

Supporting Information for

PhNCO-Enabled Synthesis of Secondary Amides from *N*-(2-aminophenyl)benzamides

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Table of Contents

1	General information	3
2	General procedure to synthesis of starting materials (1a-t)	4
3	Further transformations	4-5
4	Spectral characterization	5-18
5	References	18-19
6	^1H and ^{13}C spectra	20-96

1. General information

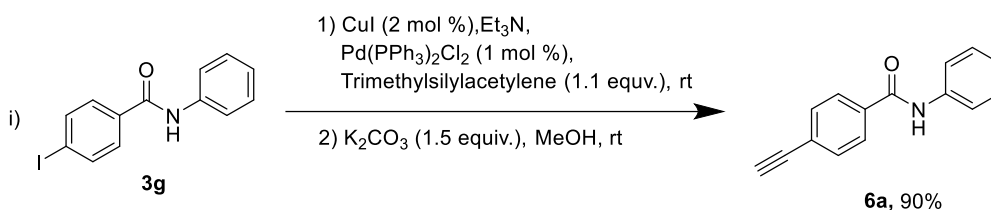
All chemicals were purchased from commercial providers (Sigma Aldrich, Alfa Aesar, TCI, and matrix scientific) and used directly without further purification, unless otherwise noted. Well cleaned and oven dried glassware was used for the experiments. Reaction was monitored by Thin Layer Chromatography (TLC), purchased as pre-coated with silica gel 60 F254 from Merck. Column chromatography was carried out using the silica gel 230-400 mesh (purchased from Merck) with mixture of ethyl acetate/hexane or hexane as the eluent. ^1H NMR spectra were recorded on 400 MHz, ^{13}C -NMR spectra were recorded on 100 MHz, Varian mercury spectrometer using CDCl_3 or $\text{DMSO}-d_6$ as solvent. The spectra were recorded and presented in chemical shifts (ppm) with tetramethylsilane (TMS) used as internal standard. Multiplicities were provided in s (singlet), d (doublet), t (triplet), q (quartet), br (broad single), m (multiplet), dd (doublet of doublet) and dt (doublet of triplet). Coupling constants (J) were reported in Hz. All the compounds were characterized by ESI mass on Thermo Finnigan (TRACEGC- POLARISQ) and HRMS (ESI+ mode) on JMS-700 spectrometer. Melting points were determined using Fargo instruments.

2. General procedure to synthesis of starting materials (1a-t) ^{1 2 3 4 5}



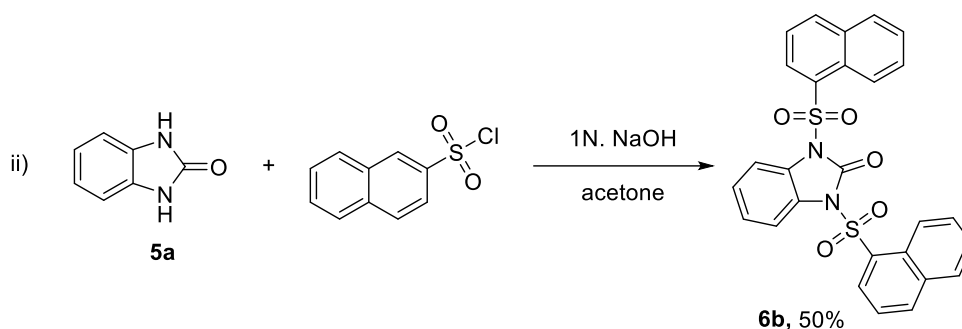
An oven-dried round-bottomed flask (100 mL) equipped with a stir bar was charged with amine (**1aa**) (5 mmol, 2.0 equiv.), triethylamine (1.0 equiv.) and dichloromethane (20 mL), placed under nitrogen, and subjected to three evacuation/backfilling cycles under high vacuum. Acyl chloride (**2aa**) (1.2 equiv.) was added dropwise to the reaction mixture with vigorous stirring at 0 °C, and the reaction mixture was stirred 2hr at reflux. After the indicated time, the reaction mixture was diluted with Et₂O (10 mL) and filtered. The organic layer was washed with HCl (1.0 N, 10 mL), brine (10 mL), and the organic layer was dried over anhydrous MgSO₄, filtered, and concentrated under vacuum. The crude product was purified by column chromatography (Hexane/EtOAc, 4/1, silica gel).

3. Further transformations ^{6,7}



In a dry round-bottomed flask, a solution of CuI (2.0 mol %), Pd(PPh₃)₂Cl₂ (1.0 mol %), and **3g** (0.2 mmol, 1.0 equiv.) in 300 μL of Et₃N was added to trimethylsilylacetylene (1.1 equiv.) dropwise under a nitrogen atmosphere. The mixture was stirred at room temperature until the starting materials were completely consumed. The reaction mixture was then filtered with a short ciliate and removed the solvent in vacuum. The resulting crude product was dissolved in 2 mL of methanol and added with K₂CO₃ (1.5 equiv.). The reaction mixture was diluted with Et₂O (2 mL) after stirred at room temperature for 2 h. After washing with water

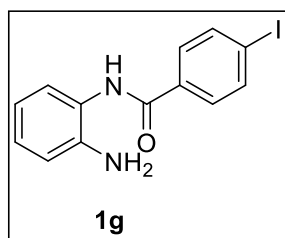
(15 mL) and drying over anhydrous Na_2SO_4 , the residue was concentrated under reduced pressure and purified by column chromatography to afford the **6a**.



1,3-dihydro-2H-benzo[d]imidazol-2-one (**5a**) (0.2 mmol) was suspended in acetone (2 ml) in a three-neck round bottomed flask fitted with an air condenser and two dropping funnels. In one dropping funnel was taken 1 N NaOH solution (2 ml) and in the other a solution of naphthalene-2-sulfonyl chloride (2.0 equiv.) in acetone. To the suspension of (**5a**) in acetone was added 1 N NaOH solution and naphthalene-2-sulfonyl chloride, dropwise with constant stirring. The temperature was maintained at 20 to 30°C. The mixture was stirred for one hour. Acetone was removed in vacuo, the residue washed with water and recrystallized from chloroform and methanol (3:1) to afford **6a**.

4. Spectral characterization

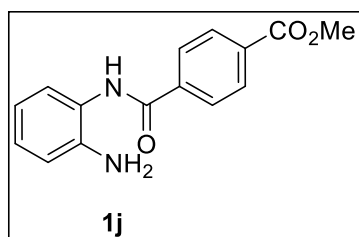
N-(2-aminophenyl)-4-iodobenzamide (**1g**): The title compound was synthesized



according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:4) and obtained as a yellow solid (1127 mg, 84%); Mp. 204- 206 °C; $^1\text{H-NMR}$ (400 MHz, DMSO-d_6) δ 9.69

(bs, 1H), 7.92-7.87 (m, 2H), 7.76-7.69 (m, 2H), 7.13 (d, $J = 4.0$ Hz, 1H), 6.96 (t, $J = 4.0$ Hz, 1H), 6.76 (d, $J = 8.0$ Hz, 1H), 6.57 (t, $J = 8.0$ Hz, 1H), 4.89 (bs, 2H); $^{13}\text{C-NMR}$ (100 MHz, DMSO-d_6) δ 164.9, 143.7, 137.6, 134.2, 131.7, 127.2, 130.4, 127.1, 123.4, 116.6, 116.5. HRMS (HR-EI) m/z : $[\text{M}]^+$ calcd for $\text{C}_{13}\text{H}_{11}\text{IN}_2\text{O}$, 337.9916; found, 337.9909.

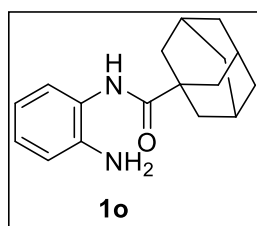
methyl 4-(2-aminophenyl)carbamoylbenzoate (1j): The title compound was



synthesized according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:4) and obtained as a yellow solid (1073 mg, 80%); Mp.

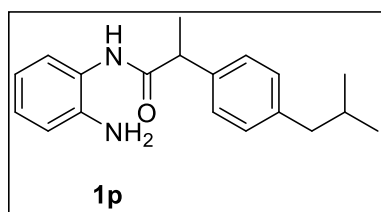
195–197 °C; $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 9.82 (bs, 1H), 8.07 (q, $J = 8.4$ Hz, 4H), 7.16 (d, $J = 8.0$ Hz, 1H), 6.97 (t, $J = 8.0$ Hz, 1H), 6.77 (d, $J = 8.0$ Hz, 1H), 6.58 (t, $J = 16.0$ Hz, 1H), 4.92 (bs, 2H), 3.88 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, $\text{DMSO-}d_6$) δ 166.2, 165.0, 143.7, 139.3, 132.3, 129.6, 129.5, 128.6, 127.2, 123.3, 116.6, 116.5, 52.8. HRMS (HR-El)m/z: $[\text{M}]^+$ calcd for $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_3$, 270.1004; found, 270.1001.

***N*-(2-aminophenyl)adamantane-1-carboxamide (1o):** The title compound was



synthesized according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:4) and obtained as a yellow solid (1087 mg, 81%); Mp. 161–163 °C; $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 8.61 (bs, 1H), 6.99 (dd, $J = 8.0$ Hz, 1.2Hz, 1H), 6.90 (t, $J = 8.0$ Hz, 1H), 6.72 (dd, $J = 8.0$ Hz, 0.8Hz, 1H), 6.54 (td, $J = 8.0$ Hz, 1.6Hz, 1H), 4.60 (bs, 2H), 2.00 (s, 3H), 1.90 (d, $J = 3.2$ Hz, 6H), 1.69 (s, 6H); $^{13}\text{C-NMR}$ (100 MHz, $\text{DMSO-}d_6$) δ 176.4, 143.4, 127.0, 126.5, 124.3, 116.9, 116.6, 41.0, 39.1, 36.6, 28.2. HRMS (HR-El)m/z: $[\text{M}]^+$ calcd for $\text{C}_{17}\text{H}_{22}\text{N}_2\text{O}$, 270.1732; found, 270.1728.

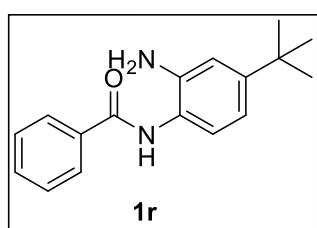
***N*-(2-aminophenyl)-2-(4-isobutylphenyl)propenamide (1p):** The title compound was



synthesized according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:4) and obtained as a yellow solid (939 mg, 70%); Mp.

176–178 °C; ¹H-NMR (400 MHz, DMSO- d₆) δ 9.21 (bs, 1H), 7.30 (d, *J* = 4.0 Hz, 2H), 7.10 (d, *J* = 4.0 Hz, 3H), 6.87 (t, *J* = 8.0 Hz, 1H), 6.68 (d, *J* = 8.0 Hz, 1H), 6.51 (t, *J* = 8.0 Hz, 1H), 4.70 (bs, 2H), 3.83 (d, *J* = 4.0 Hz, 1H), 2.40 (d, *J* = 8.0 Hz, 2H), 1.84- 1.75 (m, 1H), 1.39 (d, *J* = 8.0 Hz, 3H), 0.84 (d, *J* = 8.0 Hz, 6H); ¹³C-NMR (100 MHz, DMSO- d₆) δ 172.9, 142.3, 139.9, 139.8, 129.3, 127.4, 126.3, 125.6, 123.8, 116.7, 116.3, 45.4, 44.7, 30.1, 22.6, 19.1. HRMS (HR-EI)m/z: [M]⁺ calcd for C₁₉H₂₄N₂O, 296.1889; found, 296.1891.

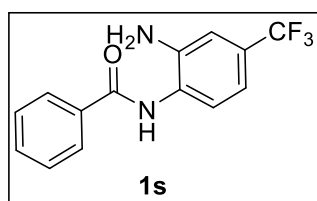
***N*-(2-amino-4-(tert-butyl)phenyl)benzamide (1r):** The title compound was



synthesized according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:4) and obtained as a yellow solid (1154 mg, 86%); Mp. 189–191 °C; ¹H-NMR

(400 MHz, DMSO- d₆) δ 9.60 (bs, 1H), 7.97 (d, *J* = 8.0 Hz, 2H), 7.57-7.49 (m, 3H), 7.08 (d, *J* = 8.0 Hz, 1H), 6.83 (d, *J* = 4.0 Hz, 1H), 6.64 (dd, *J* = 8.0 Hz, 4.0 Hz, 1H), 4.79 (bs, 2H), 1.25 (s, 9H); ¹³C-NMR (100 MHz, DMSO- d₆) δ 165.7, 149.4, 142.9, 135.1, 131.7, 128.7, 128.2, 126.6, 121.4, 113.9, 113.6, 34.5, 31. HRMS (HR-EI)m/z: [M]⁺ calcd for C₁₇H₂₀N₂O, 268.1576; found, 268.1569.

***N*-(2-amino-4-(trifluoromethyl)phenyl)benzamide (1s):** The title compound was

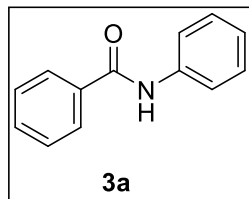


synthesized according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:4) and obtained as a yellow solid (1100 mg, 82%); Mp. 196–198 °C; ¹H-NMR (400

MHz, DMSO- d₆) δ 9.67 (bs, 1H), 7.98 (d, *J* = 8.0 Hz, 2H), 7.57-7.48 (m, 4H), 7.27 (dd, *J* = 8.0 Hz, 4.0 Hz, 1H), 6.86 (d, *J* = 8.0 Hz, 1H), 5.65 (bs, 2H); ¹³C-NMR (100 MHz, DMSO- d₆) δ 166.2, 147.3, 134.8, 132.0, 128.7, 128.3, 126.8, 124.3 (q, *J*_{C-F} = 241Hz), 123.9 (d,

$J_{C-F} = 37\text{Hz}$), 122.7, 116.0, 115.7 (d, $J_{C-F} = 32\text{Hz}$). HRMS (HR-EI)m/z: $[M]^+$ calcd for $C_{14}H_{11}F_3N_2O$, 280.0823; found, 280.0816.

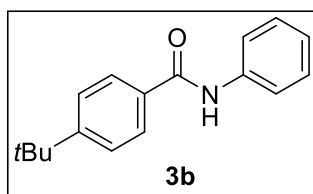
***N*-phenyl benzamide (3a)**⁸: The title compound was synthesized according to the



general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid (34 mg, 85%); ¹H-

NMR (400 MHz, DMSO- d_6) δ 10.22 (bs, 1H), 7.95-7.92 (m, 2H), 7.76 (d, $J = 7.6$ Hz, 2H), 7.59-7.49 (m, 3H), 7.33 (t, $J = 4.0$ Hz, 2H), 7.08 (t, $J = 7.6$ Hz, 1H); ¹³C-NMR (100 MHz, DMSO- d_6) δ 166.0, 139.6, 135.4, 132.0, 129.0, 128.8, 128.1, 124.1, 120.8.

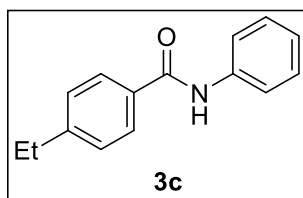
4-(*tert*-butyl)-*N*-phenyl benzamide (3b)⁸: The title compound was synthesized



according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white

solid (44 mg, 87%); ¹H-NMR (400 MHz, DMSO- d_6) δ 10.16 (bs, 1H), 7.88 (d, $J = 8.4$ Hz, 2H), 7.77 (d, $J = 7.6$ Hz, 2H), 7.54 (d, $J = 8.4$ Hz, 2H), 7.34 (t, $J = 7.6$ Hz, 2H), 7.08 (d, $J = 7.2$ Hz, 1H); ¹³C-NMR (100 MHz, DMSO- d_6) δ 165.9, 154.8, 139.7, 132.7, 129.0, 127.9, 125.6, 124.0, 120.7, 35.1, 31.4.

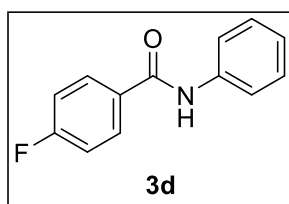
4-ethyl-*N*-phenylbenzamide (3c)⁹: The title compound was synthesized according to



the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid

(39 mg, 86%); ¹H-NMR (400 MHz, DMSO- d_6) δ 10.15 (bs, 1H), 7.88 (d, $J = 8.0$ Hz, 2H), 7.77 (d, $J = 8.4$ Hz, 2H), 7.37-7.32 (m, 4H), 7.09 (t, $J = 7.6$ Hz, 1H), 2.68 (q, $J = 7.6$ Hz, 2H), 1.21 (t, $J = 7.2$ Hz, 3H); ¹³C-NMR (100 MHz, DMSO- d_6) δ 165.4, 147.7, 139.3, 132.4, 128.6, 127.8, 127.7, 123.5, 120.3, 28.1, 15.4.

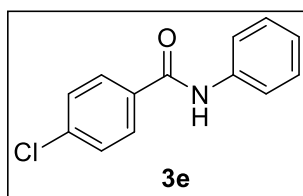
4-fluoro-*N*-phenylbenzamide (3d)⁸: The title compound was synthesized according



to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid

(40 mg, 94%); ¹H-NMR (400 MHz, DMSO- d₆) δ 10.25 (bs, 1H), 8.05-8.02 (m, 2H), 7.77-7.75 (m, 2H), 7.39-7.33 (m, 4H), 7.13-7.09 (m, 1H); ¹³C-NMR (100 MHz, DMSO-*d*₆) δ 165.7, 164.9 (d, *J*_{C-F} = 247.0Hz), 139.4, 131.8, 130.8, (d, *J*_{C-F} = 9.0Hz), 129.1, 124.2, 120.9, 115.8 (d, *J*_{C-F} = 21 Hz).

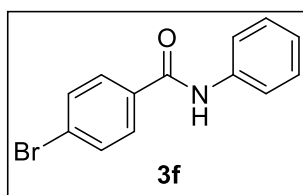
4-chloro-*N*-phenylbenzamide (3e)⁸: The title compound was synthesized according to



the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid

(39 mg, 85%); ¹H-NMR (400 MHz, DMSO- d₆) δ 10.30 (bs, 1H), 7.98 (d, *J* = 8.4 Hz, 2H), 7.76 (d, *J* = 7.2 Hz, 2H), 7.61 (d, *J* = 8.8 Hz, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.11 (t, *J* = 7.6 Hz, 1H); ¹³C-NMR (100 MHz, DMSO- d₆) δ 164, 139.0, 136.4, 133.6, 129.6, 128.6, 128.5, 123.9, 120.4.

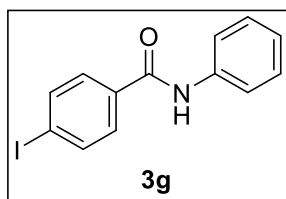
4-bromo-*N*-phenylbenzamide (3f)⁸: The title compound was synthesized according



to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid

(49 mg, 88%); ¹H-NMR (400 MHz, DMSO- d₆) δ 10.28 (bs, 1H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.75-7.72 (m, 4H), 7.34 (t, *J* = 8.0 Hz, 2H), 7.09 (t, *J* = 7.6 Hz, 1H); ¹³C-NMR (100 MHz, DMSO- d₆) δ 165.0, 139.4, 134.5, 131.8, 130.2, 129.1, 125.7, 124.3, 120.9.

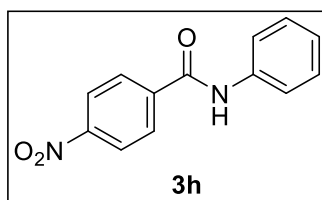
4-iodo-*N*-phenylbenzamide (3g)¹⁰: The title compound was synthesized according to



the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid (43 mg, 93%); ¹H-

NMR (400 MHz, DMSO- *d*₆) δ 10.27 (bs, 1H), 7.91-7.87 (m, 2H), 7.74-7.71 (m, 4H), 7.33 (t, *J* = 7.2 Hz, 2H), 7.09 (t, *J* = 8.0 Hz, 1H); ¹³C-NMR (100 MHz, DMSO- *d*₆) δ 165.2, 139.4, 137.7, 134.7, 131.8, 130.2, 130.0, 129.1, 124.2, 120.8, 99.7.

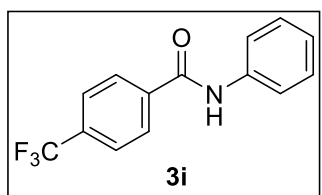
4-nitro-*N*-phenylbenzamide (3h)⁹: The title compound was synthesized according to



the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid

(42 mg, 87%); ¹H-NMR (400 MHz, DMSO- *d*₆) δ 10.60 (bs, 1H), 8.37 (d, *J* = 8.0 Hz, 2H), 8.19 (d, *J* = 12.0 Hz, 2H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.38 (t, *J* = 8.4 Hz, 2H), 7.14 (t, *J* = 7.2 Hz, 1H); ¹³C-NMR (100 MHz, DMSO- *d*₆) δ 164.3, 149.6, 141.1, 139.1, 129.6, 129.2, 124.6, 124.0, 120.9.

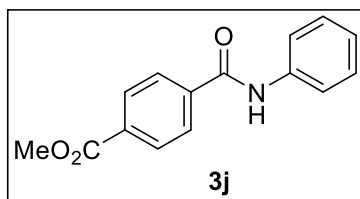
***N*-phenyl-4-(trifluoromethyl)benzamide (3i)**⁸: The title compound was synthesized



according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white

solid (38 mg, 71%); ¹H-NMR (400 MHz, DMSO- *d*₆) δ 10.55 (bs, 1H), 8.24 (d, *J* = 8.0 Hz, 2H), 8.00 (d, *J* = 8.0 Hz, 2H), 7.87 (d, *J* = 7.6 Hz, 2H), 7.46 (t, *J* = 8.0 Hz, 2H), 7.22 (t, *J* = 8.0 Hz, 1H); ¹³C-NMR (100 MHz, DMSO-*d*₆) δ 164.8, 139.2, 131.9, 131.6 (d, *J*_{C-F} = 32 Hz), 139.1, 129.0, 125.9 (q, *J*_{C-F} = 292 Hz), 125.9, 125.8, 124.5 (d, *J*_{C-F} = 7.0Hz), 120.9.

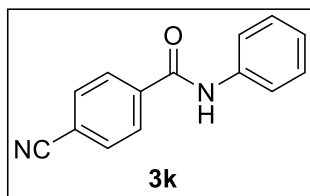
methyl 4-(phenyl carbamoyl)benzoate (3j)⁸: The title compound was synthesized



according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a

bright white solid (30 mg, 60%); ¹H-NMR (400 MHz, DMSO- d₆) δ 10.44 (bs, 1H), 8.09 (q, *J* = 8.4 Hz, 4H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.12 (t, *J* = 7.6 Hz, 1H); ¹³C-NMR (100 MHz, DMSO- d₆) δ 165.6, 164.6, 139.0, 138.8, 132.0, 129.1, 128.6, 128.0, 123.9, 120.4, 52.4.

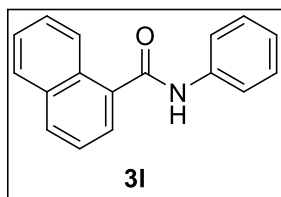
4-cyano-*N*-phenylbenzamide (3k)¹¹: The title compound was synthesized according



to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid

(36 mg, 80%); ¹H-NMR (400 MHz, DMSO- d₆) δ 10.47 (bs, 1H), 8.12-8.09 (m, 2H), 8.04-8.02 (m, 2H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.13 (t, *J* = 7.6 Hz, 1H); ¹³C-NMR (100 MHz, DMSO- d₆) δ 164.1, 139.0, 138.7, 132.5, 128.7, 128.5, 124.1, 120.4, 118.3, 113.8.

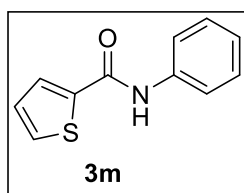
***N*-phenyl-1-naphthamide (3l)**⁹: The title compound was synthesized according to



the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid (22 mg, 45%); ¹H-

NMR (400 MHz, DMSO- d₆) δ 10.57 (bs, 1H), 8.20-8.18 (m, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 8.05-8.02 (m, 1H), 7.82 (d, *J* = 7.6 Hz, 2H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.64-7.58 (m, 3H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.13 (t, *J* = 7.2 Hz, 1H); ¹³C-NMR (100 MHz, DMSO- d₆) δ 167.2, 139.3, 134.7, 133.1, 130.0, 129.6, 128.7, 128.3, 126.9, 126.3, 125.4, 125.1, 125.0, 123.6, 119.8.

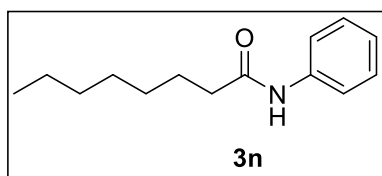
***N*-phenylthiophene-2-carboxamide (3m)**⁸: The title compound was synthesized



according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid (37

mg, 91%); ¹H-NMR (400 MHz, DMSO- d₆) δ 10.19 (bs, 1H), 8.00 (dd, *J* = 3.6 Hz, 0.8 Hz, 1H), 7.84 (dd, *J* = 4.8 Hz, 1.2 Hz, 1H), 7.70 (d, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 2H), 7.21 (q, *J* = 3.6 Hz, 1H), 7.08 (t, *J* = 7.2 Hz, 1H); ¹³C-NMR (100 MHz, DMSO- d₆) δ 160.0, 140.1, 138.7, 131.9, 129.2, 128.7, 128.1, 123.9, 120.5.

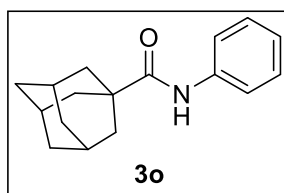
***N*-phenyloctanamide (3n)**⁹: The title compound was synthesized according to the general



procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid (26 mg, 80%);

¹H-NMR (400 MHz, DMSO- d₆) δ 9.82 (bs, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.27 (t, *J* = 7.2 Hz, 2H), 7.01 (t, *J* = 6.0 Hz, 1H), 2.28 (t, *J* = 7.6 Hz, 2H), 1.58 (t, *J* = 7.2 Hz, 2H), 1.34-1.22 (m, 8H), 0.86 (t, *J* = 6.8 Hz, 3H); ¹³C-NMR (100 MHz, DMSO- d₆) δ 171.7, 139.8, 129.0, 123.3, 119.4, 36.8, 31.6, 29.1, 28.9, 25.6, 22.5, 14.4.

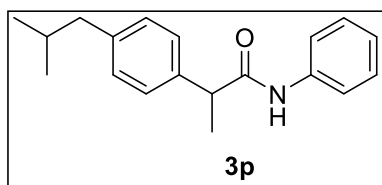
***N*-phenyladamantane-1-carboxamide (3o)**: The title compound was synthesized



according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid

(27 mg, 52%); Mp. 132–134 °C; ¹H-NMR (400 MHz, DMSO- d₆) δ 9.07 (bs, 1H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.27 (t, *J* = 8.0 Hz, 2H), 7.02 (t, *J* = 8.0 Hz, 1H), 2.02-1.90 (m, 9H), 1.71-1.70 (m, 6H); ¹³C-NMR (100 MHz, DMSO- d₆) δ 176.3, 139.8, 128.8, 123.5, 120.6, 41.3, 38.7, 36.5, 28.1. HRMS (HR-EI)m/z: [M]⁺ calcd for C₁₇H₂₁NO, 255.1623; found, 255.1621.

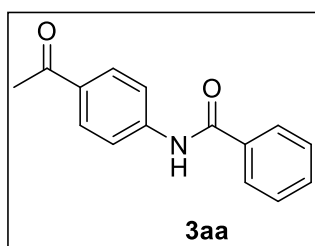
2-(4-isobutylphenyl)-*N*-phenylpropanamide (3p): The title compound was



synthesized according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane

(1:19) and obtained as a bright white solid (39 mg, 70%); Mp. 167–169 °C; ¹H-NMR (400 MHz, DMSO-*d*₆) δ 10.00 (bs, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.29–7.24 (m, 4H), 7.10 (d, *J* = 8.0 Hz, 2H), 7.01 (t, *J* = 4.0 Hz, 1H), 3.79 (q, *J* = 8.0 Hz, 1H), 2.39 (d, *J* = 8.0 Hz, 2H), 1.82–1.76 (m, 1H), 1.39 (d, *J* = 8.0 Hz, 3H), 0.84 (d, *J* = 8.0 Hz, 6H); ¹³C-NMR (100 MHz, DMSO-*d*₆) δ 172.4, 139.5, 139.3, 139.1, 128.9, 128.7, 127.0, 123.1, 119.1, 45.6, 44.2, 29.6, 22.2, 18.6. HRMS (HR-EI)*m/z*: [*M*]⁺ calcd for C₁₉H₂₃NO, 281.1780; found, 281.1785.

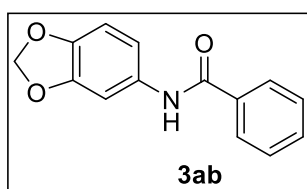
***N*-(4-acetylphenyl)benzamide (3aa)** ¹²: The title compound was synthesized



according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid (25 mg, 53%); ¹H-NMR (400 MHz, DMSO-*d*₆) δ 10.56

(bs, 1H), 7.99–7.93 (m, 6H), 7.62–7.53 (m, 3H), 2.55 (s, 3H); ¹³C-NMR (100 MHz, DMSO-*d*₆) δ 197.1, 166.4, 144.0, 135.0, 132.5, 132.3, 129.7, 128.9, 128.2, 119.9, 26.9.

***N*-(benzo[*d*][1,3]dioxol-5-yl)benzamide (3ab)** ¹³: The title compound was

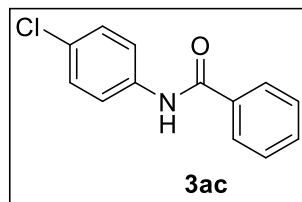


synthesized according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a

bright white solid (28 mg, 57%); ¹H-NMR (400 MHz, DMSO-*d*₆) δ 10.11 (bs, 1H), 7.89–7.87 (m, 2H), 7.54–7.46 (m, 3H), 7.40 (d, *J* = 2.0 Hz, 1H), 7.15 (dd, *J* = 8.4 Hz, 2.0 Hz,

1H), 6.86 (d, $J = 8.0$ Hz, 1H), 5.97 (s, 2H); $^{13}\text{C-NMR}$ (100 MHz, $\text{DMSO-}d_6$) δ 165.8, 147.5, 143.8, 135.5, 134.0, 132.0, 128.9, 128.1, 113.9, 108.4, 103.0, 101.5.

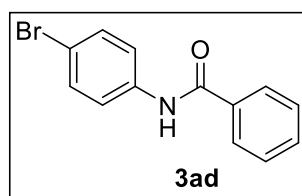
***N*-(4-chlorophenyl)benzamide (3ac)**⁸: The title compound was synthesized



according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid

(41 mg, 88%); $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 10.35 (s, 1H), 7.96- 7.93 (m, 2H), 7.82 (dt, $J = 8.7$ Hz, 3.4 Hz, 2H), 7.62- 7.52 (m, 3H), 7.41 (dt, $J = 8.8$ Hz, 3.2 Hz, 2H); $^{13}\text{C-NMR}$ (100 MHz, $\text{DMSO-}d_6$) δ 166.1, 138.6, 135.2, 132.1, 129.0, 128.9, 128.1, 127.7, 122.3.

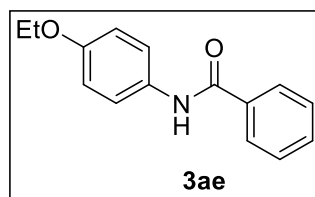
***N*-(4-bromophenyl)benzamide (3ad)**⁸: The title compound was synthesized according



to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white solid

(50 mg, 90%); $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 10.35 (s, 1H), 7.96- 7.93 (m, 2H), 7.78 (dd, $J = 8.9$ Hz, 1.6 Hz, 2H), 7.60 (tt, $J = 7.2$ Hz, 1.4 Hz, 1H), 7.55- 7.51 (m, 4H). $^{13}\text{C-NMR}$ (100 MHz, $\text{DMSO-}d_6$) δ 166.1, 139.0, 135.1, 132.2, 131.9, 128.9, 128.1, 122.6, 115.8.

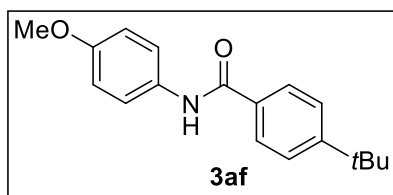
***N*-(4-ethoxyphenyl)benzamide (3ae)**¹⁴: The title compound was synthesized



according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a bright white

solid (34 mg, 70%); $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 10.09 (s, 1H), 7.95- 7.92 (m, 2H), 7.65 (dt, $J = 9.0$ Hz, 3.4 Hz, 2H), 7.60- 7.49 (m, 3H), 6.91 (dt, $J = 9.1$ Hz, 3.4 Hz, 2H), 4.01 (q, $J = 7.0$ Hz, 2H), 1.32 (t, $J = 6.9$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, $\text{DMSO-}d_6$) δ 165.5, 155.2, 135.5, 132.5, 131.8, 128.8, 128.0, 122.4, 114.7, 63.5.

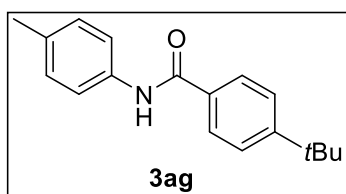
4-(tert-butyl)-N-(4-methoxyphenyl)benzamide (3af): The title compound was



synthesized according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl

acetate/hexane (1:19) and obtained as a bright white solid (45 mg, 80%); Mp. 139–141 °C; ¹H-NMR (400 MHz, DMSO-*d*₆) δ 10.01 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.64 (d, *J* = 8.9 Hz, 2H), 7.51 (d, *J* = 8.3 Hz, 2H), 6.90 (dt, *J* = 8.9 Hz, 3.3 Hz, 2H), 3.72 (s, 3H), 1.3 (s, 9H); ¹³C-NMR (100 MHz, DMSO-*d*₆) δ 165.5, 155.9, 154.6, 132.77, 132.75, 127.8, 125.5, 122.3, 114.1, 55.6, 35.1, 31.2. HRMS (HR-El)m/z: [M]⁺ calcd for C₁₈H₂₁NO₂, 283.1572; found, 283.1569.

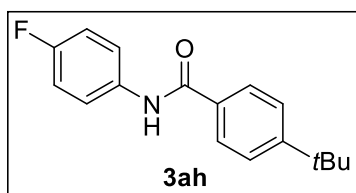
4-(tert-butyl)-N-(p-tolyl)benzamide (3ag): The title compound was synthesized



according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane (1:19) and obtained as a

bright white solid (51 mg, 95%); Mp. 128–130 °C; ¹H-NMR (400 MHz, DMSO-*d*₆) δ 10.07 (s, 1H), 7.87 (d, *J* = 8.2 Hz, 2H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.53 (d, *J* = 8.3 Hz, 2H), 7.14 (d, *J* = 8.2 Hz, 2H), 2.207 (s, 3H), 1.32 (s, 9H); ¹³C-NMR (100 MHz, DMSO-*d*₆) δ 165.7, 154.7, 137.2, 132.9, 132.8, 129.4, 127.9, 125.6, 120.7, 35.1, 31.4, 20.9. HRMS (HR-El)m/z: [M]⁺ calcd for C₁₈H₂₁NO, 267.1623; found, 267.1621.

4-(tert-butyl)-N-(4-fluorophenyl)benzamide (3ah): The title compound was

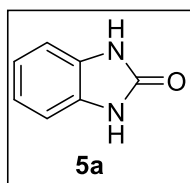


synthesized according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate/hexane

(1:19) and obtained as a bright white solid (50 mg, 92%); Mp. 134–137 °C; ¹H-NMR (400 MHz, DMSO-*d*₆) δ 10.22 (s, 1H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.78 (dd, *J* = 9.0 Hz, 4.0 Hz,

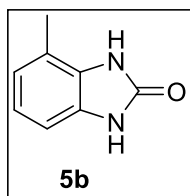
2H), 7.54 (d, $J = 8.4$ Hz, 2H), 7.18 (t, $J = 8.9$ Hz, 2H), 1.31 (s, 9H); $^{13}\text{C-NMR}$ (100 MHz, DMSO- d_6) δ 165.8, 159.8 (d, $J_{\text{C-F}} = 239$ Hz), 154.9, 136.1, 132.5, 127.9, 125.6, 122.5 (d, $J_{\text{C-F}} = 8.0$ Hz), 115.6 (d, $J_{\text{C-F}} = 22$ Hz), 35.1, 31.4. HRMS (HR-EI)m/z: $[\text{M}]^+$ calcd for $\text{C}_{17}\text{H}_{18}\text{FNO}$, 271.1372; found, 271.1374.

1,3-dihydro-2H-benzo[d]imidazol-2-one (5a) ¹⁵: The title compound was



synthesized according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate and obtained as a brown solid (23 mg, 86%); $^1\text{H-NMR}$ (400 MHz, DMSO- d_6) δ 10.54 (bs, 2H), 6.89 (s, 4H); $^{13}\text{C-NMR}$ (100 MHz, DMSO- d_6) δ 155.7, 130.1, 120.8, 108.9.

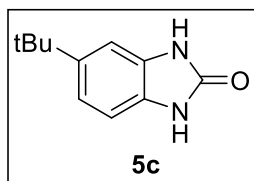
4-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (5b) ¹⁶: The title compound was



synthesized according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate and obtained as a brown solid (23 mg, 78%); $^1\text{H-NMR}$ (400 MHz, DMSO- d_6) δ 10.62 (bs, 1H), 10.50 (s, 1H), 6.84- 6.72 (m, 3H),

2.25 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, DMSO- d_6) δ 155.9, 129.7, 129.0, 122.0, 120.8, 118.6, 106.5, 16.6.

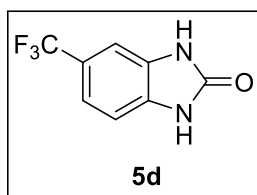
5-(tert-butyl)-1,3-dihydro-2H-benzo[d]imidazol-2-one (5c) ¹⁵: The title compound



was synthesized according to the general procedure. The crude mixture was purified using column chromatography by eluting with ethyl acetate and obtained as a brown solid (29 mg, 76%);

$^1\text{H-NMR}$ (400 MHz, DMSO- d_6) δ 10.40 (bs, 2H), 6.95-6.80 (m, 3H), 1.24 (s, 9H); $^{13}\text{C-NMR}$ (100 MHz, DMSO- d_6) δ 156.0, 143.6, 130.0, 127.8, 117.6, 108.3, 105.38, 34.7, 32.0.

5-(trifluoromethyl)-1,3-dihydro-2H-benzo[d]imidazol-2-one (5d)¹⁵: The title



compound was synthesized according to the general procedure.

The crude mixture was purified using column chromatography

by eluting with ethyl acetate and obtained as a brown solid (30

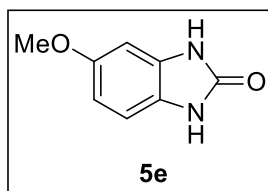
mg, 75%); ¹H-NMR (400 MHz, DMSO-*d*₆) δ 10.98 (d, *J* = 38.3 Hz, 2H), 7.28 (d, *J* = 8.2 Hz,

1H), 7.16 (s, 1H), 7.09 (d, *J* = 8.1 Hz, 1H); ¹³C-NMR (100 MHz, DMSO-*d*₆) 155.7, 133.3,

130.26, 125.0, 121.5 (d, *J*_{C-F} = 32 Hz), 118.3 (q, *J*_{C-F} = 218 Hz), 109.0 (d, *J*_{C-F} = 20 Hz),

105.3.

5-methoxy-1,3-dihydro-2H-benzo[d]imidazol-2-one (5e): The title compound was



synthesized according to the general procedure. The crude

mixture was purified using column chromatography by eluting

with ethyl acetate and obtained as a brown solid (27 mg, 81%);

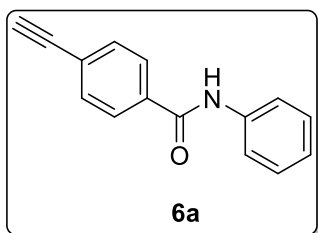
Mp. 272–274 °C; ¹H-NMR (400 MHz, DMSO-*d*₆) δ 10.42 (d, *J* = 14.6 Hz, 2H), 6.77- 6.69

(m, 3H), 2.25 (s, 3H); ¹³C-NMR (100 MHz, DMSO-*d*₆) δ 155.8, 130.3, 129.8, 127.9, 121.3,

109.4, 108.6, 21.5. HRMS (HR-EI)m/z: [M-H]⁺ calcd for C₈H₇N₂O₂, 163.0508; found,

163.0504.

4-ethynyl-*N*-phenylbenzamide (6a): The title compound was synthesized according to



the general procedure. The crude mixture was purified

using column chromatography by eluting with ethyl

acetate and obtained as a white solid (40 mg, 90%); ¹H-

NMR (400 MHz, DMSO-*d*₆) δ 10.30 (s, 1H), 7.97-7.93 (m,

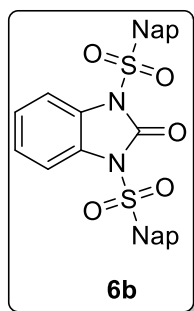
2H), 7.75 (dd, *J* = 1.4 Hz, 7.6 Hz, 2H), 7.64-7.61 (m, 2H), 7.37-7.32 (m, 2H), 7.12-7.01

(m, 1H); ¹³C-NMR (100 MHz, DMSO-*d*₆) δ 164.7, 138.9, 134.9, 131.7, 128.6, 127.9,

124.7, 123.8, 120.4, 83.0, 82.8. HRMS (HR-EI)m/z: [M+H]⁺ calcd for C₁₅H₁₂NO,

222.0919; found, 222.0924.

1,3-bis(naphthalen-1-ylsulfonyl)-1,3-dihydro-2H-benzo[d]imidazol-2-one (6b)⁷: The



title compound was synthesized according to the general procedure.

The crude mixture was purified using column chromatography by eluting with ethyl acetate and obtained as a white solid (51 mg, 50%); ¹H-NMR (400 MHz, DMSO-*d*₆) δ 8.75 (d, *J*= 1.7 Hz, 1H), 8.12 (td, *J*= 7.9 Hz, 3.2 Hz, 4H), 7.89-7.67 (m, 7H), 7.54-7.46 (m, 1H), 7.17-

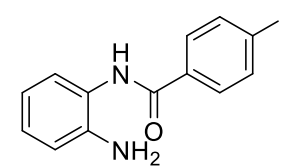
6.96 (m, 5H); ¹³C-NMR (100 MHz, DMSO-*d*₆) δ 150.9, 135.6, 131.8, 130.4, 129.9, 128.4, 126.9, 125.0, 122.5, 122.0, 112.9, 110.5.

5. References

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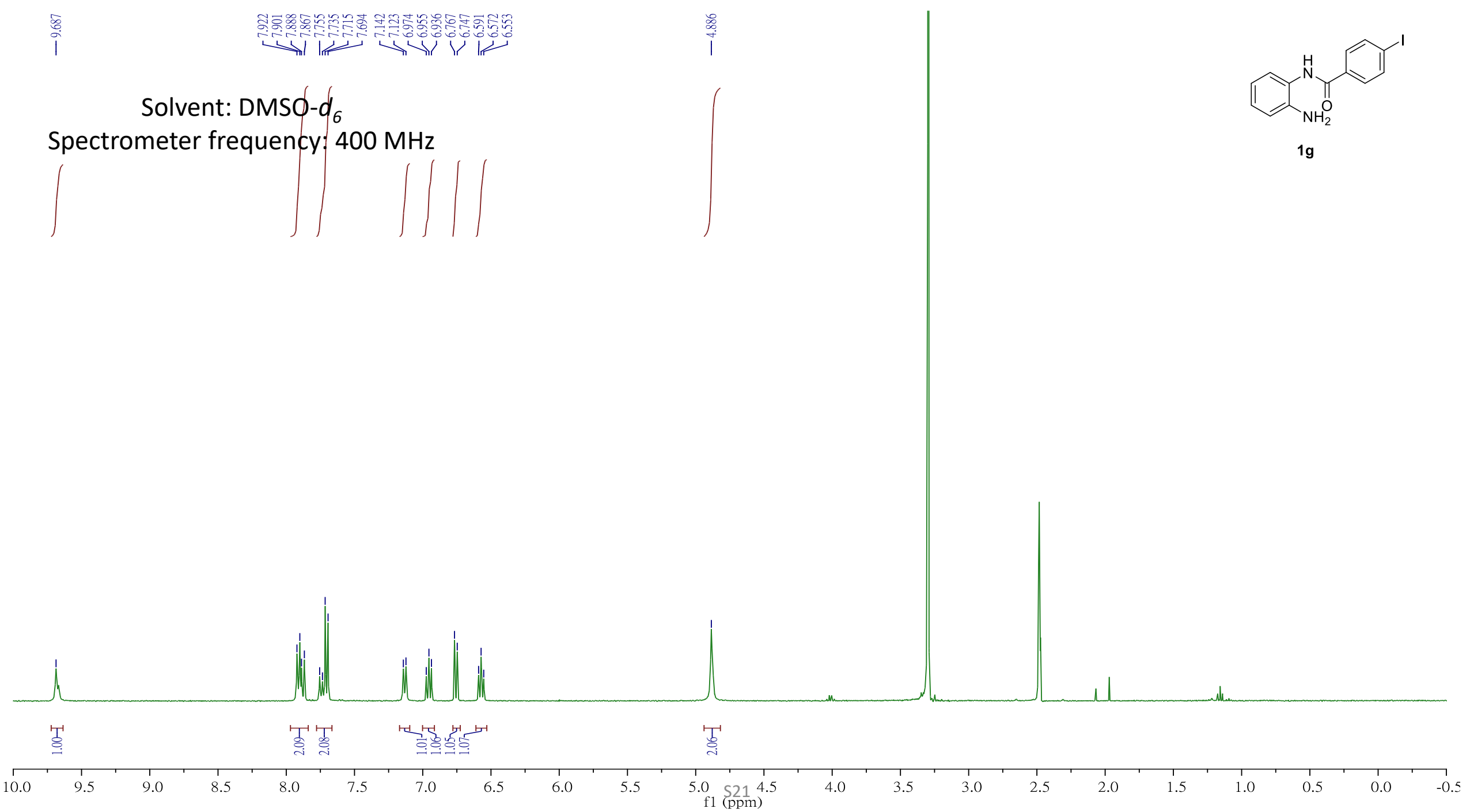
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Proton and Carbon Spectra

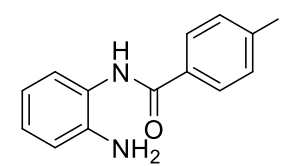


1g

Solvent: DMSO-*d*₆
Spectrometer frequency: 400 MHz



Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz

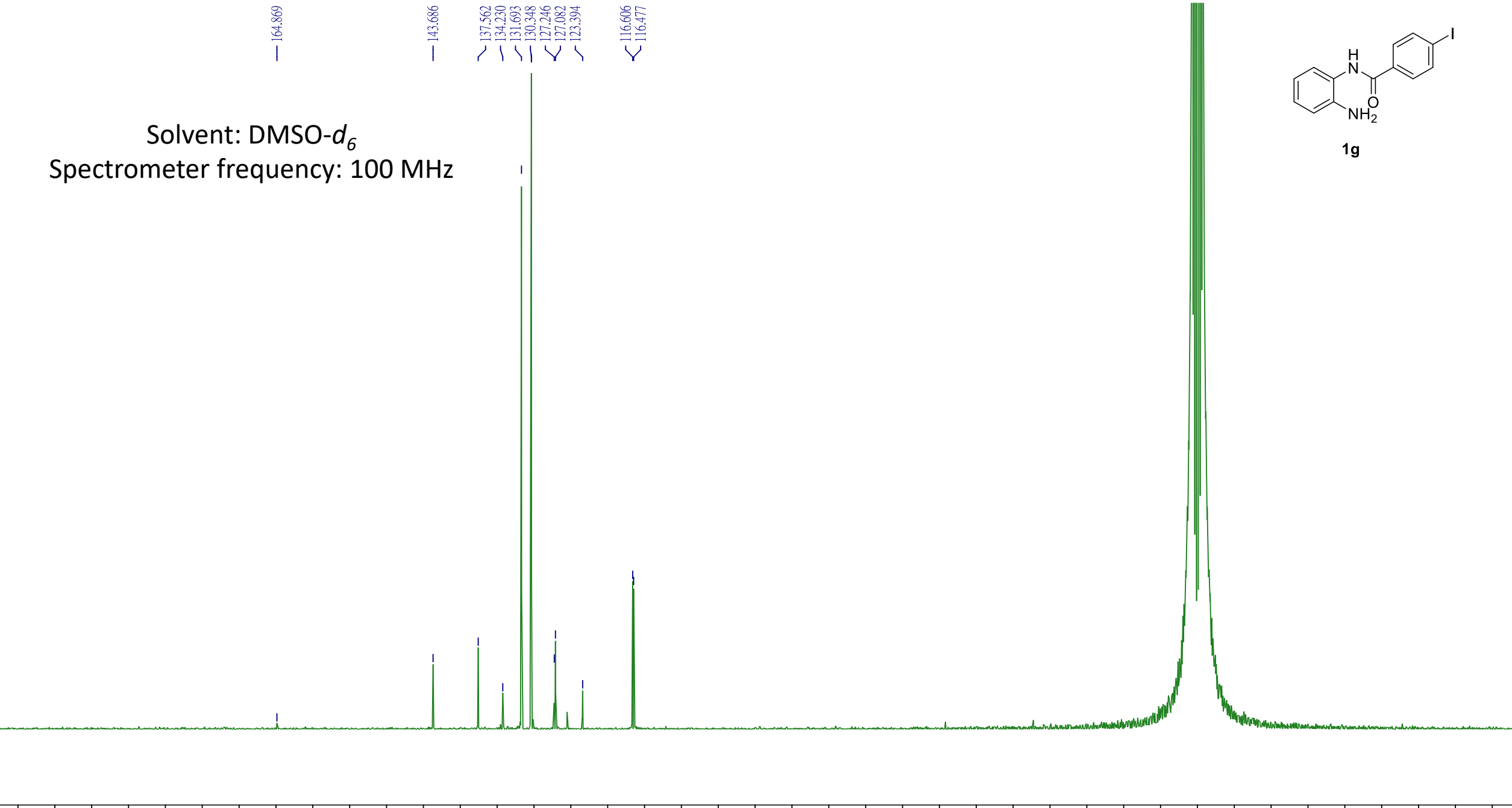


1g

164.869
143.686
137.562
134.230
131.693
130.348
127.246
127.082
123.394
116.606
116.477

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)



9.819

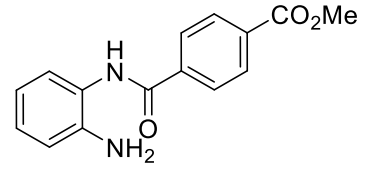
8.103
8.082
8.065
8.044

7.166
7.147
6.988
6.968
6.946
6.781
6.758
6.603
6.584
6.563

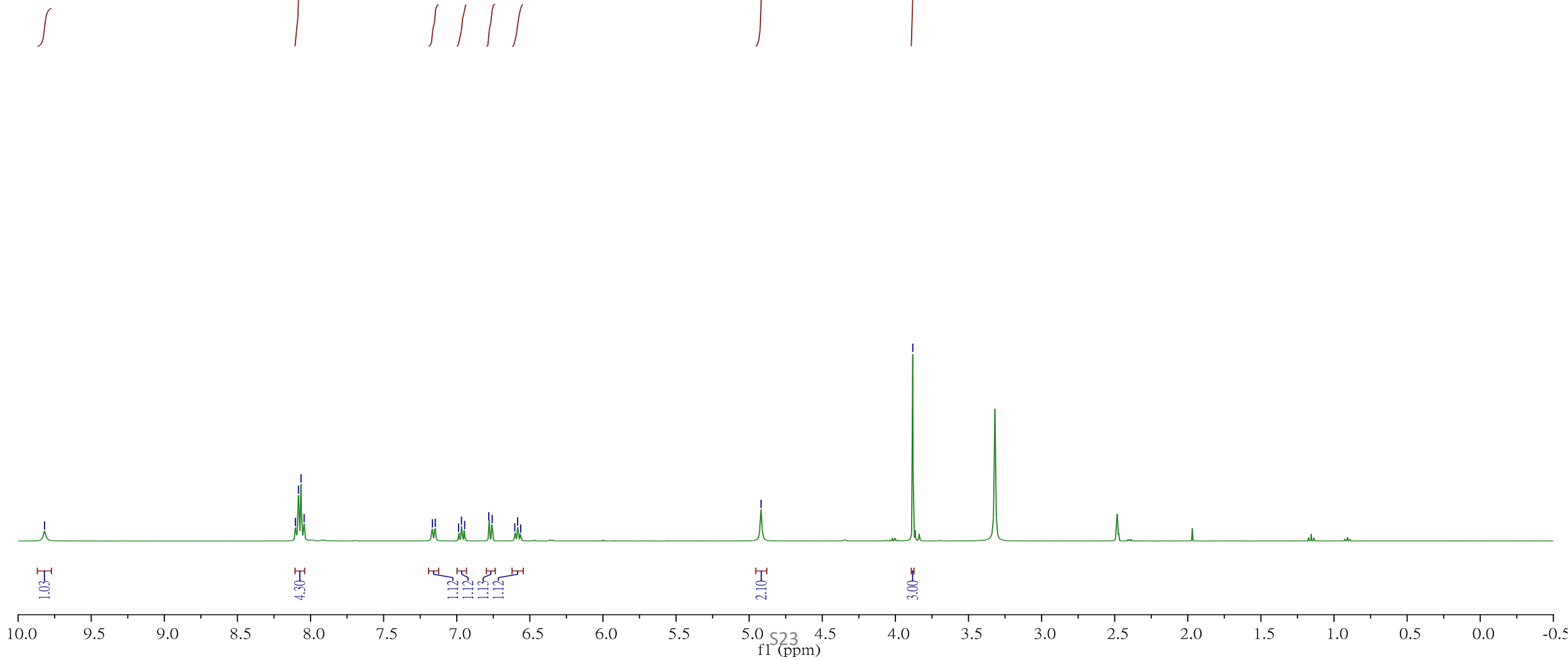
4.919

3.881

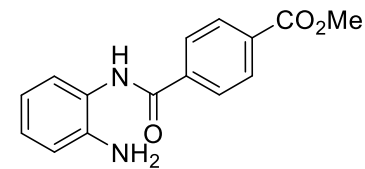
Solvent: DMSO-*d*₆
Spectrometer frequency: 400 MHz



1j



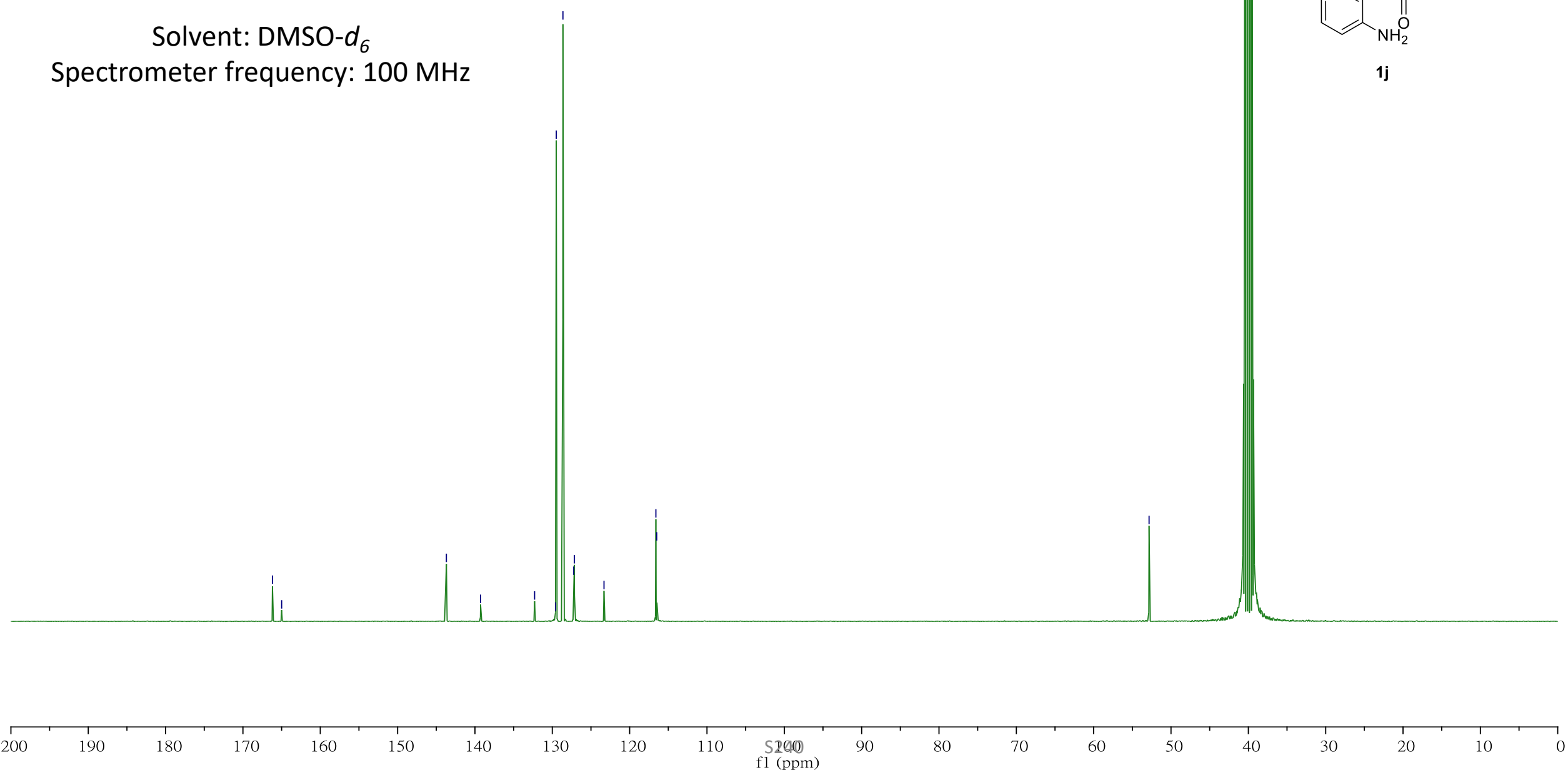
Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



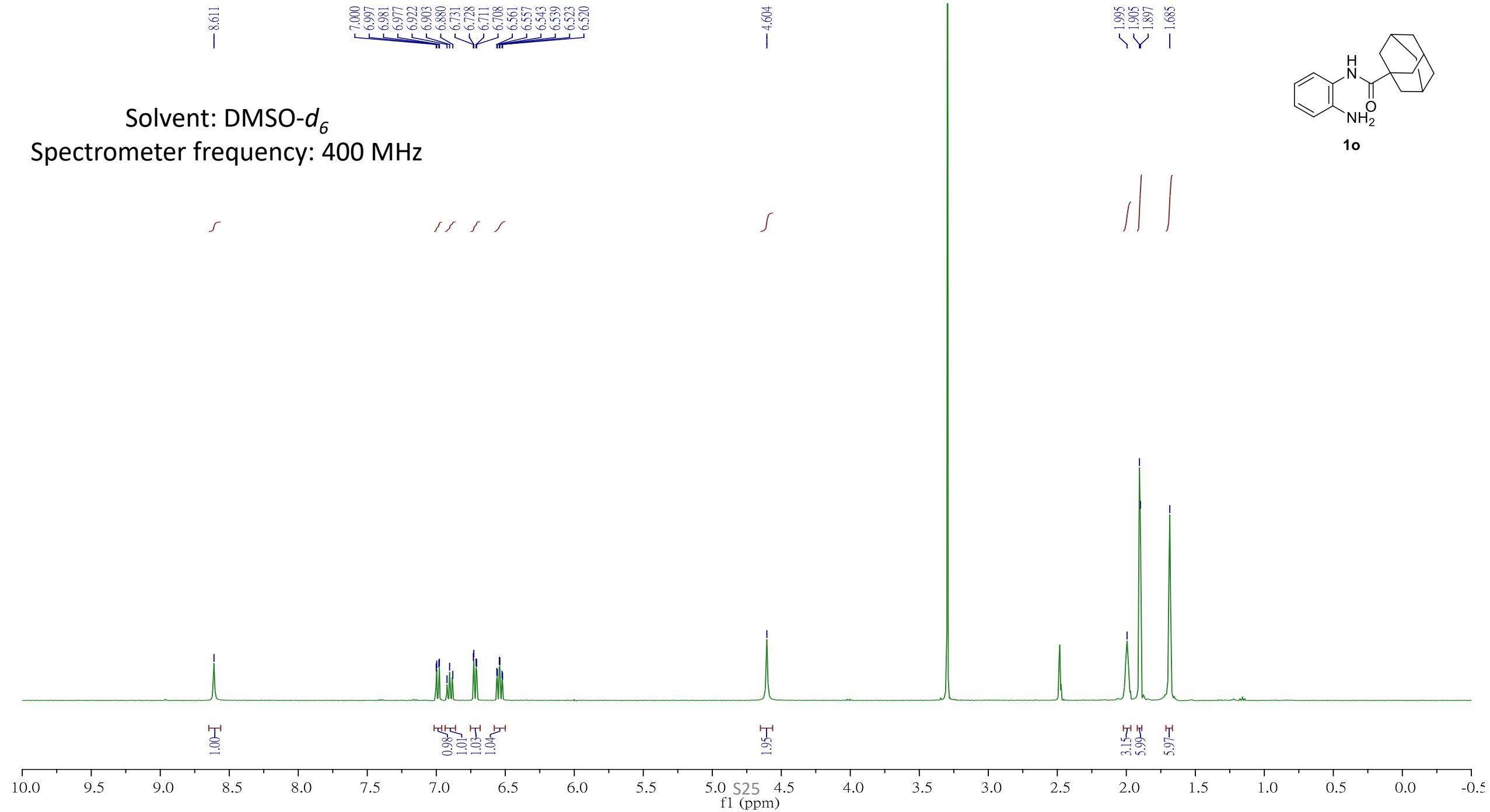
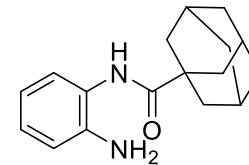
1j

166.189
164.995
143.693
139.276
132.289
129.584
129.489
128.625
127.228
127.152
123.315
116.606
116.499

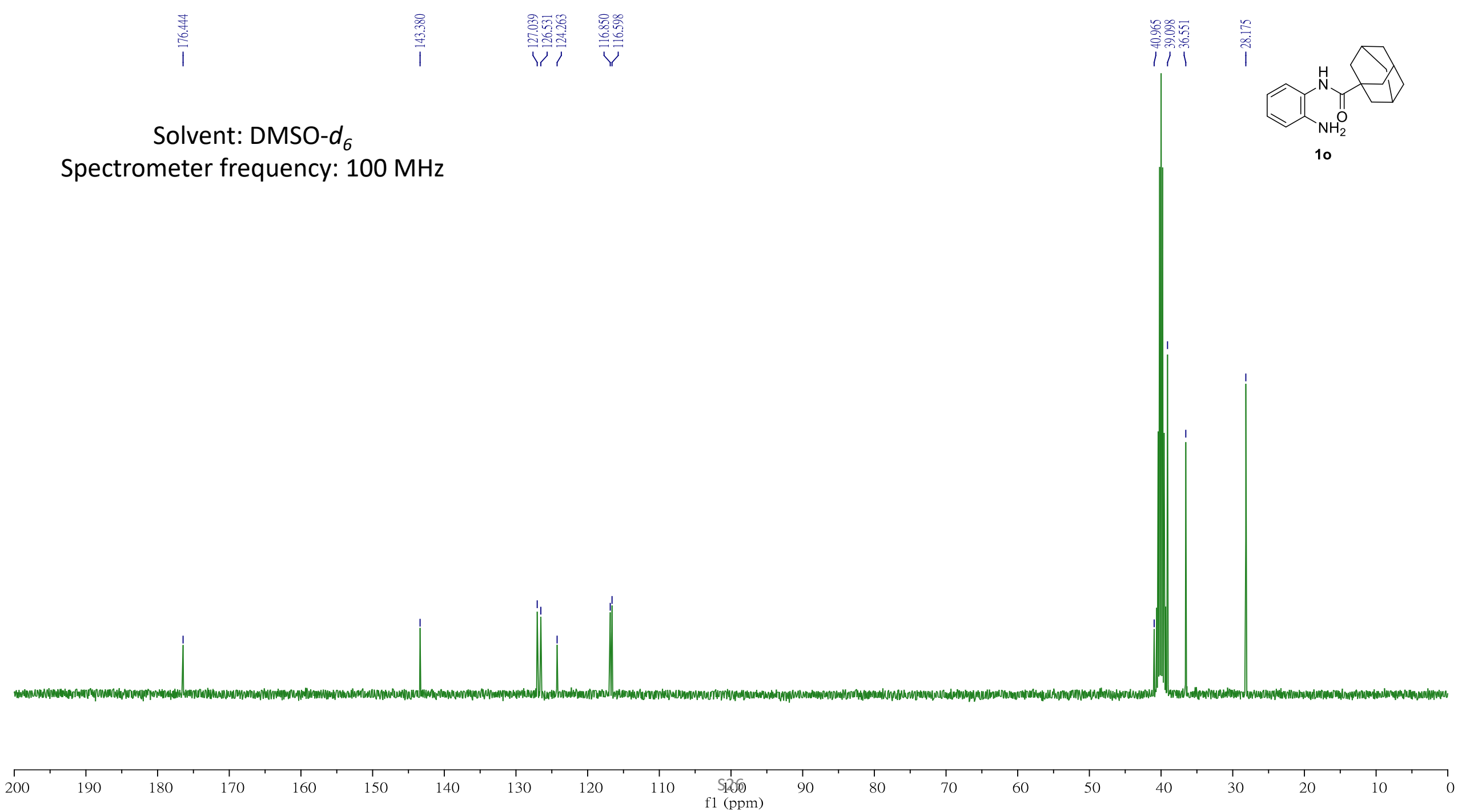
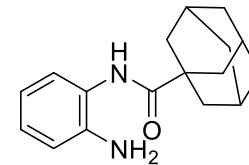
52.837



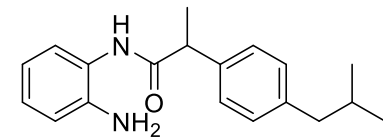
Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



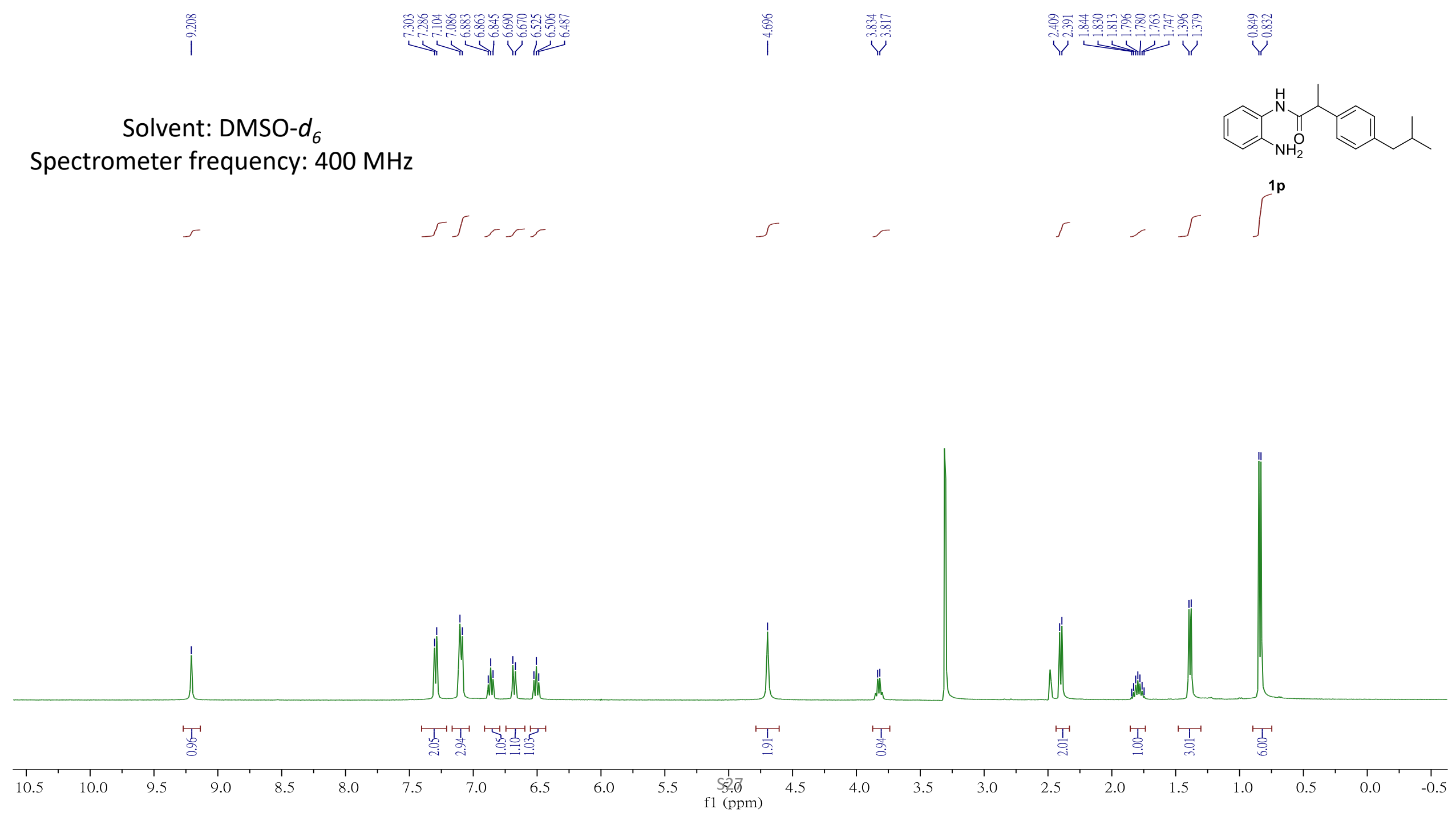
Solvent: DMSO-*d*₆
Spectrometer frequency: 100 MHz



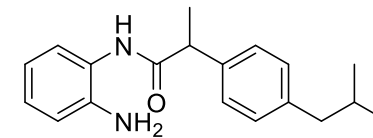
Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



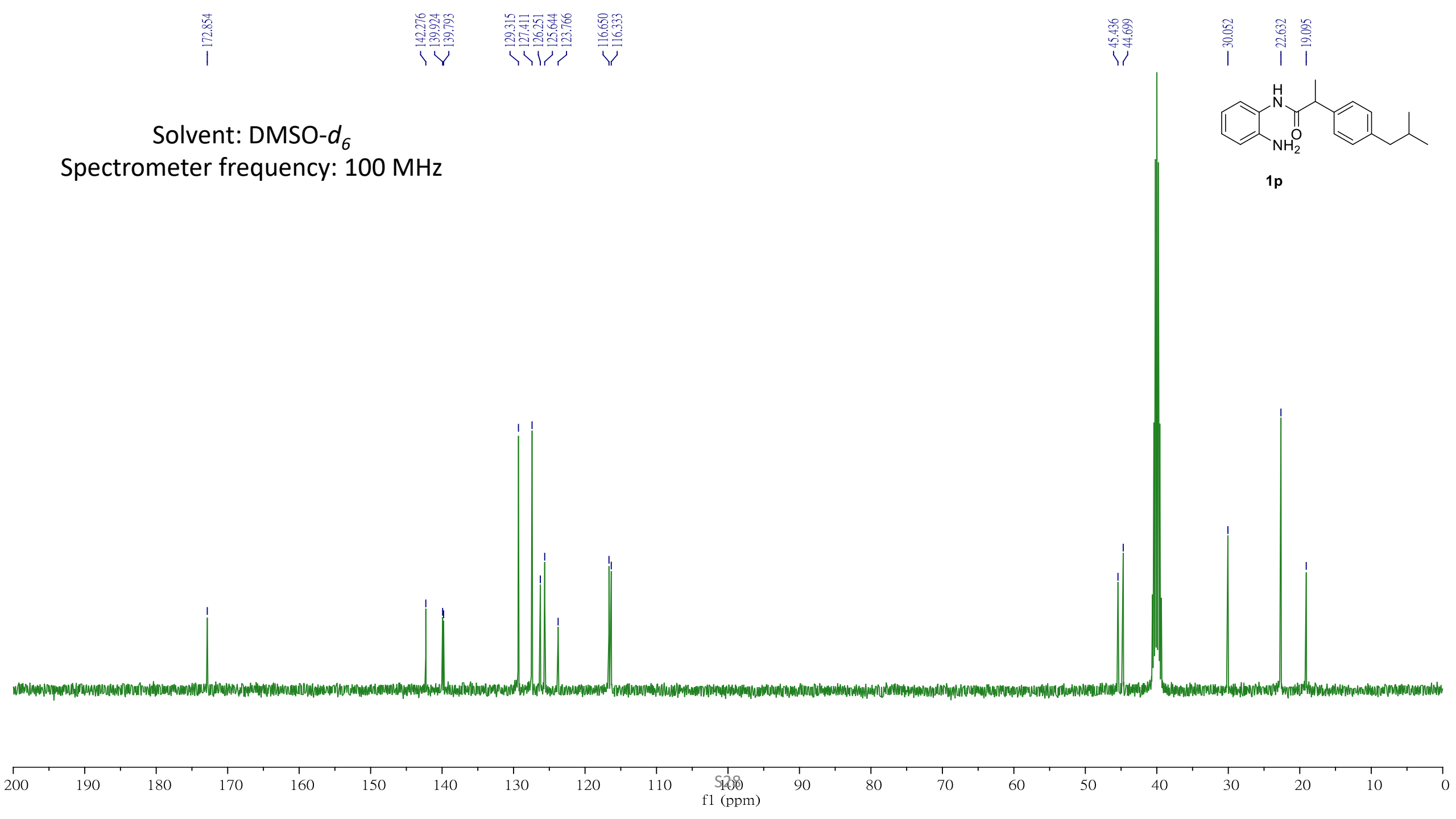
1p

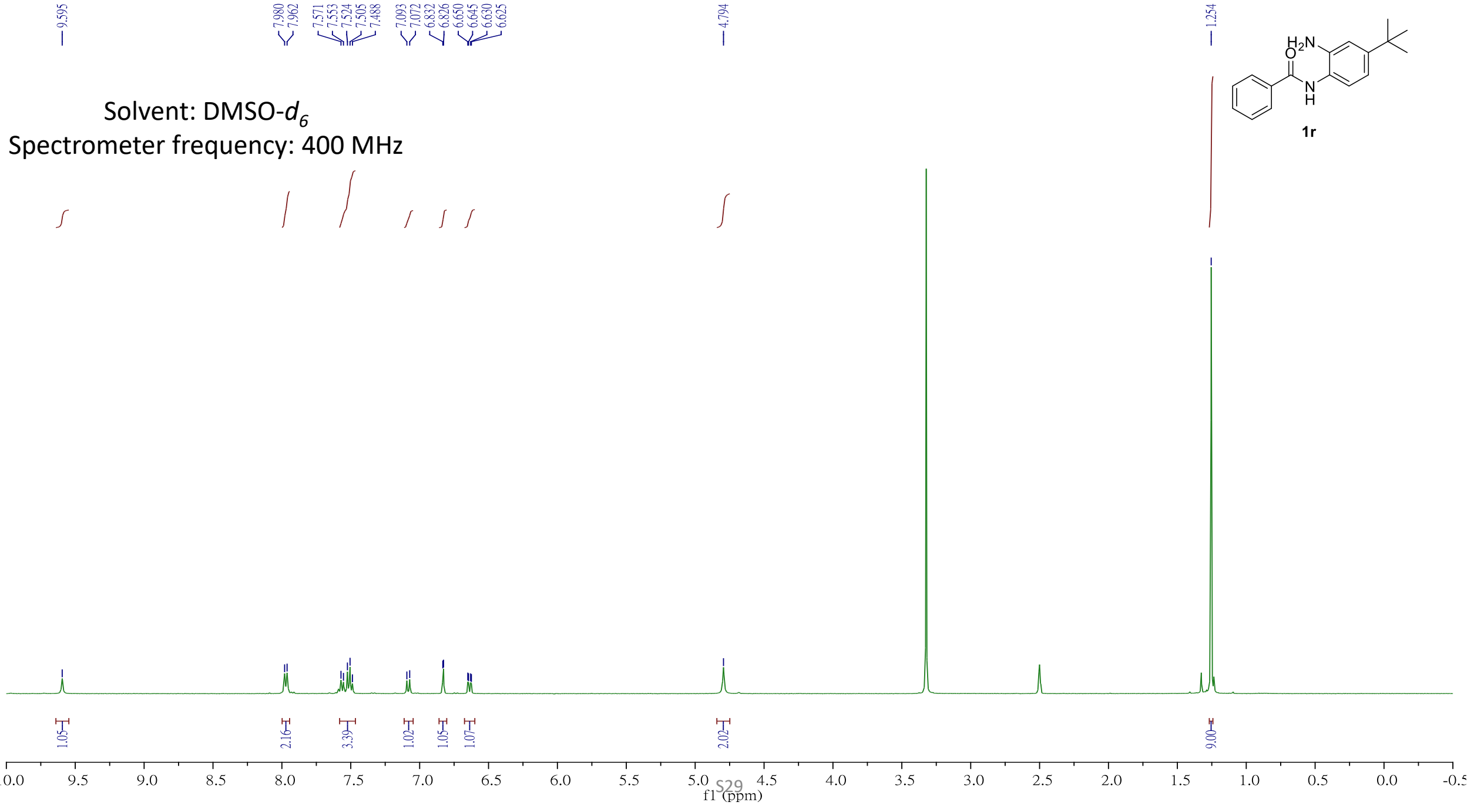


Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz

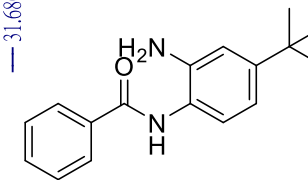


1p



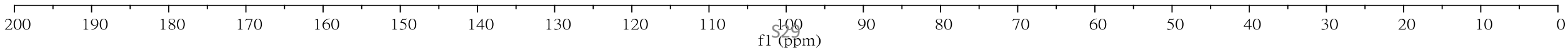


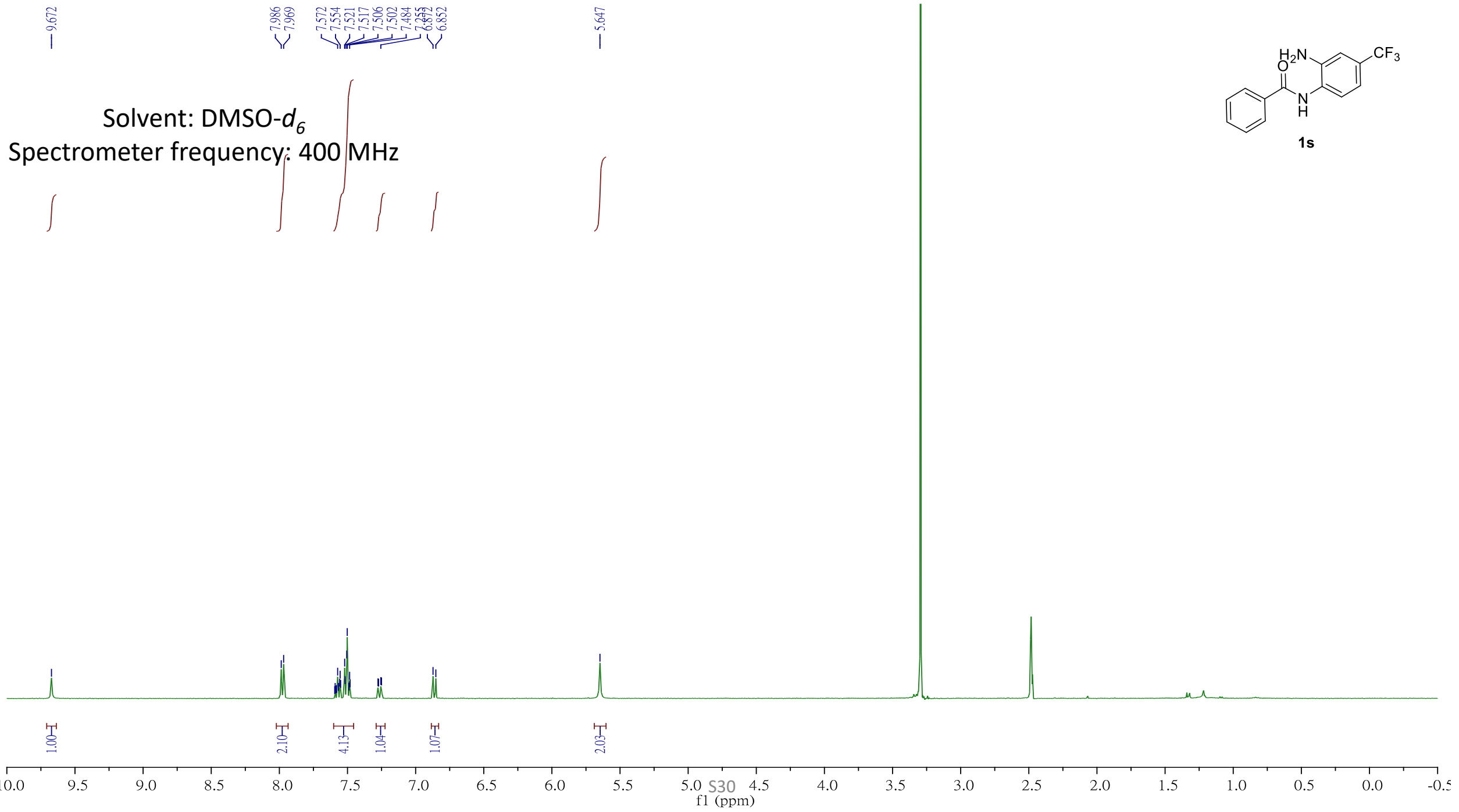
Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



165.746
149.350
142.902
135.138
131.746
128.691
128.156
126.594
121.393
113.899
113.614

34.464
31.680

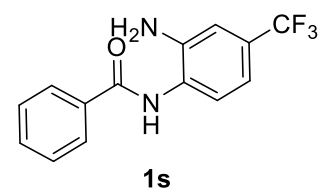




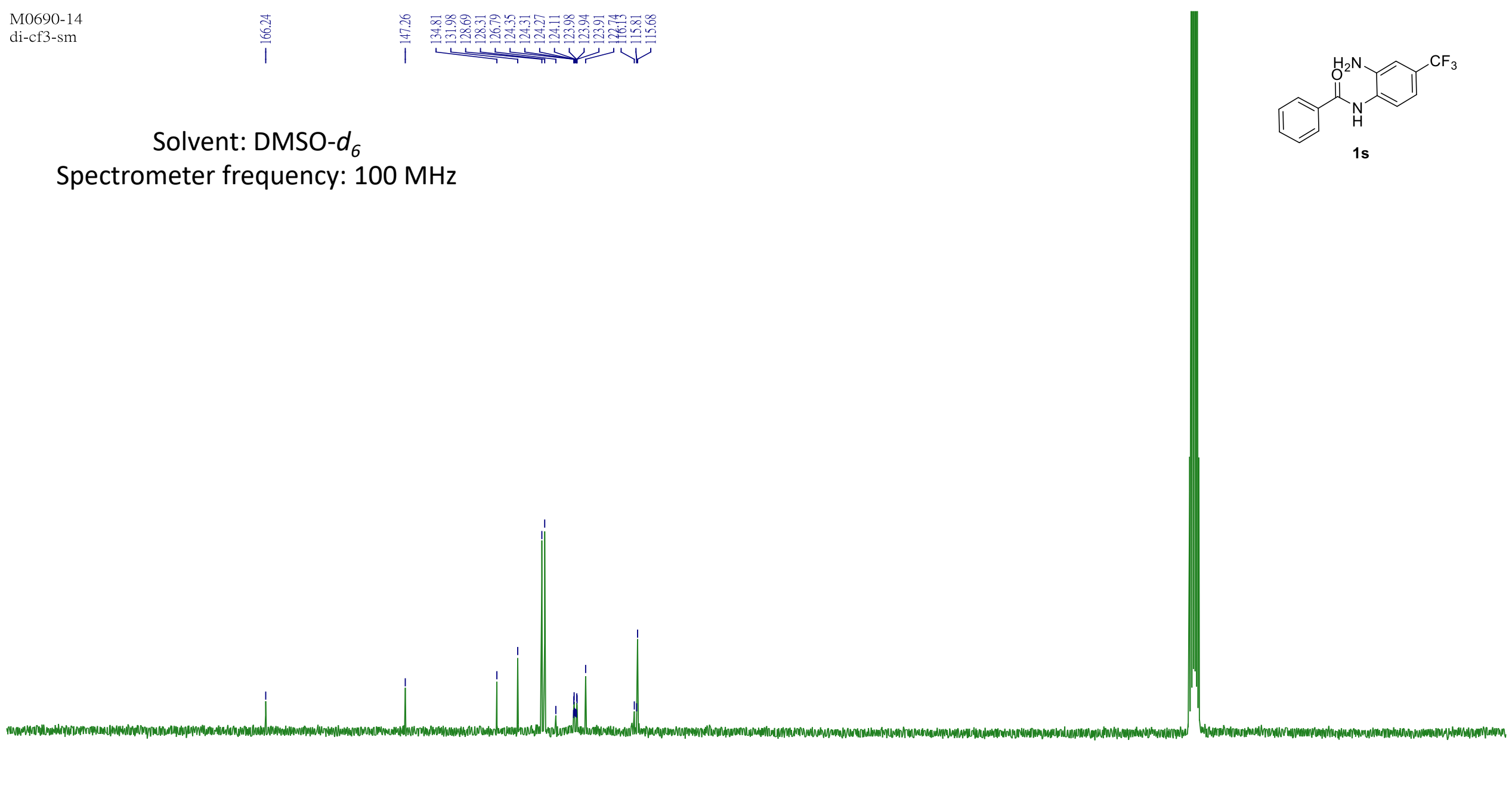
M0690-14
di-cf3-sm

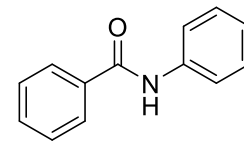
166.24
147.26
134.81
131.98
128.69
128.31
126.79
124.35
124.31
124.27
124.11
123.98
123.94
123.91
122.74
116.15
115.81
115.68

Solvent: DMSO-*d*₆
Spectrometer frequency: 100 MHz



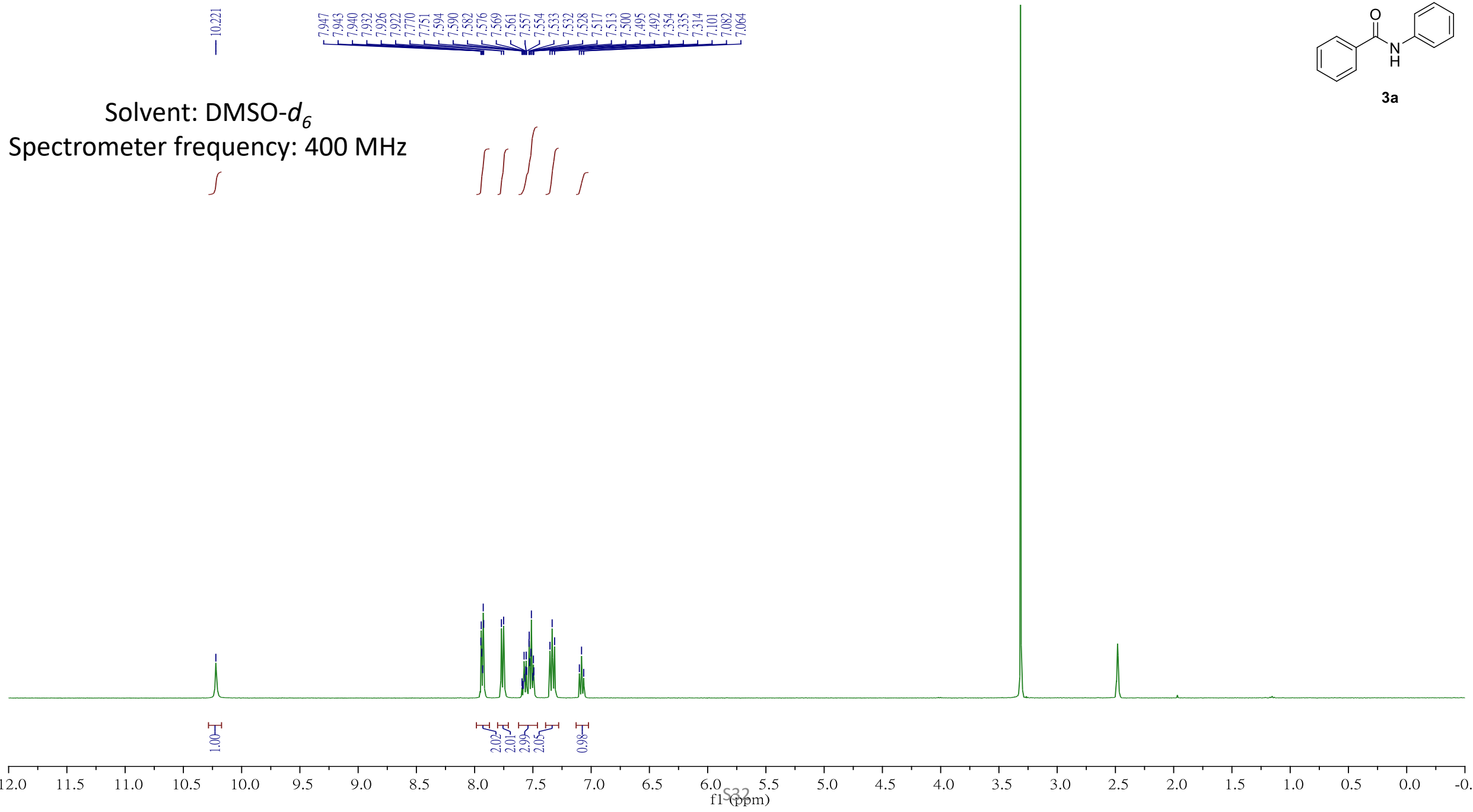
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

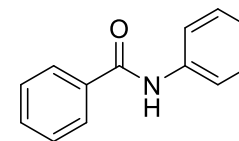




3a

Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz





3a

Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz

165.982

139.600

135.421

131.972

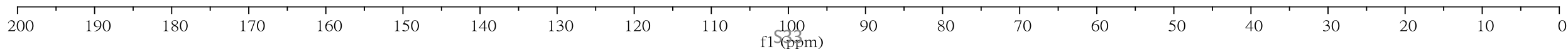
129.031

128.812

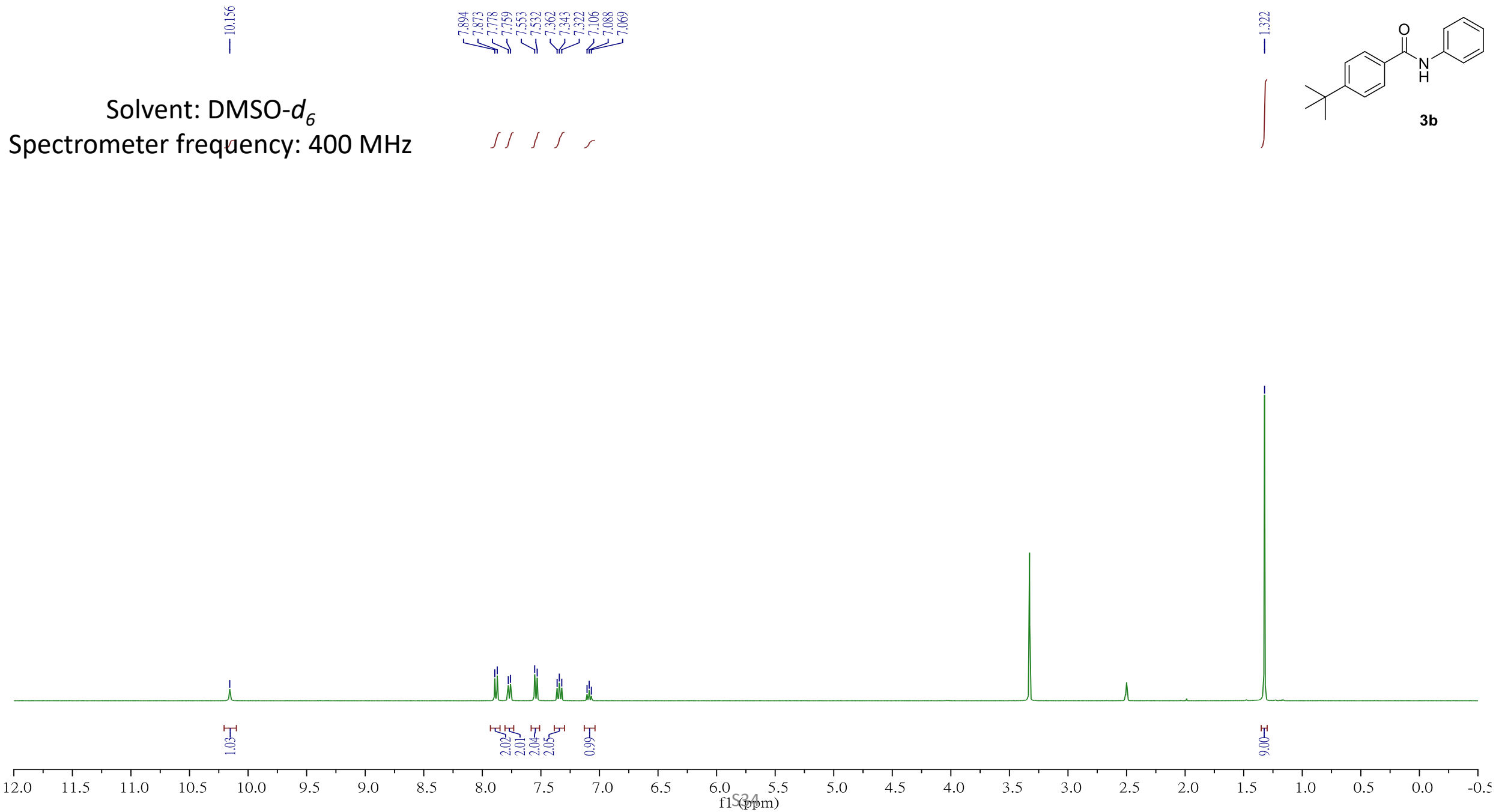
128.074

124.084

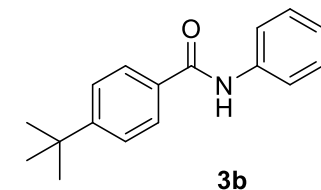
120.788



Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



165.926

154.809

139.697

132.729

129.008

127.942

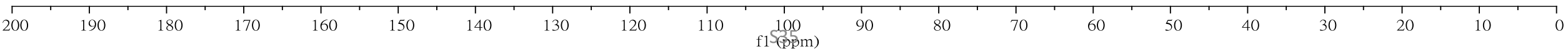
125.576

123.953

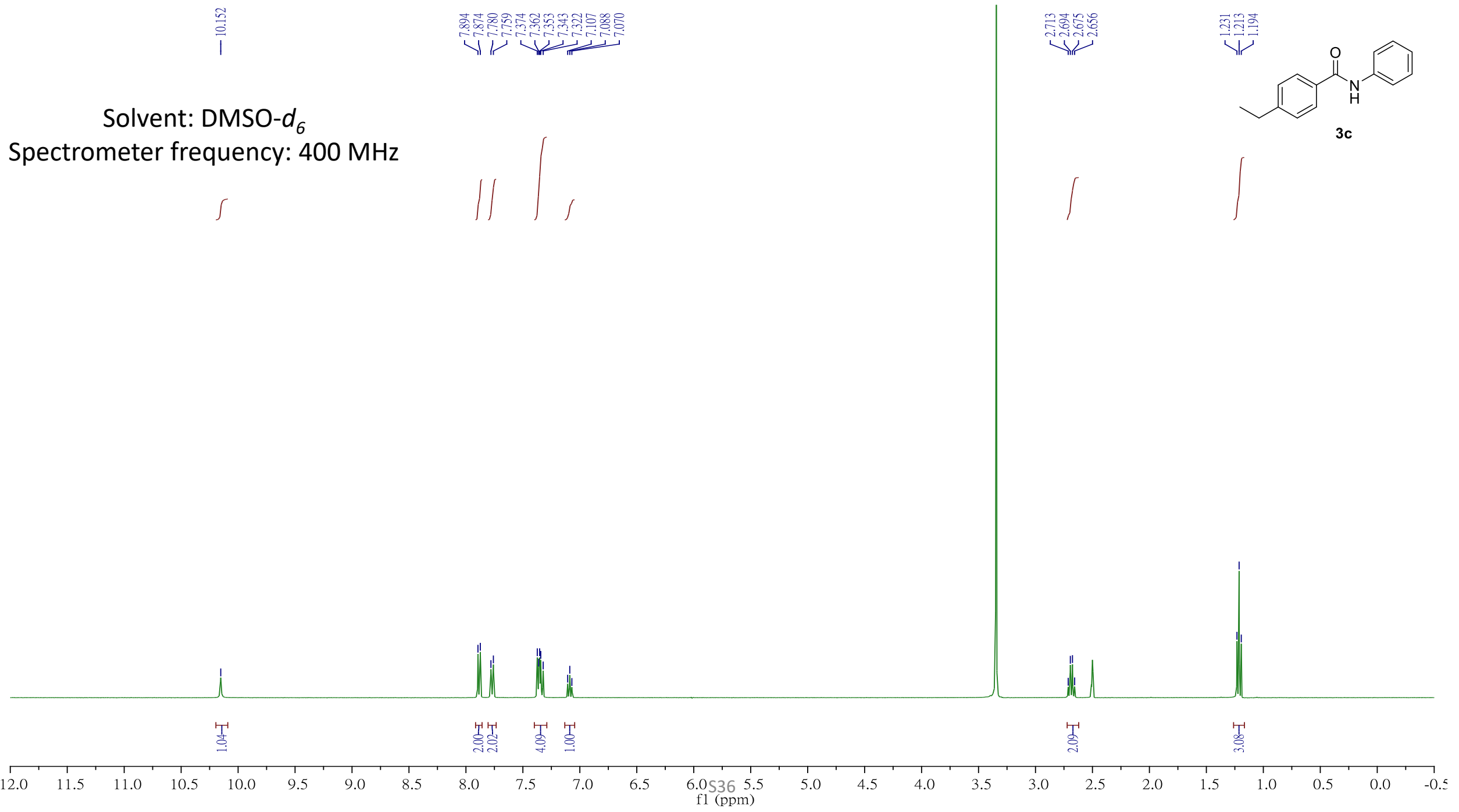
120.692

35.119

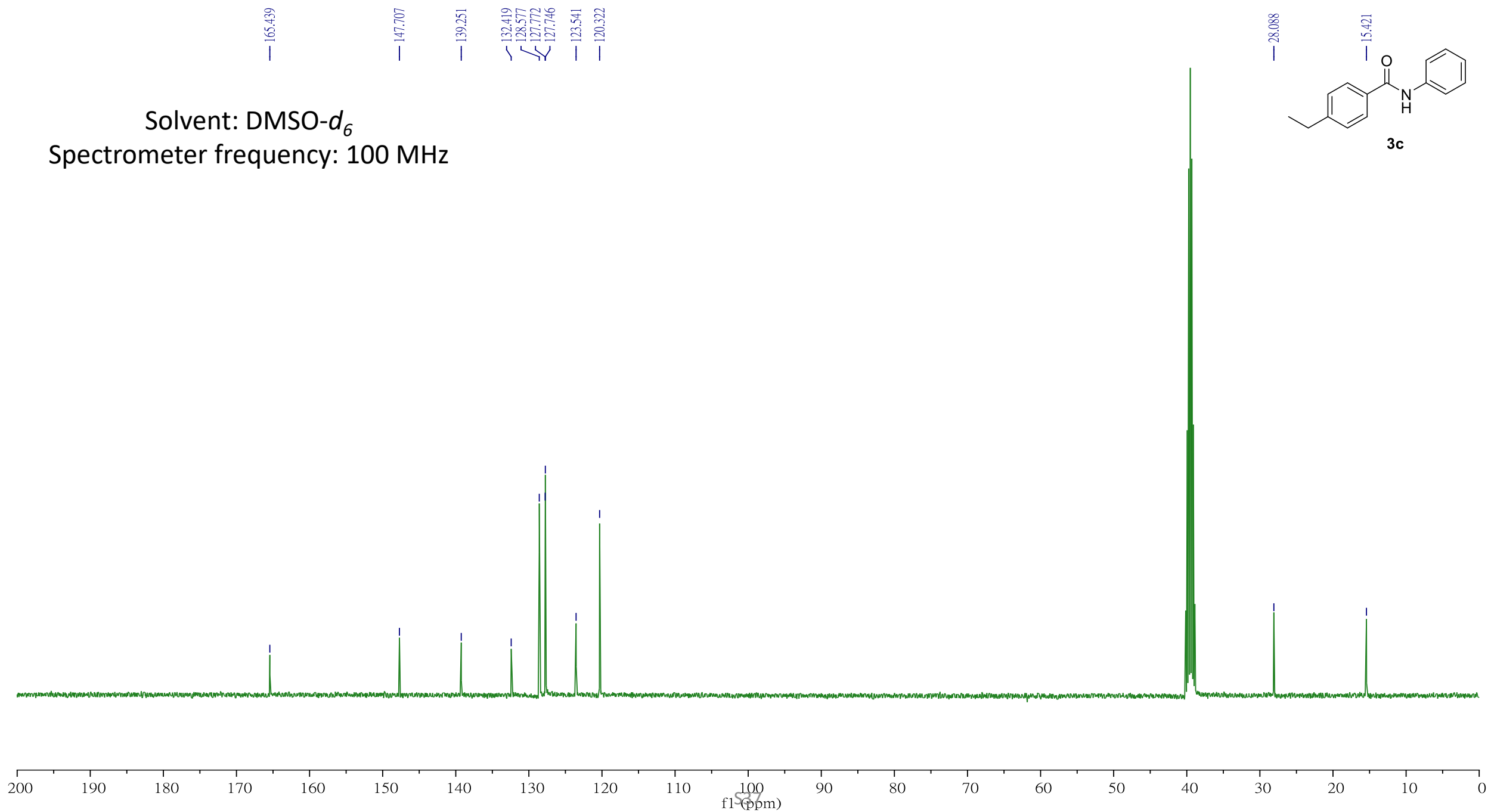
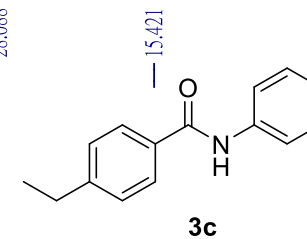
31.384



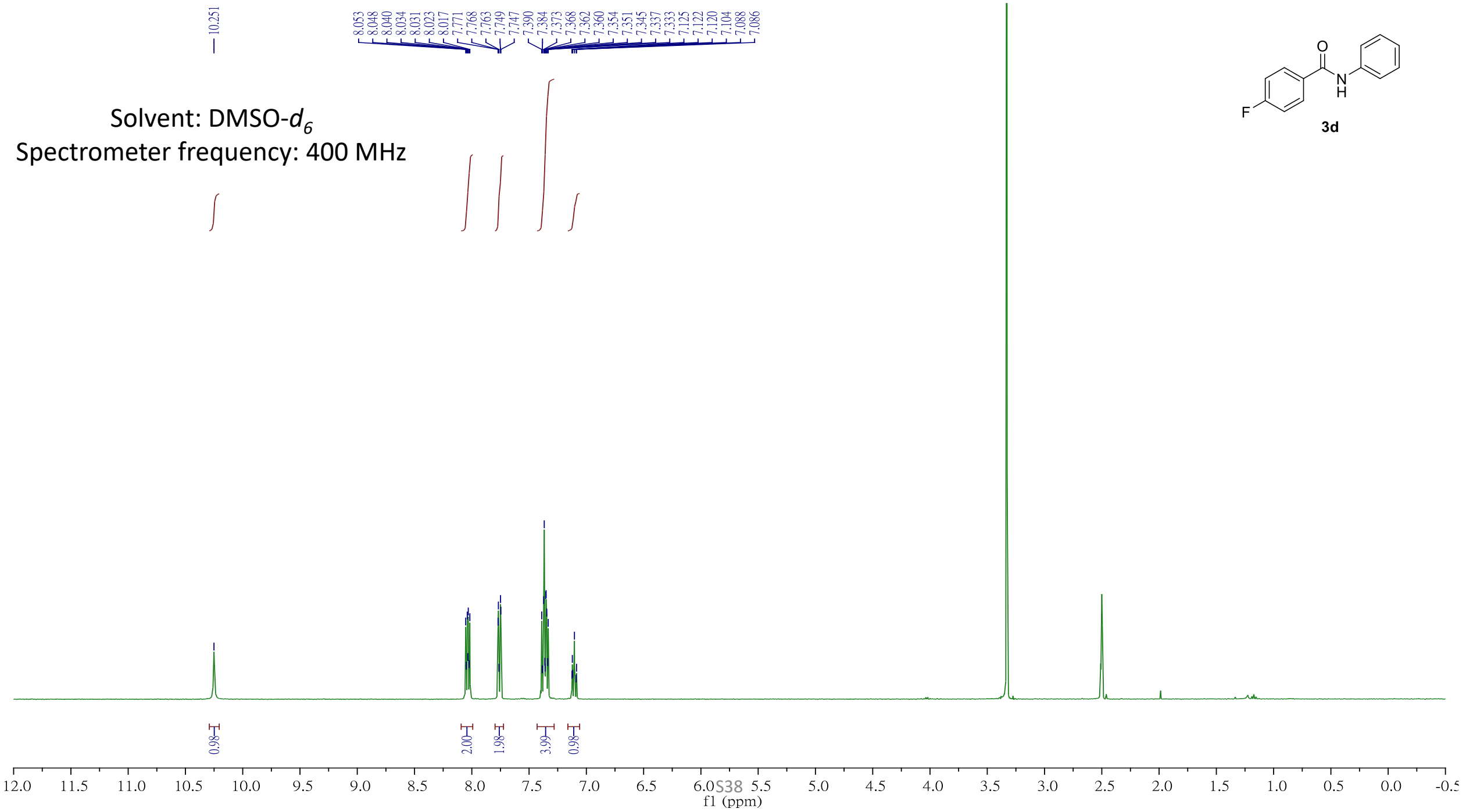
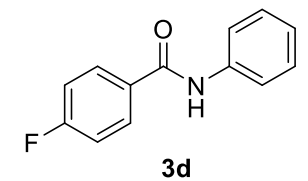
Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



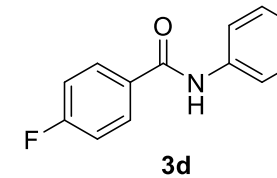
Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



Solvent: DMSO-*d*₆
Spectrometer frequency: 400 MHz



Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz

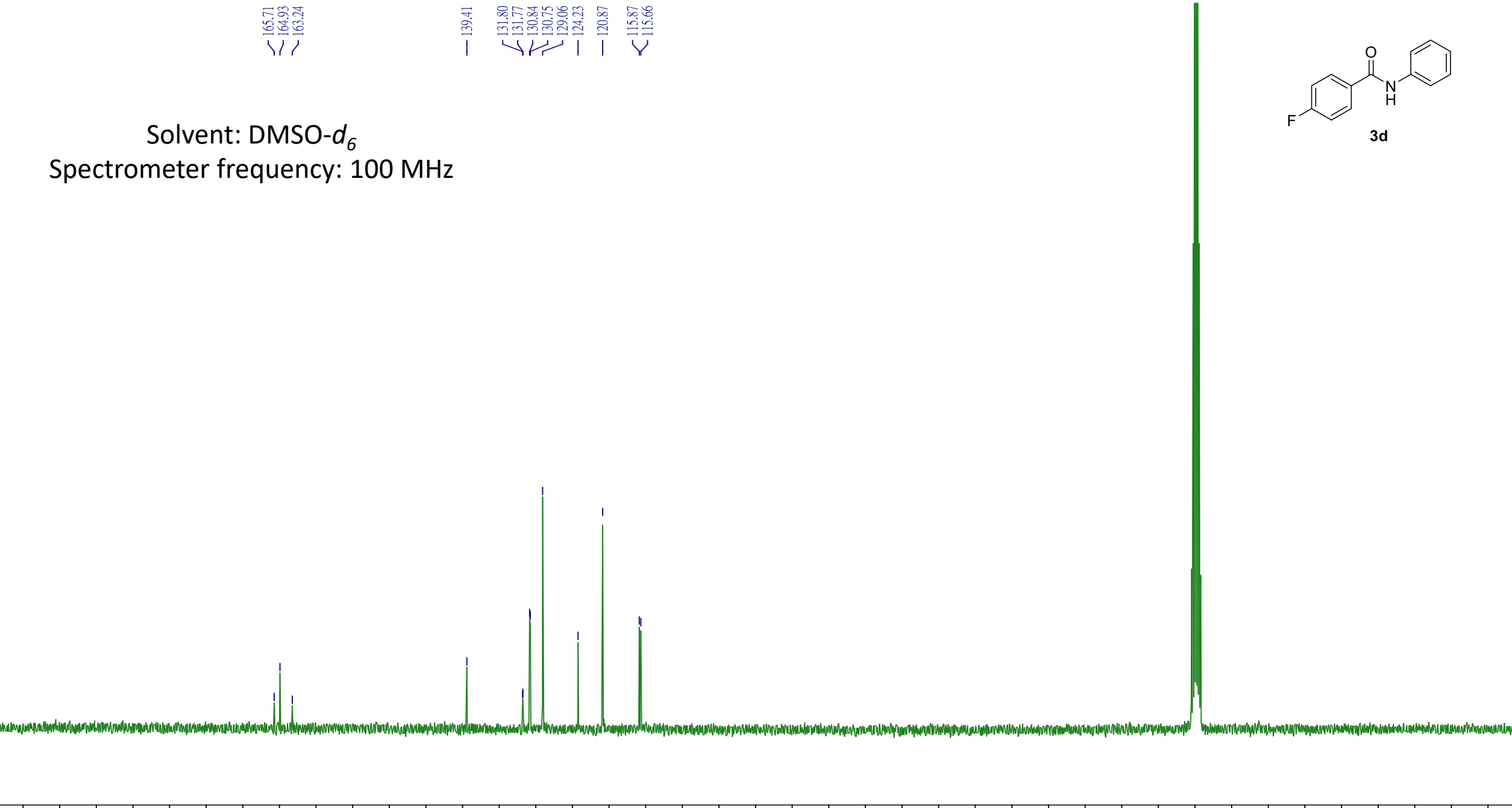


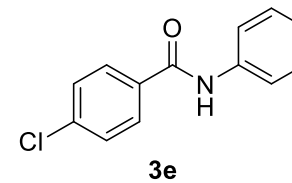
165.71
164.93
163.24

139.41
131.80
131.77
130.84
130.75
129.06
124.23
120.87
115.87
115.66

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

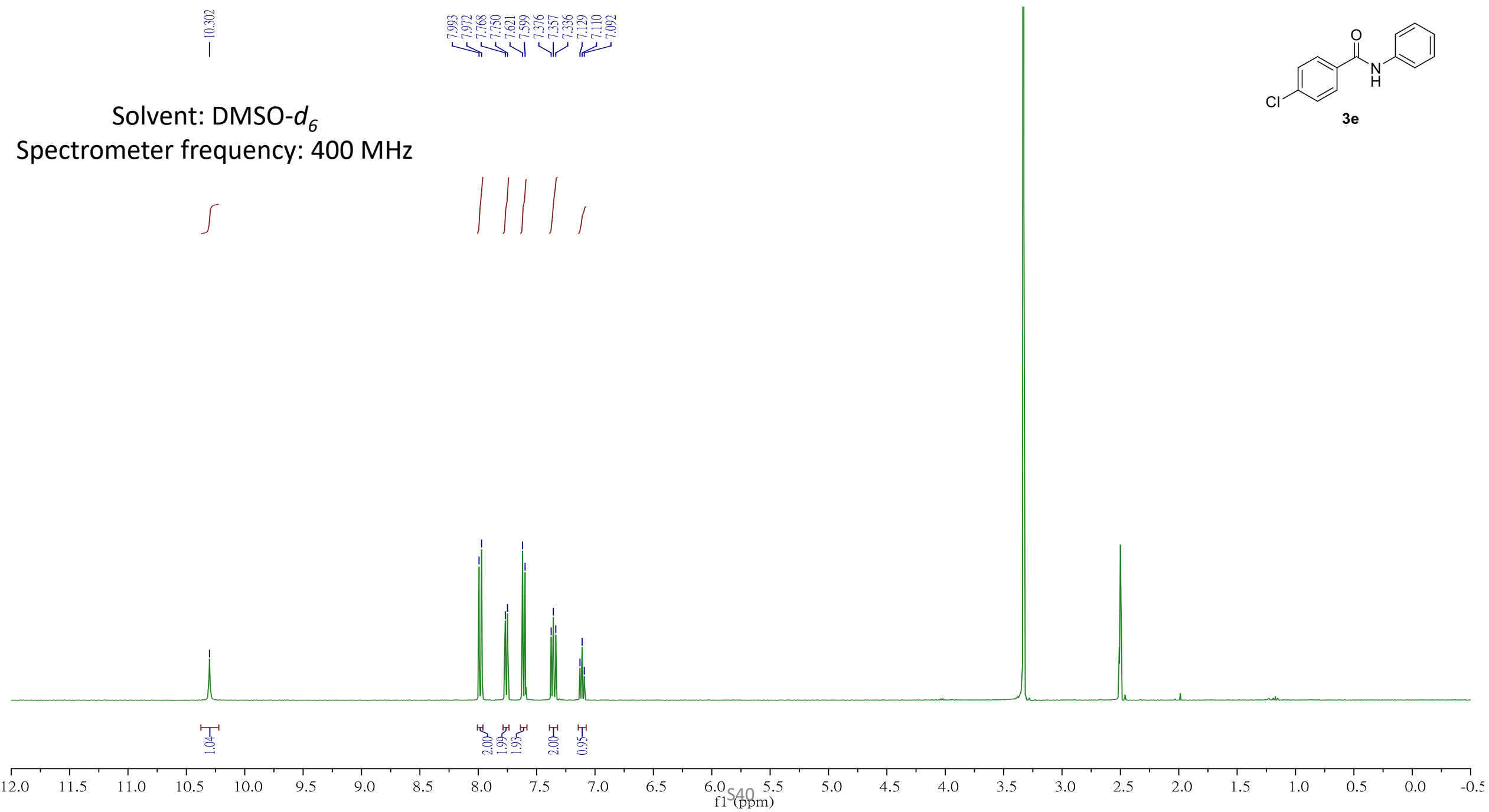
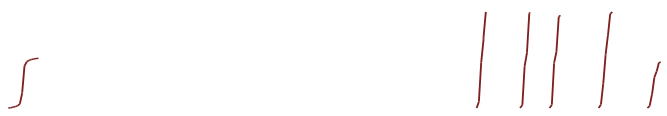
500
f1 (ppm)





Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz

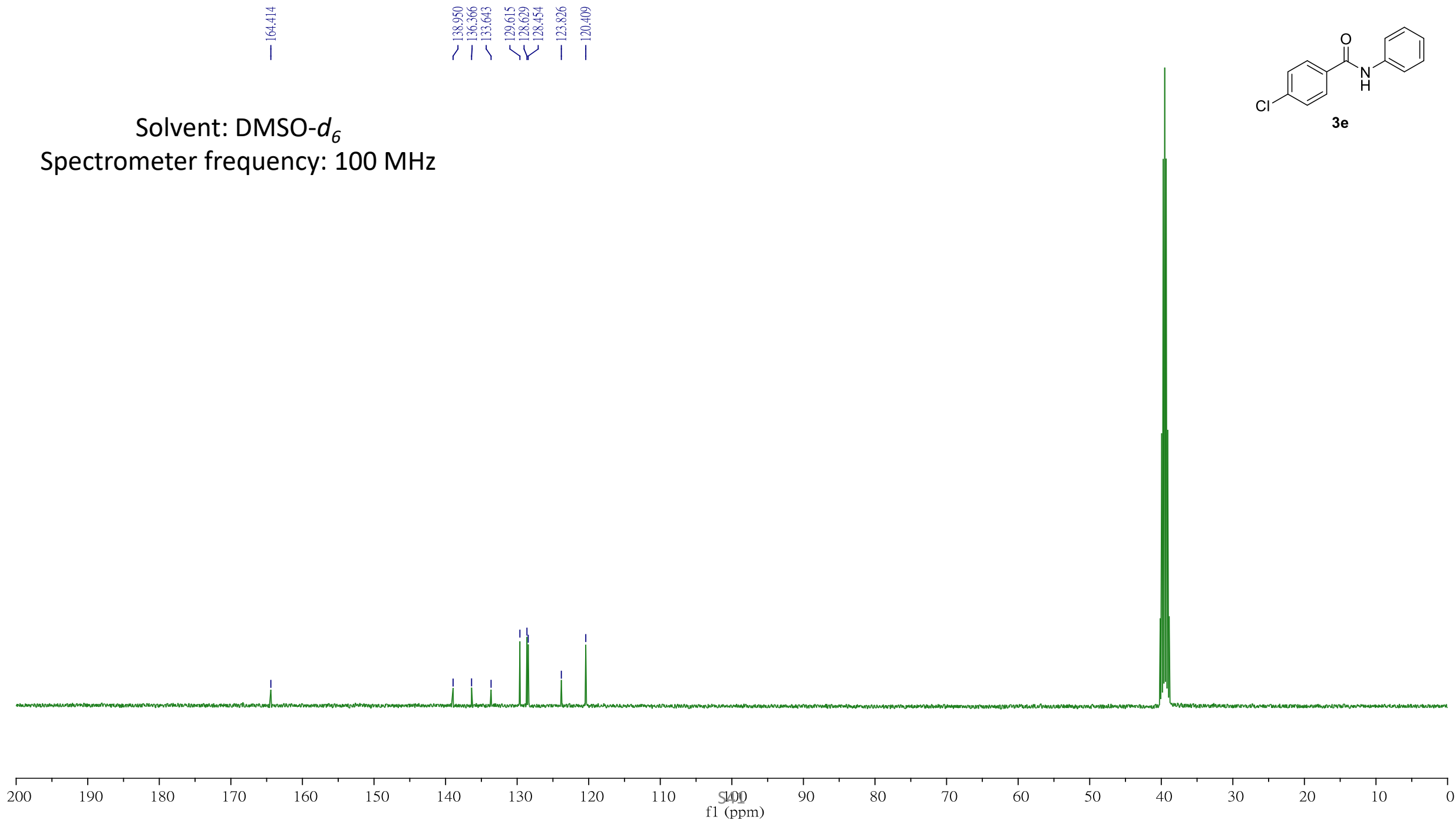
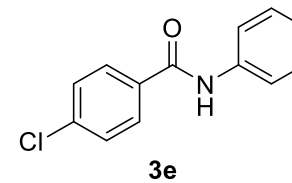
10.302
7.993
7.972
7.768
7.750
7.621
7.599
7.376
7.357
7.336
7.129
7.110
7.092



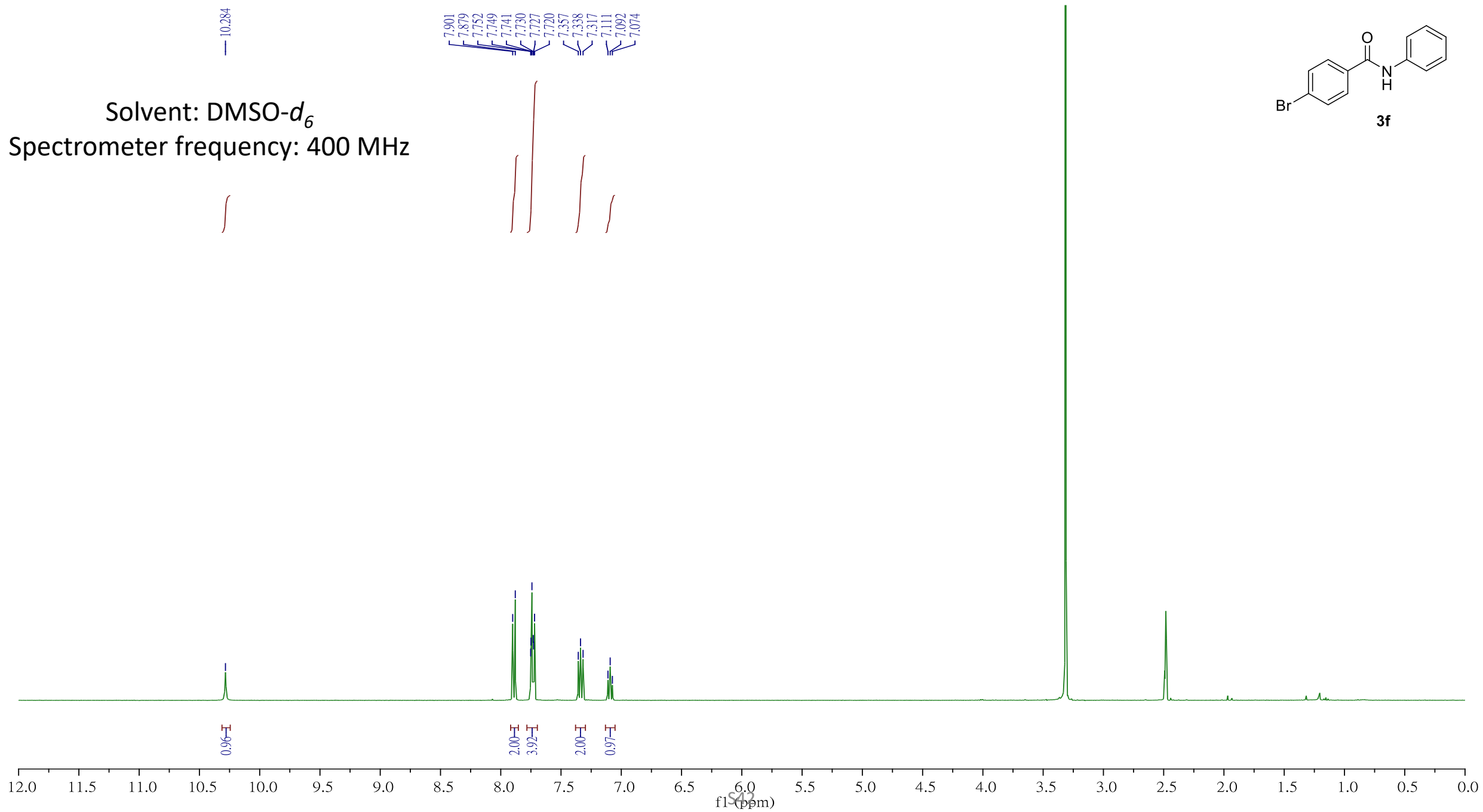
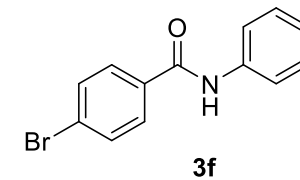
1.04
2.00
1.99
1.93
2.00
0.95

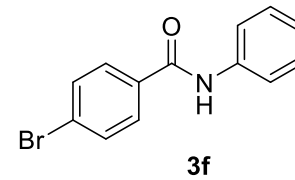
f1 (ppm)

Solvent: DMSO-*d*₆
Spectrometer frequency: 100 MHz

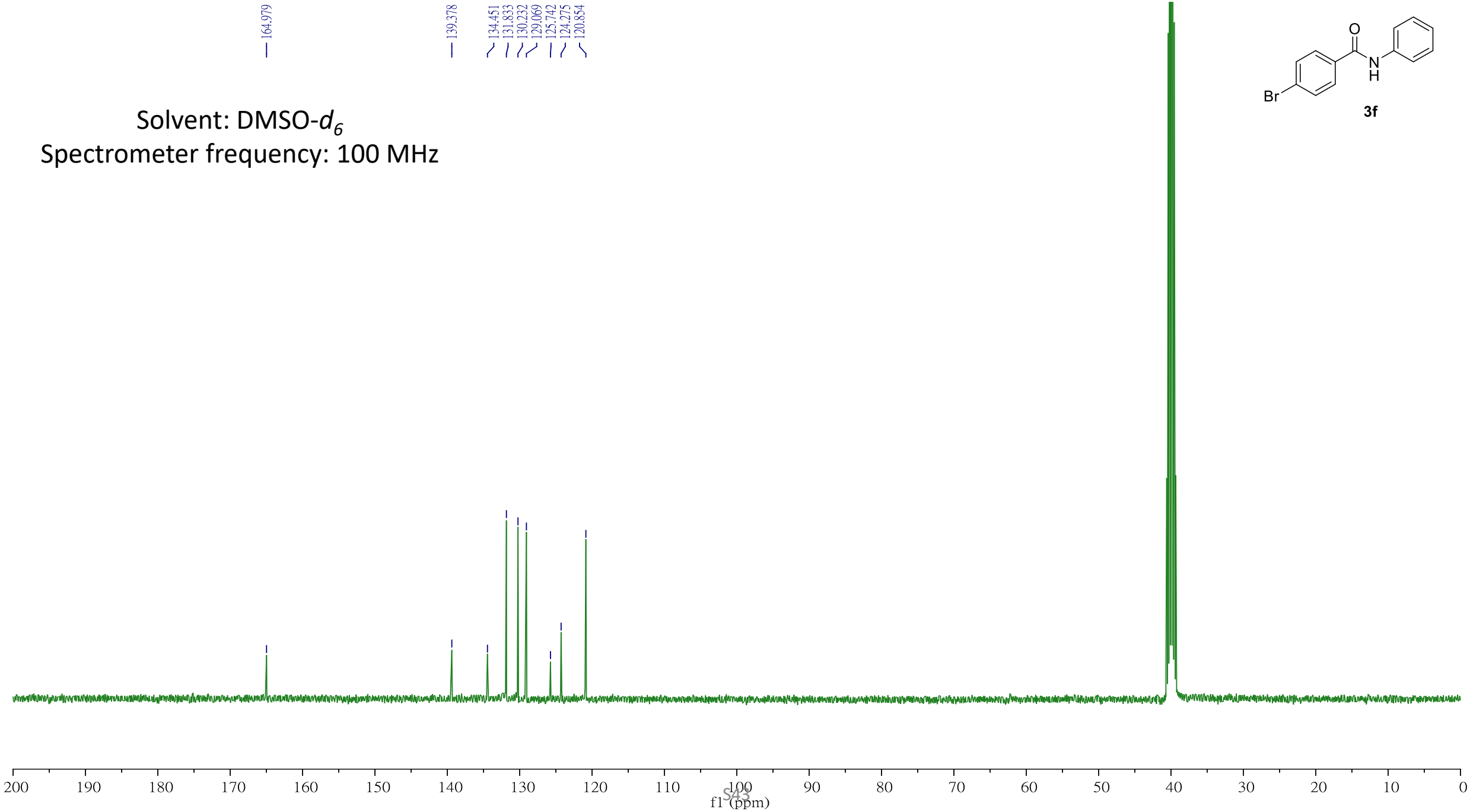


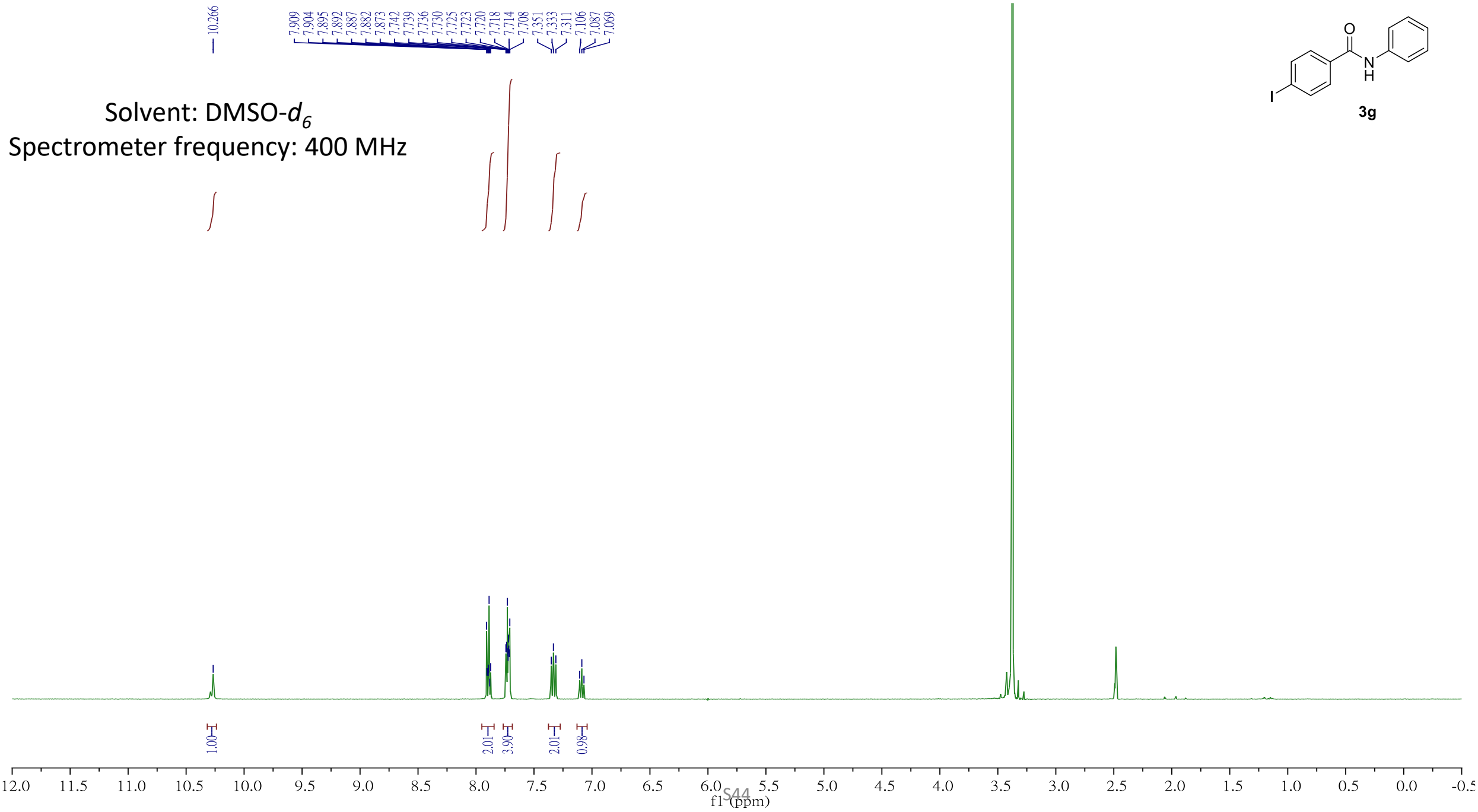
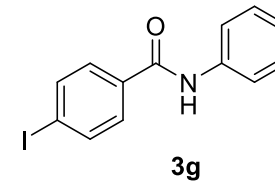
Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



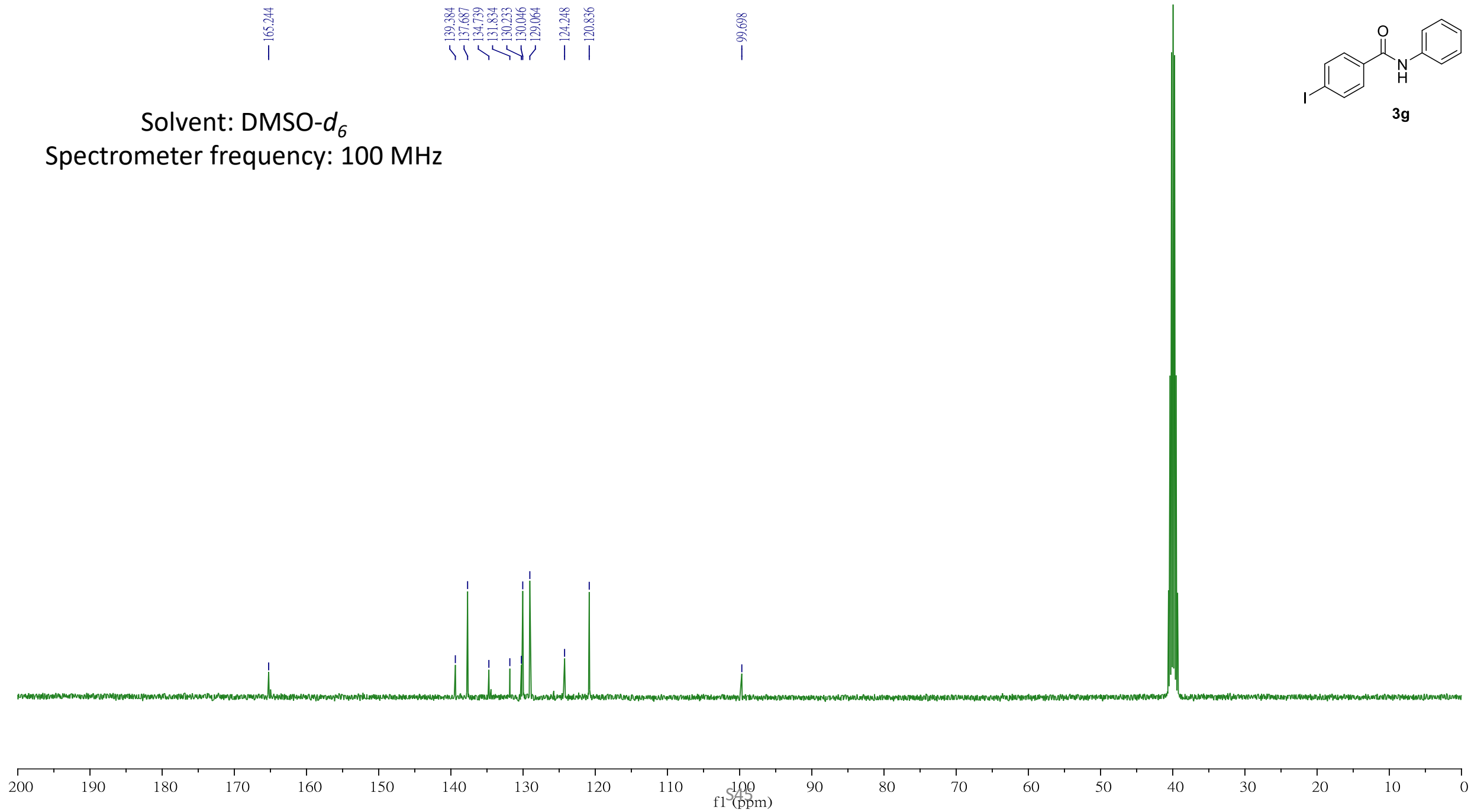
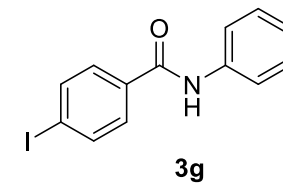


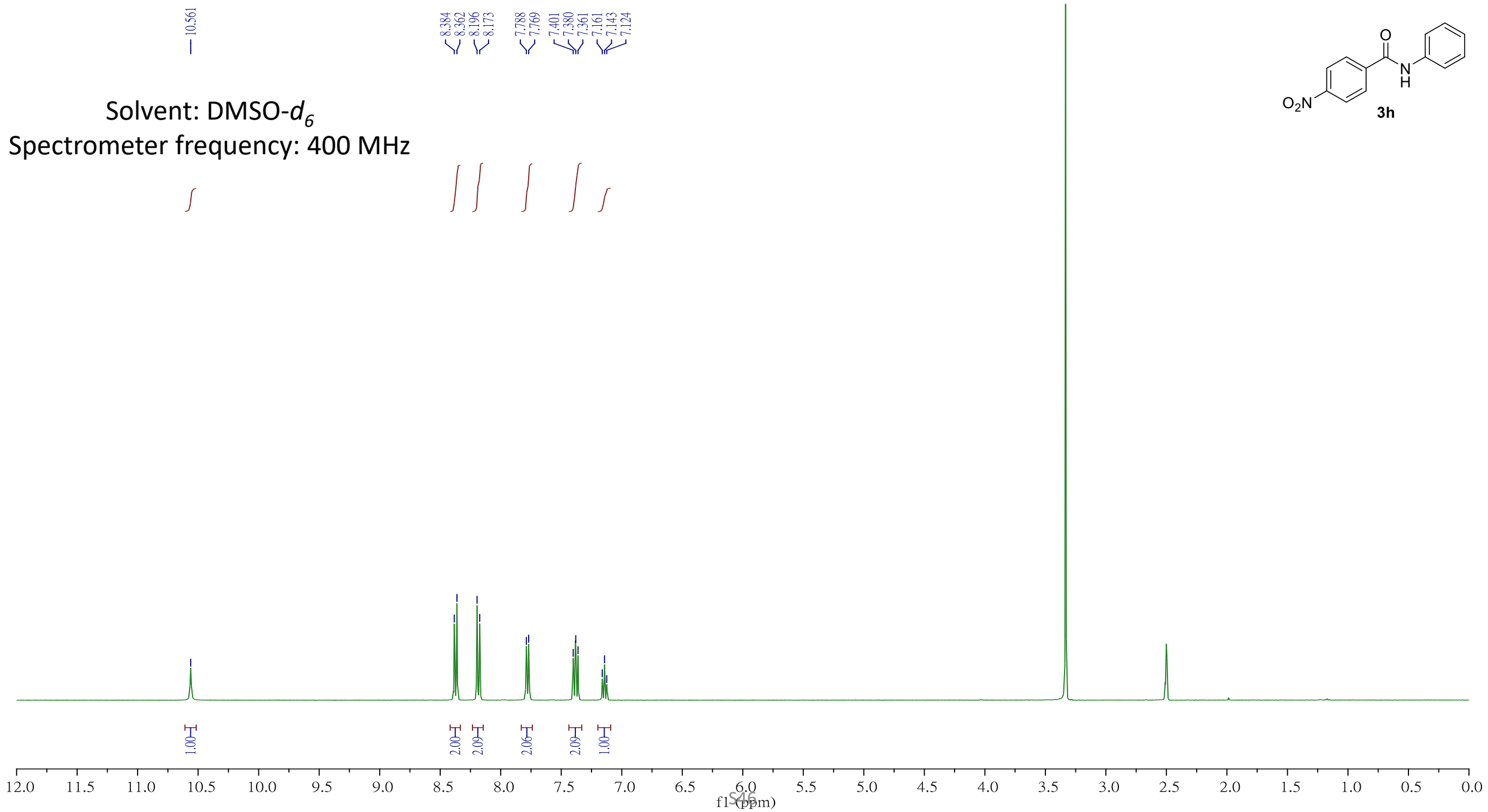
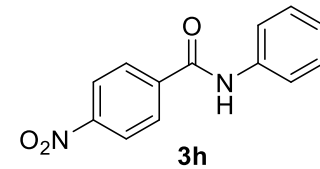
Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz

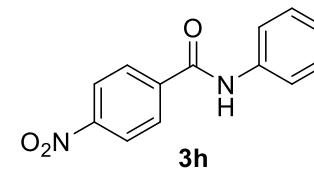




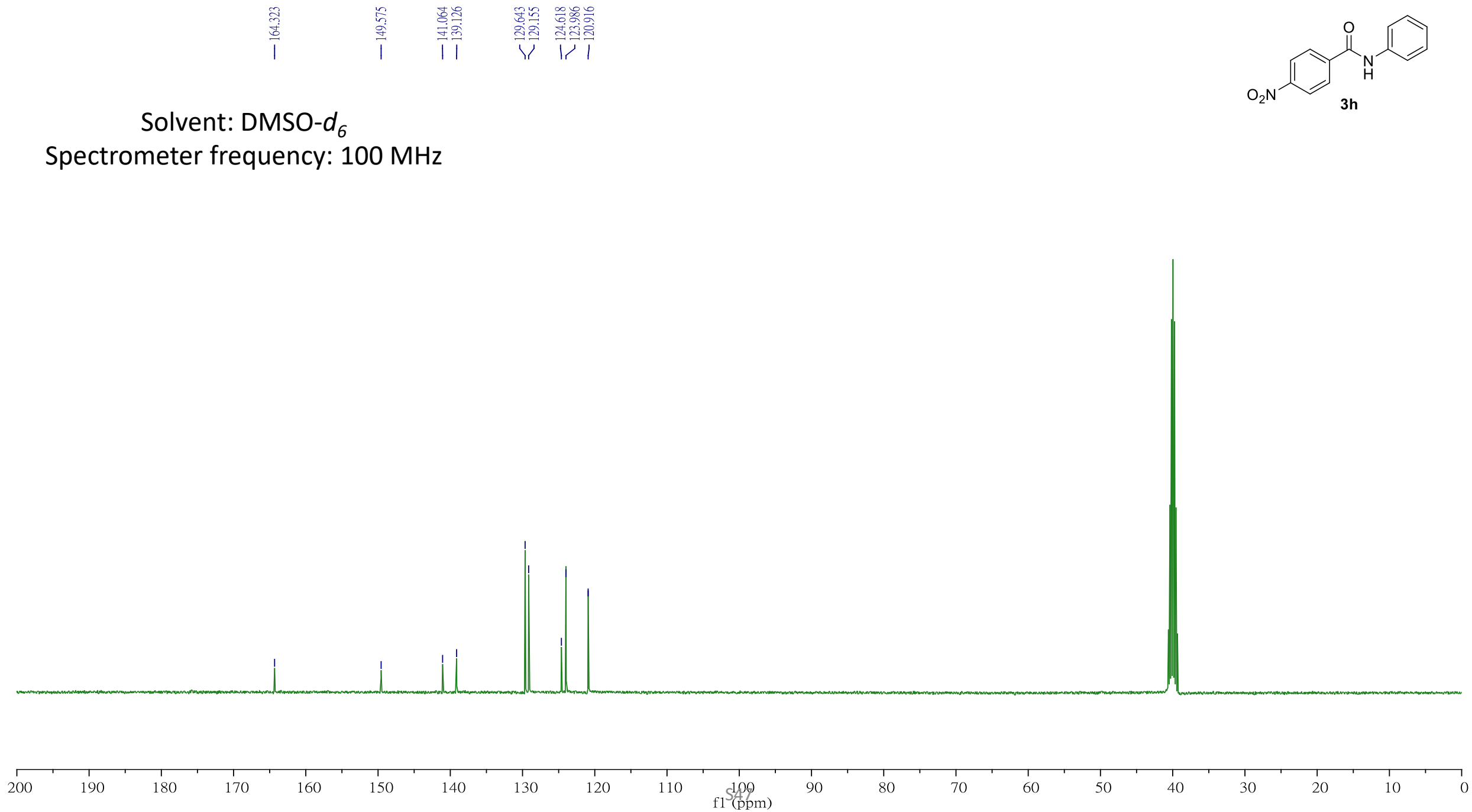
Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz

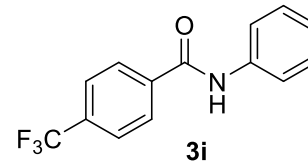




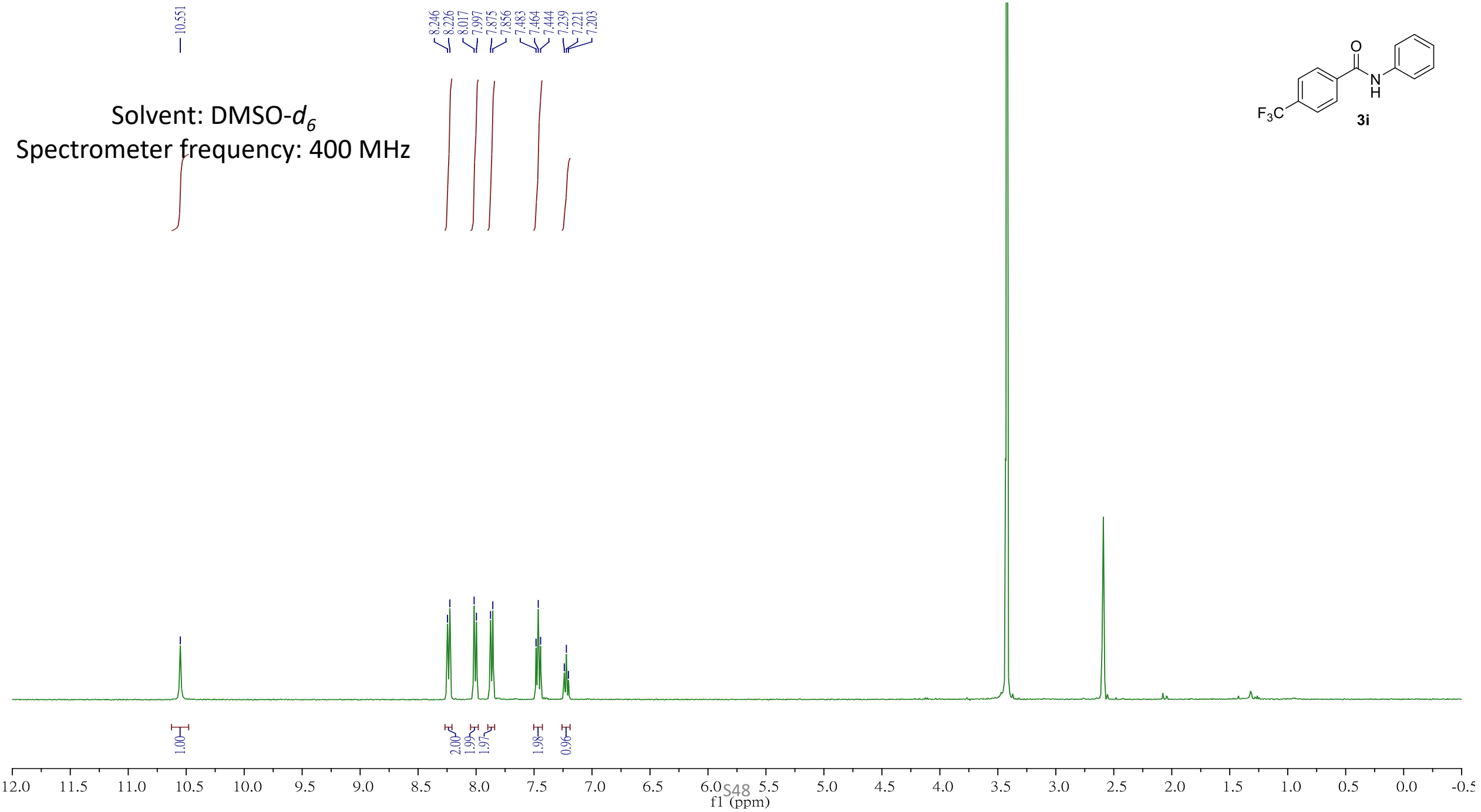


Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz





Solvent: DMSO-*d*₆
Spectrometer frequency: 400 MHz

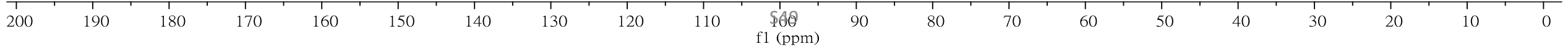
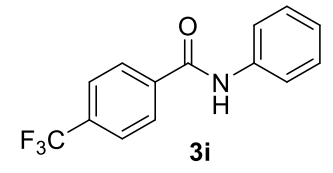


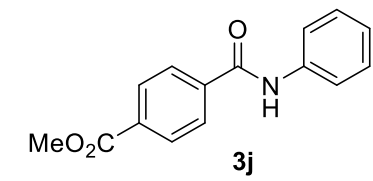
M0032-7
NQ-DI-CF3 -CARBON

164.82

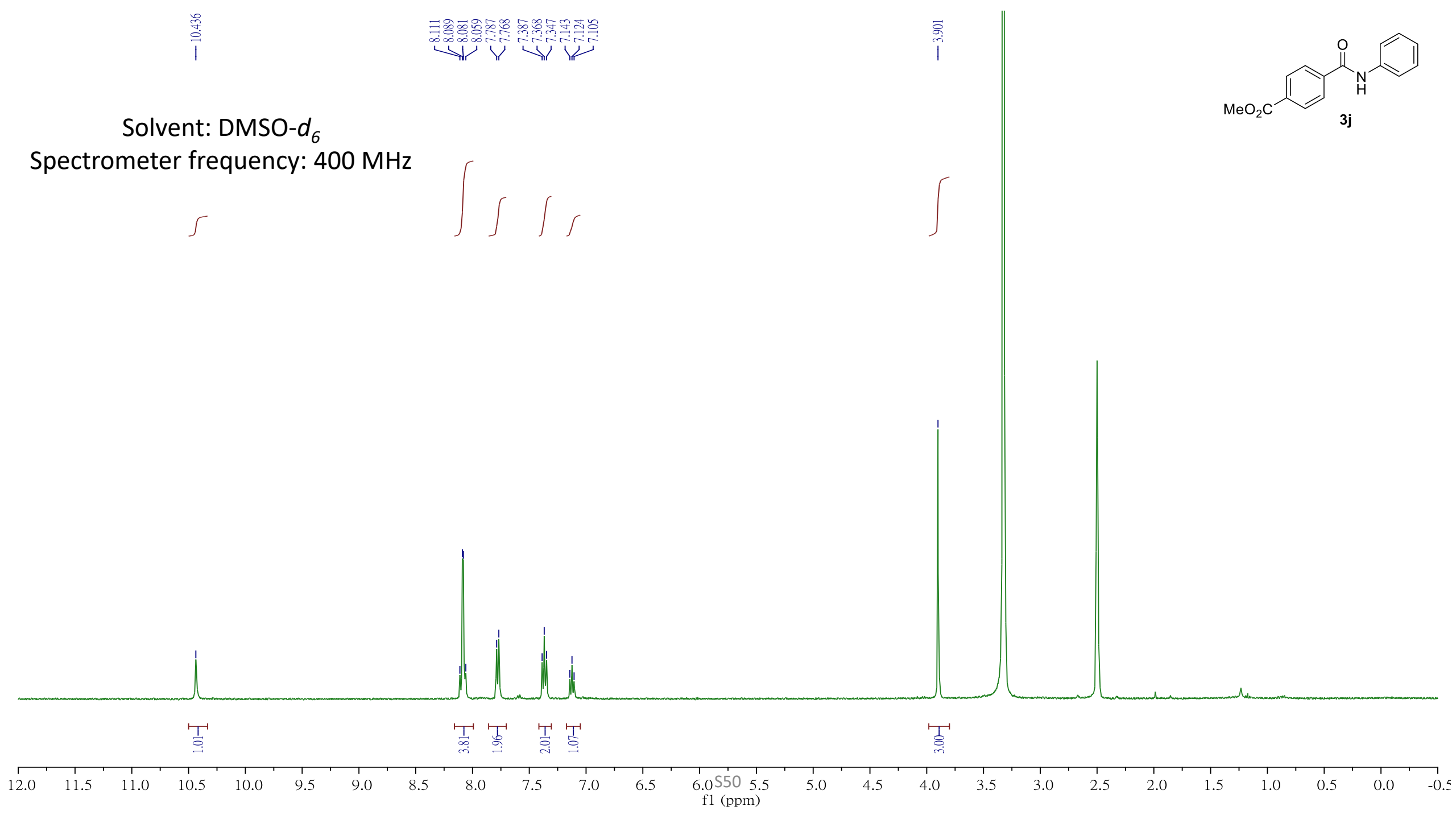
139.24
131.93
131.61
129.12
129.03
125.93
125.88
125.85
125.81
125.77
125.72
124.54
124.47
123.01
120.88

Solvent: DMSO-*d*₆
Spectrometer frequency: 100 MHz

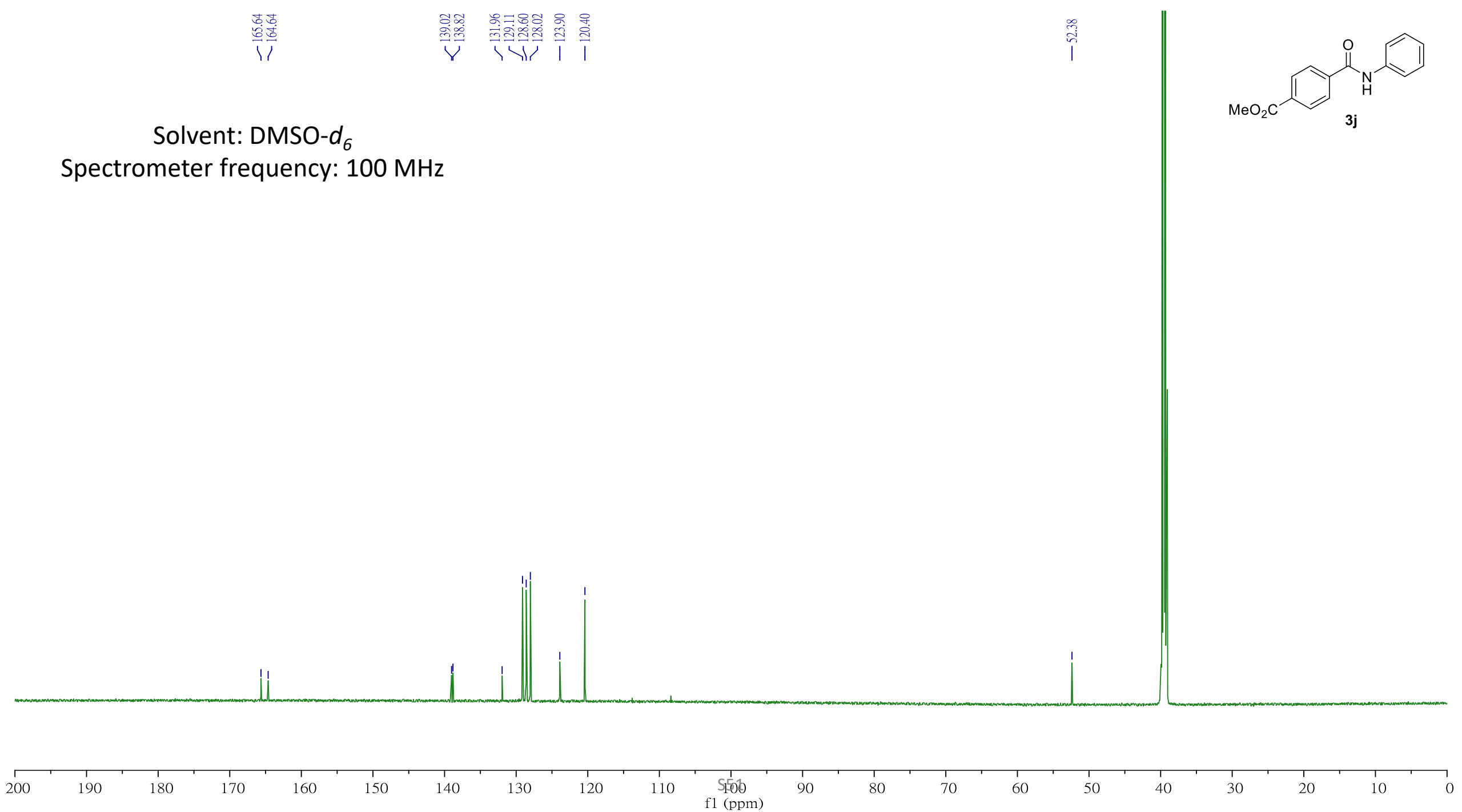
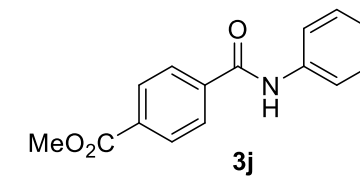


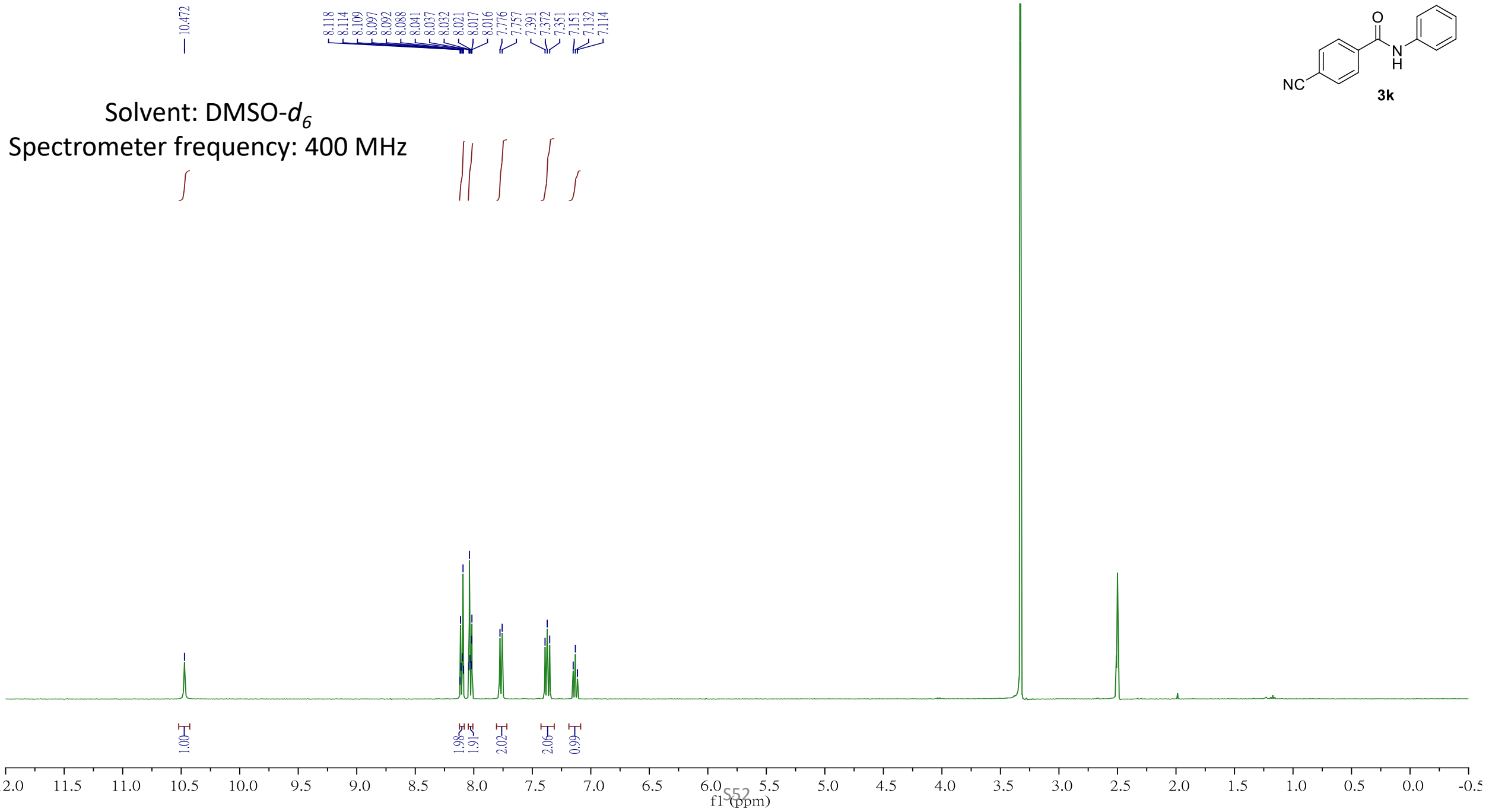
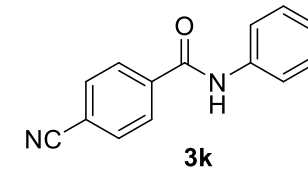


Solvent: DMSO-*d*₆
Spectrometer frequency: 400 MHz

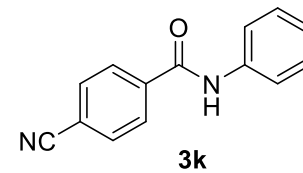


Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz

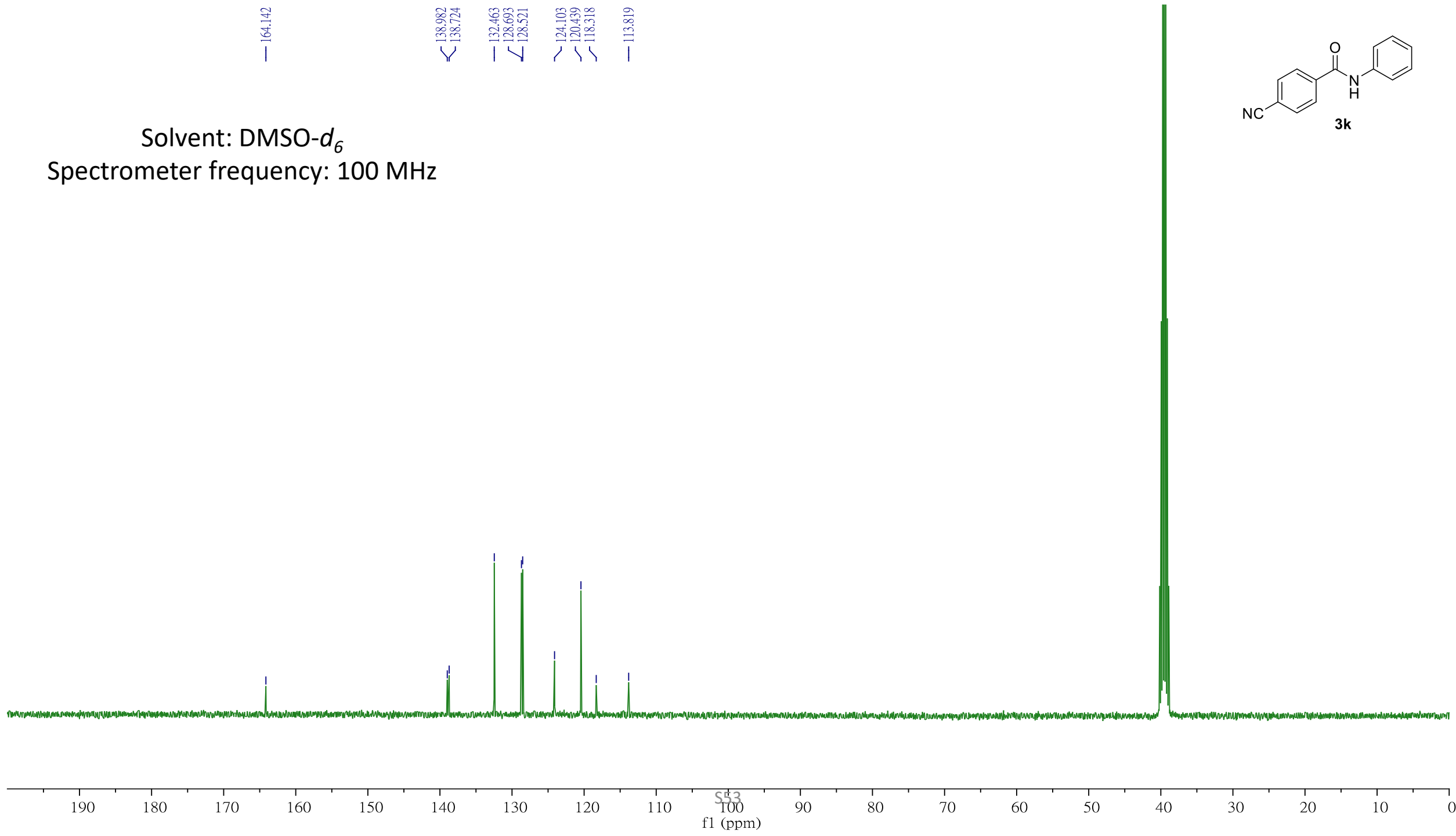


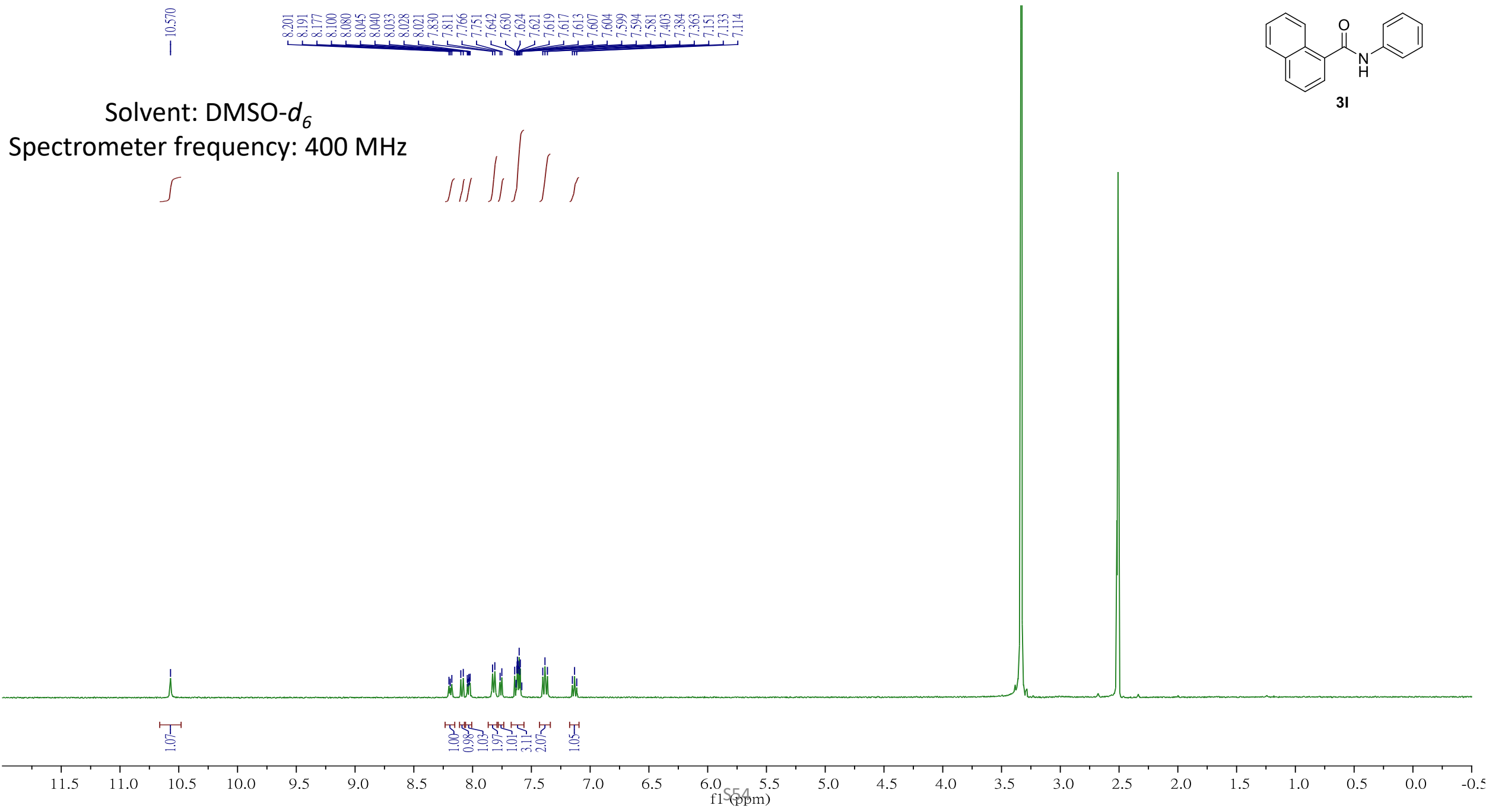
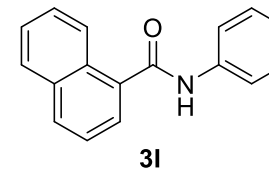


Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



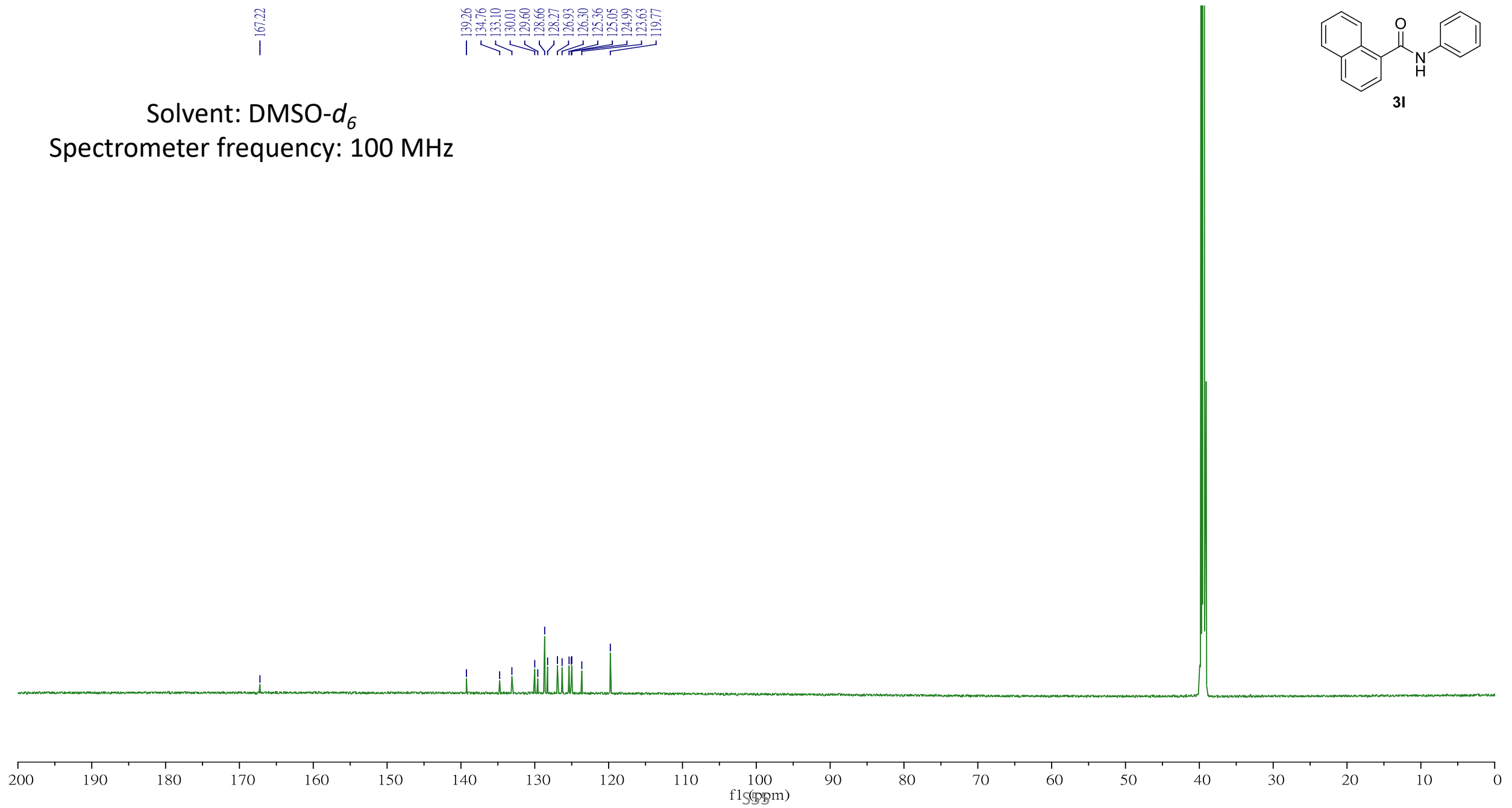
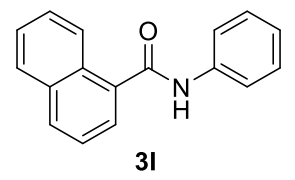
164.142
138.982 138.724
132.463 128.693 128.521
124.103 120.439 118.318
113.819

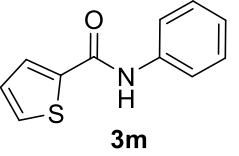




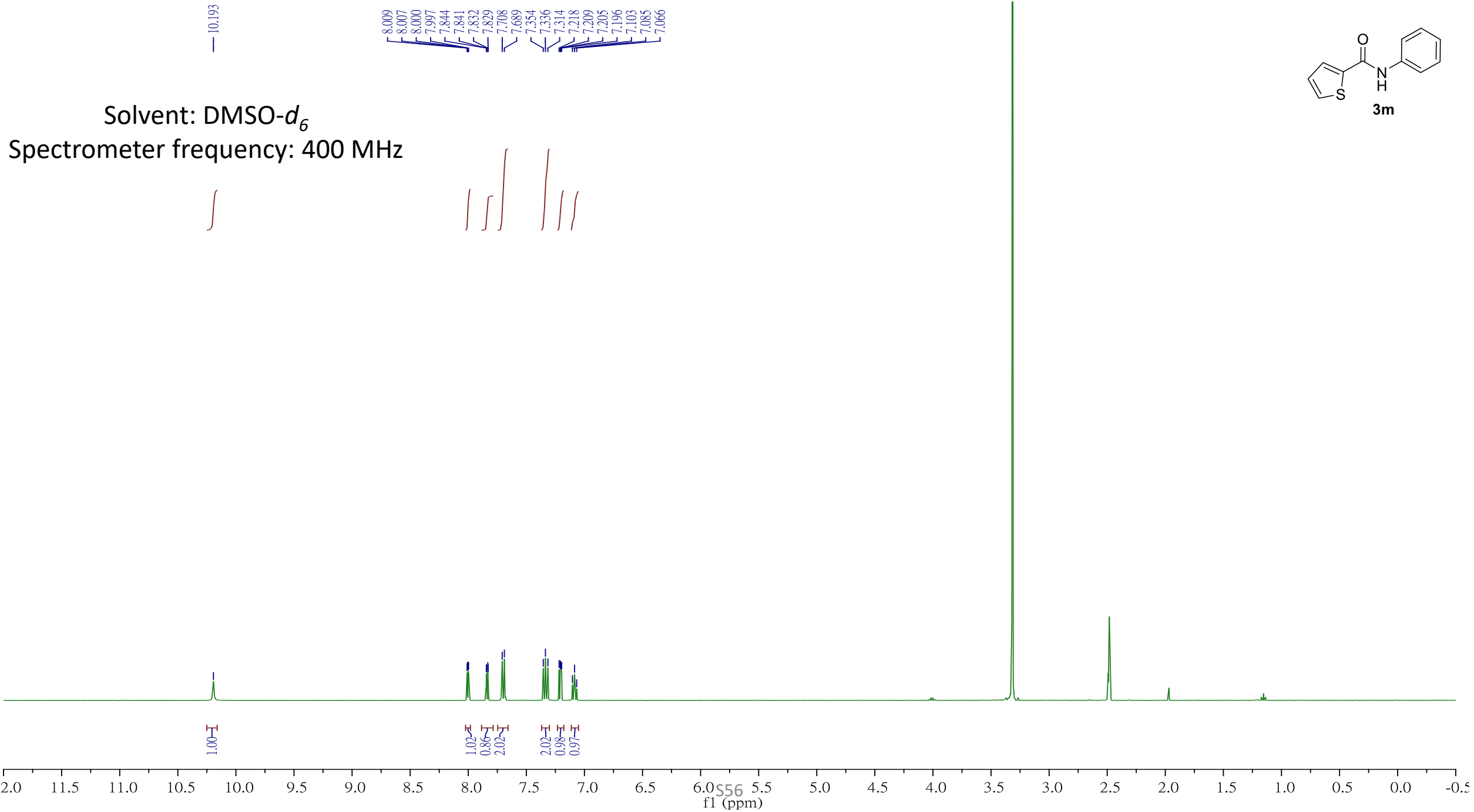
139.26
134.76
133.10
130.01
129.60
128.66
128.27
126.93
126.30
125.36
125.05
124.99
123.63
119.77

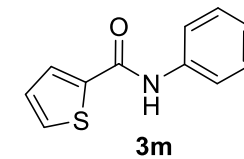
Solvent: DMSO-*d*₆
Spectrometer frequency: 100 MHz



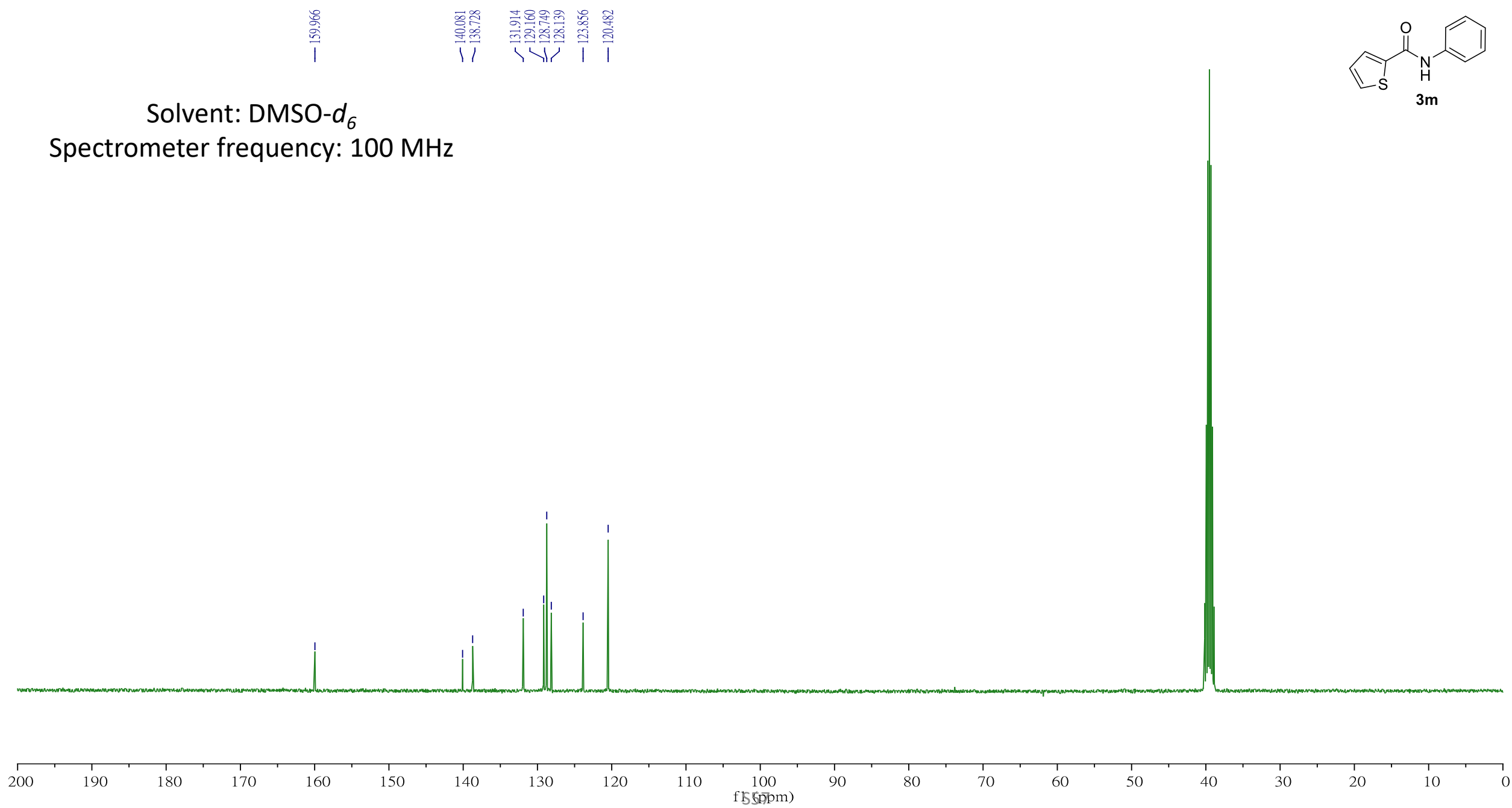


Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz





Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz

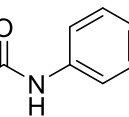
9.822

7.590
7.568
7.291
7.273
7.251
7.023
7.008
6.989

2.303
2.284
2.266

1.336
1.287
1.282
1.272
1.260
1.246
1.234
0.874
0.859
0.842

3n



0.96

1.90
1.96
1.06

2.00

2.02

8.07

3.16

0.96

1.90
1.96
1.06

2.00

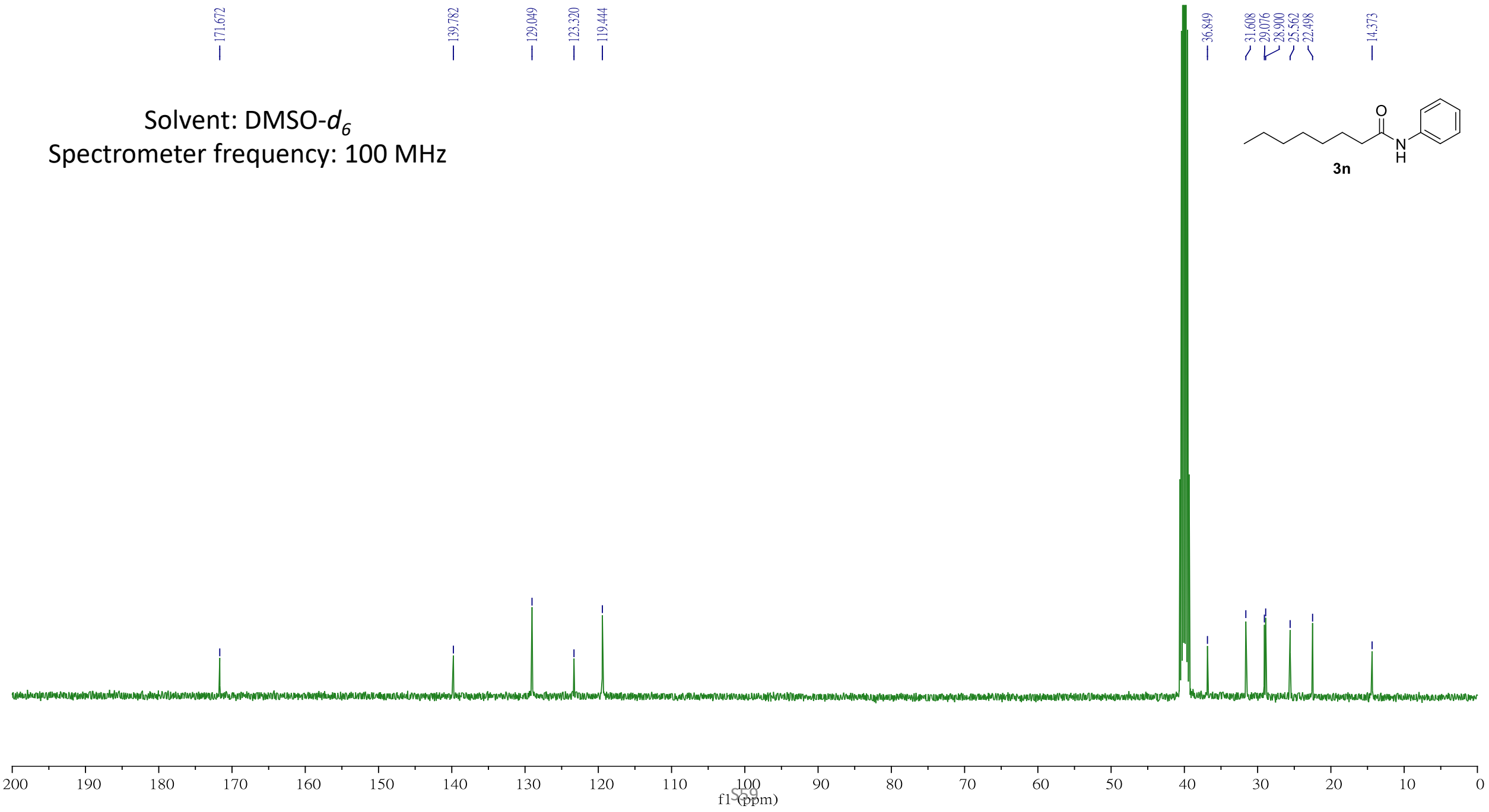
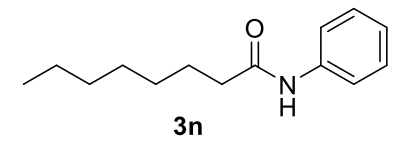
2.02

8.07

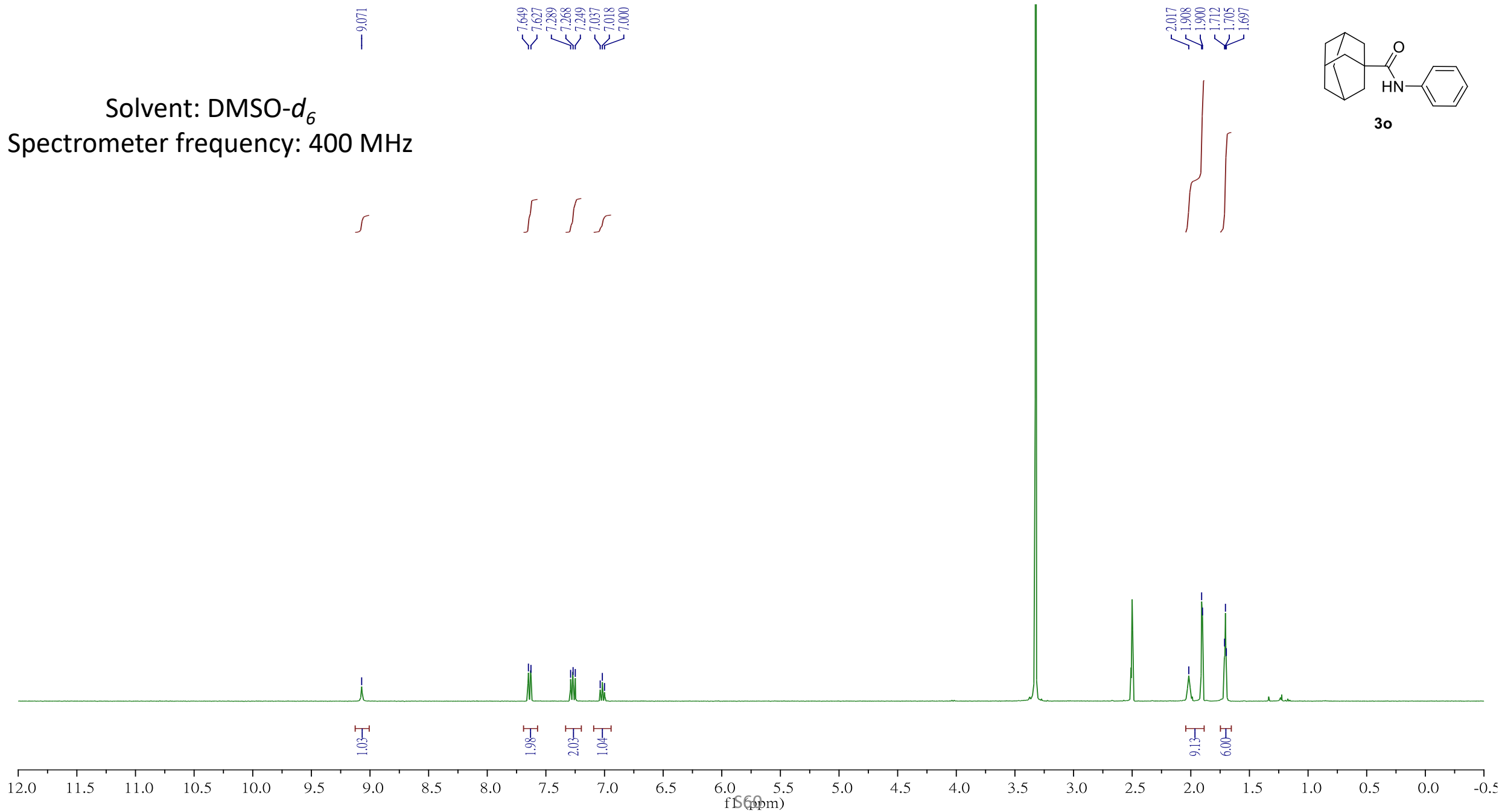
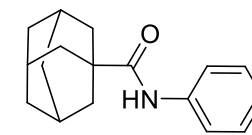
3.16

f1 (ppm)

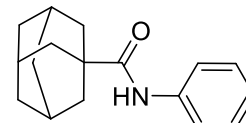
Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



176.333

139.767

128.788

123.514

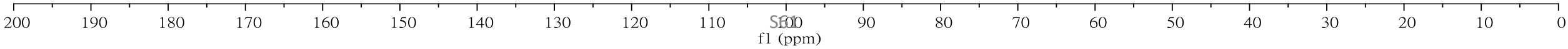
120.647

41.330

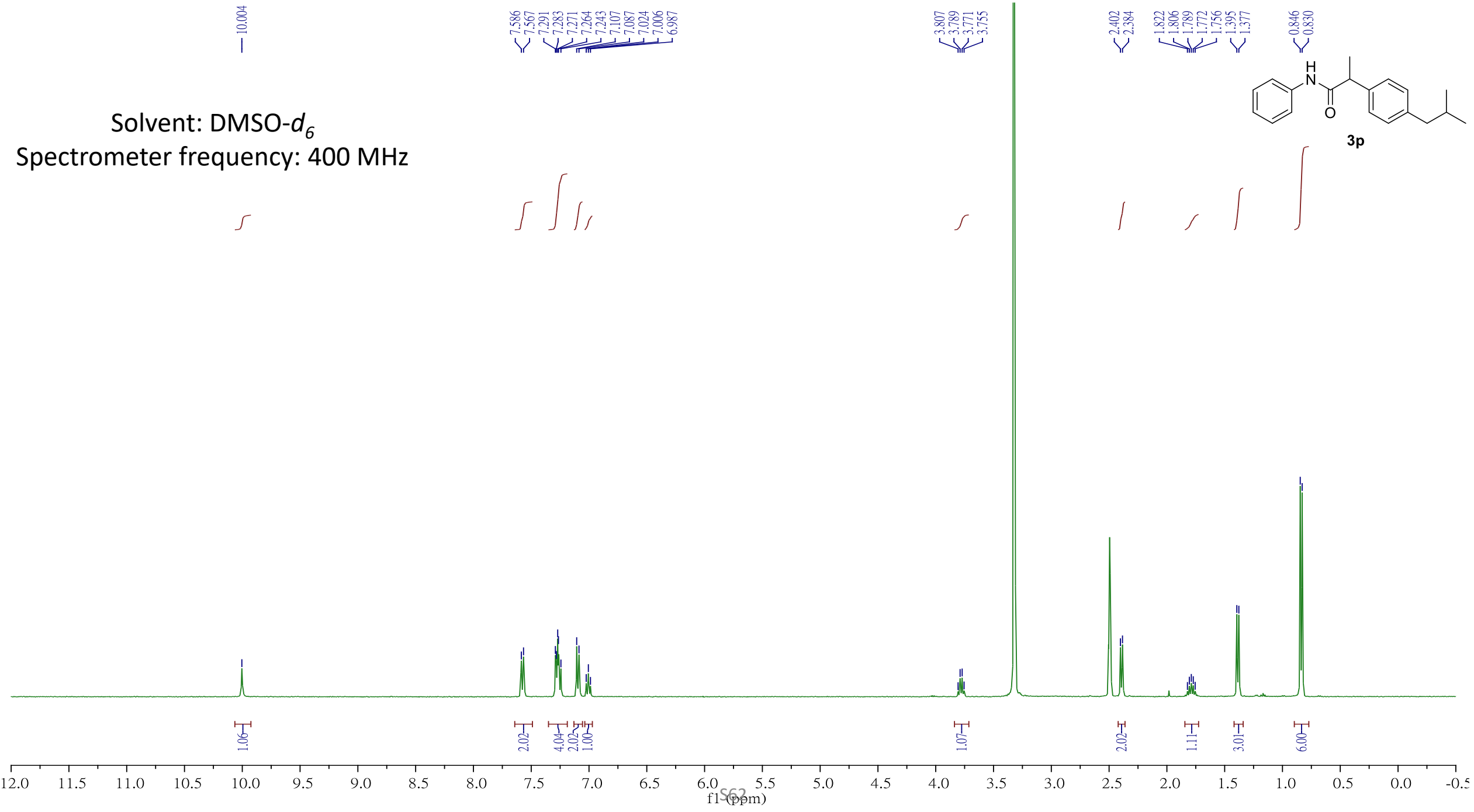
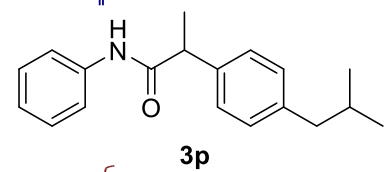
38.749

36.468

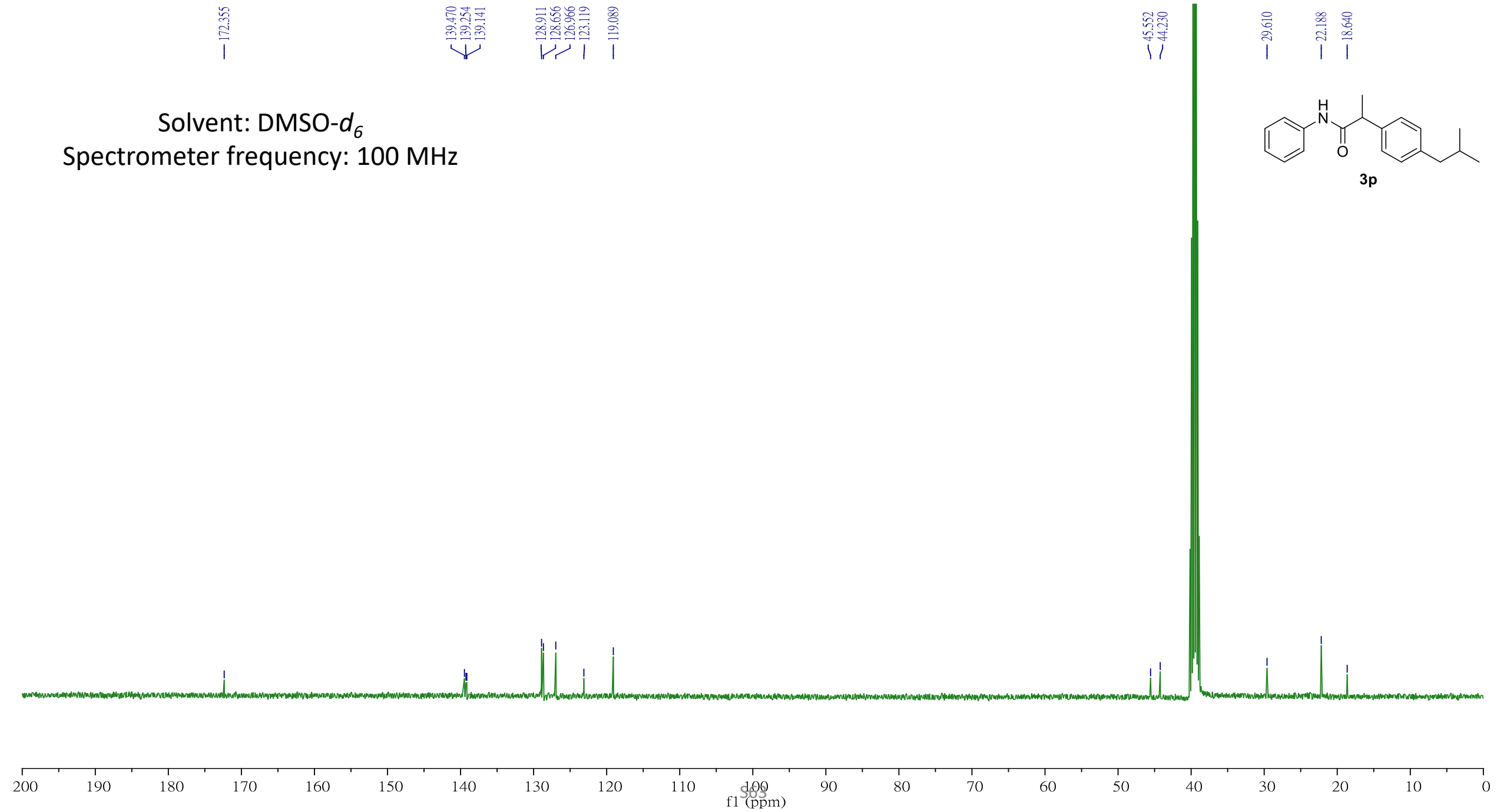
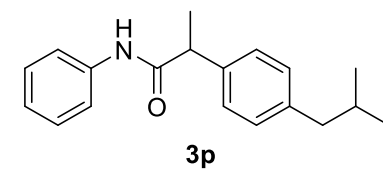
28.131

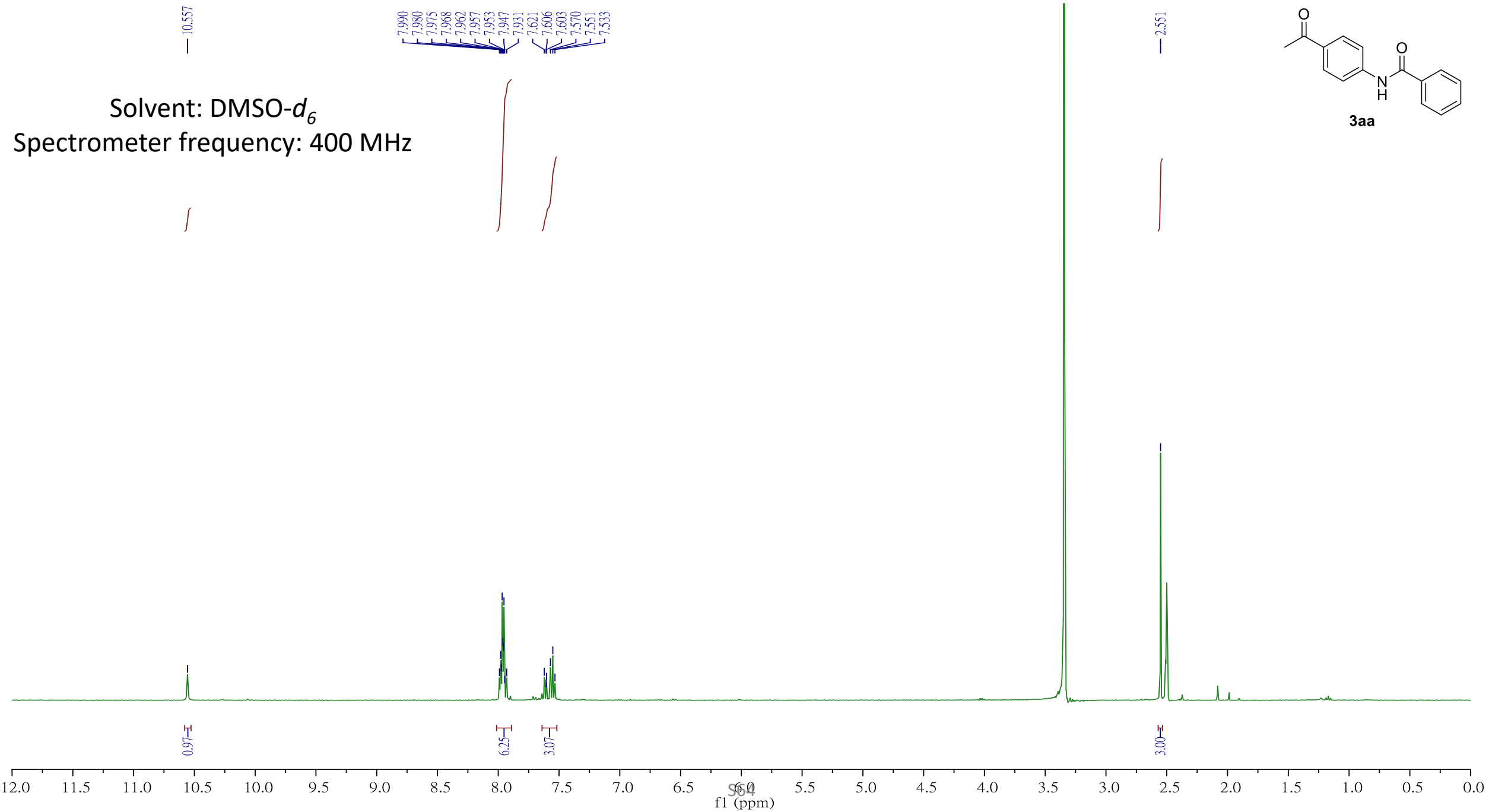


Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



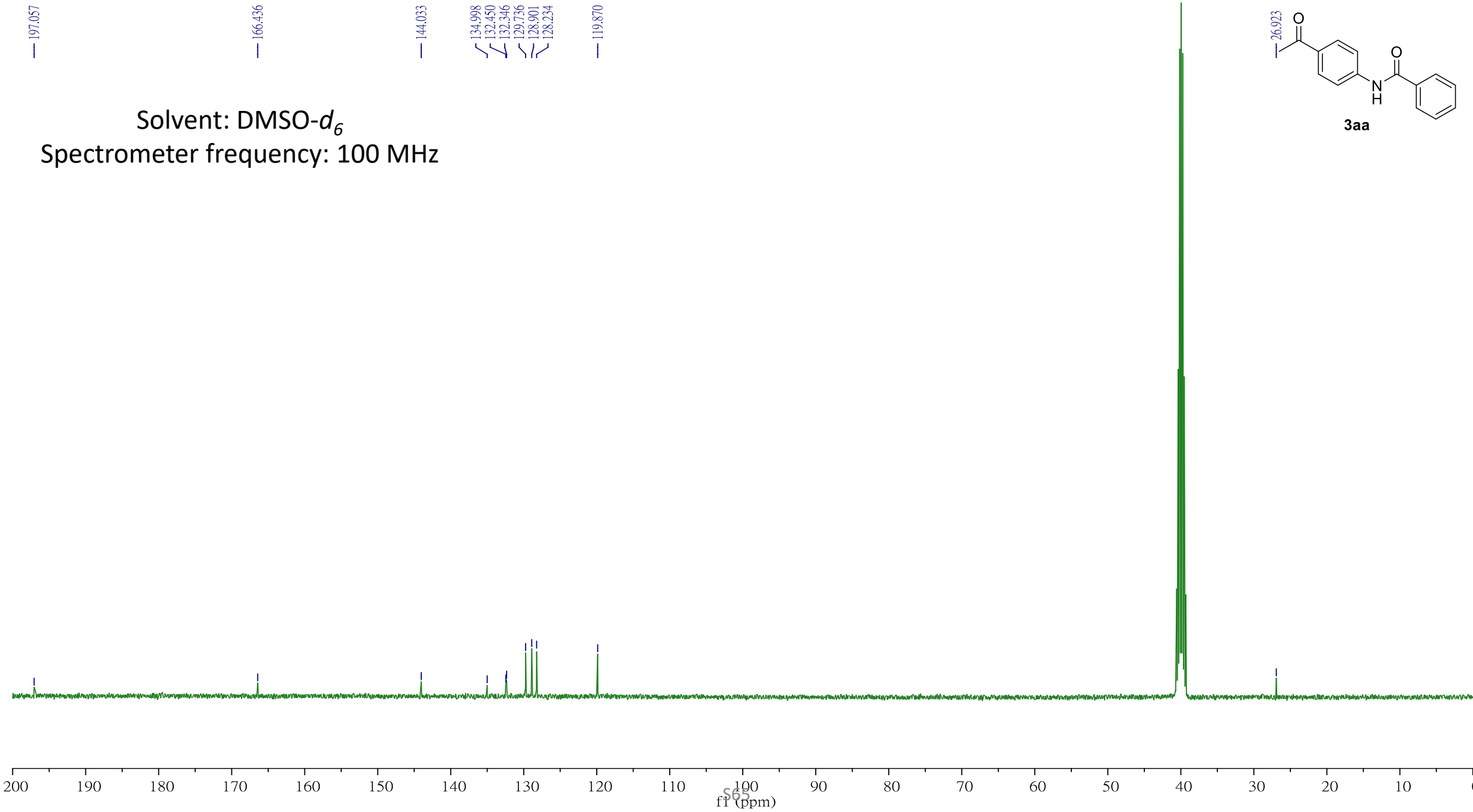
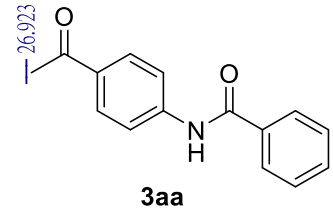
Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



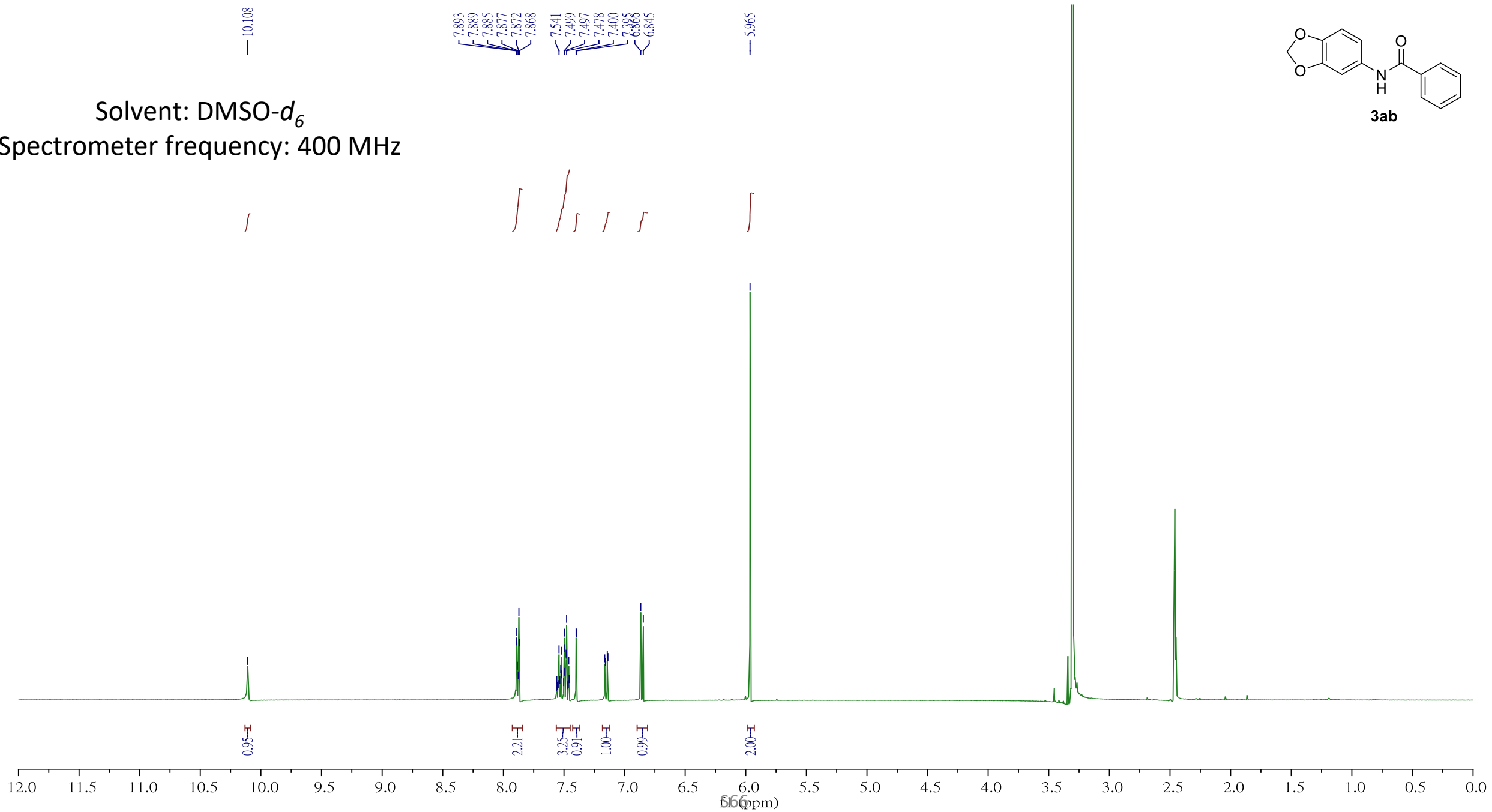
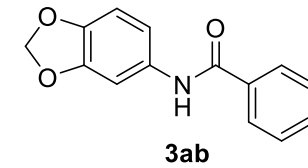


197.057
166.436
144.033
134.998
132.450
132.346
129.736
128.901
128.234
119.870

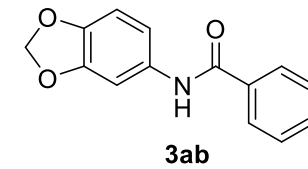
Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



165.773

147.478

143.758

135.462

133.986

132.001

128.899

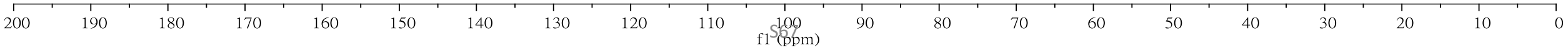
128.074

113.869

108.446

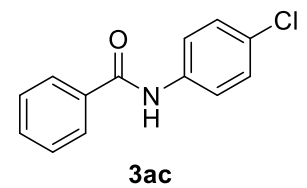
103.014

101.518

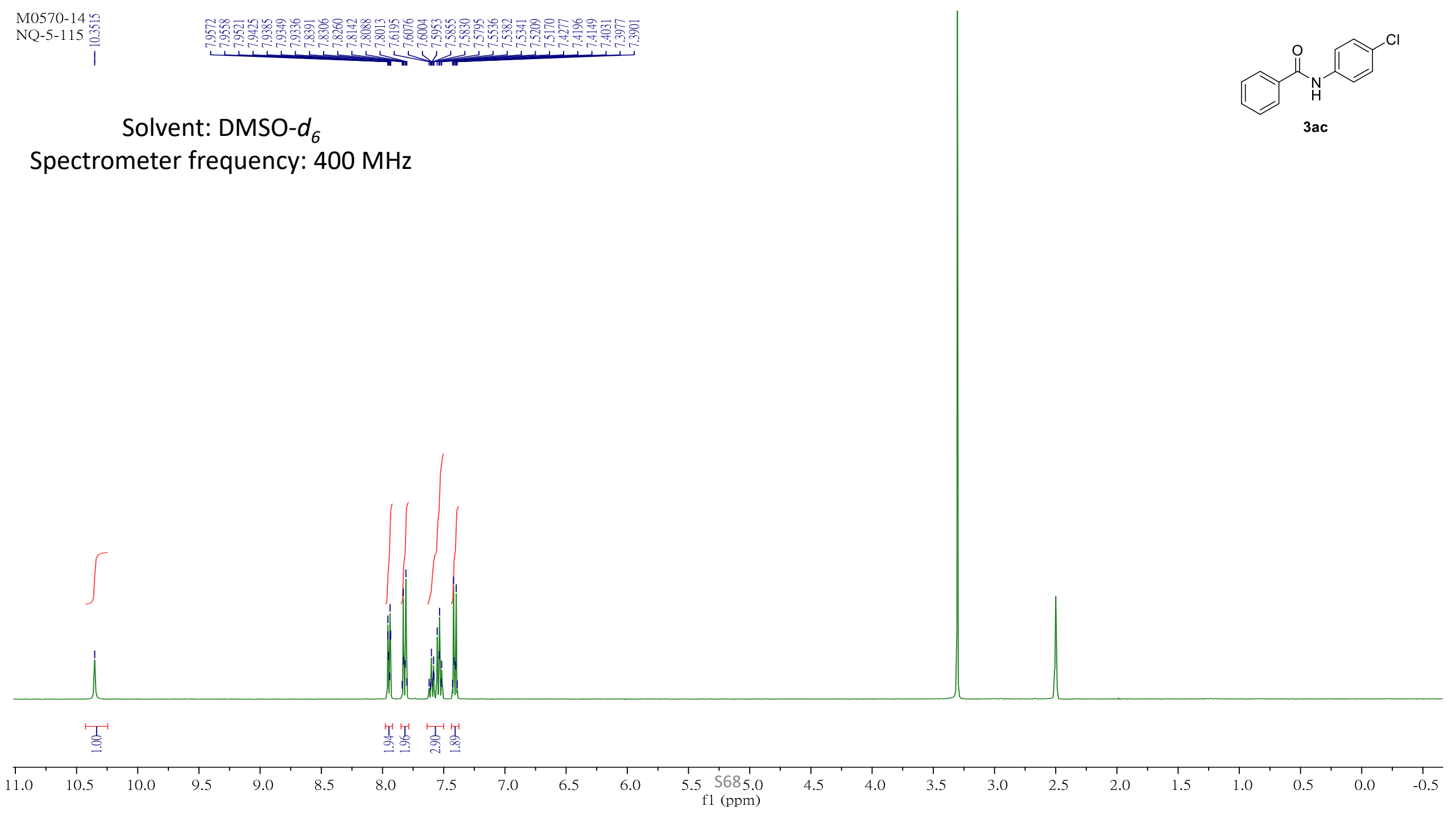


M0570-14
NQ-5-115

7.9572
7.9558
7.9521
7.9425
7.9385
7.9349
7.9336
7.8391
7.8306
7.8260
7.8142
7.8088
7.8013
7.6195
7.6076
7.6004
7.5953
7.5855
7.5830
7.5795
7.5536
7.5382
7.5341
7.5209
7.5170
7.4277
7.4196
7.4149
7.4031
7.3977
7.3901



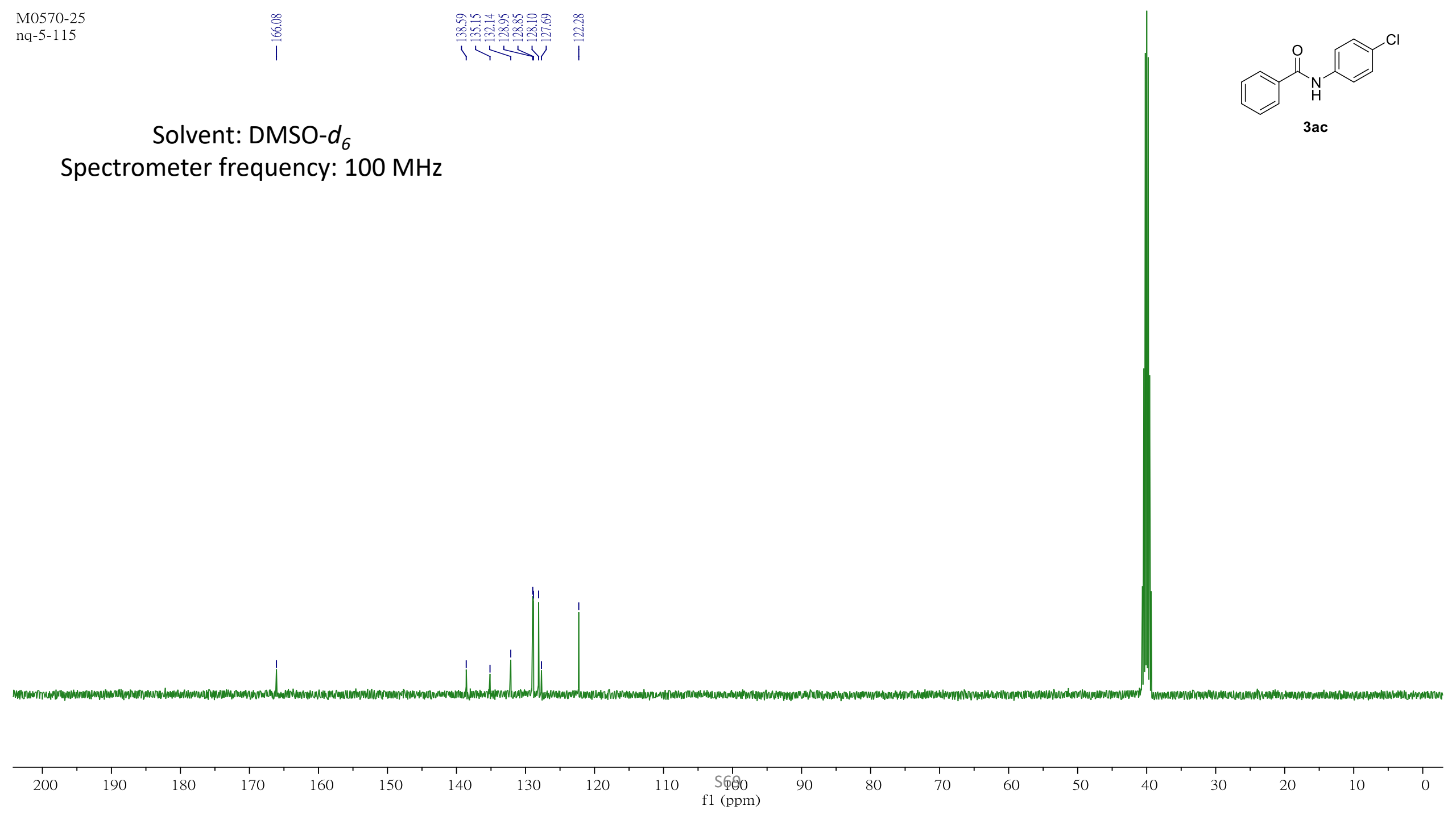
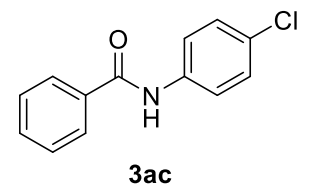
Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



M0570-25
nq-5-115

166.08
138.59
135.15
132.14
128.95
128.85
128.10
127.69
122.28

Solvent: DMSO-*d*₆
Spectrometer frequency: 100 MHz

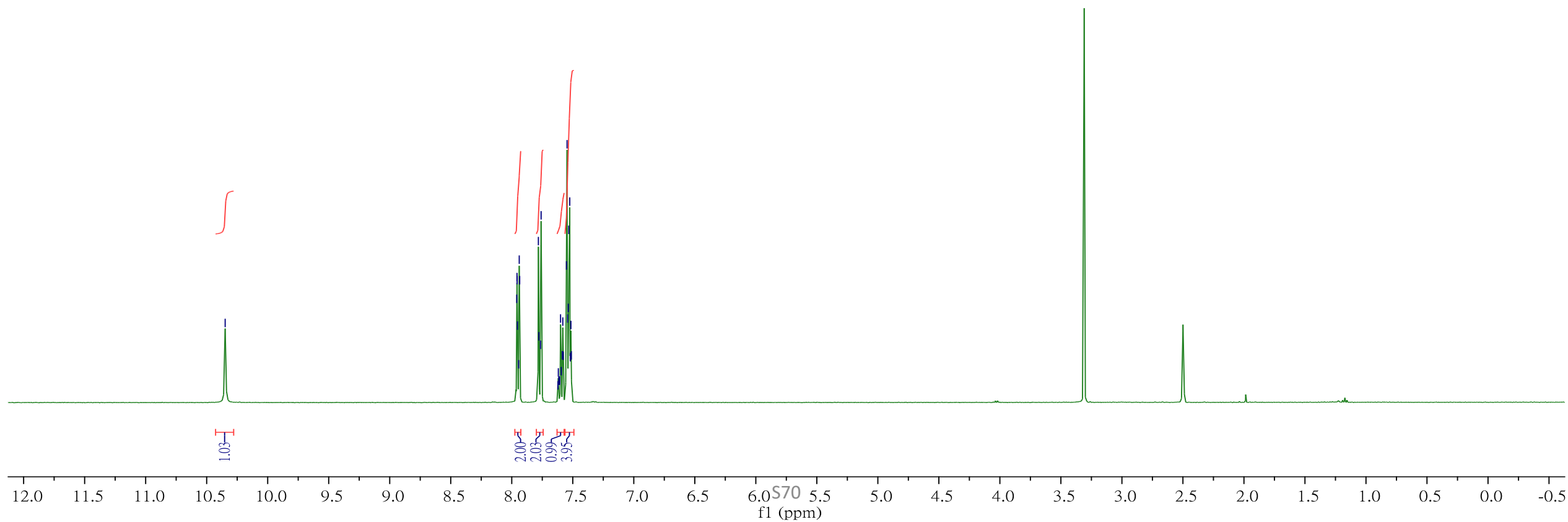
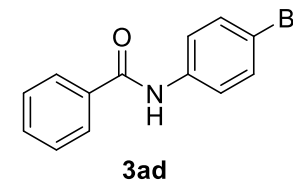


M0570-15
NQ-5-114-1

10.3485

7.9589
7.9570
7.9558
7.9538
7.9438
7.9386
7.9349
7.7818
7.7777
7.7647
7.7595
7.6216
7.6183
7.6150
7.6066
7.6001
7.5943
7.5854
7.5819
7.5784
7.5517
7.5468
7.5418
7.5367
7.5328
7.5246
7.5201
7.5154
7.5120

Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



M0570-23
NQ-5-114-1

166.09

139.01

135.13

132.15

131.87

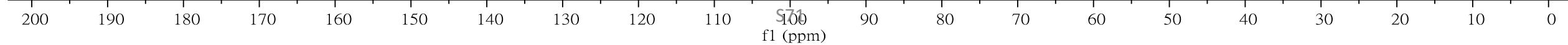
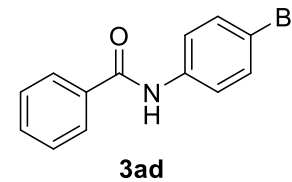
128.86

128.11

122.63

115.75

Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



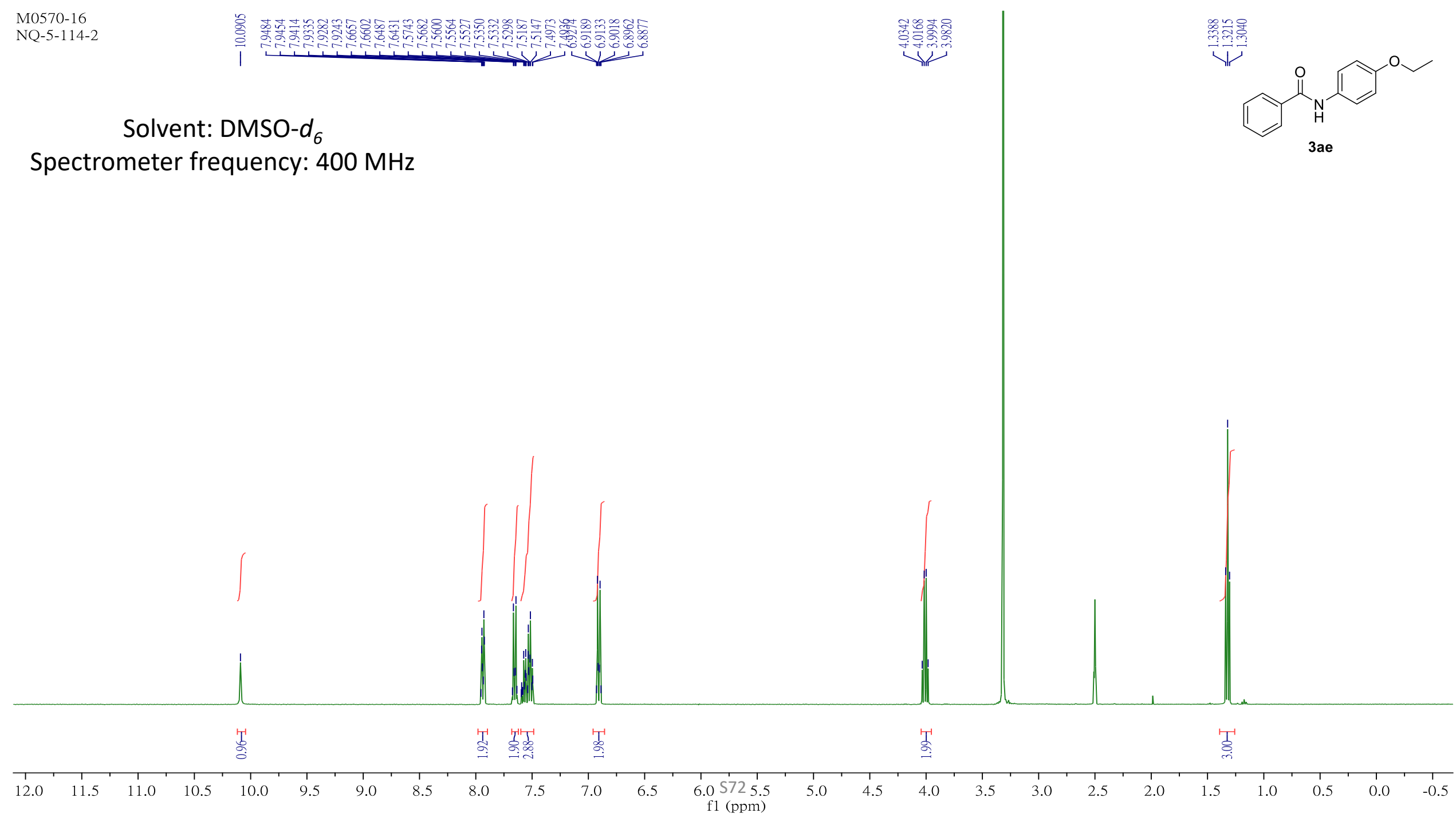
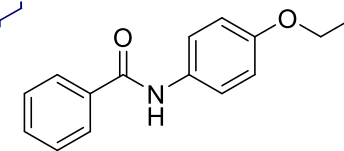
M0570-16
NQ-5-114-2

10.0905
7.9484
7.9454
7.9414
7.9335
7.9282
7.9243
7.6657
7.6602
7.6487
7.6431
7.5743
7.5682
7.5600
7.5564
7.5527
7.5350
7.5332
7.5298
7.5187
7.5147
7.4973
7.4936
6.9189
6.9133
6.9018
6.8962
6.8877

4.0342
4.0168
3.9994
3.9820

1.3388
1.3215
1.3040

Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



M0570-22
NQ-5-114-2

165.52

155.23

135.49

132.54

131.79

128.78

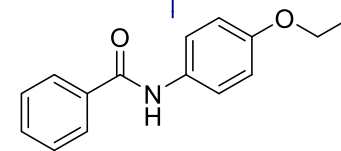
127.96

122.39

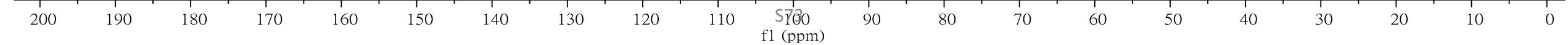
114.68

63.52

Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



15.15



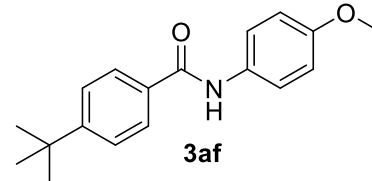
MO602-3
NQ-5-131-3

10.0197

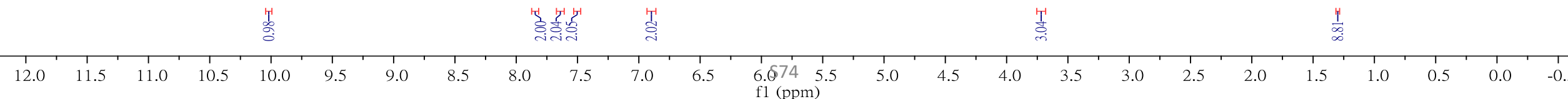
7.8609
7.8401
7.6543
7.6320
7.5200
7.4993
6.9184
6.9101
6.9054
6.8932
6.8879
6.8794

3.7229

1.2000



Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



6.74
f1 (ppm)

M0606-8
nq-5-131-3

165.4765

155.8787
154.6185

132.7731

132.7524

127.8237

125.5377

122.3055

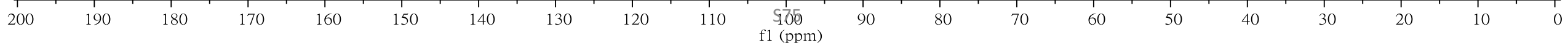
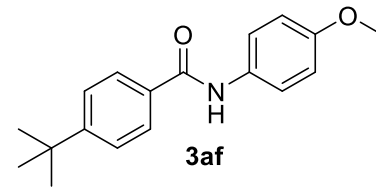
114.1404

55.6094

35.0942

31.3904

Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



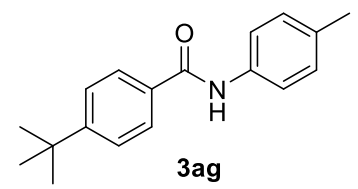
MO602-1
NQ-5-131-1

10.0784

7.8813
7.8607
7.6556
7.6350
7.5414
7.5207
7.1540
7.1335

2.2747

1.3179



Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz

12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

0.87

1.95

1.98

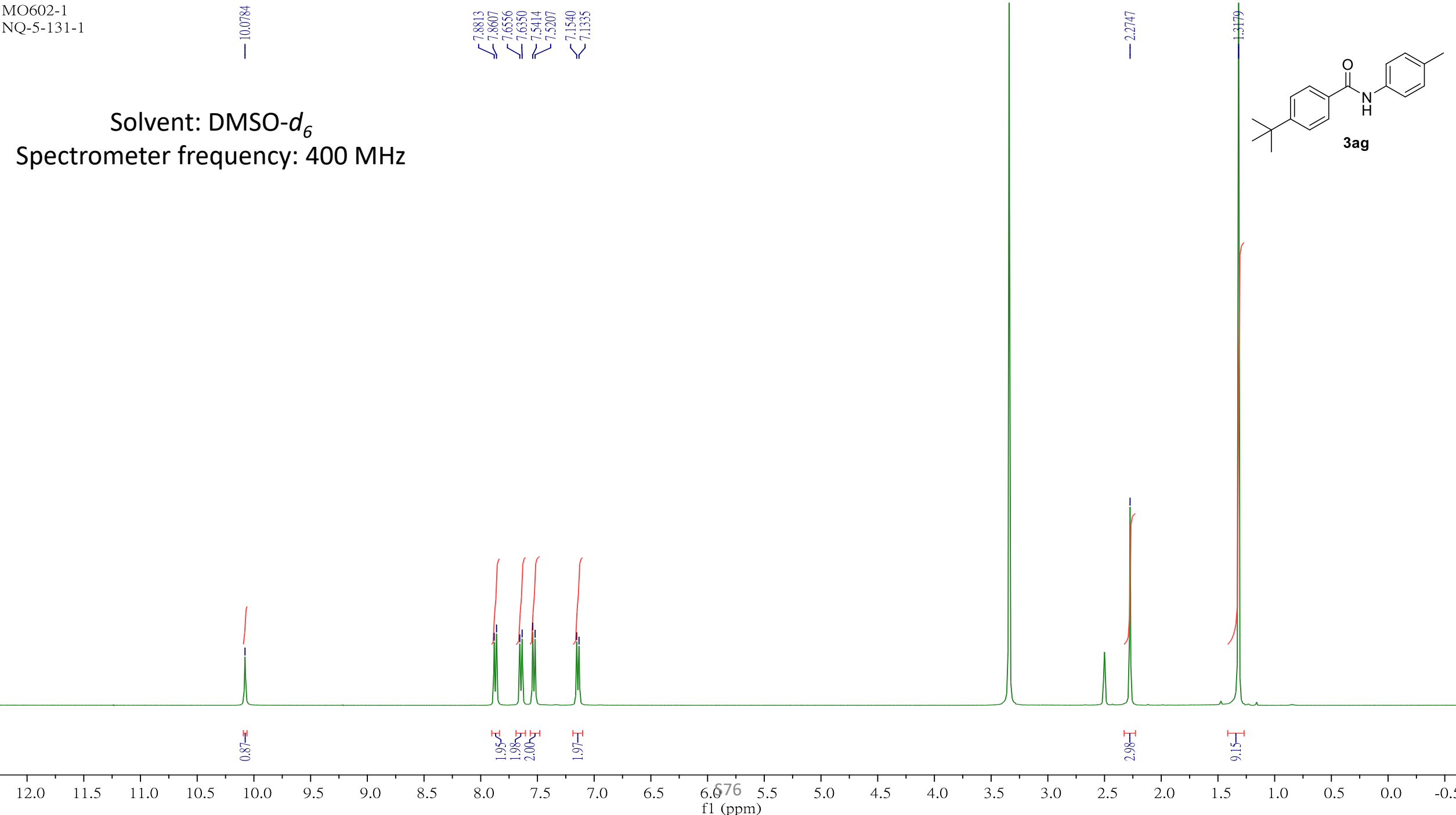
2.00

1.97

6.76

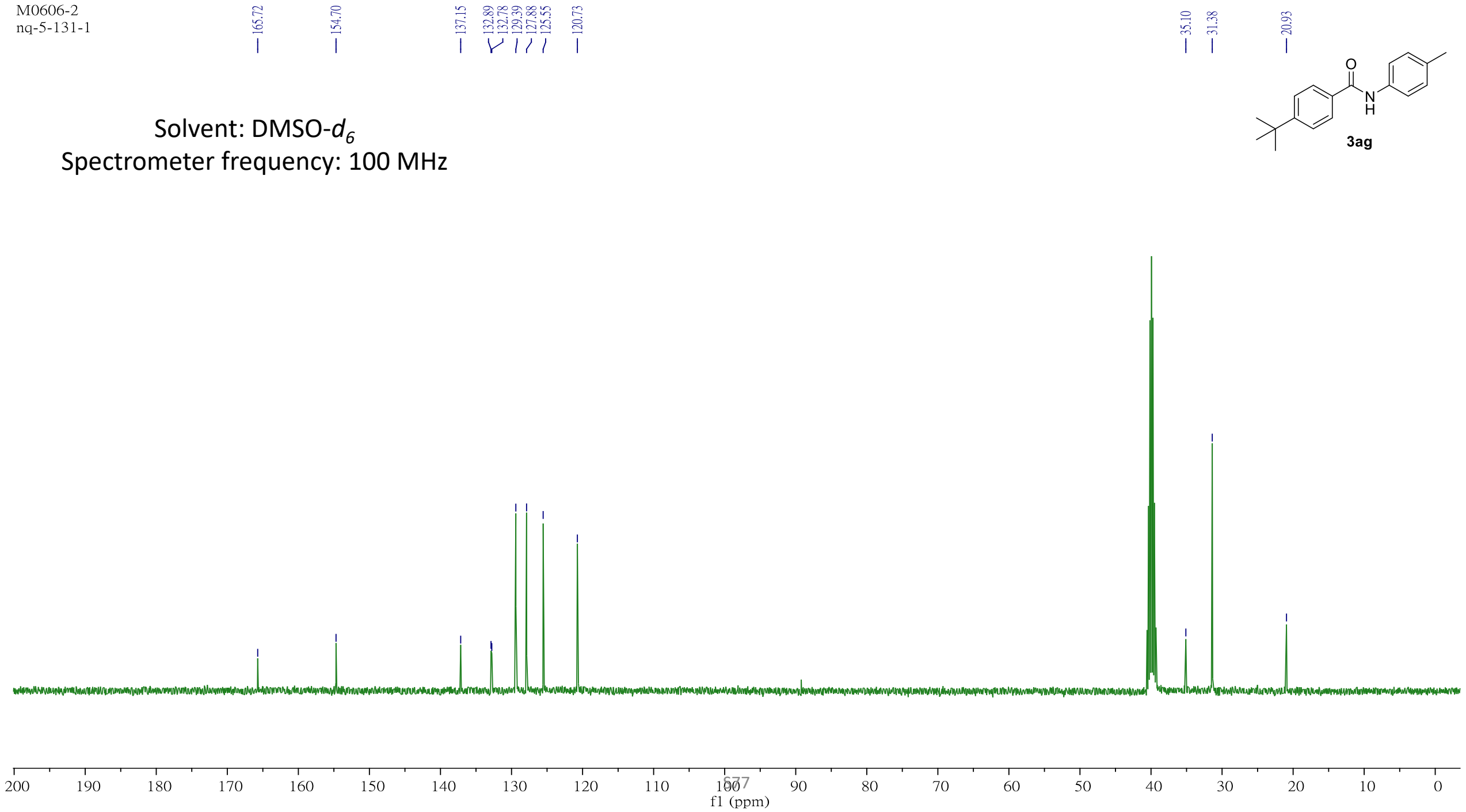
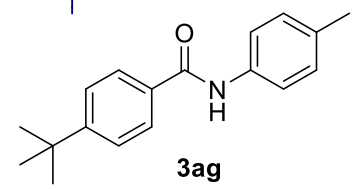
2.98

9.15



M0606-2
nq-5-131-1

Solvent: DMSO-*d*₆
Spectrometer frequency: 100 MHz

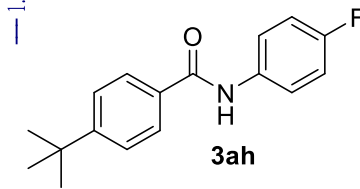


M0606-6
nq-5-131-2

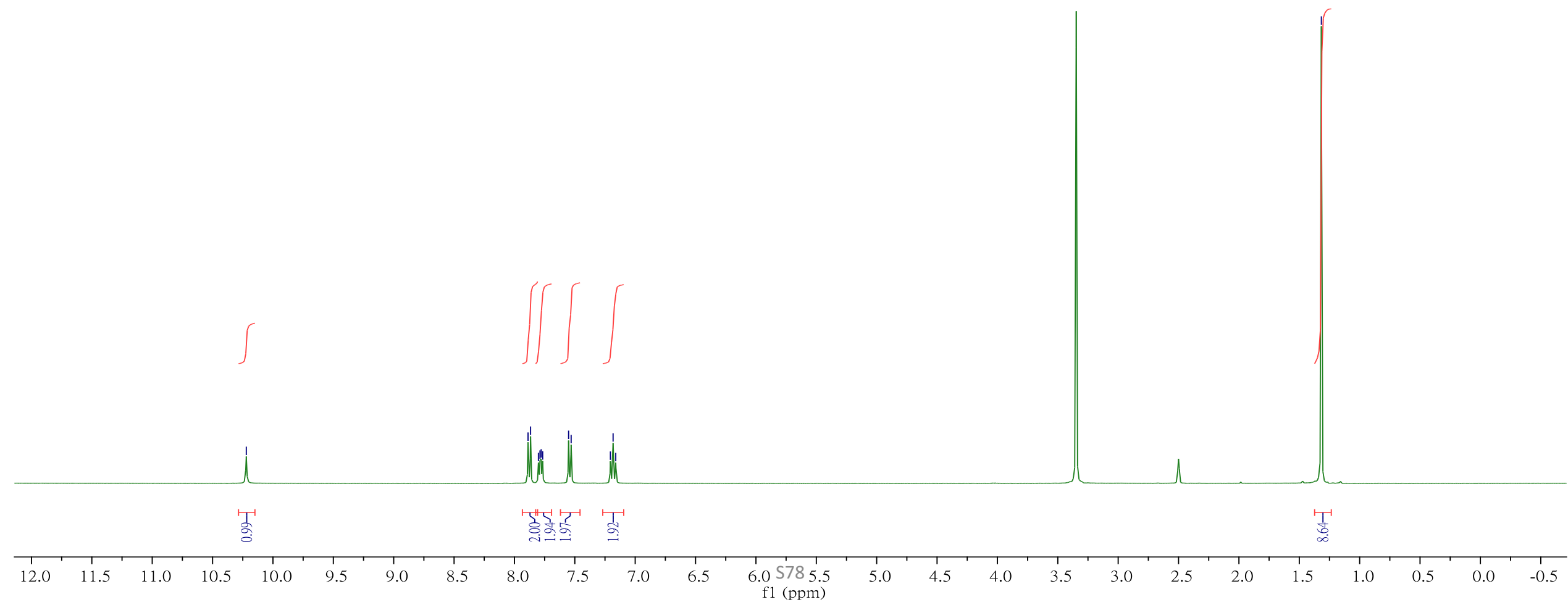
10.2210

7.8874
7.8664
7.8015
7.7888
7.7788
7.7662
7.5514
7.5304
7.2053
7.1831
7.1609

1.3173



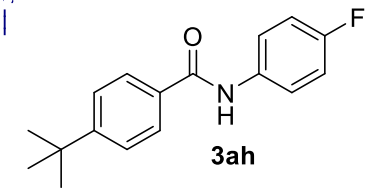
Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



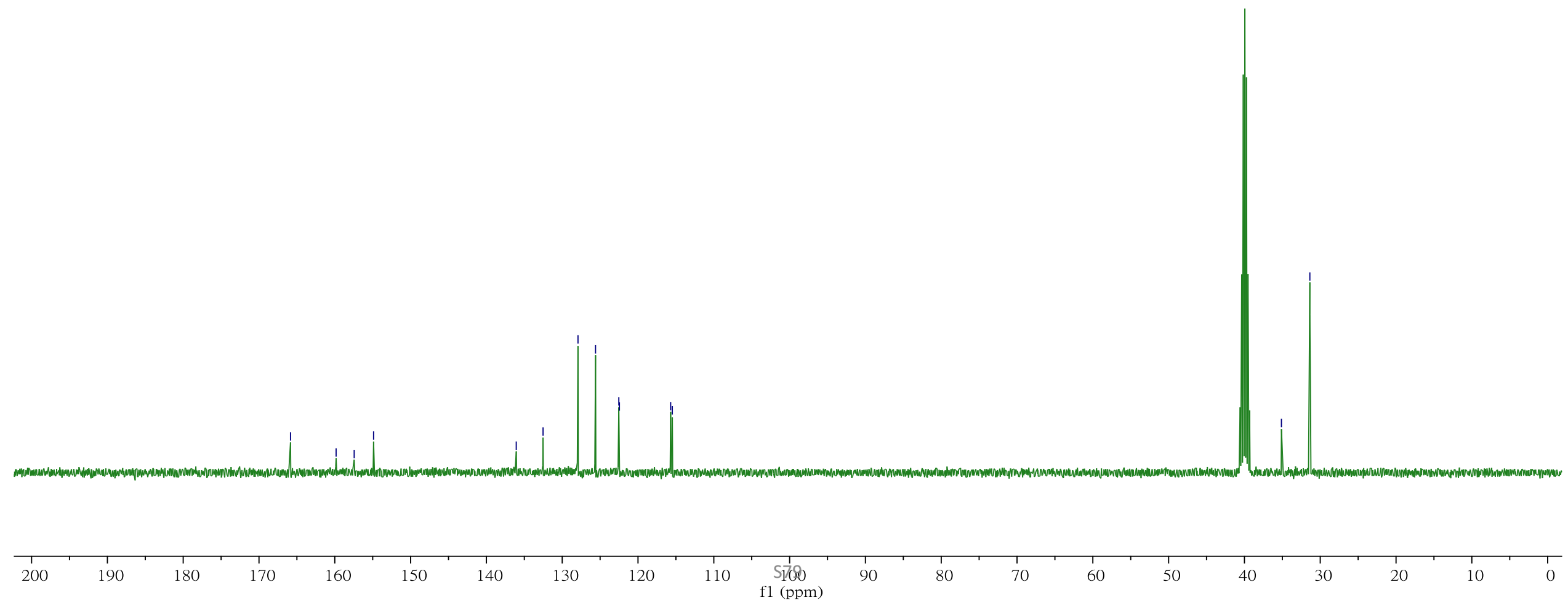
M0606-7
nq-5-131-2

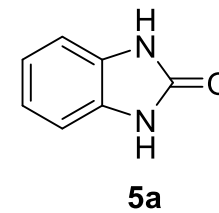
165.84
159.83
157.44
154.89
136.06
132.53
127.92
125.60
122.53
122.45
115.69
115.47

Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz

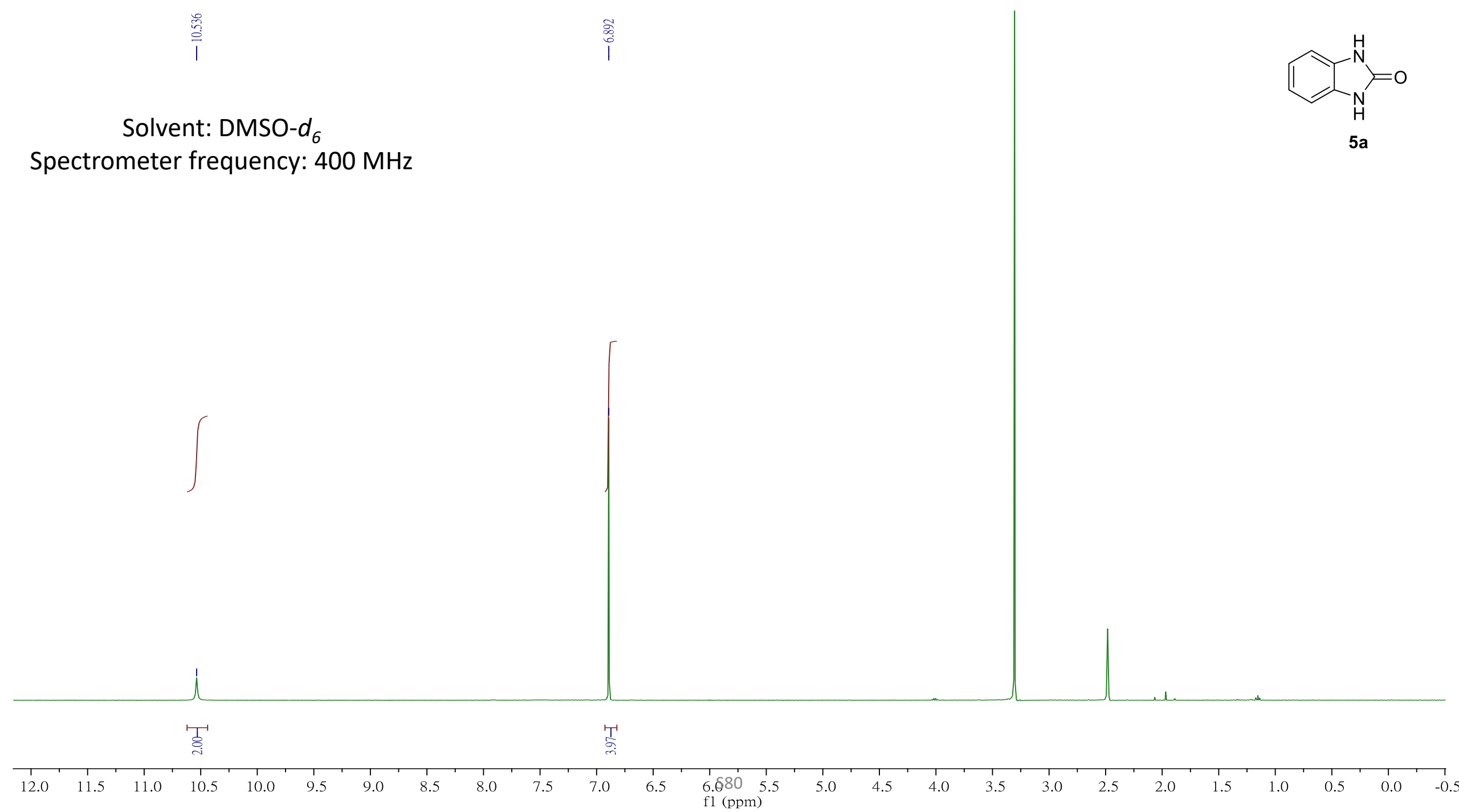


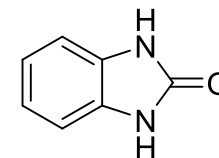
35.12
31.37





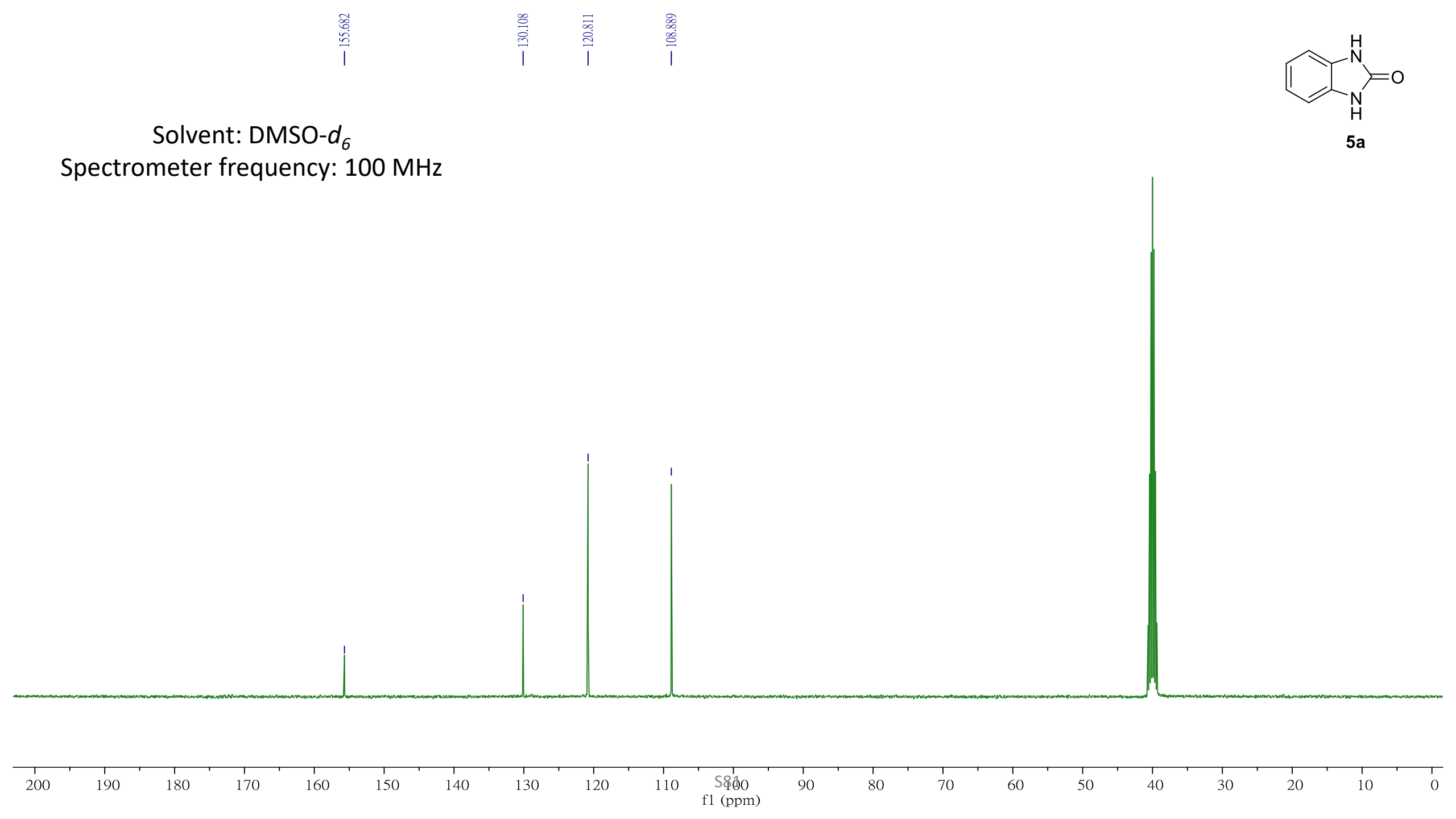
Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz





5a

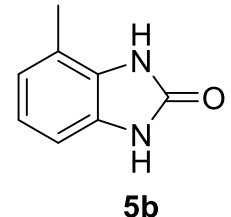
Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



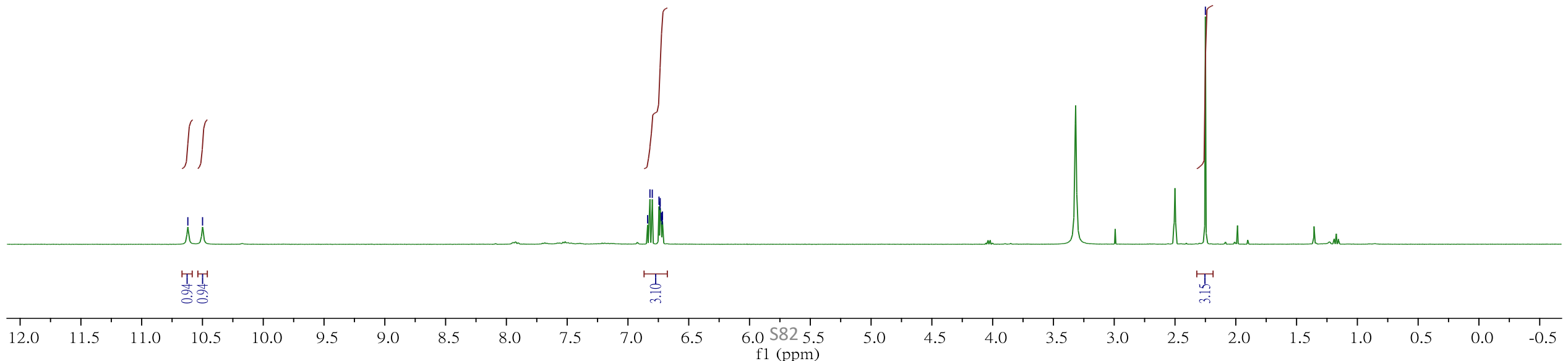
10.620
10.499

6.838
6.819
6.800
6.745
6.737
6.735
6.726
6.718
6.716

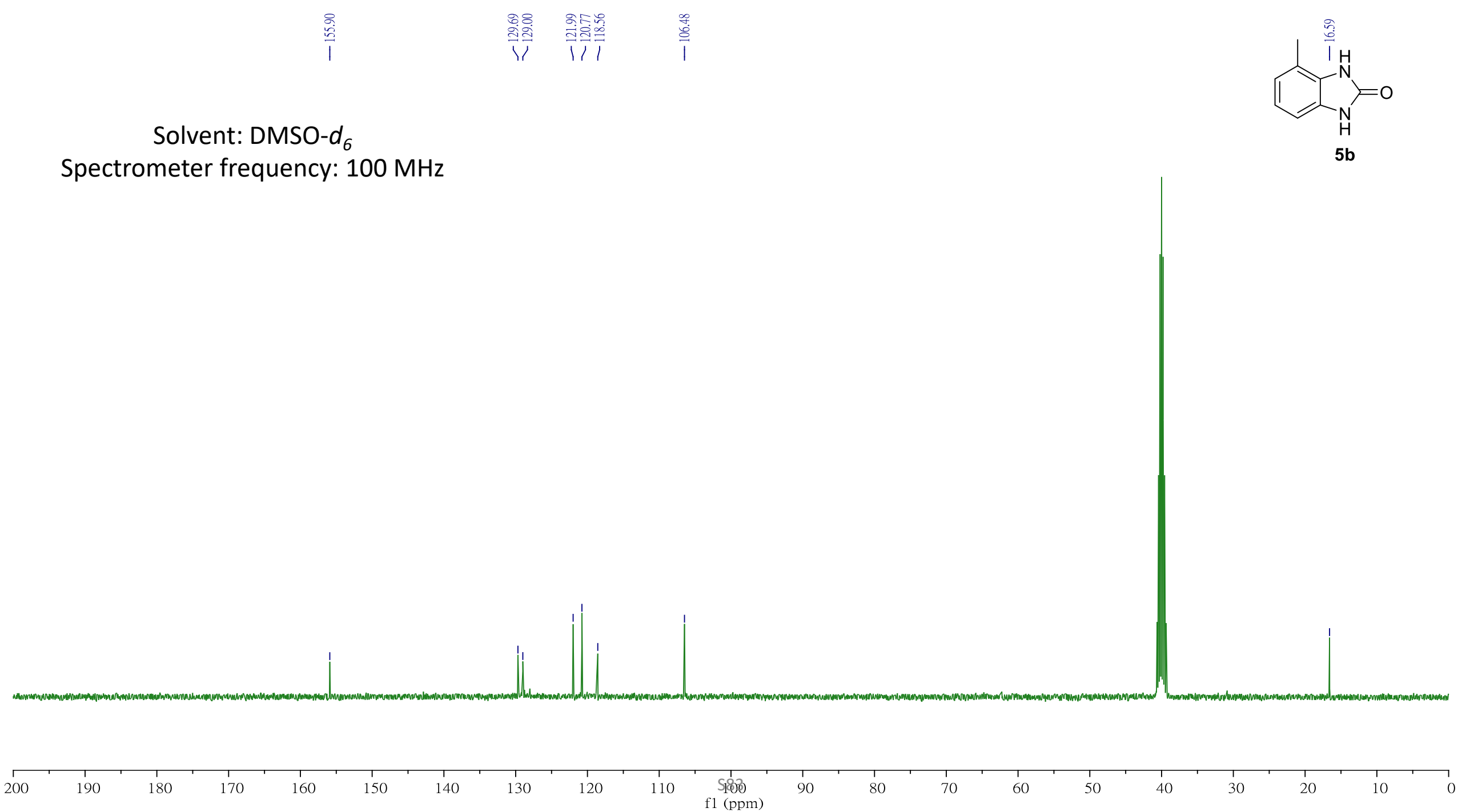
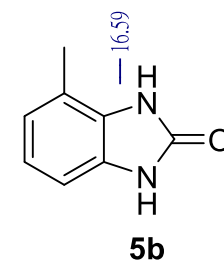
2.250



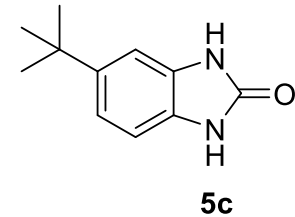
Solvent: DMSO-*d*₆
Spectrometer frequency: 400 MHz



Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



10.397

6.948
6.943
6.928
6.923
6.887
6.883
6.818
6.798

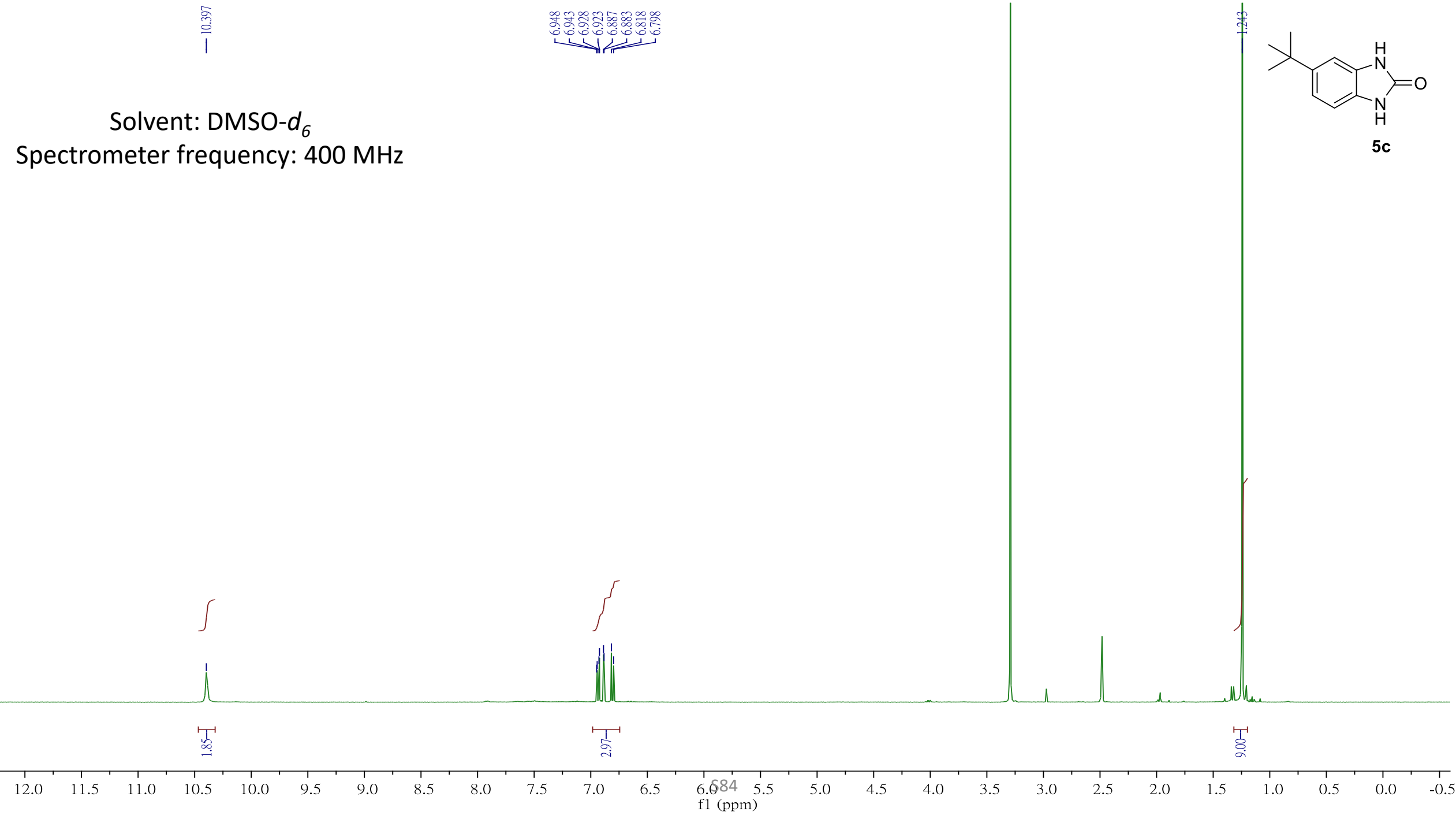
1.243

1.85

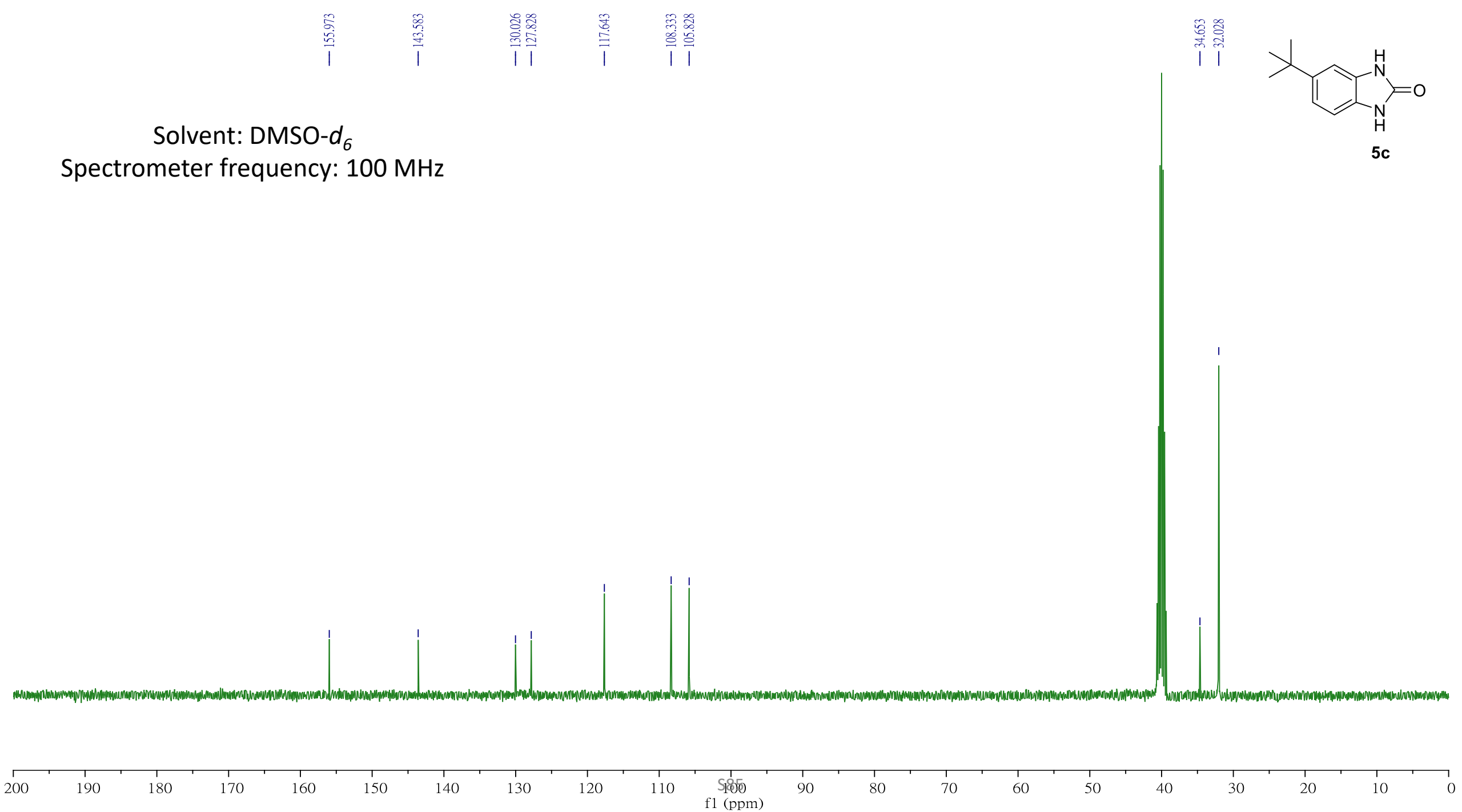
2.97

9.00

6.84
f1 (ppm)

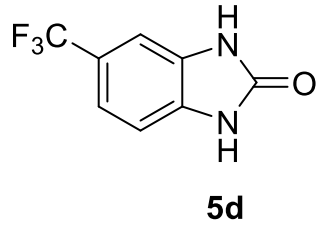


Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz

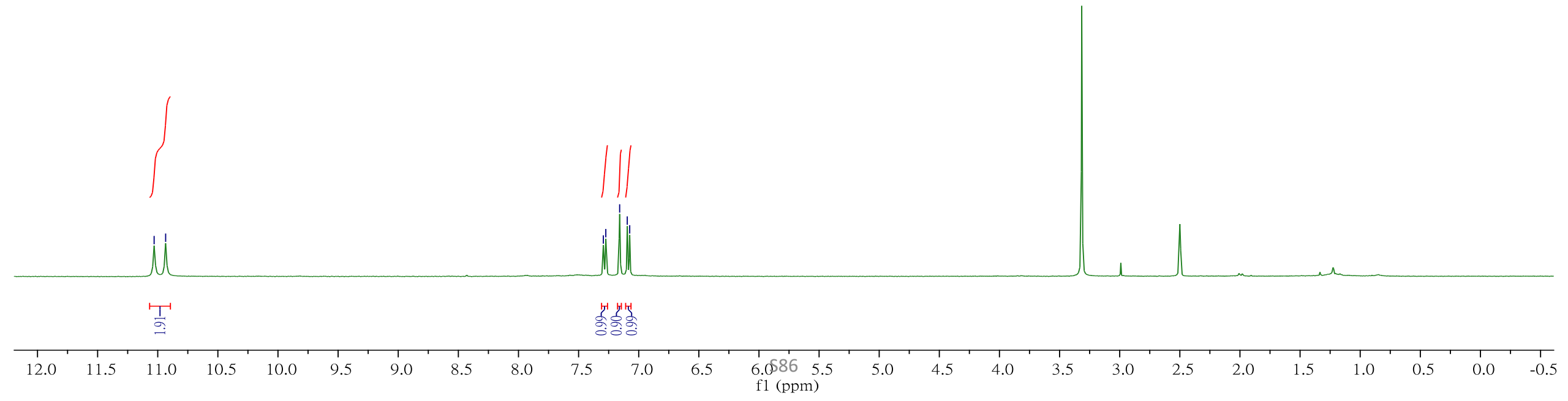


M0570-17
NQ-5-100 ALL E
11.0300
10.9343

7.2941
7.2737
7.1585
7.0953
7.0750



Solvent: DMSO-*d*₆
Spectrometer frequency: 400 MHz



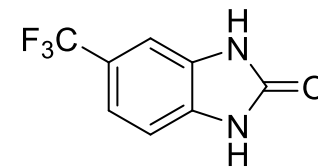
M0570-21
NQ-5-100-ALL EA

155.74

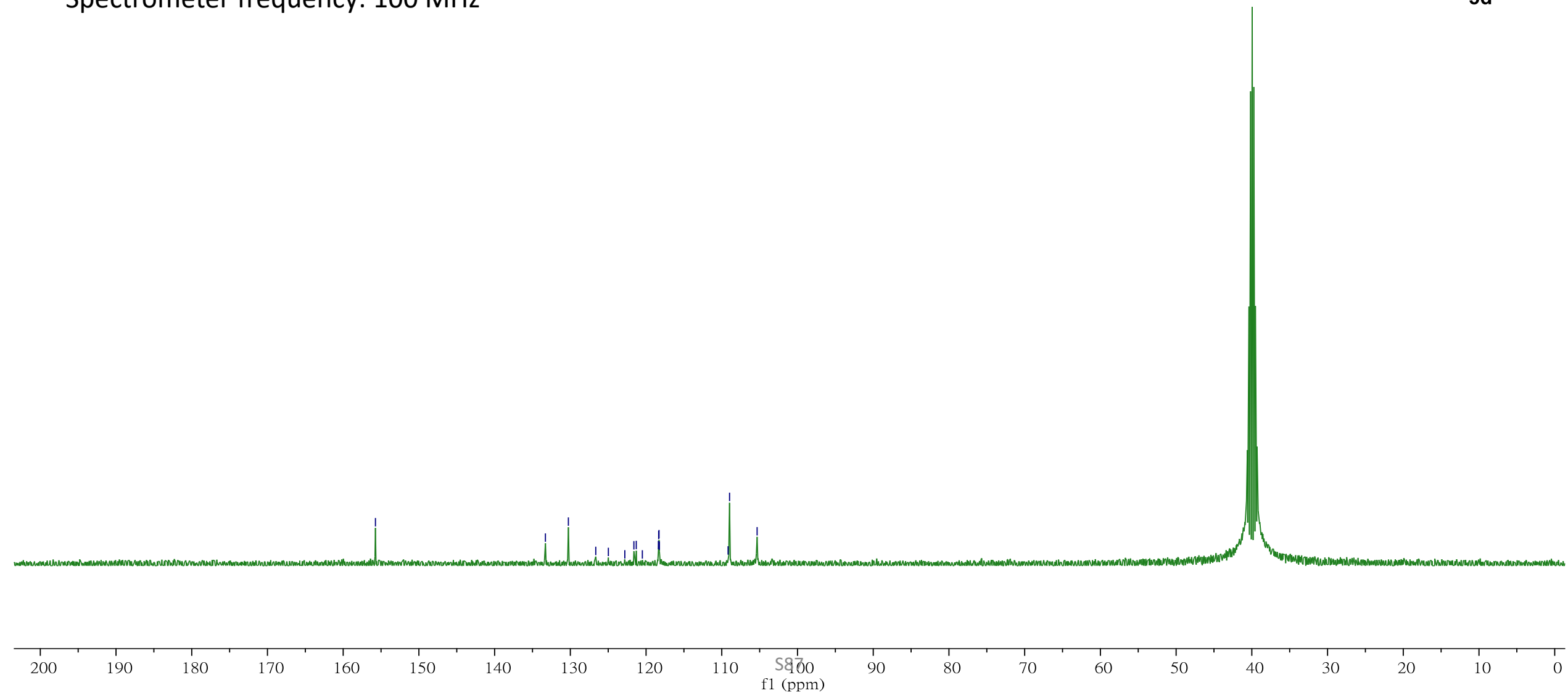
133.29
130.26
126.64
124.98
122.81
121.61
121.29
120.49
118.37
118.33
118.29
118.24

109.17
108.97
105.33

Solvent: DMSO- d_6
Spectrometer frequency: 100 MHz



5d

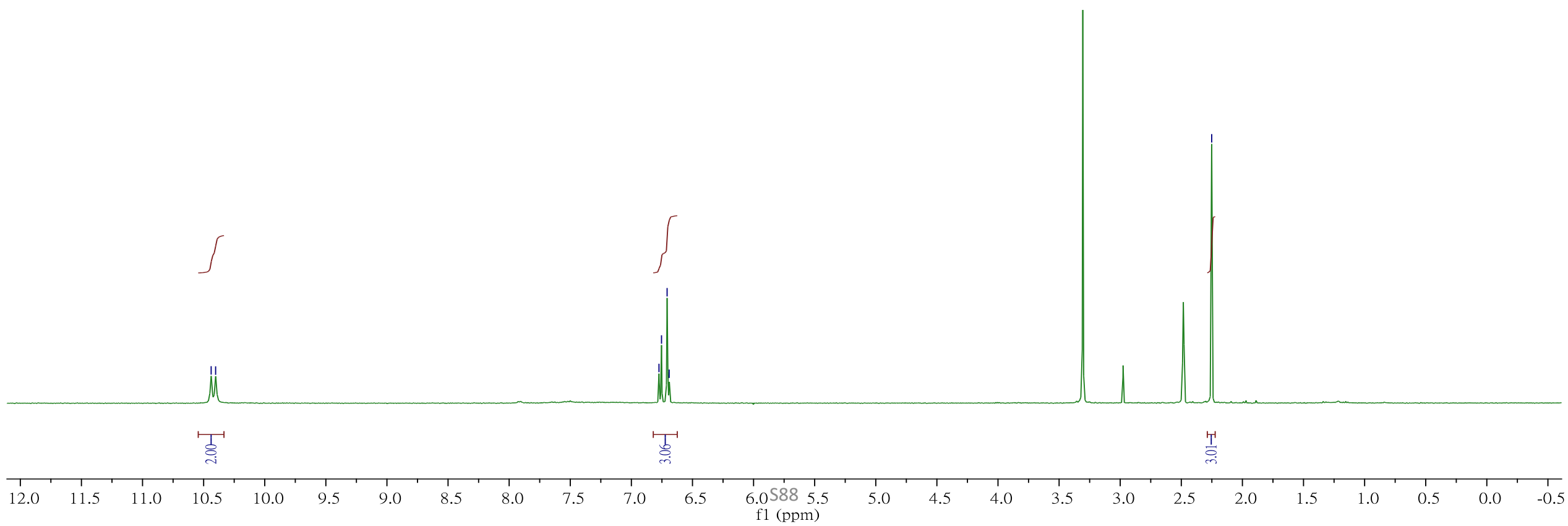
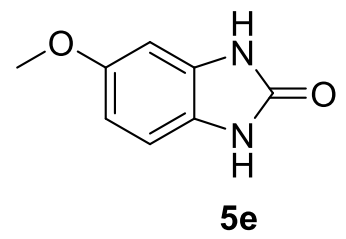


10.4384
10.4019

6.7741
6.7533
6.7075
6.6908

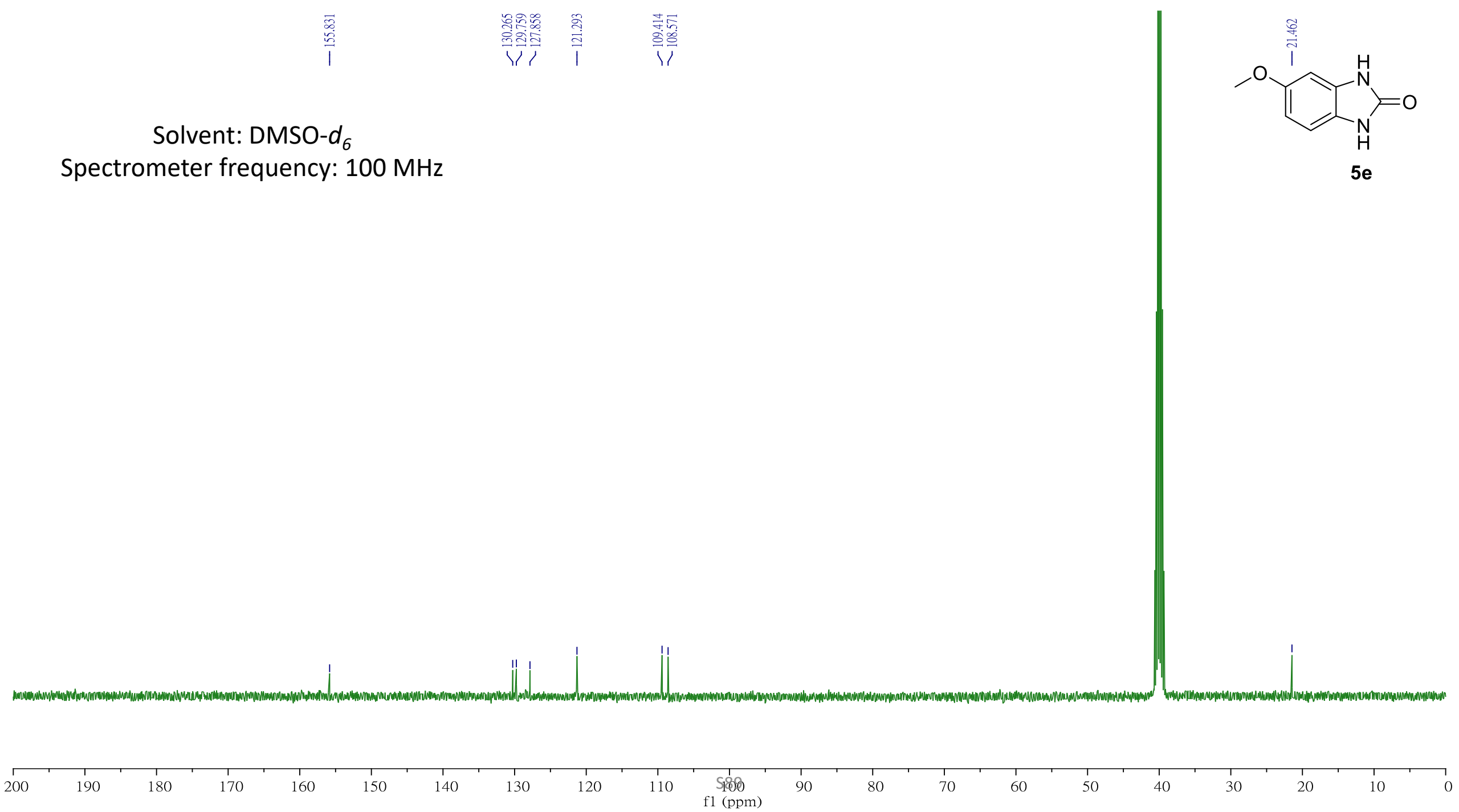
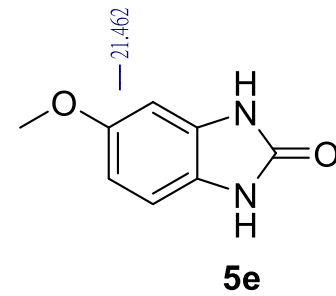
2.2513

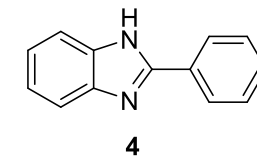
Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



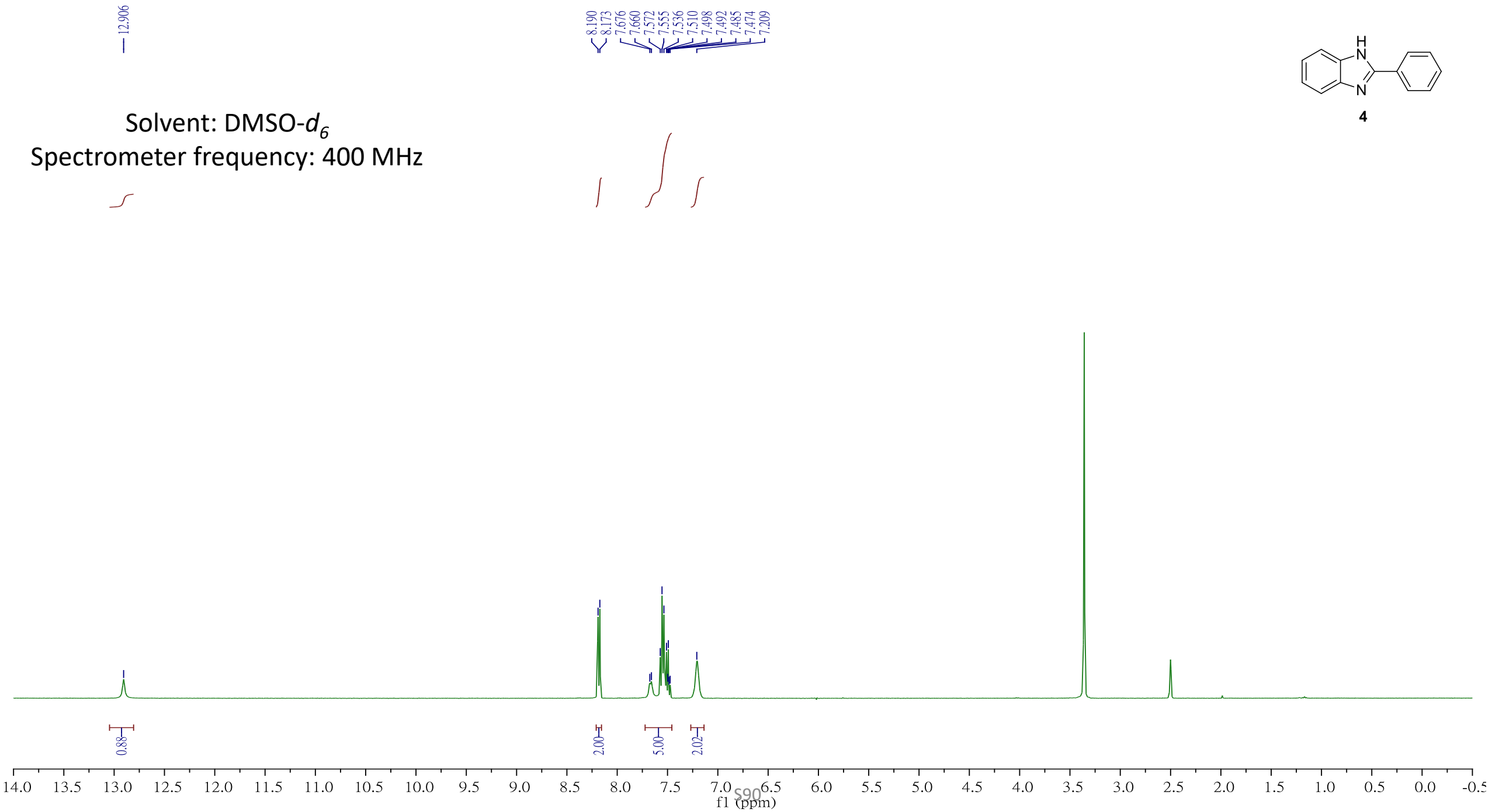
S88

Solvent: DMSO-*d*₆
Spectrometer frequency: 100 MHz

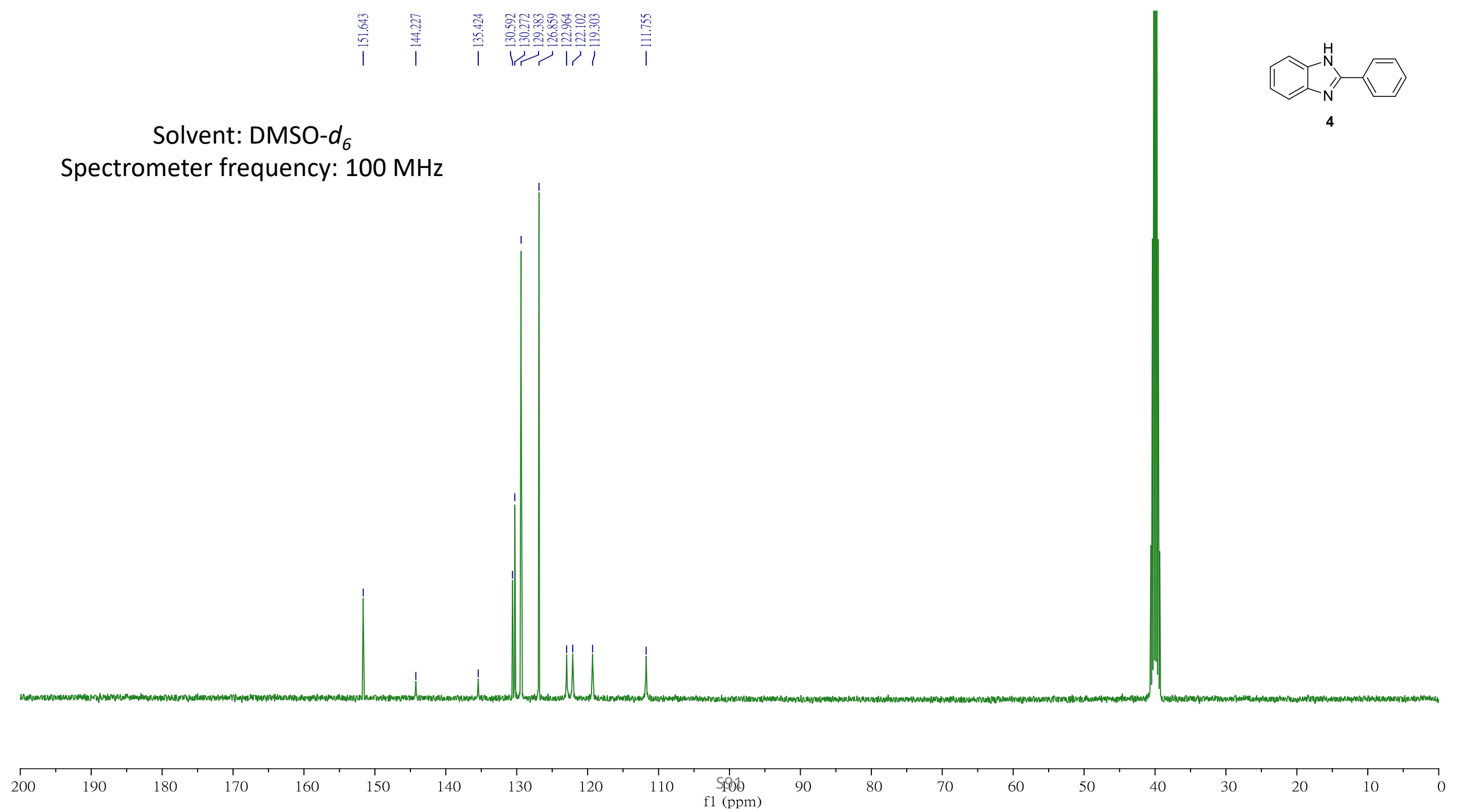
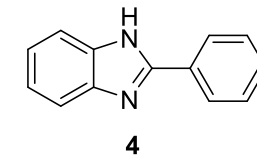




Solvent: DMSO- d_6
Spectrometer frequency: 400 MHz



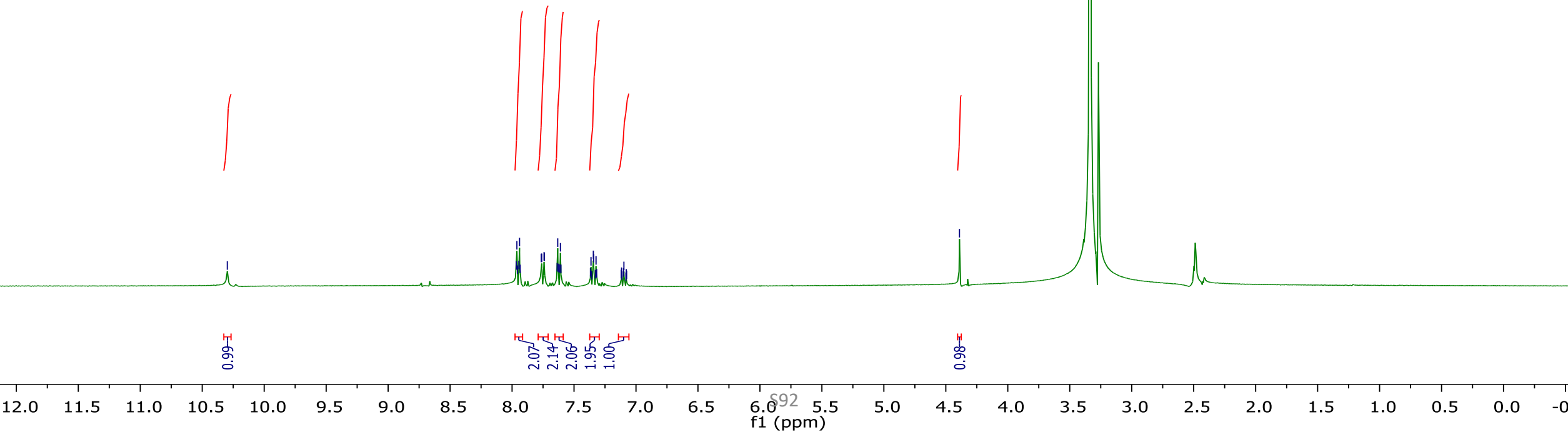
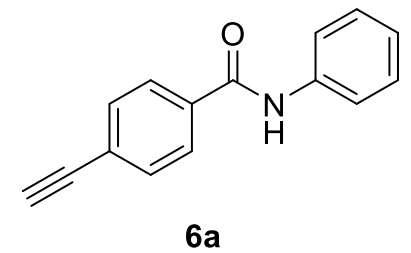
Solvent: DMSO-*d*₆
Spectrometer frequency: 100 MHz



M0843-5
aj

10.2977
7.9657
7.9610
7.9558
7.9449
7.9396
7.9347
7.7642
7.7608
7.7419
7.7389
7.6362
7.6316
7.6262
7.6151
7.6099
7.6058
7.3676
7.3631
7.3578
7.3442
7.3412
7.3274
7.3224
7.3174
7.1192
7.1162
7.1128
7.1005
7.0974
7.0815
7.0787
7.0755
4.3899

Solvent: DMSO-*d*₆
Spectrometer frequency: 400 MHz



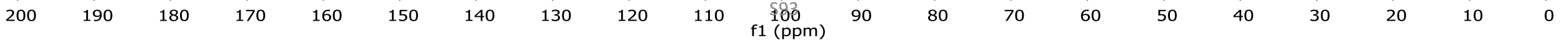
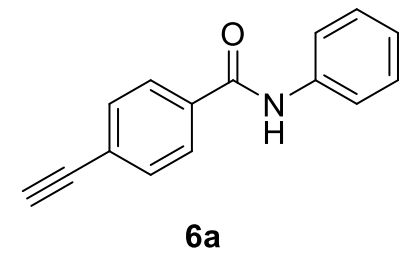
M0843-6
aj

164.6699

138.9470
134.9490
131.6785
128.6151
127.9492
124.7294
123.8202
120.3929

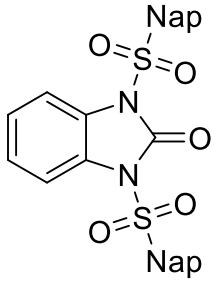
83.0476
82.8359

Solvent: DMSO-*d*₆
Spectrometer frequency: 100 MHz

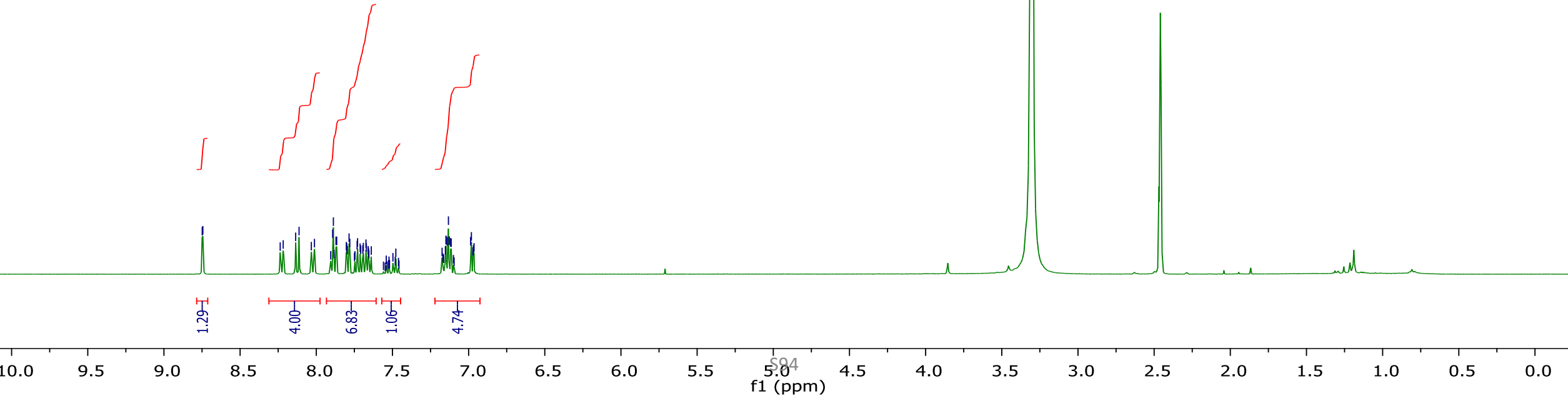


AJ-V-37
single_pulse

8.7488
8.7445
8.1351
8.1131
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7.1686
7.1642
7.1525
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7.1376
7.1324
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6.9644

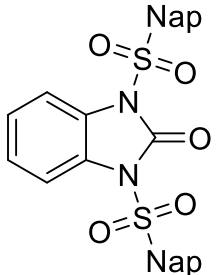


6b



M0856-11
AJ-V-37

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- 135.5818
- 131.8100
- 130.4237
- 129.8764
- 128.4009
- 126.9034
- 124.9822
- 122.4527
- 122.0069
- 112.8582
- 110.4777



6b

