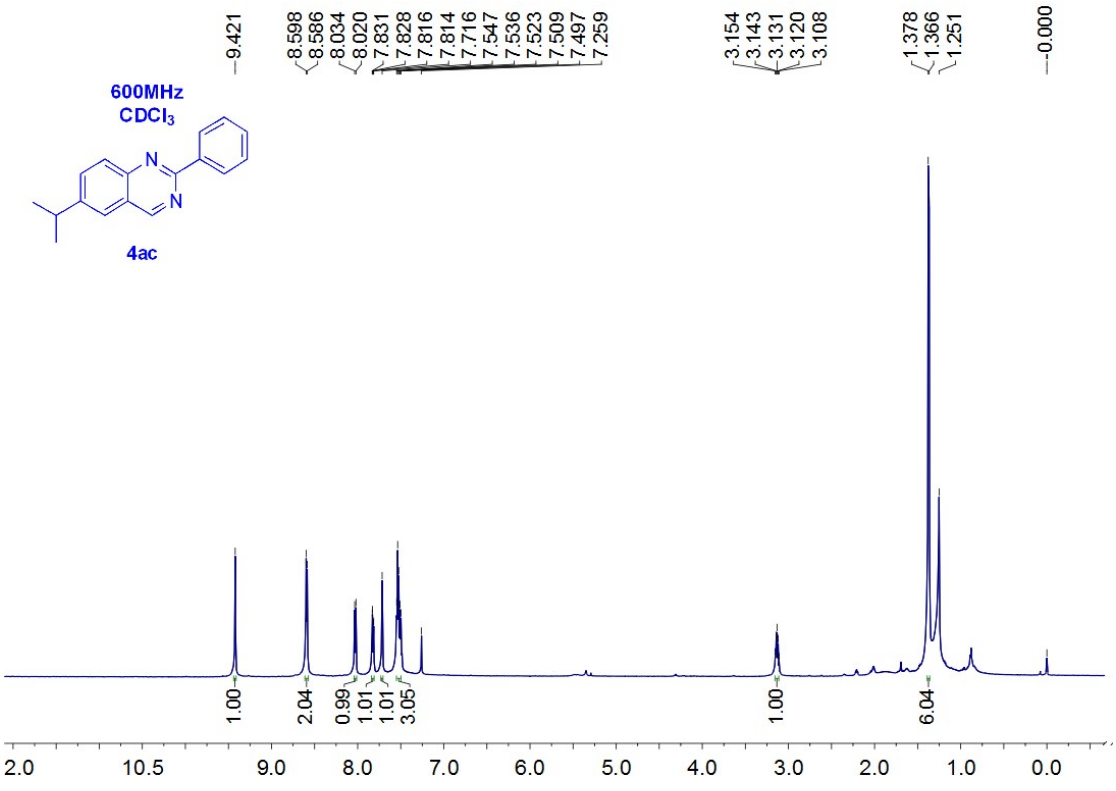
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8.020
7.831
7.828
7.816
7.814
7.716
7.547
7.536
7.523
7.509
7.497
7.259
3.154
3.143
3.131
3.120
3.108
1.378
1.366
1.251
0.000
1.00
2.04
0.99
1.01
1.01
3.05
1.00
6.04
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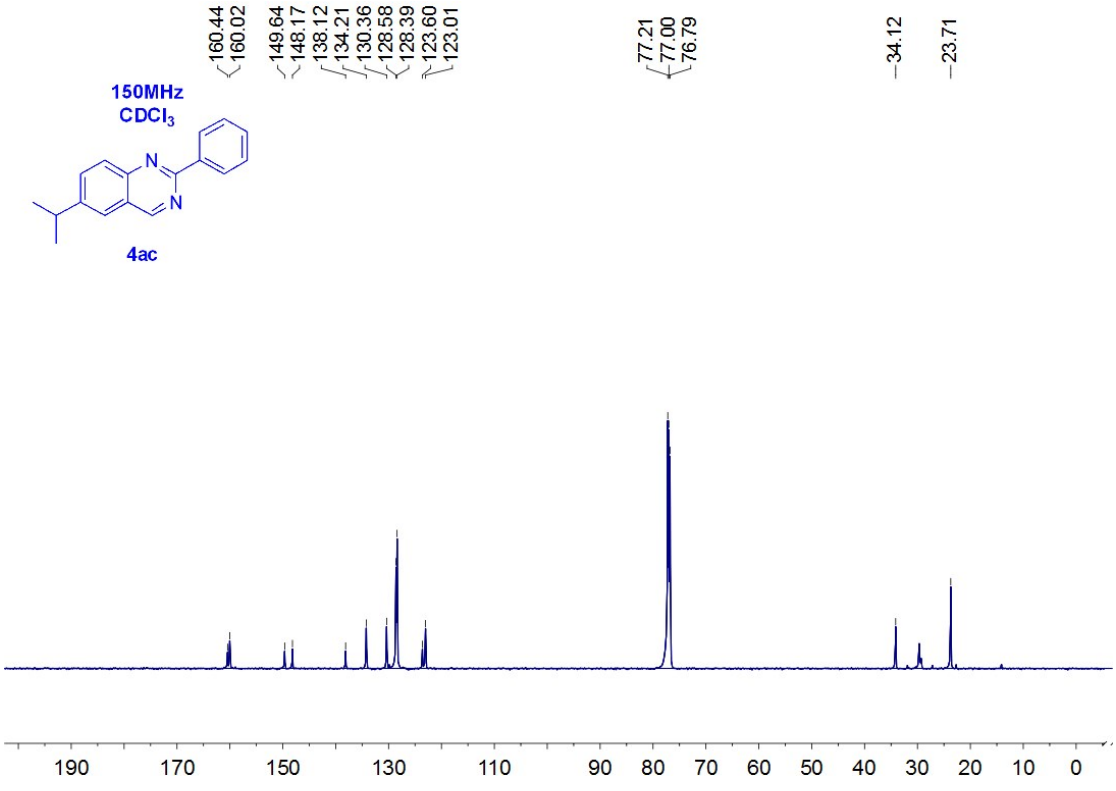
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CDCl3
4ac
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134.21
130.36
128.58
128.39
123.60
123.01
77.21
77.00
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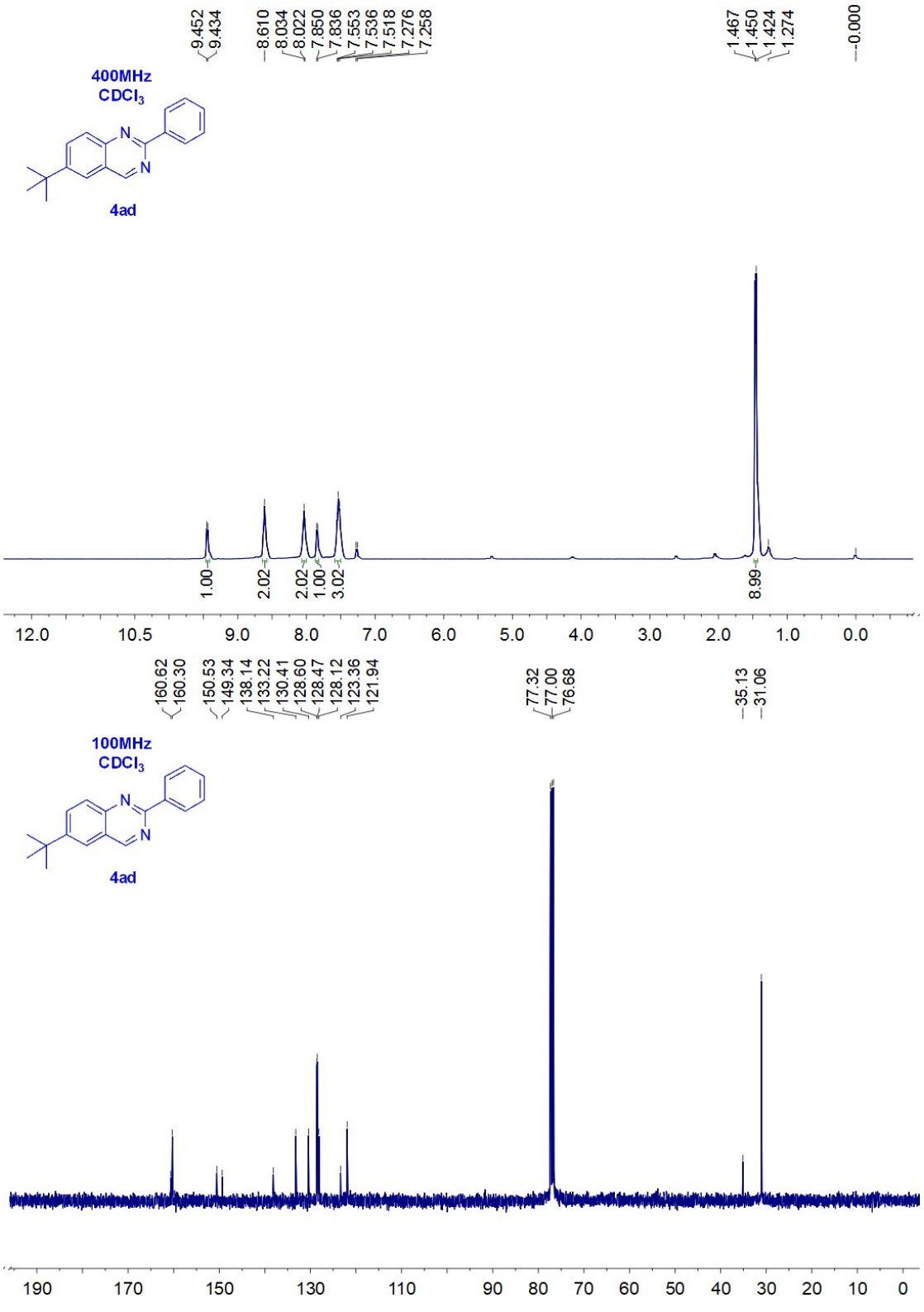
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7.553
7.536
7.518
7.276
7.258
1.467
1.450
1.424
1.274
0.000
400MHz
CDCl3
4ad
1.00
2.02
2.02
1.00
3.02
8.99
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
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160.30
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149.34
138.14
133.22
130.41
128.60
128.47
128.12
123.36
121.94
77.32
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35.13
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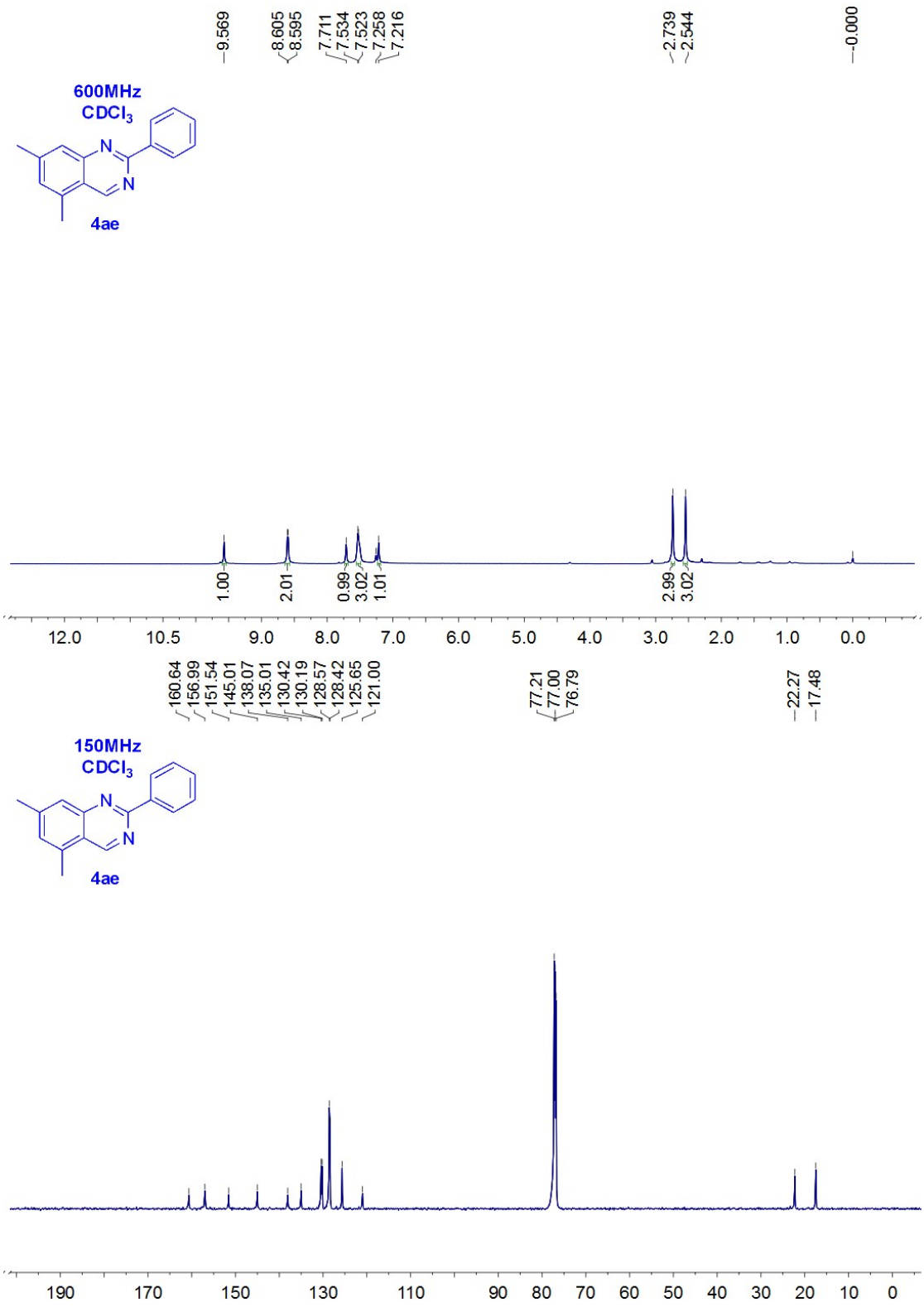
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7.534
7.523
7.258
7.216
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2.544
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2.01
0.99
3.02
1.01
2.99
3.02
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
160.64
156.99
151.54
145.01
138.07
135.01
130.42
130.19
128.57
128.42
125.65
121.00
77.21
77.00
76.79
22.27
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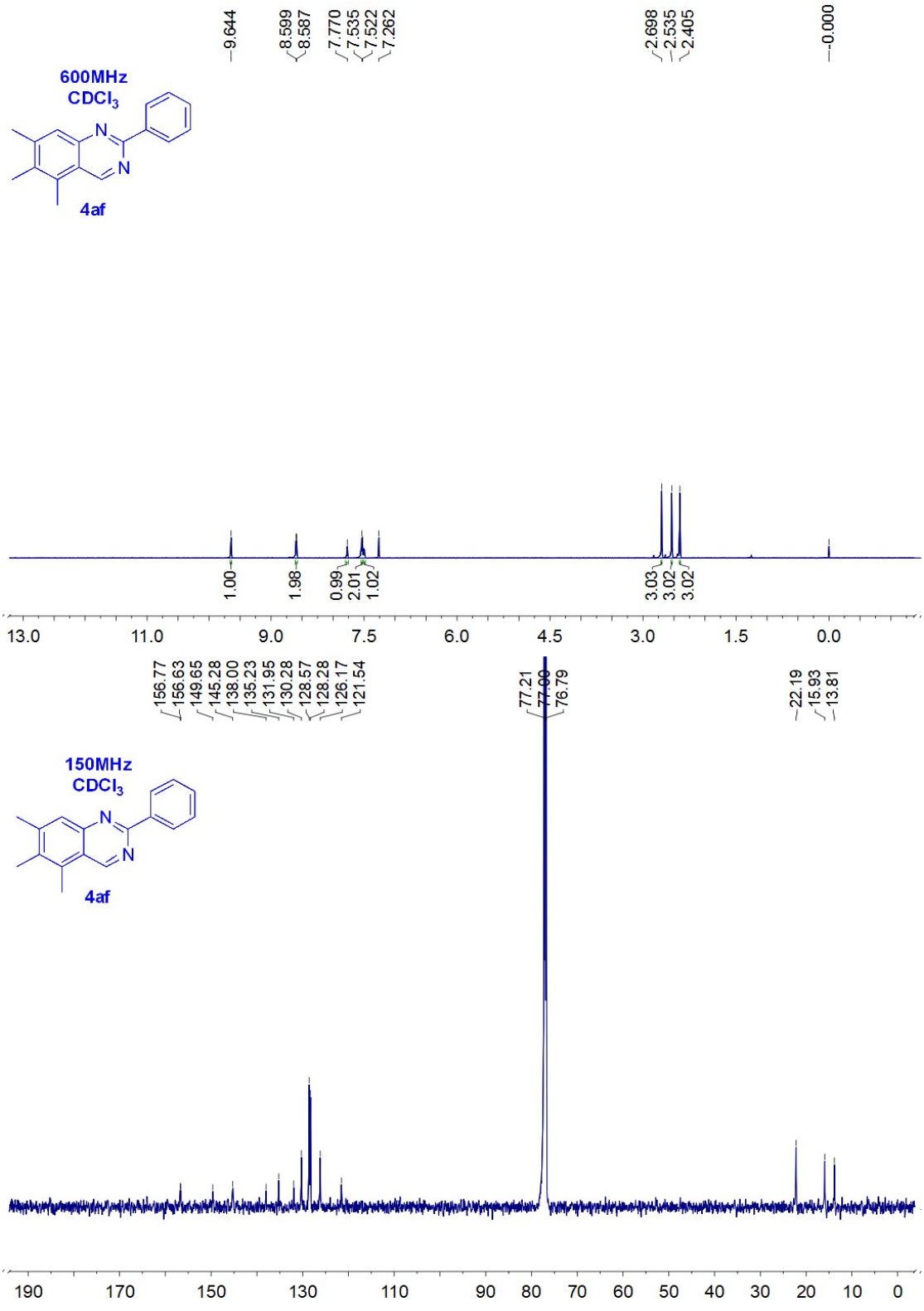
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7.522
7.262
2.698
2.535
2.405
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4af
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1.98
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2.01
1.02
3.03
3.02
3.02
13.0
11.0
9.0
7.5
6.0
4.5
3.0
1.5
0.0
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156.63
149.65
145.28
138.00
135.23
131.95
130.28
128.57
128.28
126.17
121.54
77.21
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76.79
22.19
15.93
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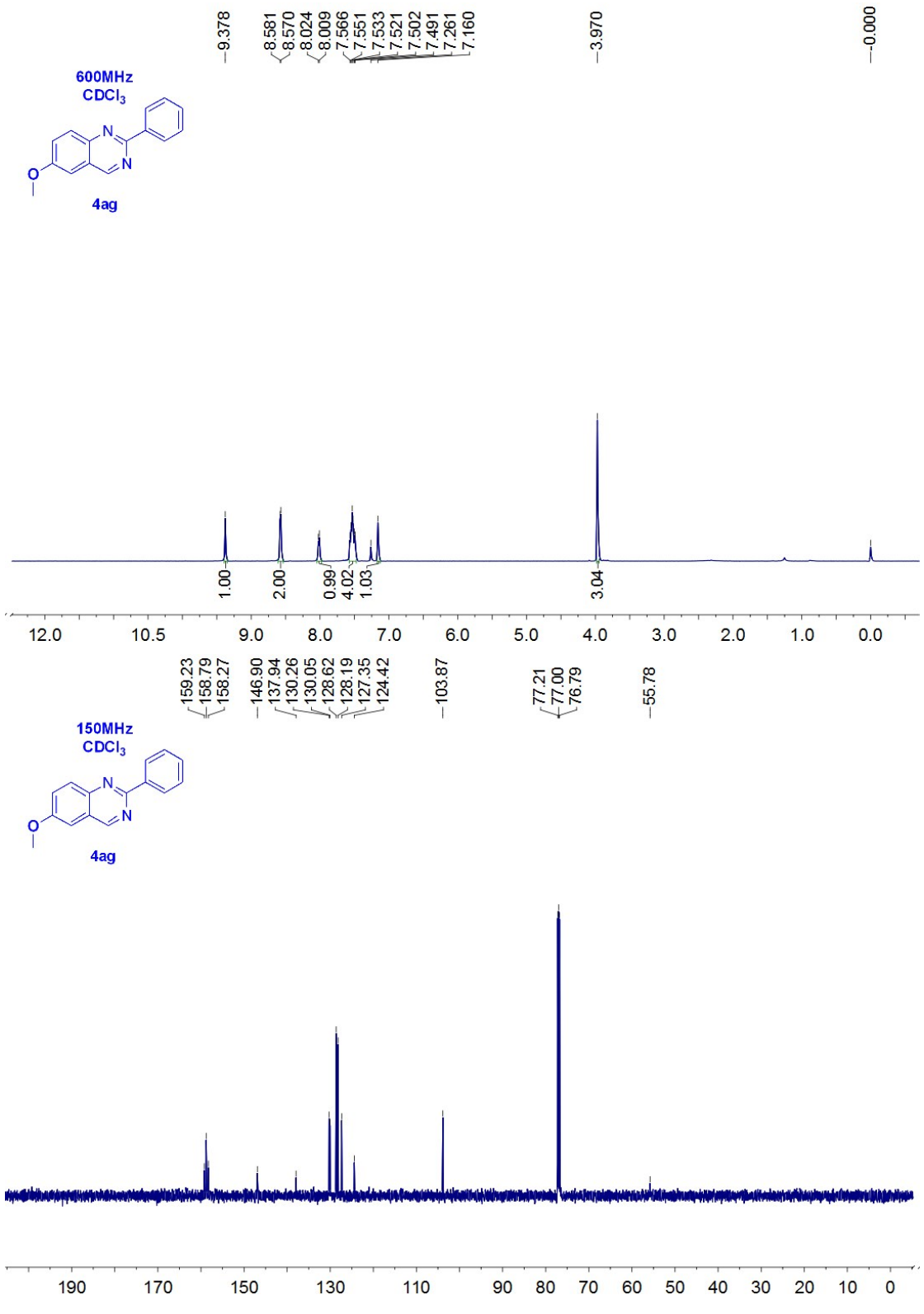
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7.533
7.521
7.502
7.491
7.261
7.160
3.970
0.000
600MHz
CDCl3
4ag
1.00
2.00
0.99
4.02
1.03
3.04
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
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158.79
158.27
146.90
137.94
130.26
130.05
128.62
128.19
127.35
124.42
103.87
77.21
77.00
76.79
55.78
150MHz
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130
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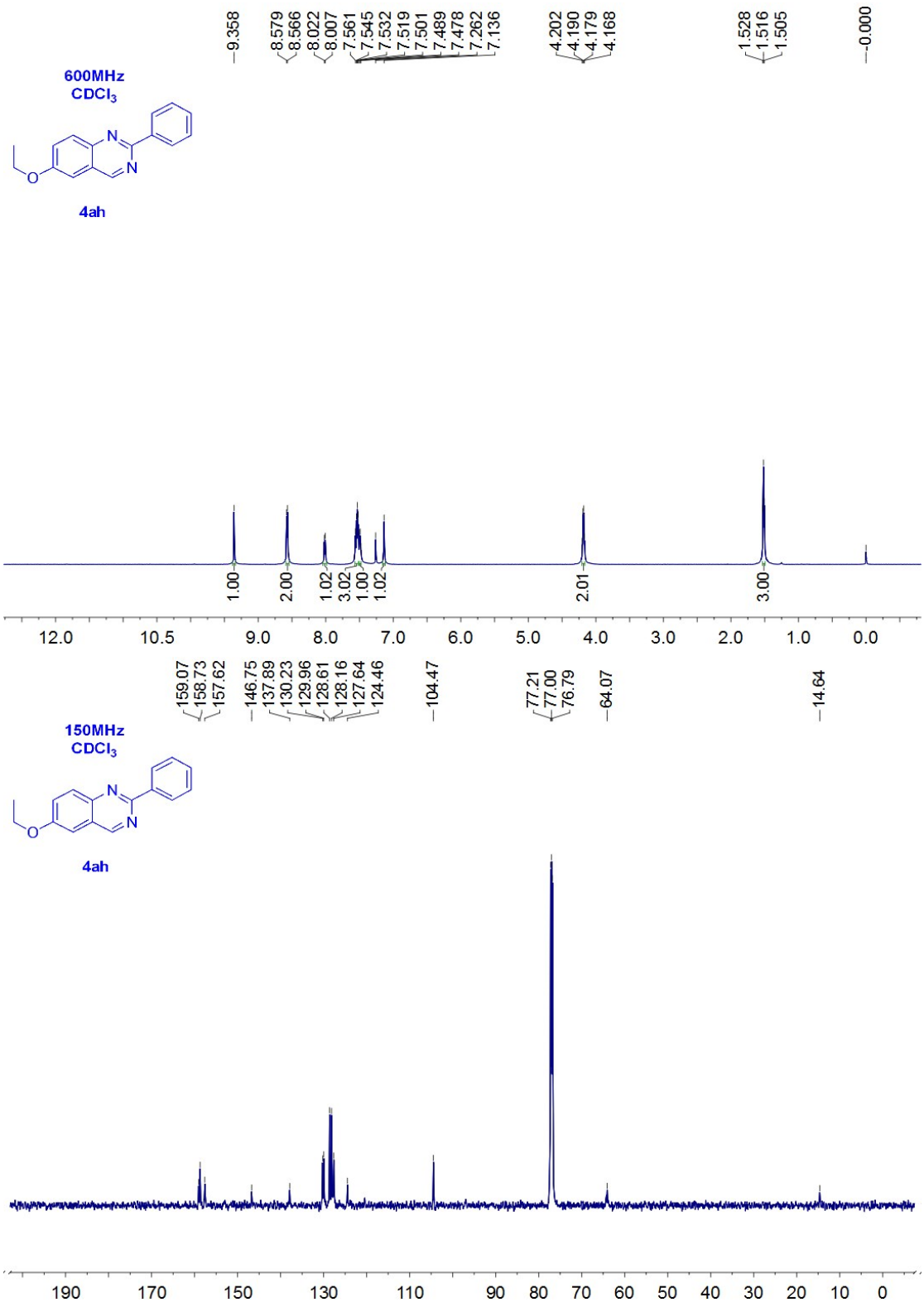
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8.566
8.022
8.007
7.561
7.545
7.532
7.519
7.501
7.489
7.478
7.262
7.136
4.202
4.190
4.179
4.168
1.528
1.516
1.505
0.000
1.00
2.00
1.02
3.02
1.00
1.02
2.01
3.00
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
159.07
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137.89
130.23
129.96
128.61
128.16
127.64
124.46
104.47
77.21
77.00
76.79
64.07
14.64
150MHz
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170
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130
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70
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10
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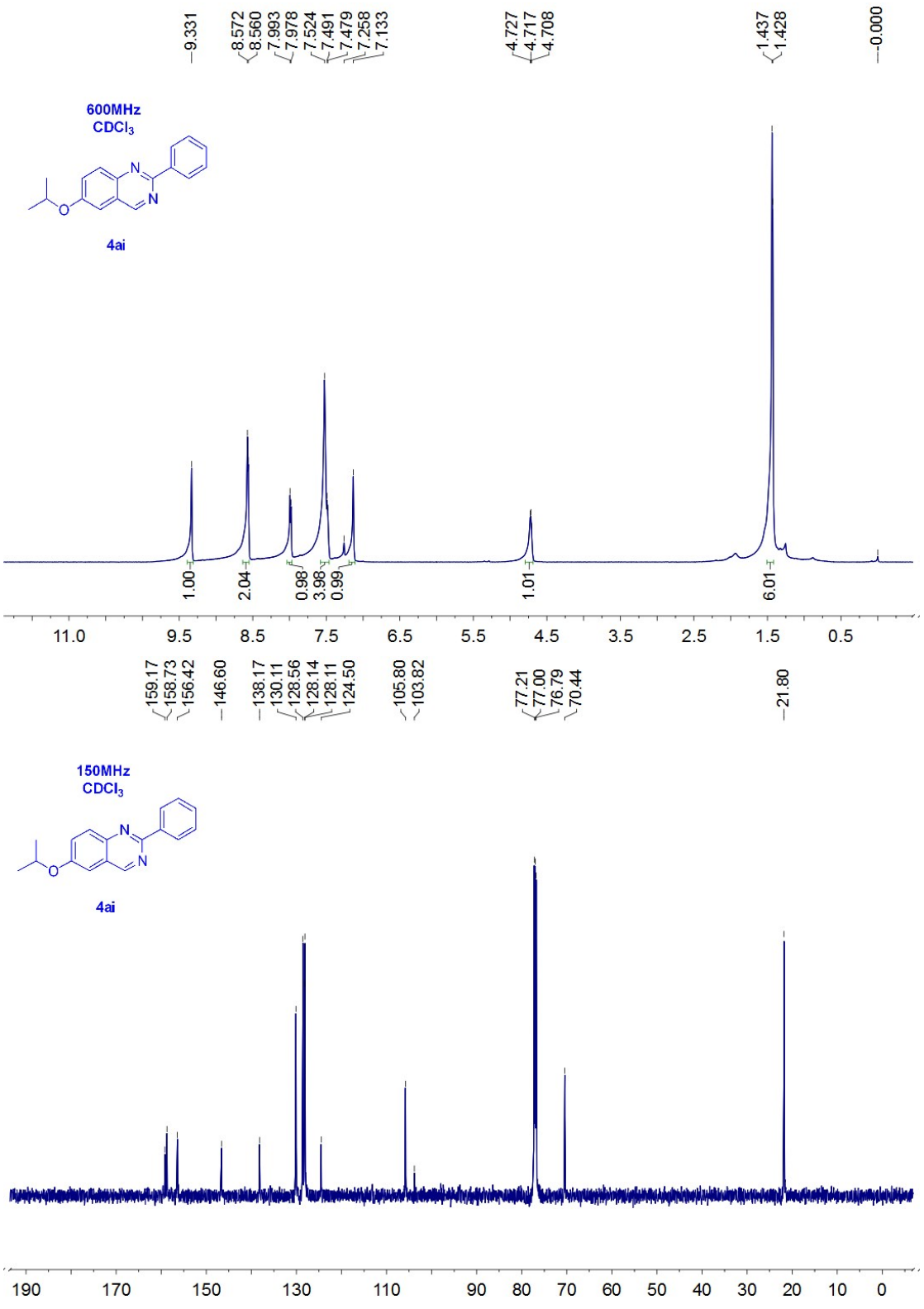
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7.491
7.479
7.258
7.133
4.727
4.717
4.708
1.437
1.428
0.000
1.00
2.04
0.98
3.98
0.99
1.01
6.01
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
159.17
158.73
156.42
146.60
138.17
130.11
128.56
128.14
128.11
124.50
105.80
103.82
77.21
77.00
76.79
70.44
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70
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30
20
10
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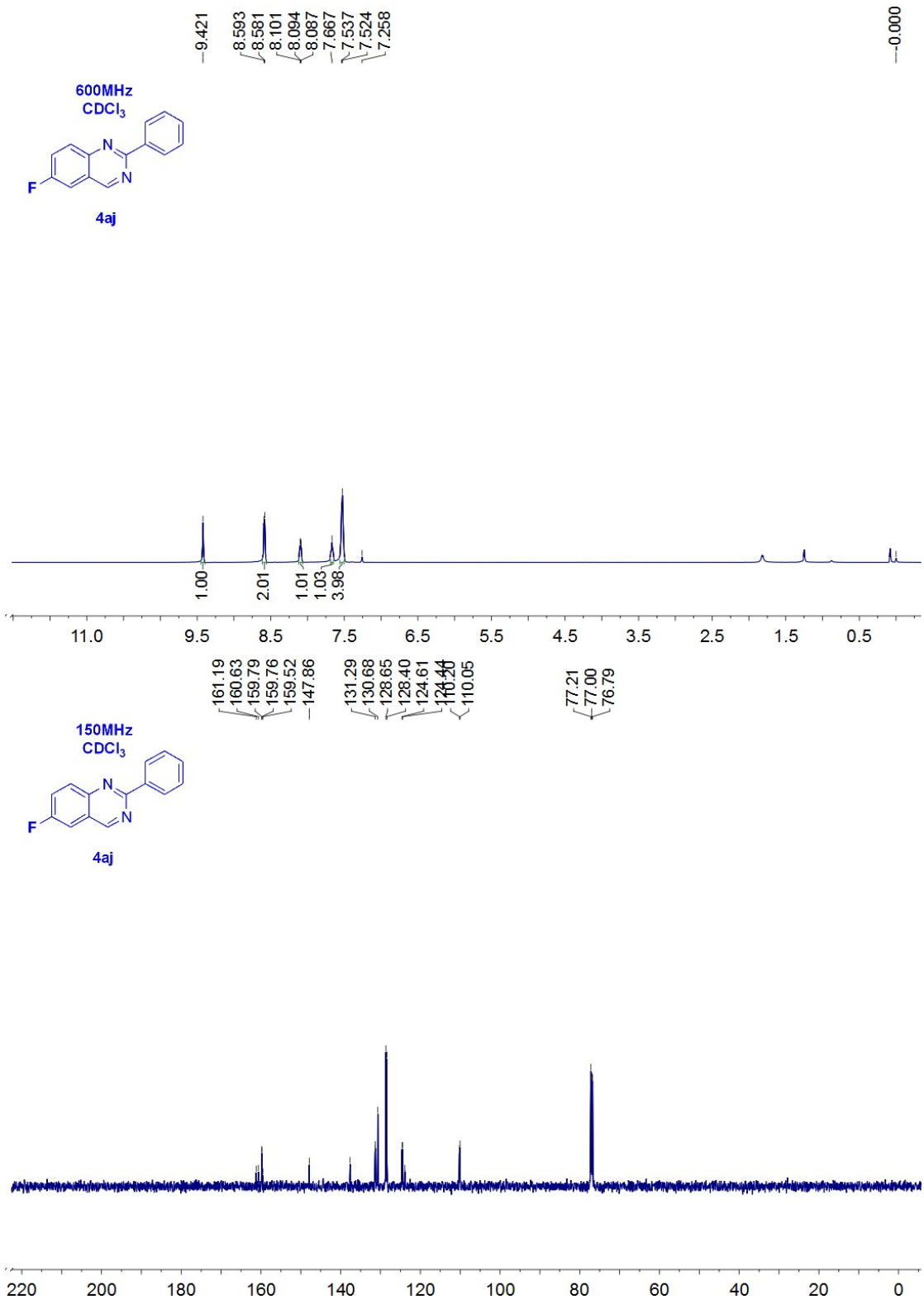
9.421
8.593
8.581
8.101
8.094
8.087
7.667
7.537
7.524
7.258
0.000
600MHz
CDCl3
4aj
1.00
2.01
1.01
1.03
3.98
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
161.19
160.63
159.79
159.76
159.52
147.86
131.29
130.68
128.65
128.40
124.61
110.05
77.21
77.00
76.79
150MHz
CDCl3
4aj
220
200
180
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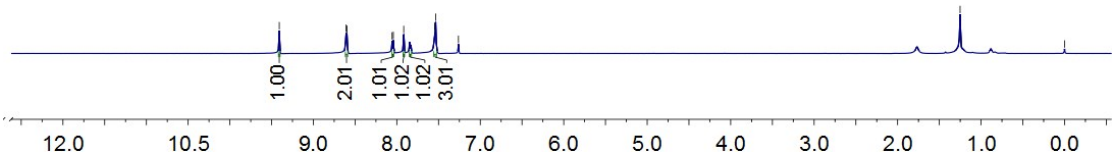
140
120
100
80
60
40
20
0

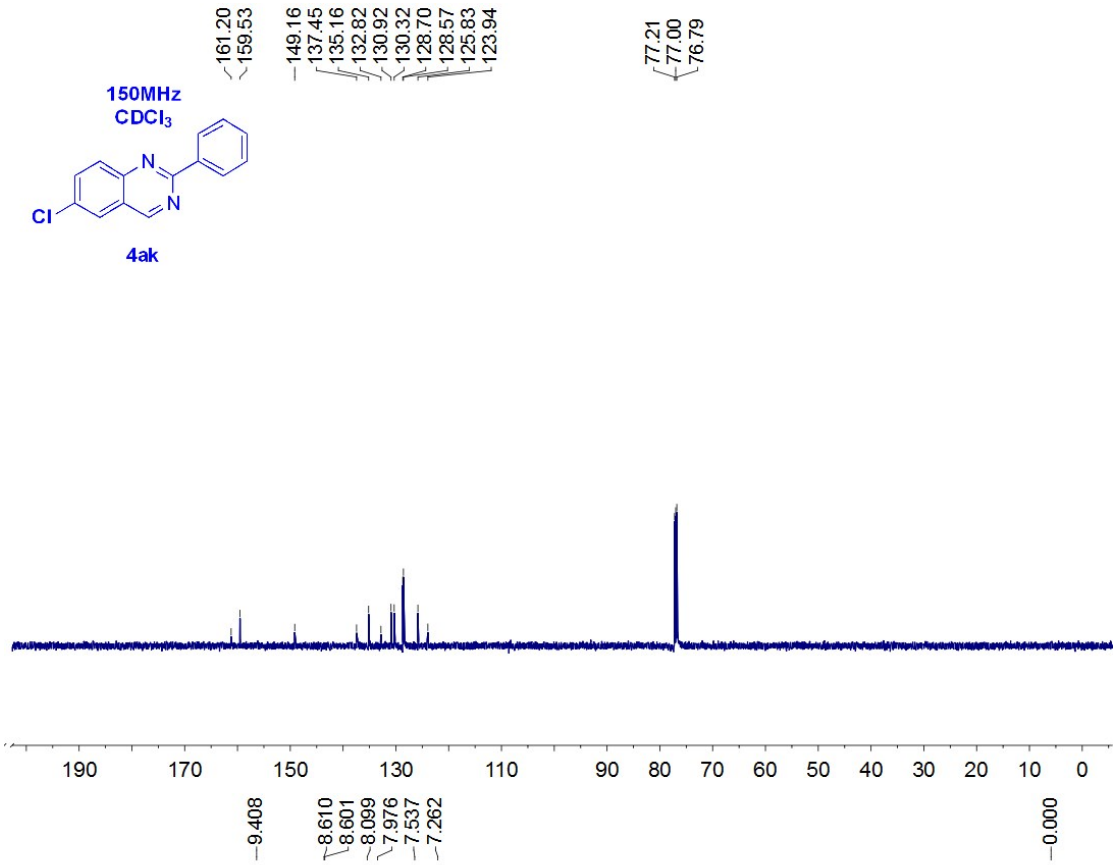
376MHz
$CDCl_3$

4aj

600MHz
$CDCl_3$

4ak

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149.16
137.45
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132.82
130.92
130.32
128.70
128.57
125.83
123.94
77.21
77.00
76.79
150MHz
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N
Cl
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190
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70
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10
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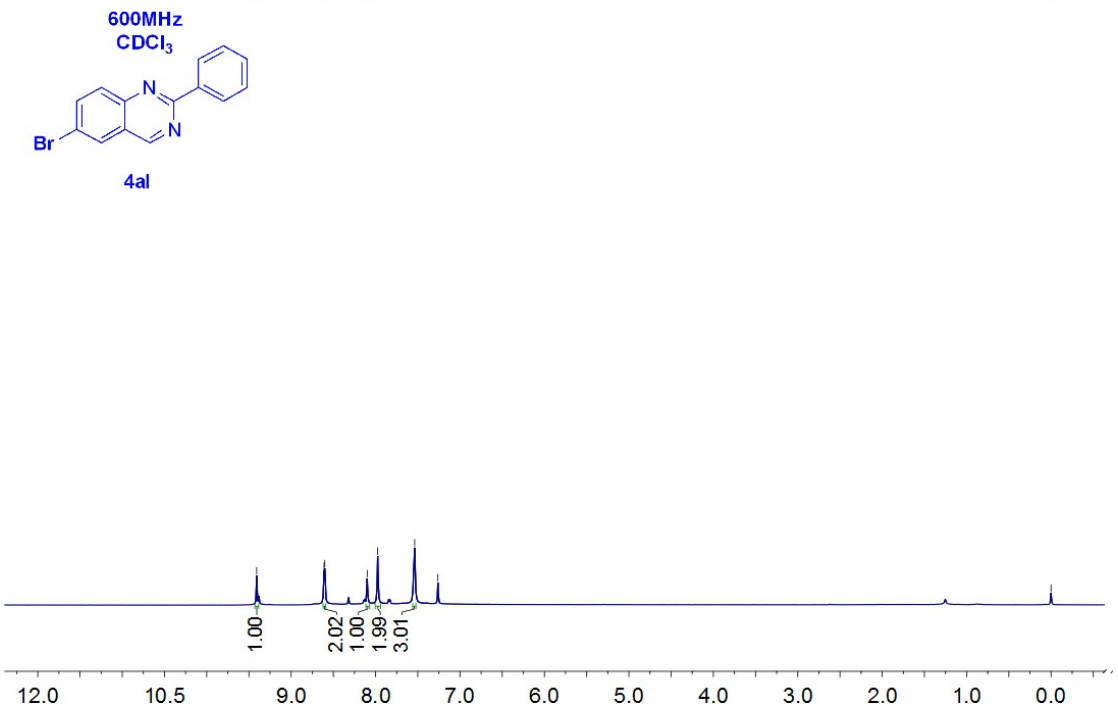
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8.099
7.976
7.537
7.262
0.000
600MHz
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N
N
Br
4al
1.00
2.02
1.00
1.99
3.01
12.0
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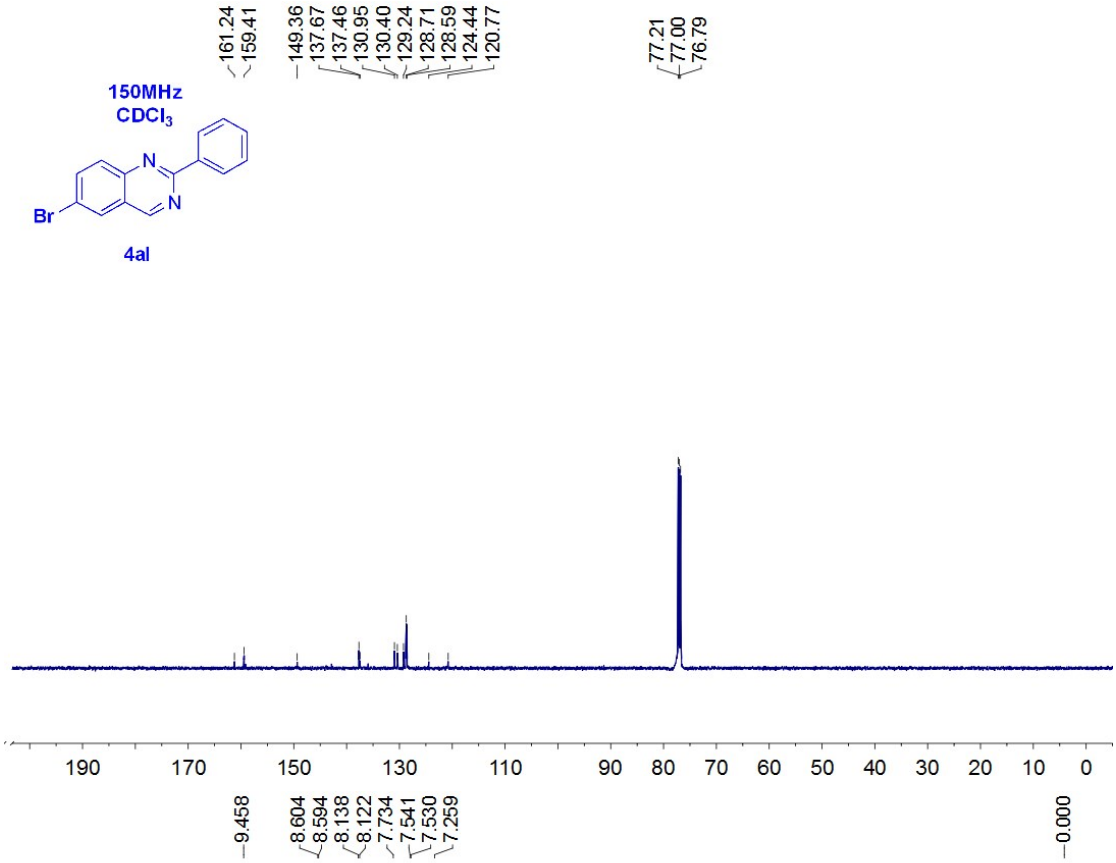
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130.40
129.24
128.71
128.59
124.44
120.77
77.21
77.00
76.79
150MHz
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Br
4al
190
170
150
130
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90
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70
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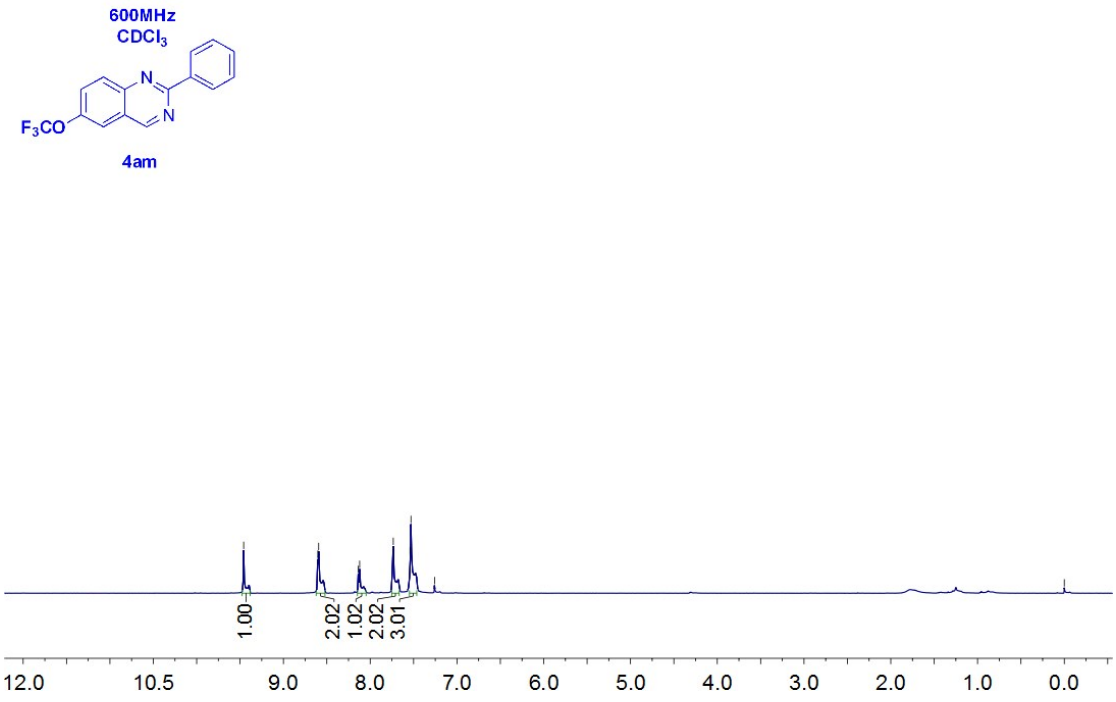
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8.604
8.594
8.138
8.122
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7.541
7.530
7.259
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600MHz
CDCl3
F3CO
4am
1.00
2.02
1.02
2.02
3.01
12.0
10.5
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7.0
6.0
5.0
4.0
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2.0
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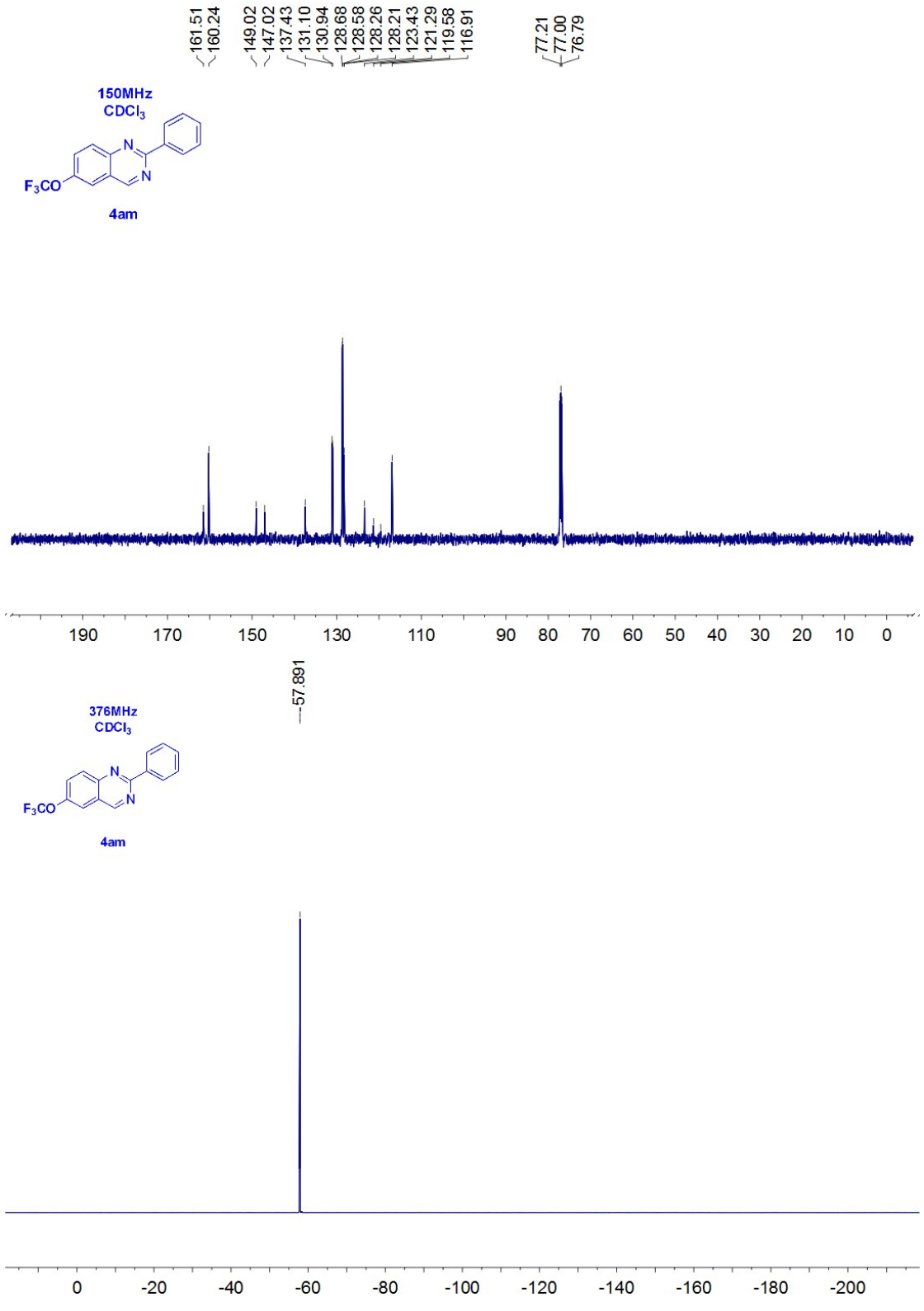
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160.24
149.02
147.02
137.43
131.10
130.94
128.68
128.58
128.26
128.21
123.43
121.29
119.58
116.91
77.21
77.00
76.79
150MHz
CDCl3
F3CO
4am
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-57.891
376MHz
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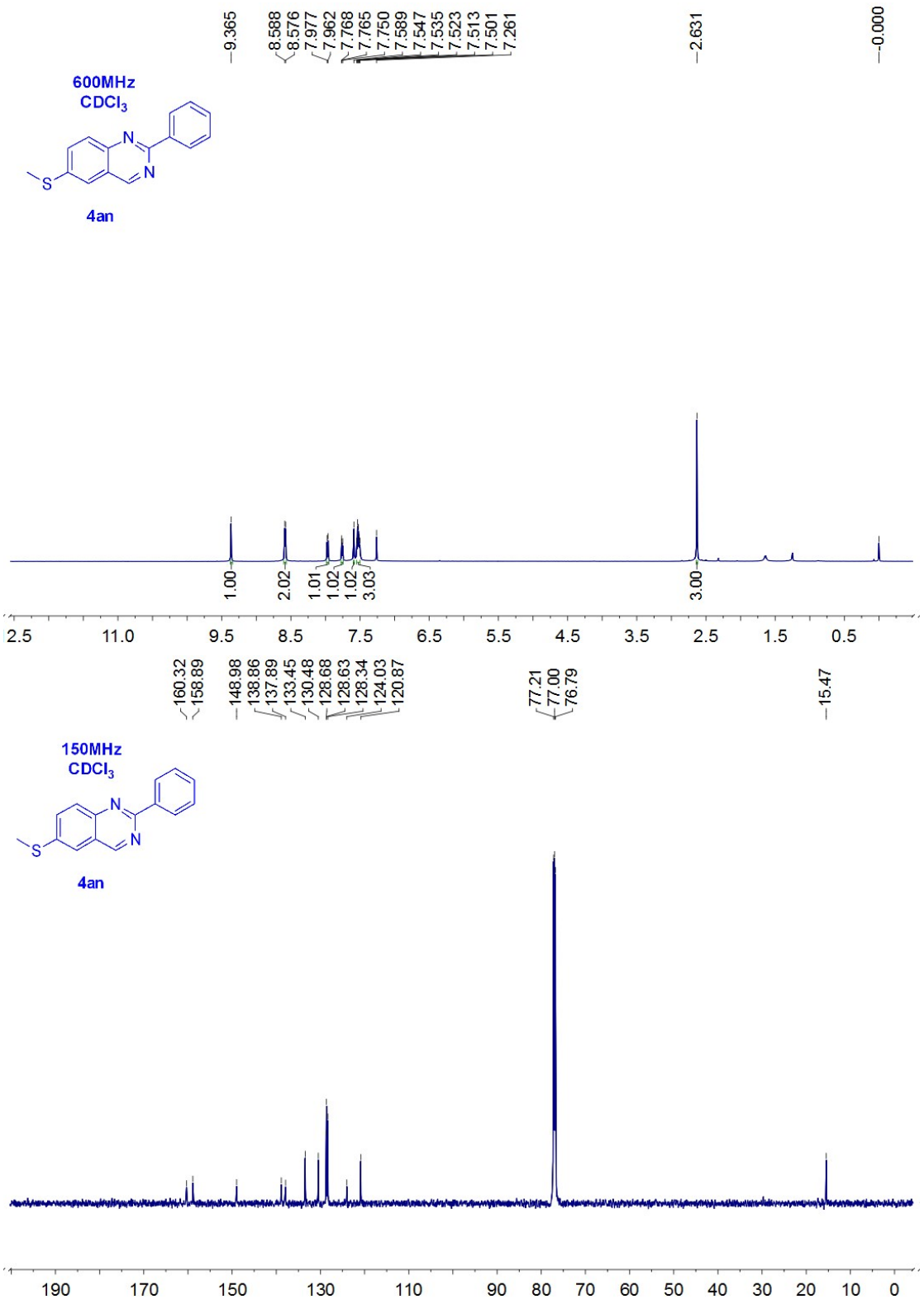
F3CO
4am
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200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4an
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8.576
7.977
7.962
7.768
7.765
7.750
7.589
7.547
7.535
7.523
7.513
7.501
7.261
2.631
0.000
1.00
2.02
1.01
1.02
1.02
3.03
3.00
2.5
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
160.32
158.89
148.98
138.86
137.89
133.45
130.48
128.68
128.63
128.34
124.03
120.87
77.21
77.00
76.79
15.47
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4an
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170
150
130
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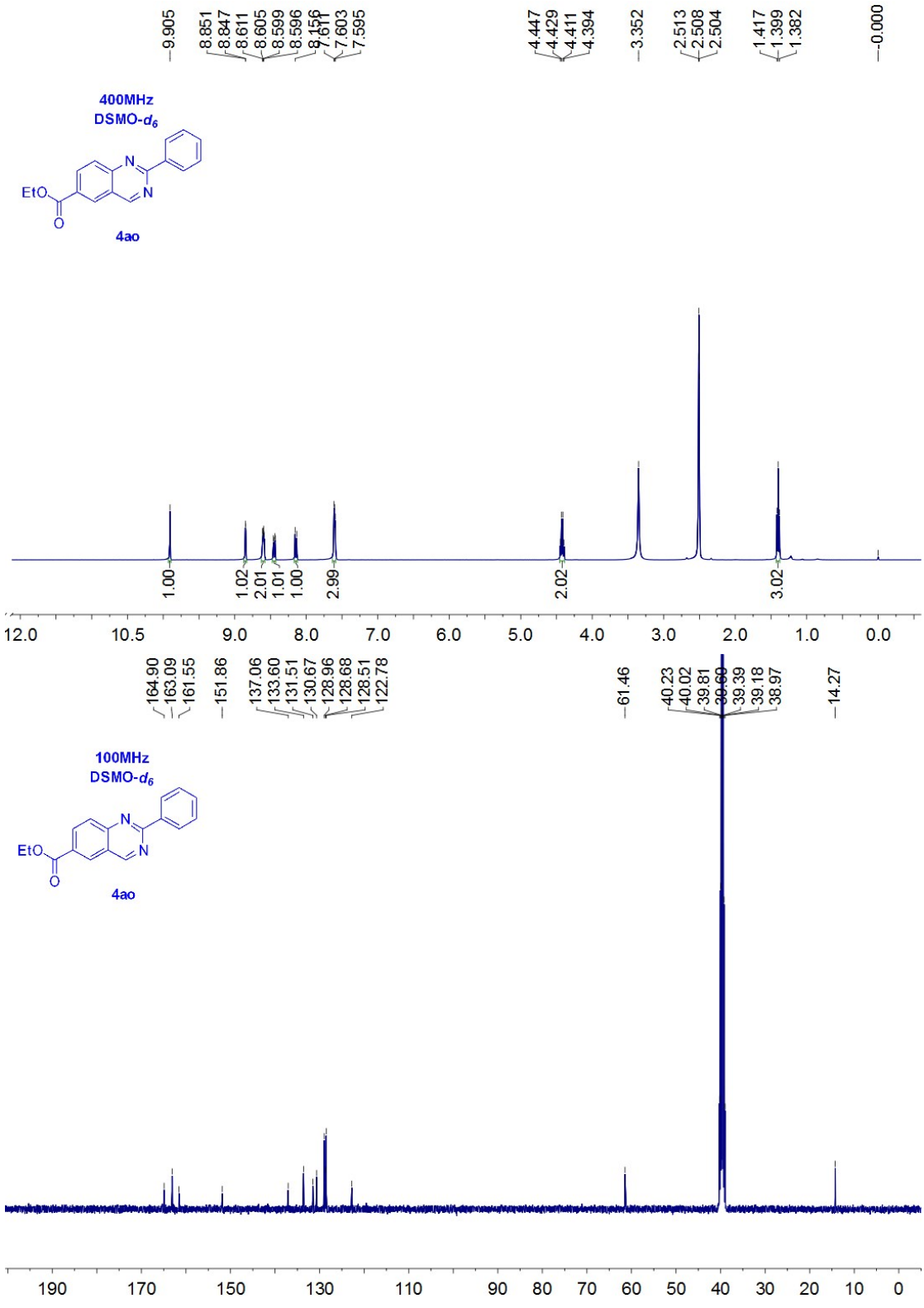
70
60
50
40
30
20
10
0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8.847
8.611
8.605
8.599
8.596
8.156
7.611
7.603
7.595
4.447
4.429
4.411
4.394
3.352
2.513
2.508
2.504
1.417
1.399
1.382
0.000
400MHz
DSMO-d6
EtO
O
N
N
4ao
1.00
1.02
2.01
1.01
1.00
2.99
2.02
3.02
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
164.90
163.09
161.55
151.86
137.06
133.60
131.51
130.67
128.96
128.68
128.51
122.78
61.46
40.23
40.02
39.81
39.60
39.39
39.18
38.97
14.27
100MHz
DSMO-d6
EtO
O
N
N
4ao
190
170
150
130
110
90
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70
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30
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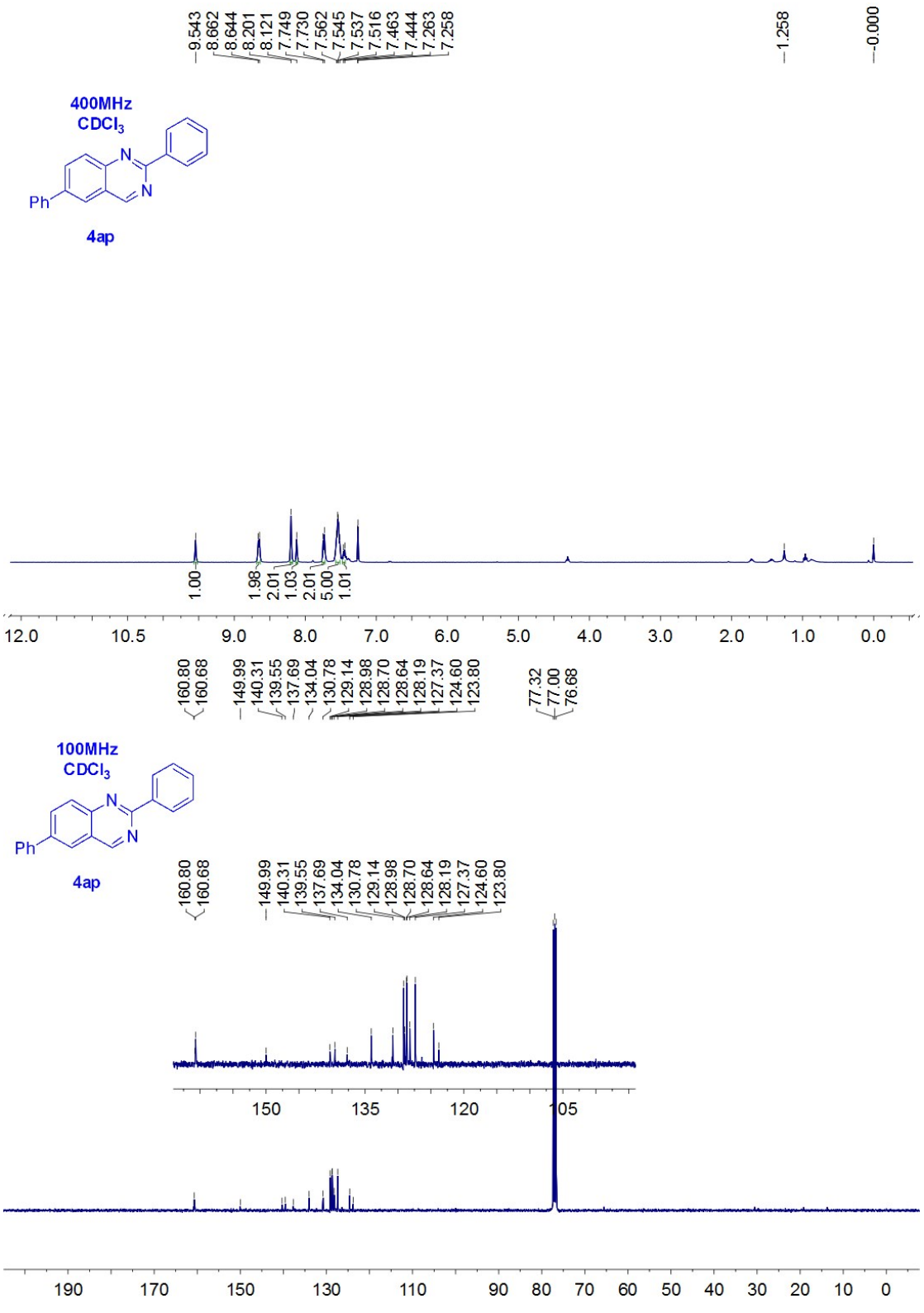
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8.644
8.201
8.121
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7.730
7.562
7.545
7.537
7.516
7.463
7.444
7.263
7.258
1.258
0.000
400MHz
CDCl3
Ph
4ap
1.00
1.98
2.01
1.03
2.01
5.00
1.01
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
160.80
160.68
149.99
140.31
139.55
137.69
134.04
130.78
129.14
128.98
128.70
128.64
128.19
127.37
124.60
123.80
77.32
77.00
76.68
100MHz
CDCl3
Ph
4ap
160.80
160.68
149.99
140.31
139.55
137.69
134.04
130.78
129.14
128.98
128.70
128.64
128.19
127.37
124.60
123.80
150
135
120
105
190
170
150
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80
70
60
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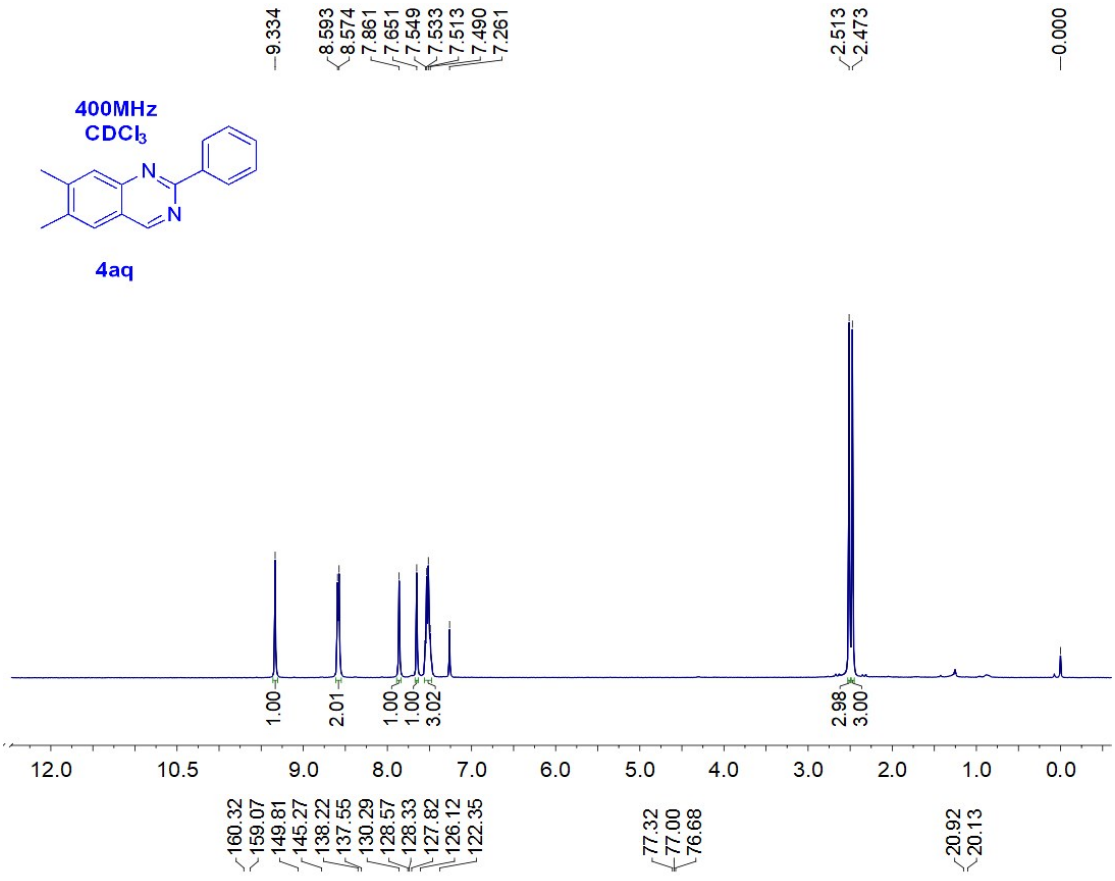
40
30
20
10
0


9.334
8.593
8.574
7.861
7.651
7.549
7.533
7.513
7.490
7.261
2.513
2.473
0.000
400MHz
CDCl3
4aq
1.00
2.01
1.00
1.00
3.02
2.98
3.00
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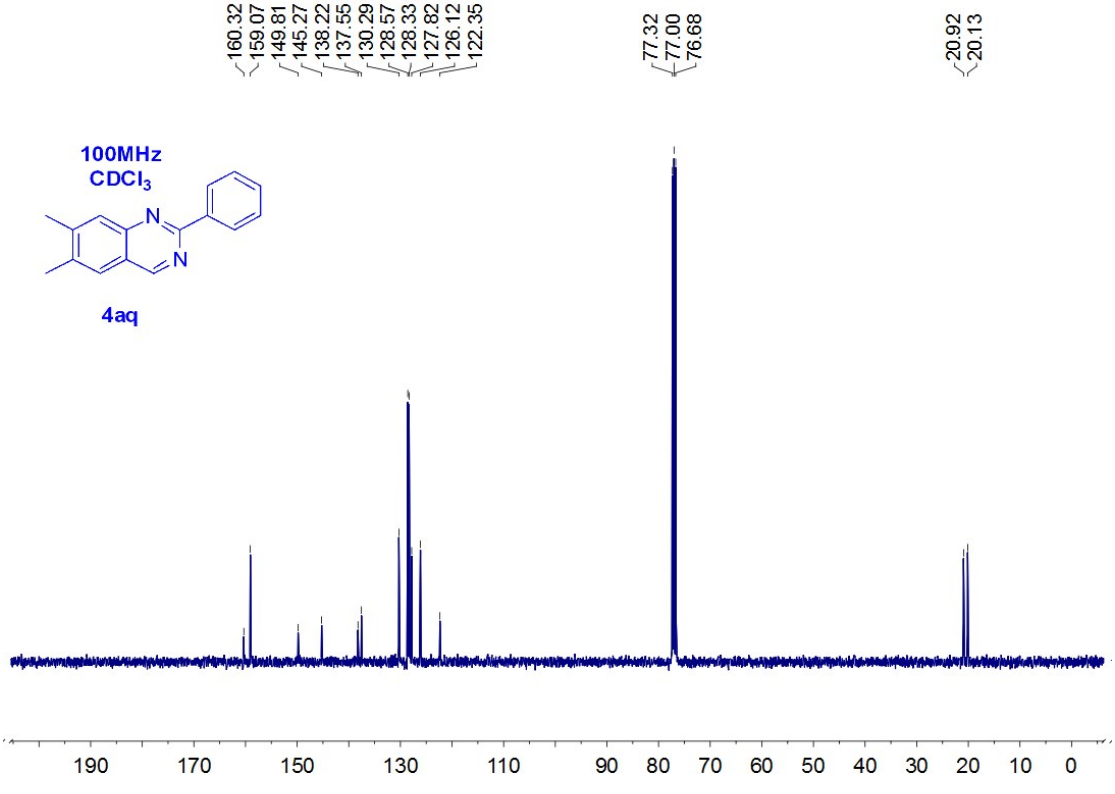
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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149.81
145.27
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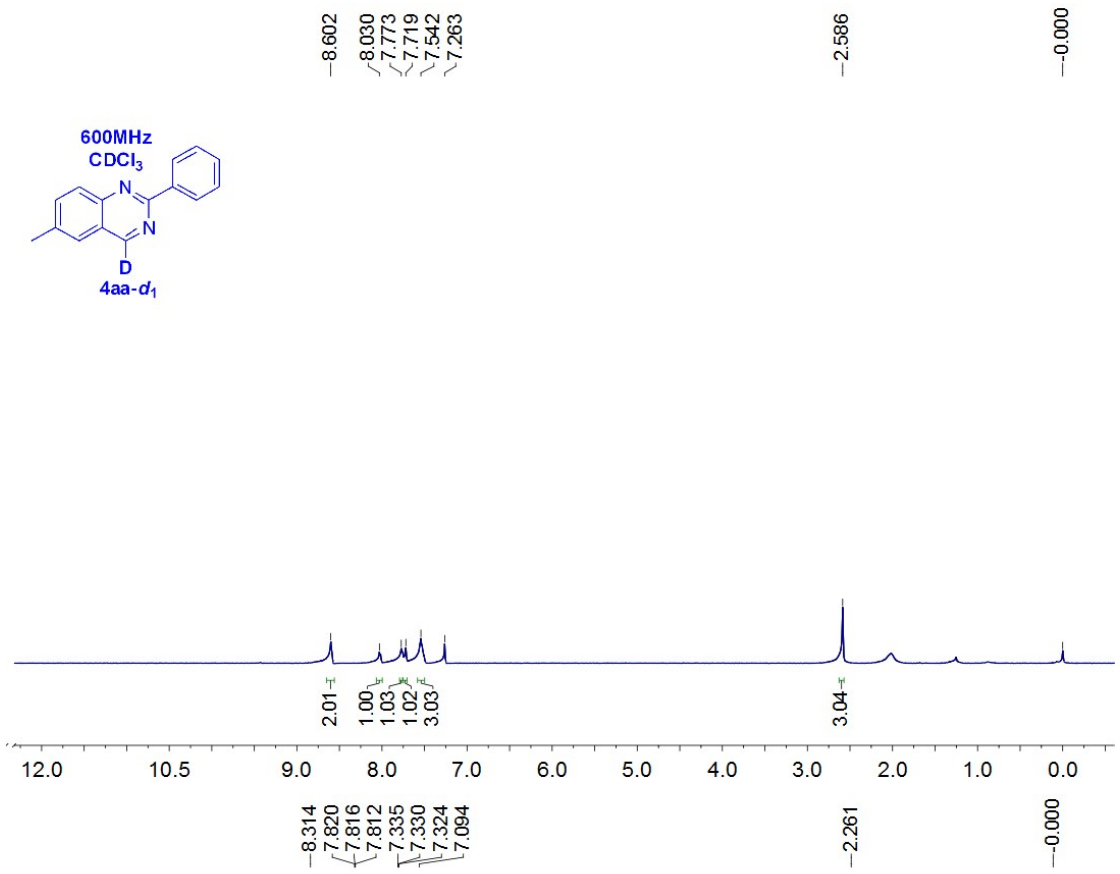
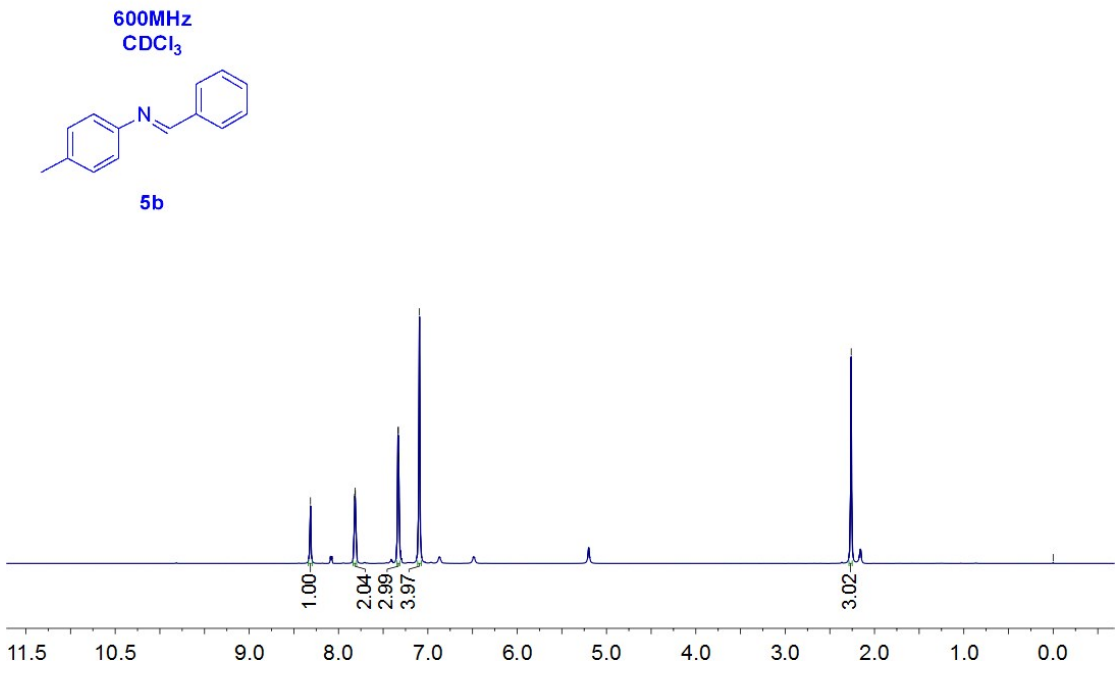
137.55
130.29
128.57
128.33
127.82
126.12
122.35
77.32
77.00
76.68
20.92
20.13
100MHz
CDCl3
4aq
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0


8.602
8.030
7.773
7.719
7.542
7.263
2.586
0.000
600MHz
CDCl3
N
N
D
4aa-d1
2.01
1.00
1.03
1.02
3.03
3.04
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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7.335
7.330
7.324
7.094
2.261
0.000
600MHz
CDCl3
N
5b
1.00
2.04
2.99
3.97
3.02
11.5
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9.0
8.0
7.0
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3.0
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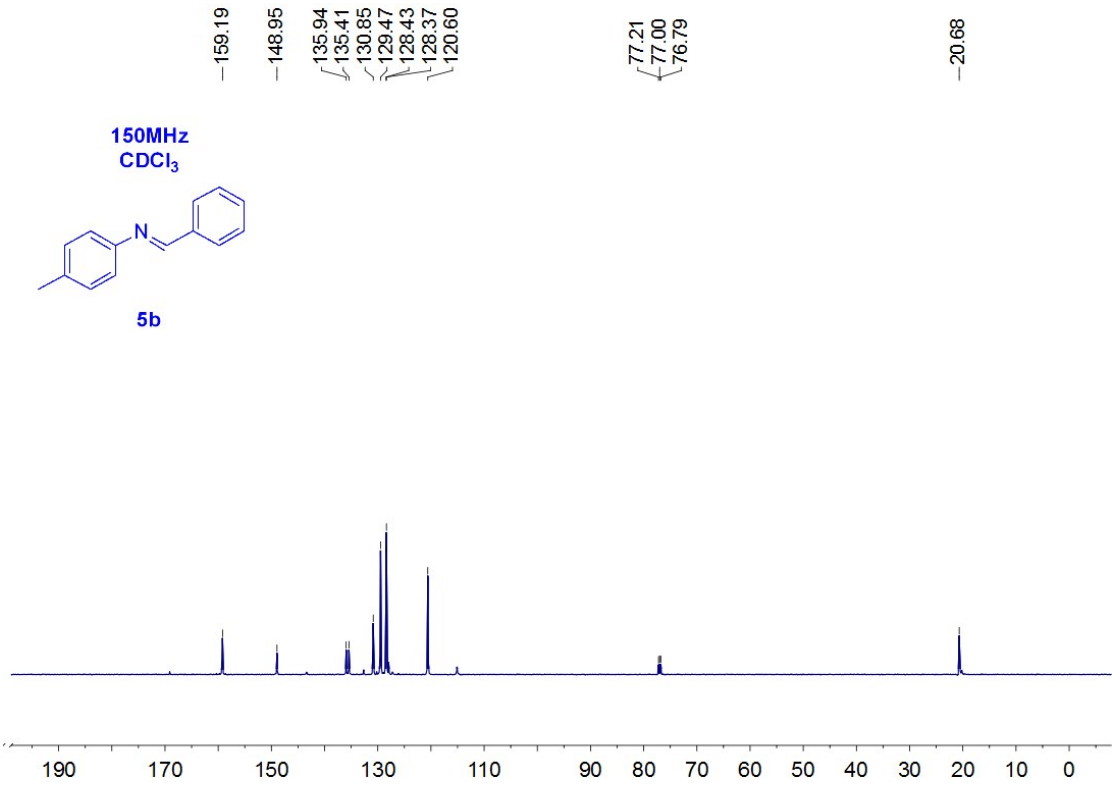
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77.21
77.00
76.79
20.68
150MHz
CDCl3
N
5b
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0