

# Late-Stage *ortho*-C–H Alkenylation of 2-Arylindazoles in Aqueous Medium by Manganese(I)-Catalysis

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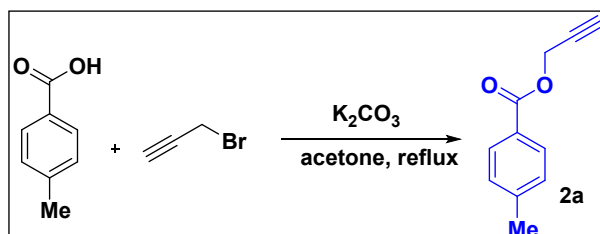
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## 1. General information:

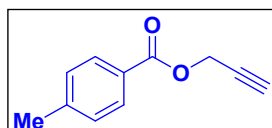
All reagents were purchased from commercial sources and used without further purification.  $^1\text{H}$  NMR spectra were determined on 400 MHz spectrometer as solutions in  $\text{CDCl}_3$ . Chemical shifts are expressed in parts per million ( $\delta$ ) and the signals were reported as s (singlet), d (doublet), t (triplet), m (multiplet) and coupling constants ( $J$ ) were given in Hz.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra were recorded at 100 MHz in  $\text{CDCl}_3$  and  $\text{DMSO}-d_6$  solution. NMR data are reported relative to residual  $\text{CHCl}_3$  ( $^1\text{H}$ ,  $\delta = 7.26$  ppm) and  $\text{CDCl}_3$  ( $^{13}\text{C}$ ,  $\delta = 77.16$  ppm) or  $\text{DMSO}-d_6$  ( $^1\text{H}$ ,  $\delta = 2.50$  ppm). TLC was done on silica gel coated glass slide. All 2-arylidazoles<sup>1</sup> were prepared by the reported methods. All solvents were dried and distilled before use. Commercially available solvents were freshly distilled before the reaction. All reactions involving moisture sensitive reactants were executed using oven dried glassware. Melting points (M.p.) were determined after recrystallization of solid compounds from a solution of dichloromethane/petroleum ether (1:3).

## 2. Experimental procedures:

### 2.1. Typical procedures for the synthesis of prop-2-yn-1-yl benzoate derivatives (2):<sup>2</sup>

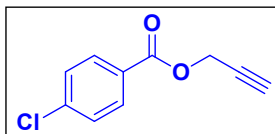


A mixture of 4-methylbenzoic acid (10.0 mmol, 1.36 g), 3-bromoprop-1-yne (12.0 mmol, 1.45 g) and anhydrous  $\text{K}_2\text{CO}_3$  (4.14 g, 3.0 equiv.) in acetone (15 mL) was stirred for 12 h in reflux. When the reaction was complete (as monitored by TLC), the solvent was evaporated under reduced pressure. The residue was purified by column chromatography over silica gel with mixtures of PE/AcOEt to give the desired product **2**.

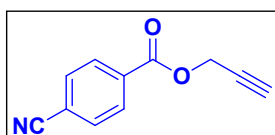


**Prop-2-yn-1-yl 4-methylbenzoate (2a):** Yellow gummy mass (91%, 1.5 g);  $R_f = 0.50$  (PE/ EA = 96 : 4);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.89 (d,  $J = 8.0$  Hz, 2H), 7.17 (d,  $J = 8.0$  Hz, 2H), 4.83 (d,  $J = 2.4$  Hz, 2H), 2.44 (t,  $J = 2.8$  Hz, 1H), 2.34 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,

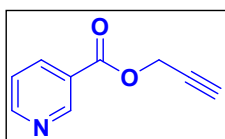
$\text{CDCl}_3$ ):  $\delta$  165.9, 144.2, 129.9, 129.2, 126.7, 77.9, 75.0, 52.3, 21.8; Anal. Calcd for  $\text{C}_{11}\text{H}_{10}\text{O}_2$ : C, 75.84; H, 5.79%; Found: C, 75.97; H, 5.75%.



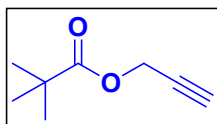
**Prop-2-yn-1-yl 4-chlorobenzoate (2b):** Yellow gummy mass (89%, 1.7 g);  $R_f = 0.50$  (PE/ EA = 97 : 3);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.98 (d,  $J = 8.4$  Hz, 2H), 7.40 (d,  $J = 8.4$  Hz, 2H), 4.90 (d,  $J = 2.4$  Hz, 2H), 2.53 (t,  $J = 2.4$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.0, 139.9, 131.2, 128.9, 127.8, 77.5, 75.3, 52.7; Anal. Calcd for  $\text{C}_{10}\text{H}_7\text{ClO}_2$ : C, 61.72; H, 3.63%; Found: C, 61.57; H, 3.68%.



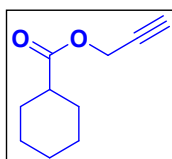
**Prop-2-yn-1-yl 4-cyanobenzoate (2c):** Yellow solid (82%, 1.5 g);  $R_f = 0.50$  (PE/ EA = 95 : 5); M.P. 85-86 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.17 (d,  $J = 8.4$  Hz, 2H), 7.76 (d,  $J = 8.4$  Hz, 2H), 4.95 (d,  $J = 2.4$  Hz, 2H), 2.55 (t,  $J = 2.4$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.3, 133.2, 132.4, 130.4, 118.0, 116.8, 75.7, 53.3; Anal. Calcd for  $\text{C}_{11}\text{H}_7\text{NO}_2$ : C, 71.35; H, 3.81; N, 7.56%; Found: C, 71.49; H, 3.78; N, 7.49%.



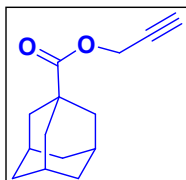
**Prop-2-yn-1-yl nicotinate (2d):** Yellow gummy mass (84%, 1.3 g);  $R_f = 0.45$  (PE/ EA = 92 : 8);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  9.15 (s, 1H), 8.71–8.69 (m, 1H), 8.25–8.21 (m, 1H), 7.35–7.31 (m, 1H), 4.92–4.87 (m, 2H), 2.53–2.52 (m, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.4, 153.6, 150.8, 137.2, 125.2, 123.3, 75.5, 52.7; Anal. Calcd for  $\text{C}_9\text{H}_7\text{NO}_2$ : C, 67.08; H, 4.38; N, 8.69%; Found: C, 66.91; H, 4.40; N, 8.81%.



**Prop-2-yn-1-yl pivalate (2e):** Yellow liquid (94%, 1.3 g);  $R_f = 0.55$  (PE/ EA = 98 : 2);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  4.62 (d,  $J = 2.4$  Hz, 2H), 2.42 (t,  $J = 2.4$  Hz, 1H), 1.18 (s, 9H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  177.7, 78.0, 74.6, 52.0, 38.7, 27.1; Anal. Calcd for  $\text{C}_8\text{H}_{12}\text{O}_2$ : C, 68.55; H, 8.63%; Found: C, 68.75; H, 8.59%.

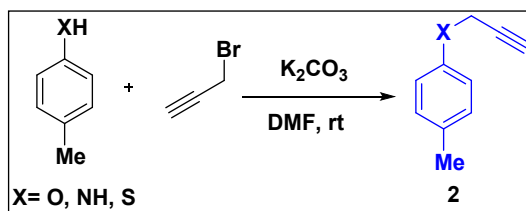


**Prop-2-yn-1-yl cyclohexanecarboxylate (2f):** Yellow liquid (92%, 1.5 g);  $R_f = 0.55$  (PE/ EA = 97 : 3);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  4.63 (d,  $J = 2.4$  Hz, 2H), 2.44 (t,  $J = 2.8$  Hz, 1H), 2.35–2.28 (m, 1H), 1.90–1.87 (m, 2H), 1.74–1.70 (m, 2H), 1.62–1.59 (m, 1H), 1.46–1.37 (m, 2H), 1.30–1.16 (m, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  175.2, 77.9, 74.7, 51.7, 42.9, 28.9, 25.7, 25.4; Anal. Calcd for  $\text{C}_{10}\text{H}_{14}\text{O}_2$ : C, 72.26; H, 8.49%; Found: C, 72.08; H, 8.53%.

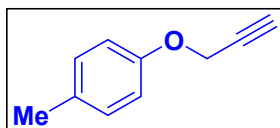


**Prop-2-yn-1-yl (3*r*,5*r*,7*r*)-adamantane-1-carboxylate (2g):** Yellow liquid (98%, 2.1 g);  $R_f = 0.50$  (PE/ EA = 96 : 4);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  4.61 (d,  $J = 2.4$  Hz, 2H), 2.43–2.42 (m, 1H), 1.98 (s, 3H), 1.87 (s, 6H), 1.68 (t,  $J = 14.8$  Hz, 6H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  176.8, 78.1, 74.5, 51.7, 40.7, 38.6, 36.4, 27.9; Anal. Calcd for  $\text{C}_{14}\text{H}_{18}\text{O}_2$ : C, 77.03; H, 8.31%; Found: C, 77.19; H, 8.28%.

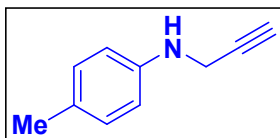
## 2.2. Typical procedures for the synthesis of 1-methyl-4-(prop-2-yn-1-yloxy)benzene (2):<sup>3</sup>



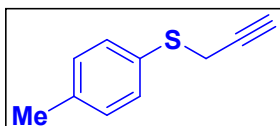
A mixture of *p*-cresol (10.0 mmol, 1.08 g), 3-bromoprop-1-yne (12.0 mmol, 1.45 g) and anhydrous  $\text{K}_2\text{CO}_3$  (4.14 g, 3.0 equiv.) in DMF (15 mL) was stirred for 12 h at room temperature. After completion of the reaction (TLC), the reaction mixture was extracted with DCM. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ . The crude residue was obtained after evaporating the solvent in vacuum and was purified by column chromatography on silica gel using a mixture of petroleum ether and ethyl acetate as an eluting solvent to afford the pure product **2**.



**1-methyl-4-(prop-2-yn-1-yloxy)benzene (2i):** Yellow gummy mass (96%, 1.4 g);  $R_f = 0.45$  (PE/ EA = 95 : 5);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.14 (d,  $J = 8.4$  Hz, 2H), 6.93–6.89 (m, 2H), 4.68 (d,  $J = 2.4$  Hz, 2H), 2.54 (t,  $J = 2.4$  Hz, 1H), 2.33 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  155.4, 130.9, 130.0, 114.7, 78.8, 75.4, 55.8, 20.5; Anal. Calcd for  $\text{C}_{10}\text{H}_{10}\text{O}$ : C, 82.16; H, 6.90%; Found: C, 81.95; H, 6.95%.

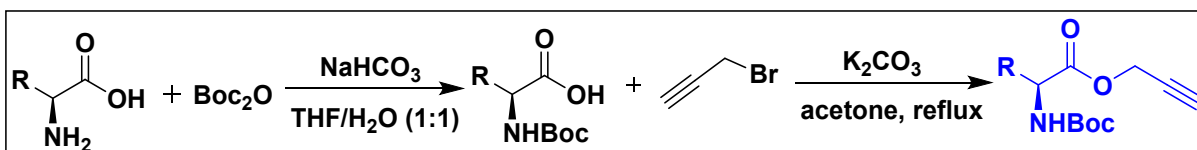


**4-methyl-N-(prop-2-yn-1-yl)aniline (2j):** Brown solid (91%, 1.3 g);  $R_f = 0.50$  (PE/ EA = 95 : 5); M.P. 46-47 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.10-7.07 (m, 2H), 6.68-6.65 (m, 2H), 3.94 (s, 2H), 3.78 (s, 1H), 2.31 (s, 3H), 2.25 (t,  $J = 2.0$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  144.6, 129.7, 127.9, 113.8, 81.3, 71.2, 33.9, 20.4; Anal. Calcd for  $\text{C}_{10}\text{H}_{11}\text{N}$ : C, 82.72; H, 7.64; N, 9.65%; Found: C, 82.85; H, 7.62, N, 9.56%.

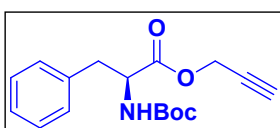


**Prop-2-yn-1-yl(p-tolyl)sulfane (2k):** Yellow gummy mass (86%, 1.3 g);  $R_f = 0.50$  (PE/ EA = 97 : 3);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.39 (d,  $J = 8.0$  Hz, 2H), 7.15 (d,  $J = 8.0$  Hz, 2H), 3.56 (d,  $J = 2.8$  Hz, 2H), 2.35 (s, 3H), 2.24 (t,  $J = 2.4$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  137.3, 131.1, 131.0, 129.8, 80.1, 71.5, 23.2, 21.1; Anal. Calcd for  $\text{C}_{10}\text{H}_{10}\text{S}$ : C, 74.03; H, 6.21%; Found: C, 73.88; H, 6.23%.

### 2.3. Typical procedures for the synthesis of (2):<sup>4</sup>

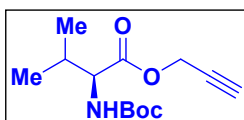


A mixture of phenylalanine (10.0 mmol, 1.65 g) and  $\text{NaHCO}_3$  (3.0 equiv., 2.52 g) in THF and  $\text{H}_2\text{O}$  (1:1 v/v) was stirred for 15 min at room temperature. After that,  $\text{Boc}_2\text{O}$  (12.0 mmol, 2.62 g) was added to the reaction mixture at 0 °C for 30 min. Then the reaction was stirred at room temperature for overnight. When the reaction was complete (as monitored by TLC), 2.0 (M) HCl was added drop wise to maintain the pH = 2-3. The reaction mixture was extracted with EtOAc. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ . The crude residue was obtained after evaporating the solvent in vacuum. The resulting crude material was used for the next step without further purification. Next step was similar to the procedure 2.1.

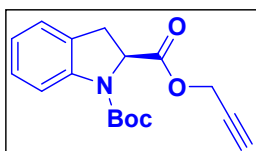


**Prop-2-yn-1-yl (tert-butoxycarbonyl)-L-phenylalaninate (2l):** Yellow liquid (82%, 2.4 g);  $R_f = 0.50$  (PE/ EA = 90 : 10);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.32-7.23 (m, 3H), 7.21-7.16 (m, 2H), 5.04 (d,  $J = 6.0$  Hz, 1H), 4.78-4.56 (m, 3H), 3.18-3.06 (m, 2H), 2.53 (t,  $J = 2.4$  Hz, 1H),

1.42 (s, 9H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.1, 155.0, 135.7, 129.4, 128.5, 127.1, 80.0, 77.0, 75.5, 54.3, 52.6, 38.0, 28.2; Anal. Calcd for  $\text{C}_{17}\text{H}_{21}\text{NO}_4$ : C, 67.31; H, 6.98; N, 4.62%; Found: C, 67.47; H, 7.01; N, 4.49%.

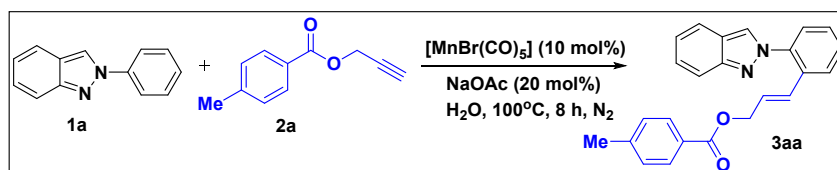


**Prop-2-yn-1-yl (tert-butoxycarbonyl)-L-valinate (2m):** Yellow liquid (67%, 1.7 g);  $R_f = 0.50$  (PE/ EA = 94 : 6);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  5.04 (d,  $J = 8.8$  Hz, 1H), 4.72-4.56 (m, 2H), 2.44 (s, 1H), 2.11-2.04 (m, 1H), 1.40-1.39 (m, 1H), 1.34 (s, 9H), 0.90-0.81 (m, 6H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.6, 155.5, 79.7, 75.3, 58.3, 52.3, 31.2, 28.2, 18.9, 17.4; Anal. Calcd for  $\text{C}_{13}\text{H}_{21}\text{NO}_4$ : C, 61.16; H, 8.29; N, 5.49%; Found: C, 61.04; H, 8.27; N, 5.57%.



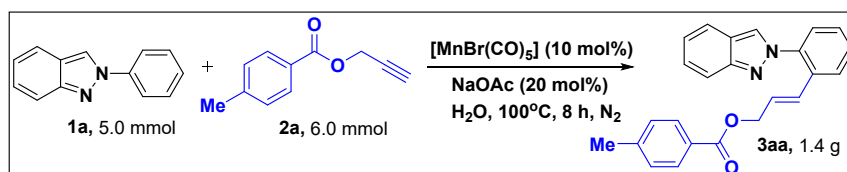
**1-(tert-butyl) 2-(prop-2-yn-1-yl) (S)-indoline-1,2-dicarboxylate (2n):** Yellow liquid (72%, 2.1 g);  $R_f = 0.45$  (PE/ EA = 90 : 10);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.89 (d,  $J = 6.8$  Hz, 1H), 7.18 (t,  $J = 7.6$  Hz, 1H), 7.09 (d,  $J = 7.2$  Hz, 1H), 6.95-6.91 (m, 1H), 4.88 (d,  $J = 8.4$  Hz, 1H), 4.78-4.67 (m, 2H), 3.53-3.46 (m, 1H), 3.13-3.08 (m, 1H), 2.49 (s, 1H), 1.50 (s, 9H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.1, 151.4, 142.4, 127.9, 127.6, 124.8, 124.3, 122.6, 114.6, 81.5, 75.4, 60.1, 52.6, 32.5, 28.2; Anal. Calcd for  $\text{C}_{17}\text{H}_{19}\text{NO}_4$ : C, 67.76; H, 6.36; N, 4.65%; Found: C, 67.93; H, 6.32; N, 4.59%.

#### 2.4. Typical experimental procedure for 3aa:



A mixture of 2-phenyl-2H-indazole (**1a**) (0.25 mmol, 48.5 mg),  $\text{MnBr}(\text{CO})_5$  (10 mol%, 6.8 mg), and NaOAc (20 mol%, 4.1 mg) was taken in an oven dried screw-capped reaction tube. Then the reaction vessel was evacuated and filled with nitrogen for three times. Then prop-2-yn-1-yl 4-methylbenzoate (**2a**) (0.3 mmol, 52.2 mg) and  $\text{H}_2\text{O}$  (2 mL) was added to the mixture and the resultant mixture was stirred at 100 °C in a preheated oil bath for 8 h. After completion of the reaction (TLC), the reaction was cooled to room temperature and extracted with ethyl acetate. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ . The crude residue was obtained after evaporating the solvent in vacuum and was purified by column chromatography on silica gel using a mixture of petroleum ether and ethyl acetate.

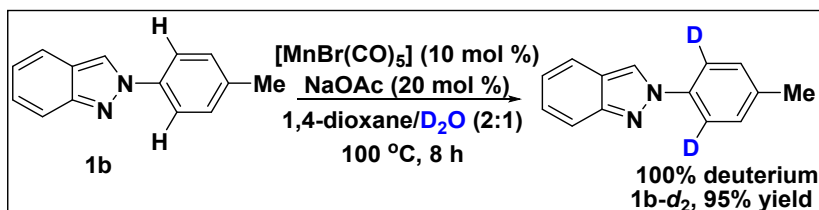
## 2.5. Synthesis of 3aa on 5 mmol scale:



A mixture of 2-phenyl-2*H*-indazole (**1a**) (5.0 mmol, 0.97 g),  $\text{MnBr}(\text{CO})_5$  (10 mol%, 137.0 mg), and NaOAc (20 mol%, 83.0 mg) was taken in an oven dried screw-capped reaction tube. Then the reaction vessel was evacuated and filled with nitrogen for three times. Then prop-2-yn-1-yl 4-methylbenzoate (**2a**) (6.0 mmol, 1.04 g) and  $\text{H}_2\text{O}$  (25 mL) was added to the mixture and the resultant mixture was stirred at 100 °C in a preheated oil bath for 8 h. After completion of the reaction (TLC), the reaction was cooled to room temperature and extracted with ethyl acetate. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ . The crude residue was obtained after evaporating the solvent in vacuum and was purified by column chromatography on silica gel using a mixture of petroleum ether and ethyl acetate (85:15) as an eluting solvent to afford the pure product **3aa** (1.4 g, 79%) as a Yellow gummy mass.

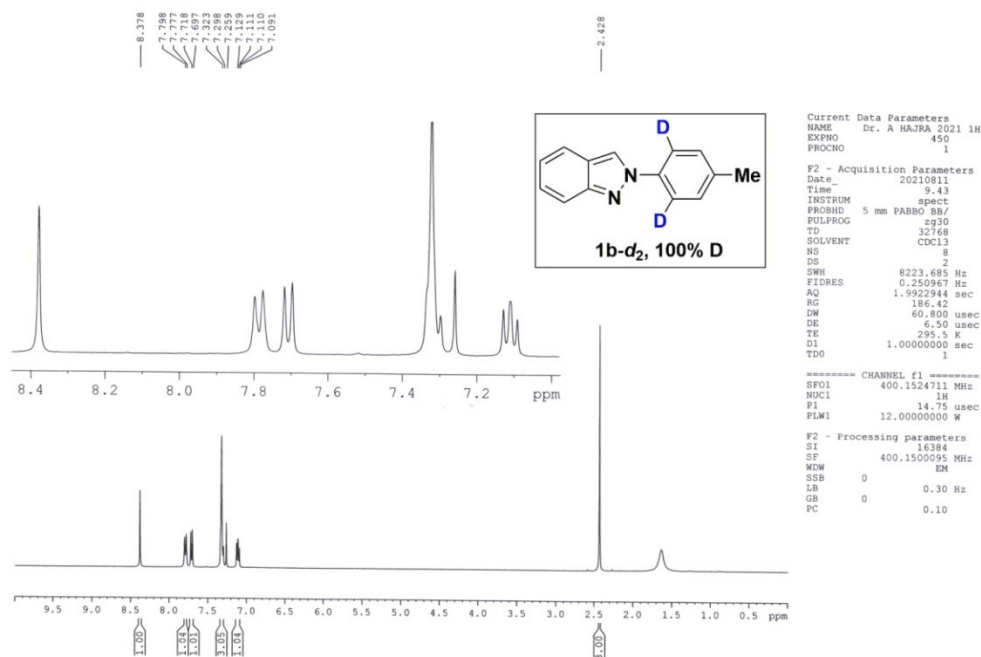
## 3. Mechanistic investigations:<sup>5</sup>

### 3.1. Preparation of 2-(4-methylphenyl-2,6-*d*<sub>2</sub>)-2*H*-indazole (**1b-d**<sub>2</sub>):

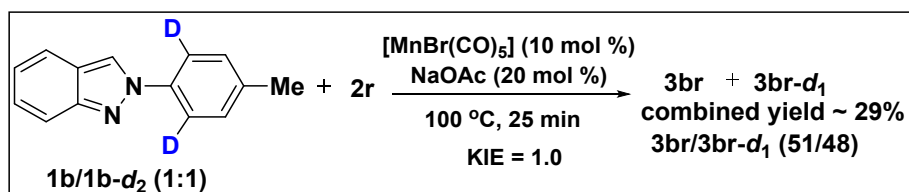


A mixture of 2-(*p*-tolyl)-2*H*-indazole (0.25 mmol, 52 mg) (**1b**),  $[\text{MnBr}(\text{CO})_5]$  (10 mol %, 6.8 mg), and NaOAc (20 mol%, 4.1 mg) was taken in an oven dried screw-capped reaction tube. Then 1,4-dioxane (2 mL) was added to the mixture and stirred for 5 min at room temperature under open atmosphere. After that,  $\text{D}_2\text{O}$  (1 mL) was added, and the resultant mixture was stirred at 100 °C for 8 h. Then, the reaction was cooled to room temperature and extracted with dichloromethane. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ . The crude residue was obtained after evaporating the solvent in vacuum and was purified by column chromatography on silica gel using a mixture of petroleum ether and ethyl acetate (85:15) as an eluting solvent to afford the pure product **1b-d**<sub>2</sub> as a white solid. The deuterium incorporation was determined using 400 MHz  $^1\text{H}$  NMR as 100%.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of **1b-d**<sub>2</sub>



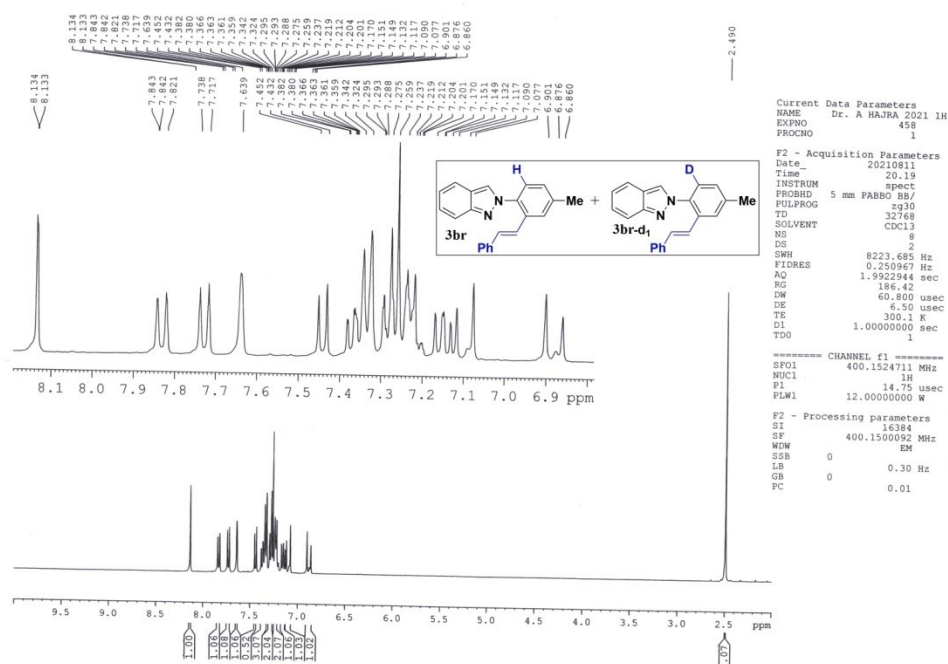
### 3.2. Intermolecular kinetic isotope effect study:



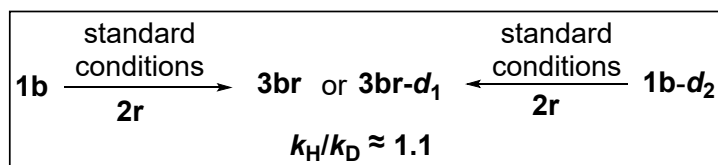
Ethynylbenzene (**2r**) (0.24 mmol, 24.5 mg) was reacted with 2-(*p*-tolyl)-2*H*-indazole (**1b**) (0.1 mmol, 20.8 mg) and 2-(4-methylphenyl-2,6-*d*<sub>2</sub>)-2*H*-indazole (**1b-d**<sub>2</sub>) (0.1 mmol, 21.0 mg) for 25 min under standard reaction condition. The resulting solution was then diluted with dichloromethane (3 x 10 mL) and washed with brine (2 x 5 mL) and water (5 mL). The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The crude residue was obtained after evaporating the solvent in vacuum and was purified by column chromatography on silica gel using a mixture of petroleum ether and ethyl acetate (95:5). The intermolecular  $k_{\text{H}}/k_{\text{D}}$  was found to be **1.0** after 25 min at ~29% conversion, based on 400 MHz <sup>1</sup>H NMR of the product **3br** and **3br-d**<sub>1</sub>.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of 3br and 3br-*d*<sub>1</sub>





### 3.3. Parallel kinetic isotope effect study:



In a set of two experiments: in first set, ethynylbenzene (**2r**) (0.12 mmol, 12.2 mg) was reacted with 2-(*p*-tolyl)-2*H*-indazole (**1b**) (0.1 mmol, 20.8 mg) under standard reaction conditions. Whereas in another set, 2-(4-methylphenyl-2,6-*d*<sub>2</sub>)-2*H*-indazole (**1b-d**<sub>2</sub>) (0.1 mmol, 21.0 mg) was used instead of **1b** in the reaction with ethynylbenzene (**2r**) under the standard reaction conditions. The reactions were quenched at 25 min, 50 min, 75 min, 100 min respectively. The resulting solution was then diluted with dichloromethane (3 x 10 mL) and washed with brine (2 x 5 mL) and water (5 mL). The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The crude residue was obtained after evaporating the solvent in vacuum and was purified by column chromatography. The calculated  $k_H/k_D$  value was found to be 1.1.

<b>t/min</b>	25	50	75	100
<b>yield</b>				

<b>3br</b>	15.5%	23.6%	28.6%	32.1%
<b>3br-<i>d</i><sub>1</sub></b>	14.1%	21.4%	26.2%	29.1%

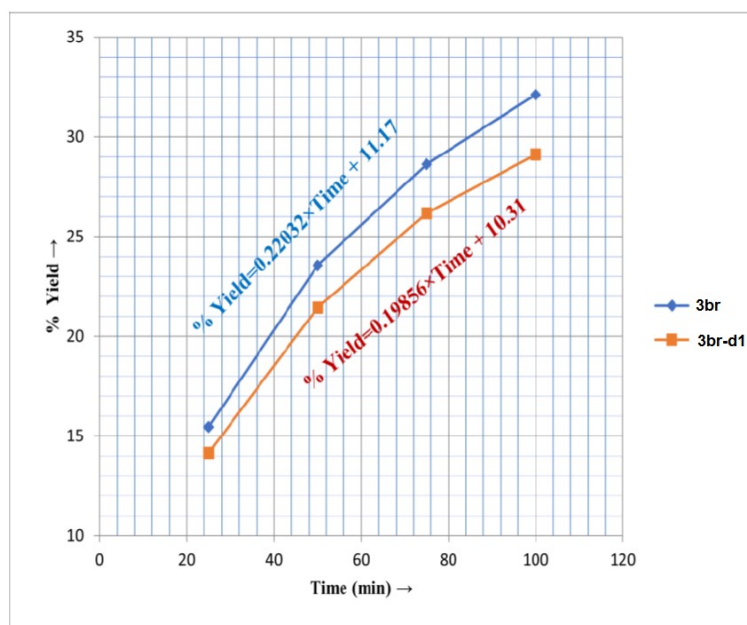
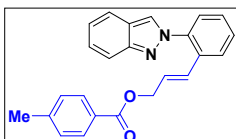
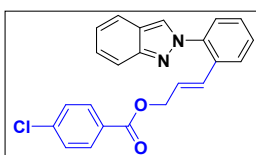


Figure S1. The reaction rate of 1b and 1b-*d*<sub>2</sub>

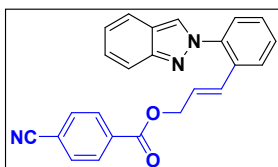
#### 4. Characterization data for the synthesized products:



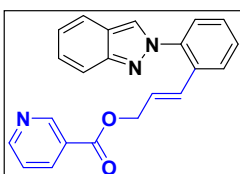
**(*E*)-3-(2-(2*H*-indazol-2-yl)phenyl)allyl 4-methylbenzoate (3aa):** Yellow gummy mass (91%, 83.8 mg);  $R_f = 0.50$  (PE/ EA = 85 : 15);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.14 (s, 1H), 7.80 (d,  $J = 8.0$  Hz, 2H), 7.74-7.71 (m, 1H), 7.53-7.40 (m, 3H), 7.38-7.34 (m, 1H), 7.17-7.12 (m, 3H), 6.55 (d,  $J = 16.0$  Hz, 1H), 6.45-6.38 (m, 1H), 4.86 (d,  $J = 5.6$  Hz, 2H), 2.38 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  166.3, 149.5, 143.7, 139.0, 132.3, 129.6, 129.3, 129.1, 128.6, 127.8, 127.2, 126.97, 126.94, 126.8, 126.7, 125.4, 122.4, 122.1, 120.5, 118.0, 64.8, 21.7; Anal. Calcd for  $\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_2$ : C, 78.24; H, 5.47; N, 7.60%; Found: C, 78.39; H, 5.50; N, 7.70%.



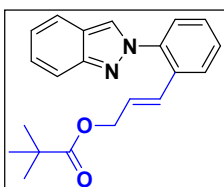
**(E)-3-(2-(2H-indazol-2-yl)phenyl)allyl 4-chlorobenzoate (3ab):** White solid (94%, 91.3 mg);  $R_f = 0.50$  (PE/ EA = 85 : 15); M.P. 81-82 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.09 (s, 1H), 7.80-7.75 (m, 3H), 7.71-7.67 (m, 2H), 7.49-7.32 (m, 4H), 7.26-7.24 (m, 2H), 7.15-7.12 (m, 1H), 6.50 (d,  $J = 16.0$  Hz, 1H), 6.40-6.33 (m, 1H), 4.85-4.83 (m, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.2, 149.5, 139.4, 138.9, 132.2, 130.9, 129.3, 128.7, 128.6, 128.3, 127.7, 126.9, 126.7, 126.6, 126.3, 125.3, 122.4, 122.0, 120.4, 117.9, 64.9; Anal. Calcd for  $\text{C}_{23}\text{H}_{17}\text{ClN}_2\text{O}_2$ : C, 71.04; H, 4.41; N, 7.20%; Found: C, 71.22; H, 4.39; N, 7.12%.



**(E)-3-(2-(2H-indazol-2-yl)phenyl)allyl 4-cyanobenzoate (3ac):** Yellow solid (90%, 85.3 mg);  $R_f = 0.50$  (PE/ EA = 80 : 20); M.P. 107-108 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.11 (s, 1H), 7.94 (d,  $J = 8.0$  Hz, 2H), 7.82-7.69 (m, 3H), 7.58 (d,  $J = 8.4$  Hz, 2H), 7.50-7.46 (m, 2H), 7.44-7.42 (m, 1H), 7.38-7.34 (m, 1H), 7.18-7.14 (m, 1H), 6.51 (d,  $J = 16.0$  Hz, 1H), 6.42-6.35 (m, 1H), 4.91-4.89 (m, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.5, 149.5, 139.0, 133.6, 132.2, 132.1, 130.0, 129.4, 128.7, 127.8, 126.9, 126.8, 126.6, 125.7, 125.3, 122.4, 122.0, 120.4, 118.0, 117.9, 116.3, 65.4; Anal. Calcd for  $\text{C}_{24}\text{H}_{17}\text{N}_3\text{O}_2$ : C, 75.98; H, 4.52; N, 11.08%; Found: C, 75.78; H, 4.57; N, 10.96%.

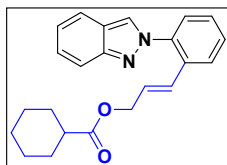


**(E)-3-(2-(2H-indazol-2-yl)phenyl)allyl isonicotinate (3ad):** Yellow gummy mass (78%, 69.3 mg);  $R_f = 0.45$  (PE/ EA = 80 : 20);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  9.16 (d,  $J = 1.2$  Hz, 1H), 8.73-8.72 (m, 1H), 8.12-8.09 (m, 2H), 7.77 (d,  $J = 9.0$  Hz, 1H), 7.73-7.69 (m, 2H), 7.51-7.45 (m, 2H), 7.44-7.41 (m, 1H), 7.36-7.32 (m, 1H), 7.27-7.24 (m, 1H), 7.15-7.12 (m, 1H), 6.53 (d,  $J = 16.0$  Hz, 1H), 6.42-6.35 (m, 1H), 4.90-4.88 (m, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.8, 153.3, 150.8, 149.4, 138.9, 137.0, 132.1, 129.3, 128.7, 128.6, 126.9, 126.8, 126.0, 125.3, 123.3, 122.4, 122.0, 120.4, 117.8, 65.4; Anal. Calcd for  $\text{C}_{22}\text{H}_{17}\text{N}_3\text{O}_2$ : C, 74.35; H, 4.82; N, 11.82%; Found: C, 74.51; H, 4.78; N, 11.90%.

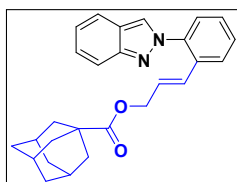


**(E)-3-(2-(2H-indazol-2-yl)phenyl)allyl pivalate (3ae):** Yellow gummy mass (96%, 80.2 mg);  $R_f = 0.50$  (PE/ EA = 92 : 8);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.10 (s, 1H), 7.79 (d,  $J = 8.4$  Hz, 1H), 7.73-7.67 (m, 2H), 7.50-7.31 (m, 4H), 7.15-7.11 (m, 1H), 6.39 (d,  $J = 16.0$  Hz, 1H), 6.32-6.25 (m, 1H), 4.63-4.61 (m, 2H), 1.05 (s, 9H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  178.0, 149.5, 138.9, 132.4, 129.3, 128.4, 127.0, 126.9, 126.7, 126.67, 126.62, 125.3, 122.3,

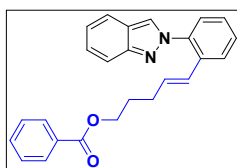
122.1, 120.3, 117.9, 64.0, 38.7, 27.0; Anal. Calcd for C<sub>21</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub>: C, 75.42; H, 6.63; N, 8.38%; Found: C, 75.61; H, 6.60; N, 8.44%.



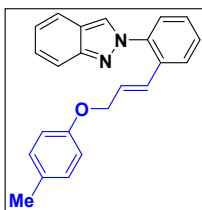
**(E)-3-(2-(2H-indazol-2-yl)phenyl)allyl cyclohexanecarboxylate (3af):** Yellow gummy mass (94%, 84.6 mg);  $R_f = 0.50$  (PE/ EA = 90 : 10); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.10 (s, 1H), 7.81-7.78 (m, 1H), 7.73 (d,  $J = 8.4$  Hz, 1H), 7.69-7.67 (m, 1H), 7.50-7.32 (m, 4H), 7.16-7.12 (m, 1H), 6.38 (d,  $J = 16.0$  Hz, 1H), 6.31-6.25 (m, 1H), 4.63-4.62 (m, 2H), 2.22-2.14 (m, 1H), 1.77-1.73 (m, 1H), 1.64-1.54 (m, 3H), 1.31-1.22 (m, 3H), 1.18-1.10 (m, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  175.6, 149.4, 138.8, 132.3, 129.2, 128.4, 127.0, 126.9, 126.7, 125.3, 122.3, 122.0, 120.4, 117.9, 63.9, 43.1, 28.9, 25.6, 25.4; Anal. Calcd for C<sub>23</sub>H<sub>24</sub>N<sub>2</sub>O<sub>2</sub>: C, 76.64; H, 6.71; N, 7.77%; Found: C, 76.87; H, 6.75; N, 7.68%.



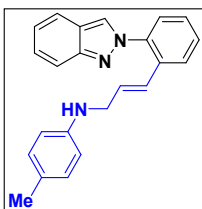
**(E)-3-(2-(2H-indazol-2-yl)phenyl)allyl (3r,5r,7r)-adamantane-1-carboxylate (3ag):** Yellow solid (89%, 91.7 mg);  $R_f = 0.50$  (PE/ EA = 90 : 10); M.P. 87-88 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.10 (s, 1H), 7.79 (d,  $J = 9.2$  Hz, 1H), 7.74-7.67 (m, 2H), 7.50-7.38 (m, 3H), 7.35-7.31 (m, 1H), 7.13 (t,  $J = 8.4$  Hz, 1H), 6.37 (d,  $J = 14.4$  Hz, 1H), 6.32-6.25 (m, 1H), 4.64-4.63 (m, 2H), 1.90-1.86 (m, 3H), 1.70 (d,  $J = 2.4$  Hz, 6H), 1.63 (d,  $J = 12.4$  Hz, 3H), 1.53 (d,  $J = 11.6$  Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  177.2, 149.5, 138.9, 132.5, 129.3, 128.4, 127.2, 126.9, 126.7, 126.6, 126.2, 125.4, 122.4, 122.1, 120.4, 117.9, 63.6, 40.7, 38.7, 36.4, 27.8; Anal. Calcd for C<sub>27</sub>H<sub>28</sub>N<sub>2</sub>O<sub>2</sub>: C, 78.61; H, 6.84; N, 6.79%; Found: C, 78.44; H, 6.86; N, 6.89%.



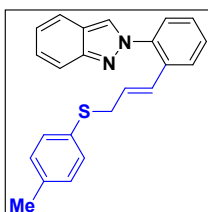
**(E)-5-(2-(2H-indazol-2-yl)phenyl)pent-4-en-1-yl benzoate (3ah):** Yellow gummy mass (49%, 46.8 mg);  $R_f = 0.45$  (PE/ EA = 90 : 10); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.11 (s, 1H), 8.00-7.97 (m, 2H), 7.80 (d,  $J = 8.4$  Hz, 1H), 7.72 (d,  $J = 8.4$  Hz, 1H), 7.65 (d,  $J = 7.6$  Hz, 1H), 7.53 (t,  $J = 7.6$  Hz, 1H), 7.48-7.45 (m, 2H), 7.43-7.33 (m, 4H), 7.12 (t,  $J = 8.0$  Hz, 1H), 6.30-6.23 (m, 1H), 6.19 (d,  $J = 15.6$  Hz, 1H), 4.31 (t,  $J = 6.4$  Hz, 2H), 2.31-2.26 (m, 2H), 1.90-1.83 (m, 2H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  166.7, 149.4, 138.5, 133.6, 133.1, 133.0, 130.3, 129.6, 129.3, 128.4, 127.7, 127.0, 126.7, 126.6, 125.6, 125.3, 122.3, 122.1, 120.5, 118.0, 64.3, 29.7, 28.3; Anal. Calcd for C<sub>25</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub>: C, 78.51; H, 5.80; N, 7.32%; Found: C, 78.38; H, 5.76; N, 7.25%.



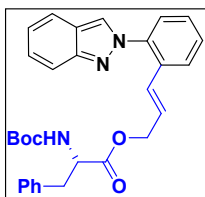
**(E)-2-(2-(3-(p-tolyloxy)prop-1-en-1-yl)phenyl)-2H-indazole (3ai):** Yellow gummy mass (95%, 80.8 mg);  $R_f = 0.50$  (PE/ EA = 90 : 10);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.07 (s, 1H), 7.85 (d,  $J = 8.8$  Hz, 1H), 7.73 (d,  $J = 8.0$  Hz, 2H), 7.53 (d,  $J = 7.6$  Hz, 1H), 7.49-7.37 (m, 3H), 7.18 (t,  $J = 7.6$  Hz, 1H), 7.07 (d,  $J = 8.4$  Hz, 2H), 6.77 (d,  $J = 8.4$  Hz, 2H), 6.54 (d,  $J = 16.0$  Hz, 1H), 6.47-6.42 (m, 1H), 4.58 (d,  $J = 5.6$  Hz, 2H), 2.30 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  156.2, 149.4, 138.8, 132.3, 130.1, 129.9, 129.2, 128.45, 128.41, 127.5, 126.9, 126.8, 126.6, 125.3, 122.3, 122.0, 120.4, 117.9, 114.6, 68.4, 20.5; Anal. Calcd for  $\text{C}_{23}\text{H}_{20}\text{N}_2\text{O}$ : C, 81.15; H, 5.92; N, 8.23%; Found: C, 81.34; H, 5.97; N, 8.31%.



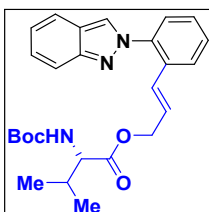
**(E)-N-(3-(2-(2H-indazol-2-yl)phenyl)allyl)-4-methylaniline (3aj):** Yellow gummy mass (79%, 67.0 mg);  $R_f = 0.50$  (PE/ EA = 90 : 10);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.02 (s, 1H), 7.79 (d,  $J = 9.2$  Hz, 1H), 7.68-7.66 (m, 2H), 7.51-7.48 (m, 1H), 7.46-7.33 (m, 3H), 7.16-7.12 (m, 1H), 6.95 (d,  $J = 8.4$  Hz, 2H), 6.50 (d,  $J = 8.4$  Hz, 2H), 6.41 (d,  $J = 16.0$  Hz, 1H), 6.35-6.29 (m, 1H), 3.82 (d,  $J = 5.2$  Hz, 2H), 2.24 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  149.5, 145.1, 138.7, 132.8, 130.9, 129.8, 129.2, 128.2, 127.2, 127.0, 126.9, 126.7, 126.4, 125.4, 122.3, 122.1, 120.5, 118.0, 113.5, 46.5, 20.5; Anal. Calcd for  $\text{C}_{23}\text{H}_{21}\text{N}_3$ : C, 81.38; H, 6.24; N, 12.38%; Found: C, 81.52; H, 6.21; N, 12.27%.



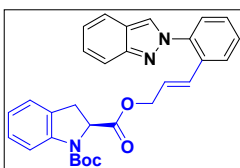
**(E)-2-(2-(3-(p-tolylthio)prop-1-en-1-yl)phenyl)-2H-indazole (3ak):** Yellow gummy mass (71%, 63.2 mg);  $R_f = 0.50$  (PE/ EA = 92 : 8);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.85 (s, 1H), 7.79 (d,  $J = 8.8$  Hz, 1H), 7.69 (d,  $J = 8.4$  Hz, 1H), 7.64-7.62 (m, 1H), 7.49-7.47 (m, 1H), 7.45-7.41 (m, 1H), 7.39-7.33 (m, 2H), 7.21 (d,  $J = 8.0$  Hz, 2H), 7.17-7.13 (m, 1H), 7.06 (d,  $J = 8.0$  Hz, 2H), 6.30-6.22 (m, 1H), 6.16 (d,  $J = 15.6$  Hz, 1H), 3.53 (d,  $J = 7.2$  Hz, 2H), 2.32 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  149.5, 138.7, 136.9, 132.5, 131.6, 131.4, 129.7, 129.3, 129.2, 128.2, 127.1, 127.0, 126.9, 126.6, 125.3, 122.3, 122.1, 120.4, 118.0, 37.9, 21.2; Anal. Calcd for  $\text{C}_{23}\text{H}_{20}\text{N}_2\text{S}$ : C, 77.49; H, 5.66; N, 7.86%; Found: C, 77.34; H, 5.64; N, 7.76%.



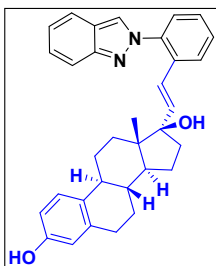
**(E)-3-(2-(2H-indazol-2-yl)phenyl)allyl (tert-butoxycarbonyl)-L-phenylalaninate (3al):** Yellow gummy mass (82%, 100.0 mg);  $R_f = 0.50$  (PE/ EA = 75 : 25);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.09 (s, 1H), 7.79 (d,  $J = 8.4$  Hz, 1H), 7.73 (d,  $J = 8.4$  Hz, 1H), 7.69-7.67 (m, 1H), 7.53-7.42 (m, 3H), 7.36-7.32 (m, 1H), 7.24-7.18 (m, 3H), 7.16-7.12 (m, 1H), 7.07-7.05 (m, 2H), 6.44 (d,  $J = 16.0$  Hz, 1H), 6.25-6.18 (m, 1H), 4.94 (d,  $J = 8.0$  Hz, 1H), 4.66-4.63 (m, 2H), 4.56-4.51 (m, 1H), 3.05-2.89 (m, 2H), 1.40 (s, 9H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.6, 155.1, 149.6, 139.0, 136.0, 132.1, 129.4, 129.3, 129.2, 128.8, 128.5, 127.07, 127.00, 126.9, 126.8, 126.1, 125.4, 122.5, 122.1, 120.4, 118.0, 80.0, 65.6, 54.5, 38.3, 28.3; Anal. Calcd for  $\text{C}_{30}\text{H}_{31}\text{N}_3\text{O}_4$ : C, 72.41; H, 6.28; N, 8.44%; Found: C, 72.57; H, 6.24; N, 8.56%.



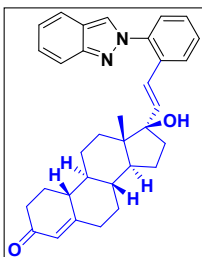
**(E)-3-(2-(2H-indazol-2-yl)phenyl)allyl (tert-butoxycarbonyl)-L-valinate (3am):** Yellow gummy mass (77%, 86.5 mg);  $R_f = 0.50$  (PE/ EA = 80 : 20);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.10 (s, 1H), 7.80-7.77 (m, 1H), 7.73 (d,  $J = 8.8$  Hz, 1H), 7.68-7.66 (m, 1H), 7.50-7.40 (m, 3H), 7.36-7.32 (m, 1H), 7.16-7.12 (m, 1H), 6.45 (d,  $J = 15.6$  Hz, 1H), 6.31-6.24 (m, 1H), 4.99 (d,  $J = 8.8$  Hz, 1H), 4.72-4.61 (m, 2H), 4.18-4.15 (m, 1H), 2.05-1.97 (m, 1H), 1.41 (s, 9H), 0.86 (d,  $J = 7.2$  Hz, 3H), 0.76 (d,  $J = 6.8$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  172.1, 155.7, 149.5, 138.9, 132.1, 129.3, 128.8, 128.7, 126.9, 126.8, 126.7, 126.1, 125.3, 122.4, 122.1, 120.4, 117.9, 79.7, 65.2, 58.5, 31.2, 28.3, 19.0, 17.4; Anal. Calcd for  $\text{C}_{26}\text{H}_{31}\text{N}_3\text{O}_4$ : C, 69.47; H, 6.95; N, 9.35%; Found: C, 69.27; H, 6.97; N, 9.27%.



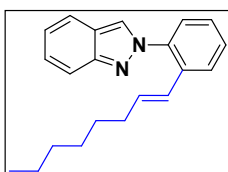
**(E)-2-(3-(2-(2H-indazol-2-yl)phenyl)allyl) 1-(tert-butyl) (S)-indoline-1,2-dicarboxylate (3an):** Yellow gummy mass (72%, 89.1 mg);  $R_f = 0.50$  (PE/ EA = 75 : 25);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.10 (s, 1H), 7.89-7.66 (m, 4H), 7.51-7.41 (m, 3H), 7.36 (t,  $J = 8.4$  Hz, 1H), 7.19-7.13 (m, 2H), 7.02 (d,  $J = 7.2$  Hz, 1H), 6.91 (t,  $J = 7.2$  Hz, 1H), 6.45 (d,  $J = 16.0$  Hz, 1H), 6.32-6.25 (m, 1H), 4.87-4.73 (m, 2H), 4.68-4.64 (m, 1H), 3.38-3.31 (m, 1H), 2.99-2.94 (m, 1H), 1.45 (s, 9H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.5, 151.5, 149.4, 142.4, 138.9, 131.9, 129.2, 128.9, 128.7, 127.8, 126.8, 126.7, 126.3, 125.9, 125.3, 124.7, 124.3, 122.5, 122.4, 122.1, 120.4, 117.8, 114.5, 81.2, 65.3, 60.2, 32.5, 28.2; Anal. Calcd for  $\text{C}_{30}\text{H}_{29}\text{N}_3\text{O}_4$ : C, 72.71; H, 5.90; N, 8.48%; Found: C, 72.57; H, 5.93; N, 8.54%.



**(8R,9S,13S,14S,17R)-17-((E)-2-(2H-indazol-2-yl)styryl)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene-3,17-diol (3ao):** White solid (68%, 83.3 mg);  $R_f = 0.45$  (PE/ EA = 70 : 30), M.P. 109-110 °C;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  9.03 (s, 1H), 8.53 (s, 1H), 7.76 (t,  $J = 8.8$  Hz, 2H), 7.68 (d,  $J = 8.8$  Hz, 1H), 7.56-7.48 (m, 2H), 7.43 (t,  $J = 8.0$  Hz, 1H), 7.30 (t,  $J = 8.4$  Hz, 1H), 7.09 (t,  $J = 7.6$  Hz, 1H), 7.99 (d,  $J = 8.4$  Hz, 1H), 6.50-6.48 (m, 1H), 6.43 (s, 1H), 6.32 (d,  $J = 16.0$  Hz, 1H), 6.21 (d,  $J = 16.0$  Hz, 1H), 4.65 (s, 1H), 2.66 (d,  $J = 4.4$  Hz, 2H), 2.50 (s, 1H), 2.12 (d,  $J = 8.8$  Hz, 1H), 1.91 (s, 2H), 1.71-1.62 (m, 3H), 1.44 (d,  $J = 9.2$  Hz, 1H), 1.25-1.17 (m, 4H), 1.13-1.06 (m, 1H), 0.75 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  154.9, 148.6, 140.5, 138.4, 137.2, 133.6, 130.5, 129.5, 127.6, 127.19, 127.13, 126.3, 126.2, 126.0, 121.8, 121.0, 120.8, 117.4, 114.9, 112.7, 82.8, 48.3, 47.1, 43.1, 36.1, 32.1, 29.2, 27.0, 26.1, 22.8, 21.1, 14.2; Anal. Calcd for  $\text{C}_{33}\text{H}_{34}\text{N}_2\text{O}_2$ : C, 80.78; H, 6.99; N, 5.71%; Found: C, 80.95; H, 6.94; N, 5.80%.

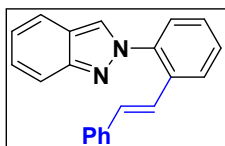


**(8R,9S,10R,13S,14S,17R)-17-((E)-2-(2H-indazol-2-yl)styryl)-17-hydroxy-13-methyl-1,2,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-3H-cyclopenta[a]phenanthren-3-one (3ap):** White solid (60%, 73.8 mg);  $R_f = 0.50$  (PE/ EA = 70 : 30); M.P. 115-116 °C;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  8.54 (s, 1H), 7.74-7.71 (m, 2H), 7.66 (d,  $J = 8.8$  Hz, 1H), 7.53 (t,  $J = 8.0$  Hz, 1H), 7.49-7.41 (m, 2H), 7.29 (t,  $J = 8.4$  Hz, 1H), 7.08 (t,  $J = 8.0$  Hz, 1H), 6.25 (d,  $J = 16.0$  Hz, 1H), 6.17 (d,  $J = 16.0$  Hz, 1H), 5.74 (s, 1H), 4.61 (s, 1H), 2.48 (d,  $J = 14.4$  Hz, 1H), 2.21-2.06 (m, 5H), 1.72-1.58 (m, 4H), 1.47-1.33 (m, 3H), 1.29-1.22 (m, 3H), 1.08-0.98 (m, 2H), 0.86-0.82 (m, 1H), 0.78 (s, 3H), 0.65-0.57 (m, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  198.5, 167.0, 148.5, 140.6, 138.3, 133.5, 129.5, 127.5, 127.16, 127.11, 126.3, 126.1, 123.6, 121.75, 121.71, 121.0, 120.8, 117.3, 82.7, 59.7, 48.5, 48.0, 46.8, 41.6, 36.1, 36.0, 34.7, 31.8, 30.2, 26.0, 25.6, 22.9, 14.1; Anal. Calcd for  $\text{C}_{33}\text{H}_{36}\text{N}_2\text{O}_2$ : C, 80.45; H, 7.37; N, 5.69%; Found: C, 80.22; H, 7.41; N, 5.62%.

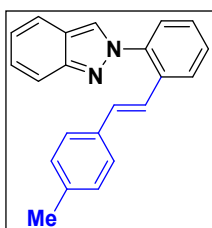


**(E)-2-(2-(Oct-1-en-1-yl)phenyl)-2H-indazole (3aq):** Yellow gummy mass (57%, 43.3 mg);  $R_f = 0.55$  (PE/ EA = 97 : 3);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.12 (s, 1H), 7.82-7.80 (m, 1H),

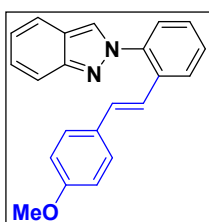
7.74 (d,  $J = 8.4$  Hz, 1H), 7.66-7.64 (m, 1H), 7.49-7.46 (m, 1H), 7.45-7.41 (m, 1H), 7.37-7.33 (m, 2H), 7.14 (t,  $J = 8.4$  Hz, 1H), 6.26-6.19 (m, 1H), 6.12 (d,  $J = 16.0$  Hz, 1H), 2.12-2.07 (m, 2H), 1.40-1.35 (m, 2H), 1.33-1.21 (m, 6H), 0.85 (t,  $J = 6.8$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  139.0, 138.4, 135.1, 134.0, 129.2, 127.4, 127.0, 126.7, 126.6, 125.3, 124.6, 122.3, 122.1, 120.4, 118.1, 33.2, 31.8, 29.2, 28.9, 22.7, 14.2; Anal. Calcd for  $\text{C}_{21}\text{H}_{24}\text{N}_2$ : C, 82.85; H, 7.95; N, 9.20%; Found: C, 82.70; H, 8.00; N, 9.30%.



**(E)-2-(2-Styrylphenyl)-2H-indazole (3ar):** Yellow gummy mass (75%, 55.5 mg);  $R_f = 0.50$  (PE / EA = 96 : 4);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.17 (s, 1H), 7.84 (d,  $J = 8.4$  Hz, 2H), 7.74 (d,  $J = 8.4$  Hz, 1H), 7.57-7.55 (m, 1H), 7.53-7.49 (m, 1H), 7.45-7.37 (m, 2H), 7.34 (d,  $J = 8.4$  Hz, 2H), 7.30-7.28 (m, 2H), 7.25-7.21 (m, 1H), 7.18-7.08 (m, 2H), 6.91 (d,  $J = 16$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  149.6, 139.1, 136.9, 133.3, 132.0, 129.3, 128.8, 128.26, 128.22, 127.1, 126.9, 126.78, 126.72, 125.5, 123.4, 122.4, 122.2, 120.5, 118.1; Anal. Calcd for  $\text{C}_{21}\text{H}_{16}\text{N}_2$ : C, 85.11; H, 5.44; N, 9.45%; Found: C, 85.25; H, 5.41; N, 9.34%.



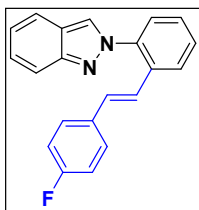
**(E)-2-(2-(4-Methylstyryl)phenyl)-2H-indazole (3as):** Yellow gummy mass (72%, 55.8 mg);  $R_f = 0.50$  (PE / EA = 95 : 5);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.07 (s, 1H), 7.75-7.72 (m, 2H), 7.63 (d,  $J = 8.4$  Hz, 1H), 7.47-7.45 (m, 1H), 7.40 (t,  $J = 7.2$  Hz, 1H), 7.33-7.28 (m, 2H), 7.15 (t,  $J = 8$  Hz, 2H), 7.08-7.04 (m, 1H), 7.00 (t,  $J = 8.8$  Hz, 3H), 6.75 (d,  $J = 16.4$  Hz, 1H), 2.22 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  149.6, 139.0, 138.2, 134.1, 133.4, 132.0, 129.5, 129.3, 128.0, 127.0, 126.8, 126.7, 126.6, 125.5, 122.4, 122.3, 122.2, 120.5, 118.1, 21.3; Anal. Calcd for  $\text{C}_{22}\text{H}_{18}\text{N}_2$ : C, 85.13; H, 5.85; N, 9.03%; Found: C, 85.29; H, 5.81; N, 8.91%.



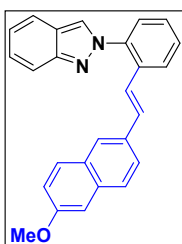
**(E)-2-(2-(4-Methoxystyryl)phenyl)-2H-indazole (3at):** Yellow gummy mass (61%, 49.7 mg);  $R_f = 0.50$  (PE : EA = 92 : 8);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.17 (s, 1H), 7.85-7.81 (m, 2H), 7.74 (d,  $J = 8.4$  Hz, 1H), 7.55-7.53 (m, 1H), 7.51-7.47 (m, 1H), 7.42-7.35 (m, 2H), 7.29 (t,  $J = 4.4$  Hz, 2H), 7.18-7.14 (m, 1H), 7.07 (d,  $J = 16.0$  Hz, 1H), 6.81 (d,  $J = 8.4$  Hz, 2H), 6.75 (d,  $J = 16.4$  Hz, 1H), 3.78 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  138.8, 133.6, 131.5, 129.7, 129.3, 128.2, 127.8, 127.1, 126.7, 126.49, 126.44, 125.6, 125.5, 122.3, 122.1,



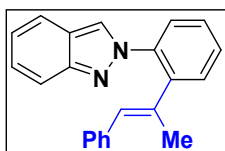
121.1, 120.5, 118.1, 114.1, 55.4; Anal. Calcd for C<sub>22</sub>H<sub>18</sub>N<sub>2</sub>O: C, 80.96; H, 5.56; N, 8.58%; Found: C, 80.81; H, 5.52; N, 8.51%.



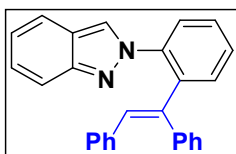
**(E)-2-(2-(4-fluorostyryl)phenyl)-2H-indazole (3au):** Yellow gummy mass (87%, 68.3 mg);  $R_f = 0.50$  (PE : EA = 95 : 5); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.16 (s, 1H), 7.86-7.81 (m, 2H), 7.75 (d,  $J = 8.8$  Hz, 1H), 7.56-7.48 (m, 2H), 7.44-7.36 (m, 2H), 7.31-7.28 (m, 2H), 7.19-7.15 (m, 1H), 7.07 (d,  $J = 16.4$  Hz, 1H), 6.99-6.94 (m, 2H), 6.83 (d,  $J = 16.4$  Hz, 1H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  162.6 (C-F, <sup>1</sup> $J_{C-F} = 246.0$  Hz), 149.6, 139.0, 133.1 (C-F, <sup>3</sup> $J_{C-F} = 8.0$  Hz), 133.0, 130.7, 129.3, 128.4 (C-F, <sup>3</sup> $J_{C-F} = 8.0$  Hz), 128.2, 127.0, 126.6 (C-F, <sup>2</sup> $J_{C-F} = 24.0$  Hz), 125.4, 123.16, 123.14, 122.4, 122.2, 120.5, 118.0, 115.7 (C-F, <sup>2</sup> $J_{C-F} = 22.0$  Hz); Anal. Calcd for C<sub>21</sub>H<sub>15</sub>FN<sub>2</sub>: C, 80.24; H, 4.81; N, 8.91%; Found: C, 80.41; H, 4.84; N, 9.03%.



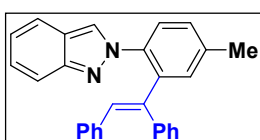
**(E)-2-(2-(2-(6-Methoxynaphthalen-2-yl)vinyl)phenyl)-2H-indazole (3av):** Yellow solid (76%, 71.5 mg);  $R_f = 0.50$  (PE : EA = 93 : 7); M.P. 98-99 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.18 (s, 1H), 7.87-7.84 (m, 2H), 7.73 (d,  $J = 8.4$  Hz, 1H), 7.65 (d,  $J = 9.2$  Hz, 2H), 7.60-7.54 (m, 2H), 7.50 (t,  $J = 7.6$  Hz, 1H), 7.43-7.35 (m, 3H), 7.23 (t,  $J = 8.0$  Hz, 1H), 7.17-7.13 (m, 1H), 7.11-7.05 (m, 2H), 6.70 (d,  $J = 16.4$  Hz, 1H), 3.88 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  158.1, 149.6, 139.0, 134.5, 133.5, 132.5, 132.3, 132.2, 129.7, 129.3, 129.0, 128.4, 128.0, 127.3, 127.2, 127.1, 126.7, 126.6, 125.6, 124.1, 122.6, 122.4, 122.2, 120.6, 119.2, 118.1, 105.9, 55.4; Anal. Calcd for C<sub>26</sub>H<sub>20</sub>N<sub>2</sub>O: C, 82.95; H, 5.36; N, 7.44%; Found: C, 82.74; H, 5.41; N, 7.36%.



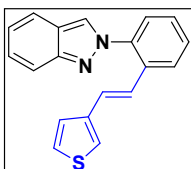
**(E)-2-(2-(1-Phenylprop-1-en-2-yl)phenyl)-2H-indazole (3aw):** Yellow gummy mass (82%, 63.6 mg);  $R_f = 0.50$  (PE/EA = 95 : 5); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.02 (s, 1H), 7.60 (d,  $J = 8.8$  Hz, 1H), 7.49-7.46 (m, 2H), 7.30-7.25 (m, 3H), 7.12 (t,  $J = 6.8$  Hz, 3H), 7.03 (d,  $J = 7.2$  Hz, 3H), 6.92-6.88 (m, 1H), 6.42 (s, 1H), 1.45 (d,  $J = 1.2$  Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  149.3, 141.0, 138.6, 137.5, 136.9, 130.9, 130.0, 129.0, 128.3, 128.2, 128.1, 126.9, 126.8, 126.7, 124.8, 122.5, 122.2, 120.5, 118.0, 18.3; Anal. Calcd for C<sub>22</sub>H<sub>18</sub>N<sub>2</sub>: C, 85.13; H, 5.85; N, 9.03%; Found: C, 85.27; H, 5.81; N, 8.93%.



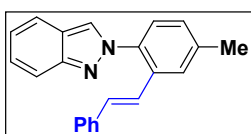
**(E)-2-(2-(1,2-diphenylvinyl)phenyl)-2H-indazole (3ax):** Yellow solid (57%, 55.2 mg);  $R_f = 0.50$  (PE : EA = 95 : 5); M.P. 139-140 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.82 (s, 1H), 7.60 (t,  $J = 9.6$  Hz, 1H), 7.54-7.45 (m, 4H), 7.19 (t,  $J = 8.4$  Hz, 1H), 7.08 (t,  $J = 2.4$  Hz, 3H), 7.03-7.00 (m, 2H), 6.97 (t,  $J = 7.2$  Hz, 1H), 6.91-6.88 (m, 1H), 6.82-6.76 (m, 5H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  149.1, 140.8, 140.2, 139.5, 138.3, 137.0, 131.7, 131.0, 129.5, 129.4, 129.1, 128.5, 128.0, 127.5, 127.3, 127.1, 127.0, 126.1, 124.8, 122.0, 121.7, 120.1, 117.7; Anal. Calcd for  $\text{C}_{27}\text{H}_{20}\text{N}_2$ : C, 87.07; H, 5.41; N, 7.52 %; Found: C, 86.92; H, 5.44; N, 7.64%.



**(E)-2-(2-(1,2-diphenylvinyl)-4-methylphenyl)-2H-indazole (3bx):** Yellow solid (55%, 53.1 mg);  $R_f = 0.50$  (PE : EA = 95 : 5); M.P. 137-138 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.78 (s, 1H), 7.59-7.57 (m, 1H), 7.44 (d,  $J = 9.4$  Hz, 1H), 7.39 (d,  $J = 8.4$  Hz, 2H), 7.28 (d,  $J = 1.6$  Hz, 1H), 7.19-7.15 (m, 1H), 7.09-7.07 (m, 3H), 7.01-6.99 (m, 2H), 6.97-6.93 (m, 1H), 6.91-6.87 (m, 1H), 6.82-6.77 (m, 5H), 2.48 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  140.5, 140.3, 139.1, 138.4, 137.2, 137.1, 132.2, 130.9, 129.5, 129.2, 129.1, 128.0, 127.8, 127.5, 127.1, 127.0, 126.9, 126.0, 124.9, 122.0, 121.6, 120.1, 117.7, 21.3; Anal. Calcd for  $\text{C}_{28}\text{H}_{22}\text{N}_2$ : C, 87.01; H, 5.74; N, 7.25%; Found: C, 87.14; H, 5.72; N, 7.14%.

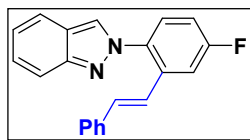


**(E)-2-(2-(2-(thiophen-3-yl)vinyl)phenyl)-2H-indazole (3ay):** Yellow gummy mass (76%, 57.3 mg);  $R_f = 0.50$  (PE : EA = 95 : 5);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.16 (s, 1H), 7.86 (d,  $J = 8.8$  Hz, 1H), 7.79 (d,  $J = 7.6$  Hz, 1H), 7.74 (d,  $J = 8.4$  Hz, 1H), 7.55 (d,  $J = 8.0$  Hz, 1H), 7.51-7.47 (m, 1H), 7.43-7.36 (m, 2H), 7.21-7.11 (m, 4H), 7.07 (t,  $J = 3.6$  Hz, 1H), 6.75 (d,  $J = 16.0$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  149.5, 139.7, 138.8, 133.2, 129.2, 128.0, 127.0, 126.7, 126.3, 125.9, 125.4, 125.0, 123.4, 123.2, 122.3, 122.1, 120.5, 118.0; Anal. Calcd for  $\text{C}_{19}\text{H}_{14}\text{N}_2\text{S}$ : C, 75.47; H, 4.67; N, 9.26%; Found: C, 75.28; H, 4.62; N, 9.33%.

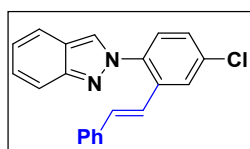


**(E)-2-(4-methyl-2-styrylphenyl)-2H-indazole (3br):** Yellow solid (78%, 60.5 mg);  $R_f = 0.50$  (PE / EA = 95 : 5); M.P. 108-109 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.02 (s, 1H), 7.72 (d,  $J$

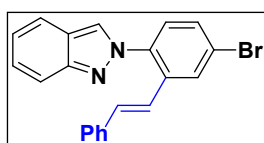
= 9.2 Hz, 1H), 7.62 (d,  $J = 8.4$  Hz, 1H), 7.53 (s, 1H), 7.33 (d,  $J = 8.4$  Hz, 1H), 7.27-7.22 (m, 3H), 7.18-7.11 (m, 4H), 7.06-6.97 (m, 2H), 6.77 (d,  $J = 16.0$  Hz, 1H), 2.38 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  149.5, 139.2, 136.99, 136.90, 132.9, 131.7, 129.0, 128.7, 128.1, 127.0, 126.8, 126.6, 125.5, 123.5, 122.3, 122.1, 120.5, 118.0, 21.4; Anal. Calcd for  $\text{C}_{22}\text{H}_{18}\text{N}_2$ : C, 85.13; H, 5.85; N, 9.03%; Found: C, 84.96; H, 5.90; N, 9.15%.



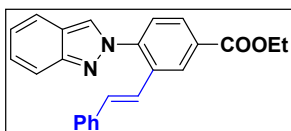
**(E)-2-(4-fluoro-2-styrylphenyl)-2H-indazole (3cr):** Yellow gummy mass (80%, 62.8 mg);  $R_f = 0.45$  (PE / EA = 95 : 5);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.13 (s, 1H), 7.82 (d,  $J = 8.4$  Hz, 1H), 7.73 (d,  $J = 8.4$  Hz, 1H), 7.54-7.50 (m, 2H), 7.40-7.36 (m, 1H), 7.33-7.28 (m, 3H), 7.26-7.24 (m, 2H), 7.19-7.15 (m, 1H), 7.14-7.09 (m, 2H), 6.82 (d,  $J = 16$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  162.9 (C-F,  $^1J_{\text{C-F}} = 247.0$  Hz), 149.7, 136.4, 135.7, 135.6, 135.3, 133.2, 129.06 (C-F,  $^3J_{\text{C-F}} = 9.0$  Hz), 128.8, 128.6, 127.0, 126.9, 125.6, 122.5, 122.3 (C-F,  $^3J_{\text{C-F}} = 7.0$  Hz), 120.5, 118.1, 115.1 (C-F,  $^2J_{\text{C-F}} = 23.0$  Hz), 112.8 (C-F,  $^2J_{\text{C-F}} = 24.0$  Hz); Anal. Calcd for  $\text{C}_{21}\text{H}_{15}\text{FN}_2$ : C, 80.24; H, 4.81; N, 8.91%; Found: C, 80.45; H, 4.83; N, 8.83%.



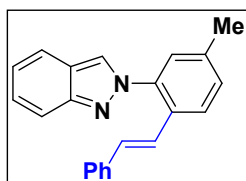
**(E)-2-(4-Chloro-2-styrylphenyl)-2H-indazole (3dr):** Yellow solid (58%, 47.9 mg);  $R_f = 0.50$  (PE / EA = 95 : 5); M.P. 101-102 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.14 (s, 1H), 7.83-7.81 (m, 2H), 7.73 (d,  $J = 8.4$  Hz, 1H), 7.50 (d,  $J = 8.4$  Hz, 1H), 7.40-7.37 (m, 2H), 7.36-7.33 (m, 2H), 7.31-7.29 (m, 1H), 7.27-7.25 (m, 2H), 7.18-7.16 (m, 1H), 7.11 (d,  $J = 16$  Hz, 1H), 6.84 (d,  $J = 16.4$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  149.8, 137.5, 136.4, 135.2, 134.9, 133.2, 128.8, 128.6, 128.4, 128.1, 127.08, 127.02, 126.5, 125.5, 122.6, 122.36, 122.30, 120.5, 118.1; Anal. Calcd for  $\text{C}_{21}\text{H}_{15}\text{ClN}_2$ : C, 76.25; H, 4.57; N, 8.47%; Found: C, 76.44; H, 4.53; N, 8.57%.



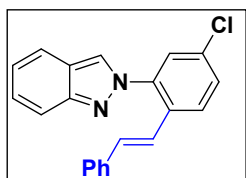
**(E)-2-(4-Bromo-2-styrylphenyl)-2H-indazole (3er):** Yellow solid (64%, 60 mg);  $R_f = 0.50$  (PE / EA = 95 : 5); M.P. 140-141 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.10 (s, 1H), 7.93 (d,  $J = 2.4$  Hz, 1H), 7.80-7.78 (m, 1H), 7.69 (d,  $J = 8.4$  Hz, 1H), 7.52-7.49 (m, 1H), 7.40 (d,  $J = 8.4$  Hz, 1H), 7.36-7.34 (m, 1H), 7.32-7.29 (m, 2H), 7.28-7.26 (m, 1H), 7.24-7.21 (m, 2H), 7.15-7.11 (m, 1H), 7.08 (d,  $J = 16.4$  Hz, 1H), 6.81 (d,  $J = 16.4$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  149.8, 138.0, 136.4, 135.1, 133.3, 131.0, 129.5, 128.8, 128.6, 128.5, 127.08, 127.04, 125.4, 123.3, 122.6, 122.3, 122.2, 120.5, 118.1; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{21}\text{H}_{16}\text{BrN}_2$ : 375.0491; found: 375.0497.



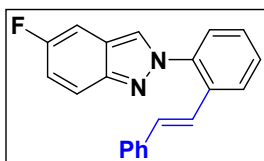
**Ethyl (E)-4-(2H-Indazol-2-yl)-3-styrylbenzoate (3fr):** Yellow solid (73%, 67.2 mg);  $R_f = 0.50$  (PE/ EA = 92 : 8); M.P. 110-111 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.51 (d,  $J = 1.6$  Hz, 1H), 8.21 (s, 1H), 8.09-8.07 (m, 1H), 7.83 (d,  $J = 8.4$  Hz, 1H), 7.73 (d,  $J = 8.8$  Hz, 1H), 7.67 (d,  $J = 8.4$  Hz, 1H), 7.40-7.36 (m, 3H), 7.32-7.27 (m, 3H), 7.24 (d,  $J = 12.0$  Hz, 1H), 7.19-7.15 (m, 1H), 6.99 (d,  $J = 16.4$  Hz, 1H), 4.49-4.44 (m, 2H), 1.46 (t,  $J = 6.8$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.8, 149.9, 142.1, 136.6, 133.1, 131.0, 129.9, 129.0, 128.87, 128.83, 128.5, 128.4, 127.1, 127.0, 125.4, 122.8, 122.7, 122.4, 120.6, 118.1, 61.9, 14.5; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{24}\text{H}_{21}\text{N}_2\text{O}_2$ : 369.1598; found: 369.1598.



**(E)-2-(5-Methyl-2-styrylphenyl)-2H-indazole (3gr):** Yellow solid (92%, 71.3 mg);  $R_f = 0.50$  (PE / EA = 95 : 5); M.P. 96-97 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.01 (s, 1H), 7.70 (d,  $J = 8.8$  Hz, 1H), 7.60-7.57 (m, 2H), 7.23-7.11 (m, 7H), 7.09-7.05 (m, 1H), 7.01 (t,  $J = 8.0$  Hz, 1H), 6.95 (d,  $J = 16$  Hz, 1H), 6.74 (d,  $J = 16.4$  Hz, 1H), 2.29 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  149.5, 138.9, 138.6, 137.0, 131.1, 130.2, 130.1, 128.7, 128.0, 127.5, 126.79, 126.72, 126.5, 125.5, 123.4, 122.3, 122.1, 120.5, 118.0, 21.1; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{22}\text{H}_{19}\text{N}_2$ : 311.1543; found: 311.1556.

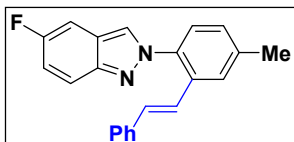


**(E)-2-(5-chloro-2-styrylphenyl)-2H-indazole (3hr):** Yellow solid (74%, 61.2 mg);  $R_f = 0.50$  (PE / EA = 95 : 5); M.P. 161-162 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.03 (s, 1H), 7.87 (d,  $J = 8.4$  Hz, 1H), 7.70-7.68 (m, 2H), 7.62-7.59 (m, 1H), 7.41-7.38 (m, 1H), 7.19 (d,  $J = 19.2$  Hz, 5H), 7.05-7.01 (m, 1H), 6.84-6.79 (m, 1H), 6.37-6.32 (m, 1H), 6.26-6.21 (m, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  149.3, 136.8, 136.5, 135.6, 135.0, 134.6, 133.0, 132.7, 131.3, 128.7, 128.5, 128.2, 126.9, 126.6, 126.5, 124.8, 122.5, 122.0, 120.6, 118.2; Anal. Calcd for  $\text{C}_{21}\text{H}_{15}\text{ClN}_2$ : C, 76.25; H, 4.57; N, 8.47%; Found: C, 76.13; H, 4.59; N, 8.54%.

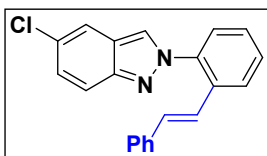


**(E)-5-Fluoro-2-(2-styrylphenyl)-2H-indazole (3ir):** Yellow gummy mass (62%, 48.7 mg);  $R_f = 0.50$  (PE / EA = 95 : 5);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.11 (s, 1H), 7.83-7.78 (m, 2H), 7.53-7.48 (m, 2H), 7.41 (t,  $J = 7.6$  Hz, 1H), 7.33-7.27 (m, 4H), 7.24-7.13 (m, 3H), 7.09 (d,  $J$

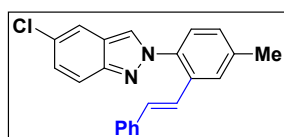
= 16.4 Hz, 1H), 6.85 (d,  $J = 16.4$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  158.7 (C-F,  $^1J_{\text{C-F}} = 239.0$  Hz), 147.1, 138.9, 136.8, 133.3, 132.2, 129.5, 128.8, 128.2, 126.99, 126.91, 126.7, 125.6 (C-F,  $^3J_{\text{C-F}} = 9.0$  Hz), 123.2, 121.5, 121.4, 120.2 (C-F,  $^3J_{\text{C-F}} = 10.0$  Hz), 118.4 (C-F,  $^2J_{\text{C-F}} = 28.0$  Hz), 102.8 (C-F,  $^2J_{\text{C-F}} = 25.0$  Hz); Anal. Calcd for  $\text{C}_{21}\text{H}_{15}\text{FN}_2$ : C, 80.24; H, 4.81; N, 8.91%; Found: C, 80.38; H, 4.78; N, 8.82%.



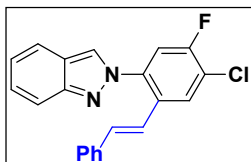
**(E)-5-fluoro-2-(4-methyl-2-styrylphenyl)-2H-indazole (3jr):** Yellow gummy mass (76%, 62.3 mg);  $R_f = 0.50$  (PE : EA = 95 : 5);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.95 (s, 1H), 7.68-7.65 (m, 1H), 7.50 (s, 1H), 7.28 (d,  $J = 8.0$  Hz, 1H), 7.21-7.18 (m, 2H), 7.17-7.13 (m, 3H), 7.11-7.07 (m, 2H), 7.05-7.00 (m, 1H), 6.95 (d,  $J = 16.4$  Hz, 1H), 6.71 (d,  $J = 16.4$  Hz, 1H), 2.35 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  158.6 (C-F,  $^1J_{\text{C-F}} = 238.0$  Hz), 147.0, 139.4, 136.9, 136.7, 132.9, 131.8, 129.0, 128.7, 128.1, 127.0, 126.8, 125.6 (C-F,  $^3J_{\text{C-F}} = 8.0$  Hz), 123.3, 121.4, 121.3, 120.1 (C-F,  $^3J_{\text{C-F}} = 10.0$  Hz), 118.2 (C-F,  $^2J_{\text{C-F}} = 29.0$  Hz), 102.8 (C-F,  $^2J_{\text{C-F}} = 24.0$  Hz), 21.4; Anal. Calcd for  $\text{C}_{22}\text{H}_{17}\text{FN}_2$ : C, 80.47; H, 5.22; N, 8.53%; Found: C, 80.29; H, 5.27; N, 8.42%.



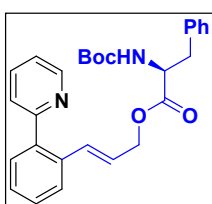
**(E)-5-chloro-2-(2-styrylphenyl)-2H-indazole (3kr):** Yellow gummy mass (52%, 43.2 mg);  $R_f = 0.50$  (PE / EA = 95 : 5);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.11 (s, 1H), 7.84 (d,  $J = 8.0$  Hz, 1H), 7.77 (d,  $J = 9.2$  Hz, 1H), 7.71 (d,  $J = 1.2$  Hz, 1H), 7.55-7.50 (m, 2H), 7.45-7.41 (m, 1H), 7.34-7.23 (m, 6H), 7.11 (d,  $J = 16.0$  Hz, 1H), 6.84 (d,  $J = 16.0$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  148.0, 138.8, 136.8, 133.3, 132.3, 129.6, 128.8, 128.35, 128.32, 128.2, 128.1, 127.0, 126.9, 126.8, 125.1, 123.1, 122.5, 119.7, 119.2; Anal. Calcd for  $\text{C}_{21}\text{H}_{15}\text{ClN}_2$ : C, 76.25; H, 4.57; N, 8.47%; Found: C, 76.05; H, 4.54; N, 8.55%.



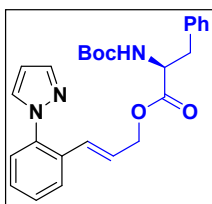
**(E)-5-Chloro-2-(4-methyl-2-styrylphenyl)-2H-indazole (3lr):** Yellow solid (79%, 68.1 mg);  $R_f = 0.50$  (PE : EA = 95 : 5); M.P. 104-105 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.06 (s, 1H), 7.75 (d,  $J = 8.8$  Hz, 1H), 7.68 (d,  $J = 1.2$  Hz, 1H), 7.62 (s, 1H), 7.41 (d,  $J = 8.0$  Hz, 1H), 7.32-7.27 (m, 5H), 7.24-7.21 (m, 2H), 7.08 (d,  $J = 16.4$  Hz, 1H), 6.80 (d,  $J = 16.0$  Hz, 1H), 2.47 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  147.8, 139.5, 136.8, 136.5, 132.8, 131.9, 129.0, 128.8, 128.2, 128.0, 127.9, 127.0, 126.8, 126.7, 125.1, 123.2, 122.5, 119.6, 119.1, 21.5; Anal. Calcd for  $\text{C}_{22}\text{H}_{17}\text{ClN}_2$ : C, 76.63; H, 4.97; N, 8.12%; Found: C, 76.76; H, 4.99; N 8.21%.



**(E)-2-(4-Chloro-5-fluoro-2-styrylphenyl)-2H-indazole (3mr):** Yellow solid (79%, 68.8 mg);  $R_f = 0.50$  (PE : EA = 94 : 6); M.P. 131-132 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.23 (s, 1H), 7.95 (d,  $J = 8.8$  Hz, 1H), 7.80 (d,  $J = 8.4$  Hz, 1H), 7.65-7.62 (m, 1H), 7.51 (t,  $J = 8.8$  Hz, 1H), 7.41-7.34 (m, 4H), 7.30-7.28 (m, 3H), 7.08 (d,  $J = 16.8$  Hz, 1H), 6.51 (d,  $J = 20.4$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  158.7 (C-F,  $^1J_{\text{C-F}} = 249.0$  Hz), 149.4, 137.1, 136.3, 136.03, 136.00, 134.9, 128.7 (C-F,  $^3J_{\text{C-F}} = 4.0$  Hz), 127.1 (C-F,  $^3J_{\text{C-F}} = 10.0$  Hz), 126.8, 125.5, 122.4 (C-F,  $^2J_{\text{C-F}} = 29.0$  Hz), 121.6, 120.5, 119.86, 119.84, 117.9, 114.8 (C-F,  $^2J_{\text{C-F}} = 23.0$  Hz); HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $\text{C}_{21}\text{H}_{15}\text{ClFN}_2$ : 349.0902; found: 349.0908.



**(E)-3-(2-(pyridin-2-yl)phenyl)allyl (tert-butoxycarbonyl)-L-phenylalaninate (3nl):** Yellow gummy mass (86%, 98.5 mg);  $R_f = 0.50$  (PE/ EA = 80 : 20);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.78 (s, 1H), 7.81 (t,  $J = 7.6$  Hz, 1H), 7.69-7.66 (m, 1H), 7.58-7.56 (m, 1H), 7.48-7.43 (m, 3H), 7.34-7.24 (m, 4H), 7.17 (d,  $J = 6.8$  Hz, 1H), 6.83 (d,  $J = 16.4$  Hz, 1H), 6.26-6.19 (m, 1H), 5.04 (d,  $J = 8.0$  Hz, 1H), 4.80-4.70 (m, 2H), 4.66-4.61 (m, 1H), 3.18-3.06 (m, 2H), 1.47 (s, 9H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.7, 158.6, 149.4, 139.5, 136.4, 136.0, 134.5, 133.4, 130.2, 129.5, 128.7, 128.6, 128.3, 127.1, 126.6, 125.0, 123.9, 122.1, 80.0, 66.0, 54.5, 38.4, 28.4; Anal. Calcd for  $\text{C}_{28}\text{H}_{30}\text{N}_2\text{O}_4$ : C, 73.34; H, 6.59; N, 6.11%; Found: C, 73.52; H, 6.56; N, 6.03%.



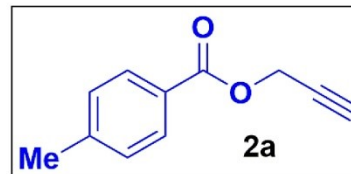
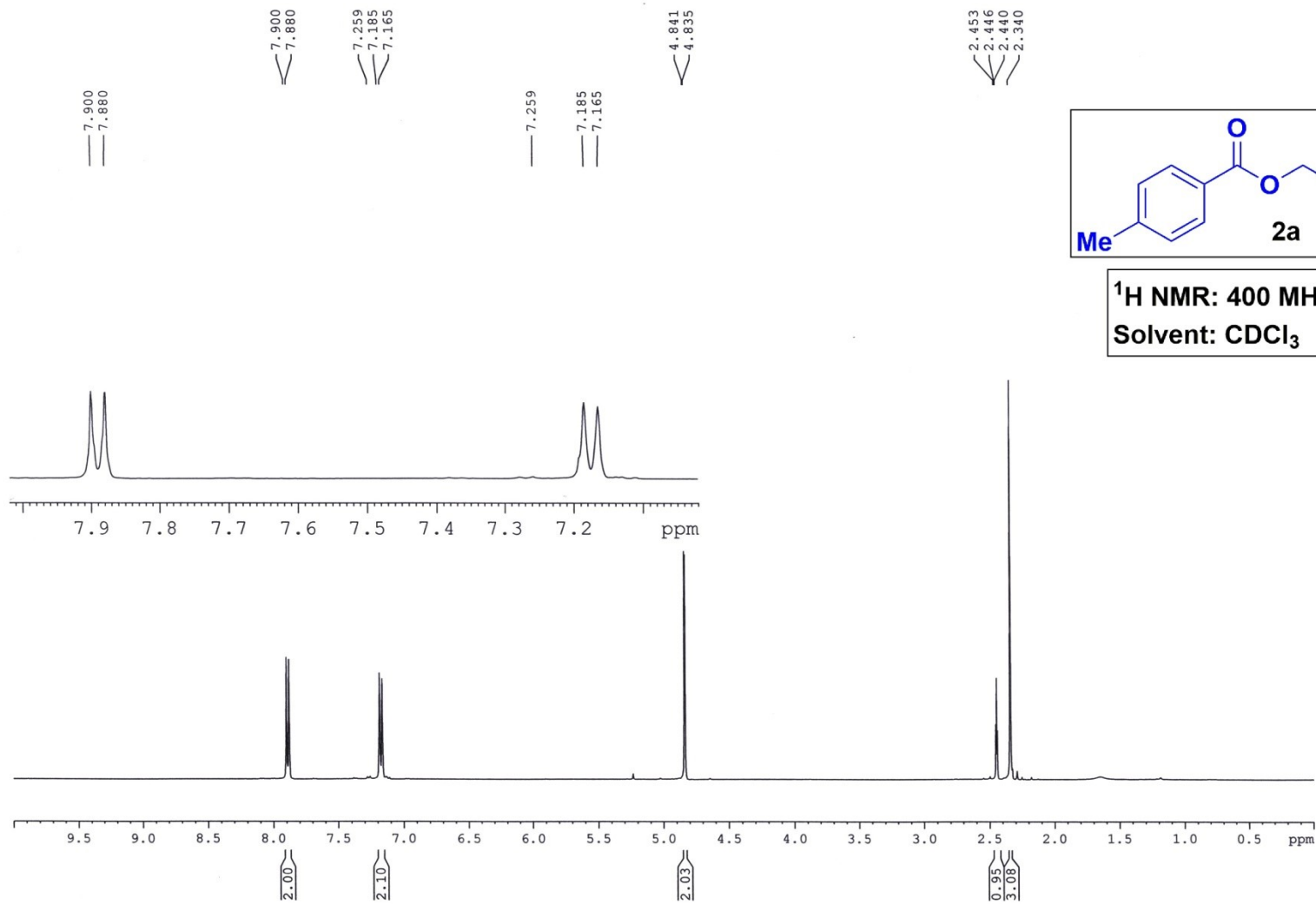
**(E)-3-(2-(1H-pyrazol-1-yl)phenyl)allyl (tert-butoxycarbonyl)-L-phenylalaninate (3ol):** White solid (88%, 98.4 mg);  $R_f = 0.50$  (PE/ EA = 80 : 20); M.P. 61-62 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.62 (s, 1H), 7.52-7.48 (m, 2H), 7.31-7.26 (m, 3H), 7.15-7.07 (m, 3H), 7.01 (d,  $J = 6.8$  Hz, 2H), 6.40 (d,  $J = 16.0$  Hz, 1H), 6.34 (t,  $J = 2.0$  Hz, 1H), 6.08-6.01 (m, 1H), 4.92 (d,  $J = 8.0$  Hz, 1H), 4.62-4.53 (m, 2H), 4.50-4.45 (m, 1H), 3.02-2.89 (m, 2H), 1.30 (s, 9H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.6, 155.1, 140.8, 138.7, 135.9, 131.7, 131.4, 129.6, 129.4, 128.8, 128.5, 128.4, 127.0, 126.9, 126.3, 125.3, 106.7, 79.9, 65.6, 54.5, 38.3, 28.3; Anal. Calcd for  $\text{C}_{26}\text{H}_{29}\text{N}_3\text{O}_4$ : C, 69.78; H, 6.53; N, 9.39%; Found: C, 69.57; H, 6.57; N, 9.27%.

## 5. References:

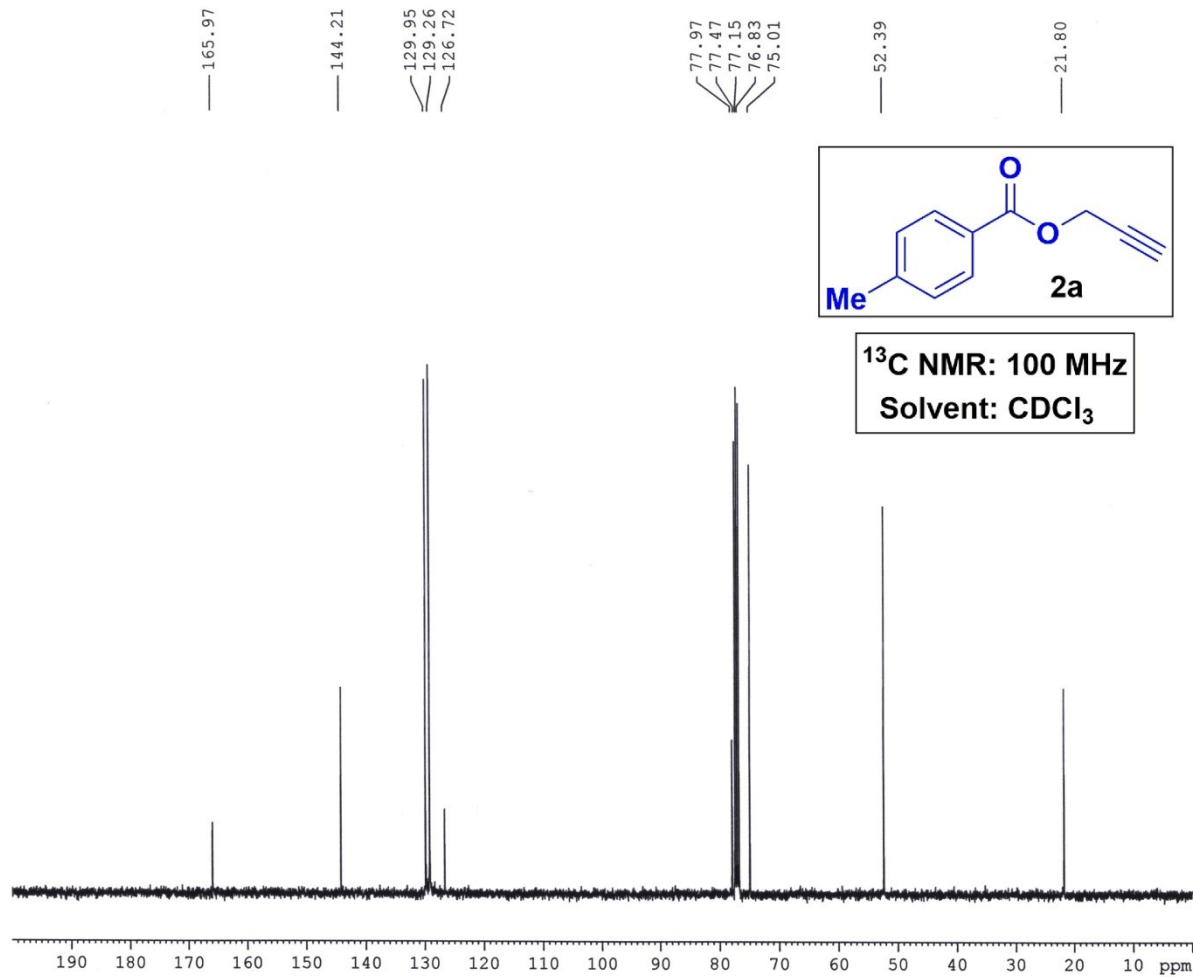
- (1) (a) M. R. Kumar, A. Park, N. Park, S. Lee, *Org. Lett.*, 2011, **13**, 3542-3545; (b) G. Bogonda, H. Y. Kim, K. Oh, *Org. Lett.*, 2018, **20**, 2711-2715. (2) P. W. Skelly, J. Sae-Jew, A. P. Kitos Vasconcelos, J. Tasnim, L. Li, J. A. Raskatov, R. Braslau, *J. Org. Chem.*, 2019, **84**, 13615-13623. (3) S. Das, A. Azim, S. K. Hota, S. P. Panda, S. Murarka, S. De Sarkar, *Chem. Commun.*, 2021, **57**, 13130-13133. (4) R. M. Borzilleri, X. Zheng, R. J. Schmidt, J. A. Johnson, S. -H. Kim, J. D. DiMarco, C. R. Fairchild, J. Z. Gougoutas, F. Y. F. Lee, B. H. Long, G. D. Vite, *J. Am. Chem. Soc.*, 2000, **122**, 8890-8897. (5) A. Maji, S. Guin, S. Feng, A. Dahiya, V. K. Singh, P. Liu, D. Maiti, *Angew. Chem. Int. Ed.*, 2017, **56**, 14903-14907.

## **6. NMR spectra for the synthesized products**





**<sup>1</sup>H NMR: 400 MHz**  
**Solvent: CDCl<sub>3</sub>**



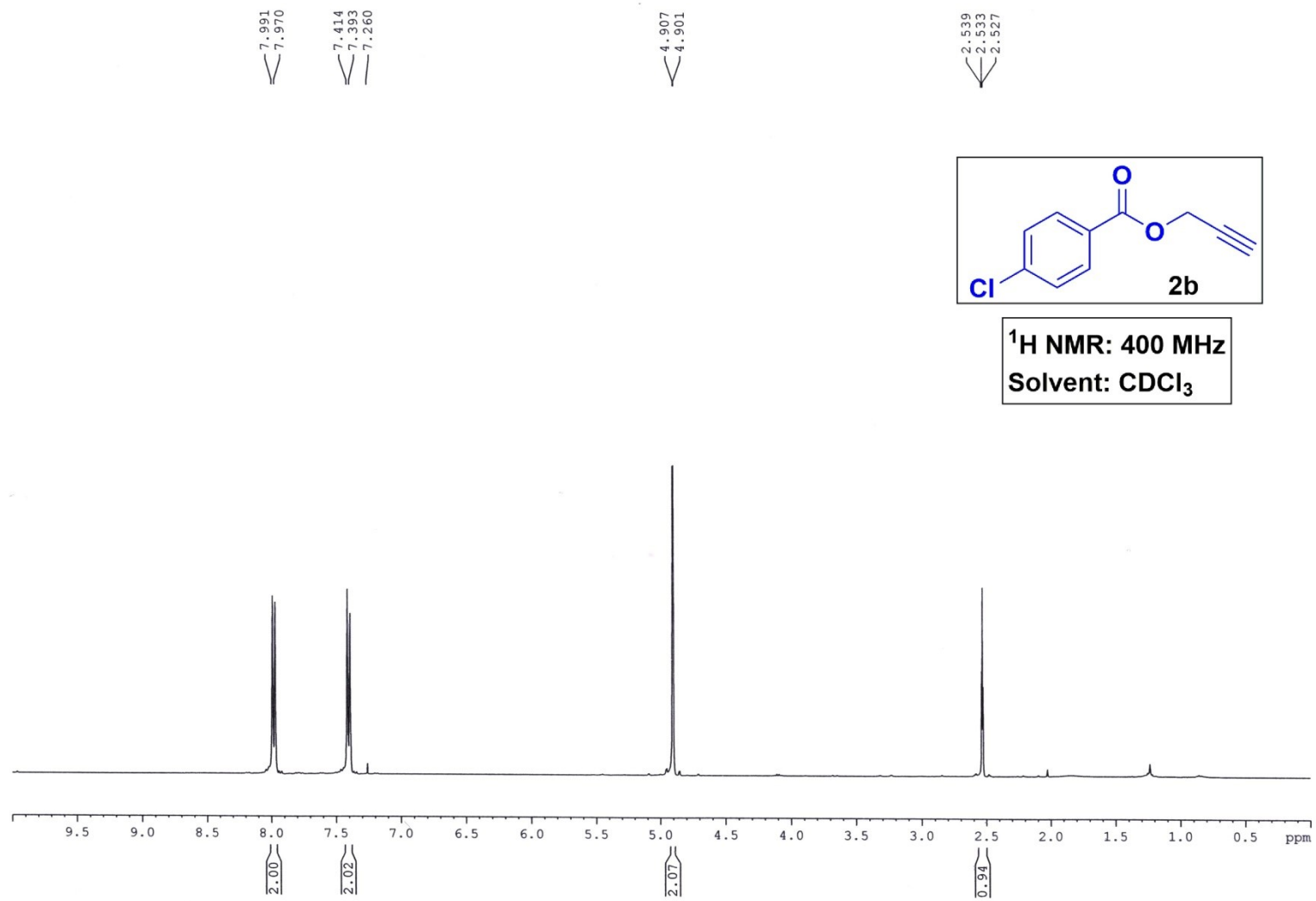
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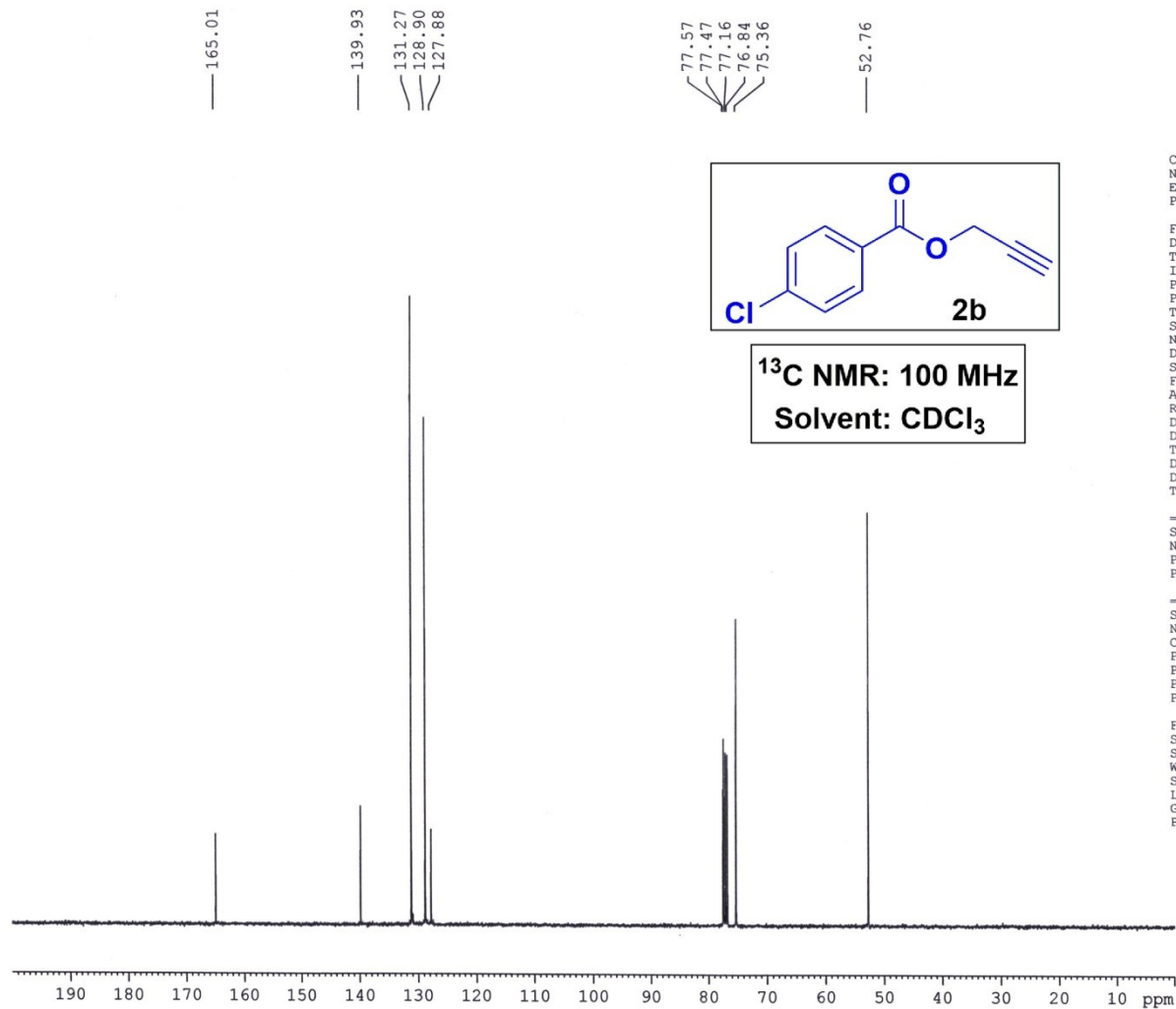
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 SOLVENT CDCl3  
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 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 77.59  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.6 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

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 NUC1 13C  
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 PLW1 54.0000000 W

----- CHANNEL f2 -----  
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 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
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 PC 1.40





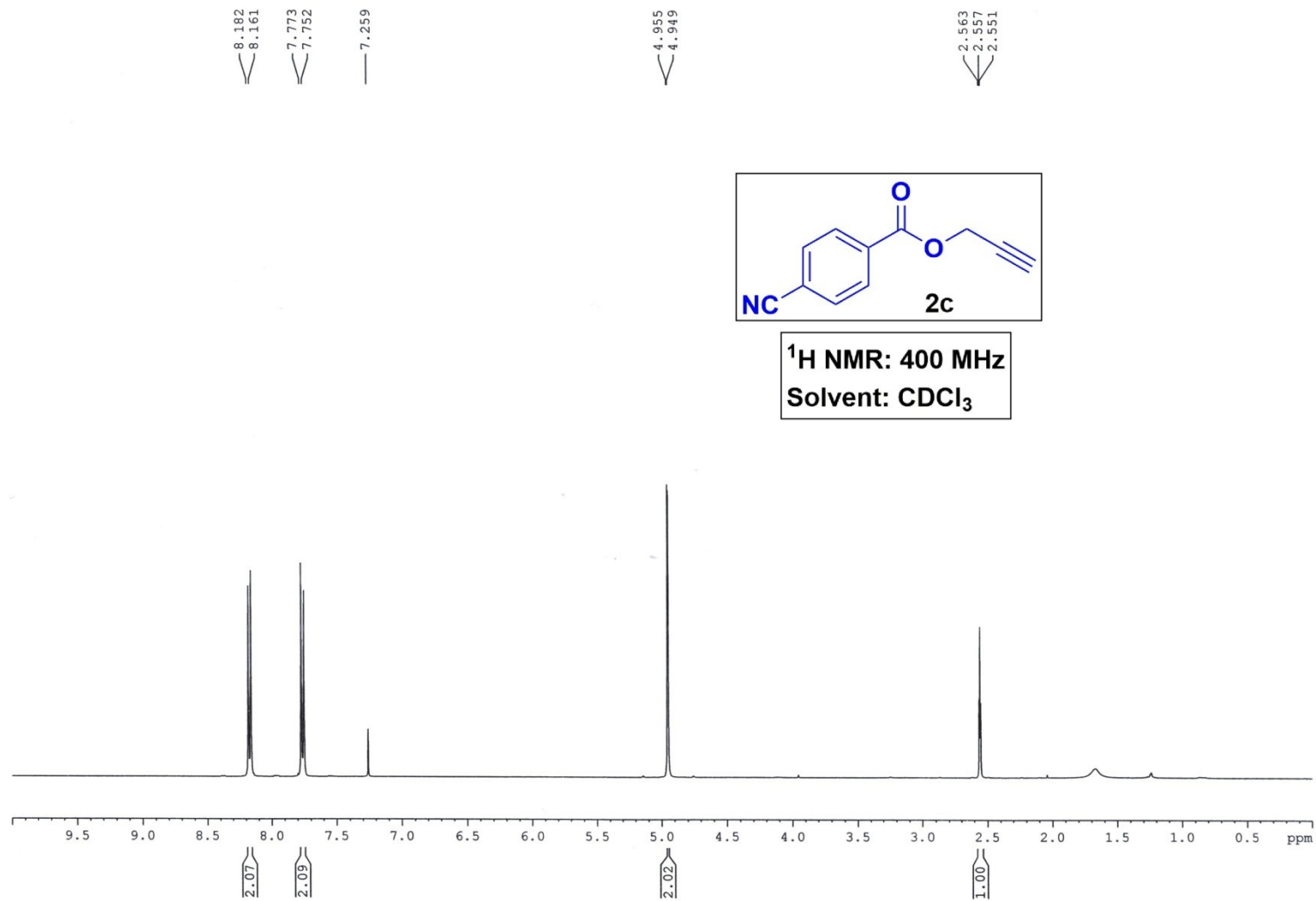
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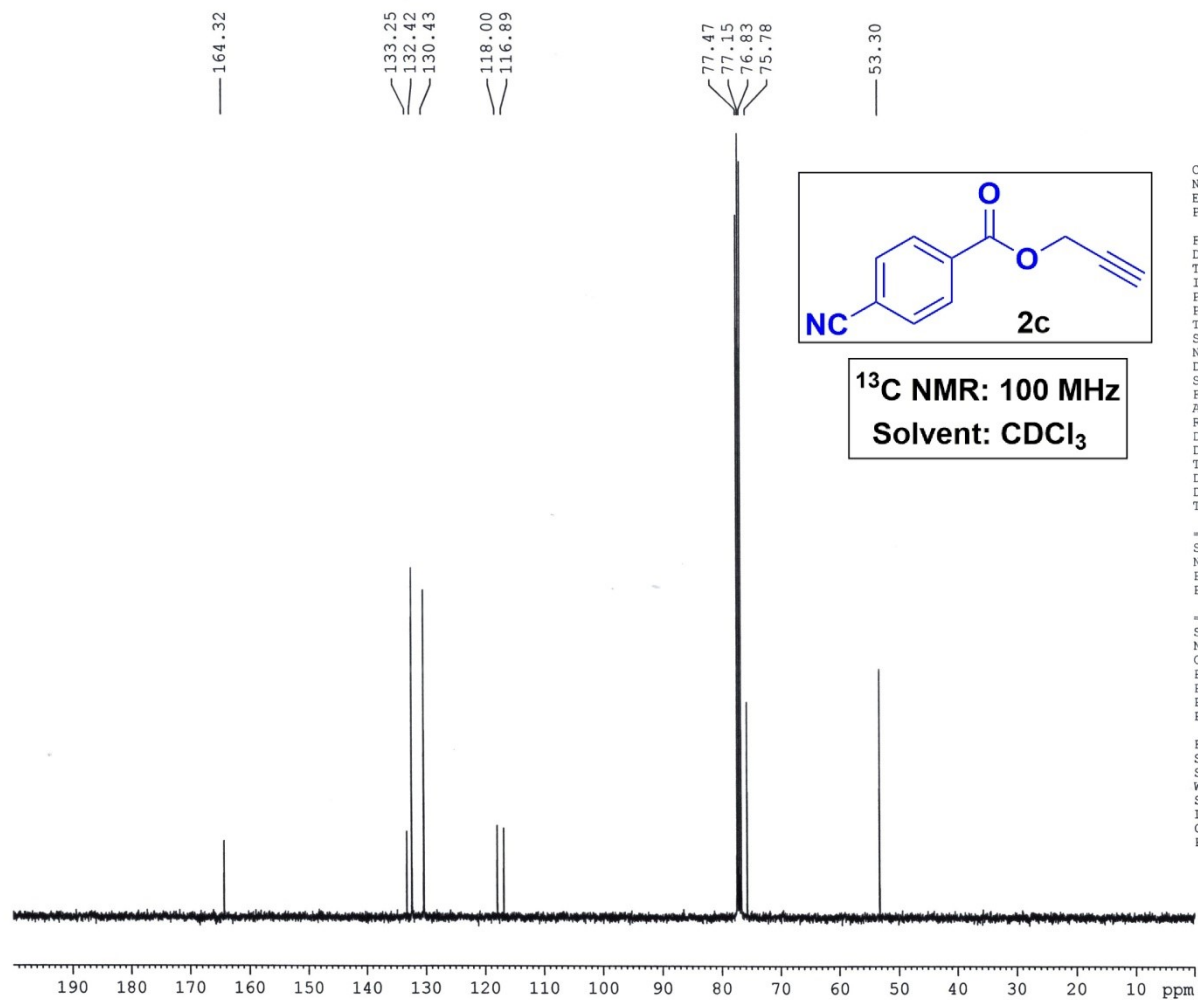
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 SOLVENT CDCl3  
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 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 62.69  
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 DE 6.50 usec  
 TE 294.3 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
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 PLW1 54.0000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

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 WDW EM  
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 LB 1.00 Hz  
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 PC 1.40





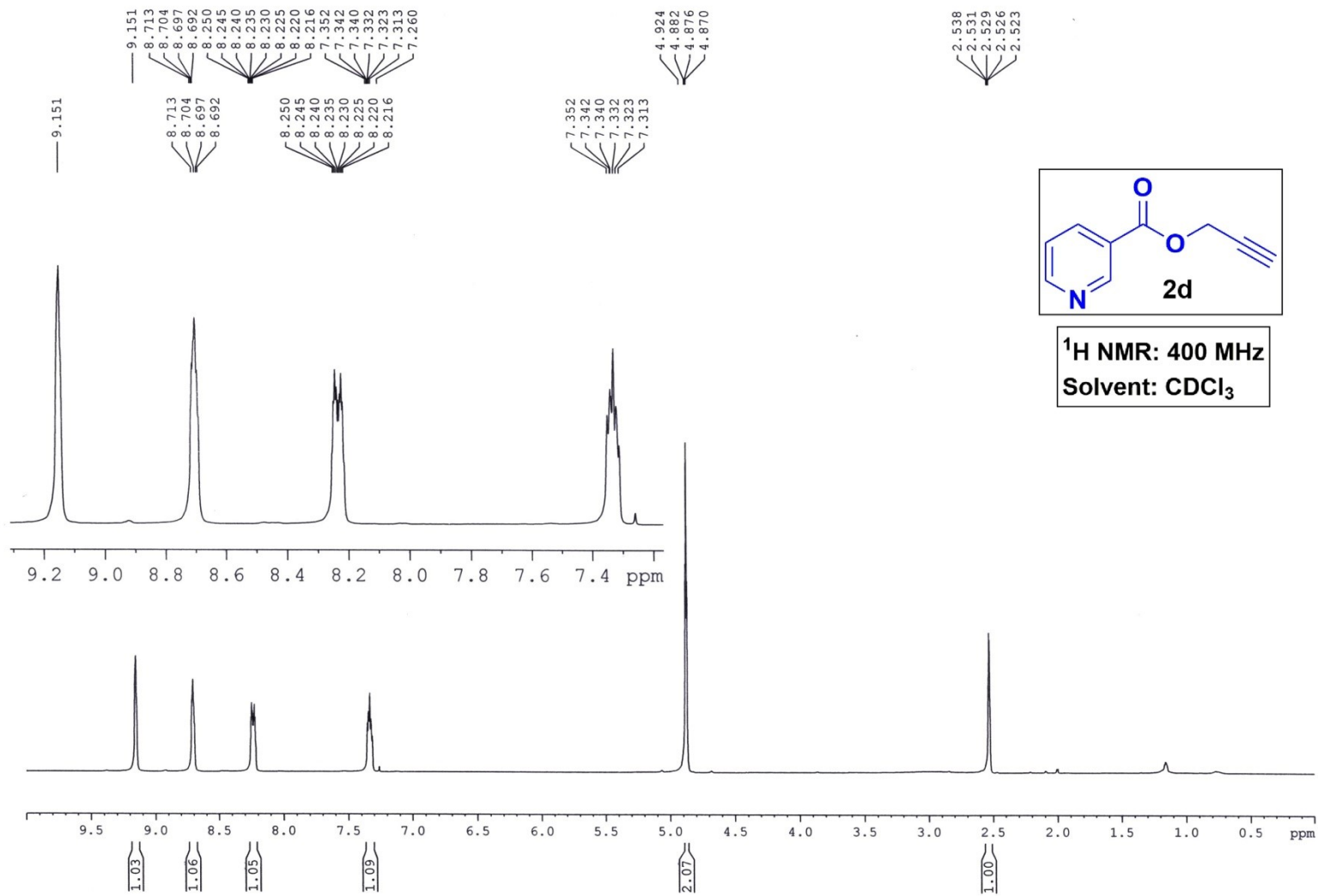
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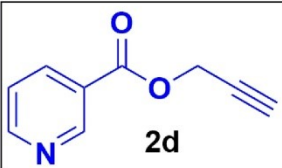
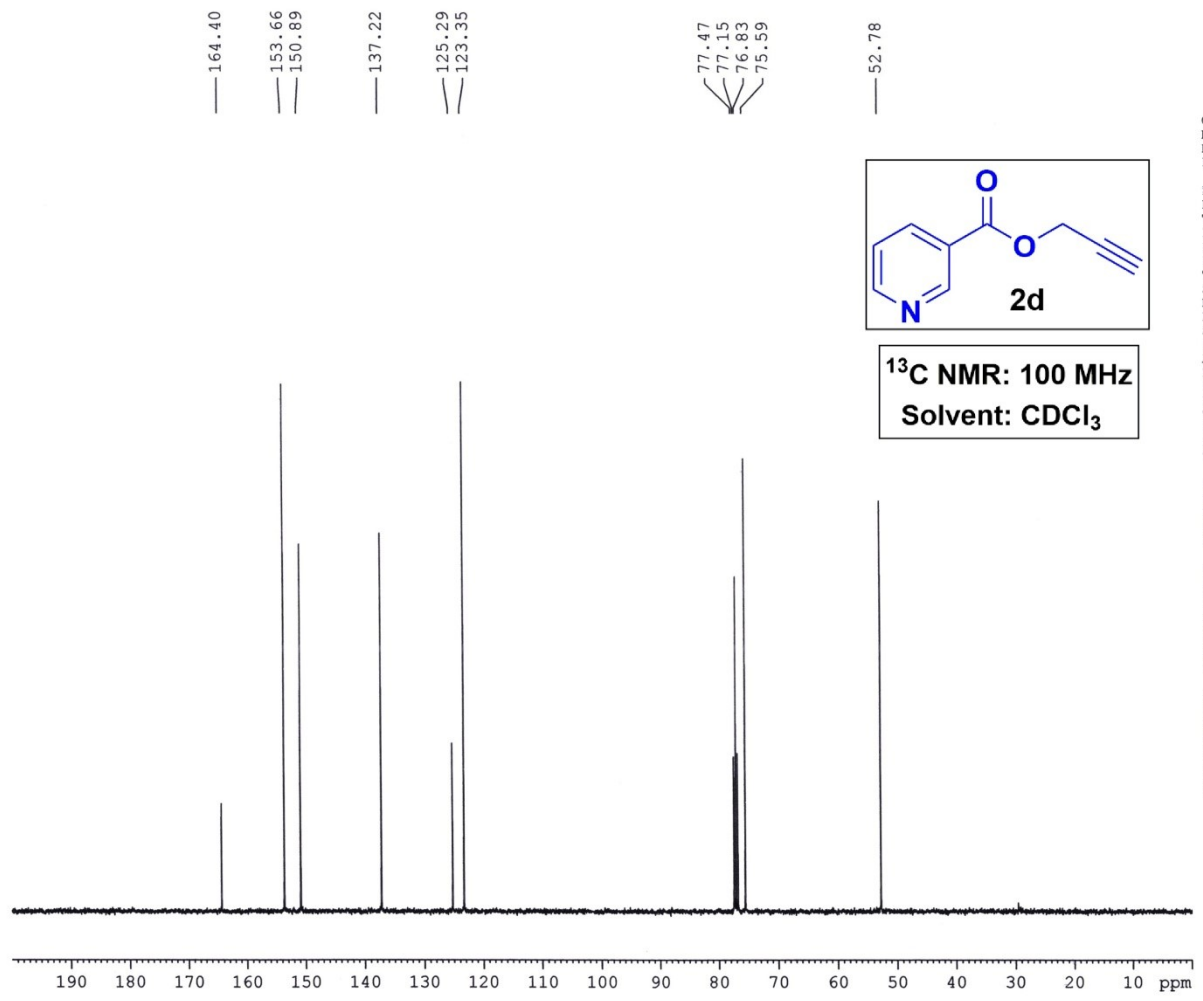
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 NS 480  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
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 DE 6.50 usec  
 TE 289.6 K  
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 TD0 1

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 NUC2 1H  
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 PLW13 0.16212000 W

F2 - Processing parameters  
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 WDW EM  
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 GB 0  
 PC 1.40





**<sup>13</sup>C NMR: 100 MHz**  
**Solvent: CDCl<sub>3</sub>**

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EXPNO     486
PROCNO    1

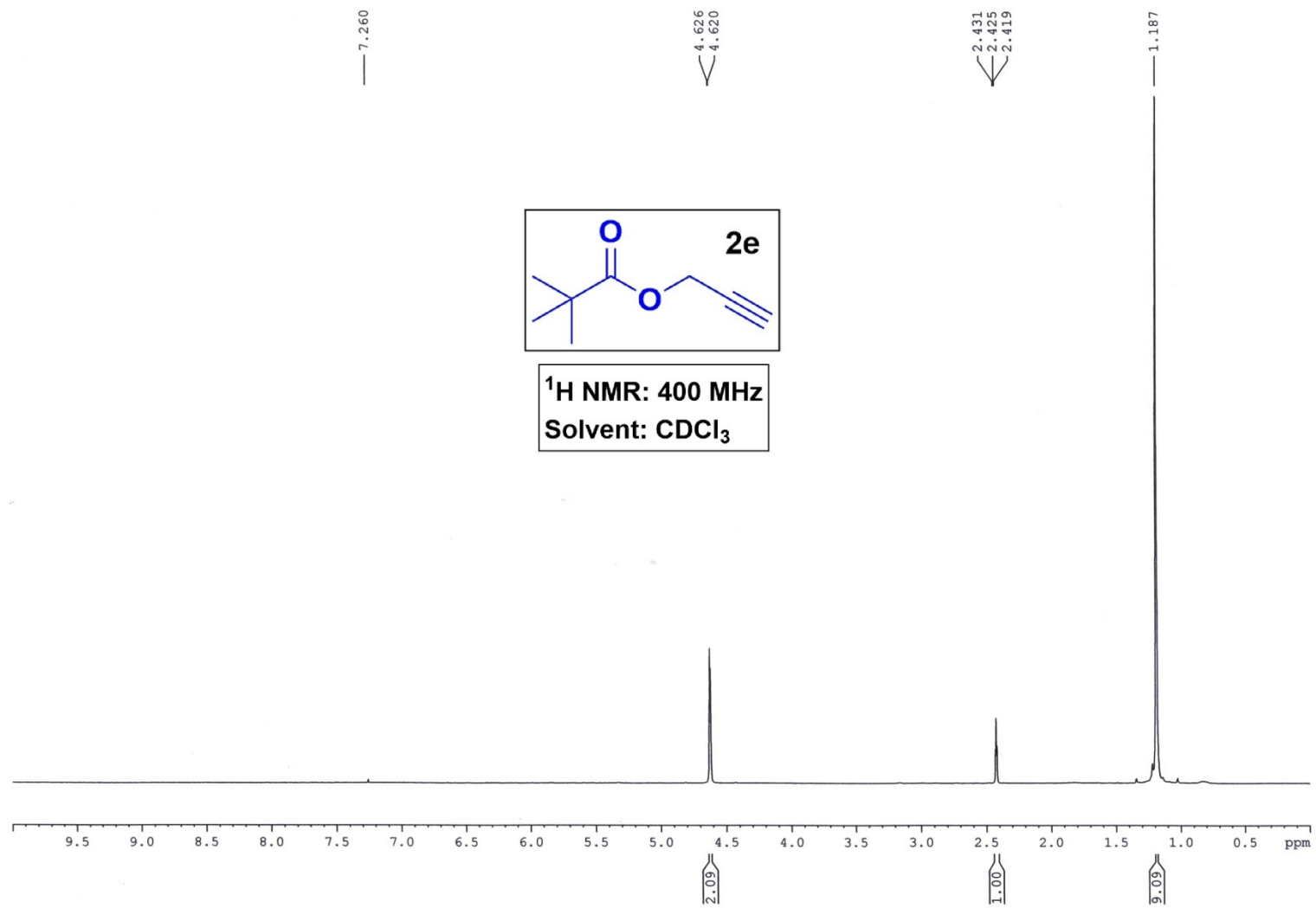
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DS         2
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FIDRES    0.733596 Hz
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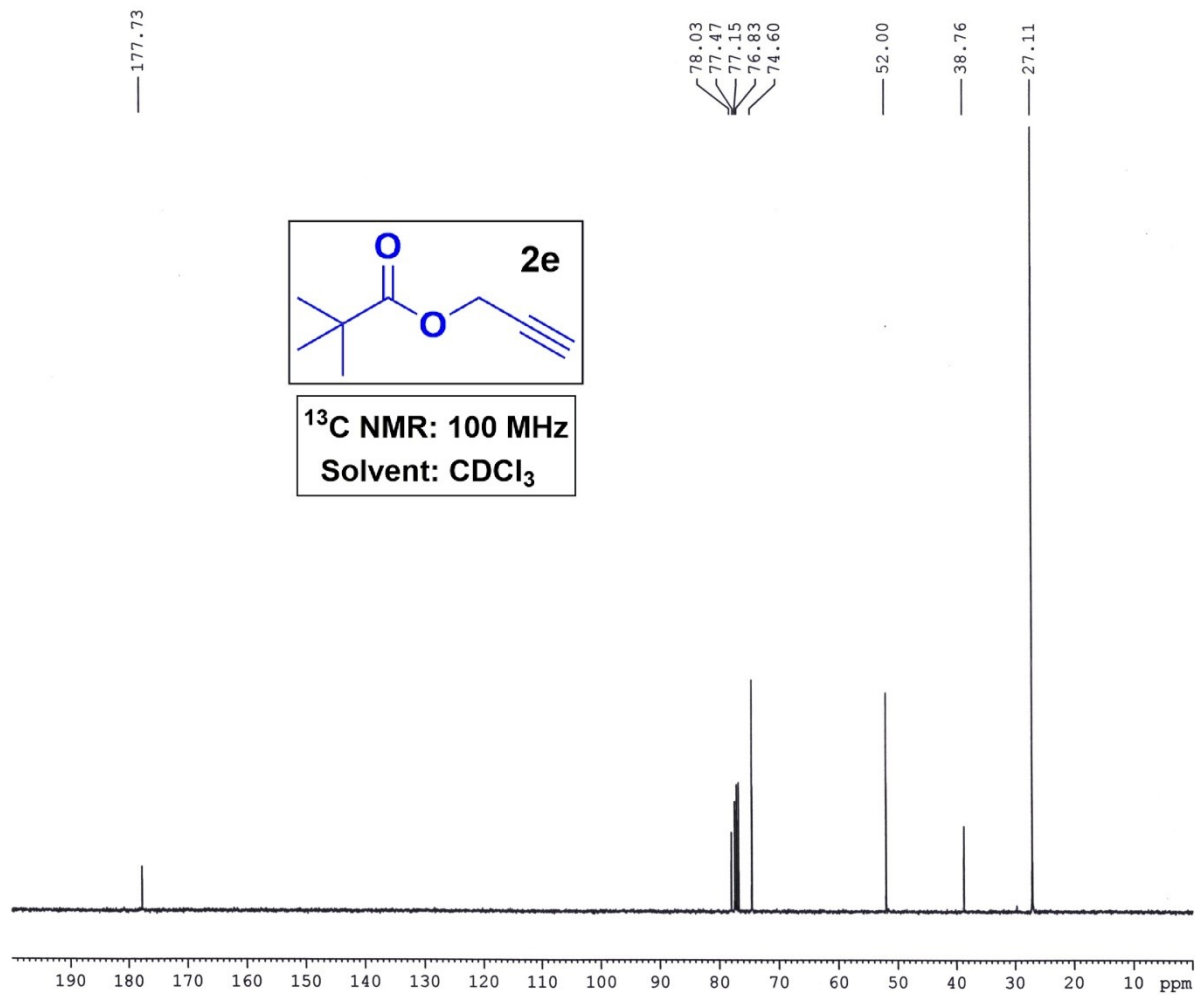
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NUC2       1H
CPDPRG[2] waltz16
PCPD2     90.00 usec
PLW2      12.00000000 W
PLW12     0.32231000 W
PLW13     0.16212000 W

F2 - Processing parameters
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LB         1.00 Hz
GB         0
PC         1.40
  
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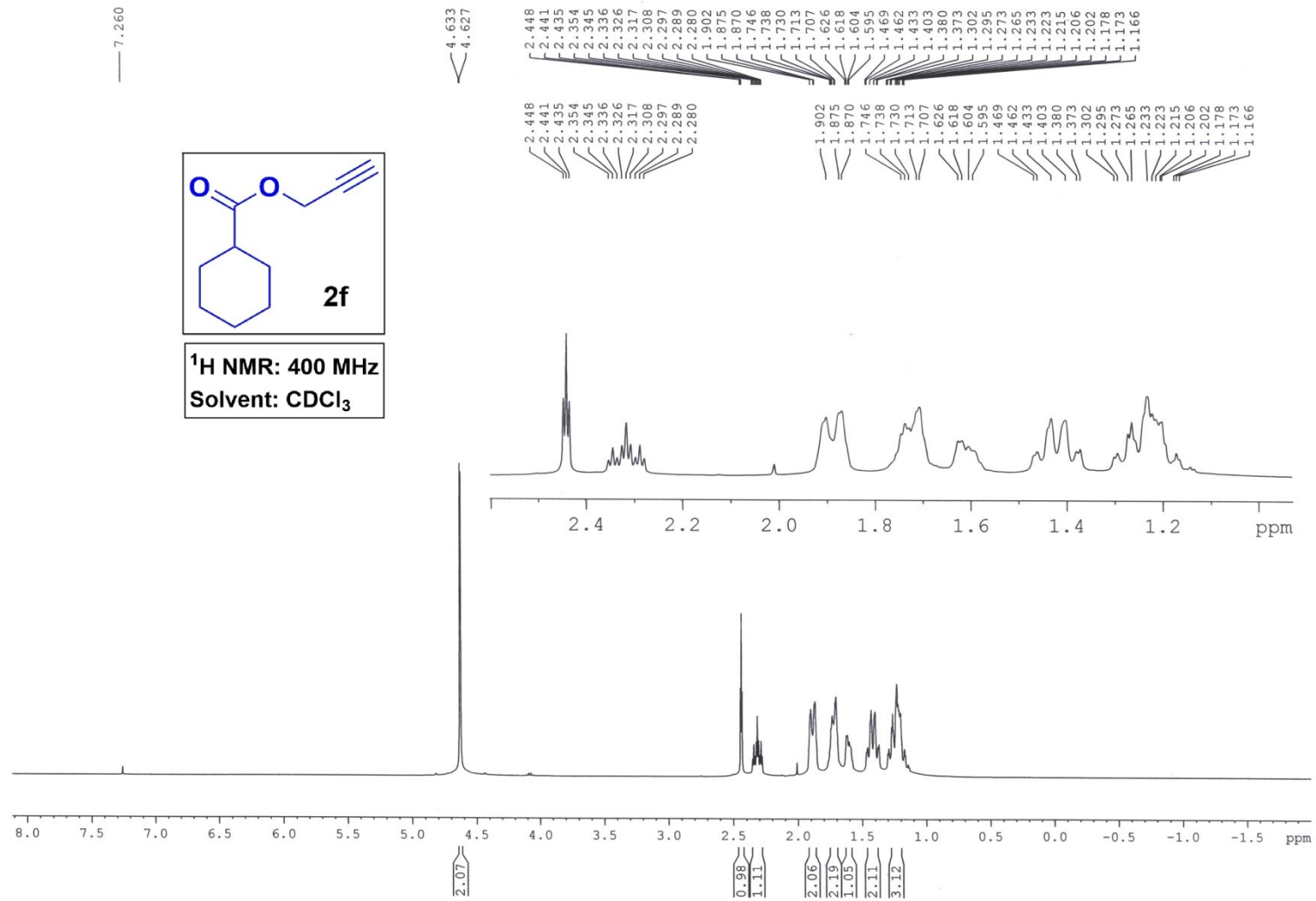
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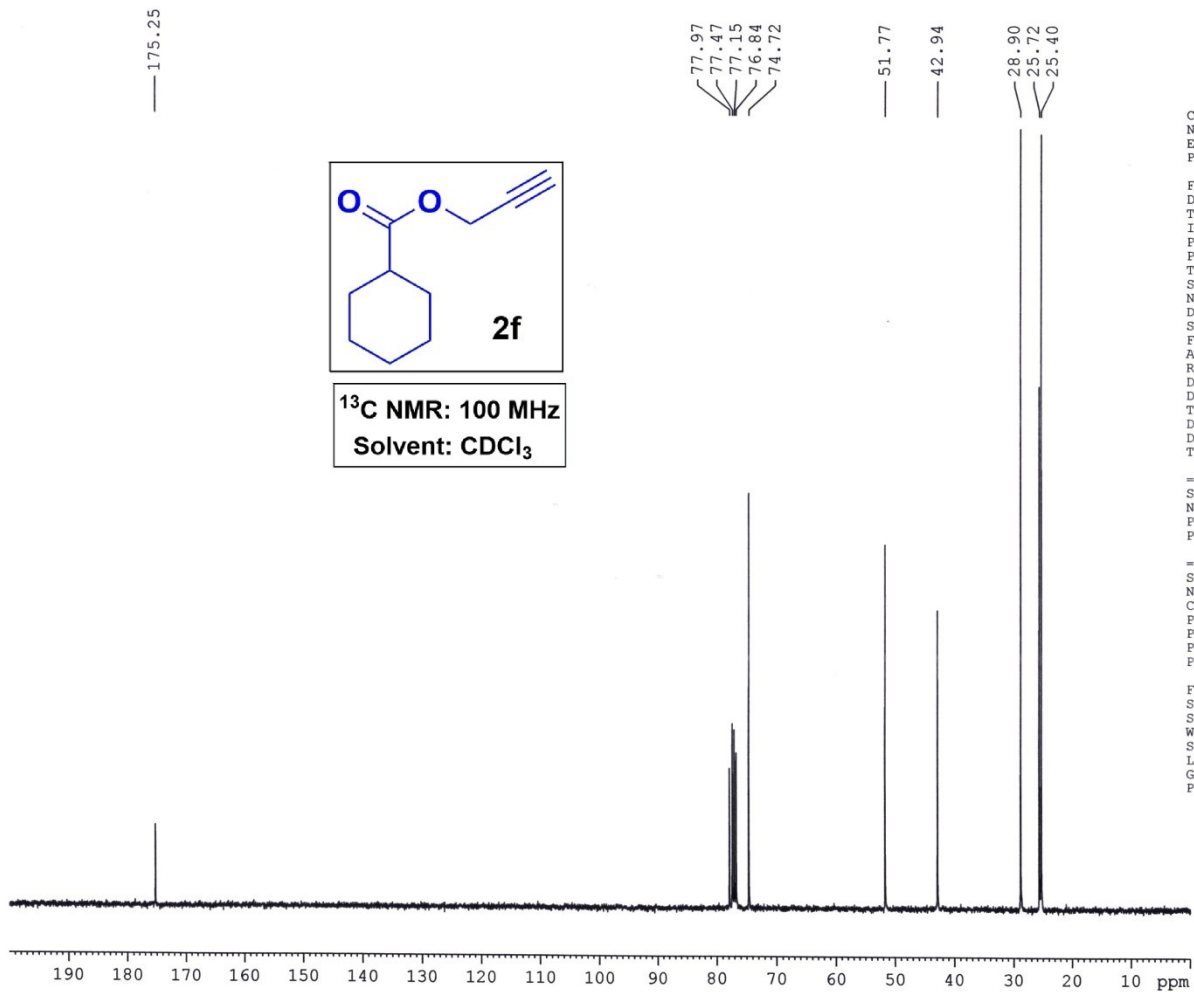
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 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 23.55  
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 DE 6.50 usec  
 TE 297.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

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 P1 8.90 usec  
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----- CHANNEL f2 -----  
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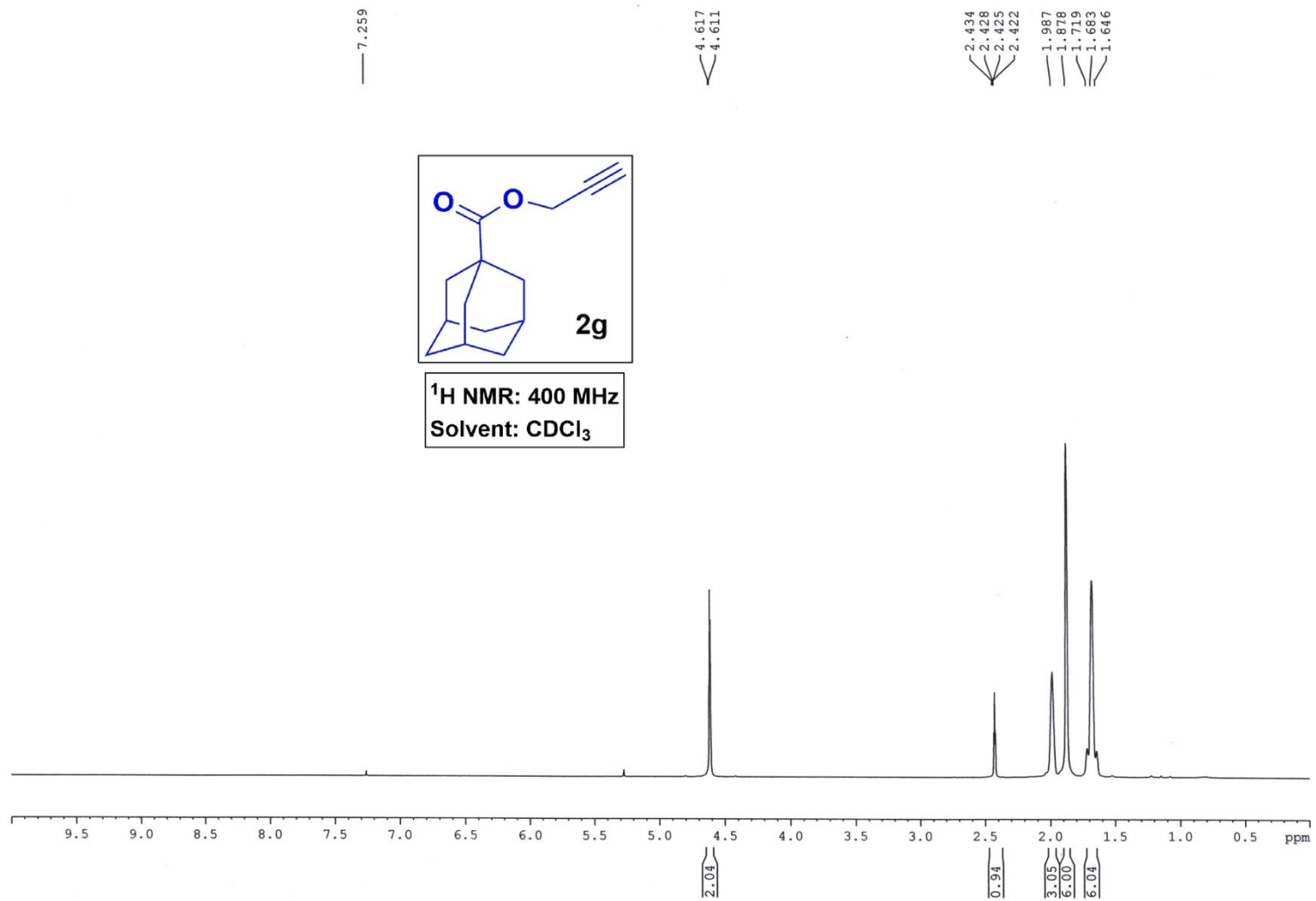
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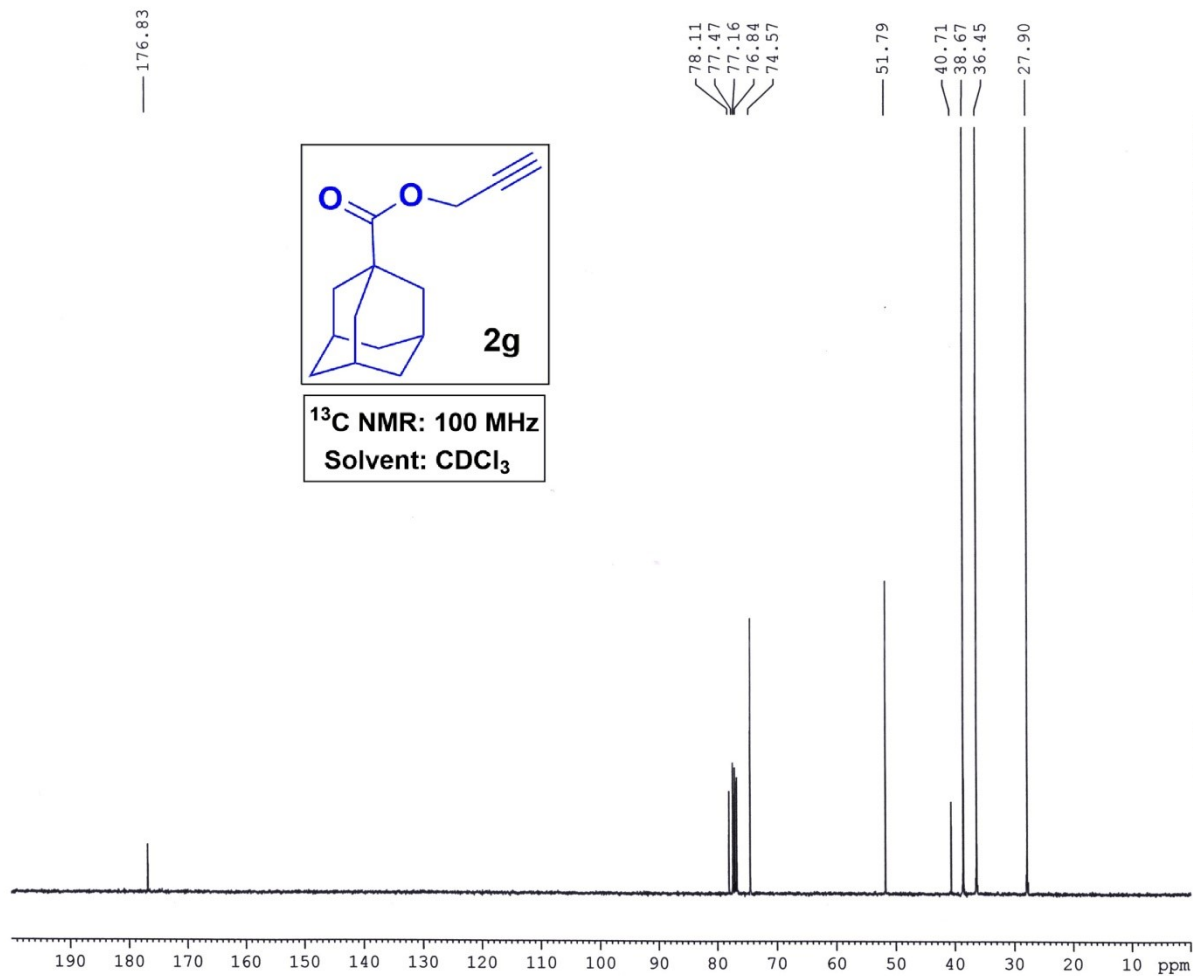
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 DE 6.50 usec  
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===== CHANNEL f2 =====  
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 FC 1.40





Current Data Parameters  
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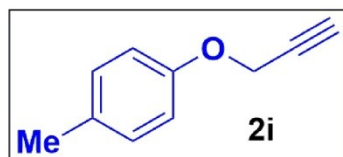
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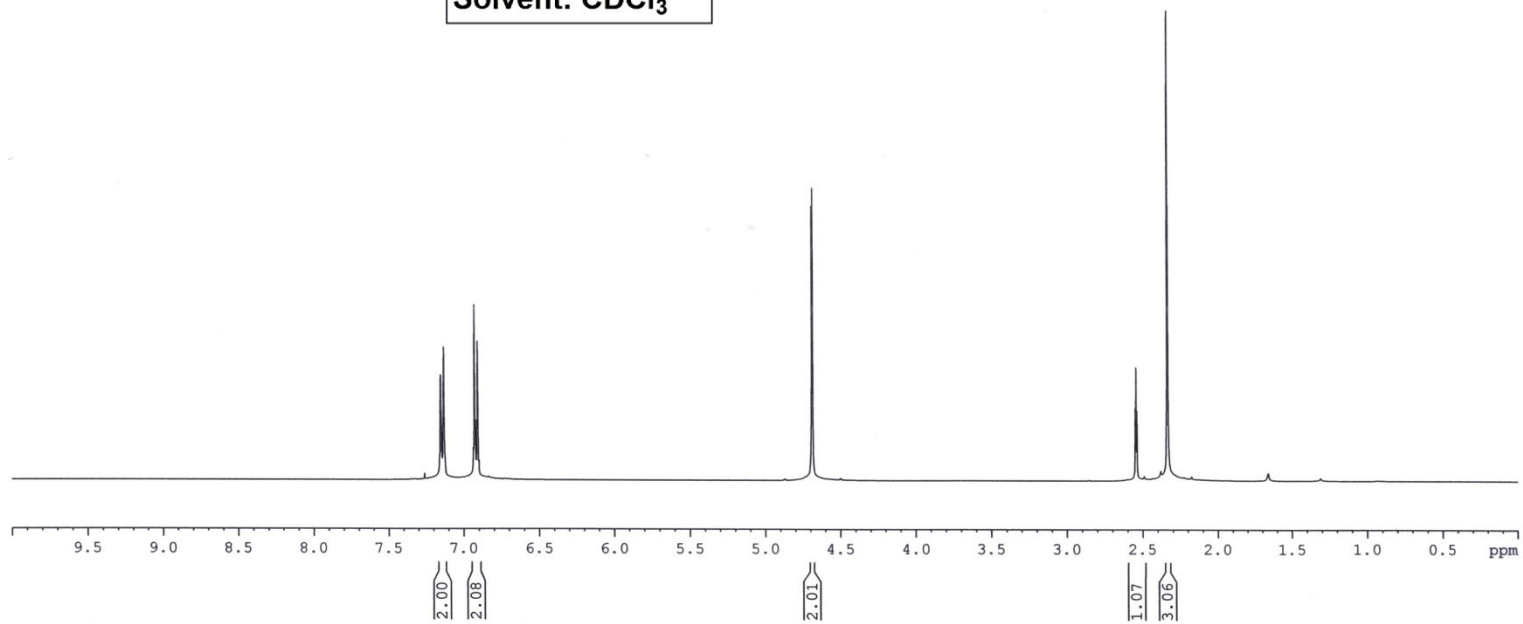
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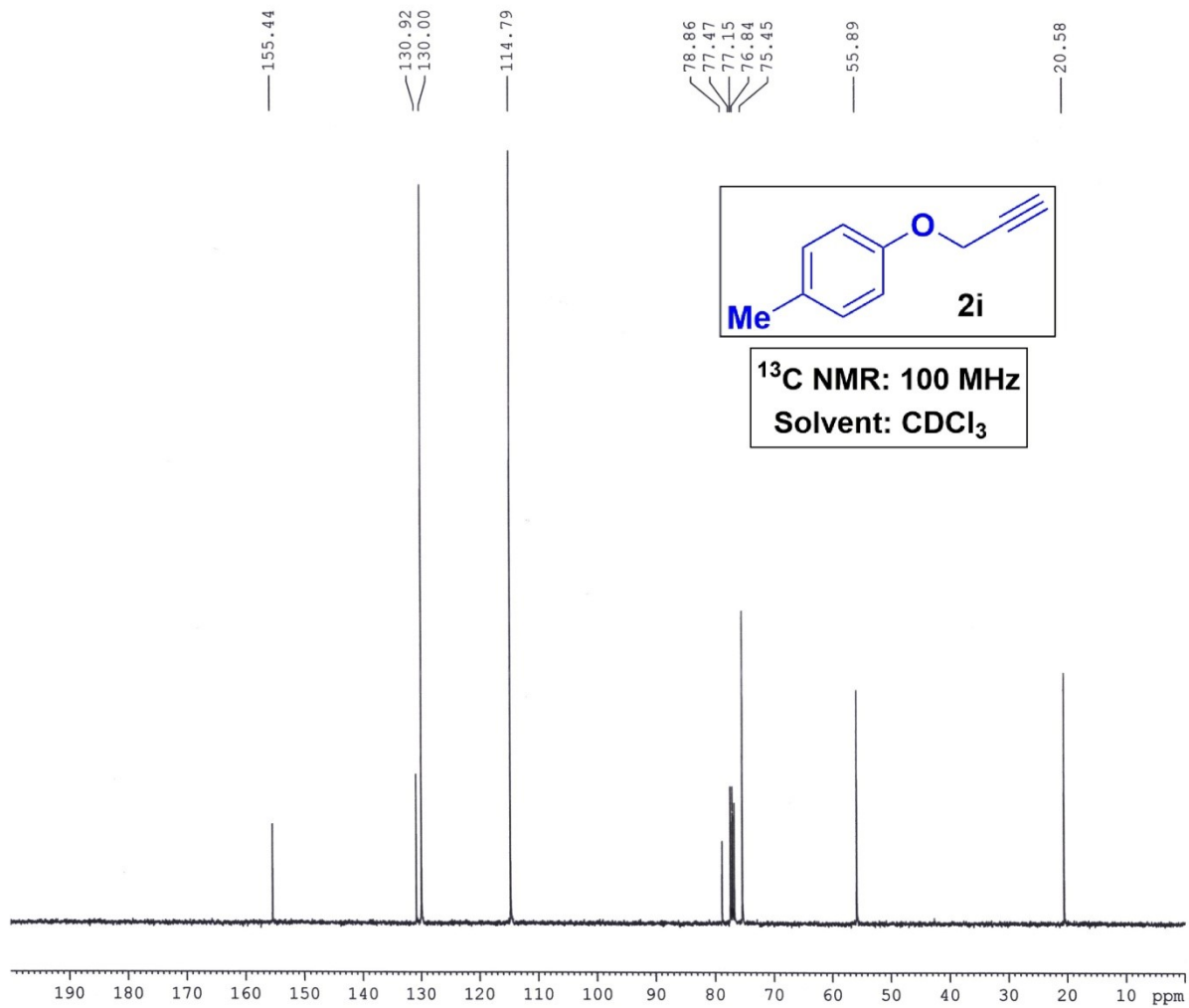
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<sup>1</sup>H NMR: 400 MHz  
Solvent: CDCl<sub>3</sub>





Current Data Parameters  
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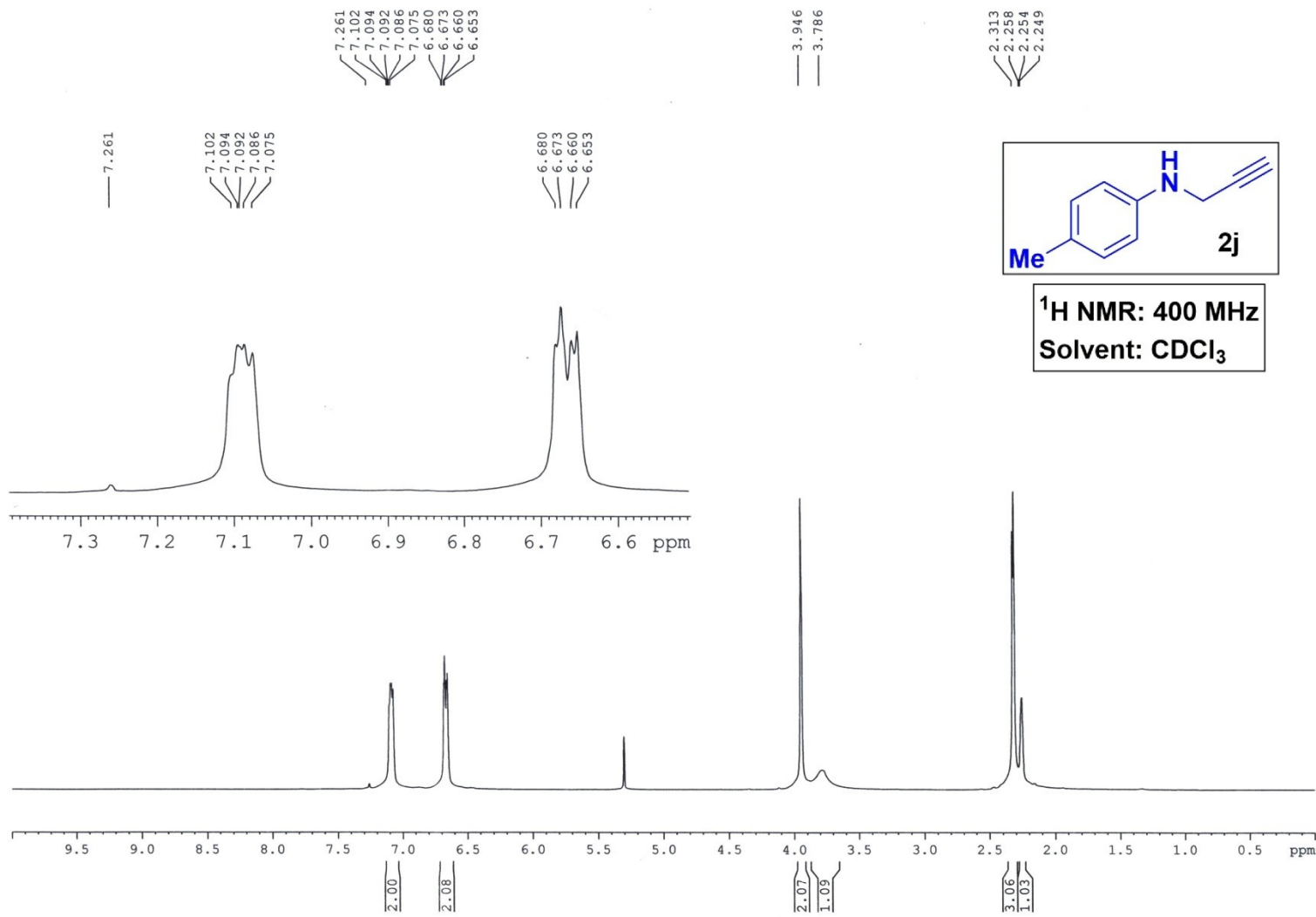
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 AQ 0.6815744 sec  
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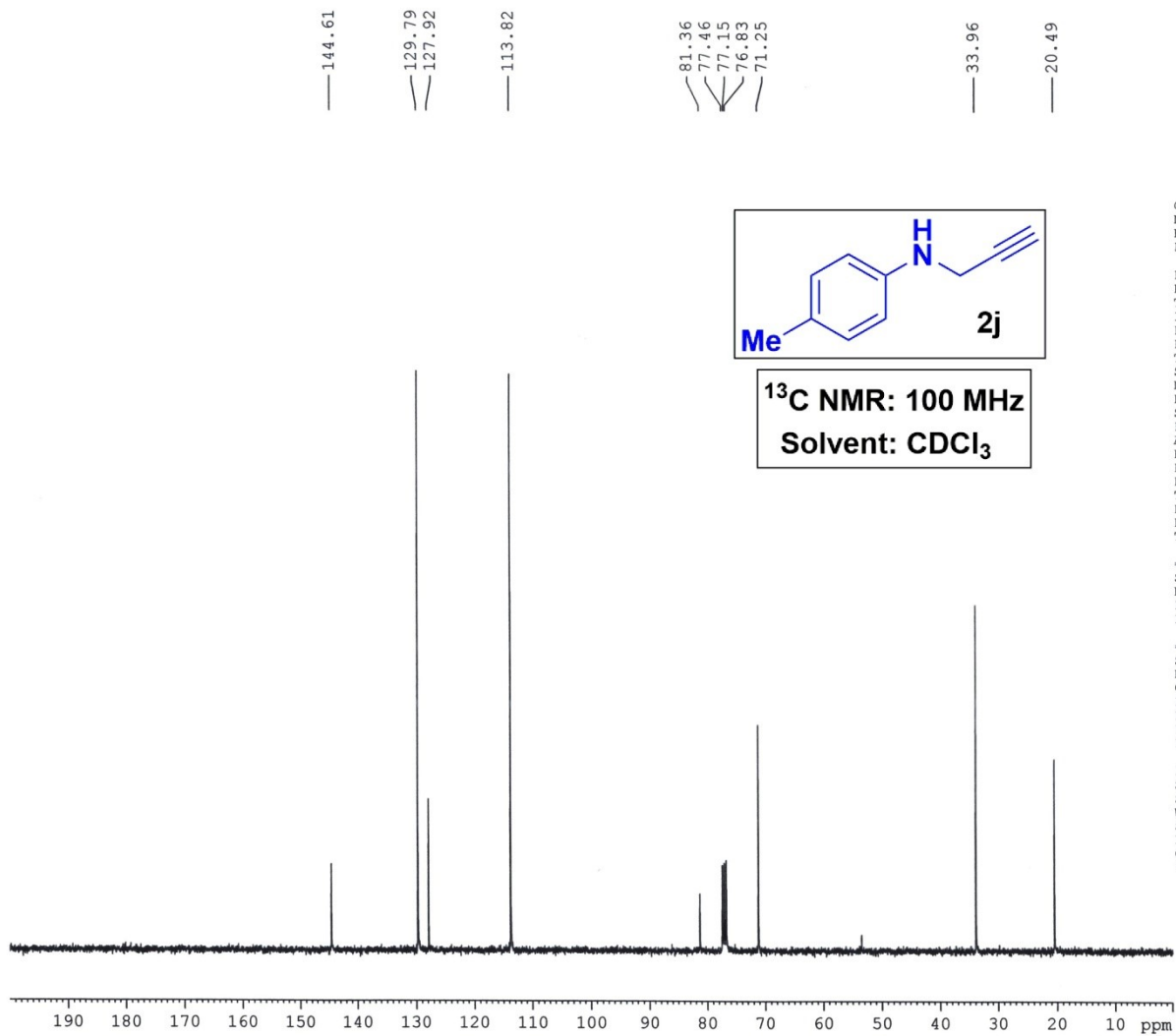
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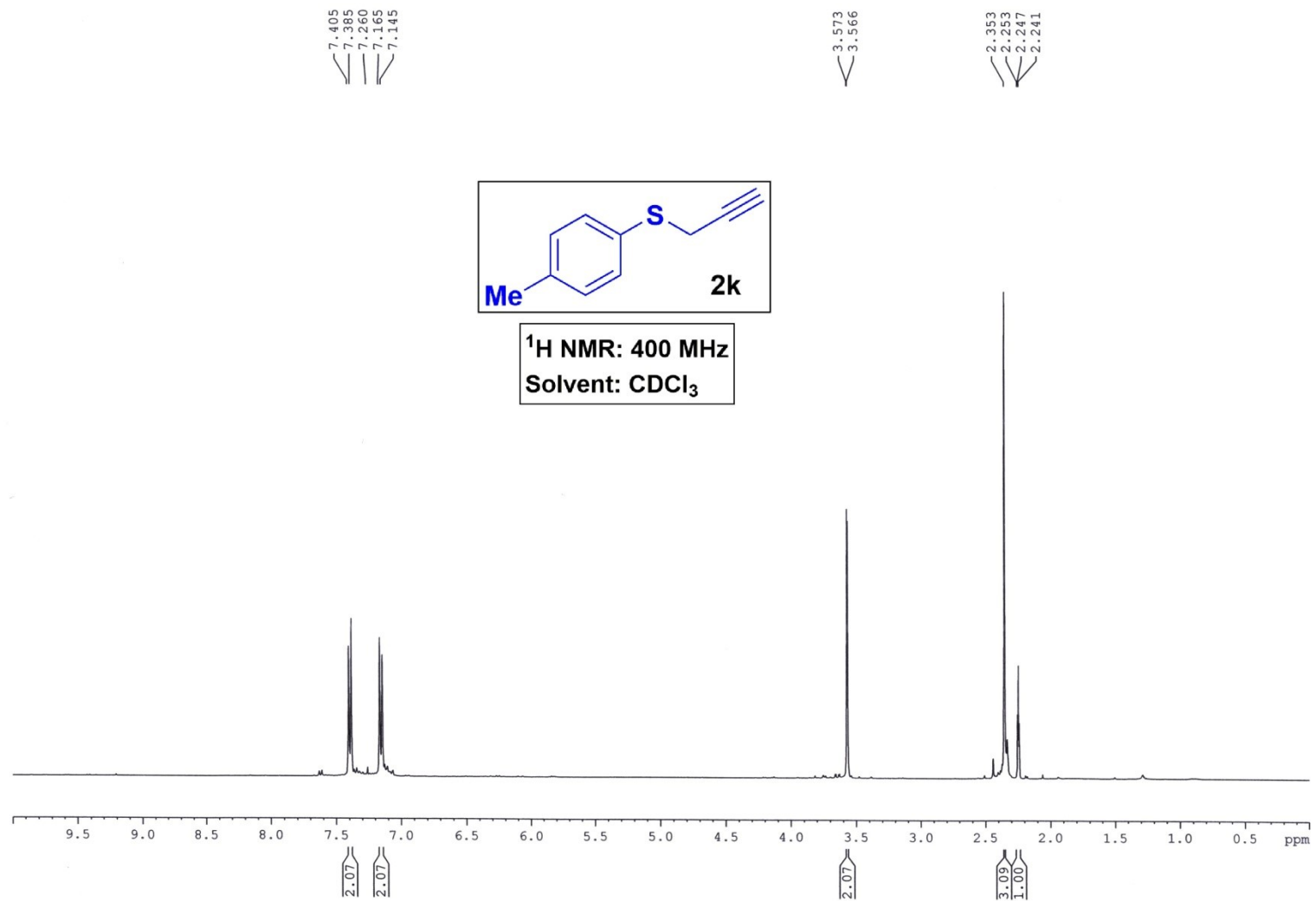
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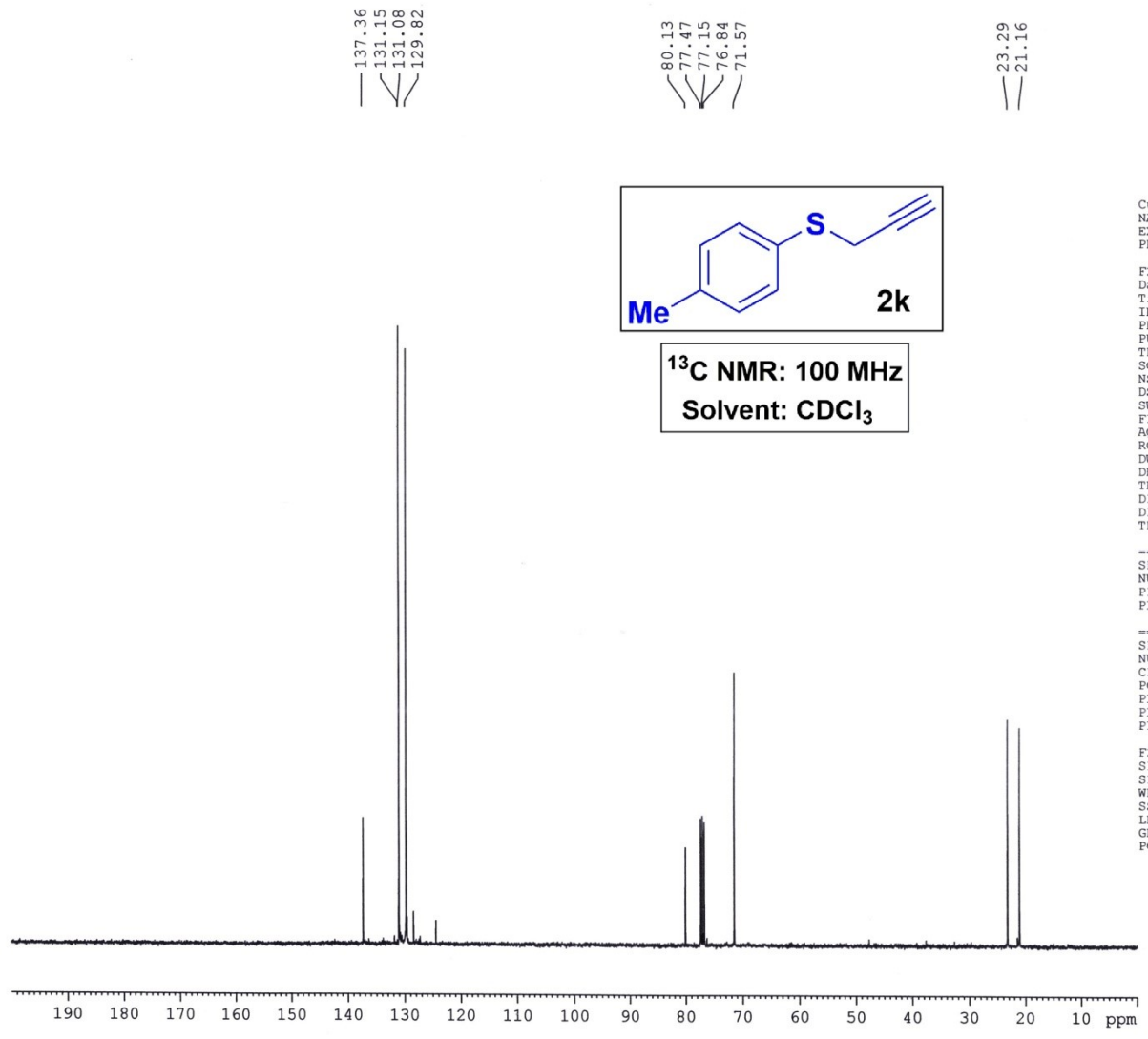
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TDO 1

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NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
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PLW12 0.32231000 W  
PLW13 0.16212000 W

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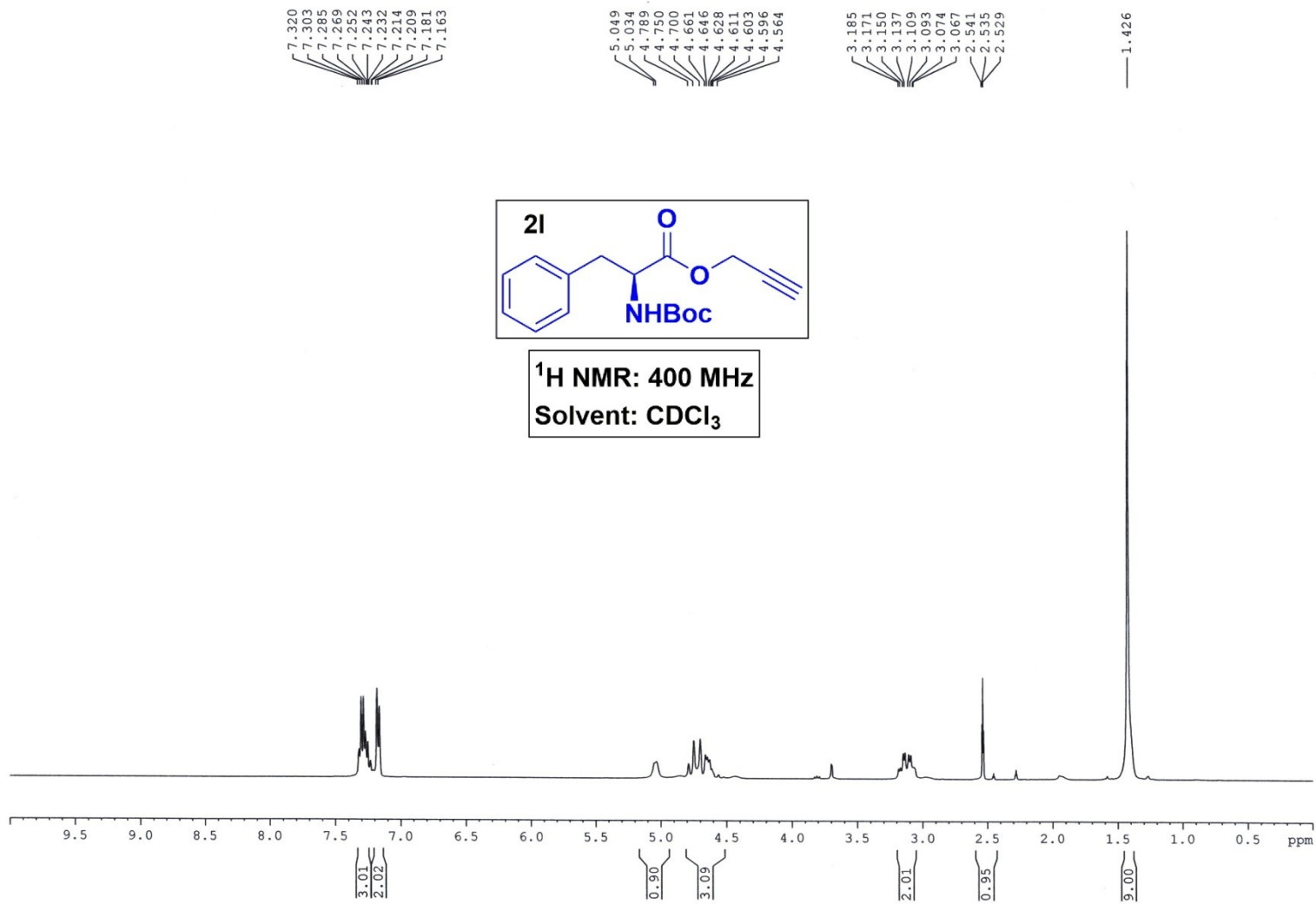
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 EXPNO 492  
 PROCNO 1

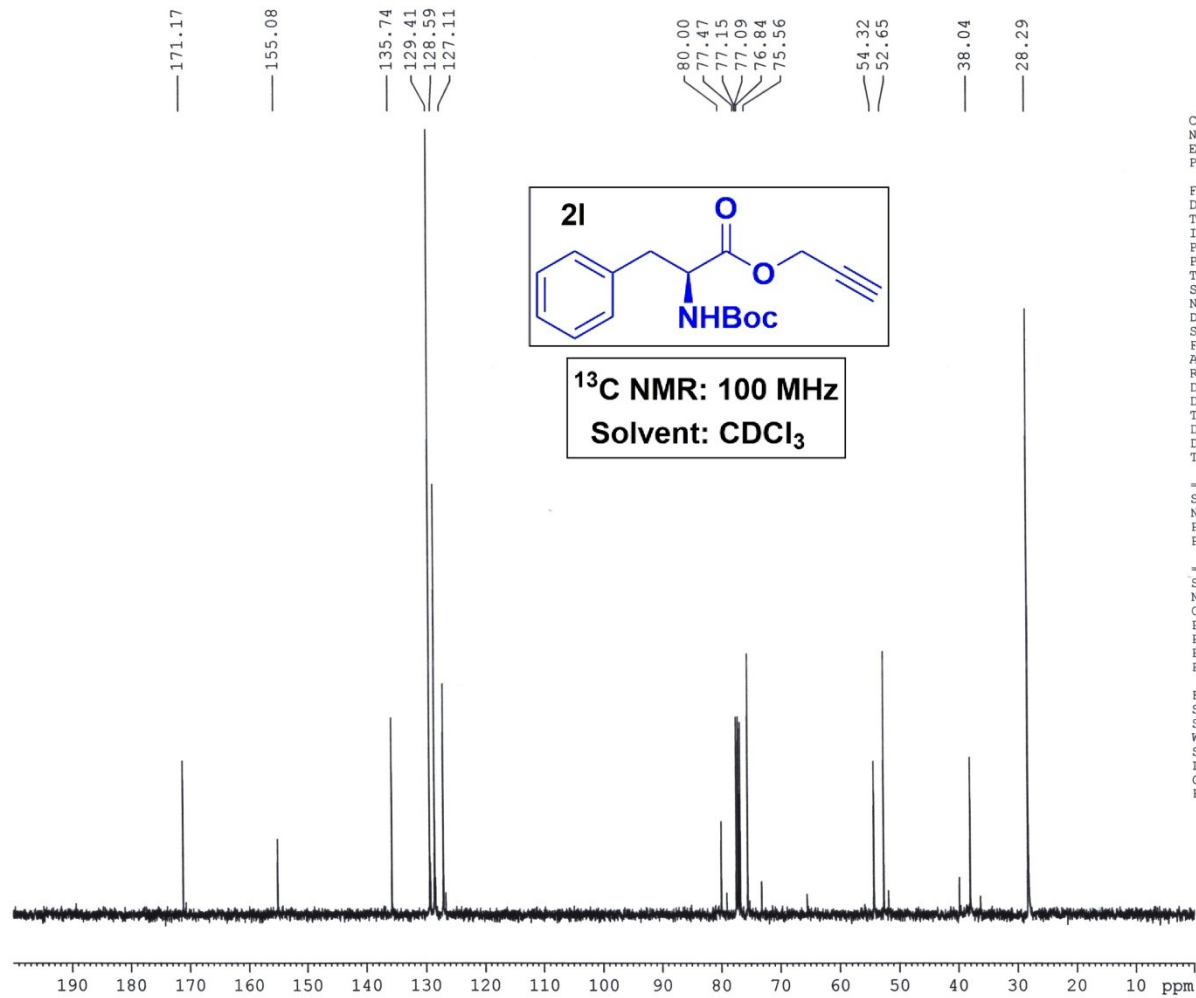
F2 - Acquisition Parameters  
 Date\_ 20211215  
 Time\_ 14.00  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 140  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 30.11  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 292.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177991 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





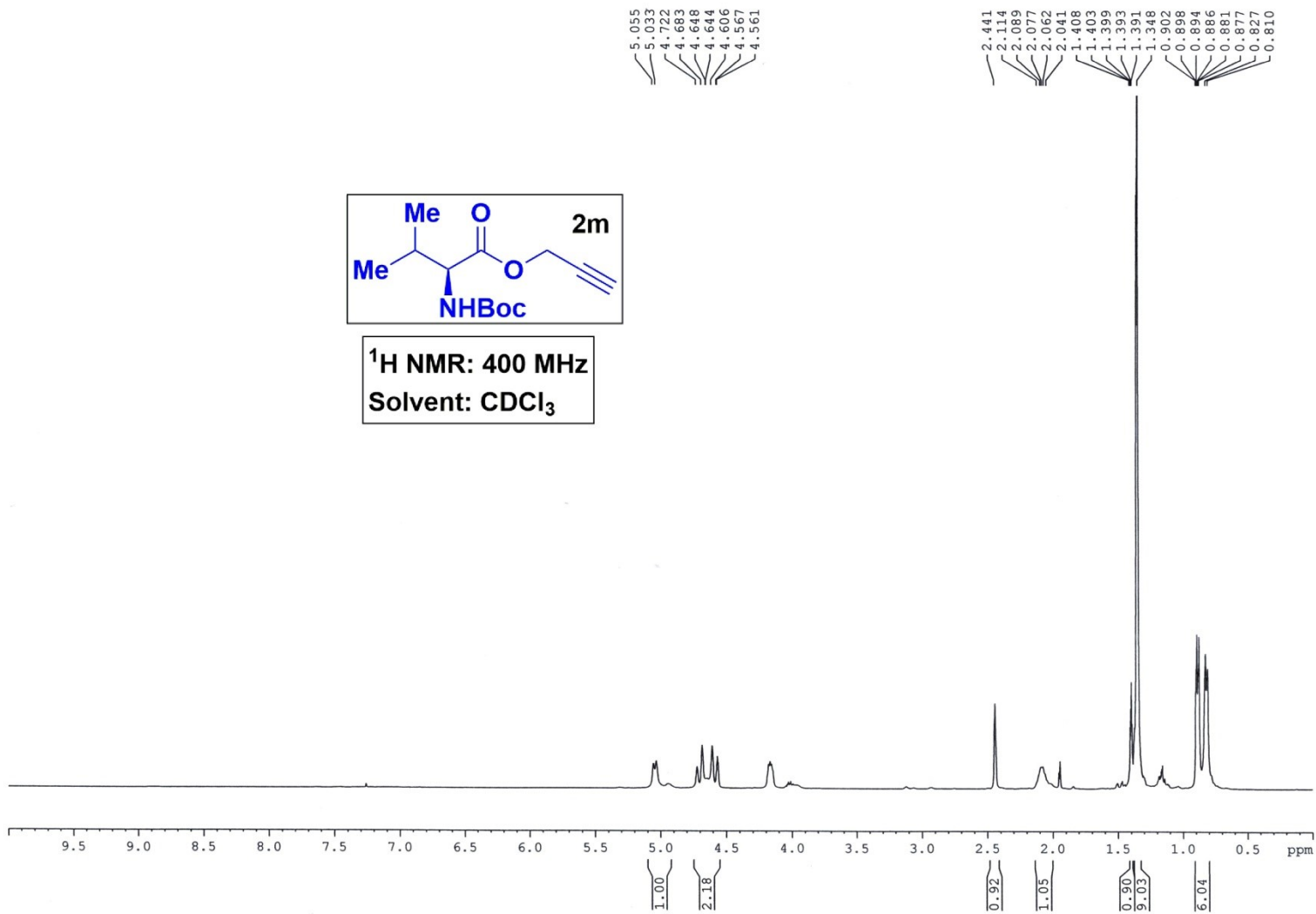
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 506  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20211226  
 Time\_ 13.28  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 50  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 20.64  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.8 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.0000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177976 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



— 171.64

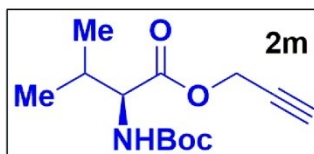
— 155.56

79.72  
77.47  
77.15  
76.83  
75.30

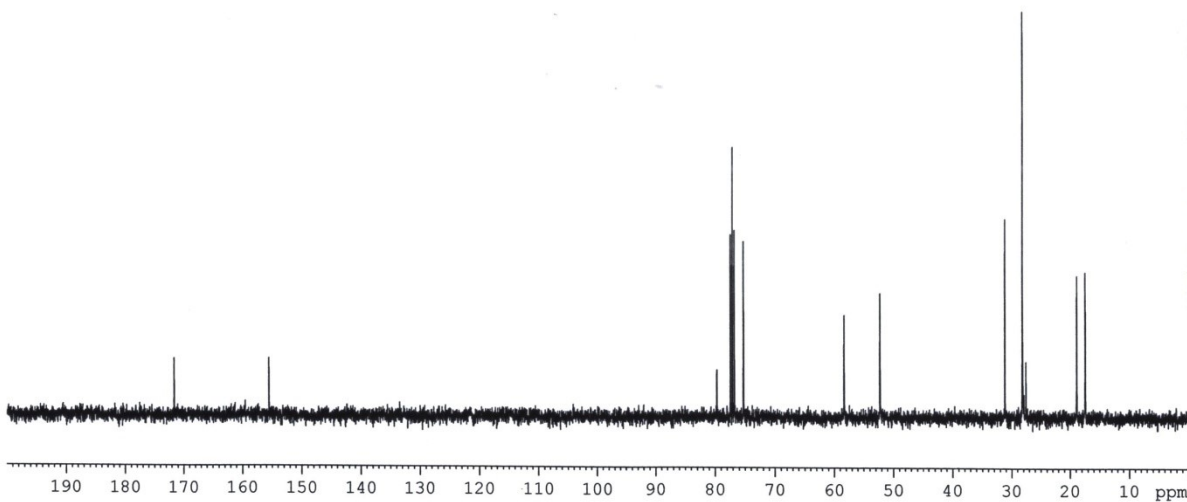
— 58.36  
— 52.31

— 31.22  
— 28.23

— 18.90  
— 17.47



**<sup>13</sup>C NMR: 100 MHz**  
**Solvent: CDCl<sub>3</sub>**



Current Data Parameters  
NAME Dr. A HAJRA-2021-13C  
EXPNO 502  
PROCNO 1

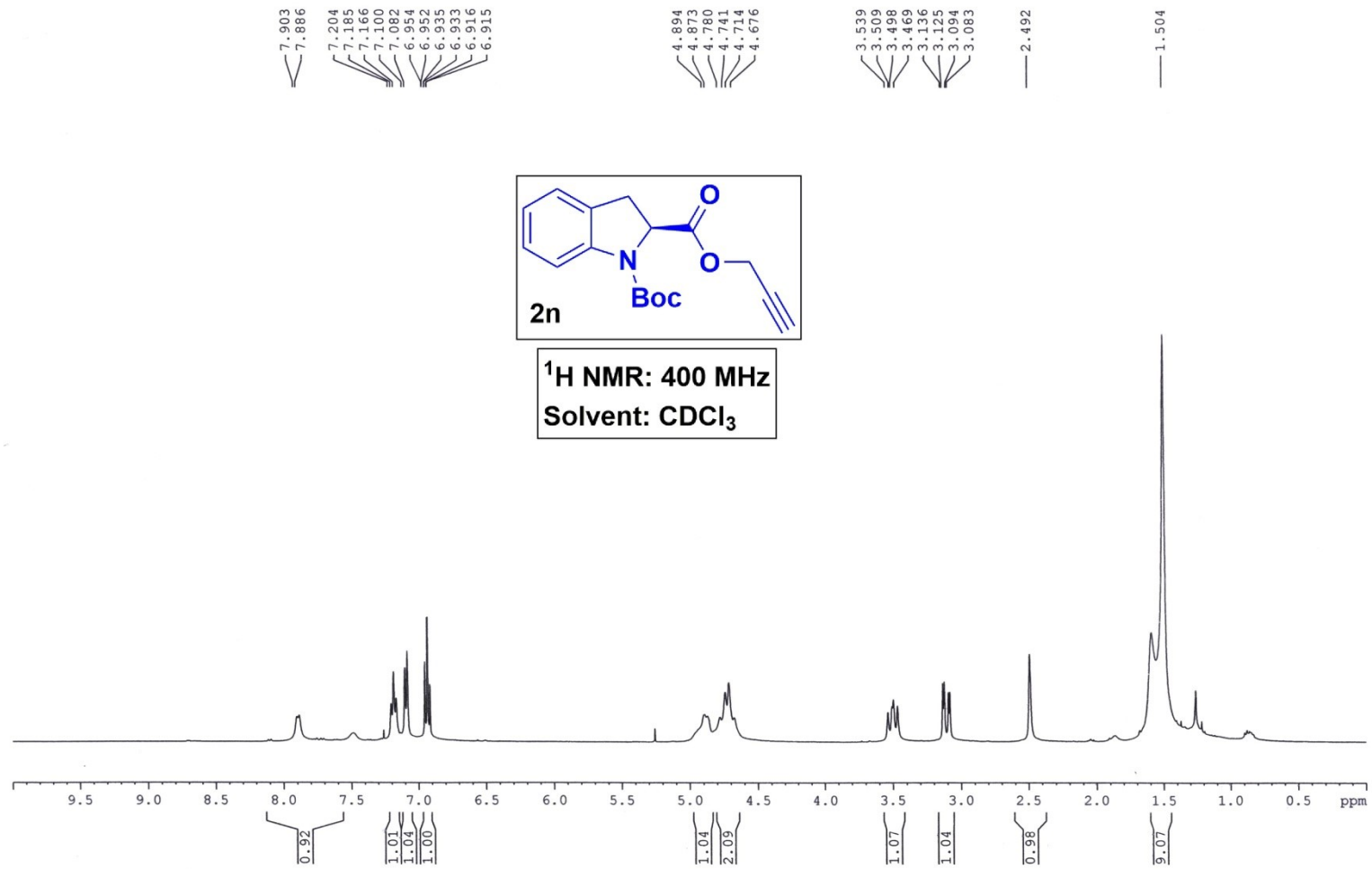
F2 - Acquisition Parameters  
Date\_ 20211219  
Time\_ 13.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 5  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 12.92  
DW 20.800 usec  
DE 6.50 usec  
TE 292.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

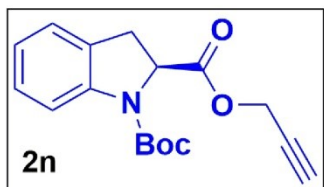
===== CHANNEL f1 =====  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.0000000 W

===== CHANNEL f2 =====  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLW2 12.0000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

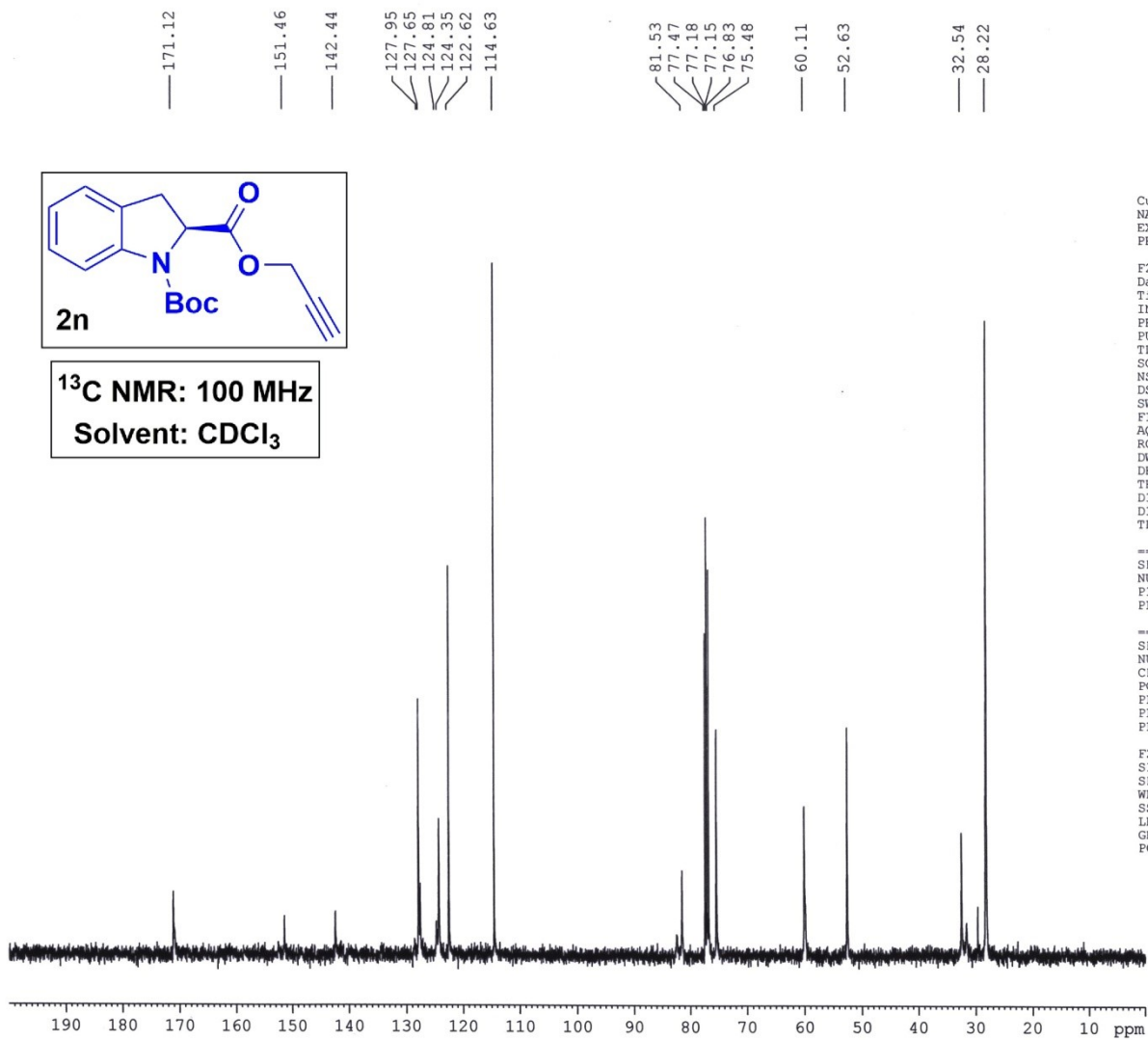
F2 - Processing parameters  
SI 16384  
SF 100.6177961 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40







**<sup>13</sup>C NMR: 100 MHz**  
**Solvent: CDCl<sub>3</sub>**



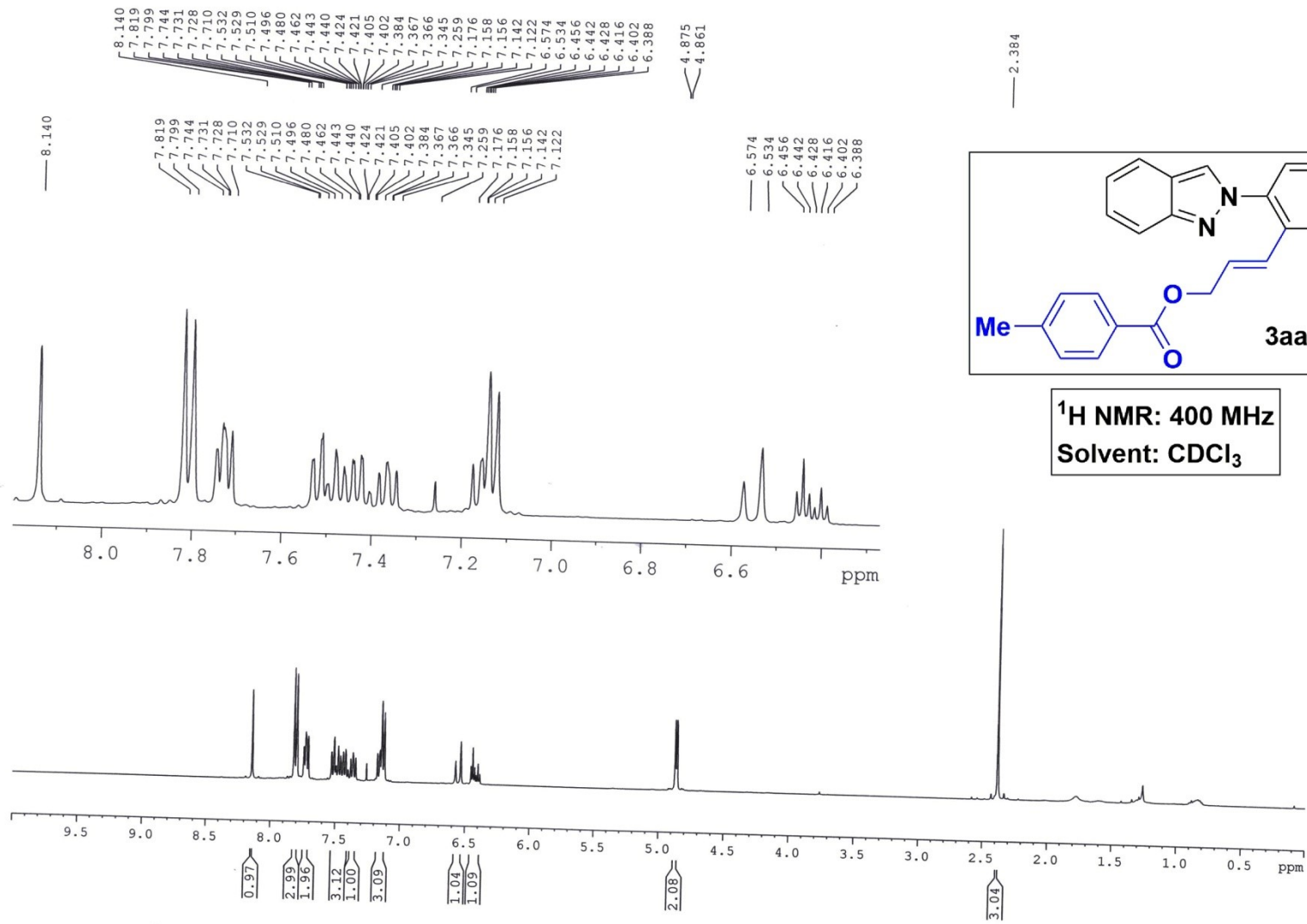
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 484  
 PROCNO 1

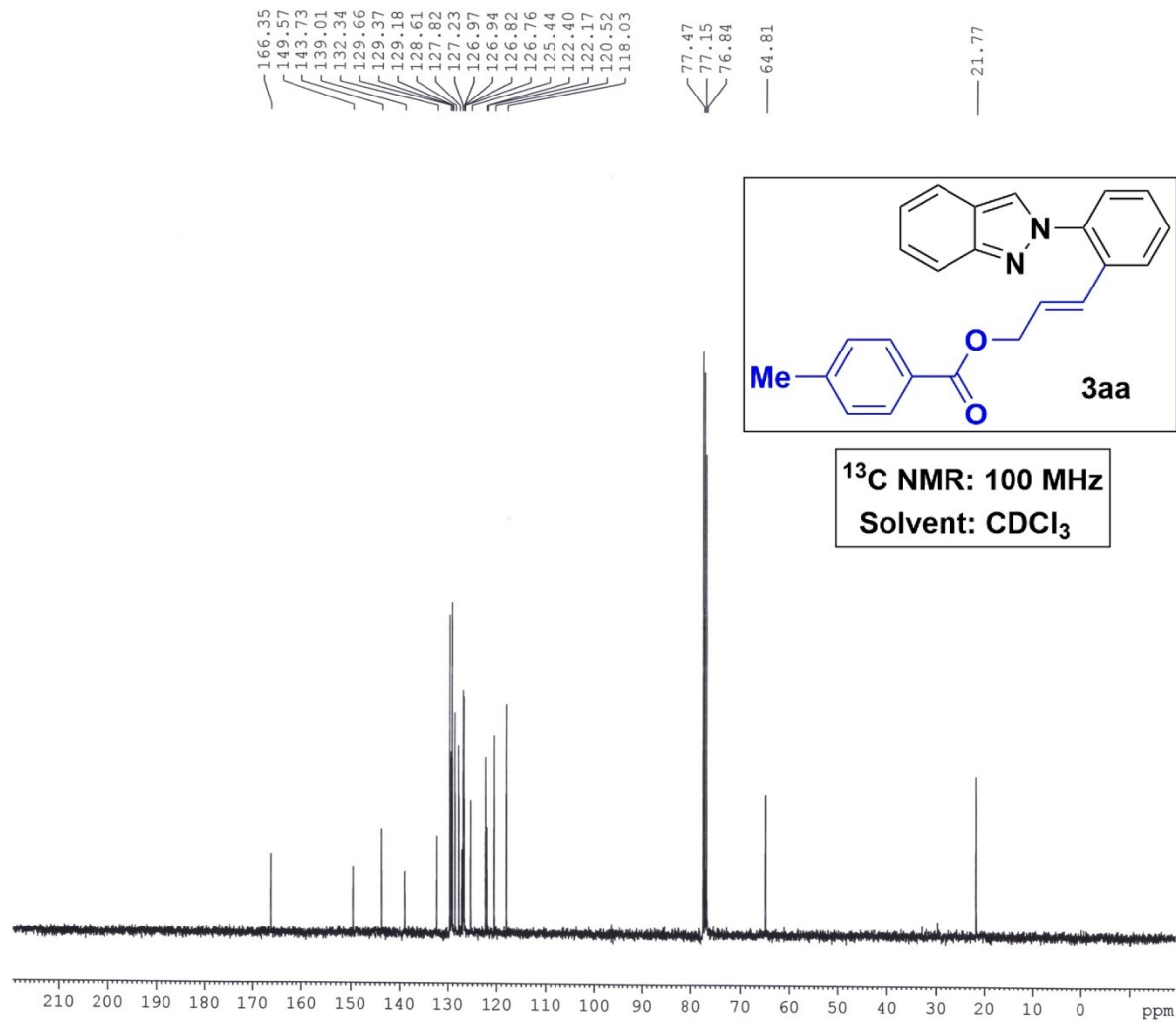
F2 - Acquisition Parameters  
 Date\_ 20211208  
 Time 16.33  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDC13  
 NS 120  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 23.55  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177990 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 1.40





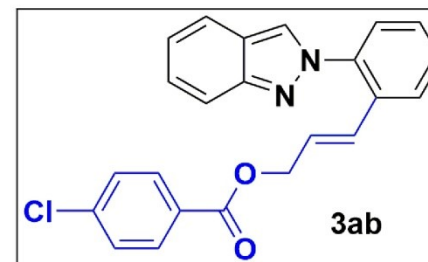
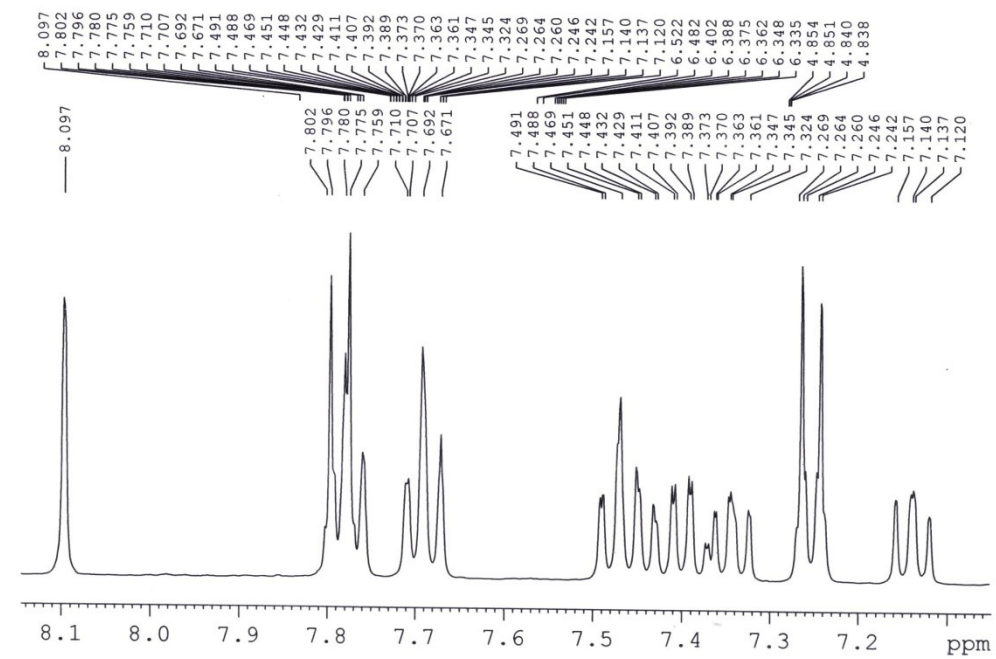
Current Data Parameters  
NAME Dr. A HAJRA-2021-13C  
EXPNO 433  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211114  
Time 11.19  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 220  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 186.42  
DW 20.800 usec  
DE 6.50 usec  
TE 293.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

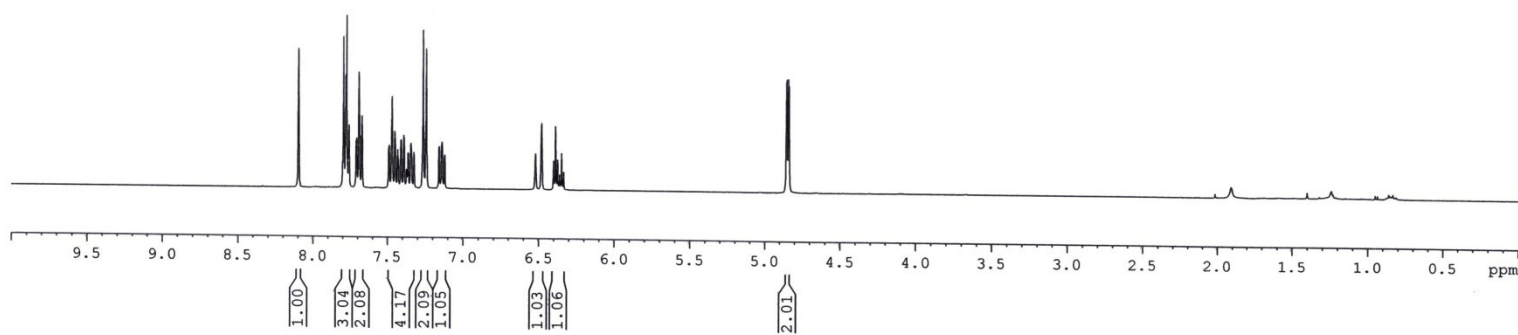
----- CHANNEL f1 -----  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W

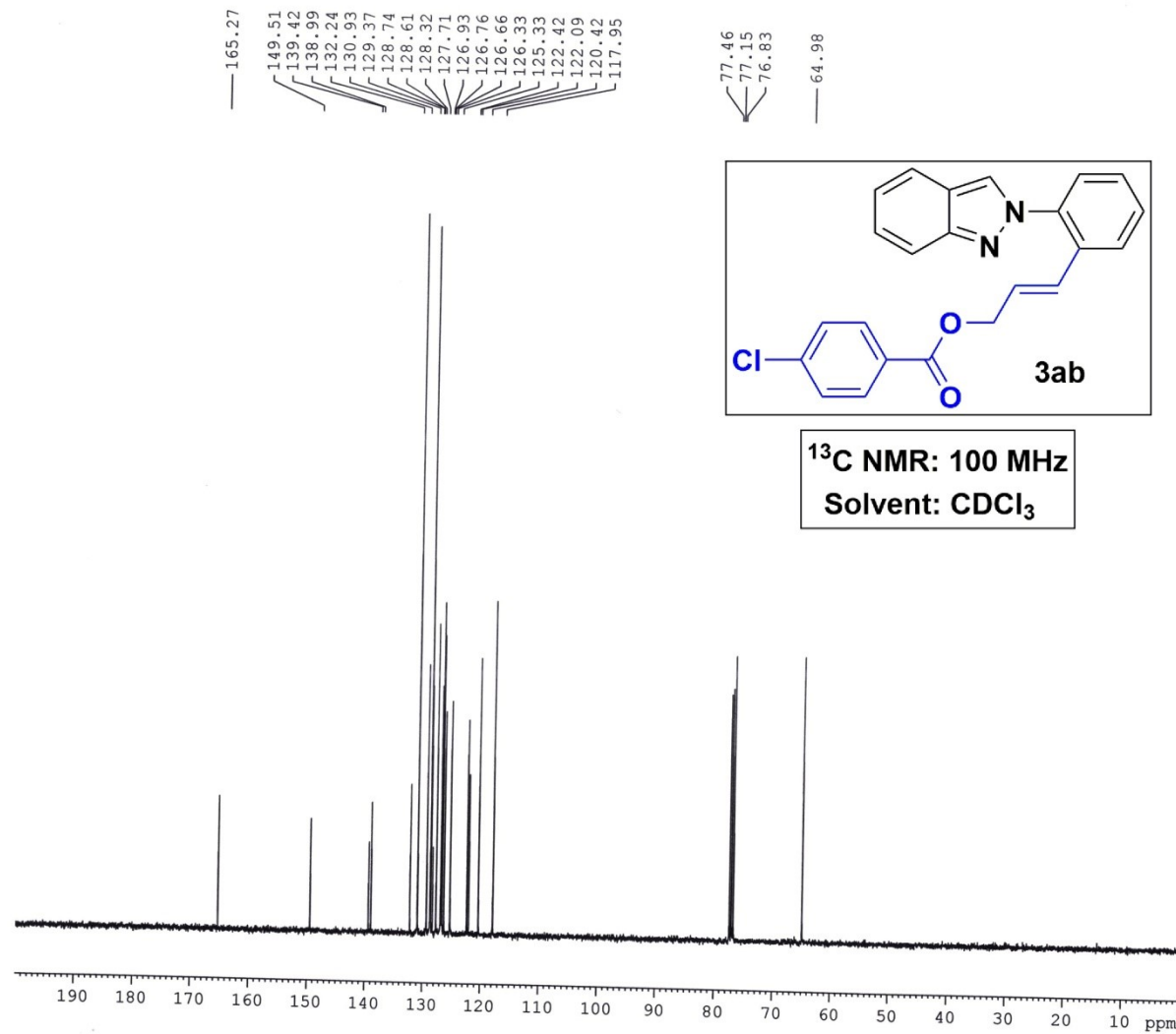
----- CHANNEL f2 -----  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

F2 - Processing parameters  
SI 16384  
SF 100.6177902 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



**<sup>1</sup>H NMR: 400 MHz**  
**Solvent: CDCl<sub>3</sub>**





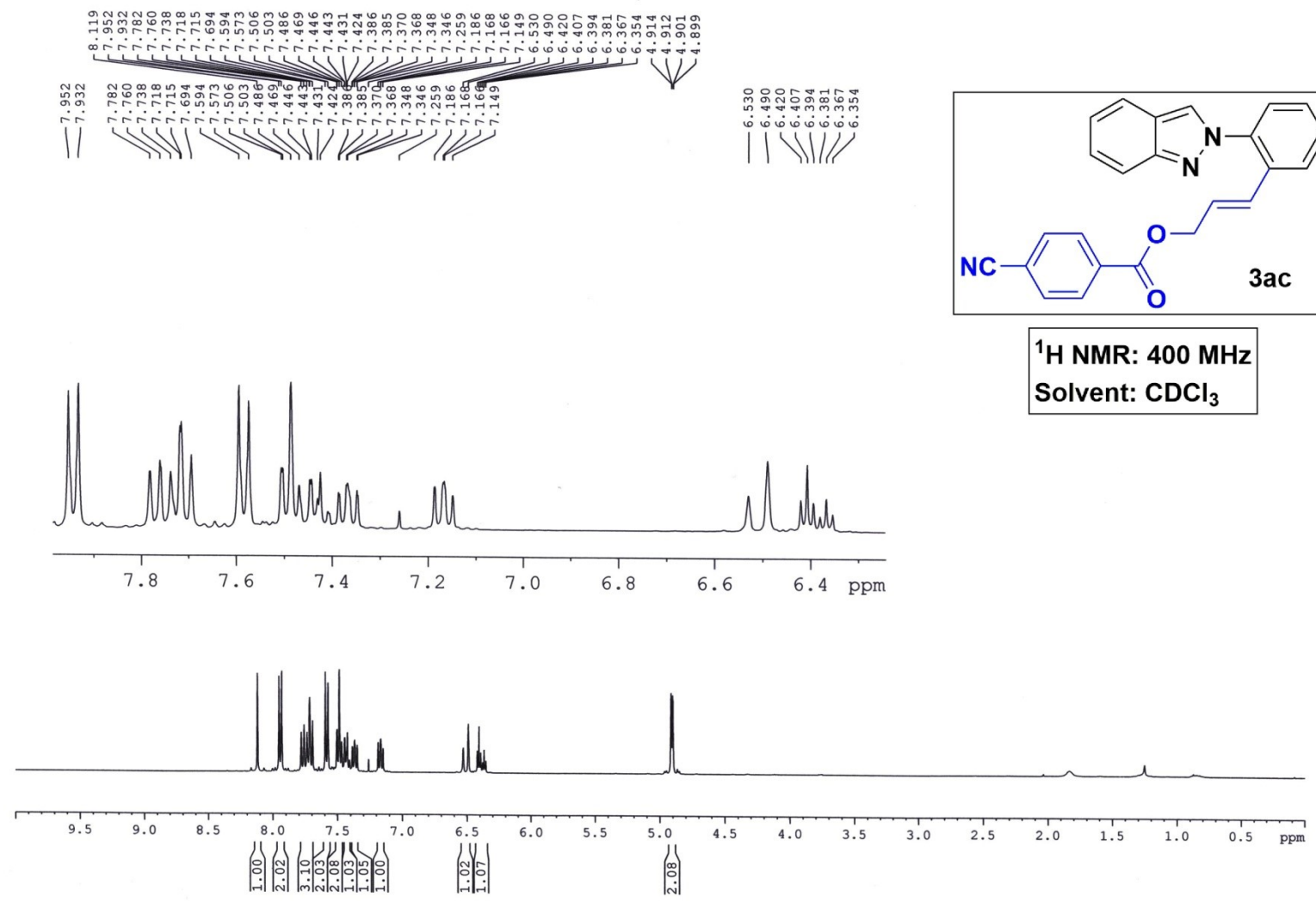
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 438  
 PROCNO 1

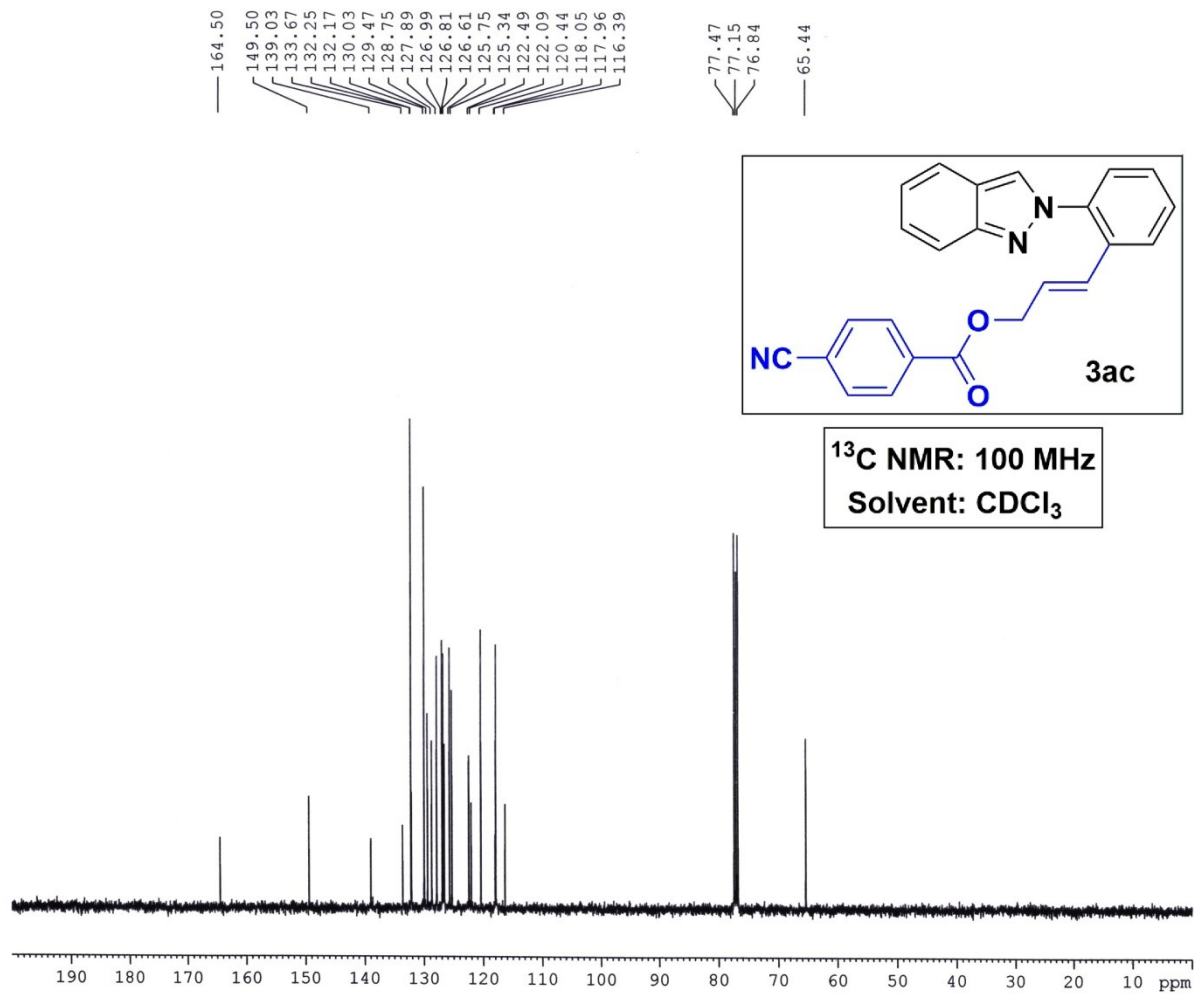
F2 - Acquisition Parameters  
 Date\_ 20211118  
 Time\_ 12.12  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 220  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 54.07  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.6 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.0000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177960 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 1.40





Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 454  
 PROCNO 1

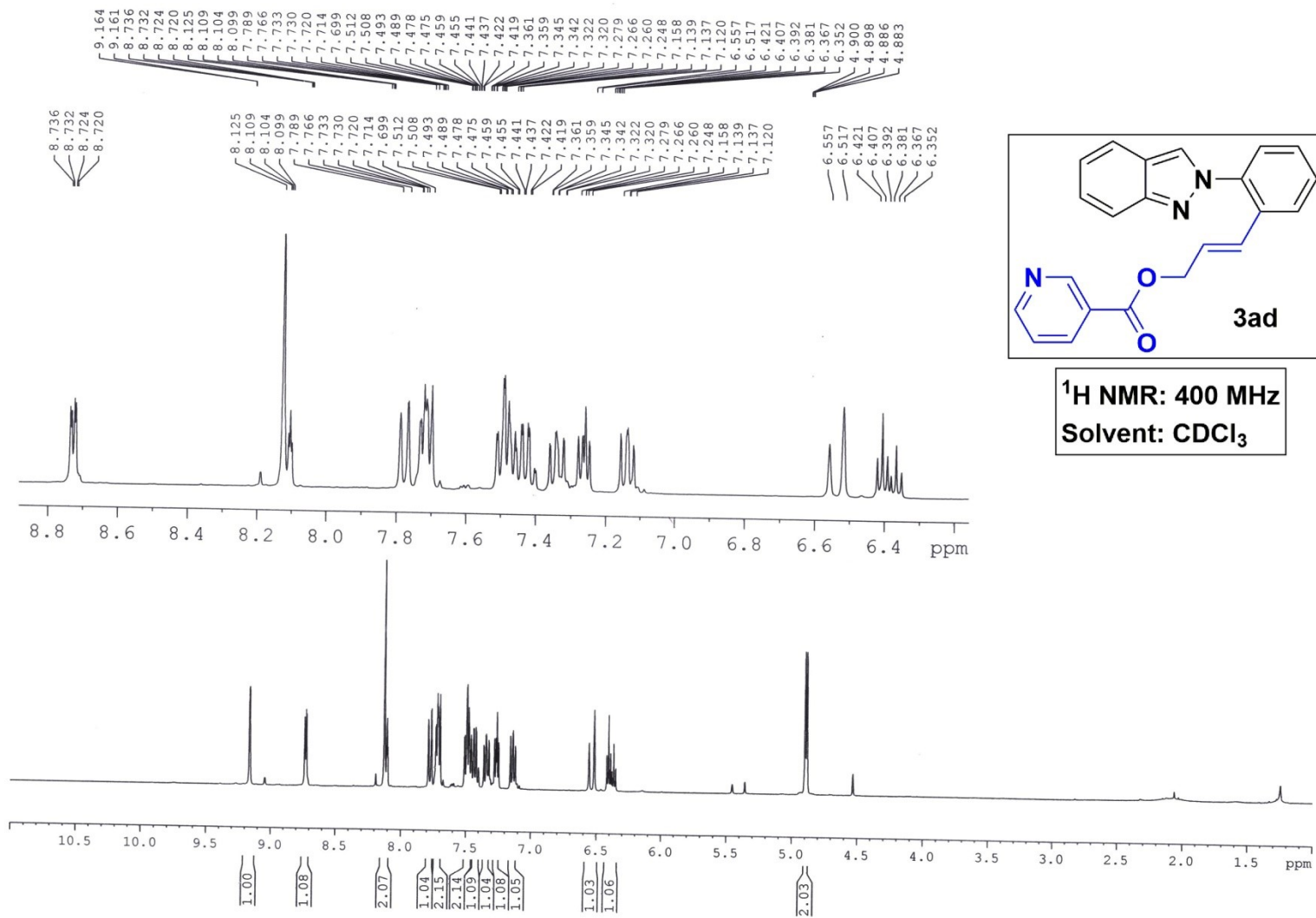
F2 - Acquisition Parameters  
 Date\_ 20211126  
 Time 12.41  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT  $\text{CDCl}_3$   
 NS 120  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 67.81  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 293.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

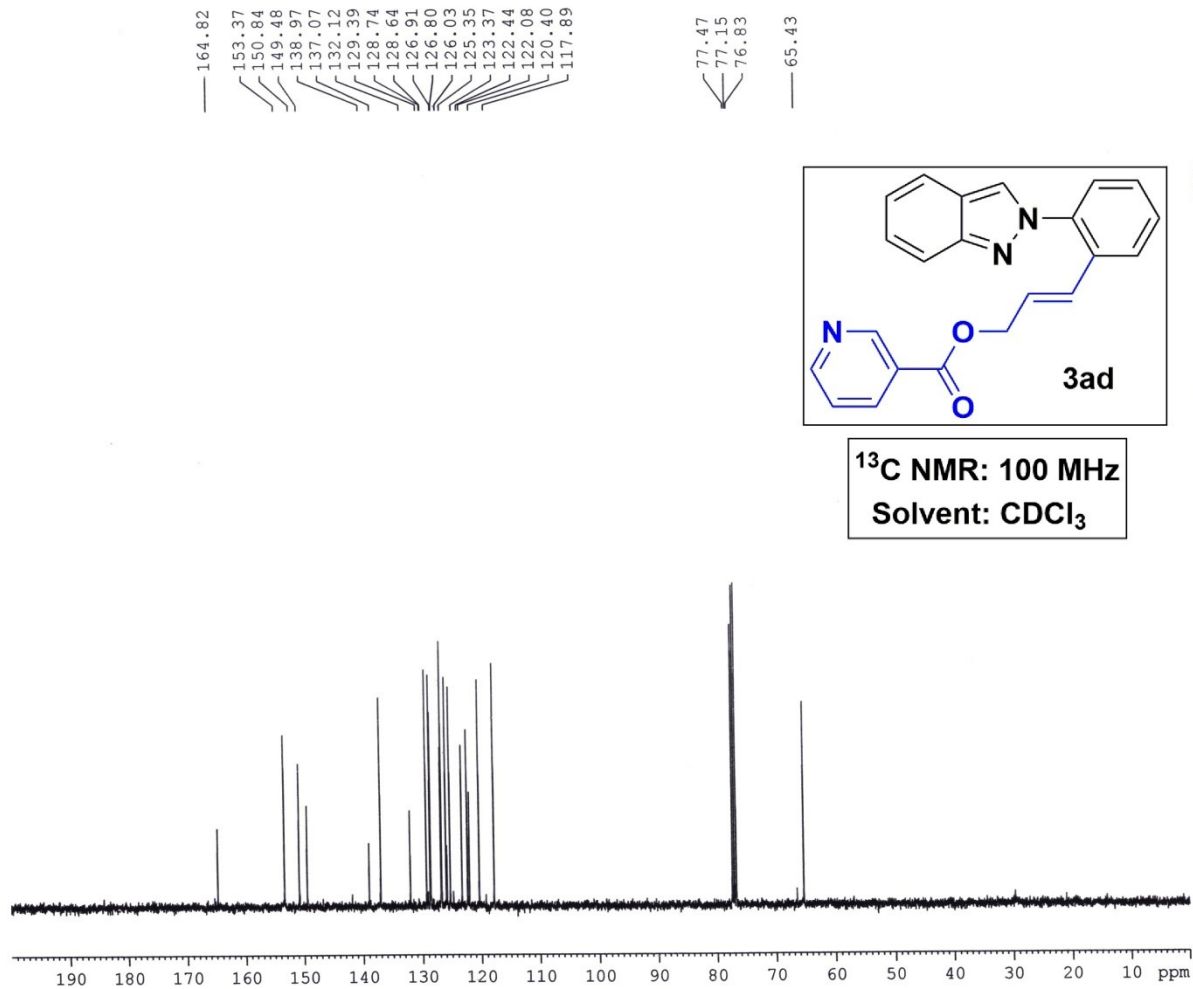
===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177936 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40







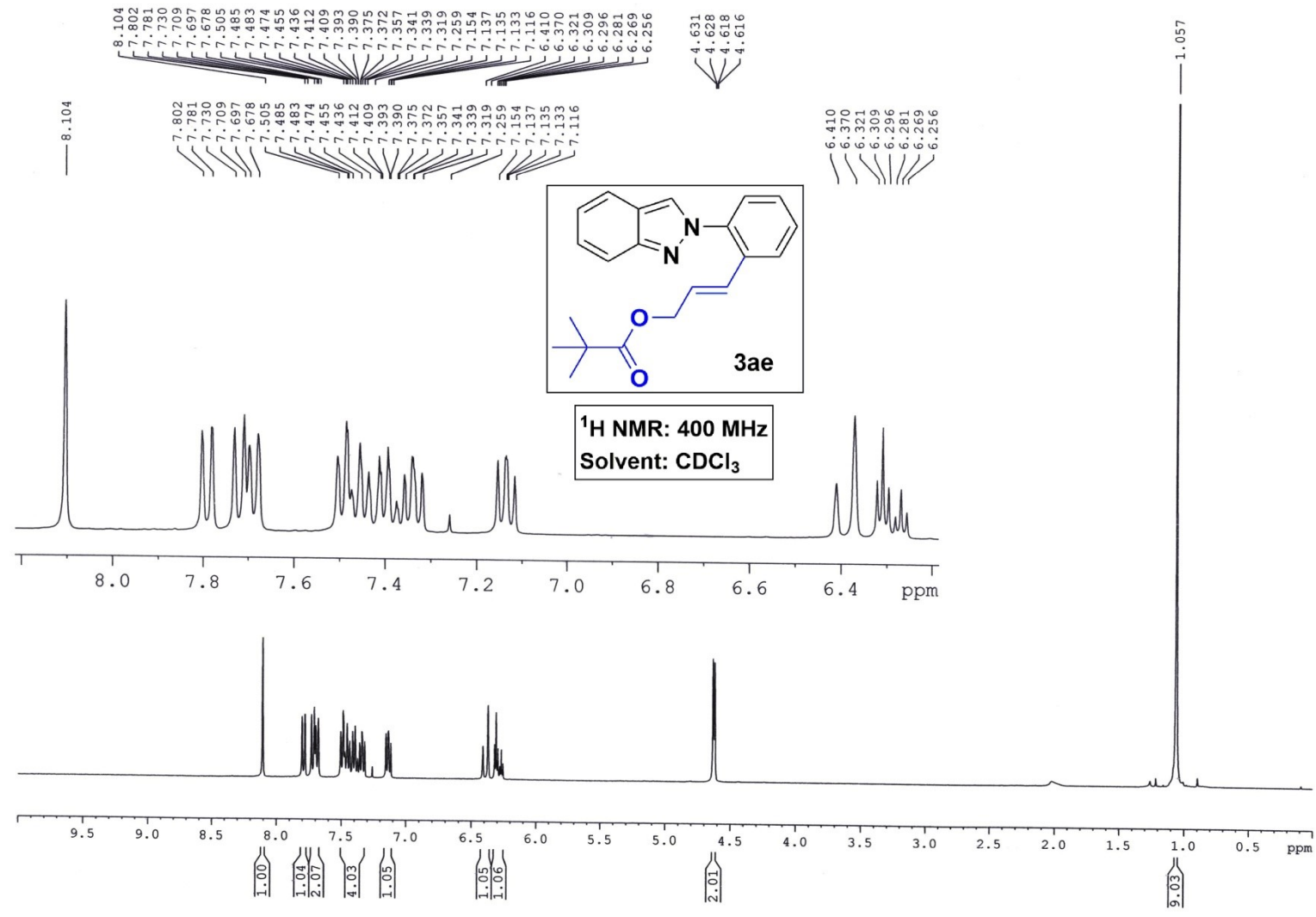
Current Data Parameters  
NAME Dr. A HAJRA-2021-13C  
EXPNO 453  
PROCNO 1

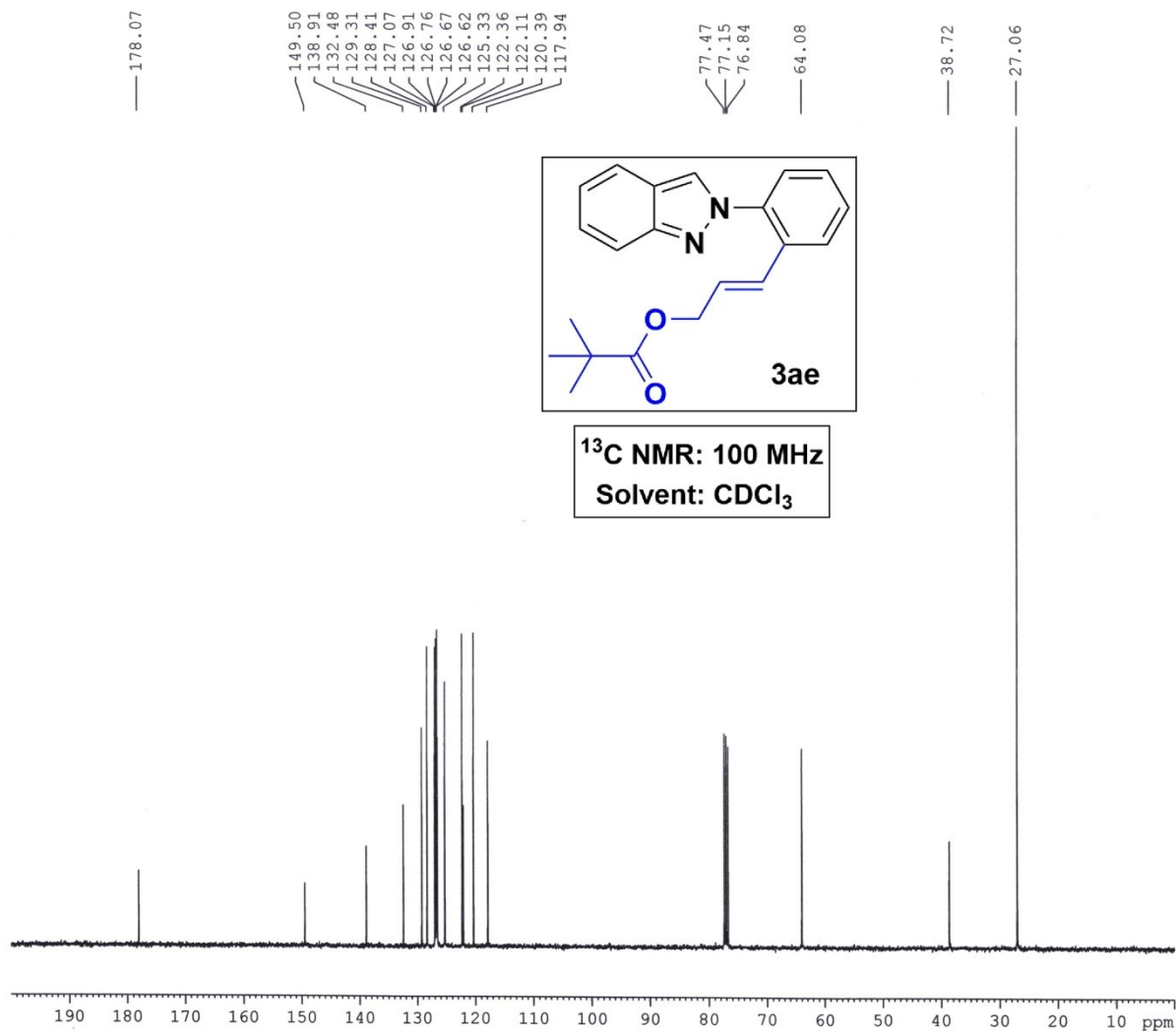
F2 - Acquisition Parameters  
Date\_ 20211126  
Time\_ 12.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 100  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 40.87  
DW 20.800 usec  
DE 6.50 usec  
TE 293.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W

===== CHANNEL f2 =====  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
FCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

F2 - Processing parameters  
SI 16384  
SF 100.6177961 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 474  
 PROCNO 1

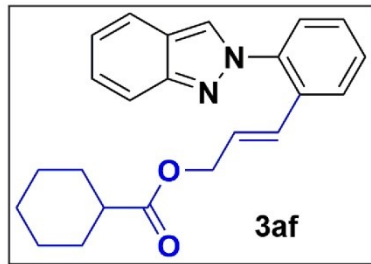
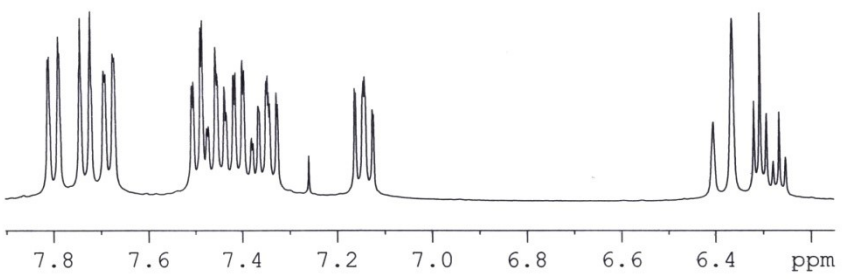
F2 - Acquisition Parameters  
 Date\_ 20211205  
 Time 18.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 230  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 30.11  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

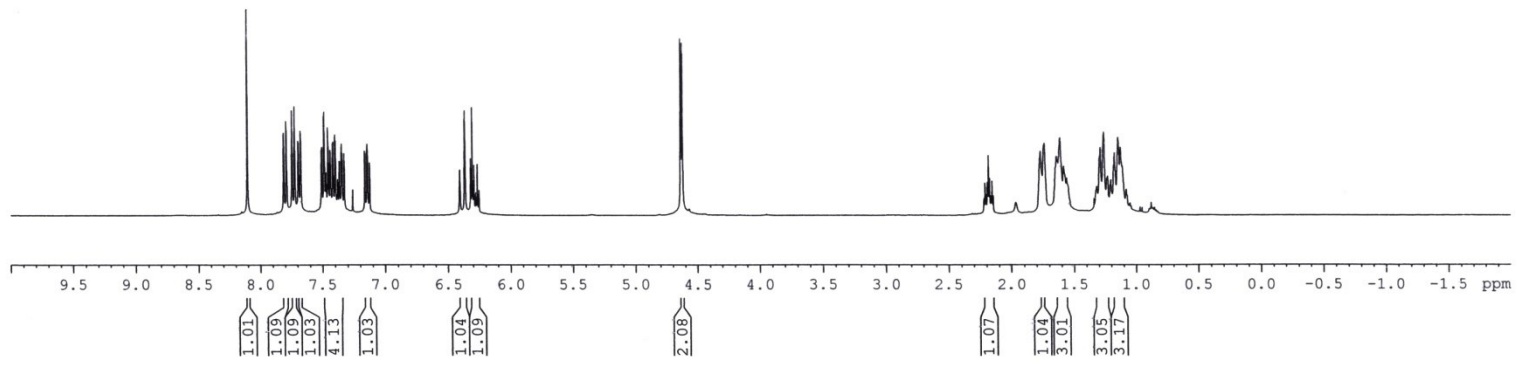
===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPMRG(2) waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

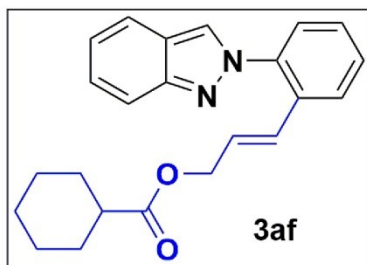
F2 - Processing parameters  
 SI 16384  
 SF 100.6177961 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

8.104  
7.811  
7.809  
7.788  
7.787  
7.772  
7.771  
7.721  
7.683  
7.690  
7.674  
7.671  
7.507  
7.507  
7.504  
7.488  
7.484  
7.475  
7.471  
7.456  
7.452  
7.437  
7.434  
7.434  
7.418  
7.414  
7.399  
7.395  
7.380  
7.377  
7.377  
7.365  
7.348  
7.346  
7.343  
7.341  
7.327  
7.325  
7.259  
7.162  
7.161  
7.144  
7.141  
7.125  
7.123  
6.404  
6.364  
6.319  
6.306  
6.319  
6.293  
6.279  
6.266  
6.253  
6.253  
4.638  
4.635  
4.625  
4.622  
2.212  
2.203  
2.192  
2.184  
2.174  
2.165  
2.155  
2.146  
1.773  
1.769  
1.741  
1.737  
1.648  
1.640  
1.633  
1.612  
1.584  
1.574  
1.560  
1.547  
1.547  
1.315  
1.287  
1.258  
1.234  
1.229  
1.209  
1.203  
1.180  
1.172  
1.143  
1.127  
1.123  
1.109

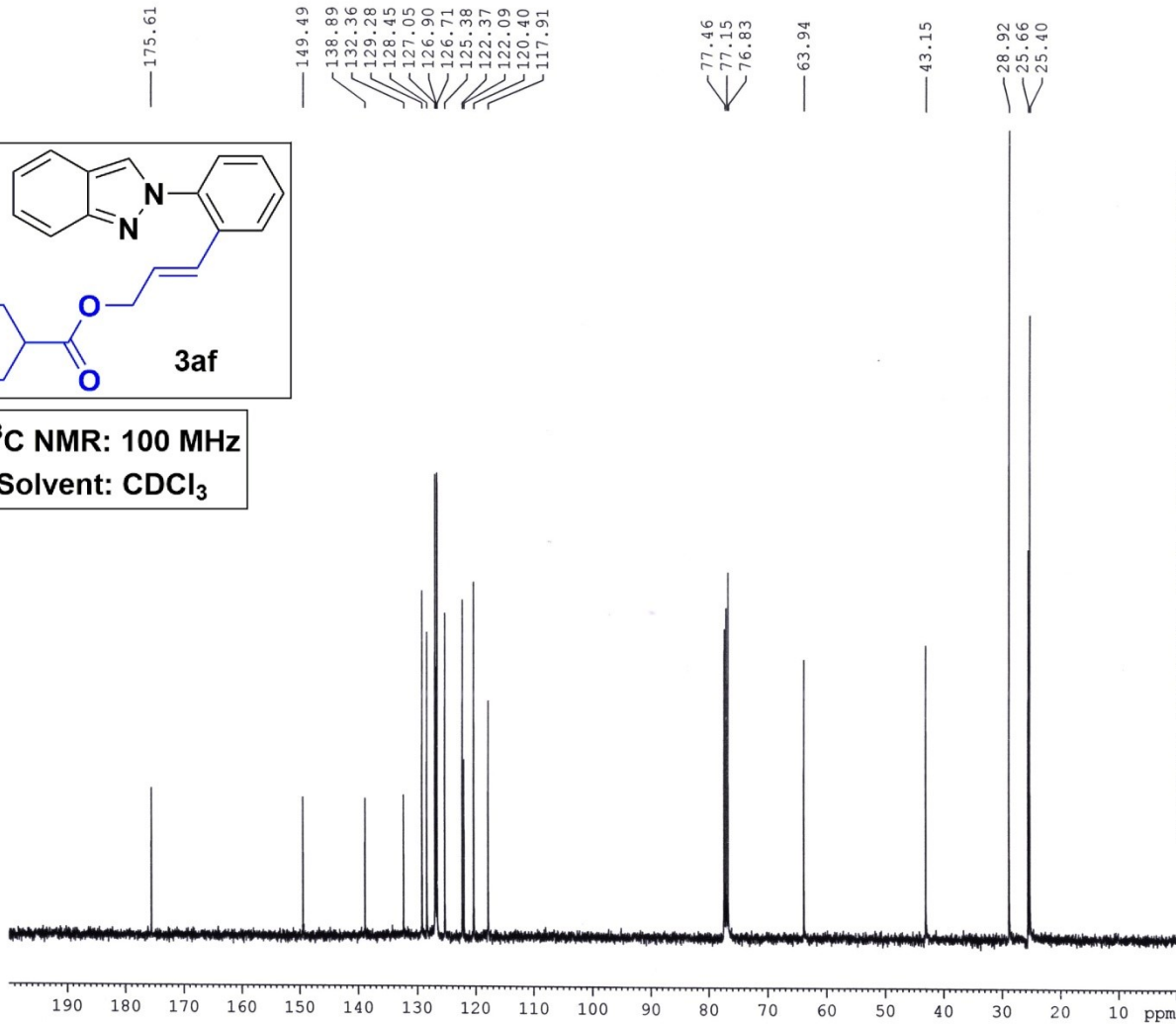


**<sup>1</sup>H NMR: 400 MHz**  
**Solvent: CDCl<sub>3</sub>**





**<sup>13</sup>C NMR: 100 MHz**  
**Solvent: CDCl<sub>3</sub>**



```

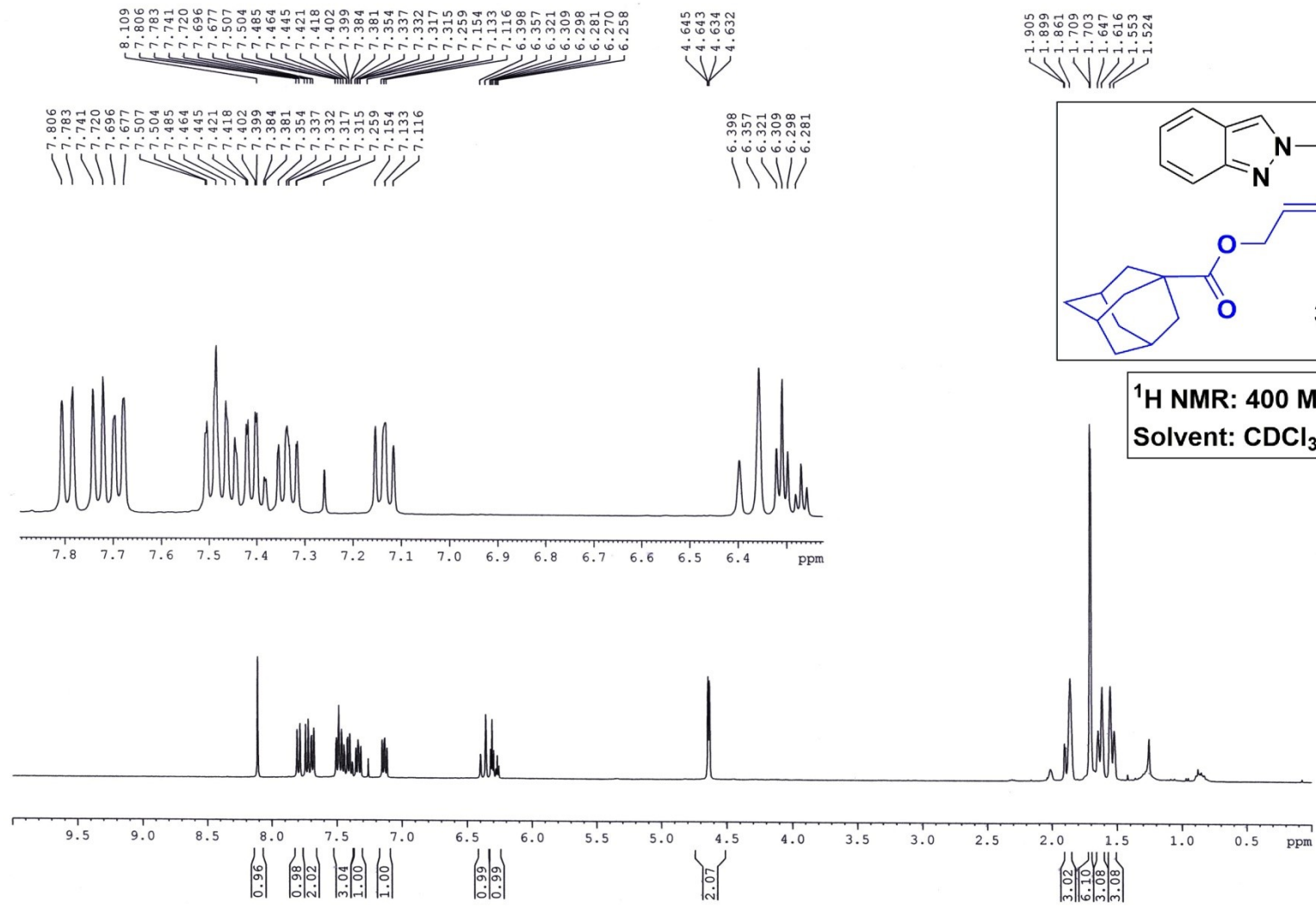
Current Data Parameters
NAME      Dr. A HAJRA-2021-13C
EXPNO     496
PROCNO    1

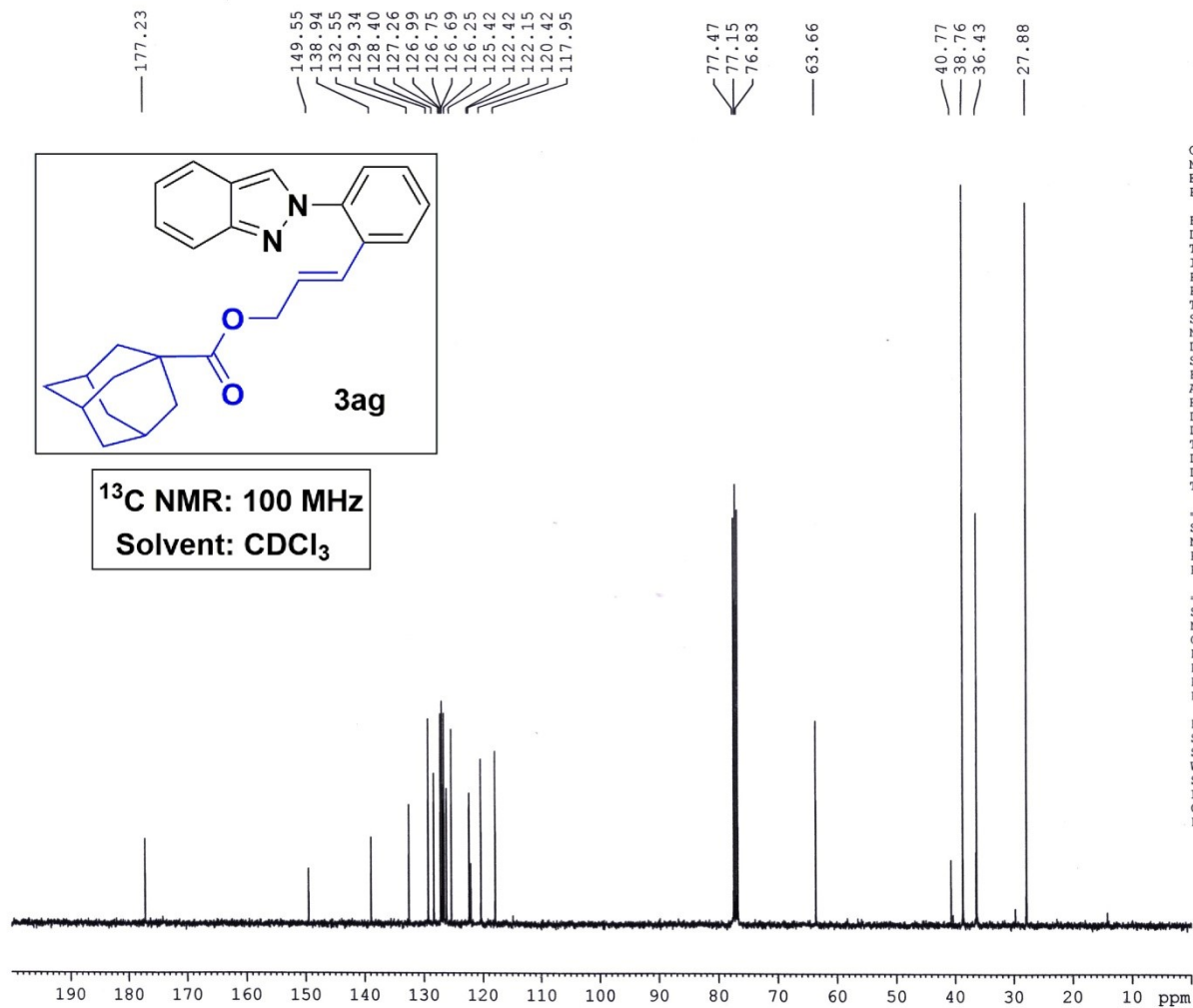
F2 - Acquisition Parameters
Date_     20211215
Time      18.59
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        32768
SOLVENT   CDCl3
NS        160
DS        2
SWH       24038.461 Hz
FIDRES    0.733596 Hz
AQ        0.6815744 sec
RG        26.53
DW        20.800 usec
DE        6.50 usec
TE        292.5 K
D1        2.0000000 sec
D11       0.0300000 sec
TD0       1

===== CHANNEL f1 =====
SFO1     100.6278588 MHz
NUC1     13C
P1       8.90 usec
PLW1     54.0000000 W

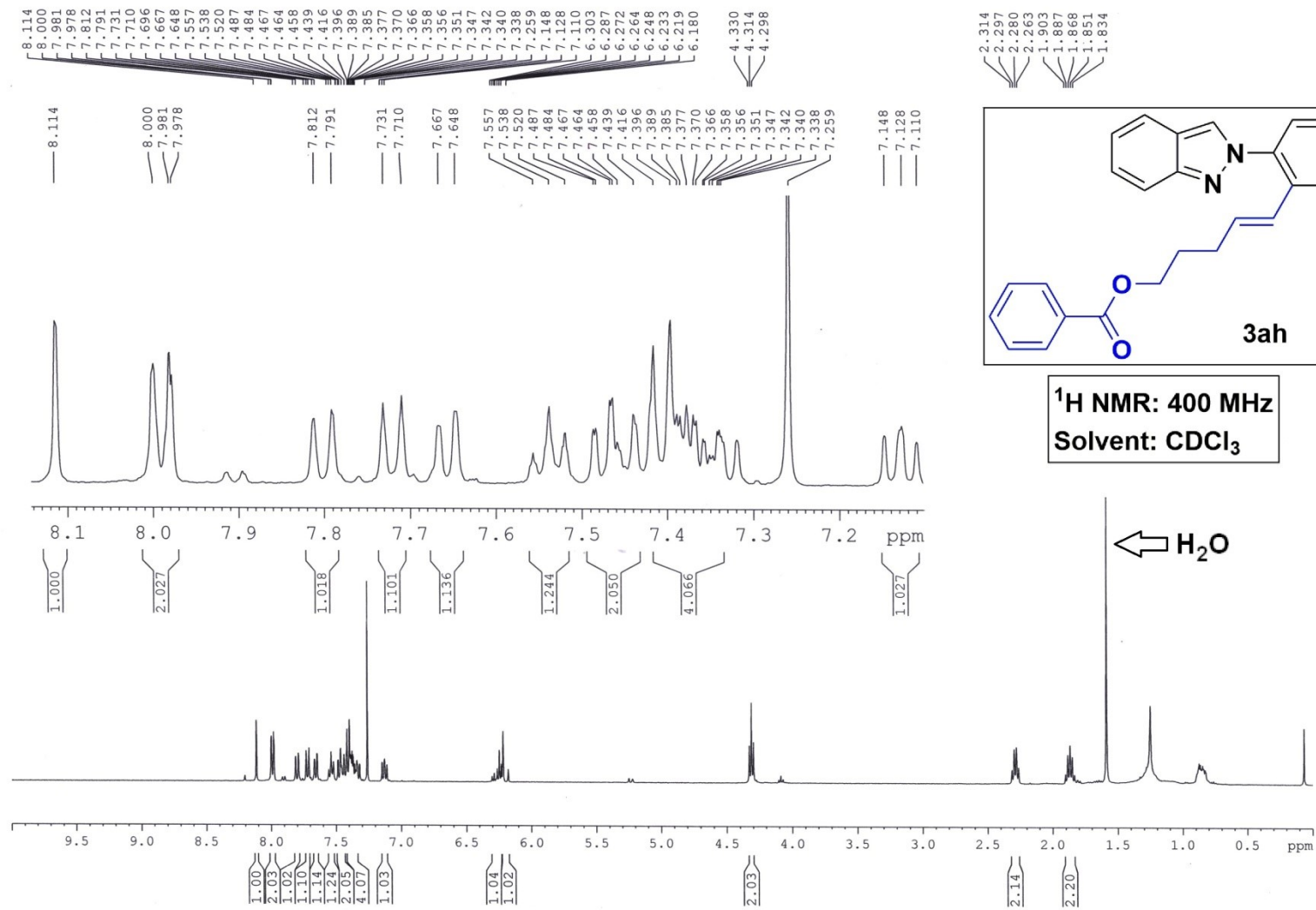
===== CHANNEL f2 =====
SFO2     400.1516006 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLW2     12.0000000 W
PLW12    0.32231000 W
PLW13    0.16212000 W

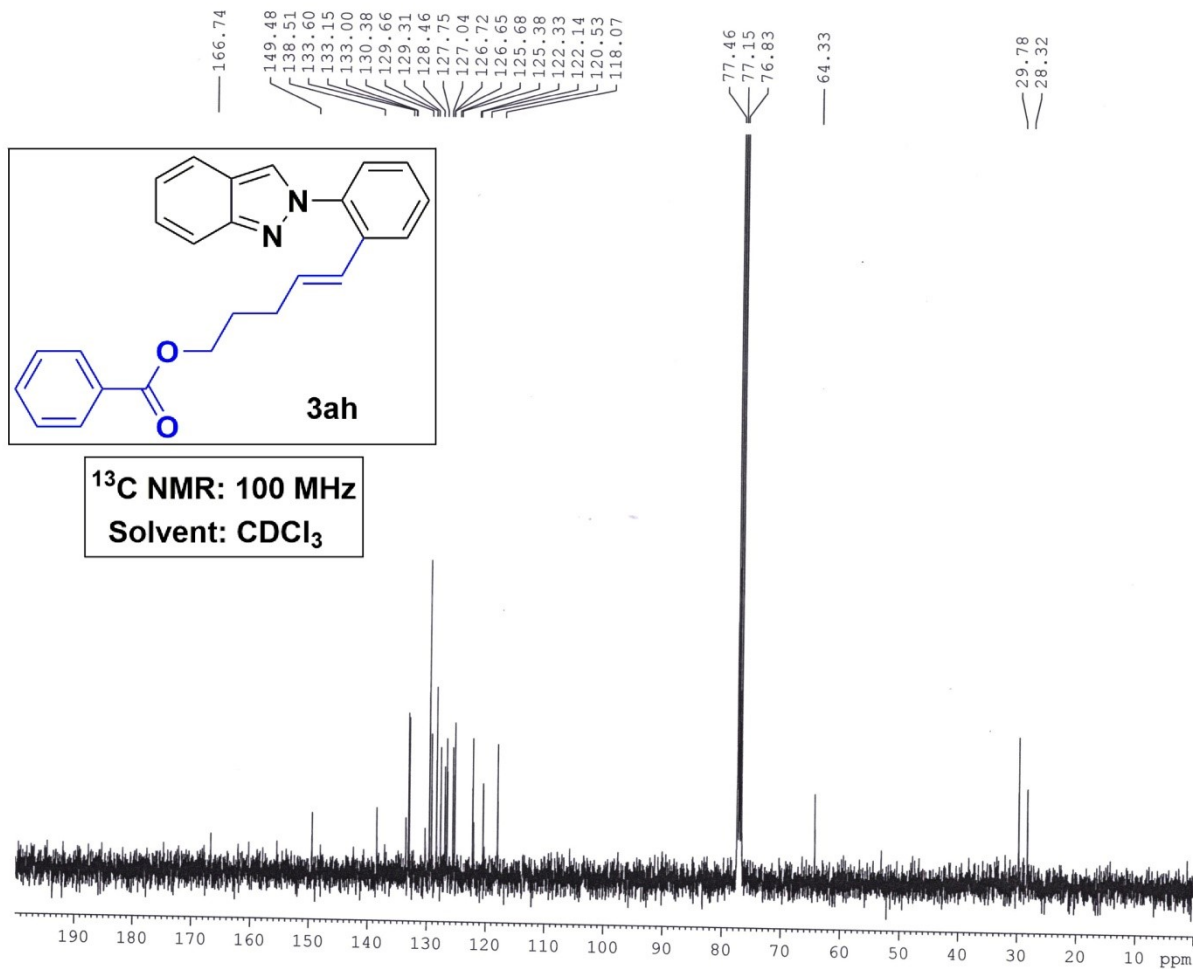
F2 - Processing parameters
SI       16384
SF       100.6177960 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```











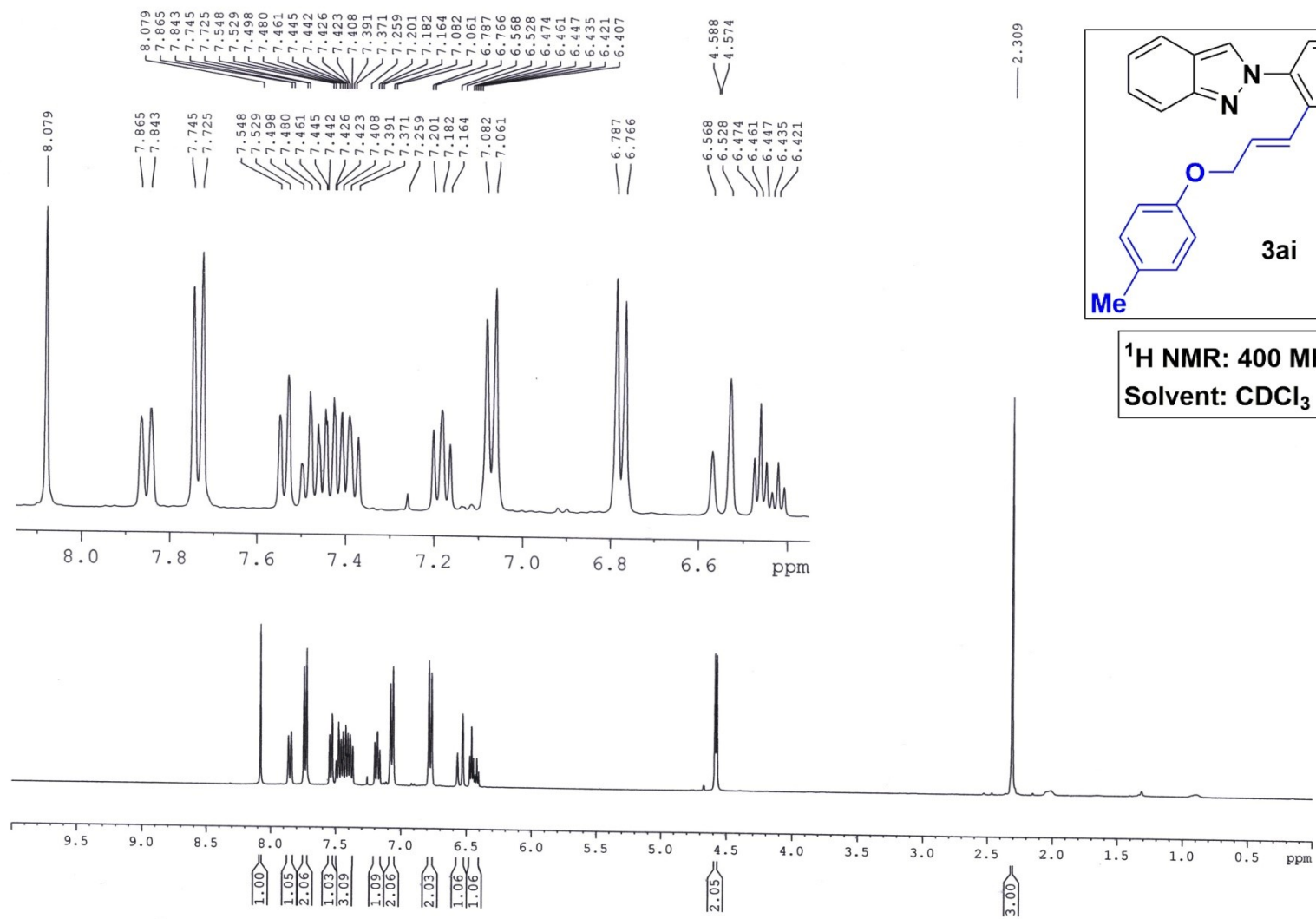
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 137  
 PROCNO 1

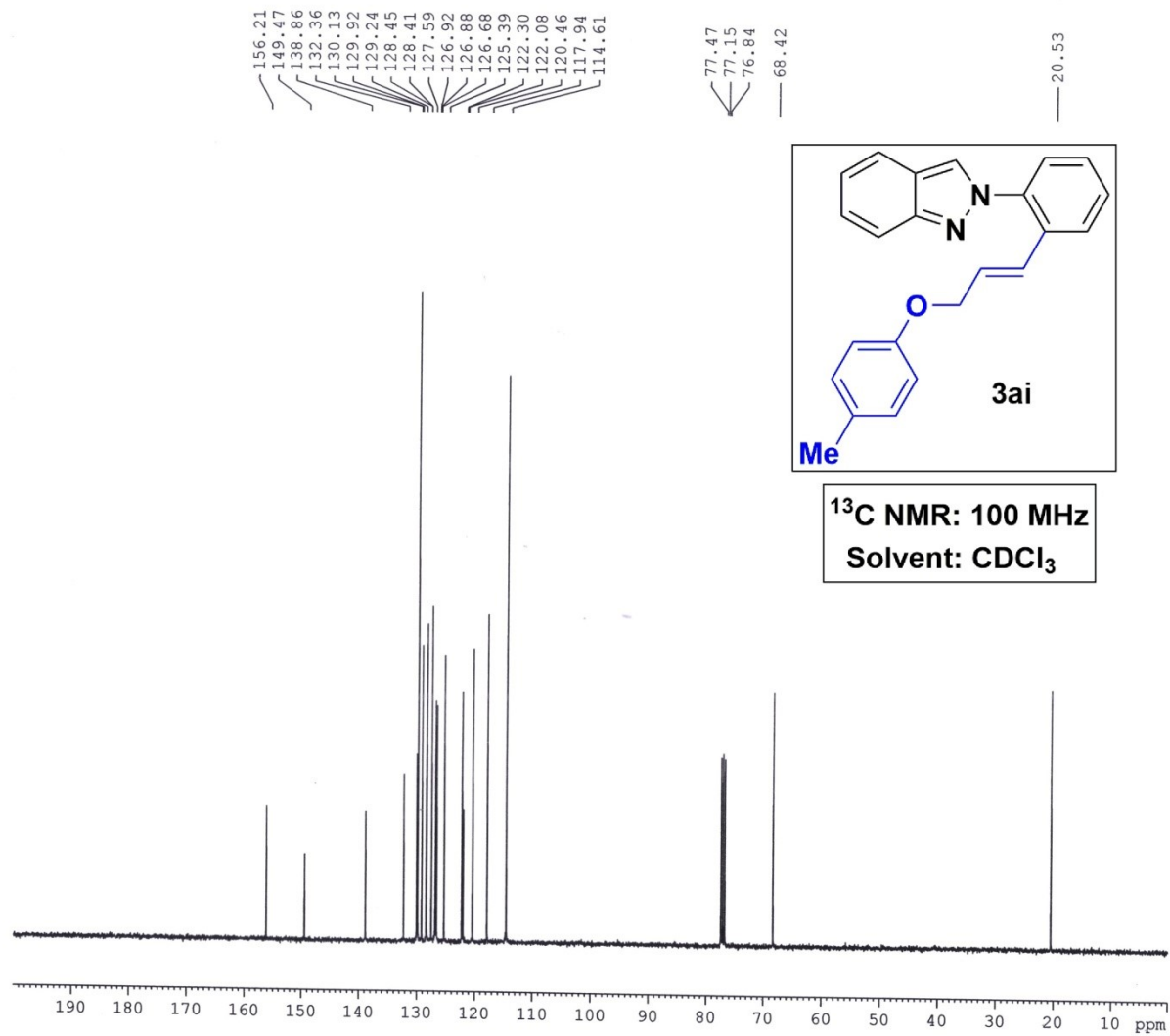
F2 - Acquisition Parameters  
 Date\_ 20210316  
 Time\_ 11.16  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 880  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177858 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





156.21  
149.47  
138.86  
132.36  
130.13  
129.92  
129.24  
128.45  
128.41  
127.59  
126.92  
126.88  
126.68  
125.39  
122.30  
122.08  
120.46  
117.94  
114.61

77.47  
77.15  
76.84  
68.42

20.53

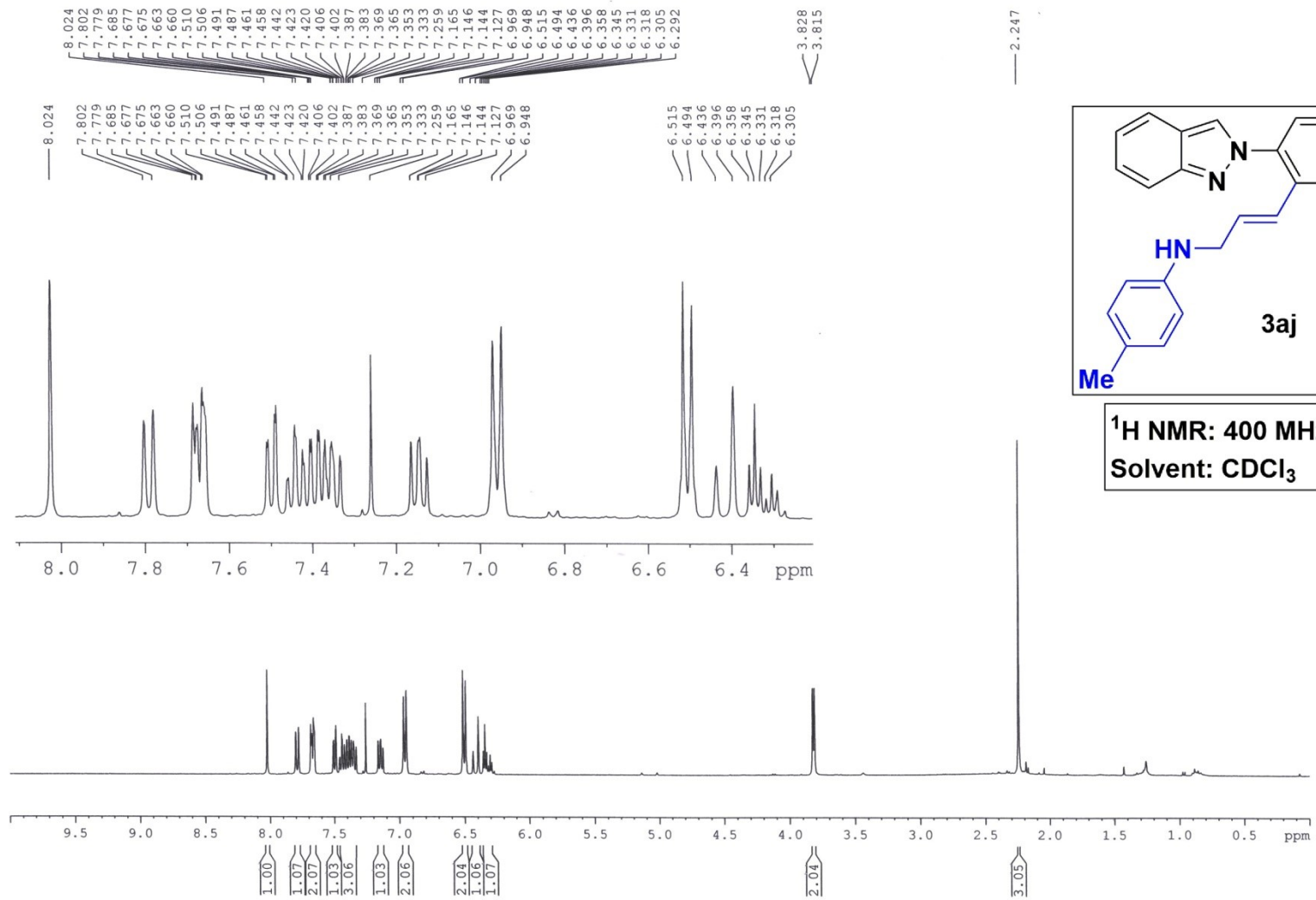
Current Data Parameters  
NAME Dr. A HAJRA-2021-13C  
EXPNO 446  
PROCNO 1

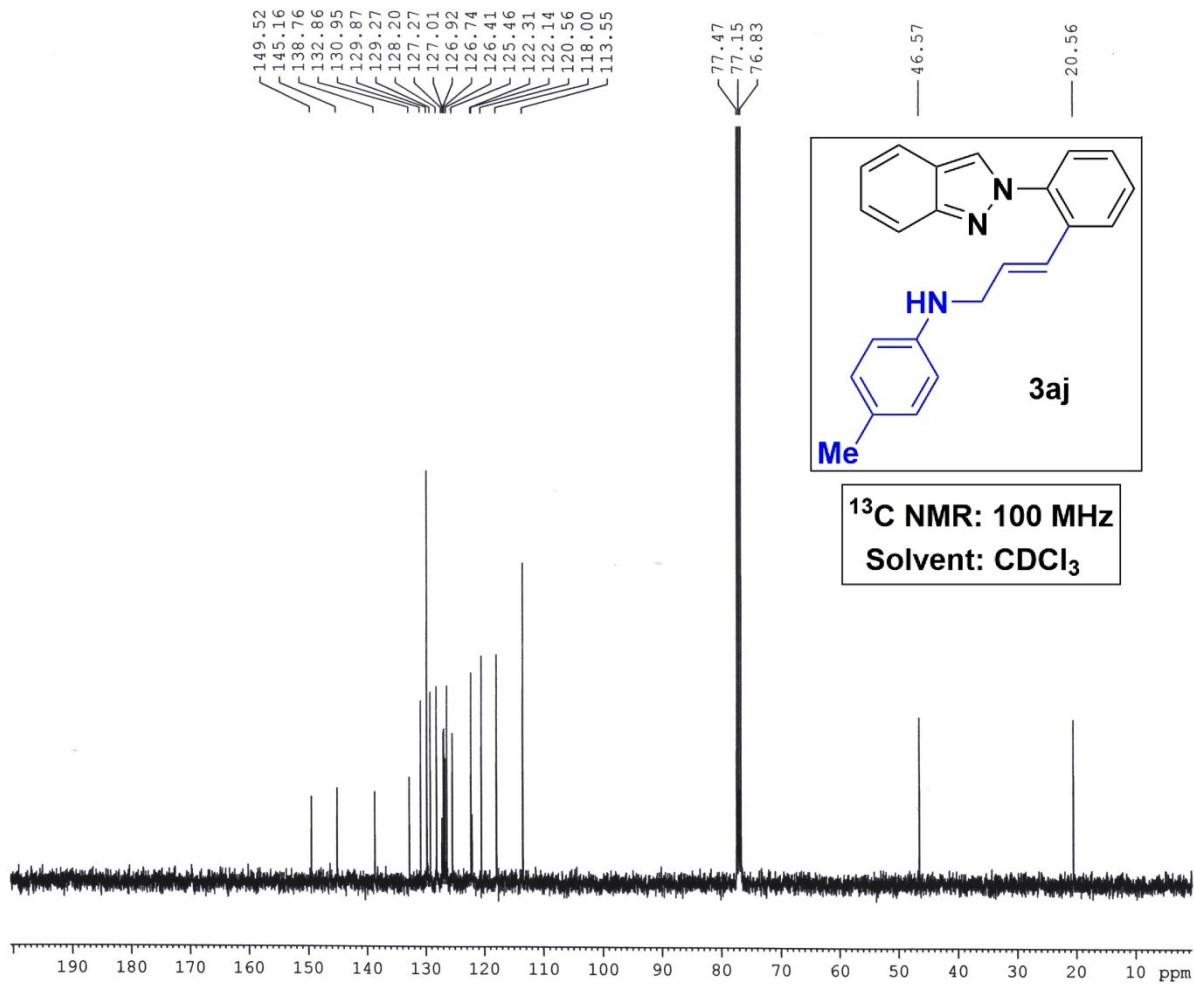
F2 - Acquisition Parameters  
Date\_ 20211121  
Time\_ 10.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
FULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 220  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 30.11  
DW 20.800 usec  
DE 6.50 usec  
TE 293.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W

===== CHANNEL f2 =====  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

F2 - Processing parameters  
SI 16384  
SF 100.6178020 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





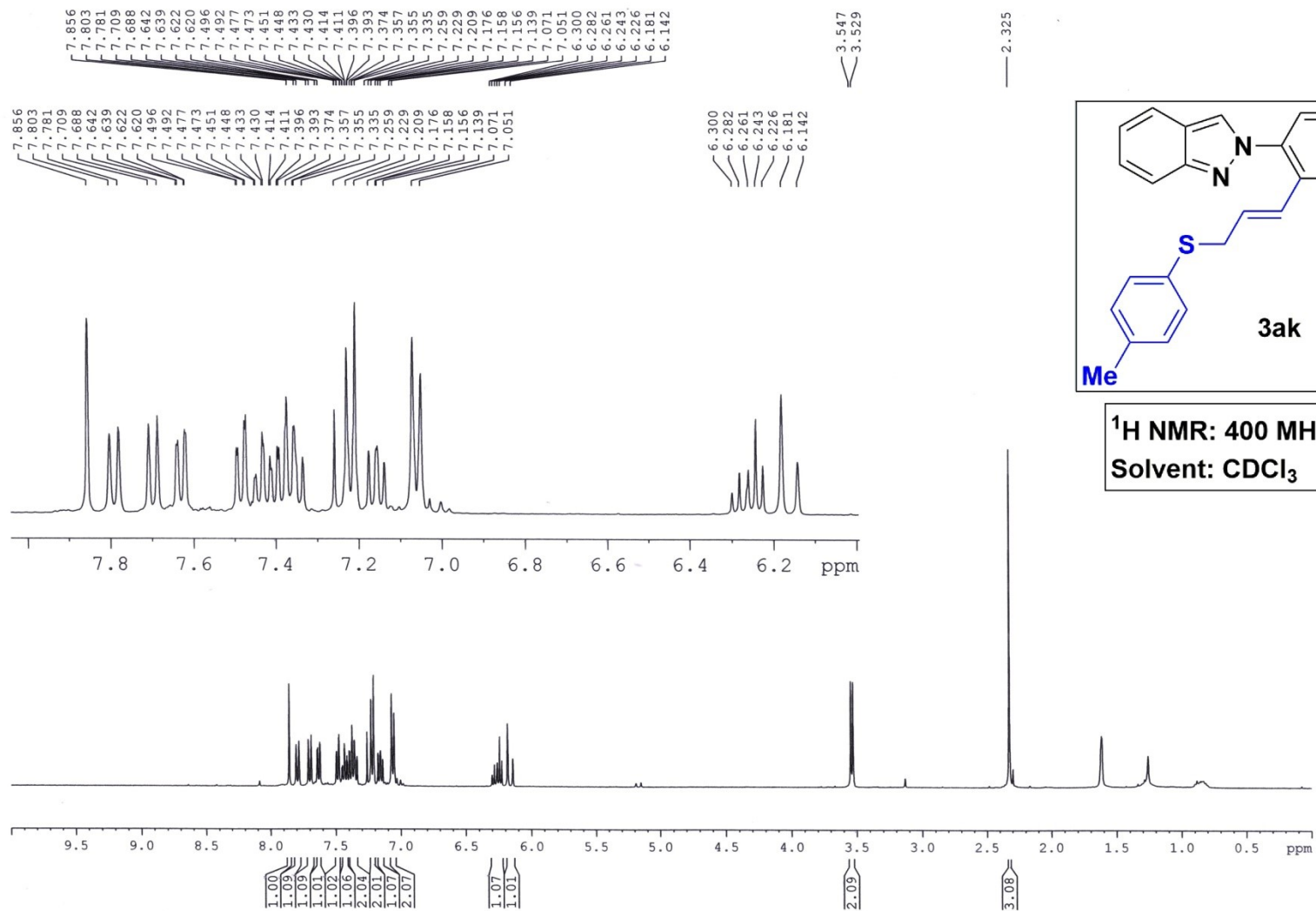
Current Data Parameters  
NAME Dr. A HAJRA-2021-13C  
EXPNO 449  
PROCNO 1

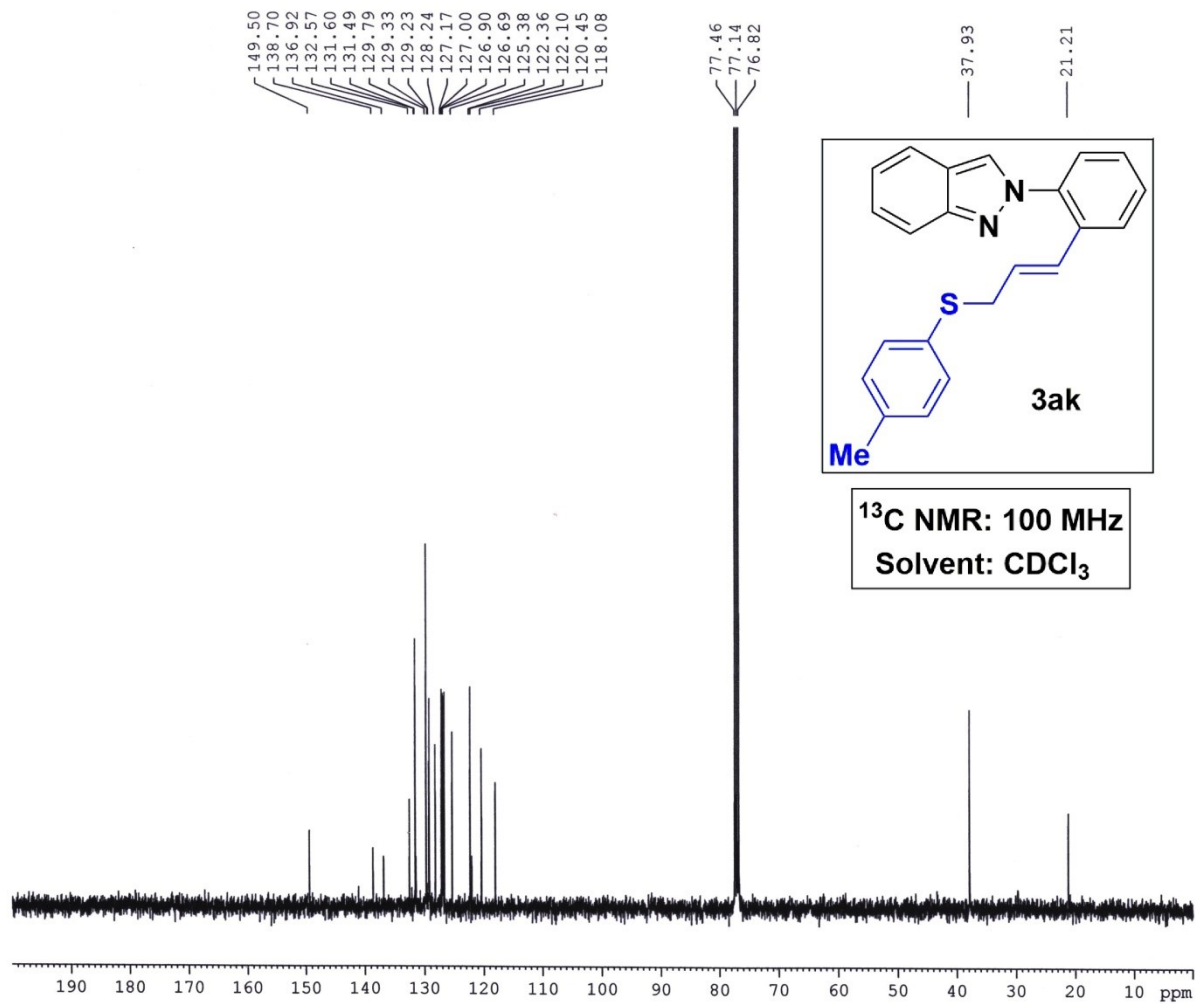
F2 - Acquisition Parameters  
Date\_ 20211121  
Time 15.49  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 450  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 168.31  
DW 20.800 usec  
DE 6.50 usec  
TE 296.6 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W

===== CHANNEL f2 =====  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

F2 - Processing parameters  
SI 16384  
SF 100.6177858 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 465  
 PROCNO 1

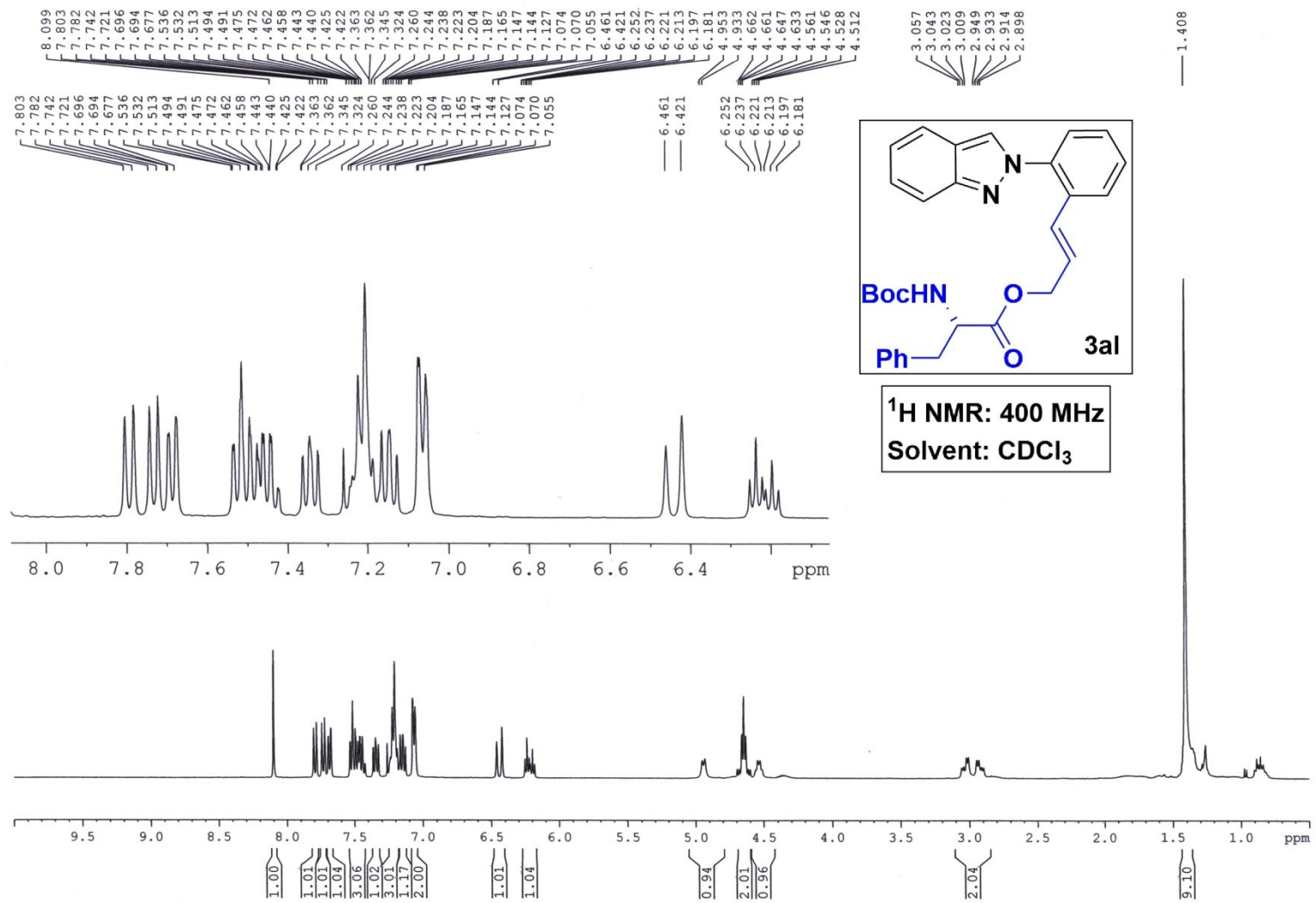
F2 - Acquisition Parameters  
 Date\_ 20211128  
 Time 20.54  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 300  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 135.7  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

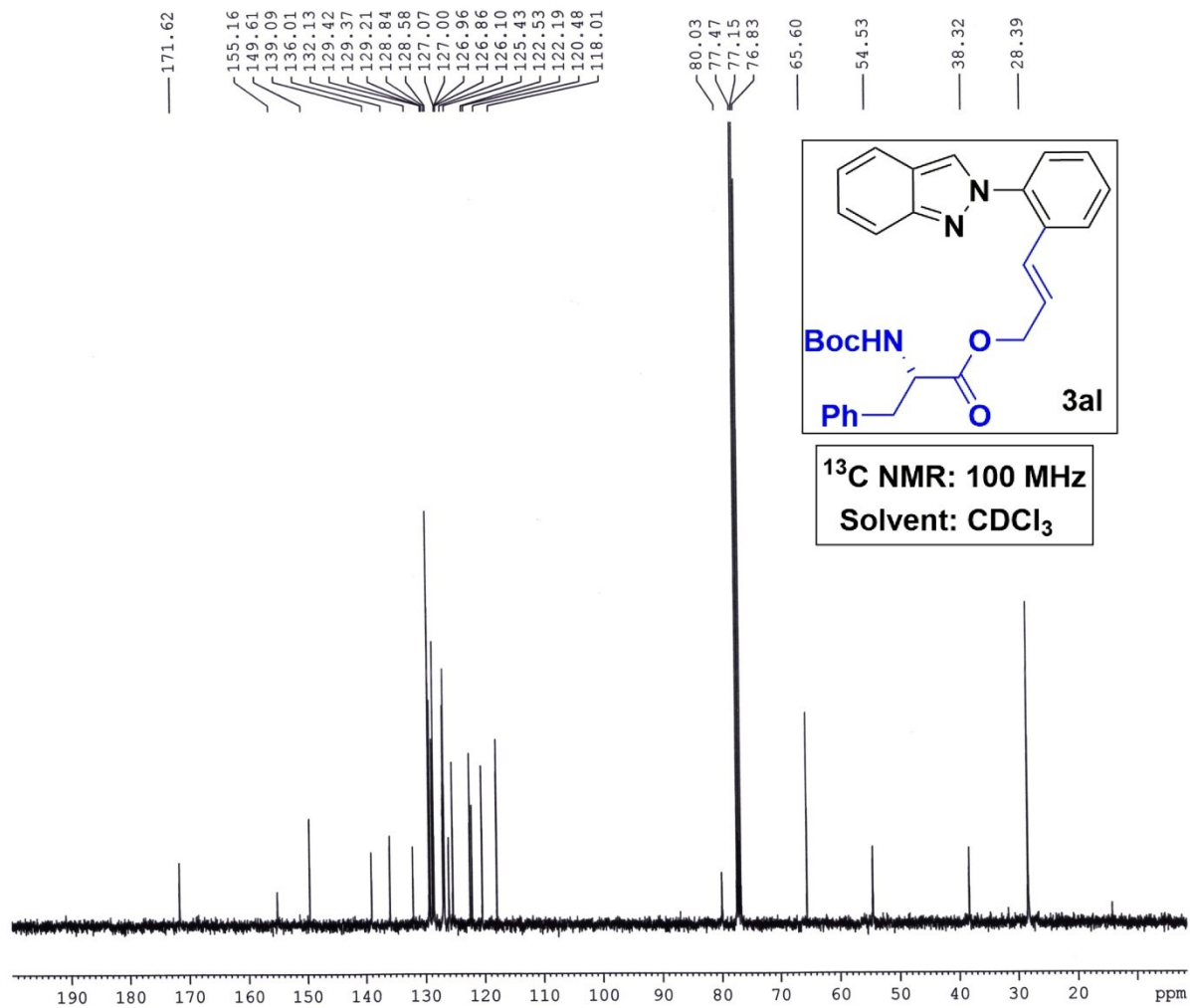
----- CHANNEL f1 -----  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177867 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40







171.62  
155.16  
149.61  
139.09  
136.01  
132.13  
129.42  
129.37  
129.21  
128.84  
128.58  
127.07  
127.00  
126.96  
126.86  
126.10  
125.43  
122.53  
122.19  
120.48  
118.01

80.03  
77.47  
77.15  
76.83  
65.60  
54.53  
38.32  
28.39

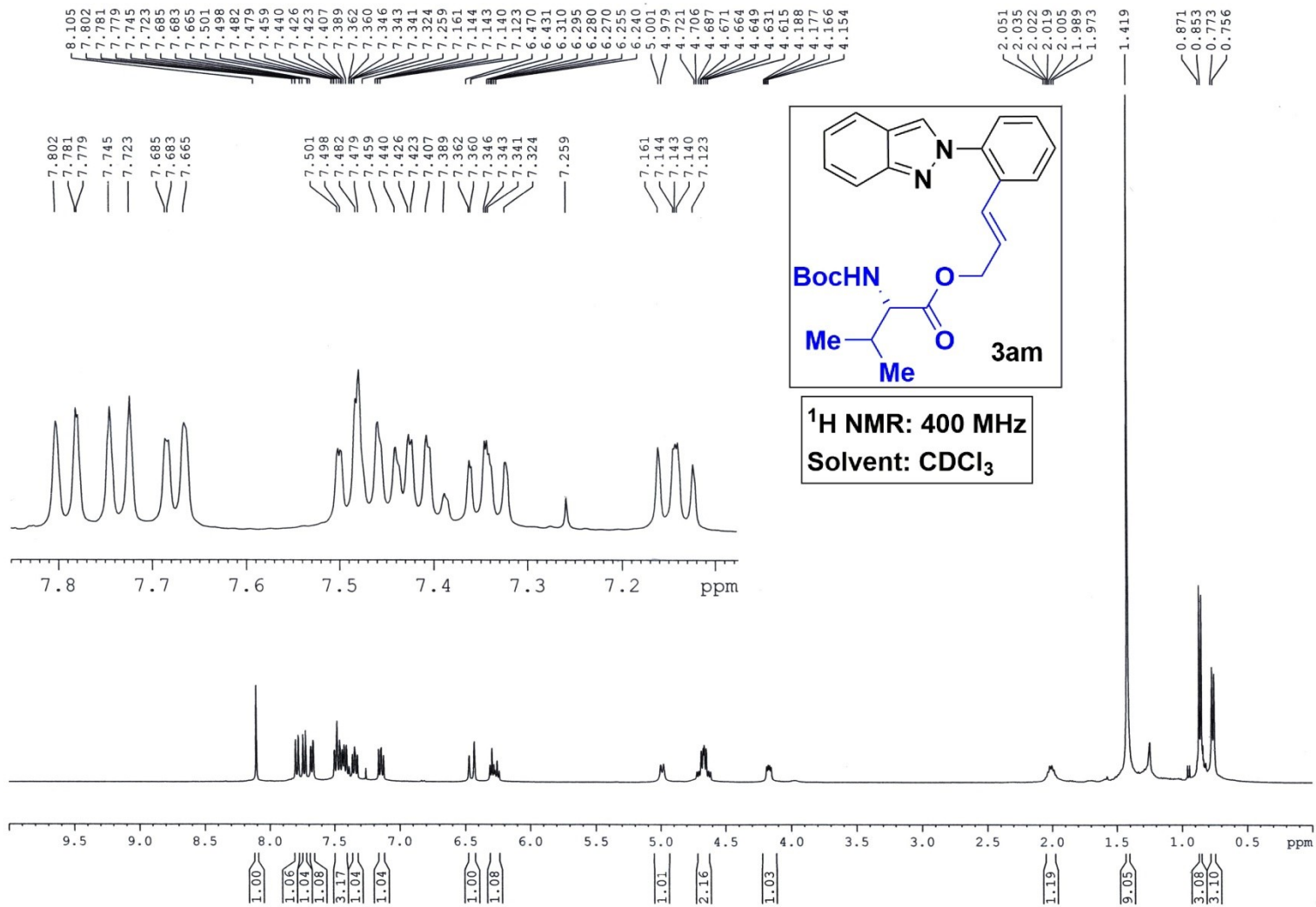
Current Data Parameters  
NAME Dr. A HAJRA-2021-13C  
EXPNO 462  
PROCNO 1

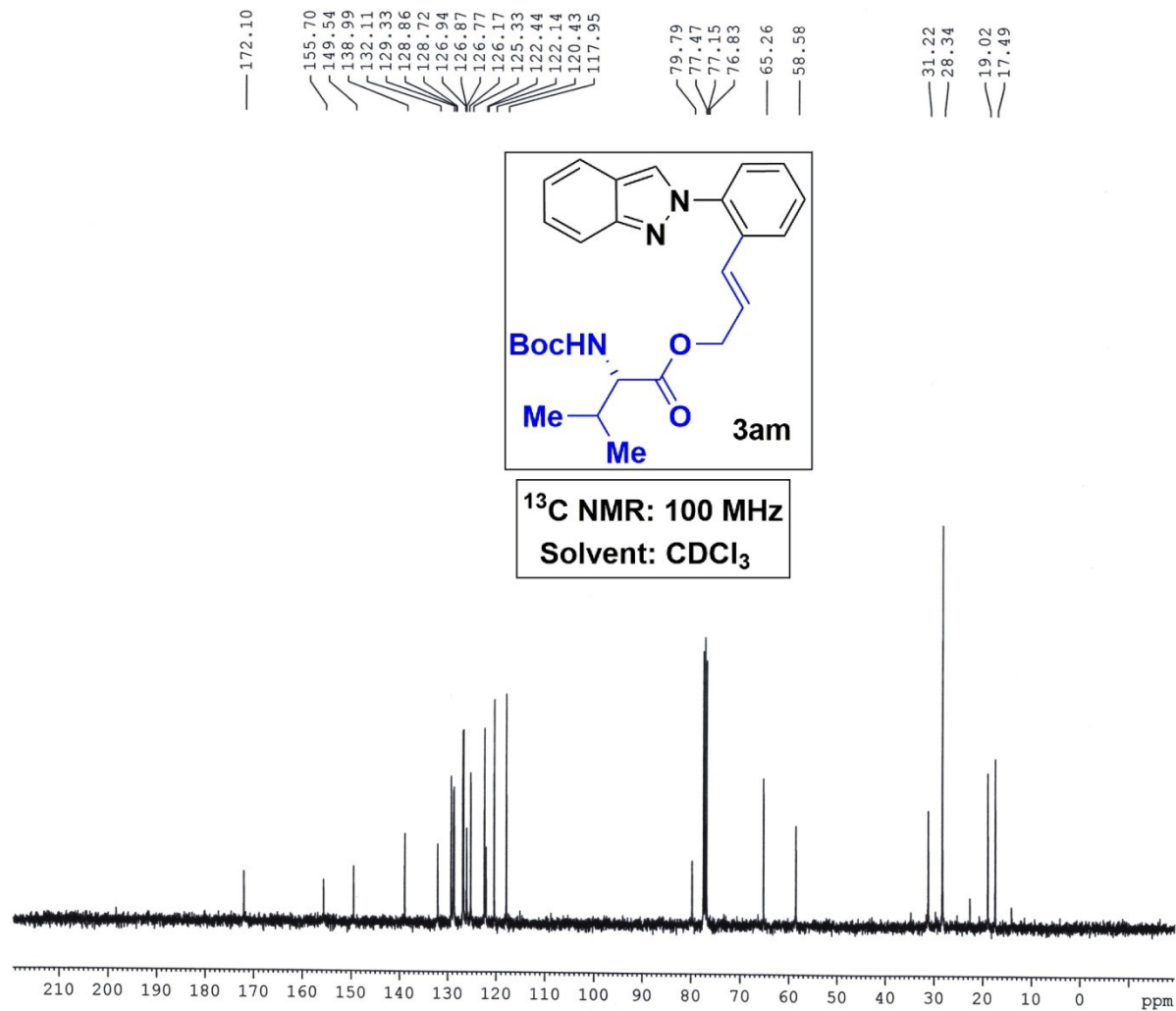
F2 - Acquisition Parameters  
Date\_ 20211128  
Time 18.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 285  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 62.69  
DW 20.800 usec  
DE 6.50 usec  
TE 297.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W

===== CHANNEL f2 =====  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

F2 - Processing parameters  
SI 16384  
SF 100.6177889 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





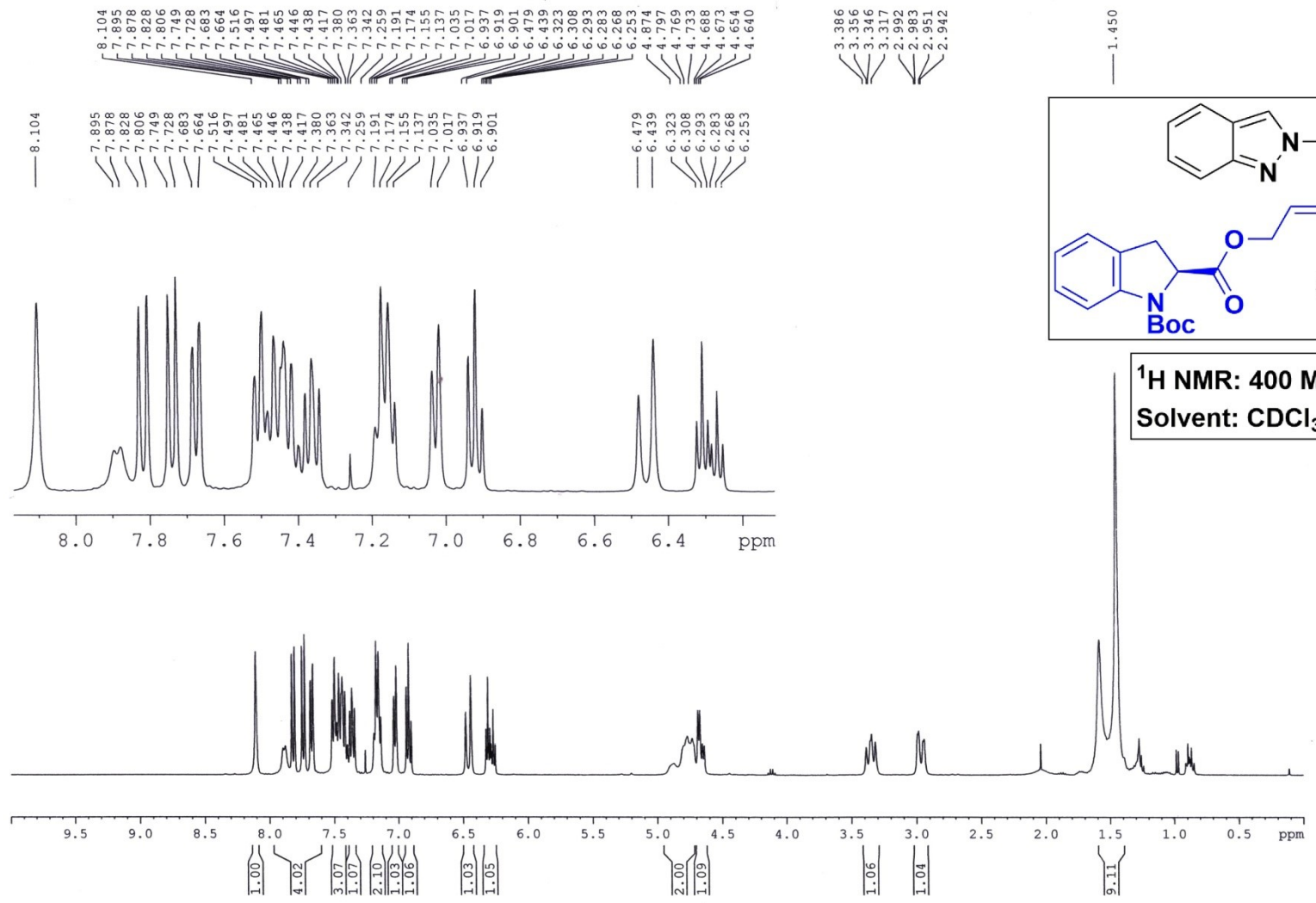
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 505  
 PROCNO 1

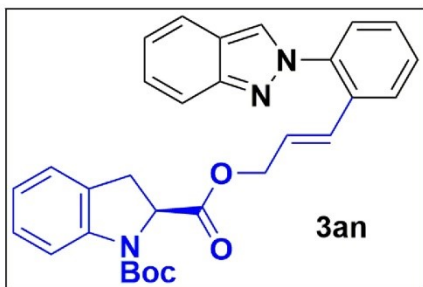
F2 - Acquisition Parameters  
 Date 20211226  
 Time 13.11  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 80  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 20.64  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

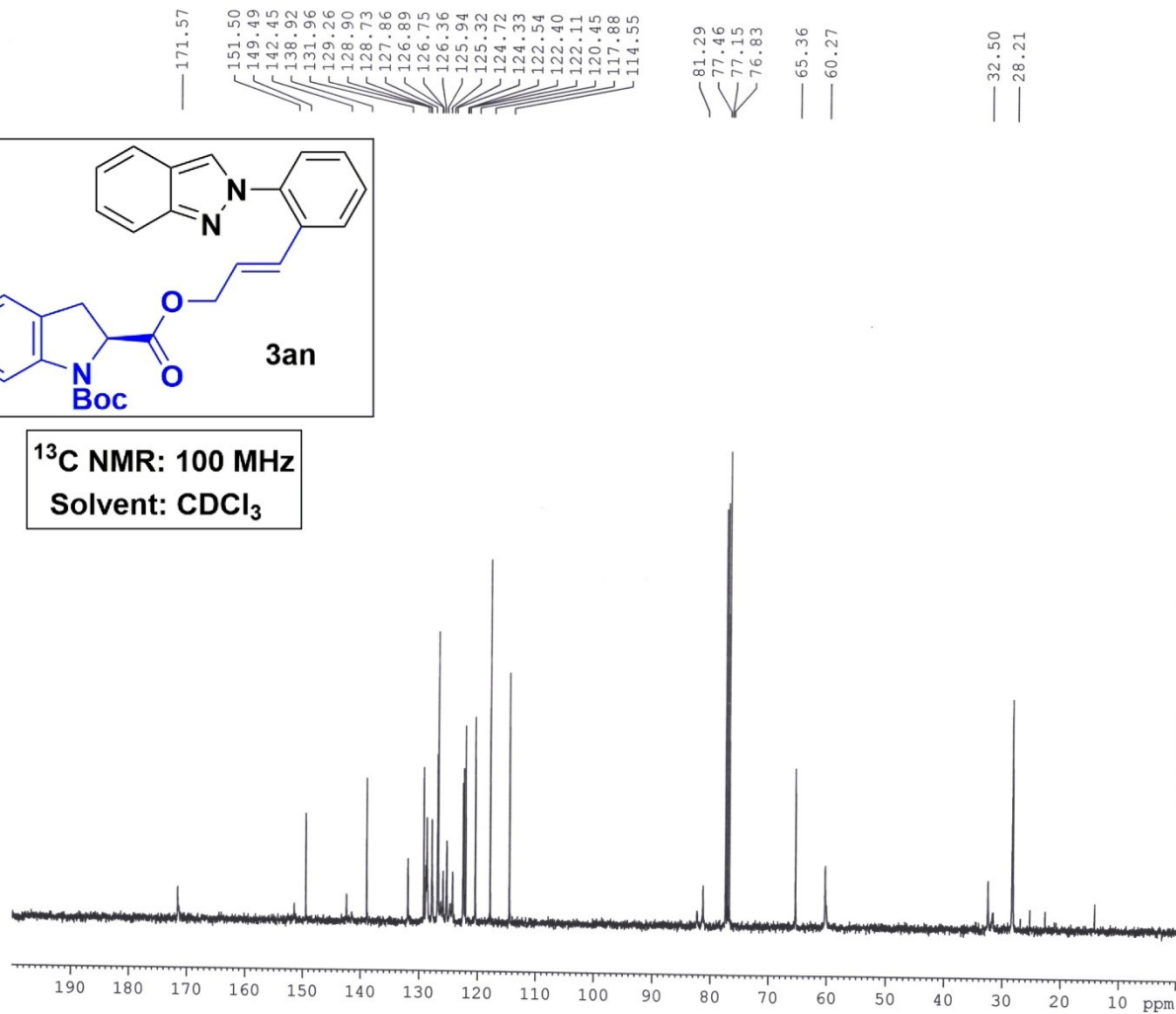
===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177947 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





**<sup>13</sup>C NMR: 100 MHz**  
**Solvent: CDCl<sub>3</sub>**



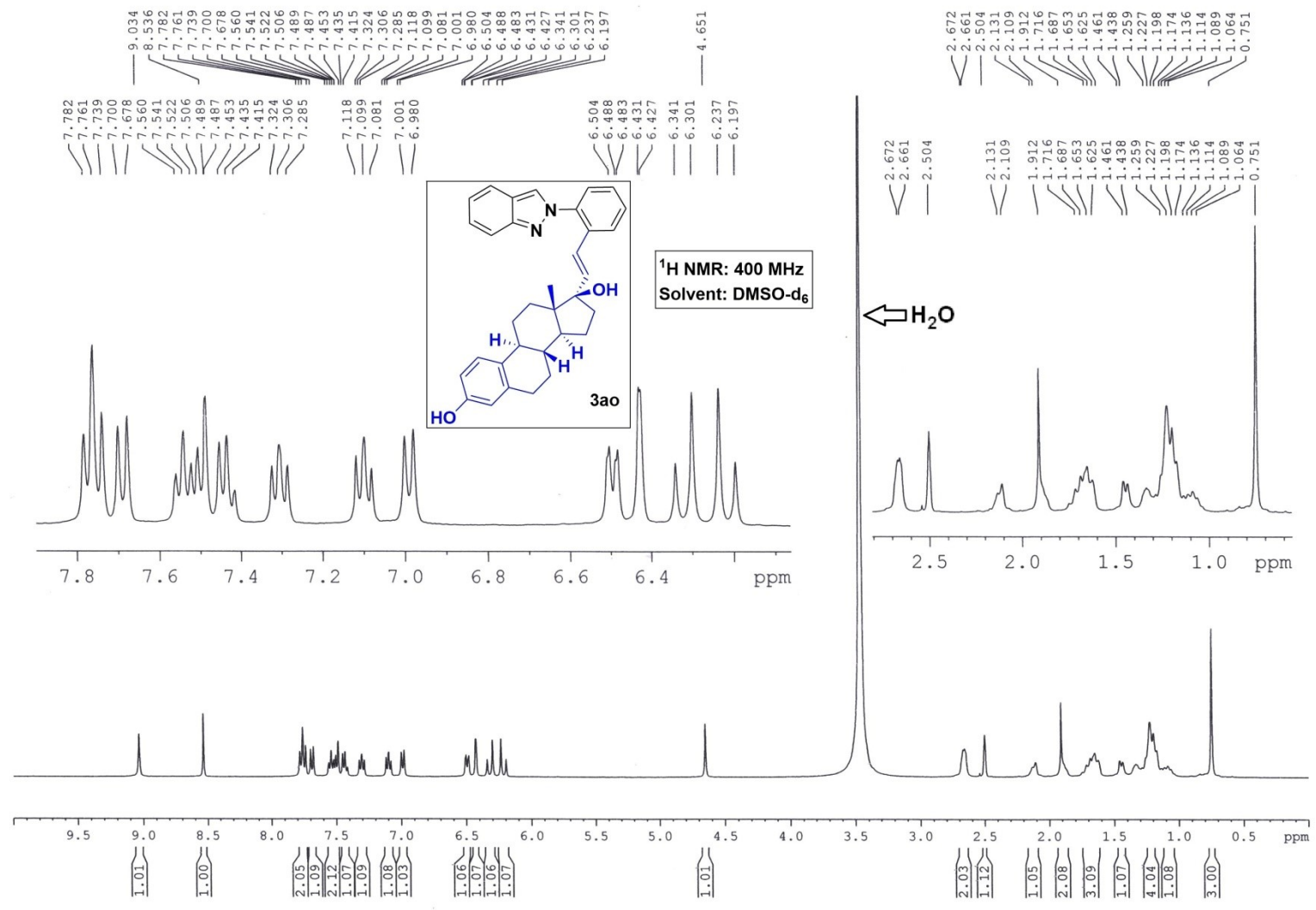
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 480  
 PROCNO 1

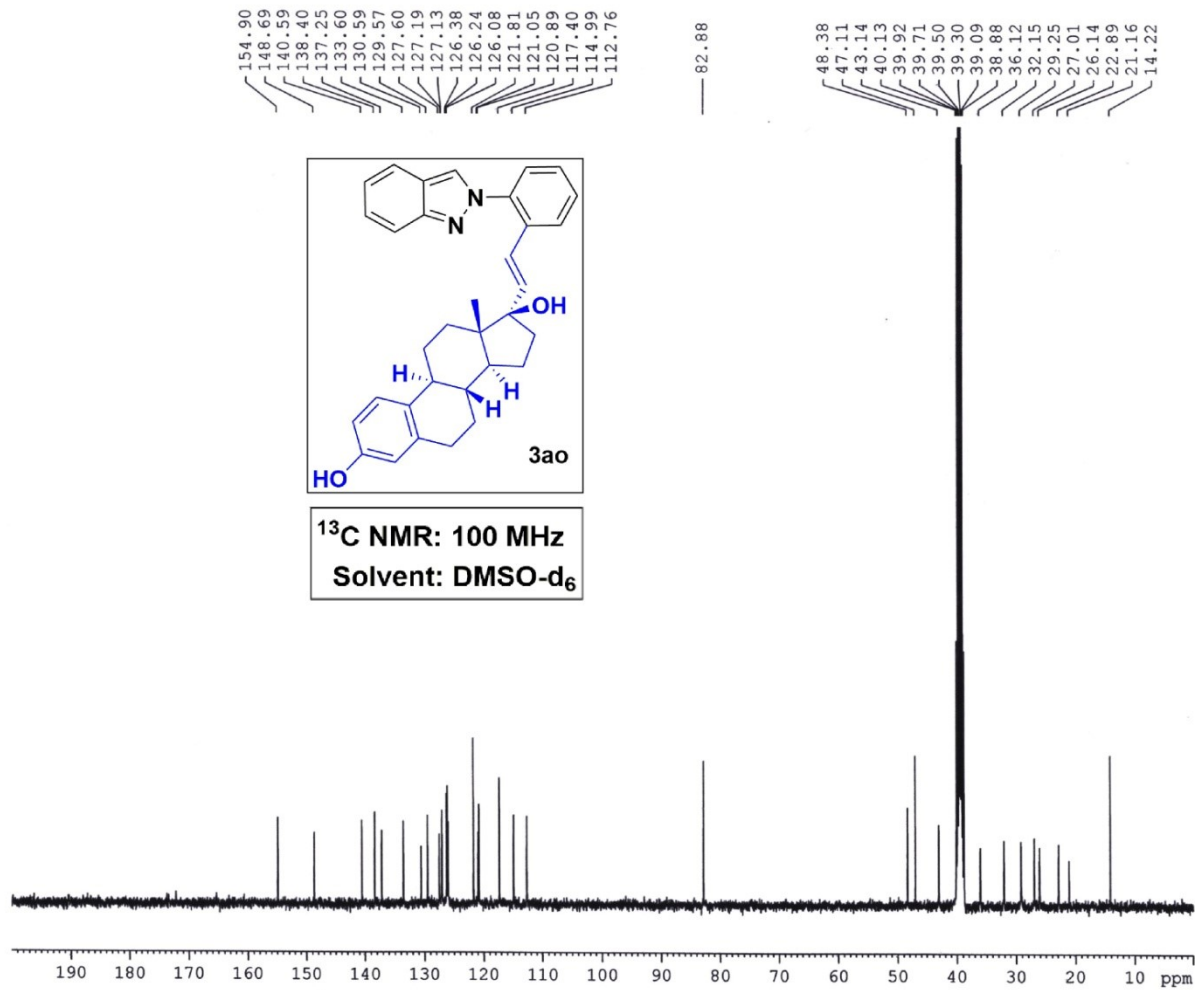
F2 - Acquisition Parameters  
 Date 20211208  
 Time 10.32  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 220  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 20.64  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.3 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 F1 8.90 usec  
 PLW1 54.0000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6178020 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





Current Data Parameters  
NAME Dr. A HAJRA-2021-13C  
EXPNO 470  
PROCNO 1

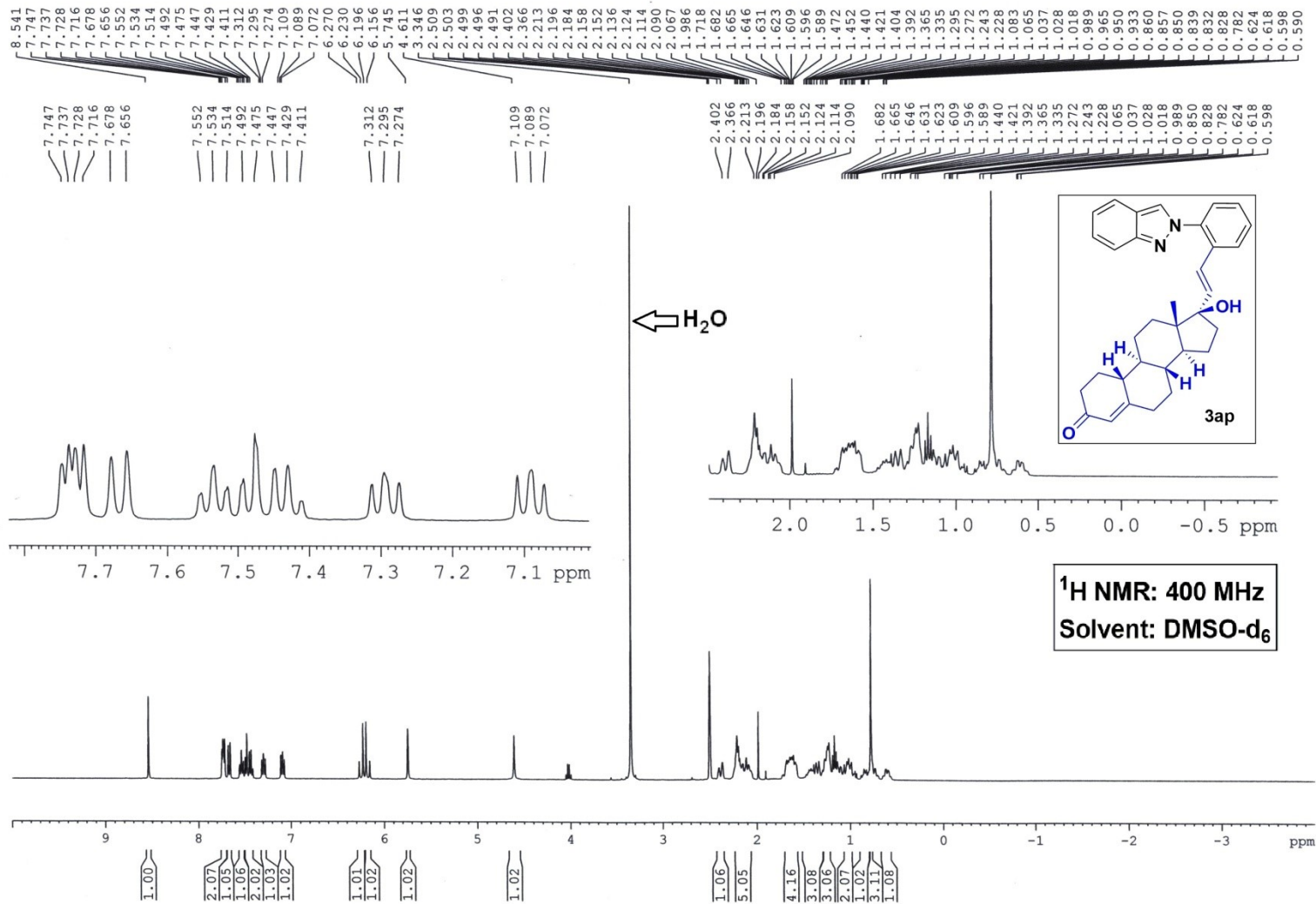
F2 - Acquisition Parameters  
Date\_ 20211201  
Time 15.13  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT DMSO  
NS 720  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 32.25  
DW 20.800 usec  
DE 6.50 usec  
TE 295.2 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

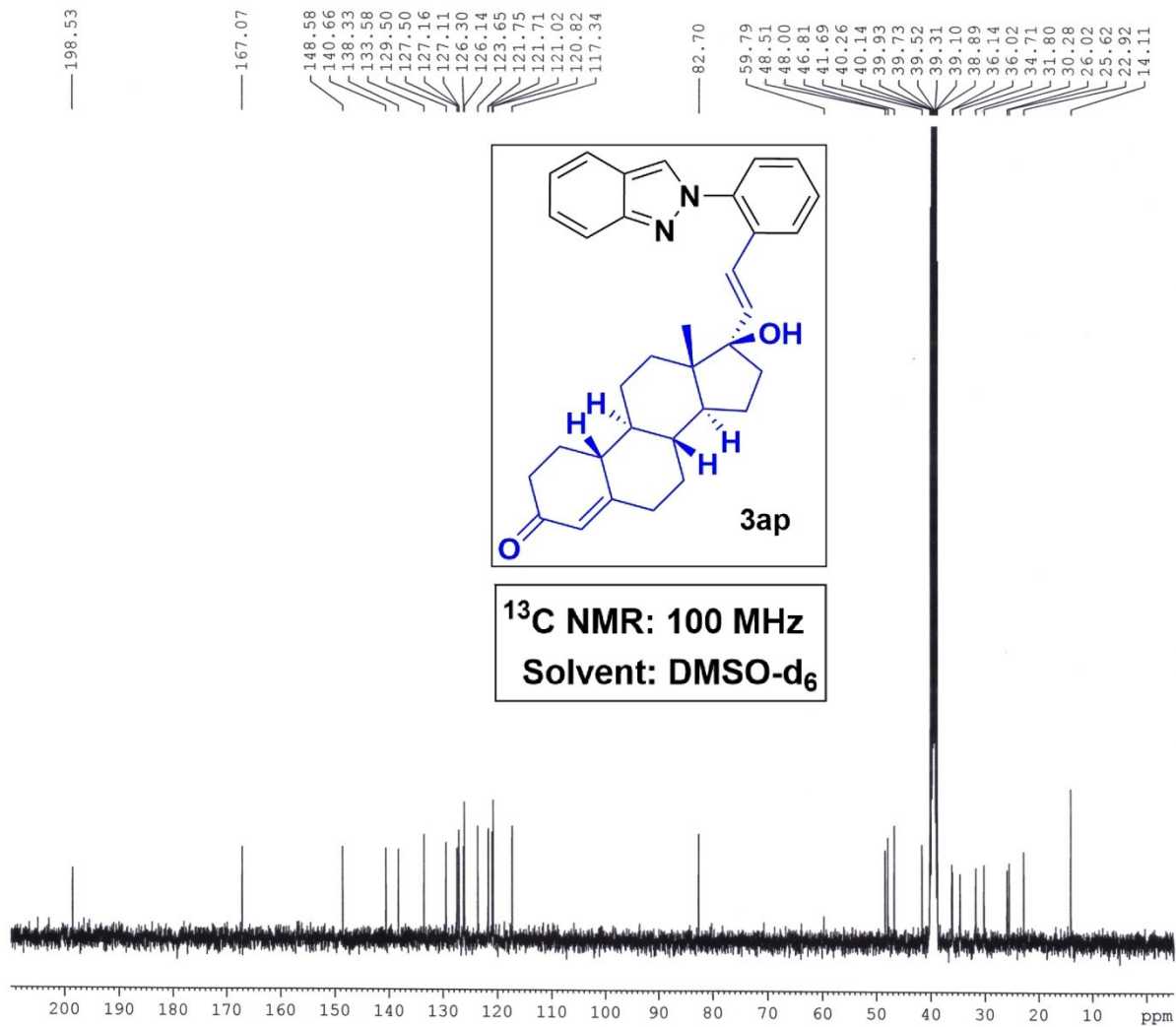
----- CHANNEL f1 -----  
SF01 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W

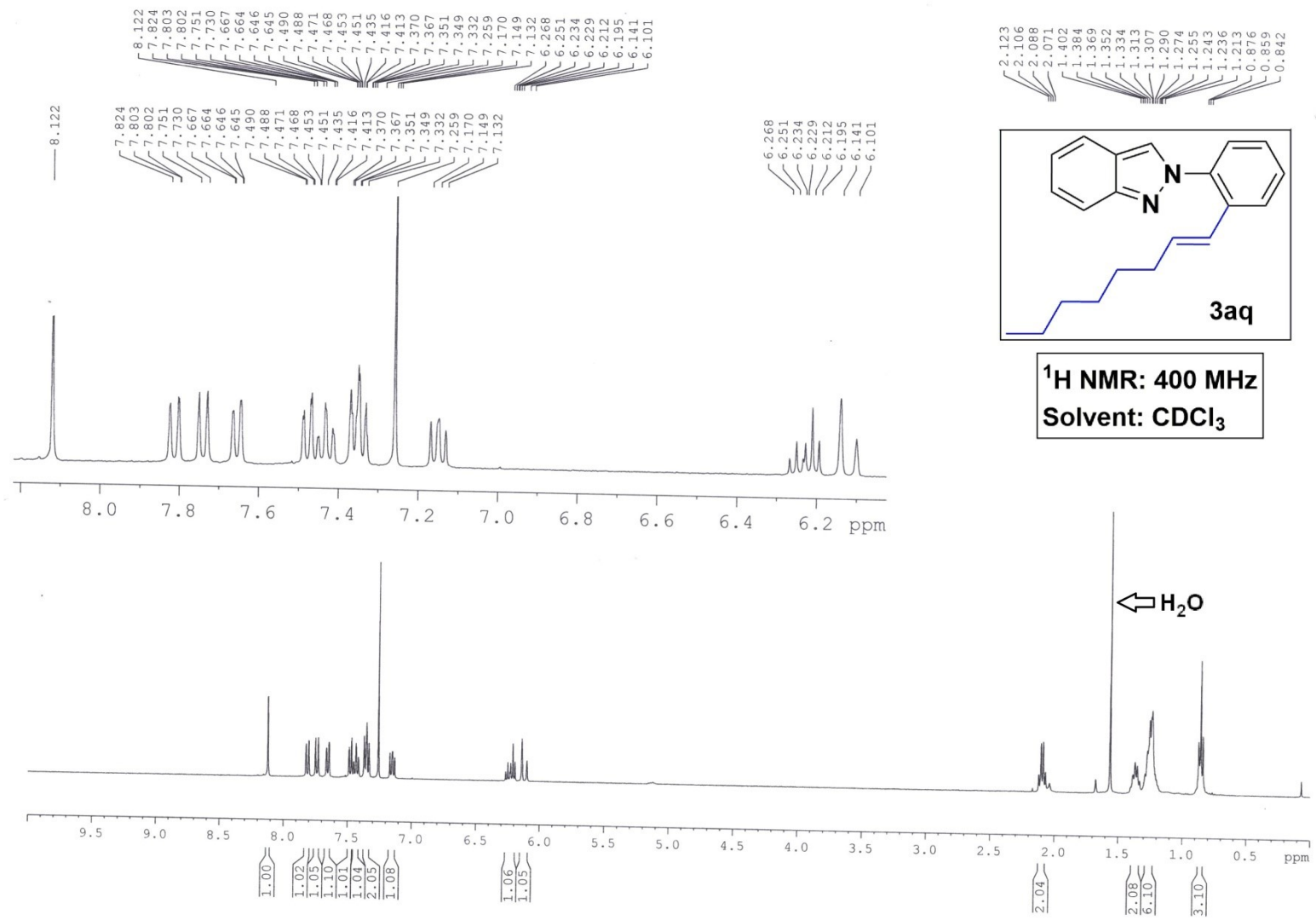
----- CHANNEL f2 -----  
SF02 400.1516006 MHz  
NUC2 1H  
PCPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

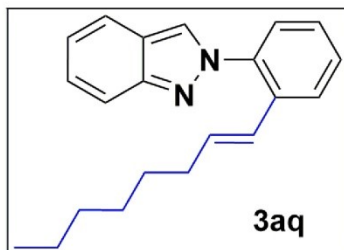
F2 - Processing parameters  
SI 16384  
SF 100.6178342 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40









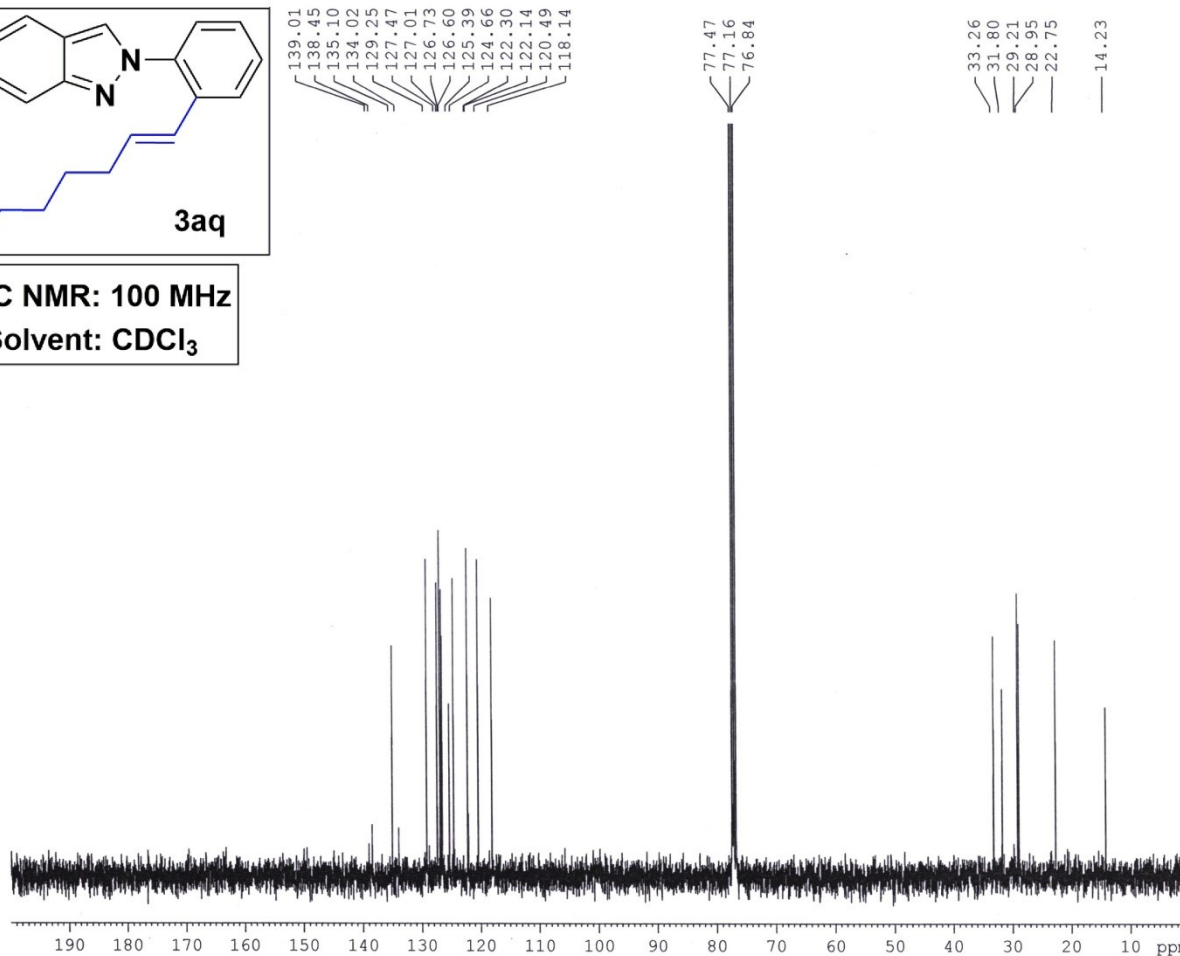


**<sup>13</sup>C NMR: 100 MHz**  
**Solvent: CDCl<sub>3</sub>**

139.01  
 138.45  
 135.10  
 134.02  
 129.25  
 127.47  
 127.01  
 126.73  
 126.60  
 125.39  
 124.66  
 122.30  
 122.14  
 120.49  
 118.14

77.47  
 77.16  
 76.84

33.26  
 31.80  
 29.21  
 28.95  
 22.75  
 14.23



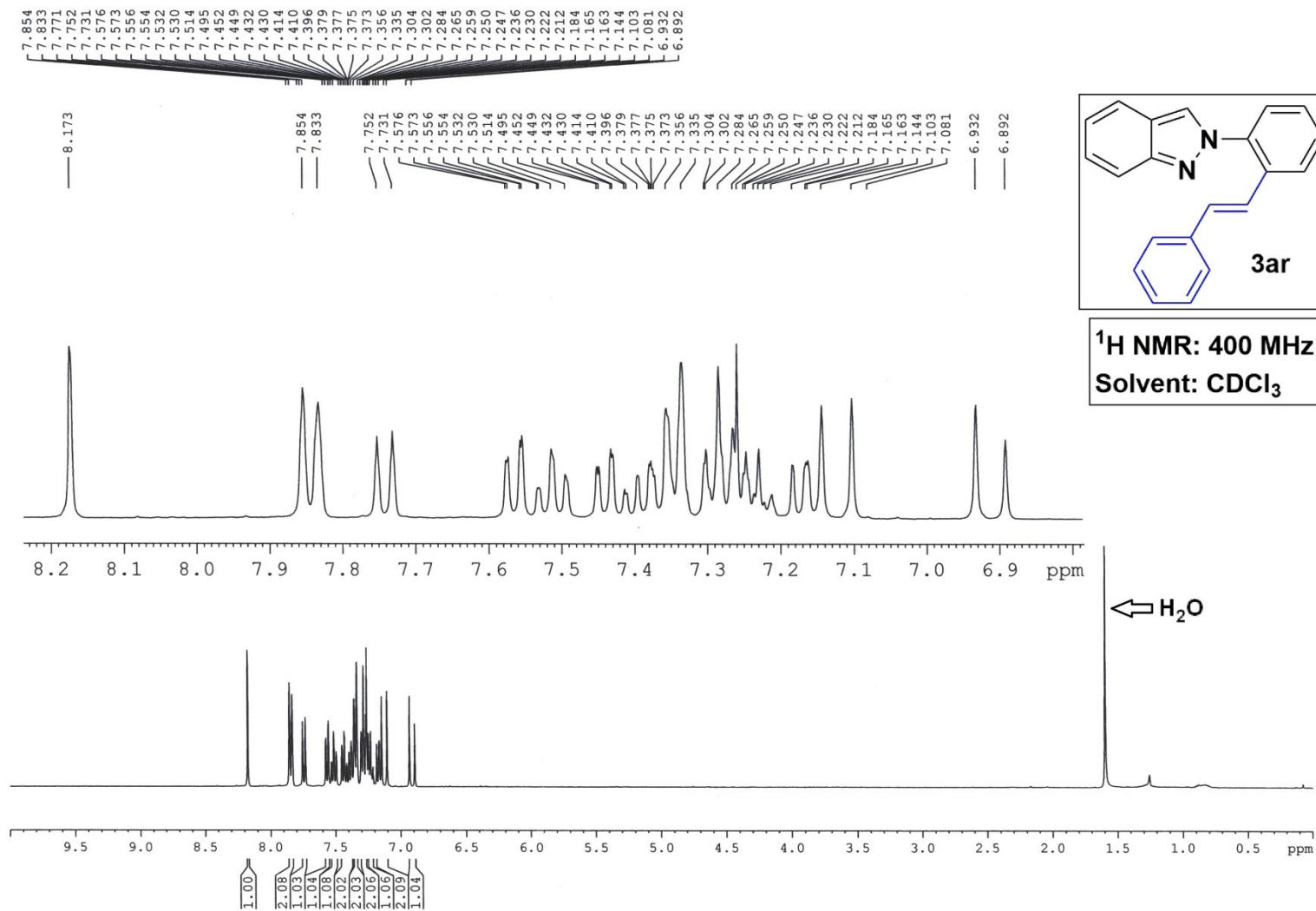
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 166  
 PROCNO 1

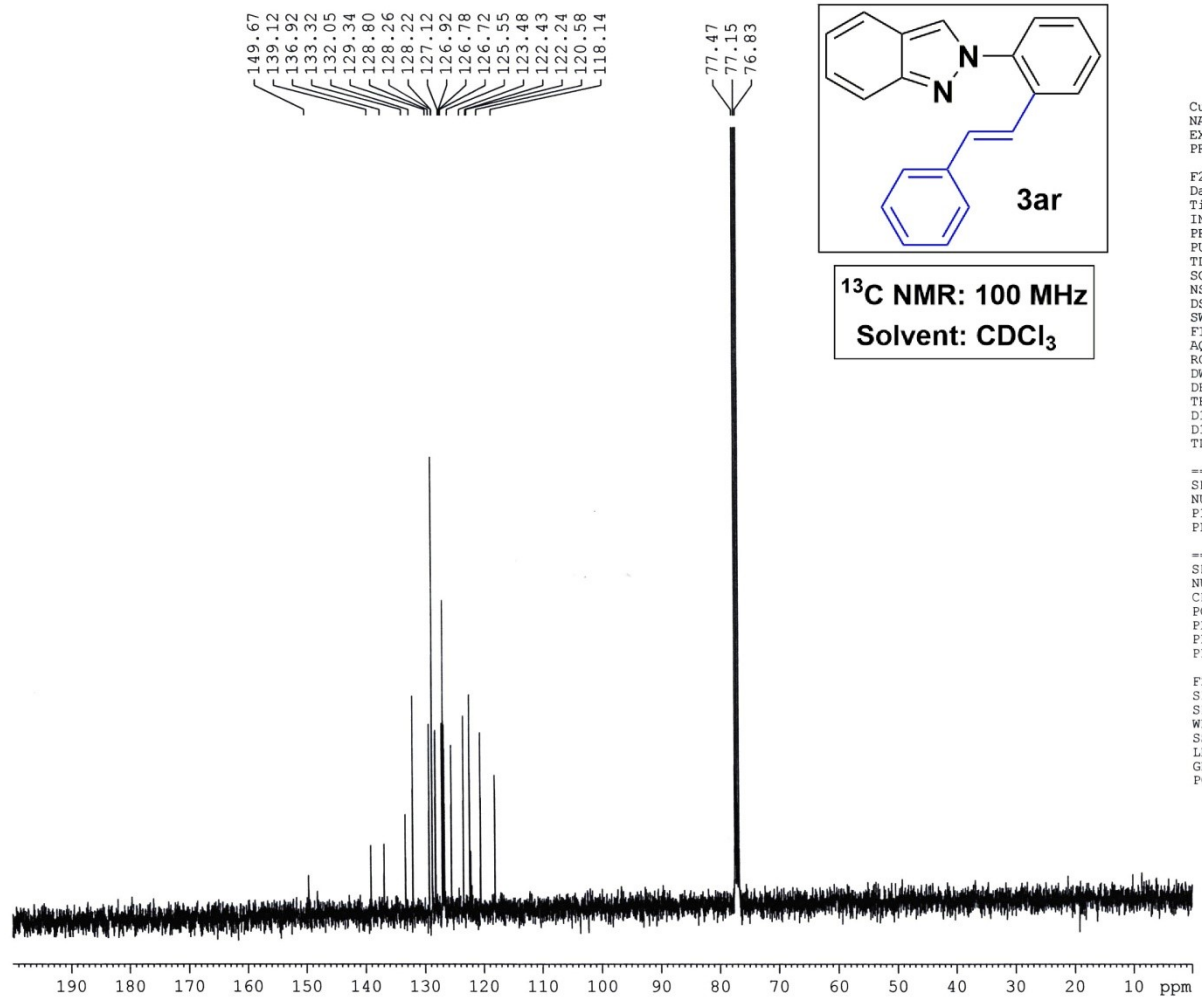
F2 - Acquisition Parameters  
 Date\_ 20210325  
 Time 12.06  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgdc  
 TD 32768  
 SOLVENT CDCl3  
 NS 880  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.5 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177830 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00





```

Current Data Parameters
NAME      Dr. A HAJRA-2021-13C
EXPNO    50
PROCNO   1

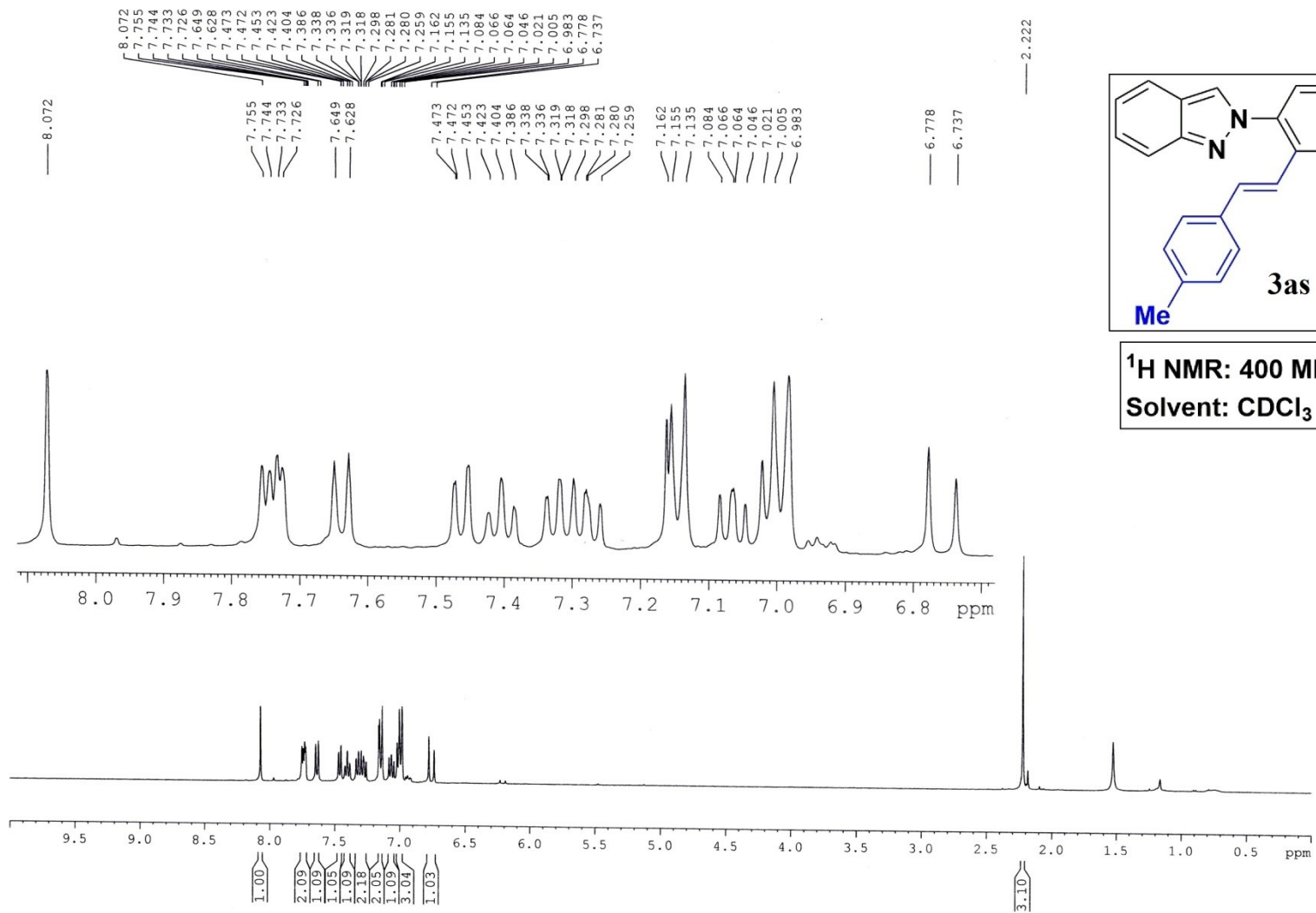
F2 - Acquisition Parameters
Date_    20210126
Time     21.12
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       32768
SOLVENT  CDCl3
NS       380
DS       2
SWH      24038.461 Hz
FIDRES   0.733596 Hz
AQ       0.6815744 sec
RG       186.42
DW       20.800 usec
DE       6.50 usec
TE       295.4 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1

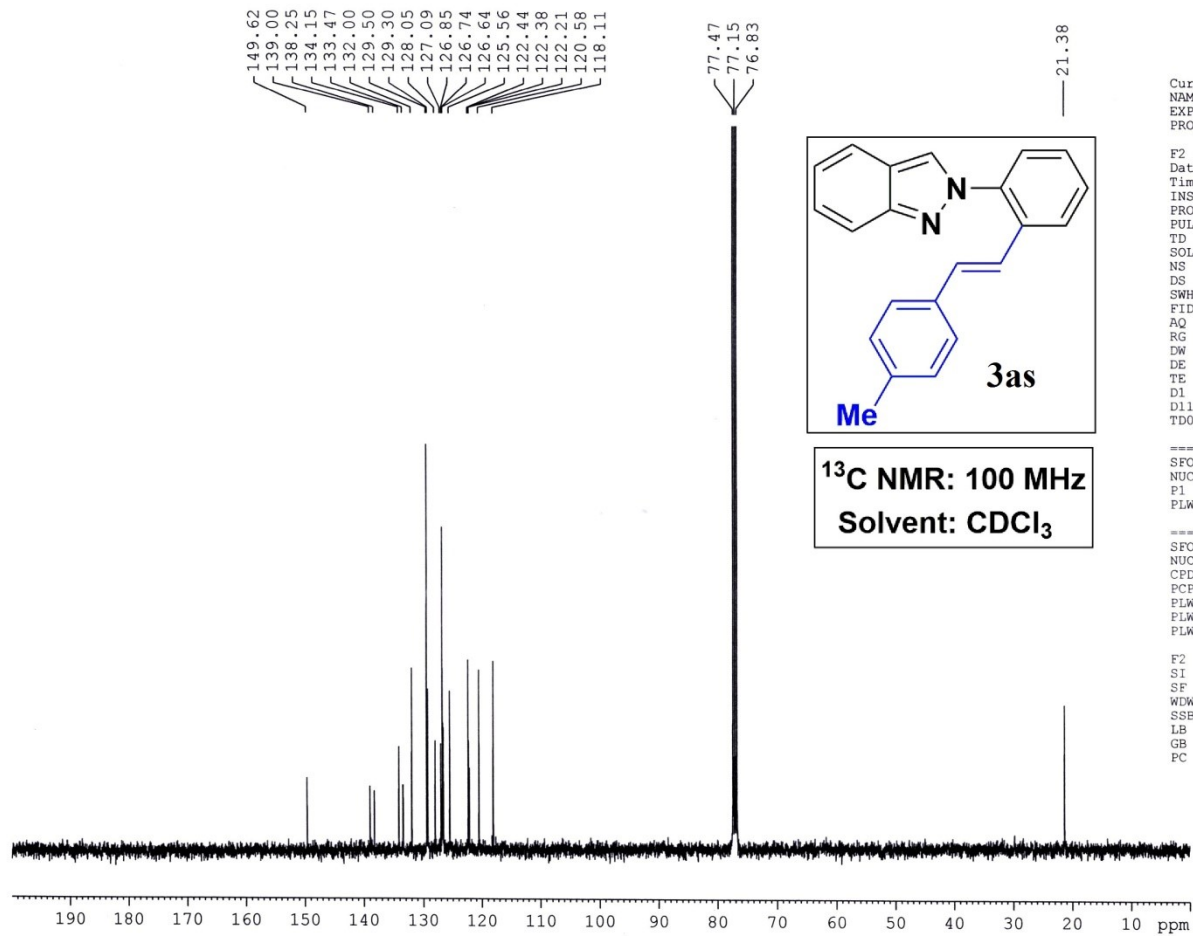
===== CHANNEL f1 =====
SFO1    100.6278588 MHz
NUC1     13C
P1       8.90 usec
PLW1    54.0000000 W

===== CHANNEL f2 =====
SFO2    400.1516006 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLW2    12.0000000 W
PLW12   0.32231000 W
PLW13   0.16212000 W

F2 - Processing parameters
SI       16384
SF       100.6177858 MHz
WW       EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

```





Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 88  
 PROCNO 1

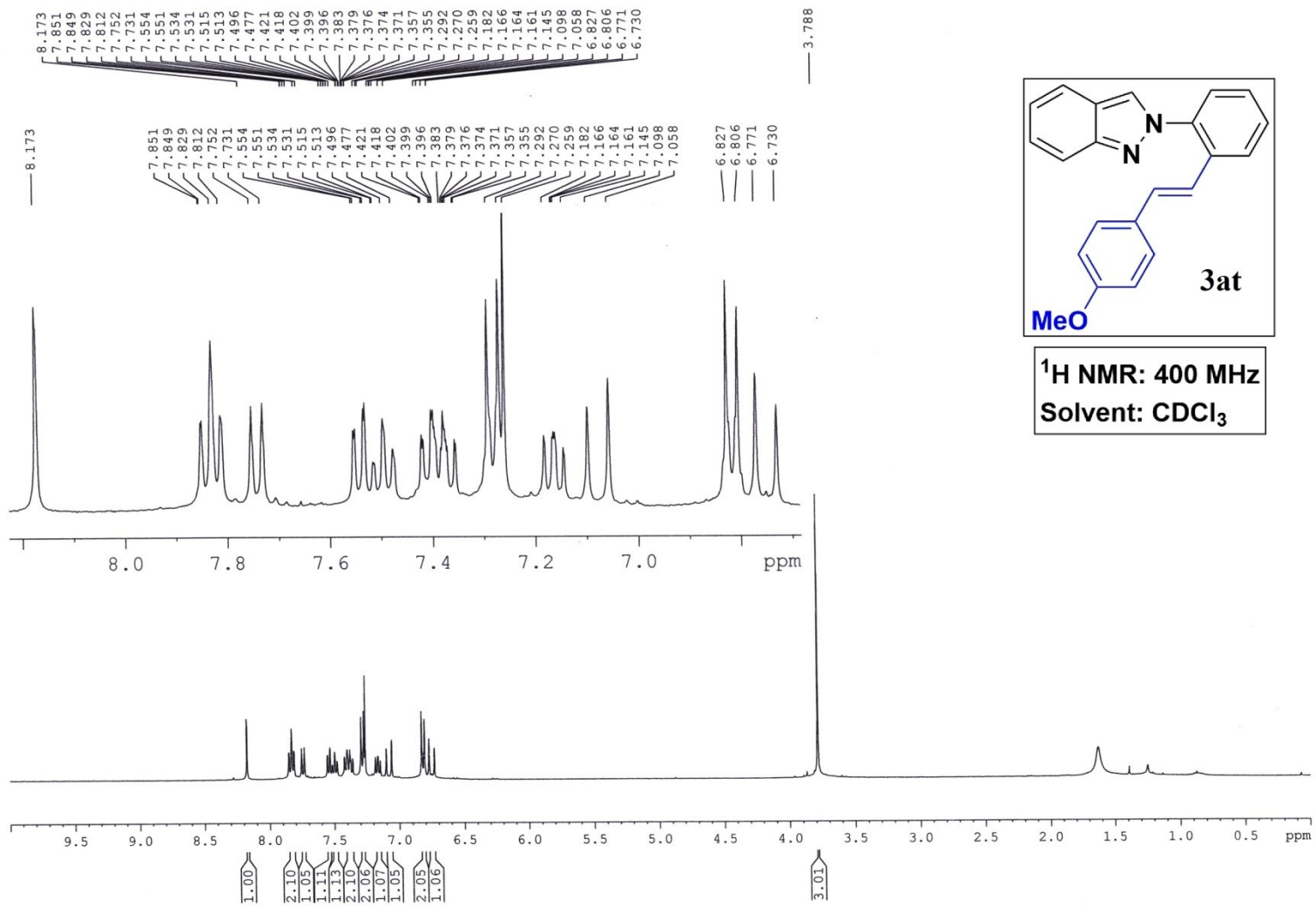
F2 - Acquisition Parameters  
 Date\_ 20210218  
 Time 0.44  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 512  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 120.16  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

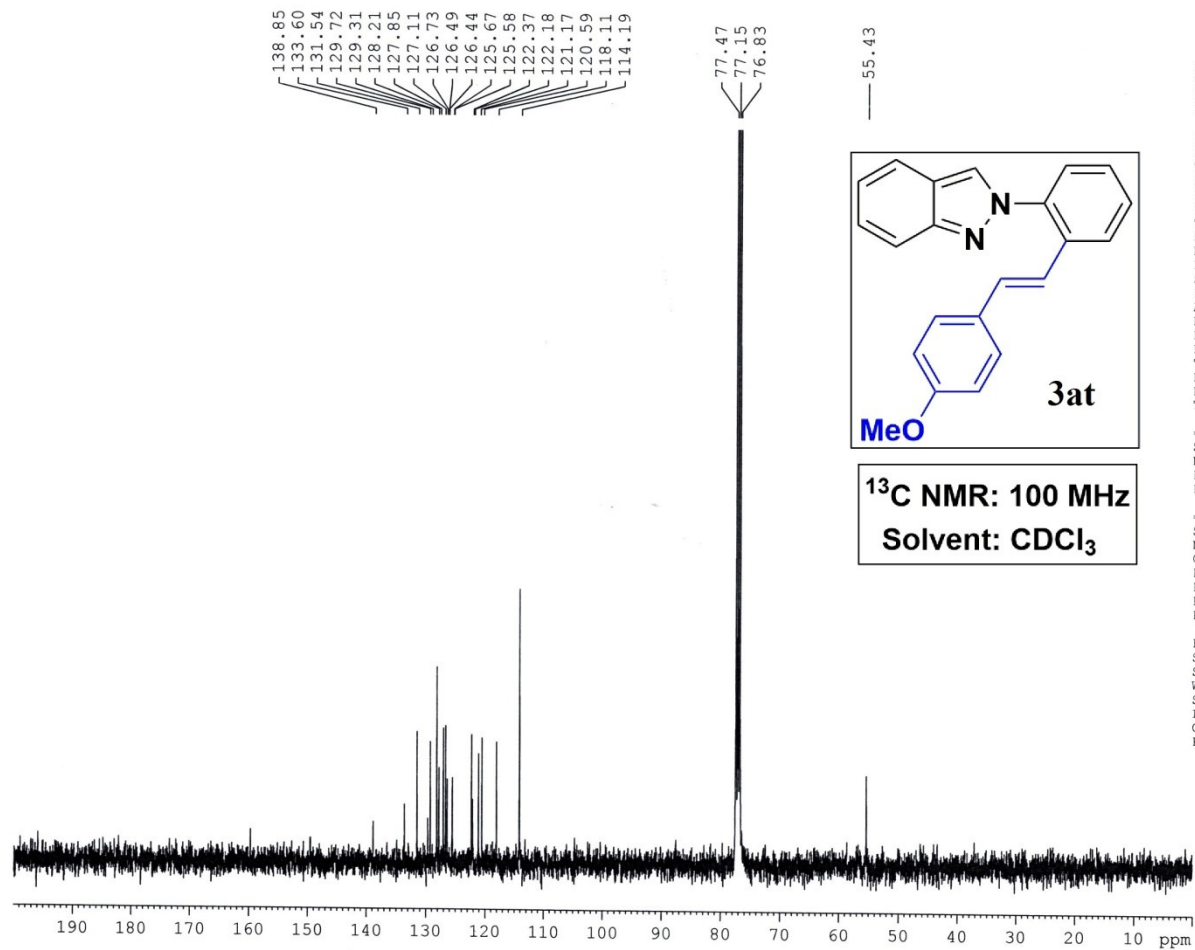
----- CHANNEL f1 -----  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

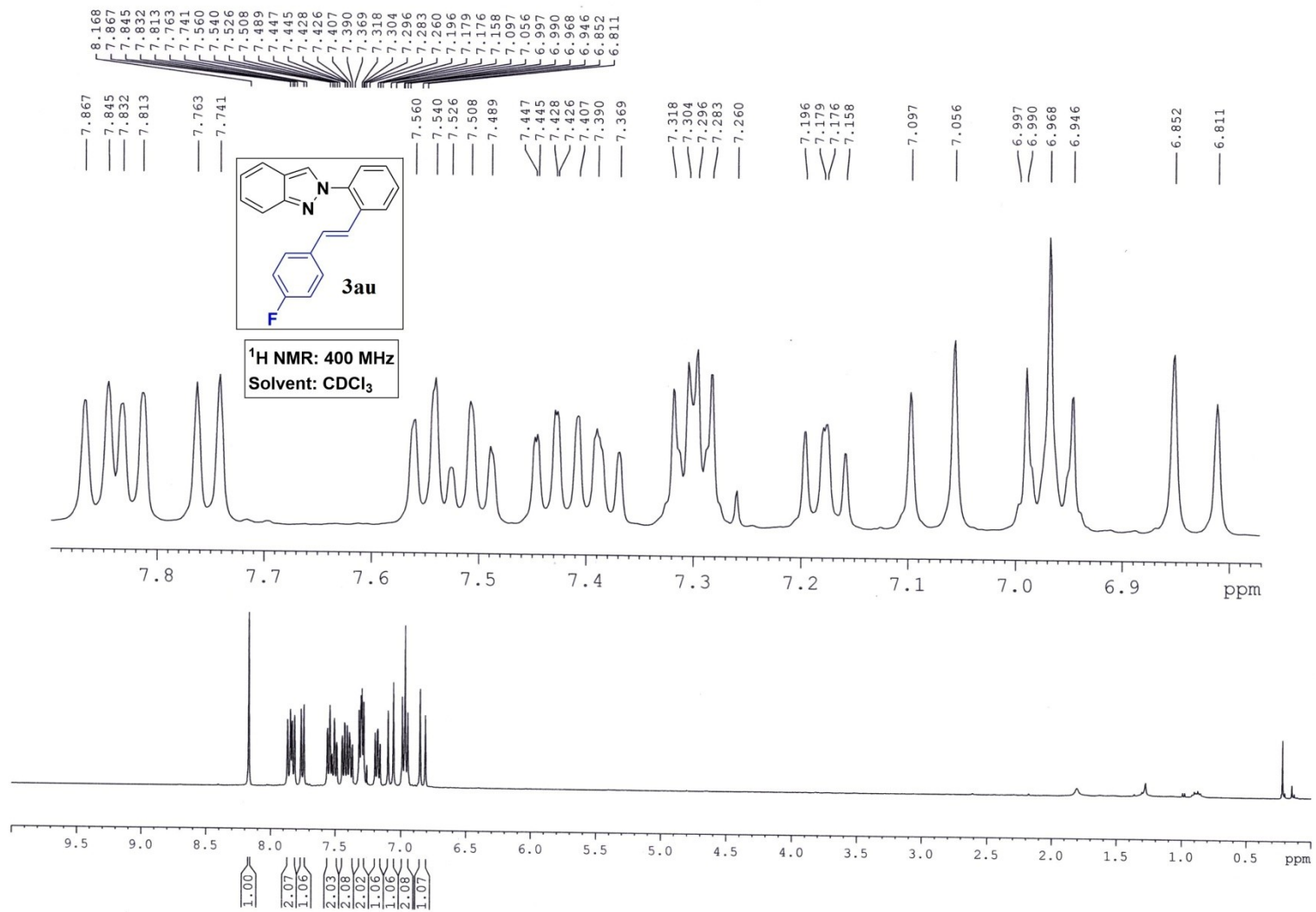
----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

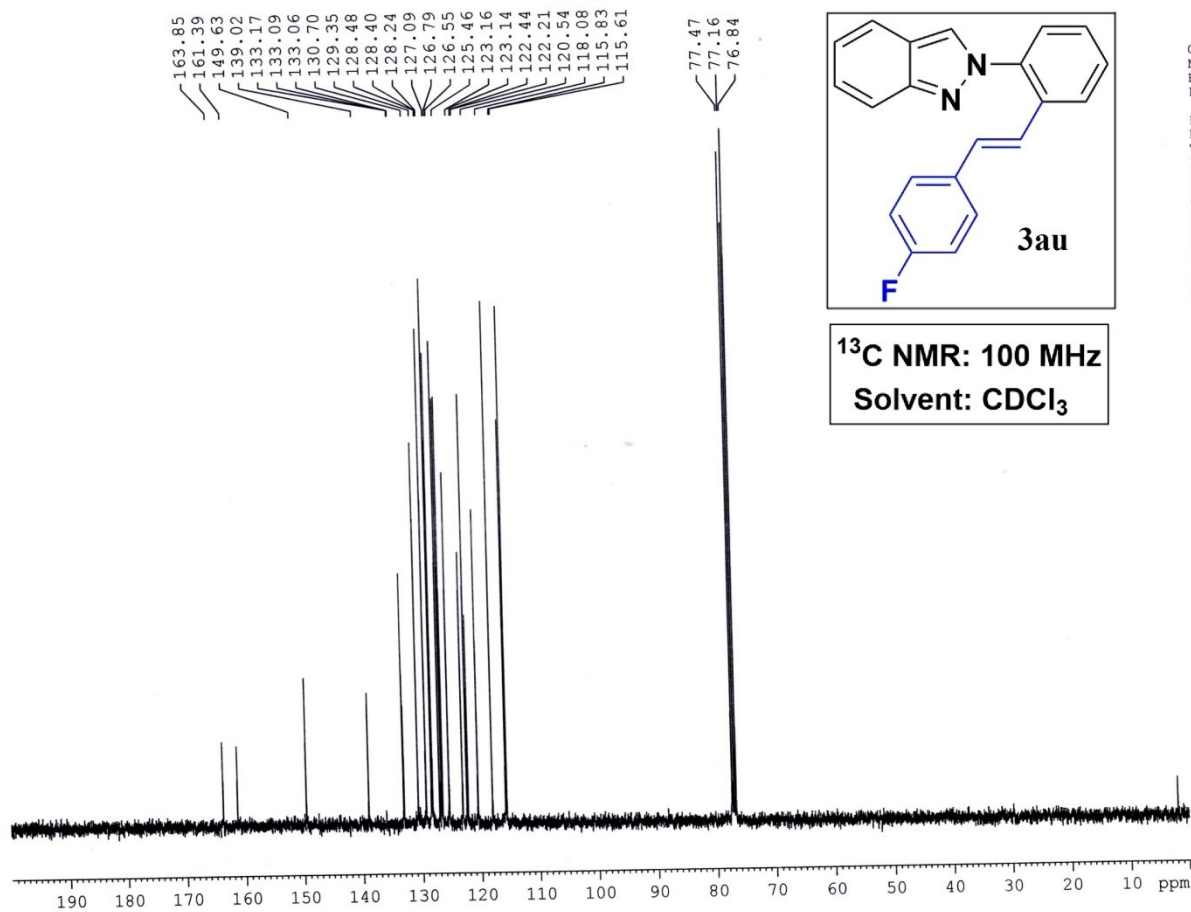
F2 - Processing parameters  
 SI 16384  
 SF 100.6177873 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40











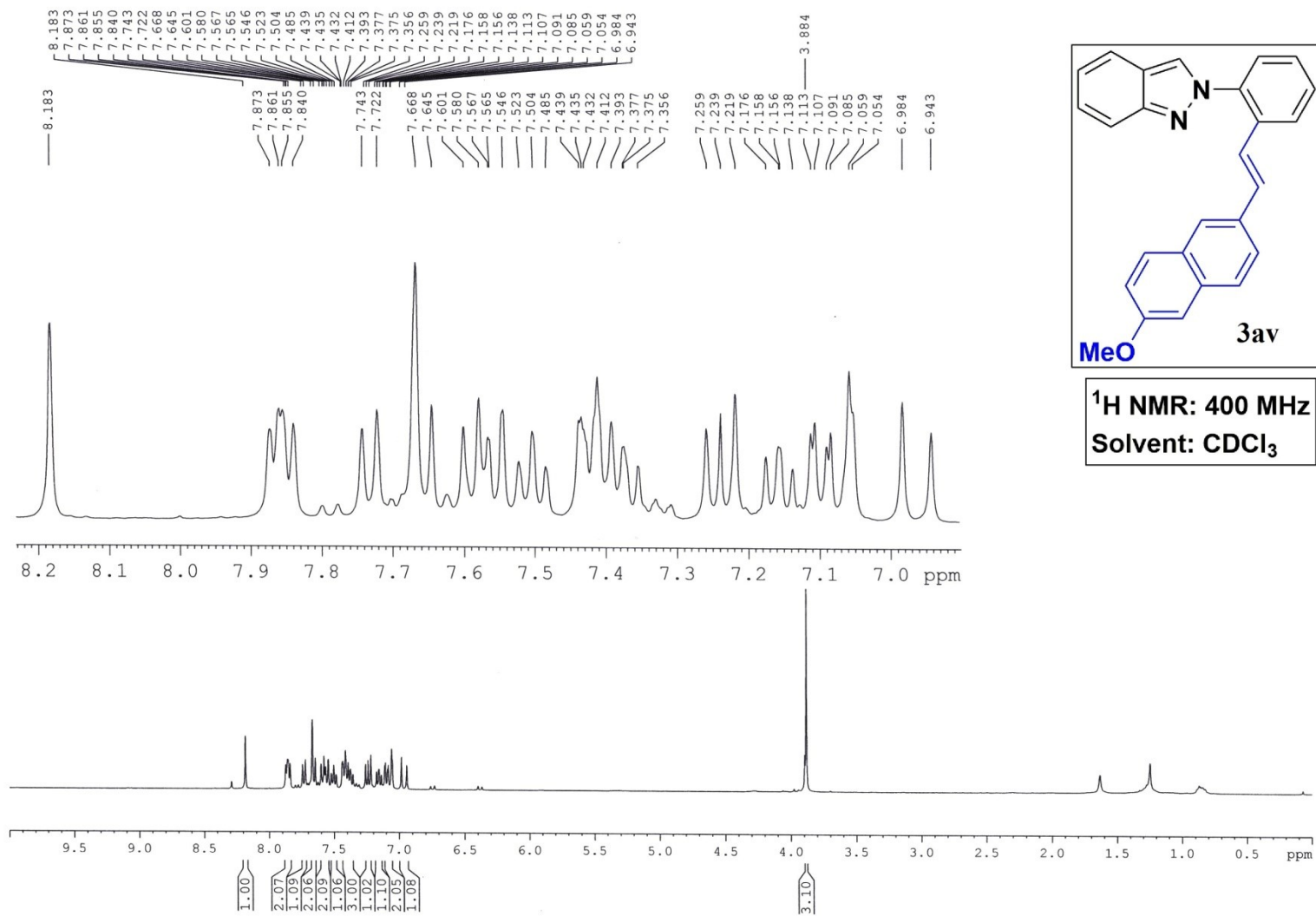
Current Data Parameters  
NAME Dr. A HAJRA-2021-13C  
EXPNO 69  
PROCNO 1

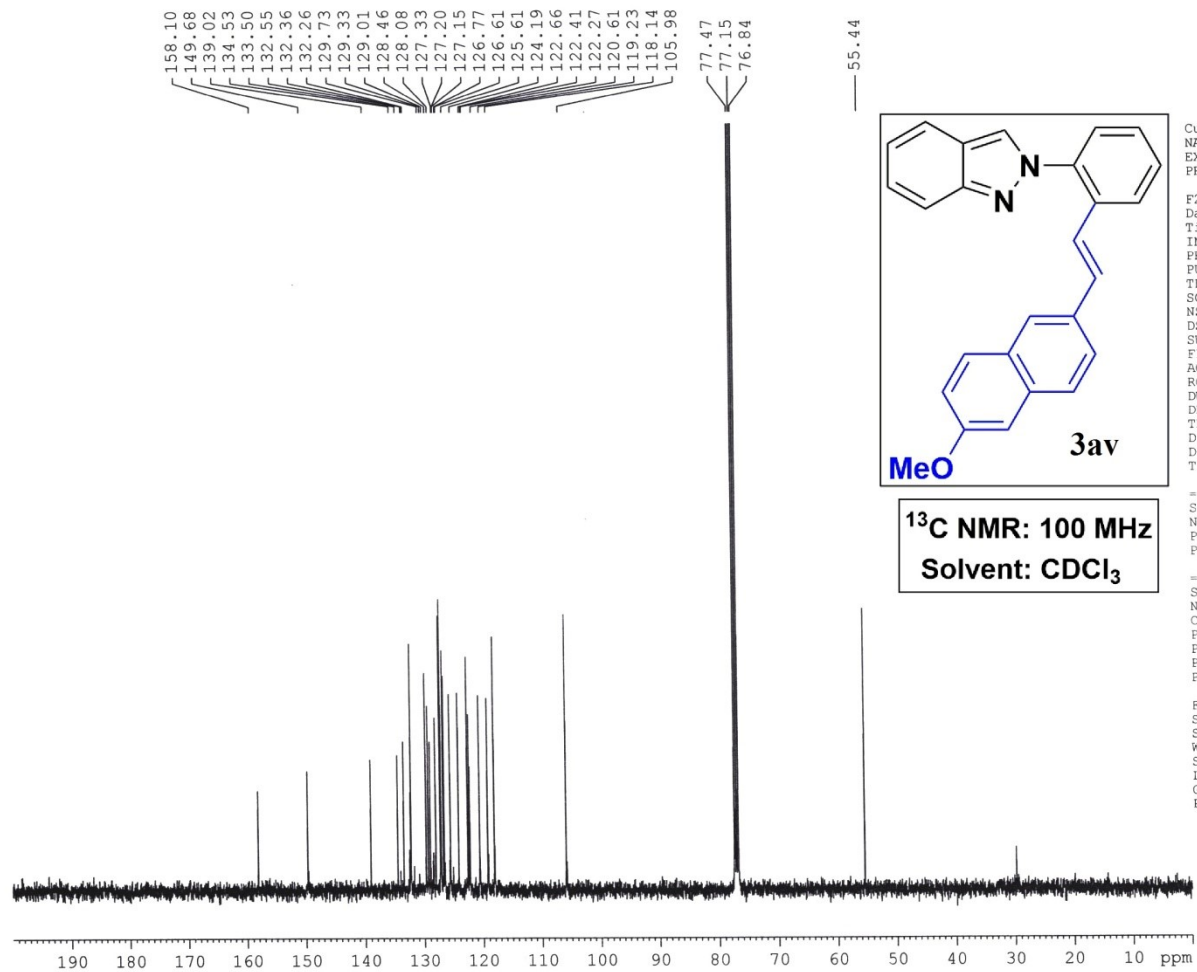
F2 - Acquisition Parameters  
Date\_ 20210209  
Time 23.49  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 220  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 57.28  
DW 20.800 usec  
DE 6.50 usec  
TE 293.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W

===== CHANNEL f2 =====  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

F2 - Processing parameters  
SI 16384  
SF 100.6177922 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





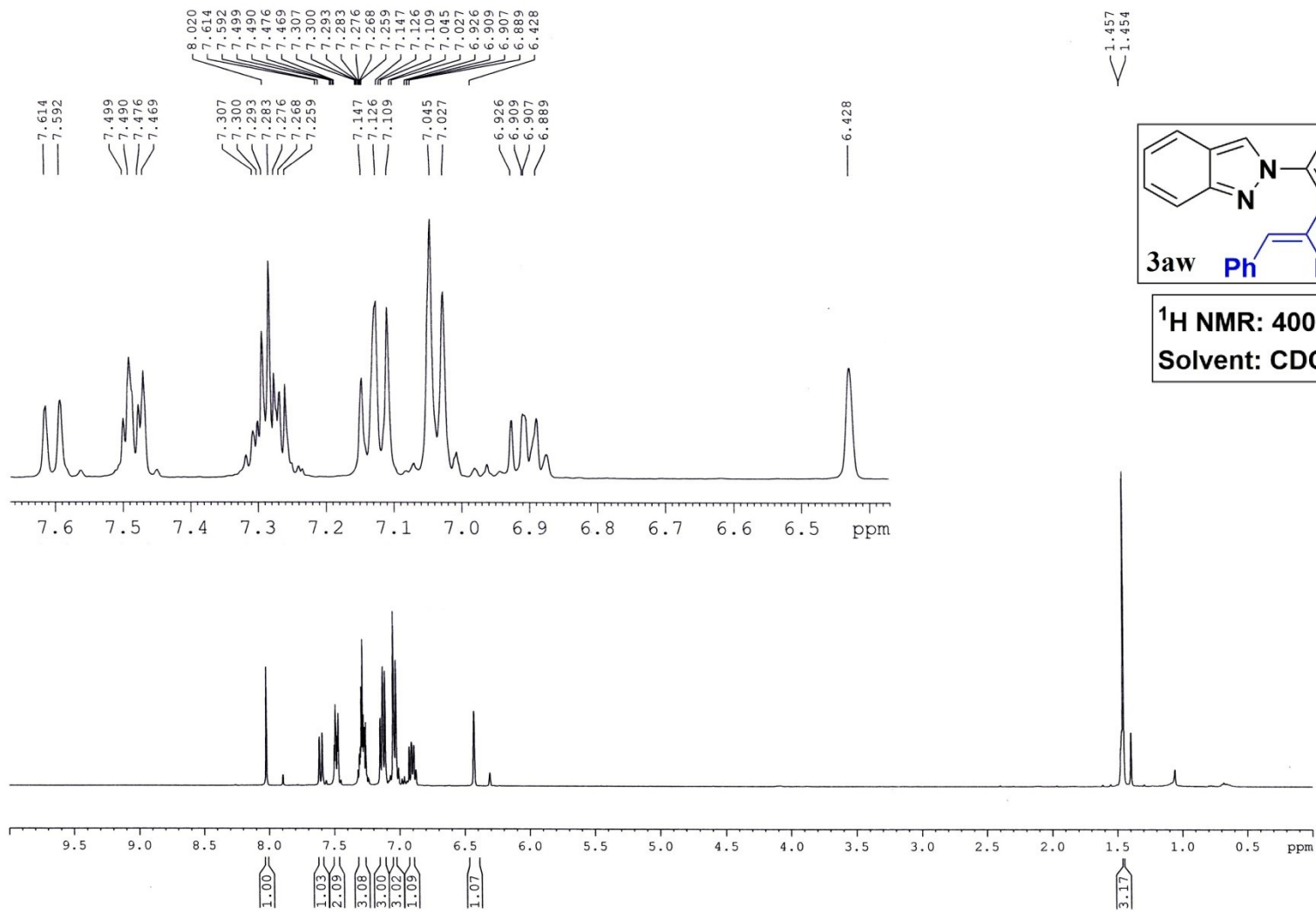
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 157  
 PROCNO 1

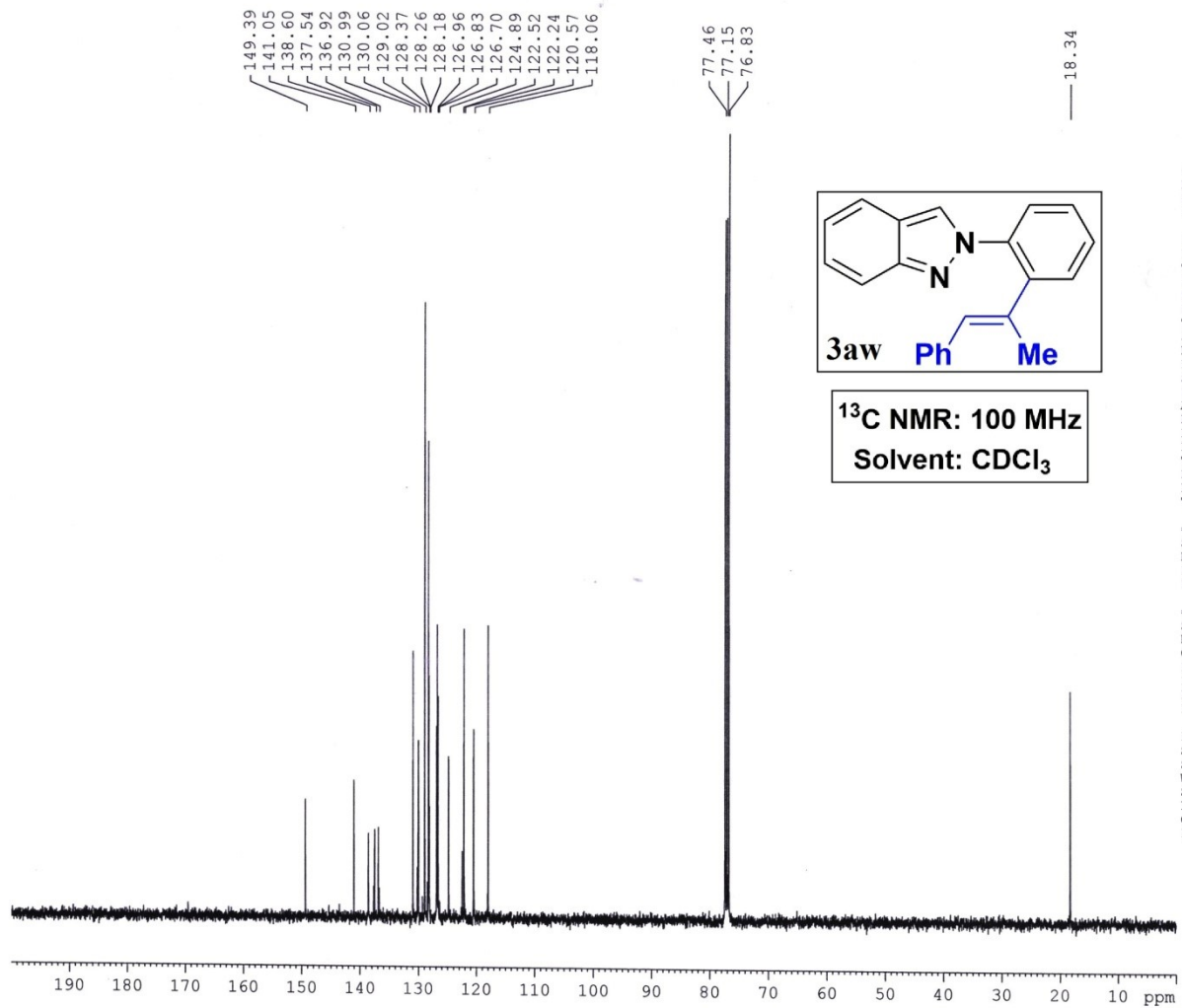
F2 - Acquisition Parameters  
 Date\_ 20210323  
 Time\_ 23.35  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 580  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 120.16  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 FCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177873 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 191  
 PROCNO 1

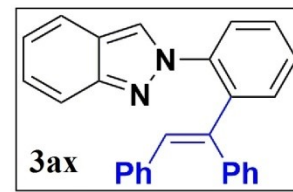
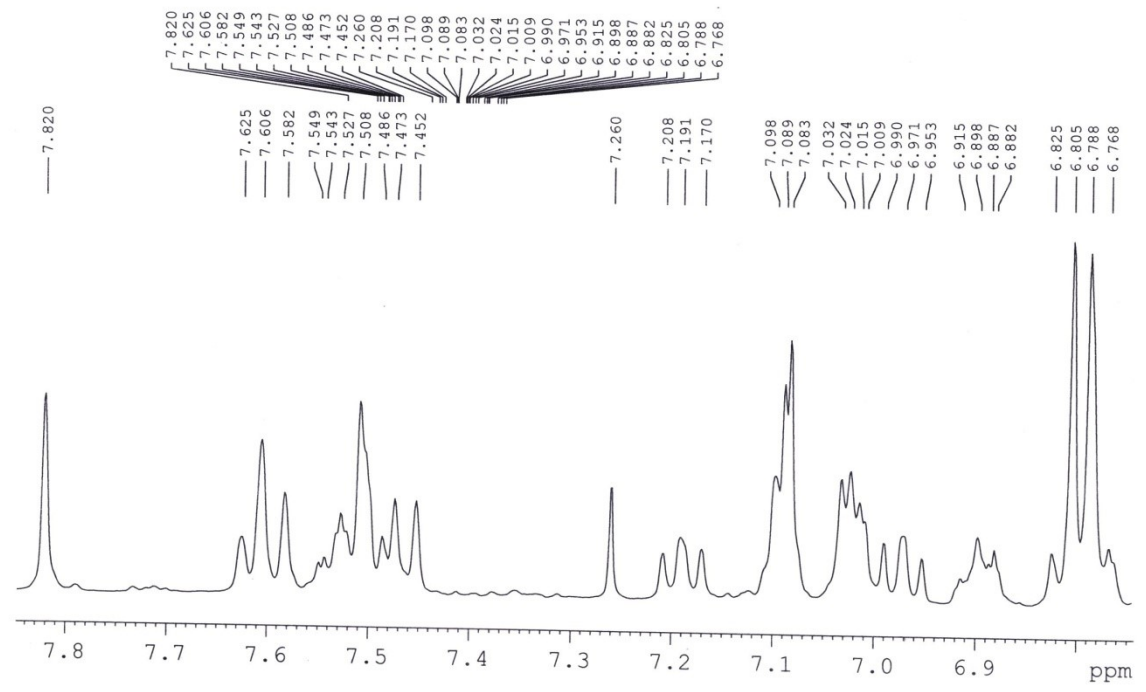
F2 - Acquisition Parameters  
 Date 20210408  
 Time 18.53  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 512  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

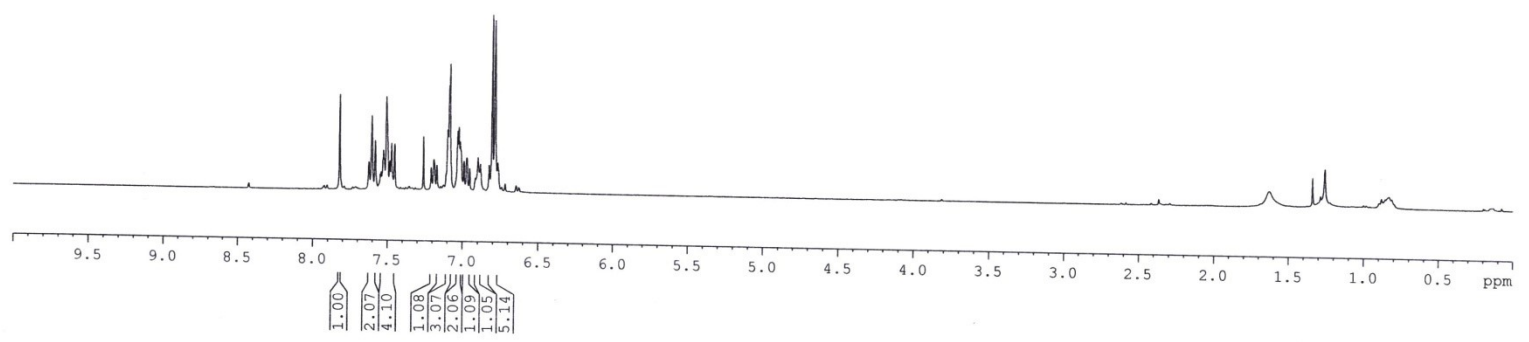
===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

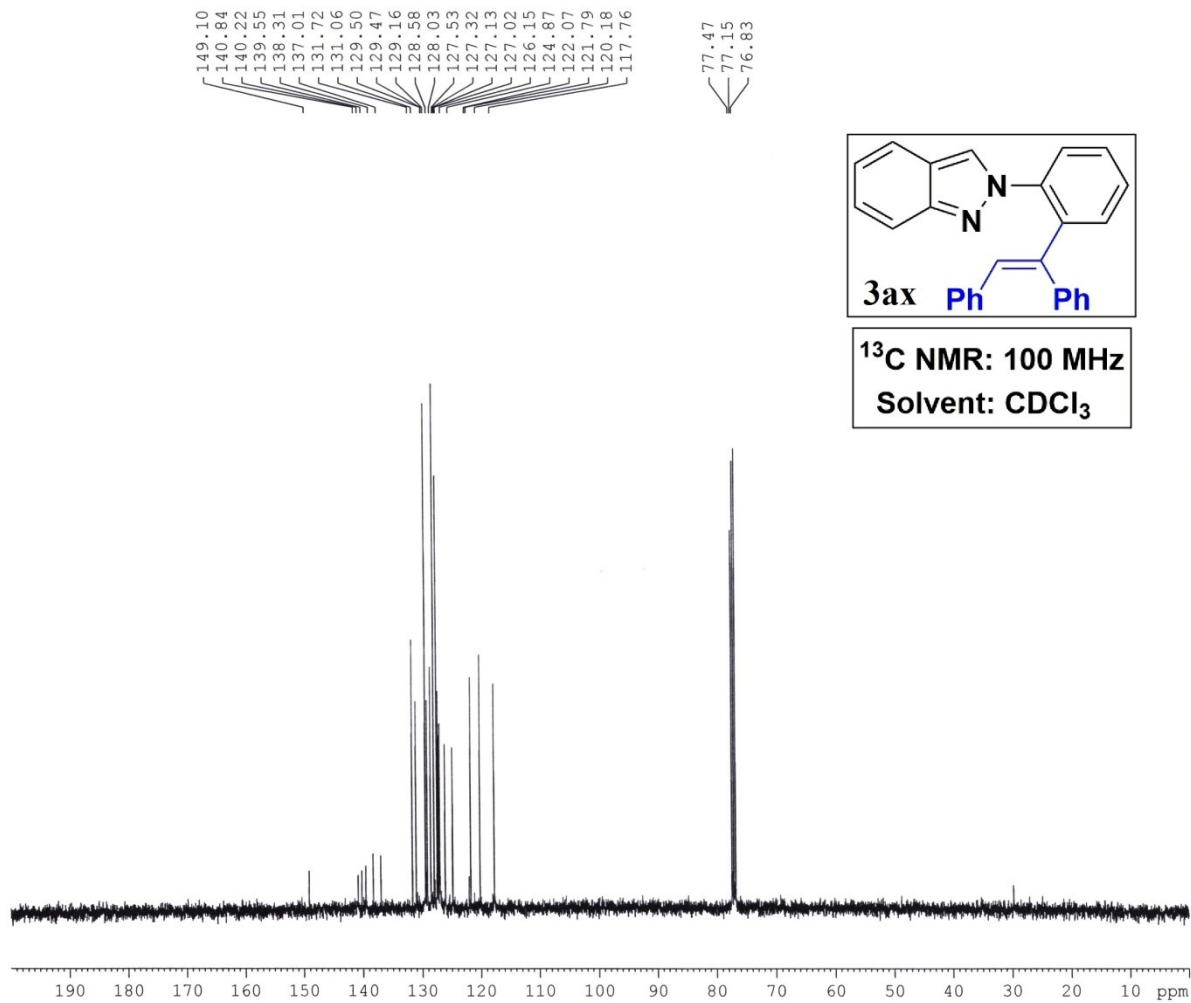
F2 - Processing parameters  
 SI 16384  
 SF 100.6177872 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





**<sup>1</sup>H NMR: 400 MHz**  
**Solvent: CDCl<sub>3</sub>**





```

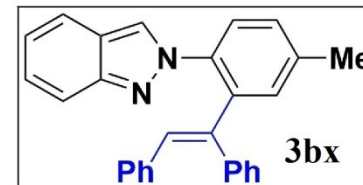
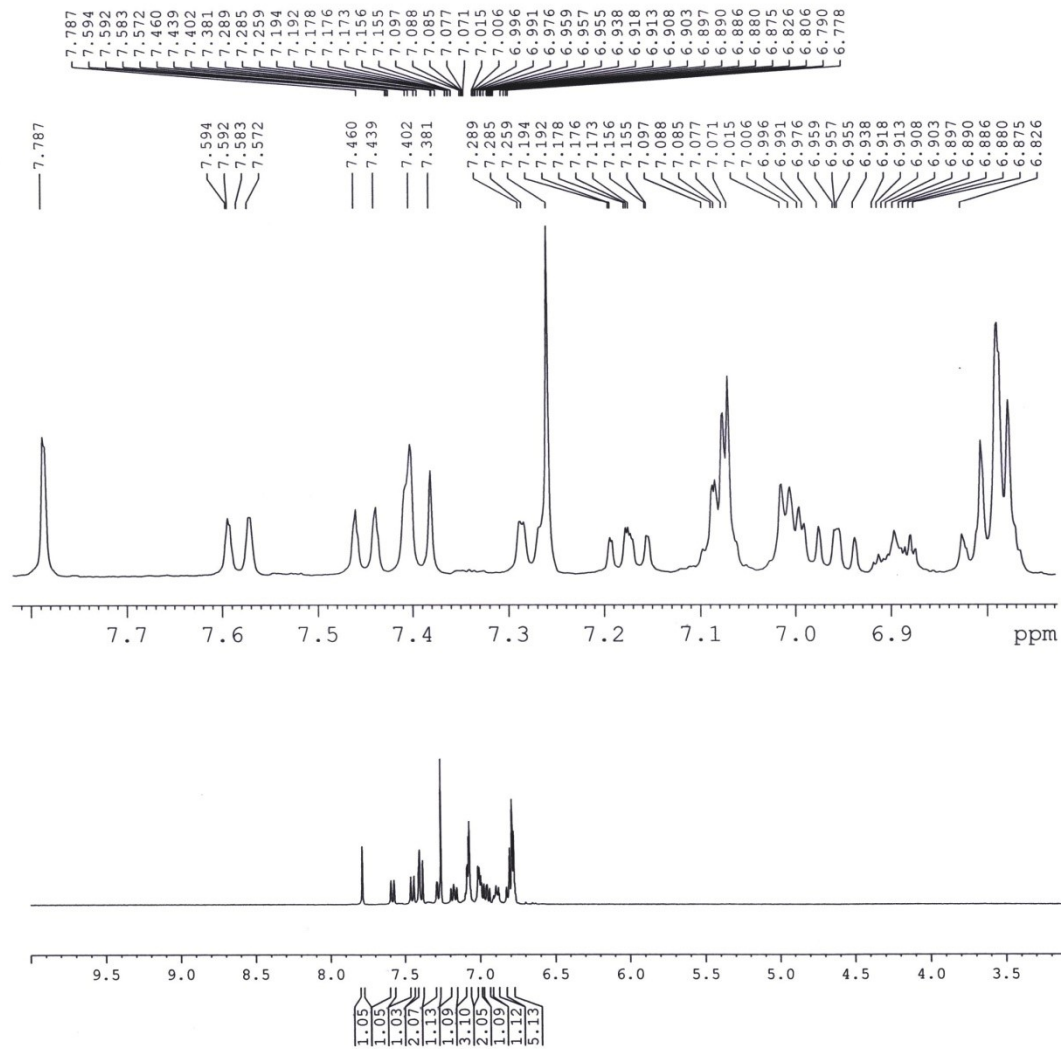
Current Data Parameters
NAME      Dr. A HAJRA-2021-13C
EXPNO     91
PROCNO    1

F2 - Acquisition Parameters
Date_     20210218
Time      2.35
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgdc
TD         32768
SOLVENT   CDCl3
NS         320
DS         2
SWH        24038.461 Hz
FIDRES     0.733596 Hz
AQ         0.6815744 sec
RG         120.16
DW         20.800 usec
DE         6.50 usec
TE         293.6 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1       100.6278588 MHz
NUC1        13C
P1          8.90 usec
PLW1        54.00000000 W

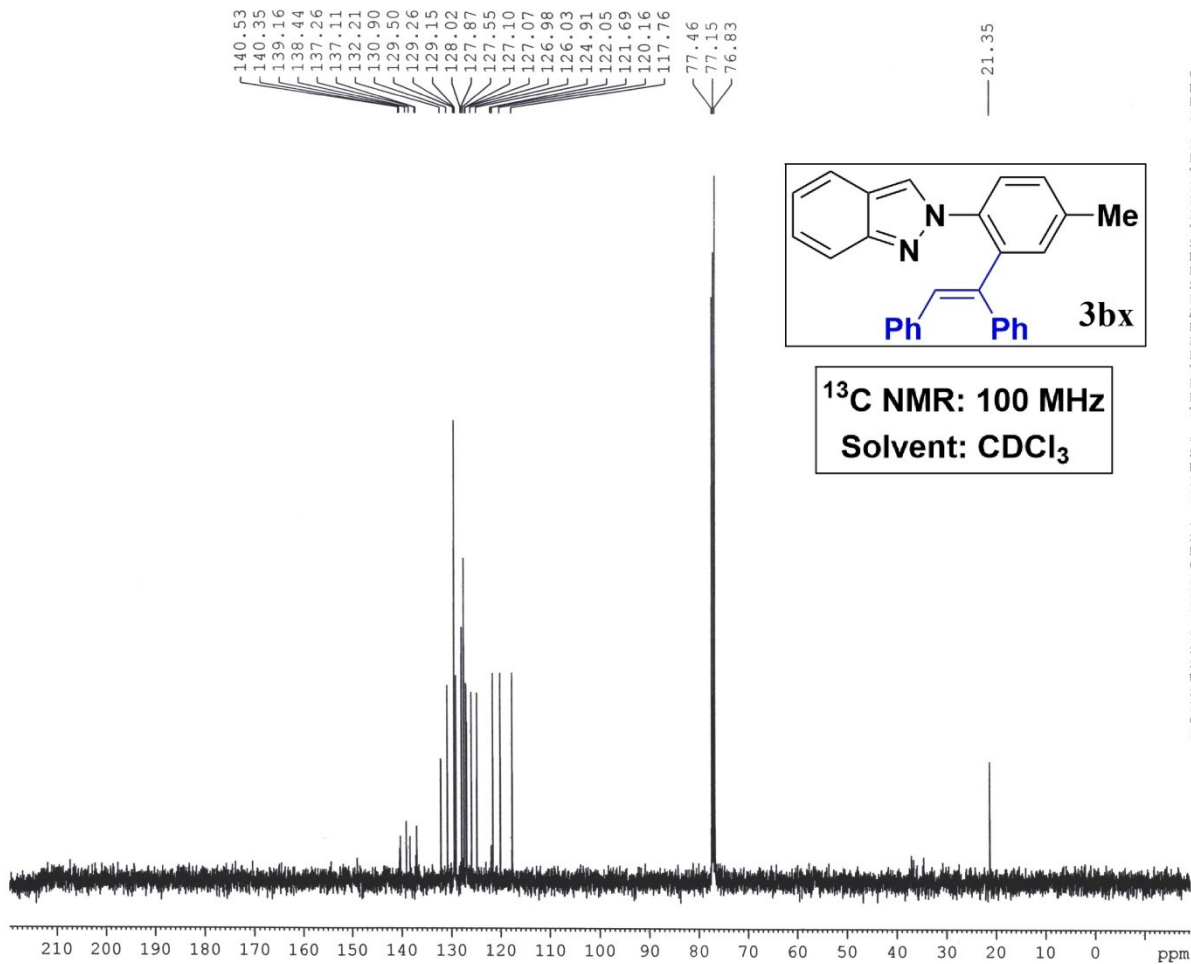
===== CHANNEL f2 =====
SFO2       400.1516006 MHz
NUC2         1H
CPDPRG[2]   waltz16
PCPD2       90.00 usec
PLW2        12.00000000 W
PLW12       0.32231000 W

F2 - Processing parameters
SI          16384
SF          100.6177873 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.00
  
```



<sup>1</sup>H NMR: 400 MHz  
Solvent: CDCl<sub>3</sub>

← H<sub>2</sub>O



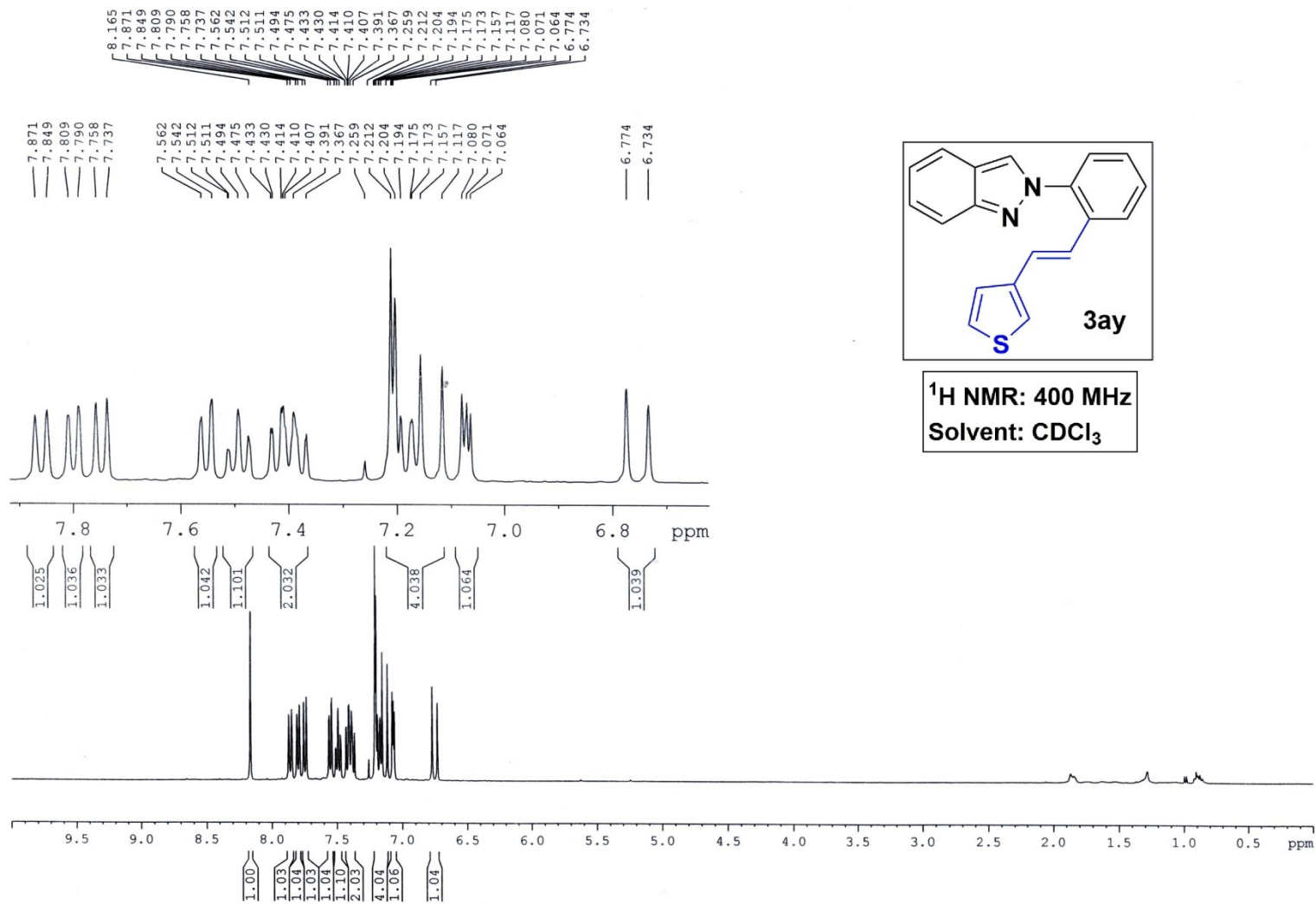
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 299  
 PROCNO 1

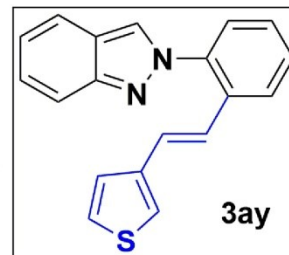
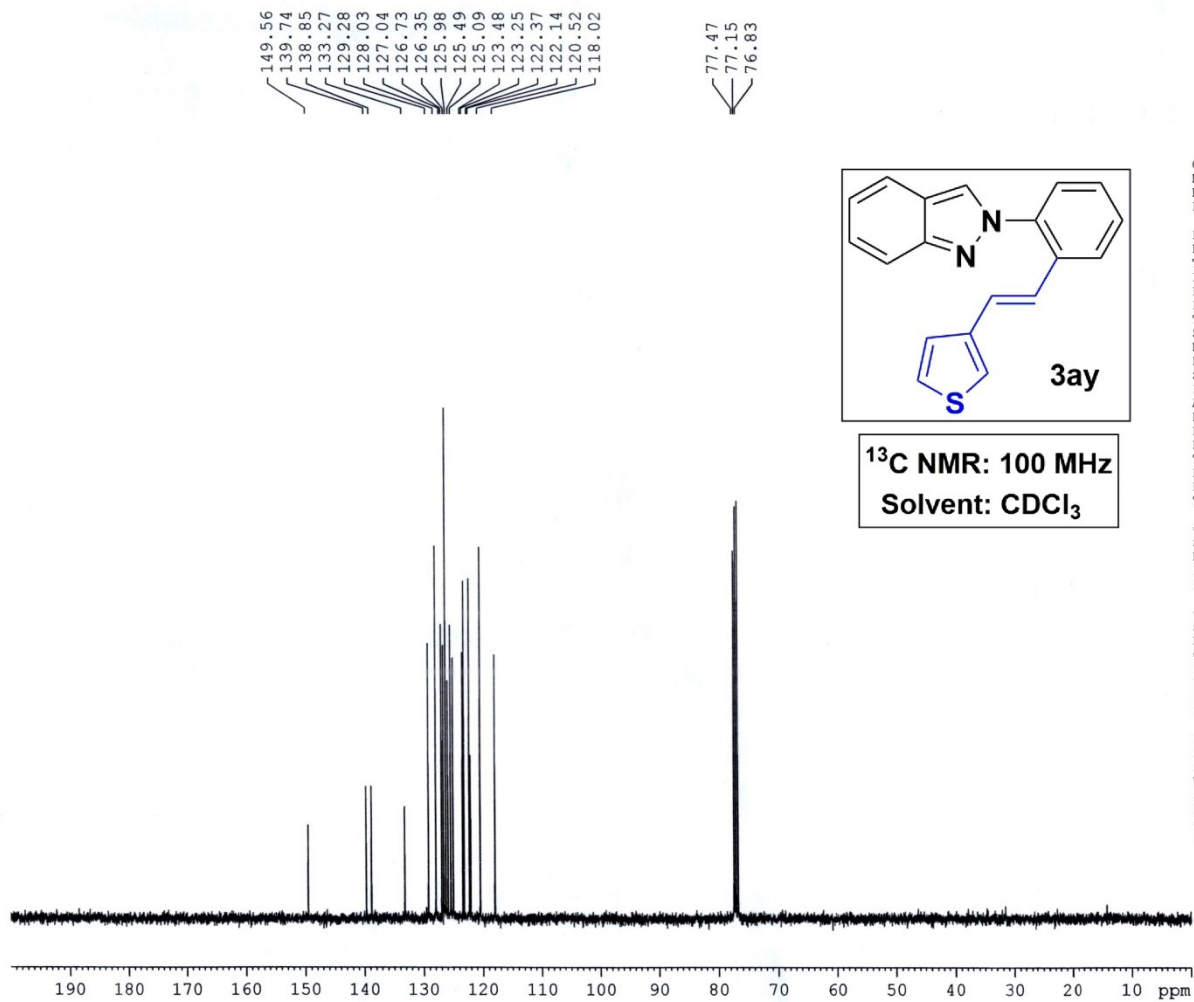
F2 - Acquisition Parameters  
 Date\_ 20210818  
 Time 19.33  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgdc  
 TD 32768  
 SOLVENT CDCl3  
 NS 640  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177842 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00





**<sup>13</sup>C NMR: 100 MHz**  
**Solvent: CDCl<sub>3</sub>**

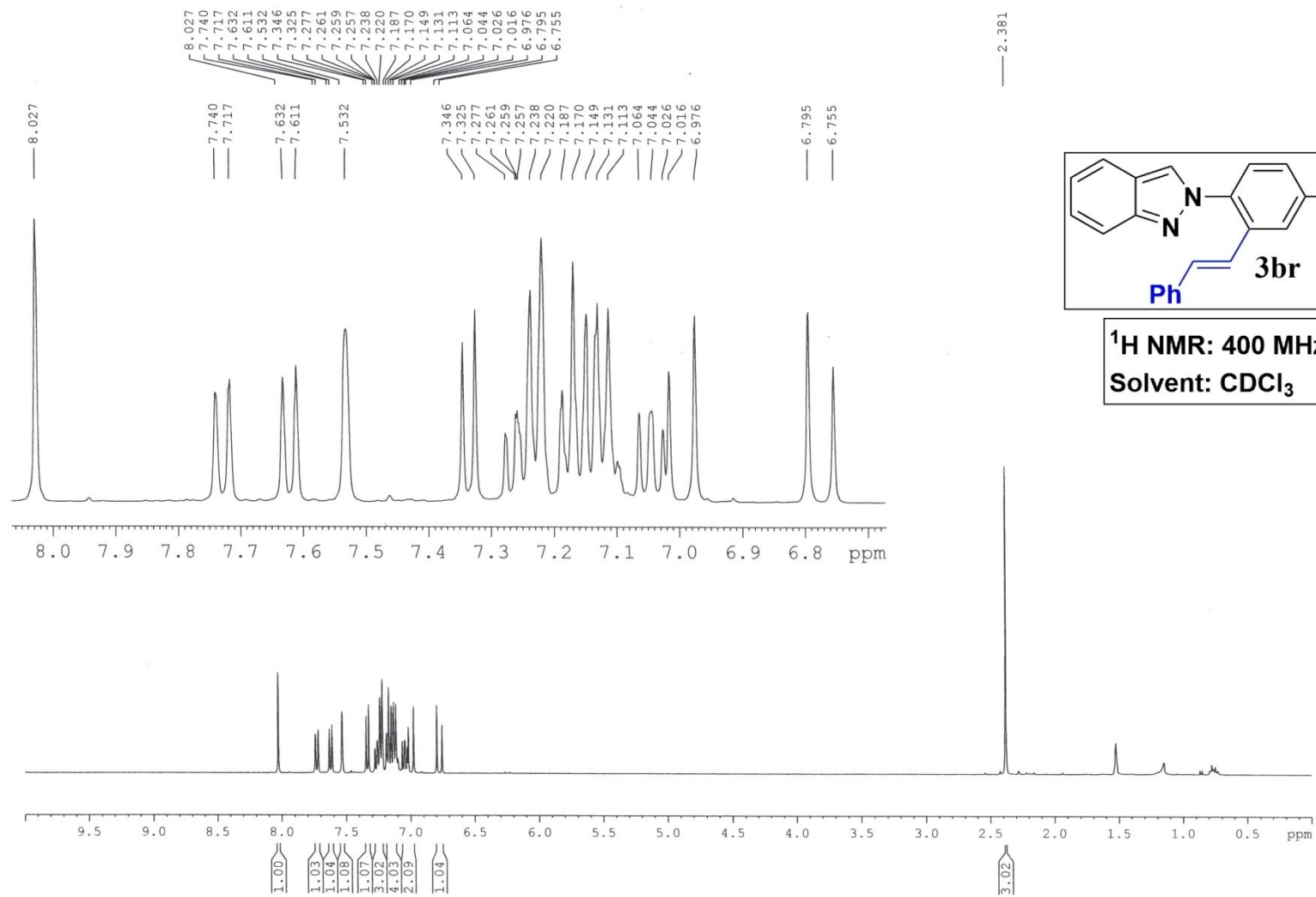
Current Data Parameters  
 NAME Dr. A HAJRA-2022-13C  
 EXPNO 9  
 PROCNO 1

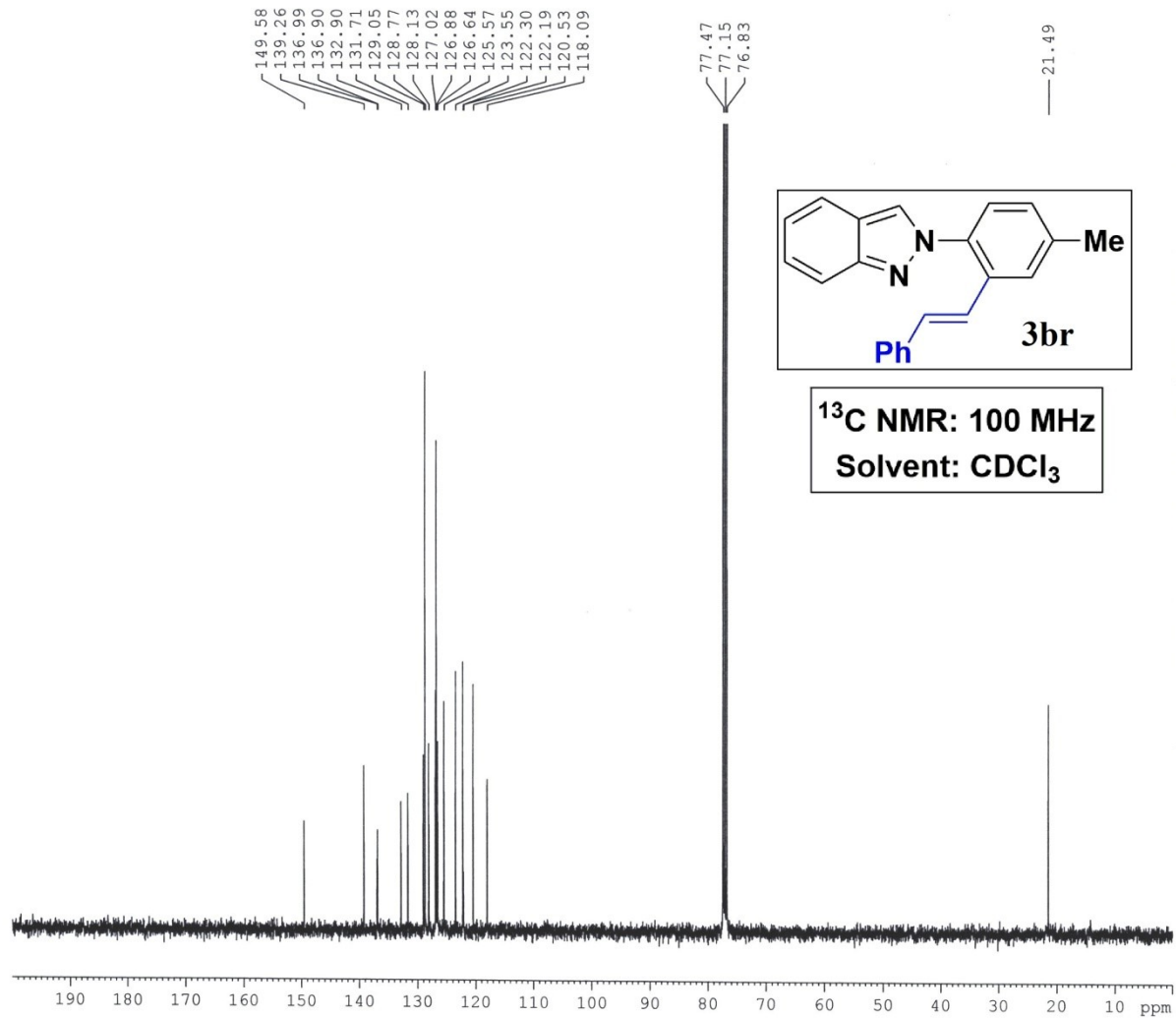
F2 - Acquisition Parameters  
 Date 20220109  
 Time 13.29  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 120  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 62.69  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 290.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177961 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





Current Data Parameters  
NAME Dr. A HAJRA-2020-13C  
EXPNO 382  
PROCNO 1

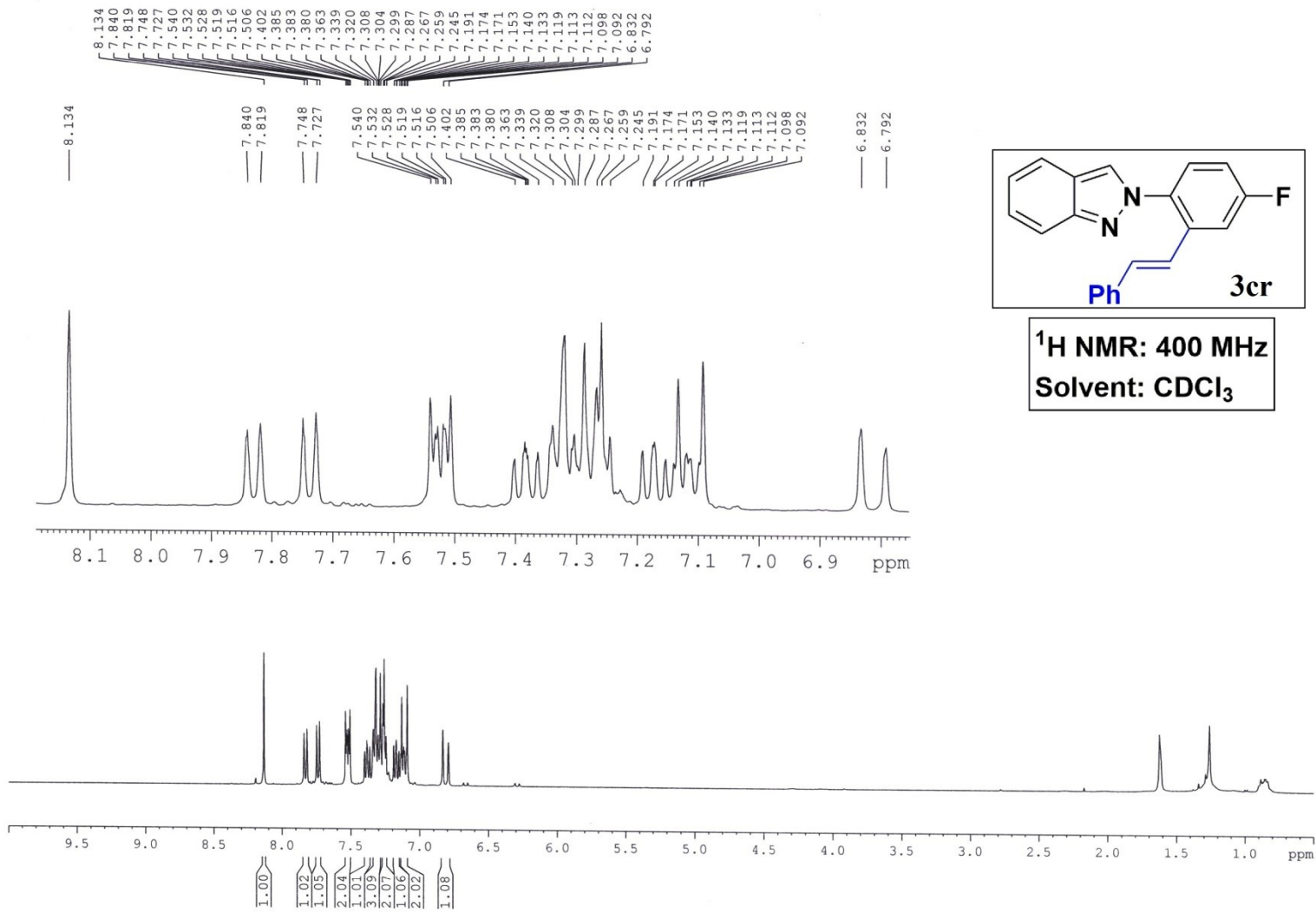
F2 - Acquisition Parameters  
Date\_ 20201230  
Time\_ 13.54  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 480  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 106.66  
DW 20.800 usec  
DE 6.50 usec  
TE 294.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

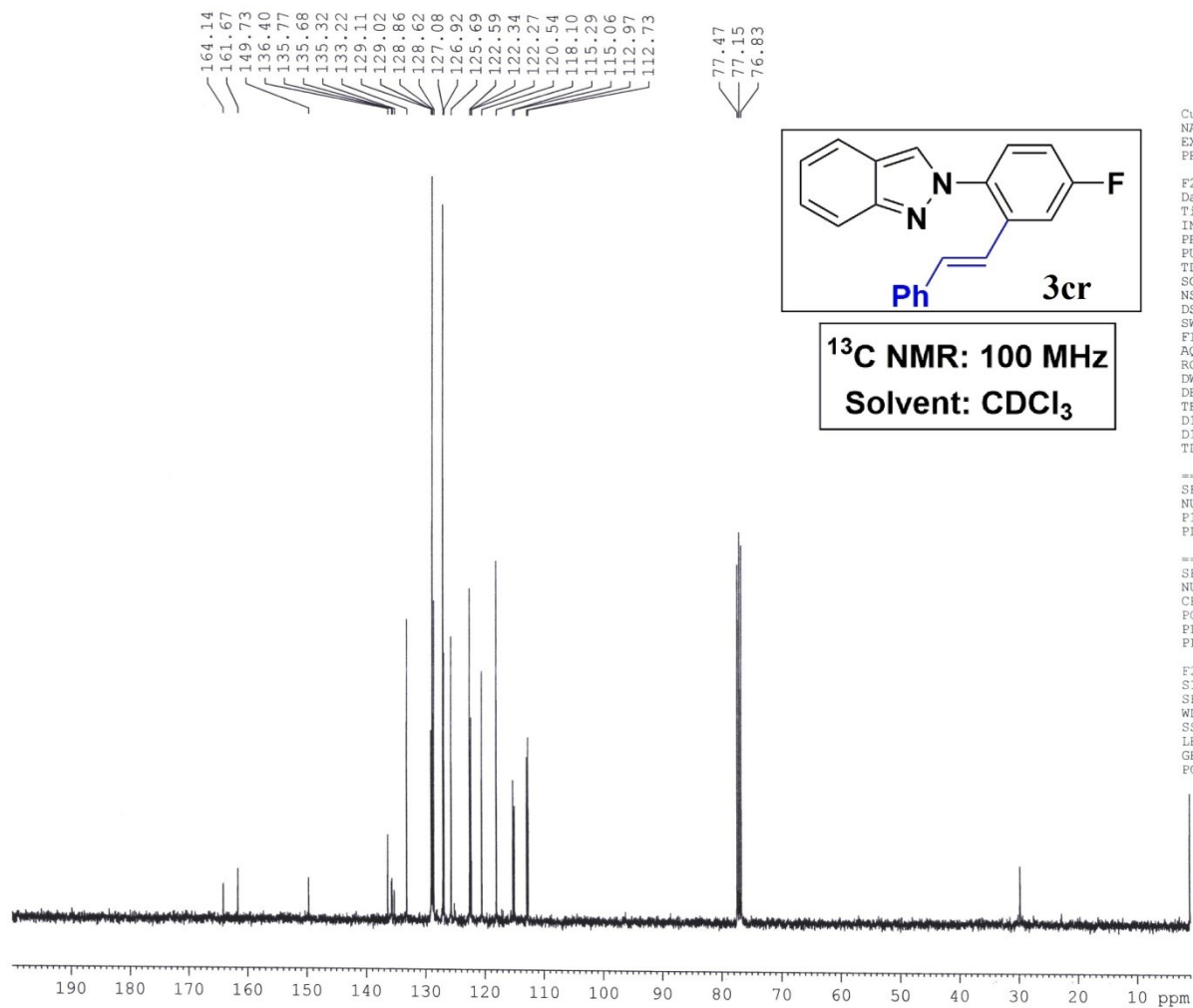
----- CHANNEL f1 -----  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W

----- CHANNEL f2 -----  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

F2 - Processing parameters  
SI 16384  
SF 100.6177872 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40







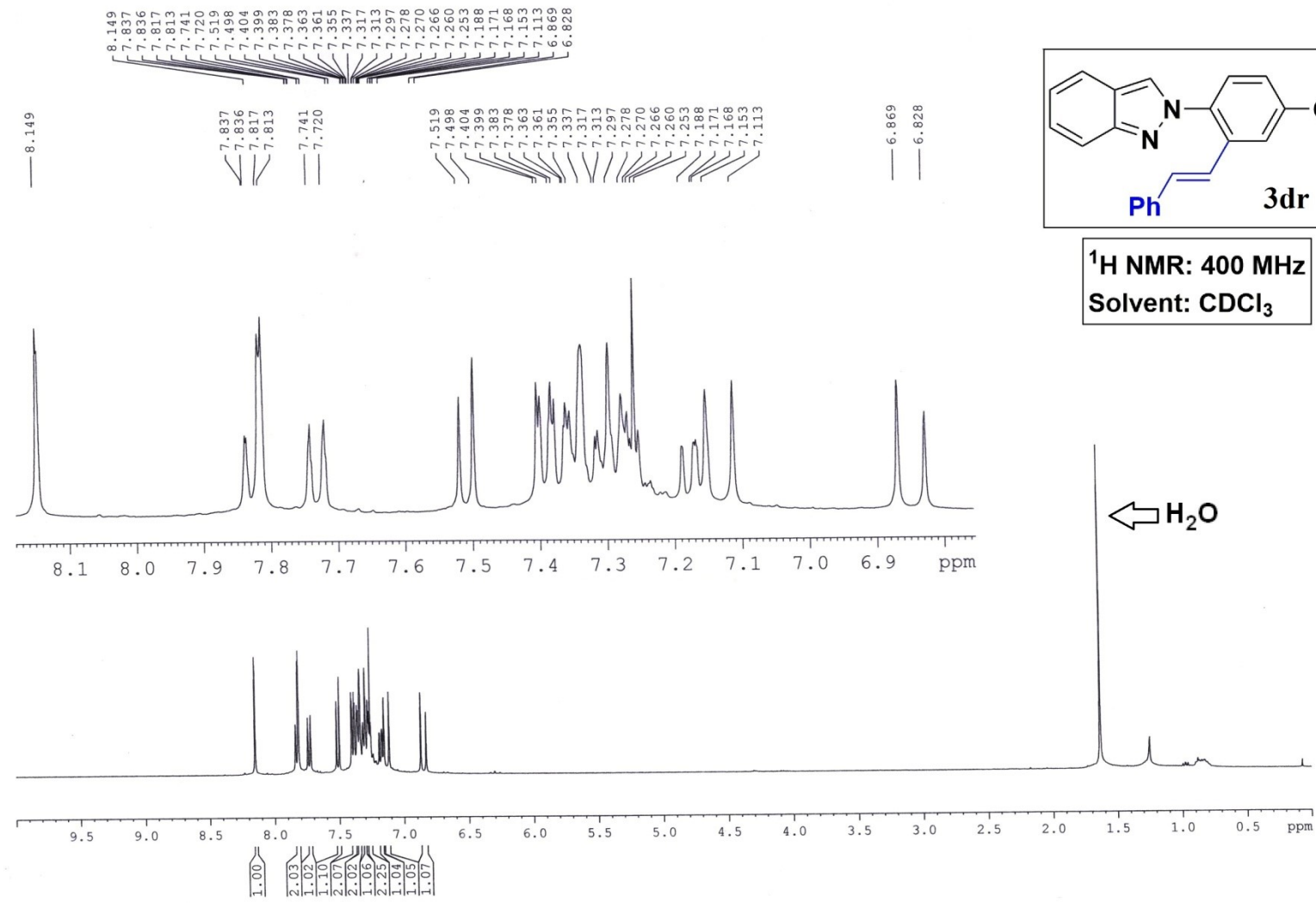
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 161  
 PROCNO 1

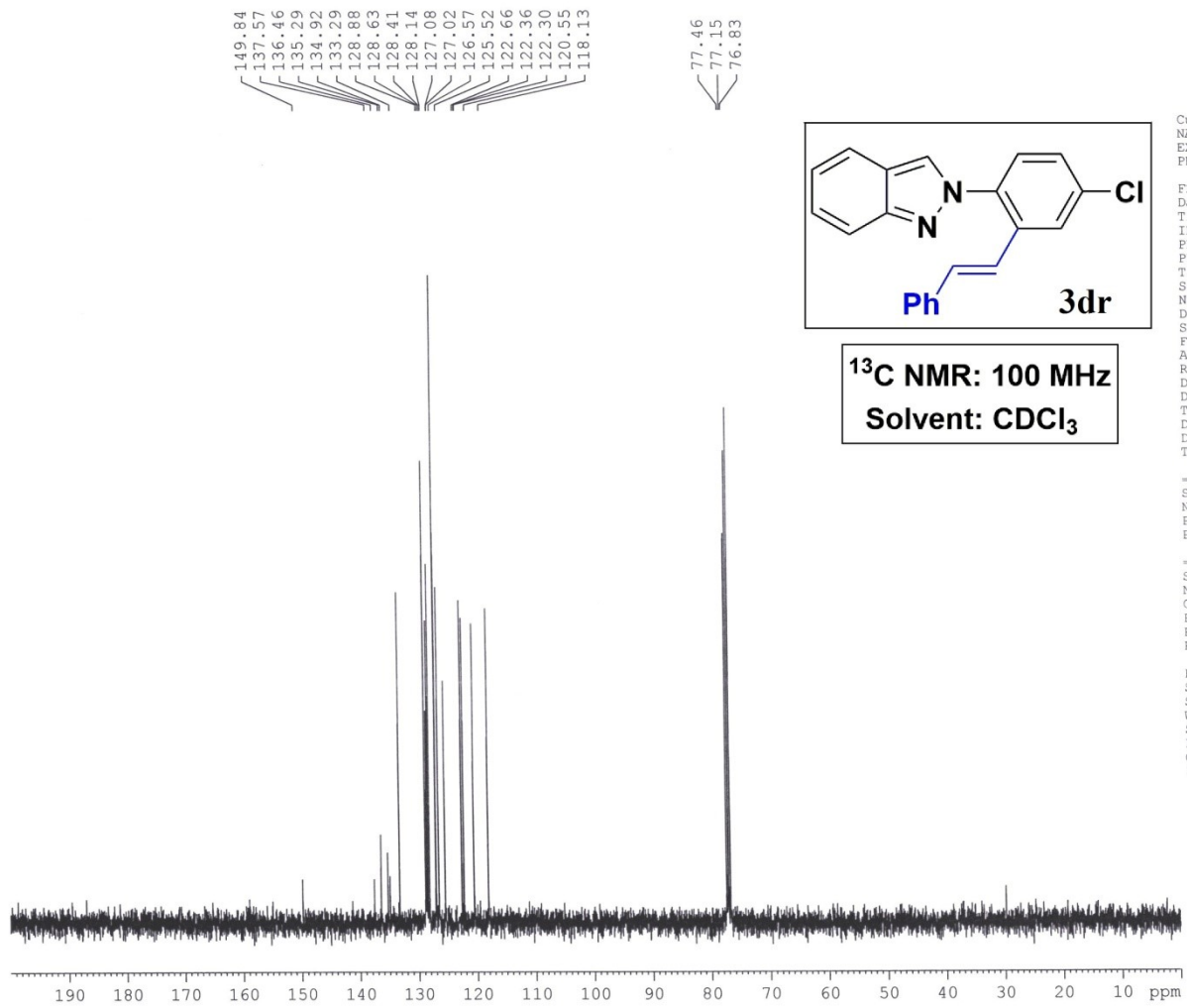
F2 - Acquisition Parameters  
 Date 20210324  
 Time 3:27  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgdc  
 TD 32768  
 SOLVENT CDCl3  
 NS 880  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 120.16  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177858 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00





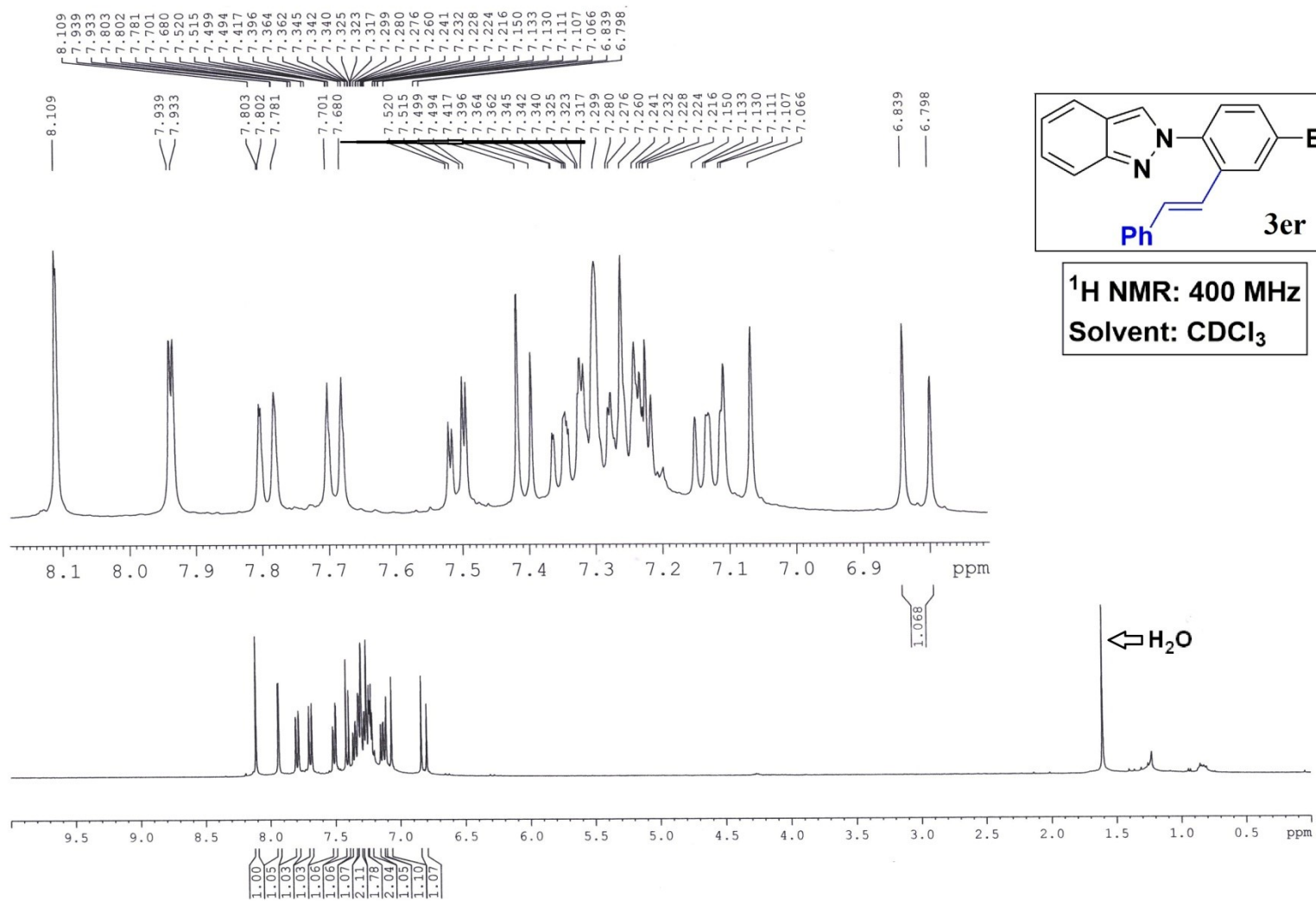
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 193  
 PROCNO 1

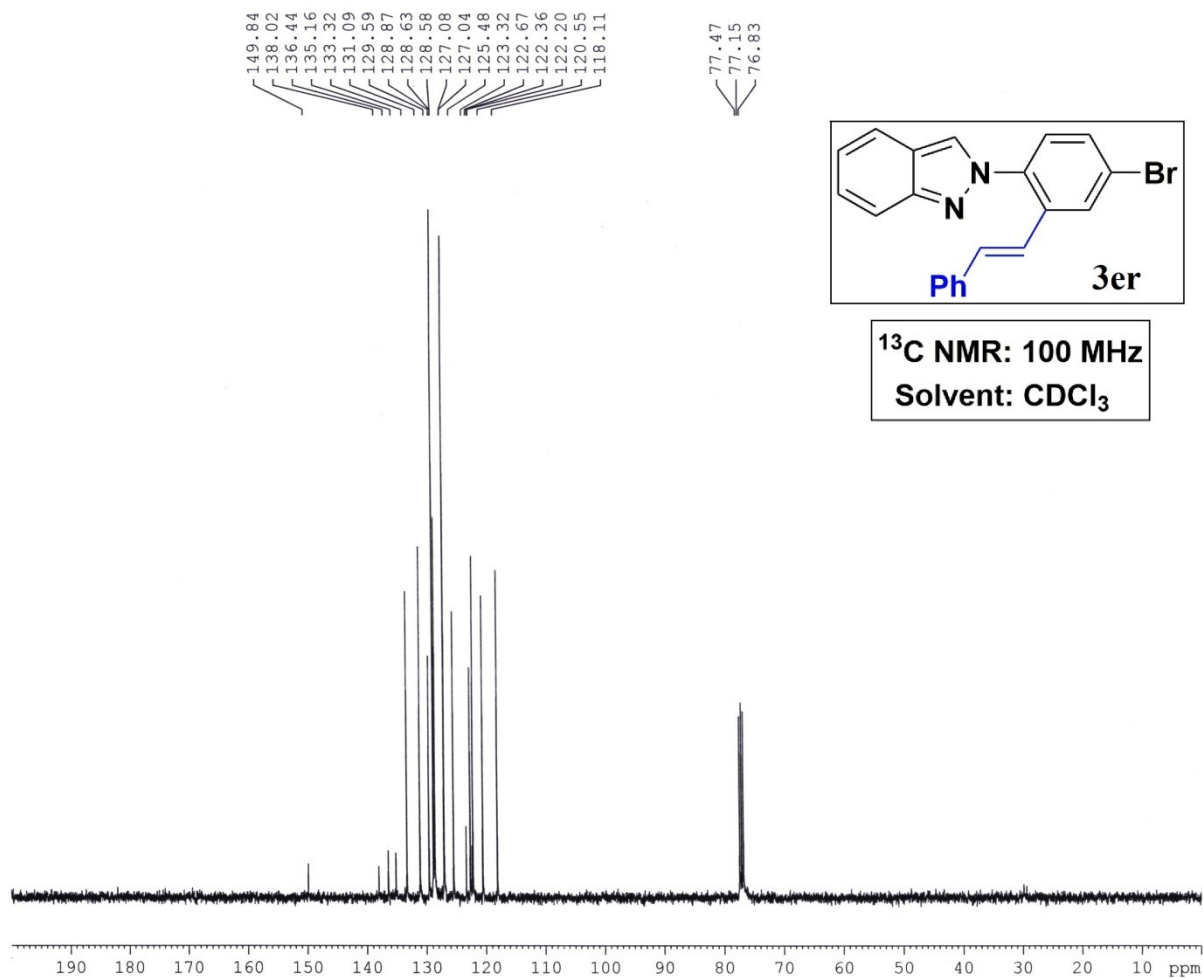
F2 - Acquisition Parameters  
 Date\_ 20210408  
 Time 20.23  
 INSTRUM spect  
 FROBHD 5 mm PABBO BB/  
 PULPROG zgdc  
 TD 32768  
 SOLVENT CDCl3  
 NS 256  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177844 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00





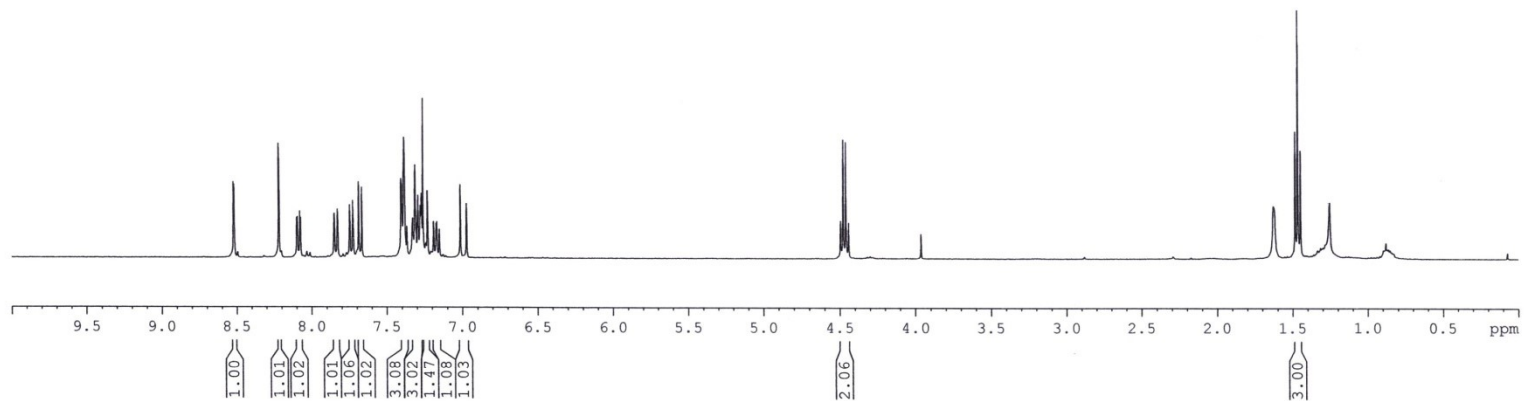
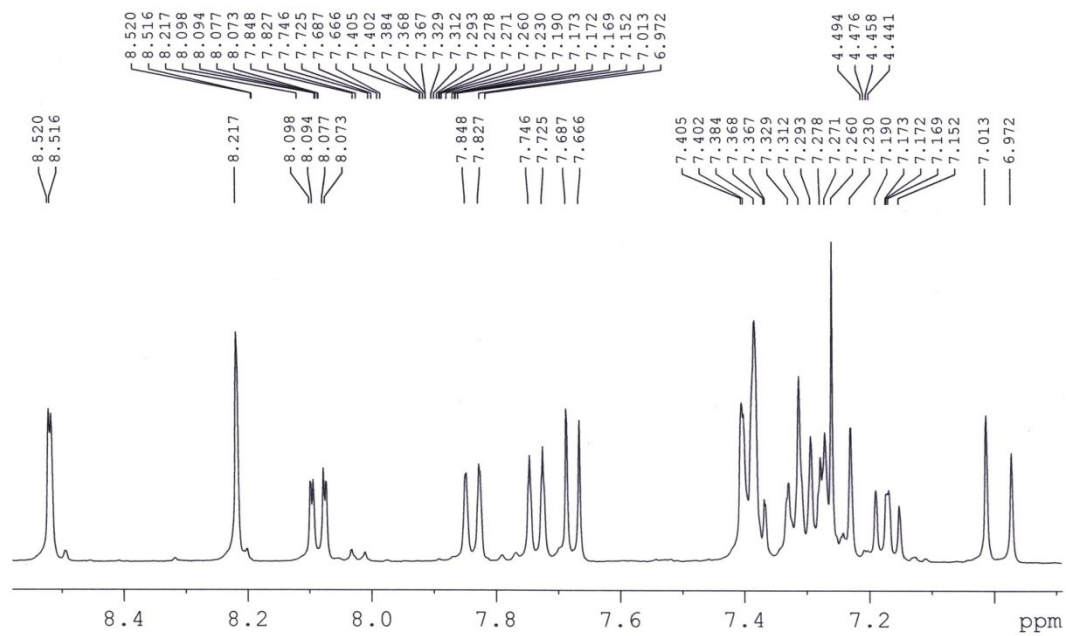
Current Data Parameters  
NAME Dr. A HAJRA-2021-13C  
EXPNO 190  
PROCNO 1

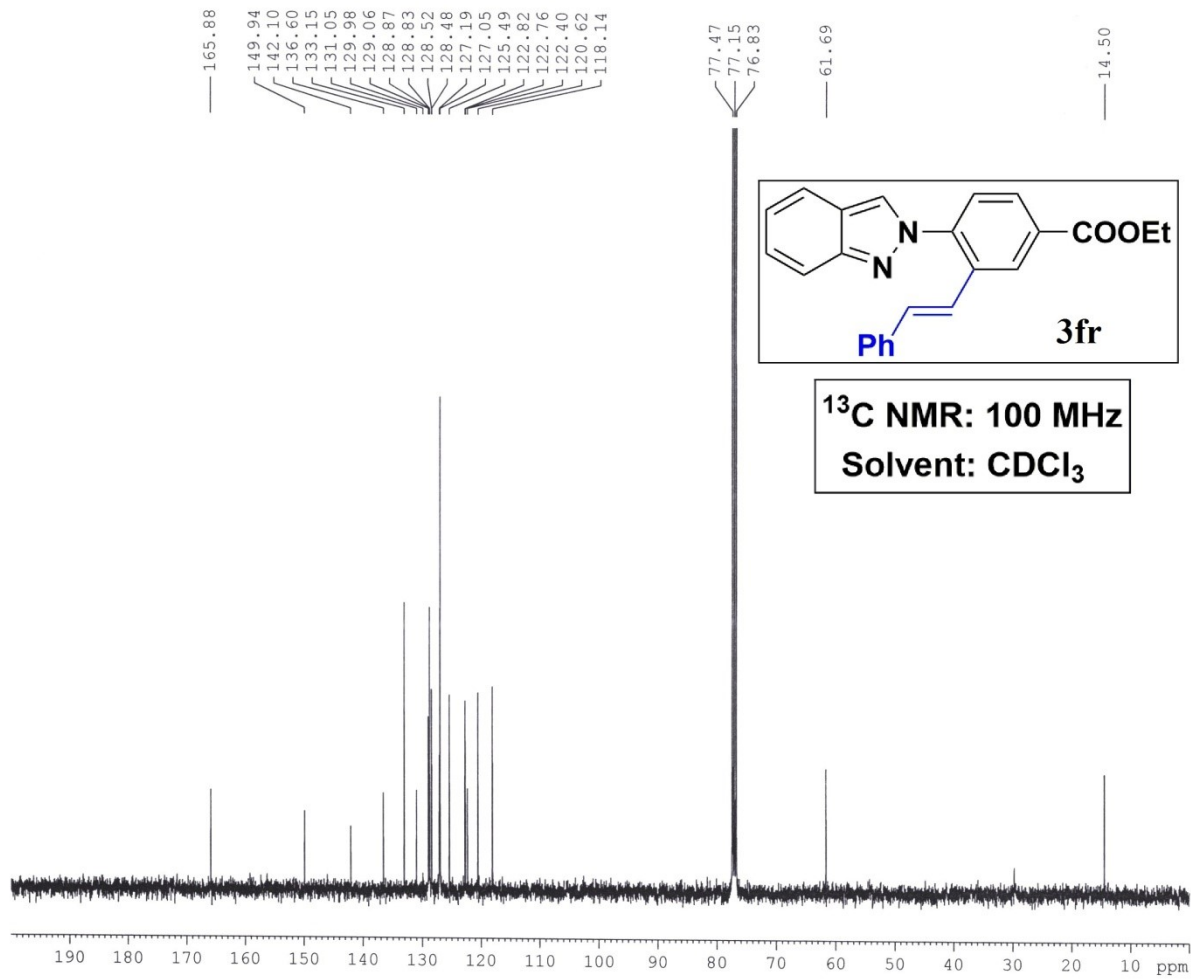
F2 - Acquisition Parameters  
Date\_ 20210408  
Time\_ 14.12  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgdc  
TD 32768  
SOLVENT CDC13  
NS 640  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 148.91  
DW 20.800 usec  
DE 6.50 usec  
TE 298.8 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W

===== CHANNEL f2 =====  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W

F2 - Processing parameters  
SI 16384  
SF 100.6177858 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.00





Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 151  
 PROCNO 1

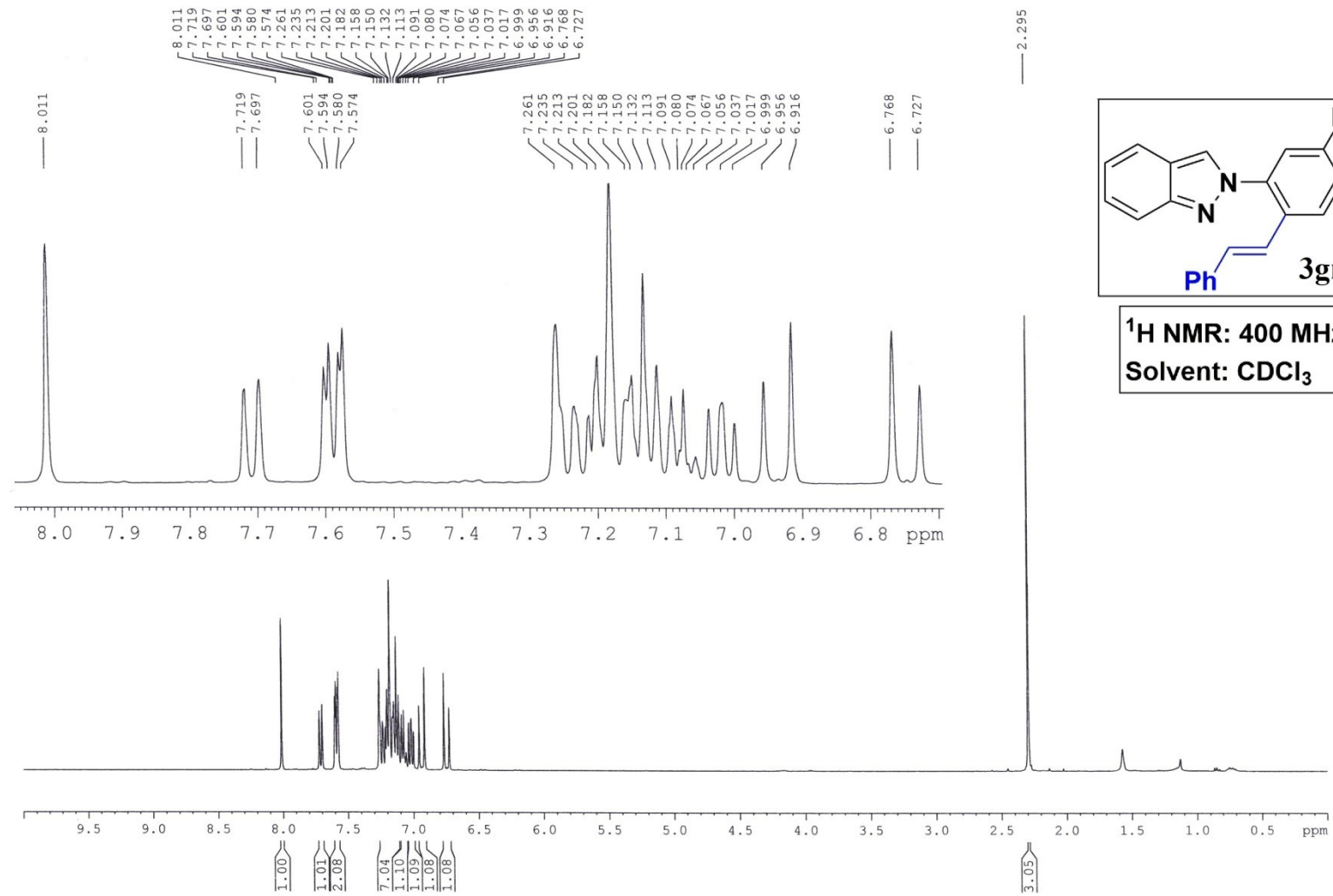
F2 - Acquisition Parameters  
 Date\_ 20210323  
 Time\_ 9:51  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 640  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 135.7  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 293.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

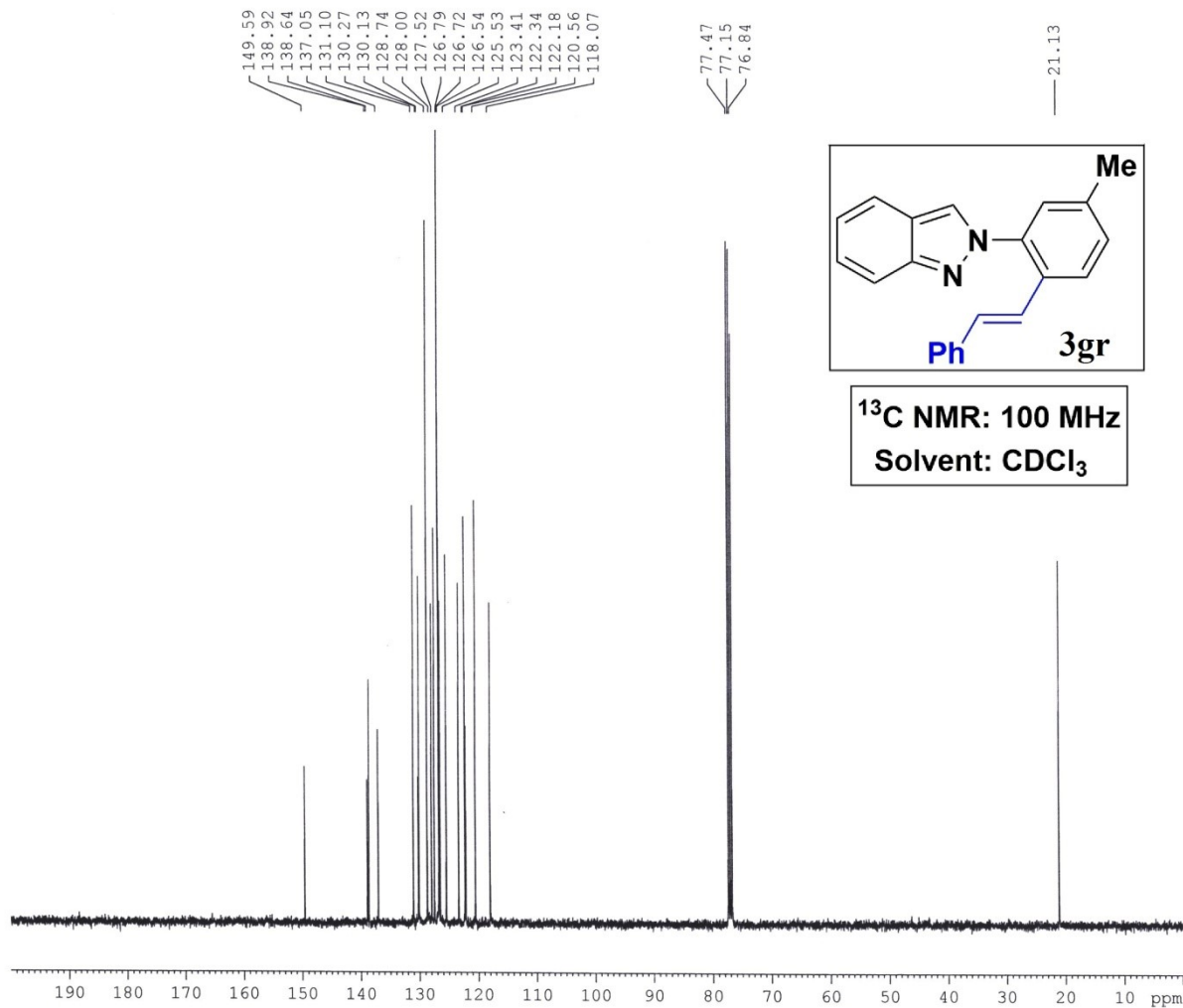
----- CHANNEL f1 -----  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177873 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40







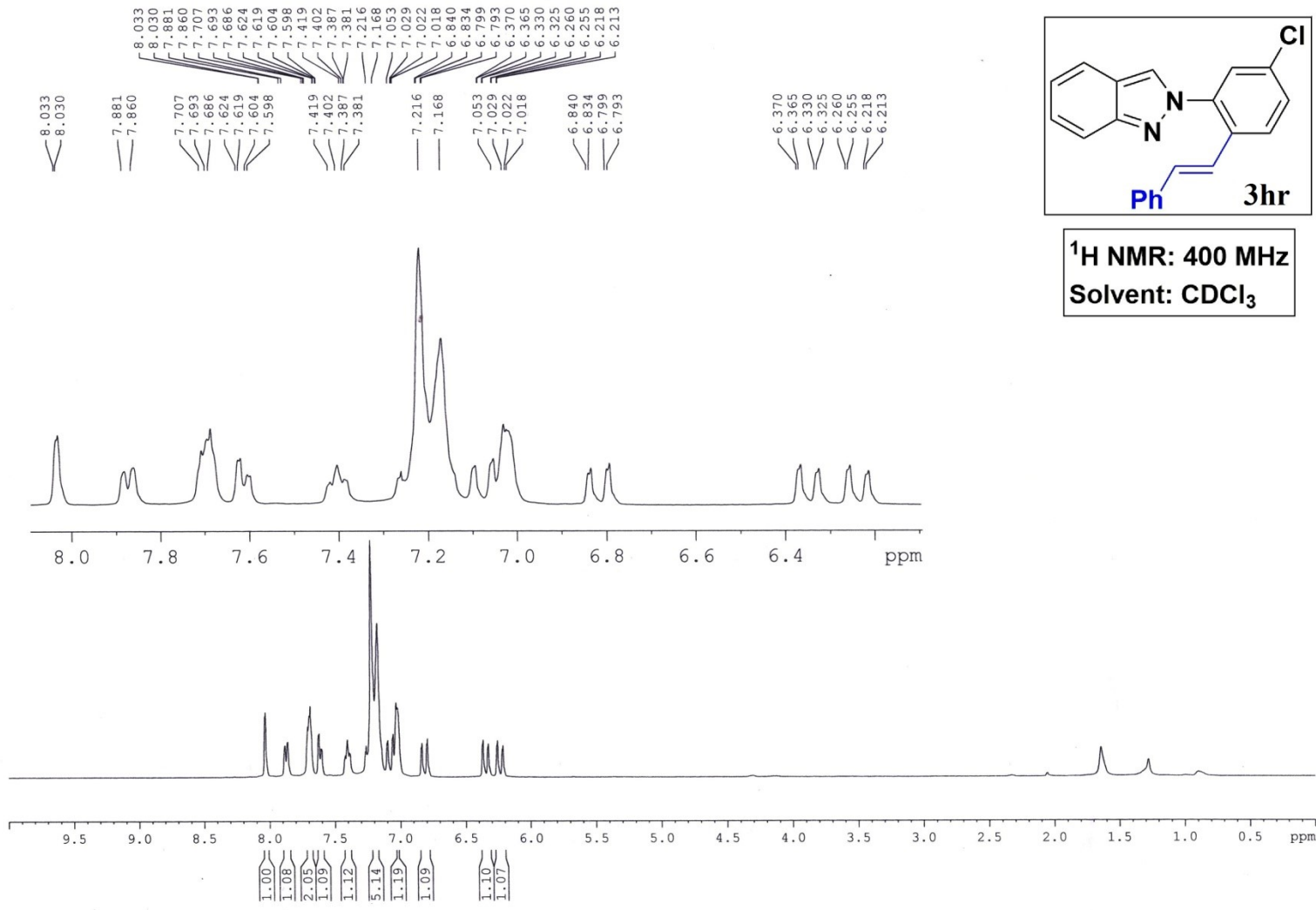
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 209  
 PROCNO 1

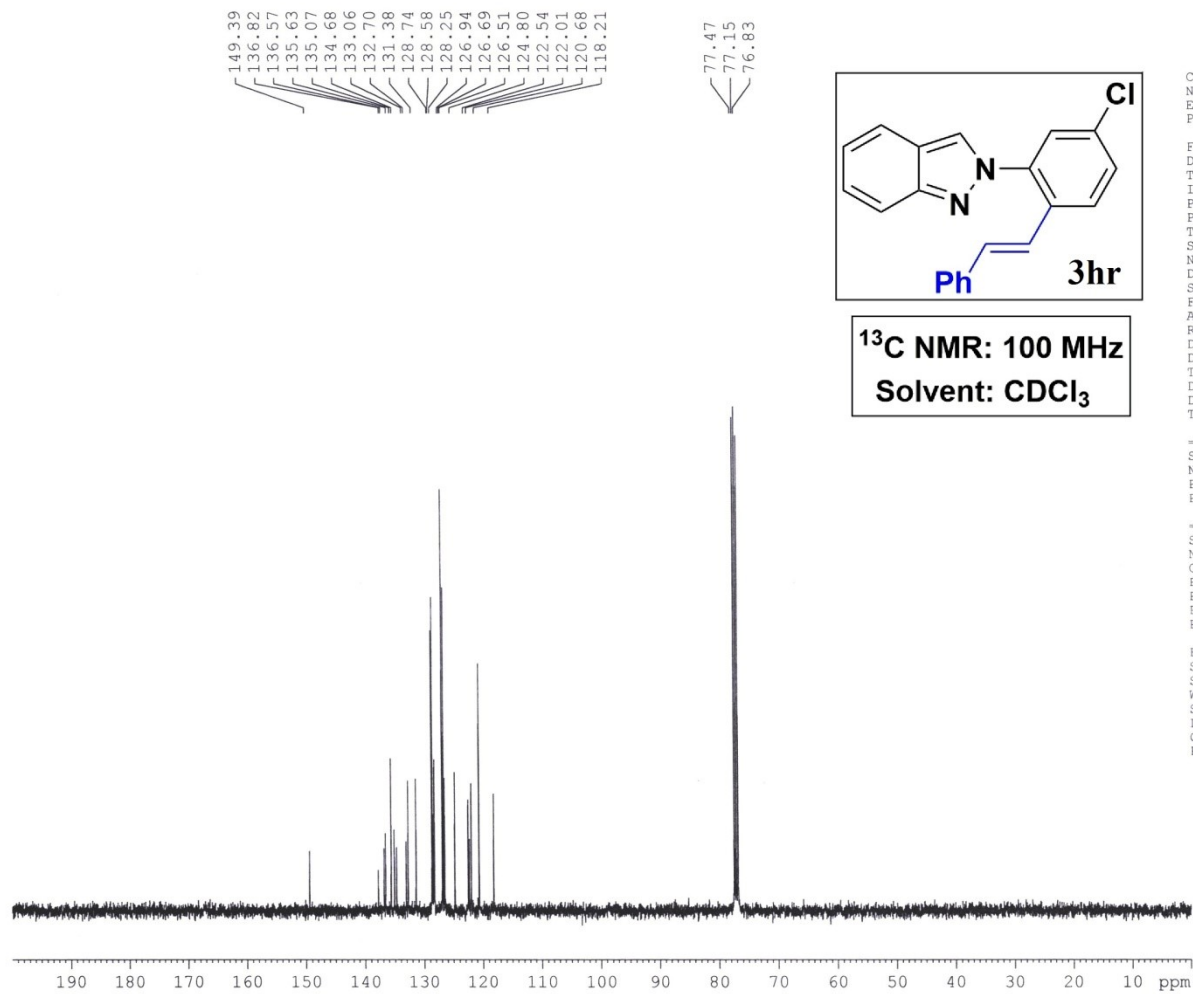
F2 - Acquisition Parameters  
 Date 20210414  
 Time 2.38  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 512  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 77.59  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.4 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.0000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177903 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





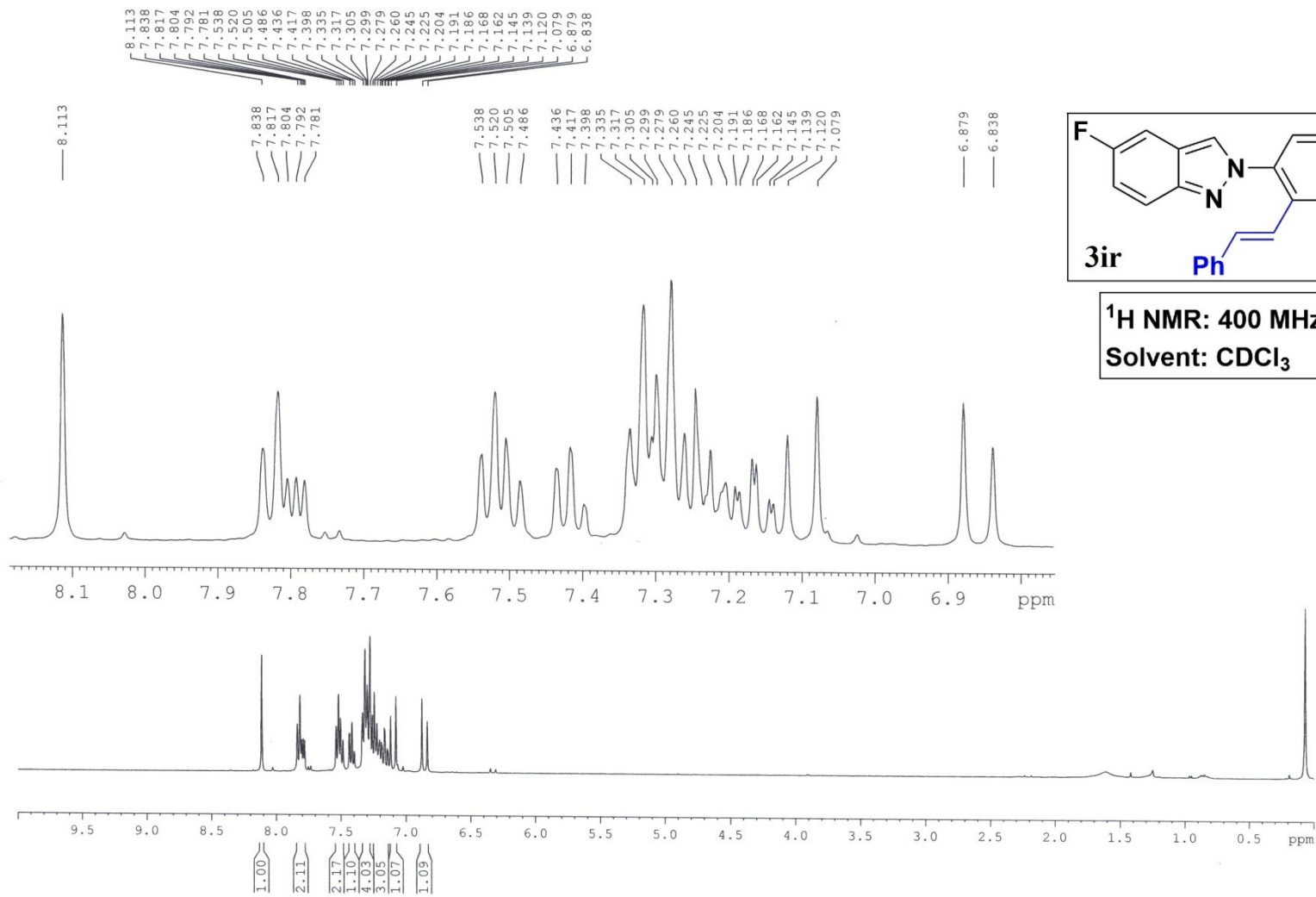
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 257  
 PROCNO 1

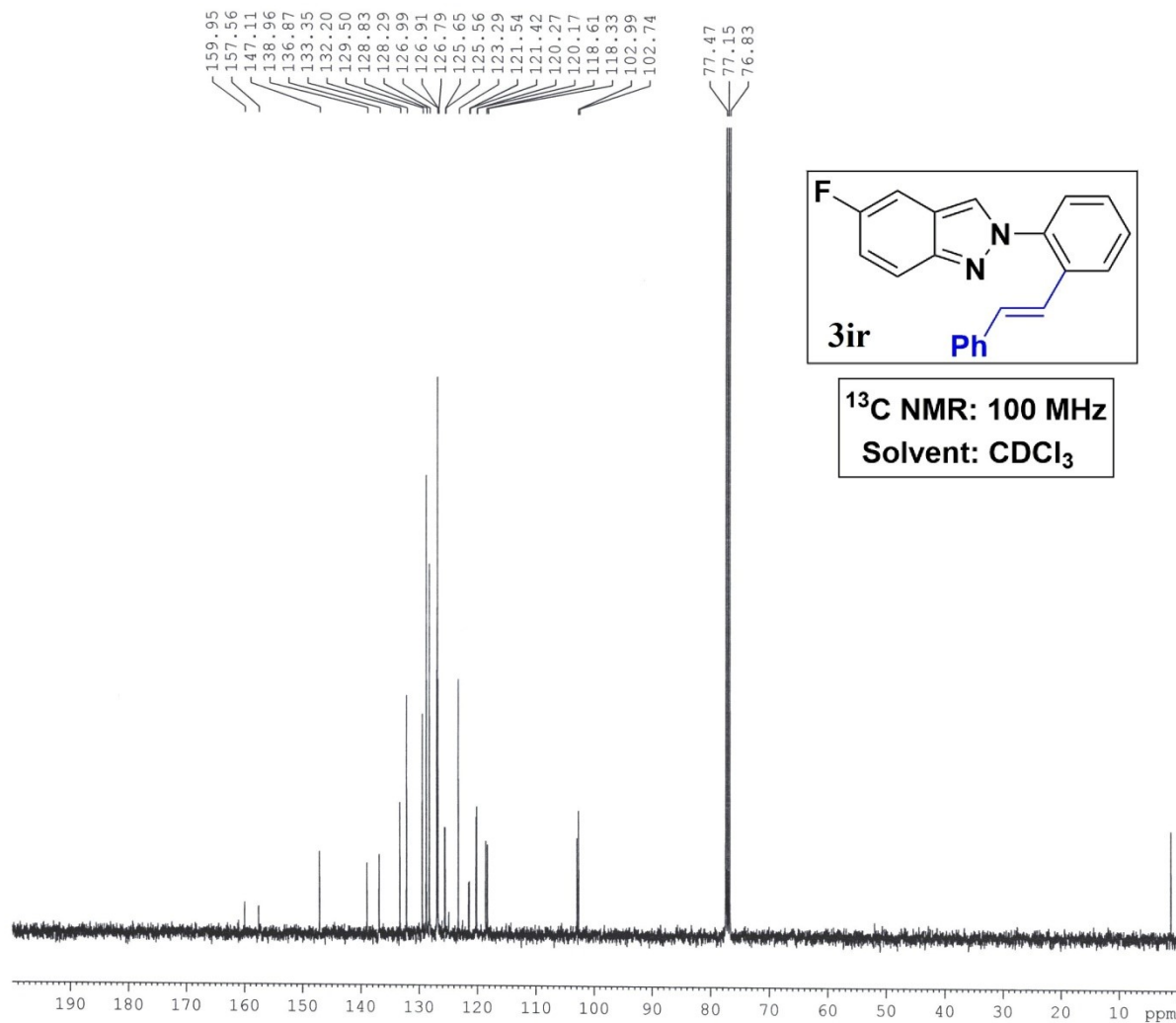
F2 - Acquisition Parameters  
 Date\_ 20210621  
 Time 13.18  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 220  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 106.66  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177872 MHz  
 NDUW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





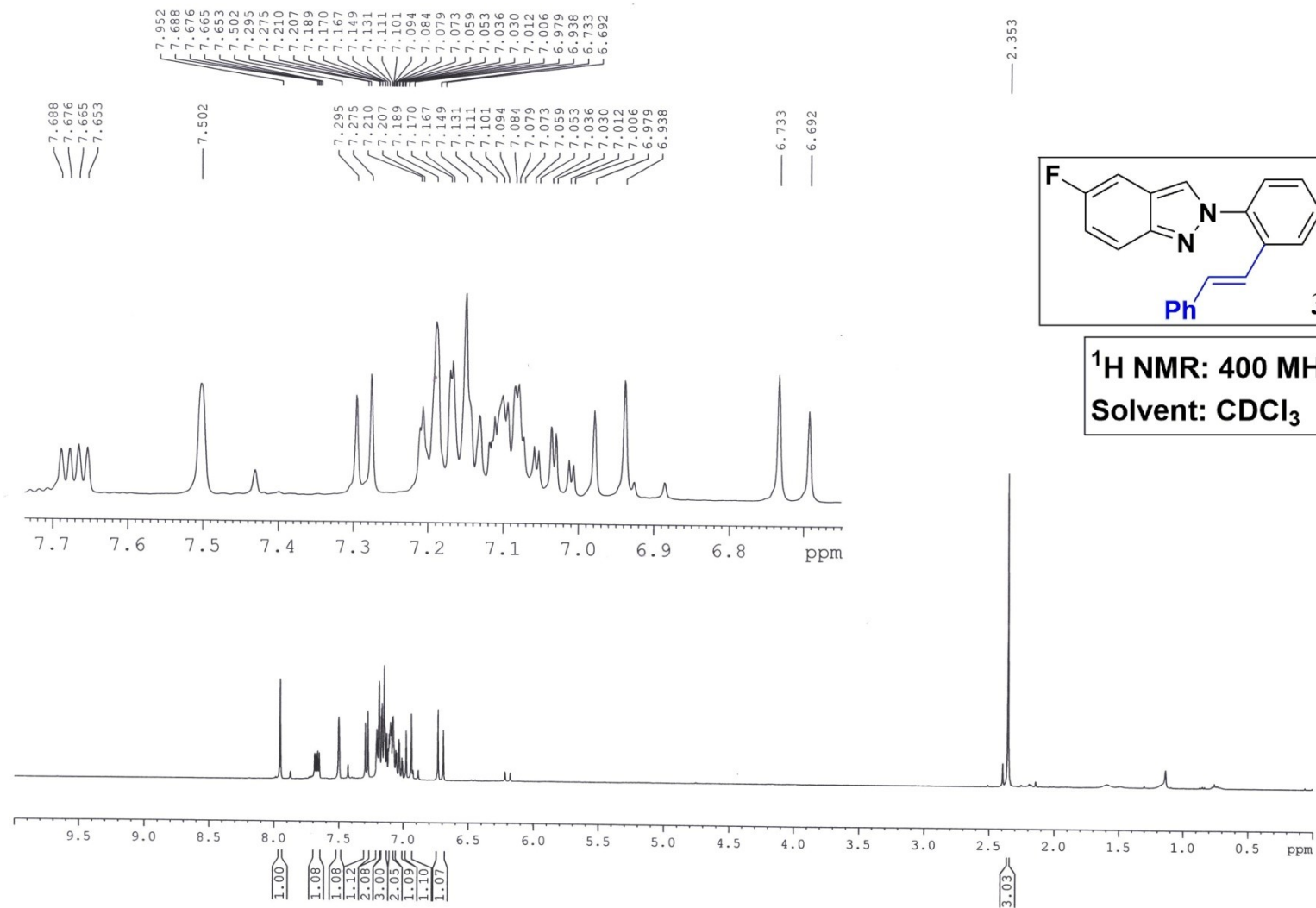
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 23  
 PROCNO 1

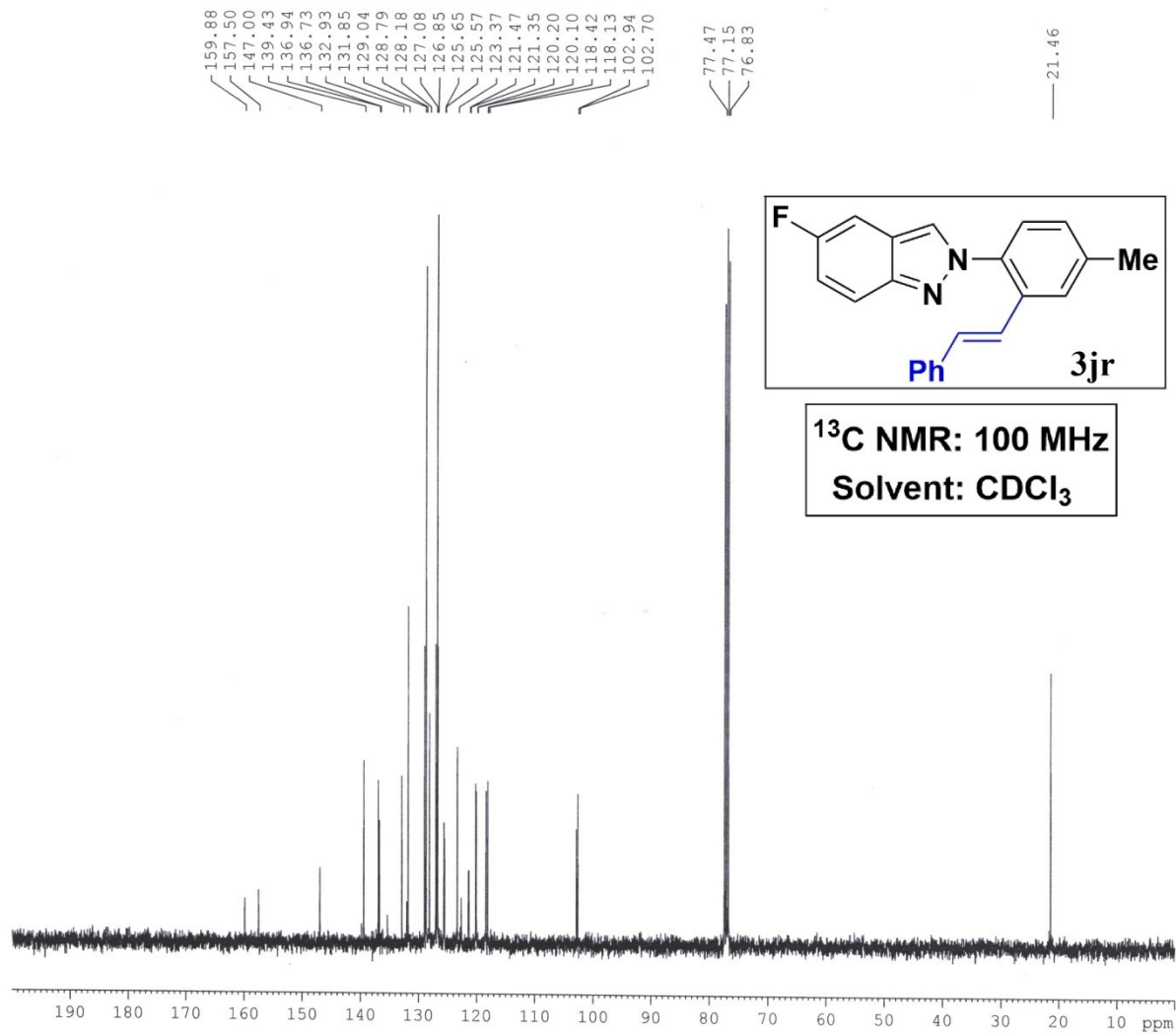
F2 - Acquisition Parameters  
 Date\_ 20210113  
 Time\_ 2.01  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 420  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 120.16  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177859 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





Current Data Parameters  
NAME Dr. A HAJRA-2021-13C  
EXPNO 122  
PROCNO 1

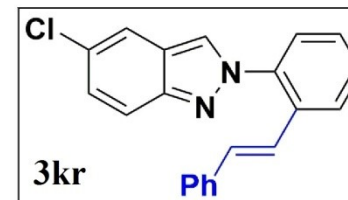
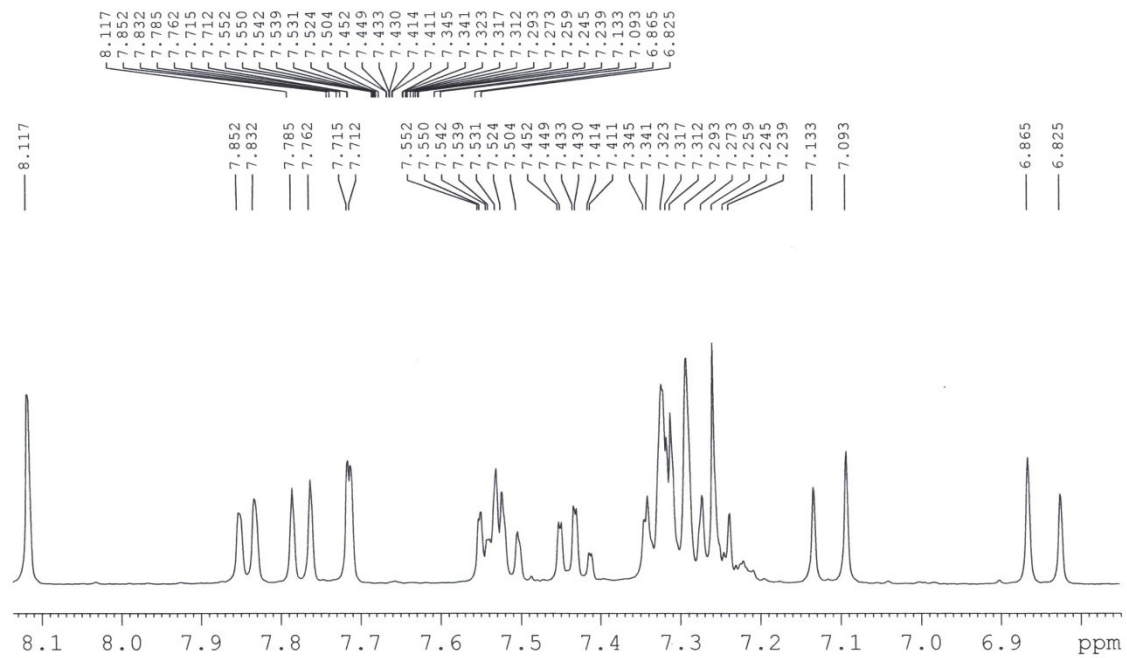
F2 - Acquisition Parameters  
Date\_ 20210304  
Time 18.44  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 120  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 54.07  
DW 20.800 usec  
DE 6.50 usec  
TE 298.6 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDD 1

===== CHANNEL f1 =====  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.0000000 W

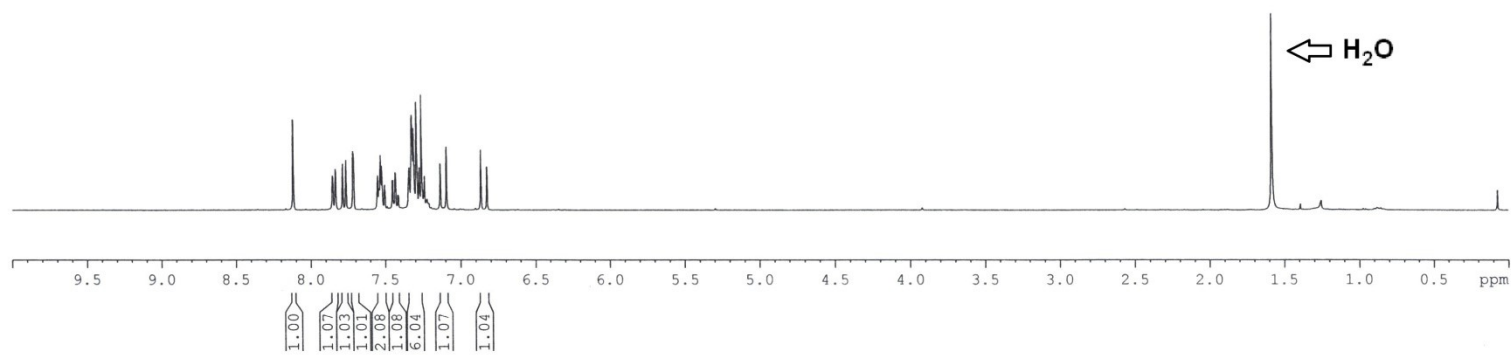
===== CHANNEL f2 =====  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLW2 12.0000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

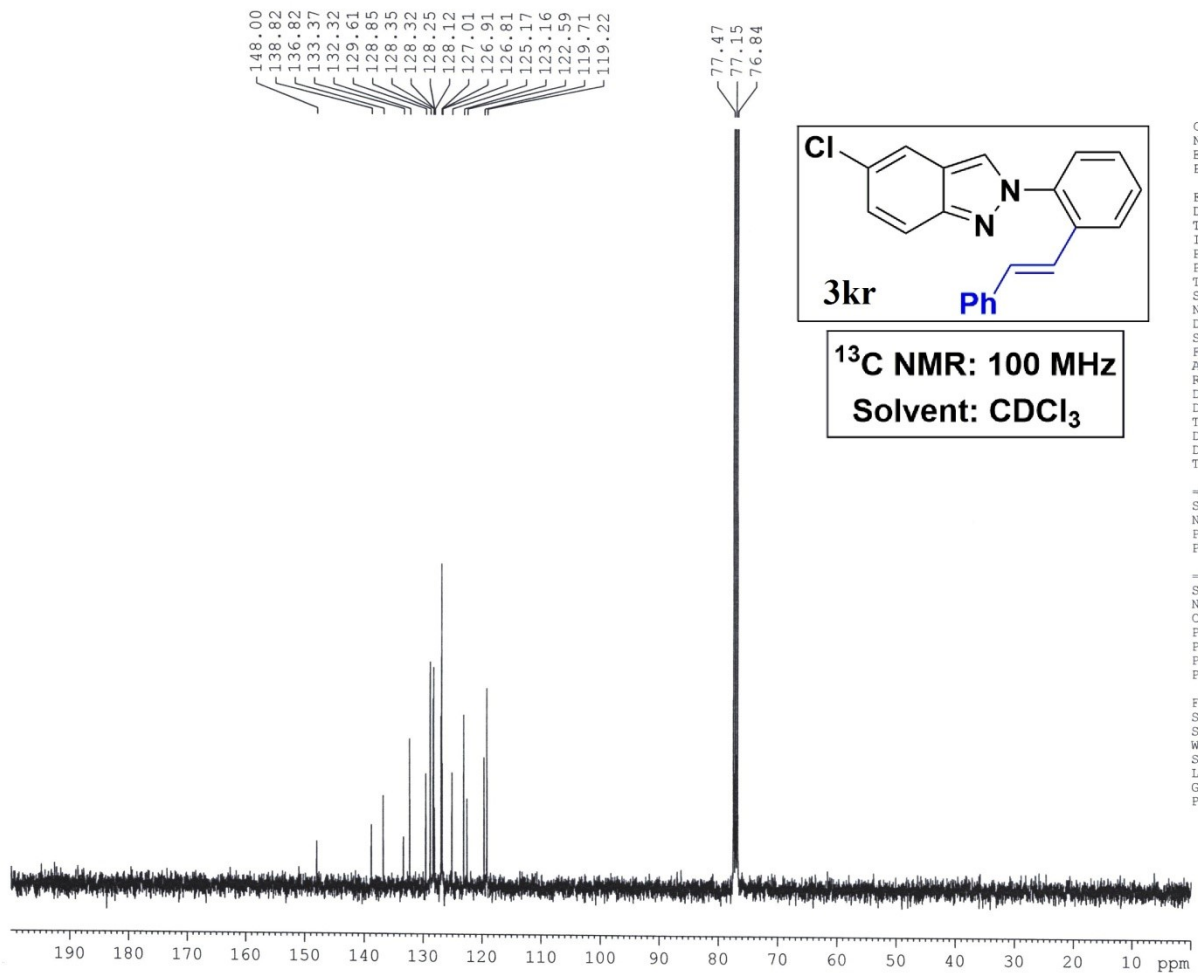
F2 - Processing parameters  
SI 16384  
SF 100.6177888 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





<sup>1</sup>H NMR: 400 MHz  
Solvent: CDCl<sub>3</sub>





```

Current Data Parameters
NAME      Dr. A HAJRA-2021-13C
EXPNO    13
PROCNO   1

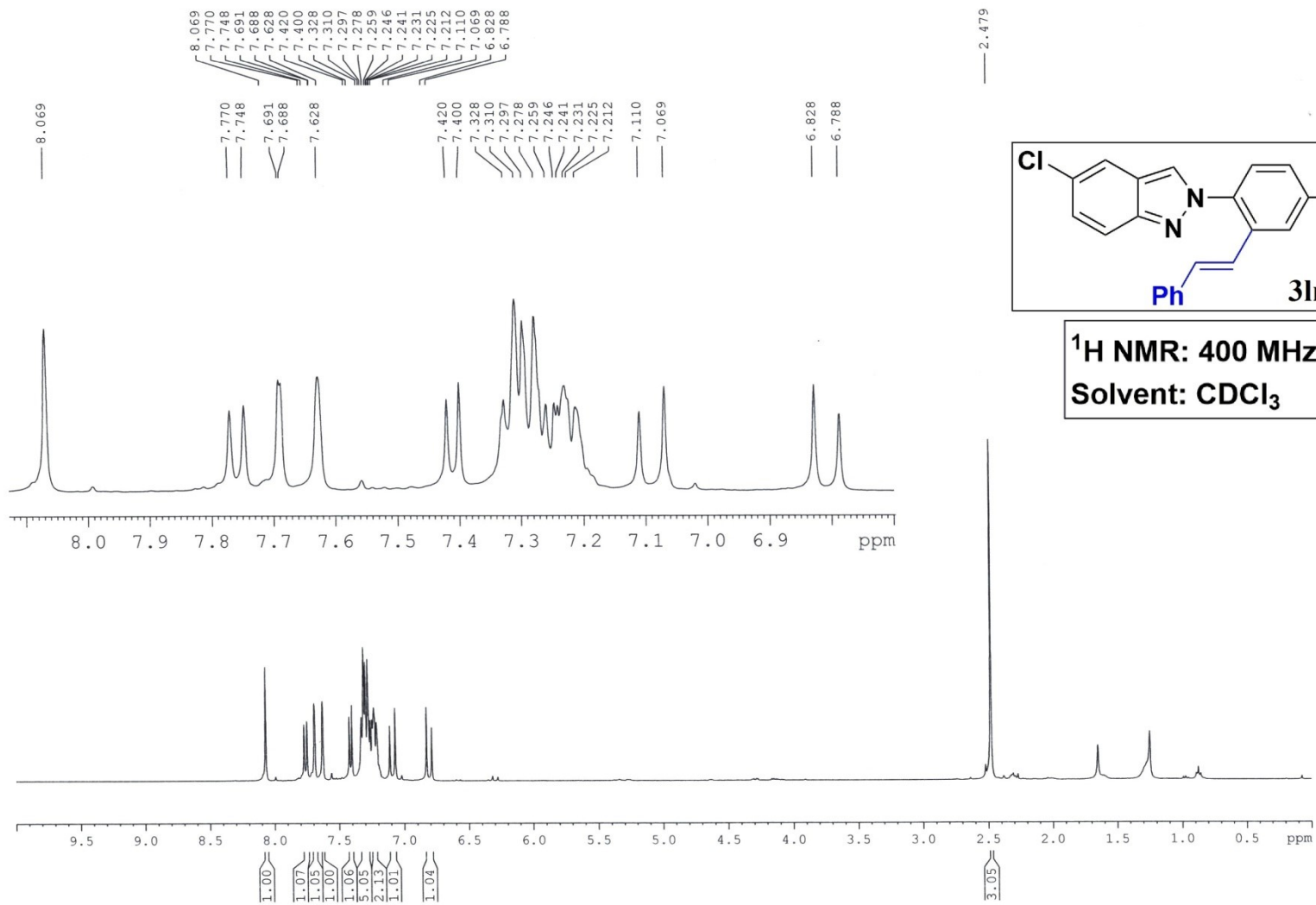
F2 - Acquisition Parameters
Date_    20210106
Time     10.03
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        32768
SOLVENT  CDC13
NS        650
DS        2
SWH       24038.461 Hz
FIDRES    0.733596 Hz
AQ        0.6815744 sec
RG        186.42
DW        20.800 usec
DE        6.50 usec
TE        297.2 K
D1        2.00000000 sec
D11       0.03000000 sec
TDO       1

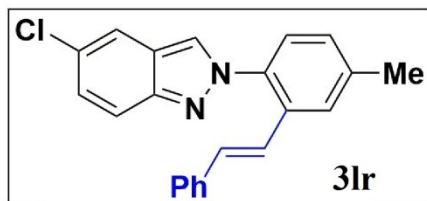
===== CHANNEL f1 =====
SFO1     100.6278588 MHz
NUC1     13C
P1       8.90 usec
PLW1     54.00000000 W

===== CHANNEL f2 =====
SFO2     400.1516006 MHz
NUC2     1H
CPDPRG[2] waltz16
PCPD2    90.00 usec
PLW2     12.00000000 W
PLW12    0.32231000 W
PLW13    0.16212000 W

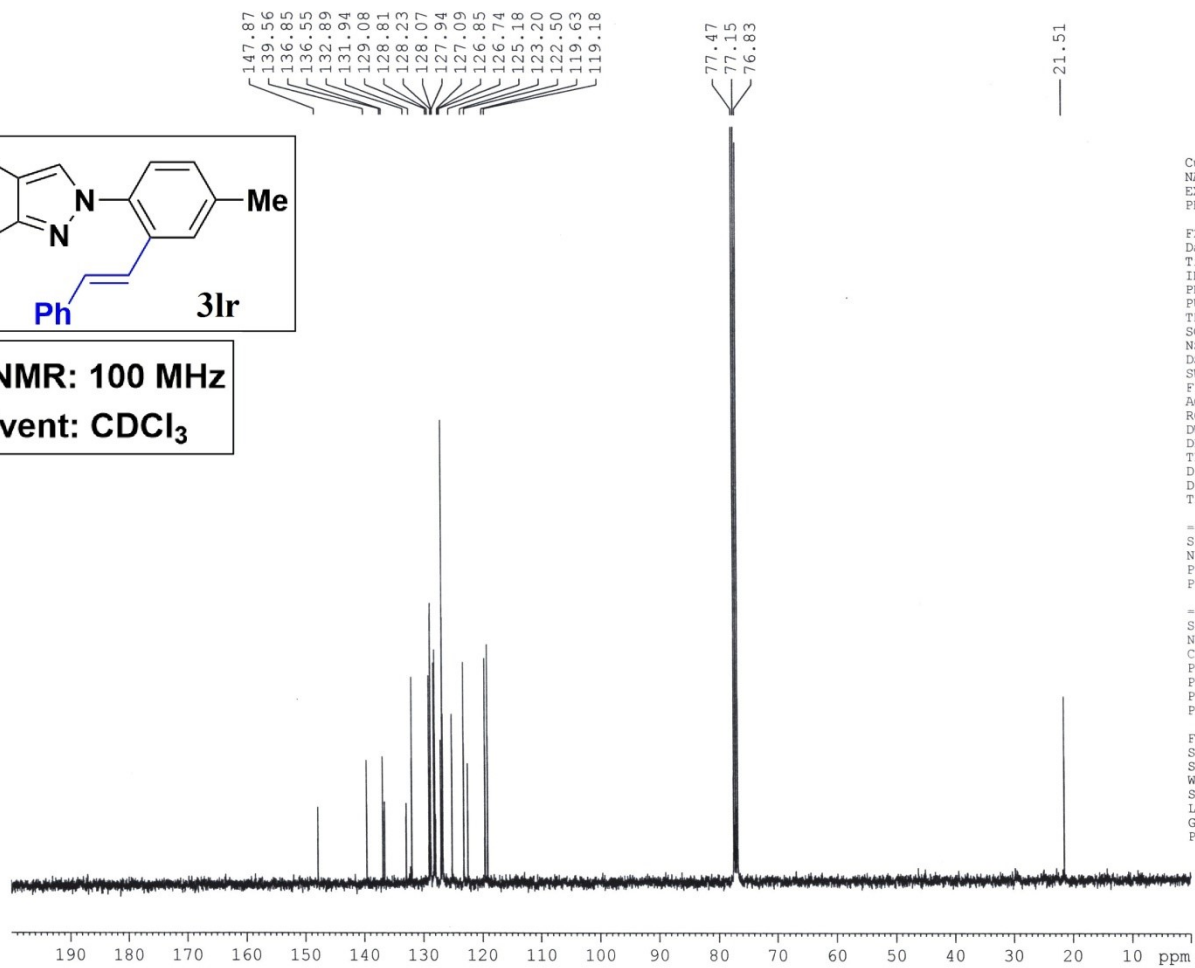
F2 - Processing parameters
SI        16384
SF        100.6177843 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```





**<sup>13</sup>C NMR: 100 MHz**  
**Solvent: CDCl<sub>3</sub>**



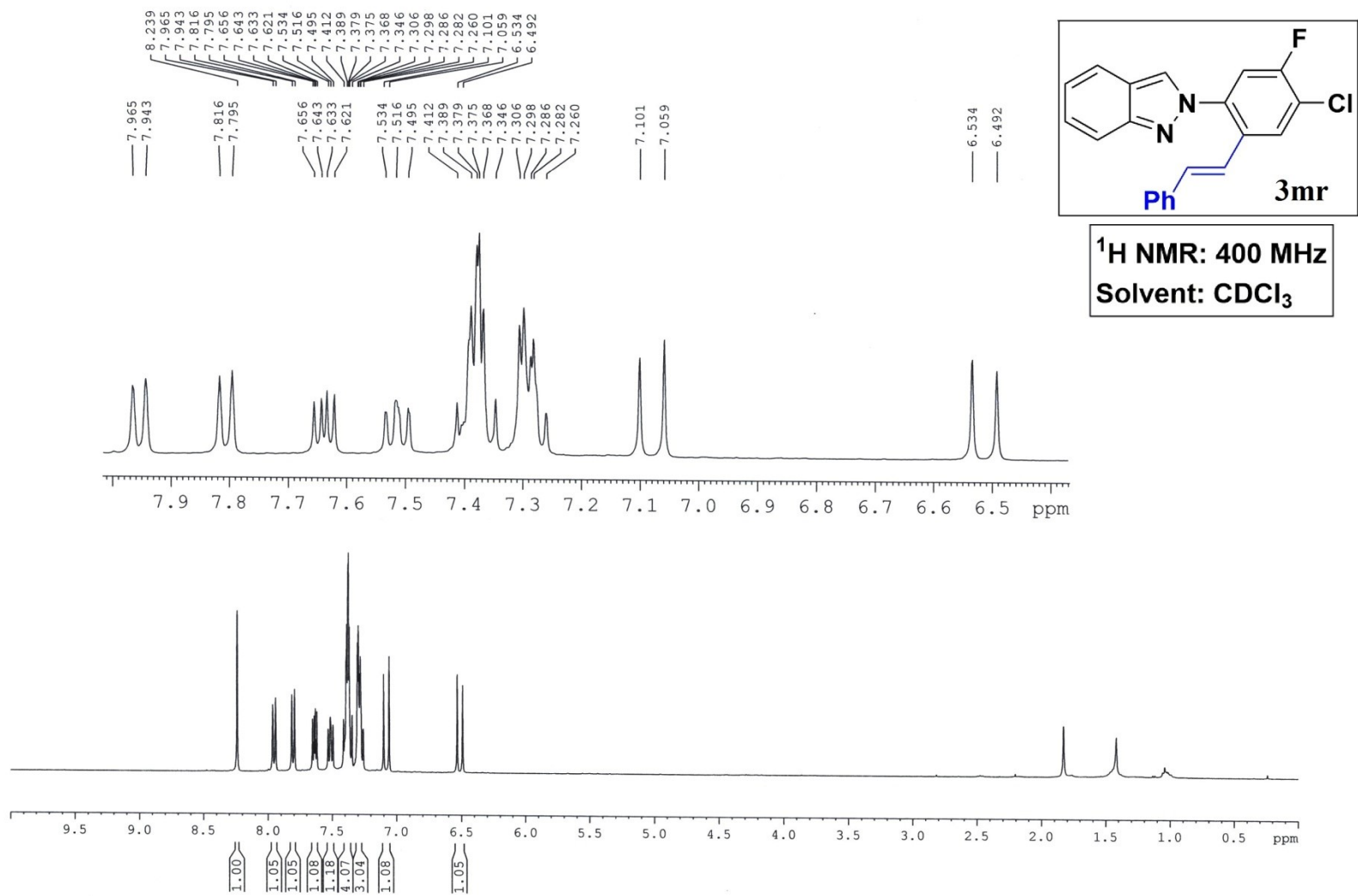
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 58  
 PROCNO 1

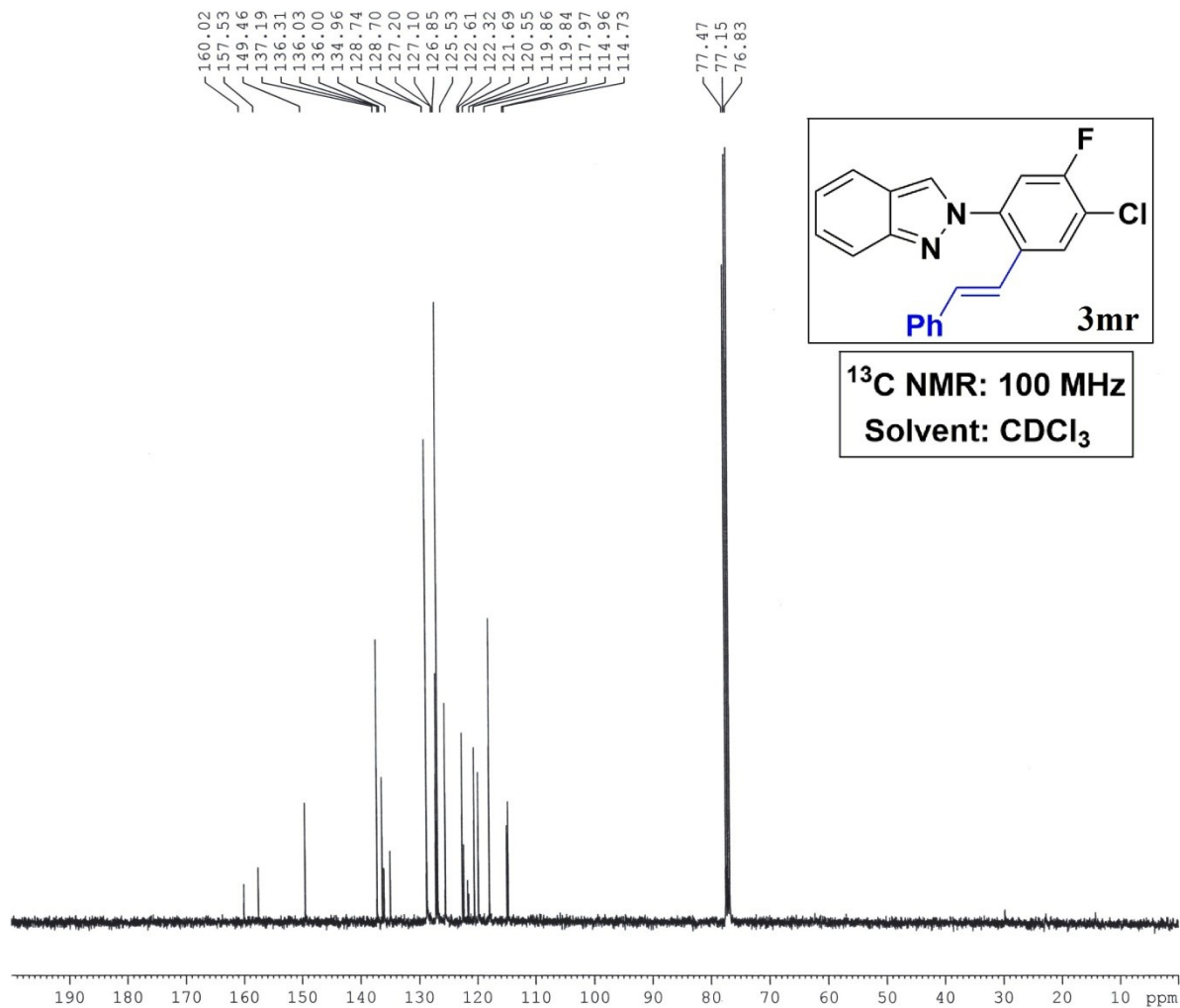
F2 - Acquisition Parameters  
 Date\_ 20210203  
 Time 2.02  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 410  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 93.46  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 291.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

----- CHANNEL f1 -----  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG(2) waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177887 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





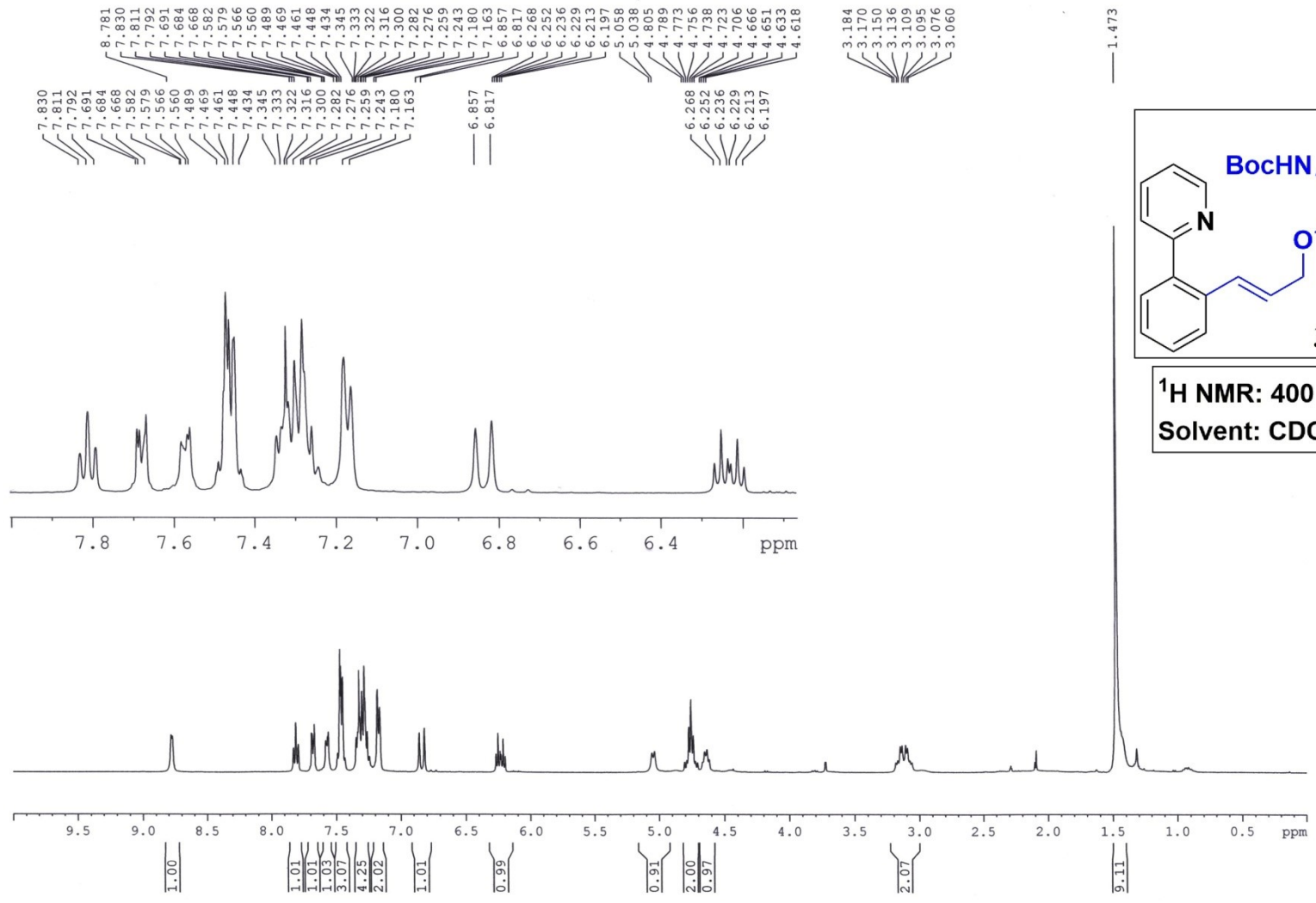
Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 5  
 PROCNO 1

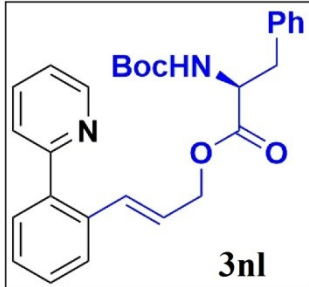
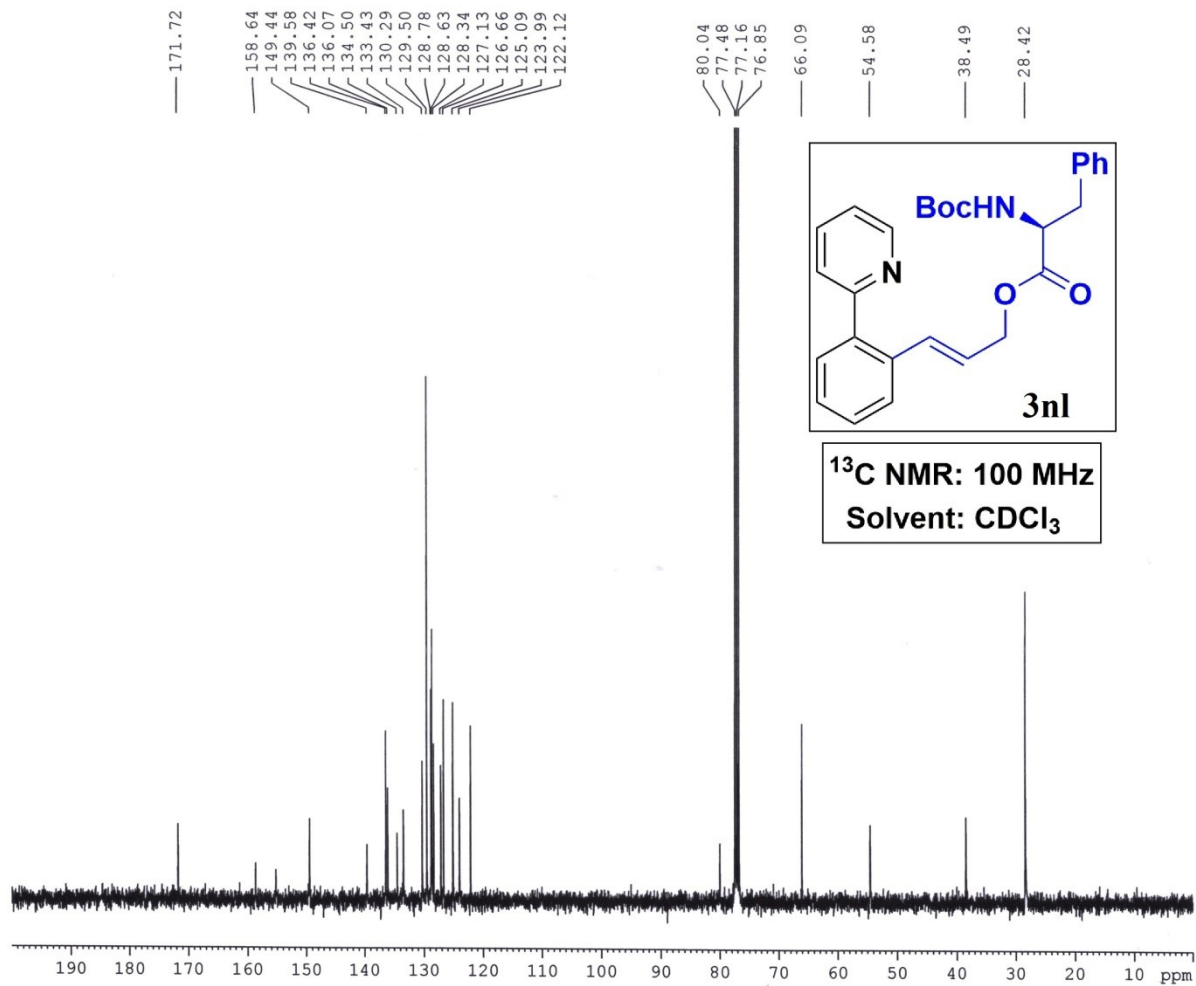
F2 - Acquisition Parameters  
 Date\_ 20210105  
 Time 13.22  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 480  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 106.66  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 293.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177887 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





**<sup>13</sup>C NMR: 100 MHz**  
**Solvent: CDCl<sub>3</sub>**

Current Data Parameters  
NAME Dr. A HAJRA-2021-13C  
EXPNO 463  
PROCNO 1

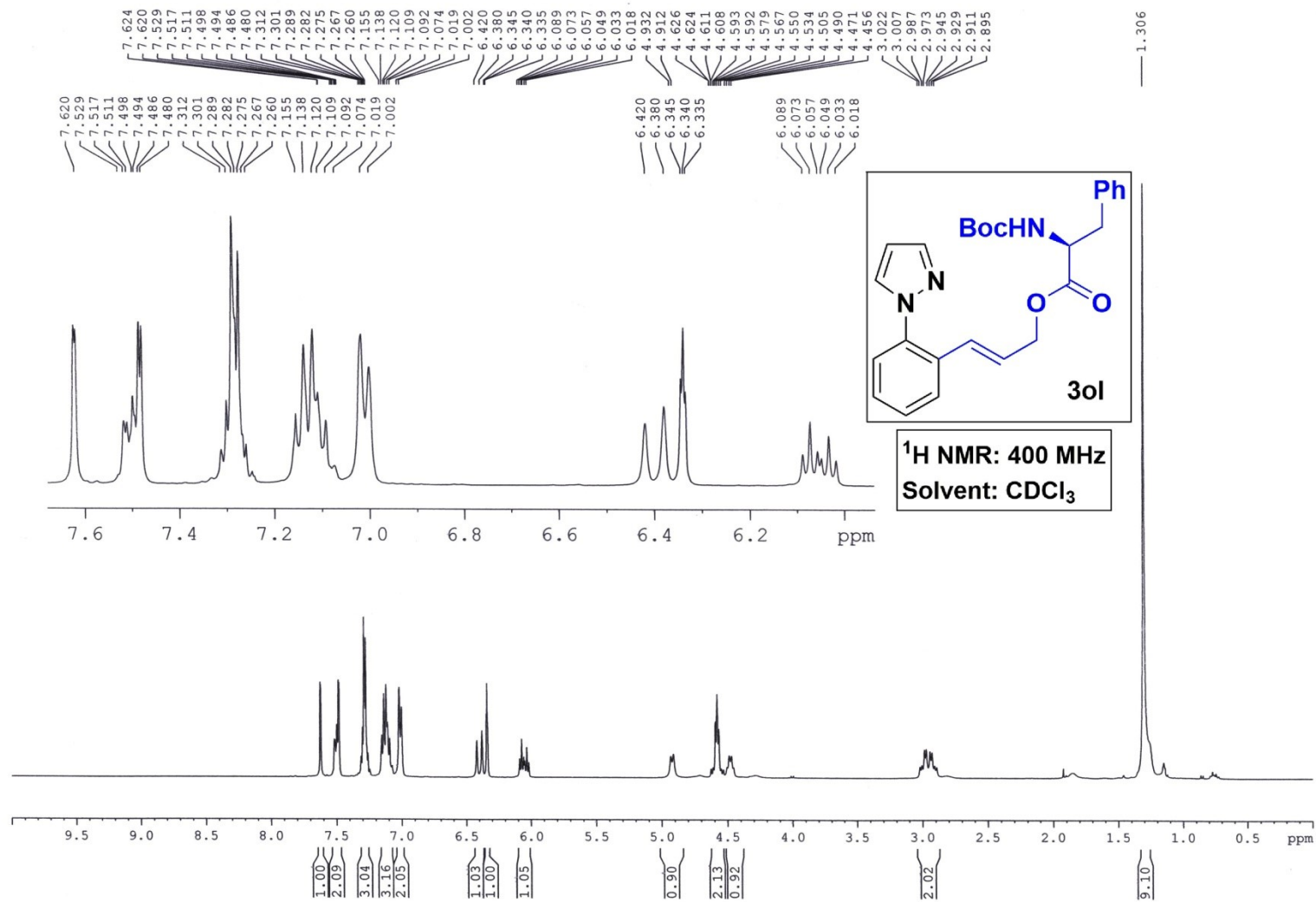
F2 - Acquisition Parameters  
Date\_ 20211128  
Time 19.21  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 400  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 106.66  
DW 20.800 usec  
DE 6.50 usec  
TE 297.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

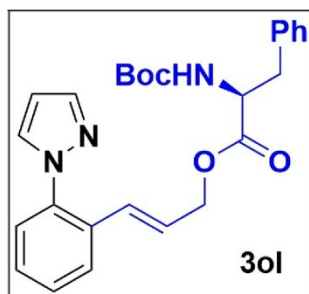
----- CHANNEL f1 -----  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.0000000 W

----- CHANNEL f2 -----  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG12 waltz16  
PCPD2 90.00 usec  
PLW2 12.0000000 W  
PLW12 0.3223100 W  
PLW13 0.1621200 W

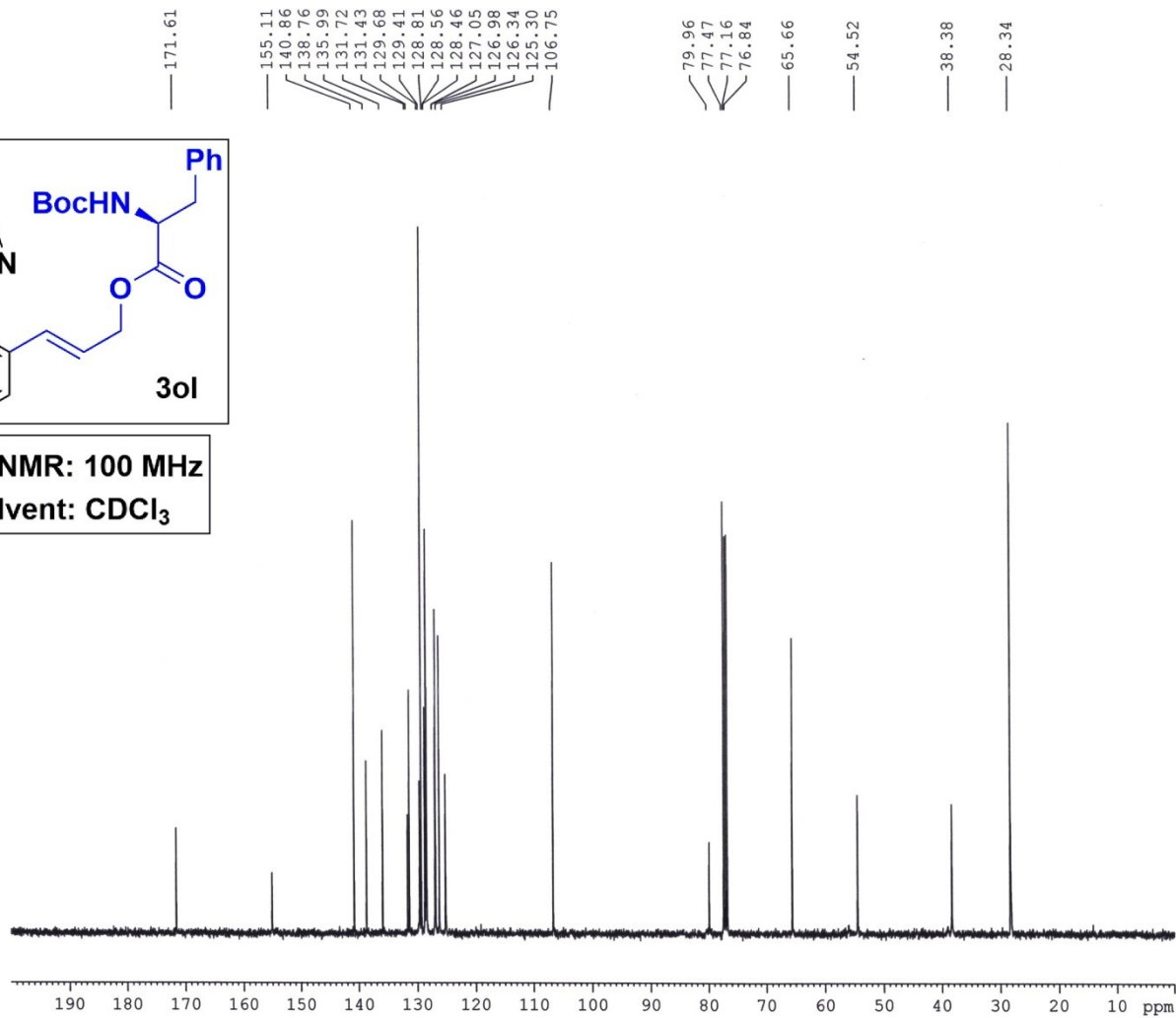
F2 - Processing parameters  
SI 16384  
SF 100.6177855 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40







**<sup>13</sup>C NMR: 100 MHz**  
**Solvent: CDCl<sub>3</sub>**



Current Data Parameters  
 NAME Dr. A HAJRA-2021-13C  
 EXPNO 473  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20211205  
 Time 17.34  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 380  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 30.11  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 PCPD2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177948 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40