

**Electronic Supporting Information**

**Hypervalent Iodine(III)-Mediated Oxidative  
Dearomatization of 2*H*-Indazoles towards Indazolyl  
Indazolones**

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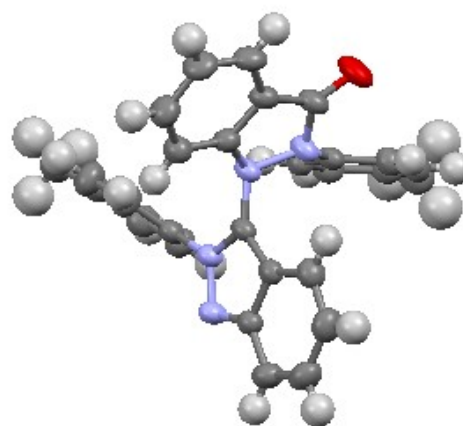
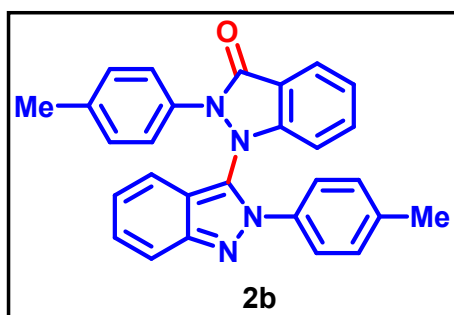
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## 1. General information:

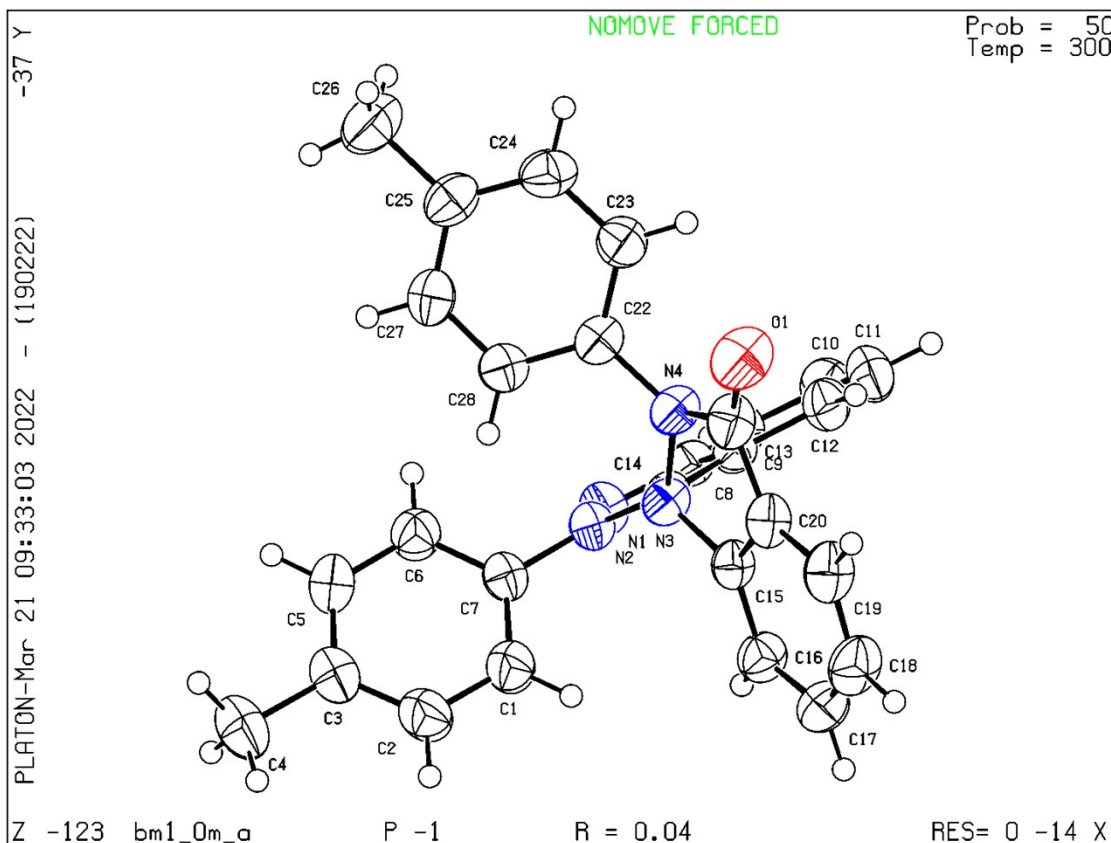
All reagents were purchased from commercial sources and used without further purification.  $^1\text{H}$  NMR spectra were determined on a 400 MHz spectrometer as solutions in  $\text{CDCl}_3$ . Chemical shifts are expressed in parts per million ( $\delta$ ) and the signals were reported as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and coupling constants ( $J$ ) were given in Hz.  $^{13}\text{C}\{^1\text{H}\}$  NMR and  $^{19}\text{F}$  NMR spectra were recorded at 100 MHz and at 376 MHz in  $\text{CDCl}_3$  solution respectively. Chemical shifts are referenced to  $\text{CDCl}_3$  ( $\delta = 7.26$  for  $^1\text{H}$  and  $\delta = 77.16$  for  $^{13}\text{C}\{^1\text{H}\}$  NMR) as internal standard. TLC was done on a silica gel-coated glass slide. All solvents were dried and distilled before use. Commercially available solvents were freshly distilled before the reaction. Melting points (M.p.) were determined after the recrystallization of solid compounds from a solution of dichloromethane/petroleum ether (1:3). All the 2*H*-indazoles were prepared by the reported methods.<sup>1</sup>

## 2. Structure determination (X-ray crystallographic data for 2b):

The brown crystal of **2b** was obtained by crystallization from a solution in dichloromethane/petroleum ether after purification by column chromatography. The chemical formula of compound **2b**:  $\text{C}_{28}\text{H}_{22}\text{N}_4\text{O}$ .



**X-ray structure of 2b**



View of ORTEP diagram for the crystal structure of the compound **2,2'-Di-*p*-tolyl-2'*H*-[1,3'-biindazol]-3(2*H*)-one (2b)** (Thermal ellipsoid contour at 50% probability level).

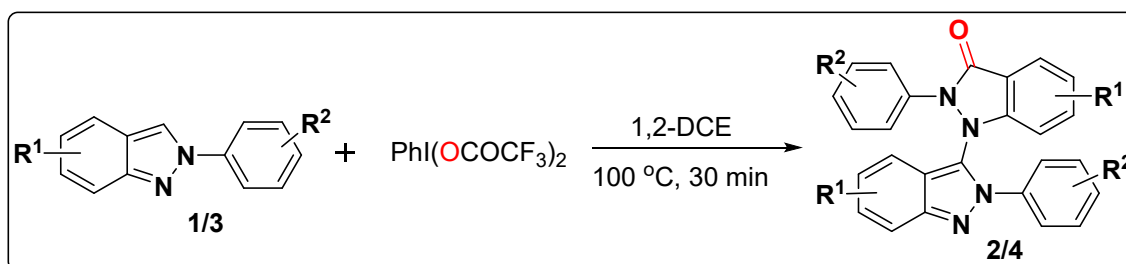
<b>Wavelength</b>	0.71073 Å	
<b>Formula</b>	C <sub>28</sub> H <sub>22</sub> N <sub>4</sub> O	
<b>Crystal system</b>	Triclinic	
<b>Space group</b>	P -1	
<b>Unit cell dimensions</b>	a = 9.1723(4) Å	α = 65.036(10)°
	b = 10.9238(5) Å	β = 78.334(10)°
	c = 12.8796(6) Å	γ = 71.536(10)°
<b>Volume</b>	1106.17 Å <sup>3</sup>	
<b>Z</b>	2	



<b>R-factor (%)</b>	3.91
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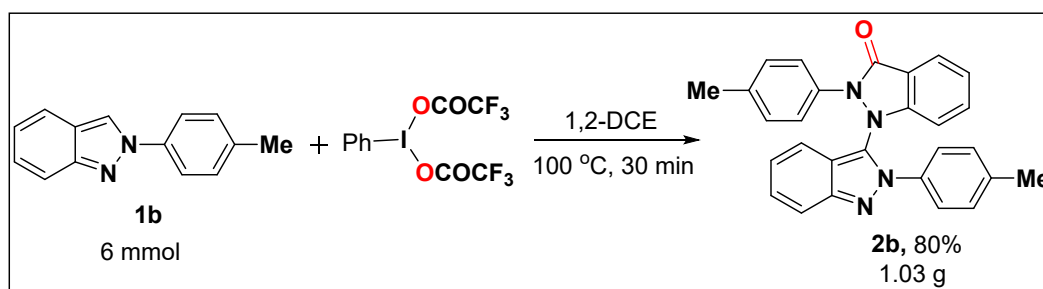
The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication with a CCDC reference number CCDC 2174840.

### 3. General experimental procedure for the synthesis of 2a-4k:



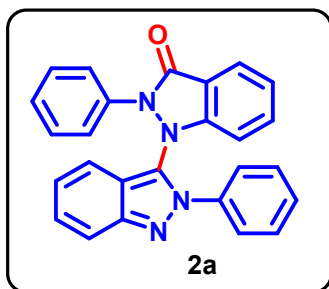
2-Arylidazoles (**1/3**, 0.2 mmol) and PIFA (0.4 mmol, 172.0 mg) in 2.0 mL 1,2-DCE solvent were added to an oven-dried reaction tube equipped with a magnetic stirrer bar, and the reaction tube was heated in an oil bath at 100 °C for 30 min in an open atmosphere. The progress of the reaction was monitored by TLC. After completion of the reaction, the reaction was cooled to room temperature and extracted with DCM (10 mL). The combined organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure to get the crude residue which was purified by column chromatography on silica gel (60–120 mesh) using a mixture of petroleum ether and ethyl acetate as an eluent to afford their corresponding products (**2/4**).

### 4. Gram scale synthesis of 2,2'-Di-*p*-tolyl-2'*H*-[1,3'-biindazol]-3(2*H*)-one (**2b**):

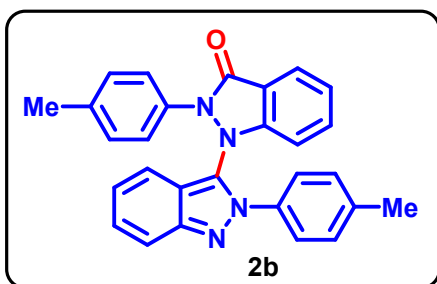


To an oven dried 100 mL round bottom flask equipped with a stir bar were charged with 2-(*p*-tolyl)-2*H*-indazole (**1b**, 6.0 mmol, 1.24 g) and PIFA (12 mmol, 5.16 g) in 40 mL 1,2-DCE were added, and the round bottom flask was heated in an oil bath at 100 °C for 30 min in an open atmosphere. The progress of the reaction was monitored by TLC. After completion of the reaction, the reaction was cooled to room temperature and extracted with 50 mL DCM. The combined organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure to get the crude residue which was purified by column chromatography on silica gel (60–120 mesh) using a mixture of petroleum ether and ethyl acetate (84 : 16) as an eluent to afford the product **2b** (80%, 1.03 g) as brown solid.

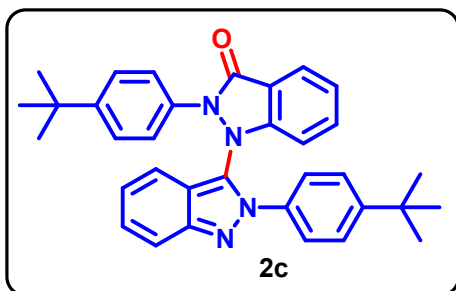
## 5. Characterization data of the synthesized compounds (2a–4k):



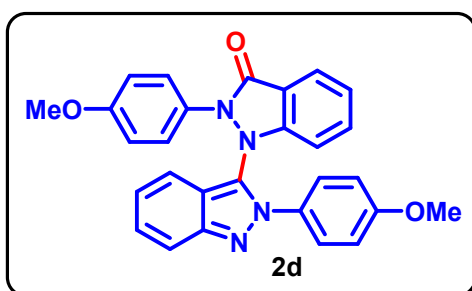
**2,2'-Diphenyl-2'*H*-[1,3'-biindazol]-3(2*H*)-one (2a):** Grey solid (32.5 mg, 81%); M.p. 150-151 °C;  $R_f = 0.50$  (PE : EA = 70 : 30);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.05 (d,  $J = 8.0$  Hz, 1H), 7.72 (d,  $J = 8.8$  Hz, 1H), 7.64-7.60 (m, 1H), 7.47-7.37 (m, 4H), 7.35-7.31 (m, 1H), 7.29-7.27 (m, 3H), 7.13-7.07 (m, 5H), 6.91-6.88 (m, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  161.5, 149.0, 148.2, 138.5, 134.1, 133.7, 129.4, 129.1, 129.0, 128.9, 127.9, 127.4, 125.6, 125.04, 125.00, 124.2, 124.1, 118.9, 118.58, 118.55, 118.2, 112.1; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{26}\text{H}_{19}\text{N}_4\text{O}]^+$ : 403.1553; found: 403.1559.



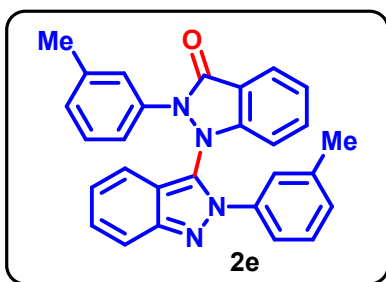
**2,2'-Di-*p*-tolyl-2'*H*-[1,3'-biindazol]-3(2*H*)-one (2b):** Brown solid (37.0 mg, 86%); M.p. 165-166 °C;  $R_f = 0.45$  (PE : EA = 75 : 25);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.04 (d,  $J = 8.0$  Hz, 1H), 7.71 (d,  $J = 8.4$  Hz, 1H), 7.62-7.58 (m, 1H), 7.37 (d,  $J = 7.2$  Hz, 1H), 7.34-7.29 (m, 1H), 7.27-7.25 (m, 1H), 7.20-7.15 (m, 4H), 7.11-7.07 (m, 2H), 6.90 (d,  $J = 8.4$  Hz, 2H), 6.78 (d,  $J = 8.4$  Hz, 2H), 2.41 (s, 3H), 2.22 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  161.4, 148.8, 148.0, 139.5, 138.1, 136.1, 133.5, 131.4, 129.66, 129.62, 128.7, 127.2, 125.7, 124.8, 124.7, 124.0, 123.9, 118.8, 118.59, 118.50, 118.2, 112.0, 21.3, 21.1; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{28}\text{H}_{23}\text{N}_4\text{O}]^+$ : 431.1866; found: 431.1874.



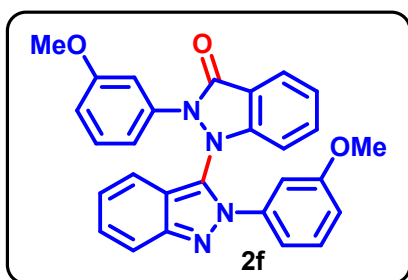
**2,2'-Bis(4-(*tert*-butyl)phenyl)-2'*H*-[1,3'-biindazol]-3(2*H*)-one (2c):** Brown solid (46.3 mg, 90%); M.p. 171-172 °C;  $R_f = 0.55$  (PE : EA = 80 : 20);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.05 (d,  $J = 8.0$  Hz, 1H), 7.73 (d,  $J = 8.8$  Hz, 1H), 7.61-7.57 (m, 1H), 7.37-7.30 (m, 4H), 7.17 (d,  $J = 8.8$  Hz, 3H), 7.09-7.06 (m, 4H), 6.74-6.72 (m, 2H), 1.35 (s, 9H), 1.22 (s, 9H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  161.7, 152.5, 151.3, 148.7, 148.2, 136.0, 133.4, 131.5, 128.7, 127.2, 126.0, 125.99, 125.90, 124.8, 124.6, 123.9, 123.8, 118.9, 118.6, 118.36, 118.34, 112.0, 34.9, 34.6, 31.4, 31.3; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{34}\text{H}_{35}\text{N}_4\text{O}]^+$ : 515.2805; found: 515.2778.



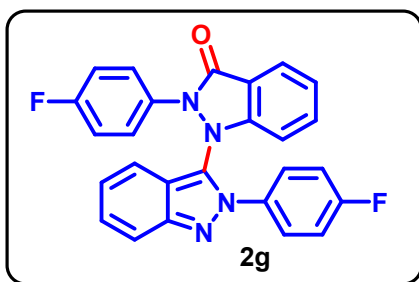
**2,2'-Bis(4-methoxyphenyl)-2'*H*-[1,3'-biindazol]-3(2*H*)-one (2d):** Grey solid (42.0 mg, 91%); M.p. 181-182 °C;  $R_f = 0.40$  (PE : EA = 55 : 35);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.04 (d,  $J = 7.6$  Hz, 1H), 7.72 (d,  $J = 8.8$  Hz, 1H), 7.61-7.57 (m, 1H), 7.37-7.30 (m, 2H), 7.21-7.18 (m, 3H), 7.10-7.06 (m, 2H), 6.89-6.85 (m, 2H), 6.80-6.76 (m, 2H), 6.64-6.60 (m, 2H), 3.84 (s, 3H), 3.71 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  161.7, 160.1, 159.5, 148.7, 148.0, 133.4, 131.6, 128.4, 128.1, 127.2, 126.8, 126.3, 124.9, 124.8, 124.0, 123.8, 118.8, 118.5, 118.1, 114.3, 114.2, 111.9, 55.7, 55.5; Anal. Calcd for  $\text{C}_{28}\text{H}_{22}\text{N}_4\text{O}_3$ : C, 72.71; H, 4.79; N, 12.11%; Found C, 72.51; H, 4.84; N, 12.20%.



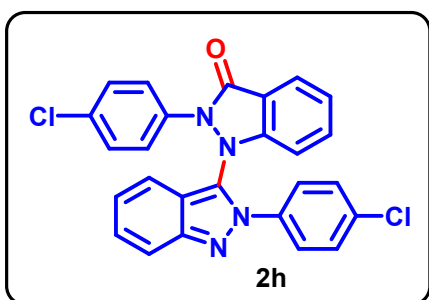
**2,2'-Di-*m*-tolyl-2'*H*-[1,3'-biindazol]-3(2*H*)-one (2e):** Brown solid (35.7 mg, 83%); M.p. 144-145 °C;  $R_f = 0.50$  (PE : EA = 78 : 22);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.22 (d,  $J = 7.6$  Hz, 1H), 7.89 (d,  $J = 8.8$  Hz, 1H), 7.81-7.77 (m, 1H), 7.55 (t,  $J = 7.6$  Hz, 1H), 7.51-7.47 (m, 1H), 7.45-7.42 (m, 3H), 7.30-7.27 (m, 3H), 7.20 (s, 1H), 7.18-7.14 (m, 1H), 7.11 (d,  $J = 7.6$  Hz, 1H), 6.91 (d,  $J = 7.6$  Hz, 1H), 6.85 (s, 1H), 2.50 (s, 3H), 2.25 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  161.4, 149.1, 148.1, 139.3, 138.8, 138.5, 134.0, 133.6, 130.0, 129.0, 128.8, 128.7, 128.6, 127.3, 126.3, 125.88, 125.86, 124.8, 124.0, 122.8, 122.0, 118.8, 118.65, 118.62, 118.2, 112.1, 21.3, 21.2; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{28}\text{H}_{23}\text{N}_4\text{O}]^+$ : 431.1866; found: 431.1870.



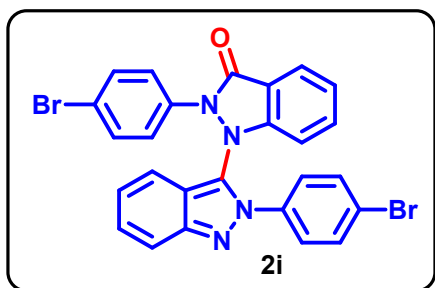
**2,2'-Bis(3-methoxyphenyl)-2'*H*-[1,3'-biindazol]-3(2*H*)-one (2f):** Yellow solid (38.8 mg, 84%); M.p. 136-137 °C;  $R_f = 0.40$  (PE : EA = 60 : 40);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.04 (d,  $J = 8.0$  Hz, 1H), 7.73 (d,  $J = 9.2$  Hz, 1H), 7.64-7.60 (m, 1H), 7.39-7.32 (m, 3H), 7.26 (t,  $J = 8.0$  Hz, 1H), 7.15-7.11 (m, 2H), 7.03-6.96 (m, 2H), 6.86-6.84 (m, 1H), 6.76-6.75 (m, 1H), 6.69-6.66 (m, 1H), 6.54 (d,  $J = 7.6$  Hz, 1H), 6.51-6.50 (m, 1H), 3.69 (s, 3H), 3.50 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  161.3, 160.1, 159.8, 148.8, 148.1, 139.5, 135.1, 133.7, 129.7, 129.6, 128.8, 127.5, 125.0, 124.2, 124.1, 118.9, 118.8, 118.4, 118.2, 117.7, 117.0, 115.9, 114.6, 112.0, 110.4, 110.3, 55.5, 55.1; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{28}\text{H}_{23}\text{N}_4\text{O}_3]^+$ : 463.1765; found: 463.1781.



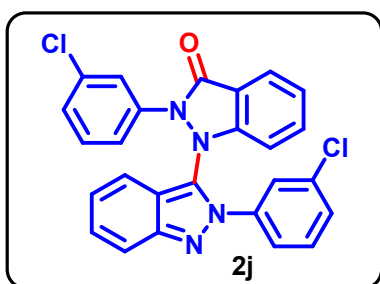
**2,2'-Bis(4-fluorophenyl)-2'H-[1,3'-biindazol]-3(2H)-one (2g):** Brown solid (34.2 mg, 78%); M.p. 178-179 °C;  $R_f = 0.50$  (PE : EA = 80 : 20);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.04 (d,  $J = 7.6$  Hz, 1H), 7.71 (d,  $J = 8.8$  Hz, 1H), 7.64-7.60 (m, 1H), 7.39 (t,  $J = 7.6$  Hz, 1H), 7.35-7.31 (m, 1H), 7.28-7.24 (m, 2H), 7.19 (d,  $J = 8.4$  Hz, 1H), 7.12-7.06 (m, 4H), 6.86-6.78 (m, 4H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  162.7 ( $J_{\text{C-F}} = 249$  Hz), 162.0 ( $J_{\text{C-F}} = 248$  Hz), 161.8, 149.0, 148.3, 134.66, 134.63, 133.9, 130.26, 130.23, 128.7, 128.0 ( $J_{\text{C-F}} = 8$  Hz), 127.6, 126.8 ( $J_{\text{C-F}} = 9$  Hz), 125.0, 124.4 ( $J_{\text{C-F}} = 10$  Hz), 119.0, 118.4, 118.0, 116.2 ( $J_{\text{C-F}} = 22$  Hz), 116.1 ( $J_{\text{C-F}} = 23$  Hz), 112.0;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ):  $\delta$  -110.7, -112.0; Anal. Calcd for  $\text{C}_{26}\text{H}_{16}\text{F}_2\text{N}_4\text{O}$ : C, 71.23; H, 3.68; N, 12.78%; Found C, 71.39; H, 3.65; N, 12.85%.



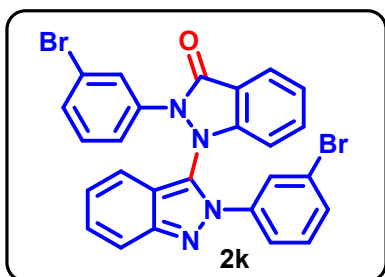
**2,2'-Bis(4-chlorophenyl)-2'H-[1,3'-biindazol]-3(2H)-one (2h):** Brown solid (35.3 mg, 75%); M.p. 199-200 °C;  $R_f = 0.50$  (PE : EA = 80 : 20);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.06 (d,  $J = 7.6$  Hz, 1H), 7.72 (d,  $J = 8.8$  Hz, 1H), 7.66-7.62 (m, 1H), 7.43-7.38 (m, 3H), 7.36-7.32 (m, 1H), 7.30-7.27 (m, 2H), 7.23 (d,  $J = 8.4$  Hz, 1H), 7.14-7.07 (m, 4H), 6.87-6.83 (m, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  161.5, 149.1, 148.4, 137.0, 135.4, 134.1, 133.8, 132.7, 129.4, 129.3, 128.8, 127.8, 126.6, 126.0, 125.1, 124.6, 124.5, 119.0, 118.5, 118.4, 118.0, 112.1; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{26}\text{H}_{17}\text{Cl}_2\text{N}_4\text{O}]^+$ : 471.0774; found: 471.0763.



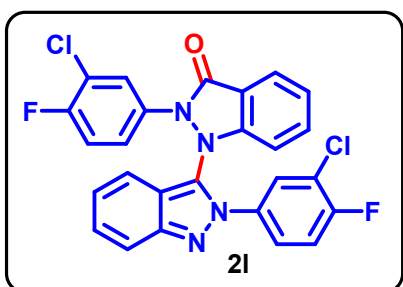
**2,2'-Bis(4-bromophenyl)-2'H-[1,3'-biindazol]-3(2H)-one (2i):** Black solid (36.9 mg, 66%); M.p. 204-205 °C;  $R_f = 0.50$  (PE : EA = 84 : 16);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.06 (d,  $J = 7.6$  Hz, 1H), 7.72 (d,  $J = 8.8$  Hz, 1H), 7.66-7.62 (m, 1H), 7.58-7.54 (m, 2H), 7.41 (t,  $J = 7.6$  Hz, 1H), 7.36-7.32 (m, 1H), 7.25-7.21 (m, 5H), 7.13-7.10 (m, 2H), 6.81-6.78 (m, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  161.5, 149.0, 148.4, 137.5, 134.1, 133.3, 132.4, 132.28, 132.20, 127.8, 126.8, 126.2, 125.2, 124.66, 124.62, 123.4, 121.8, 119.0, 118.5, 118.4, 118.0, 112.1; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{26}\text{H}_{17}\text{Br}_2\text{N}_4\text{O}]^+$ : 558.9764; found: 558.9764.



**2,2'-Bis(3-chlorophenyl)-2'H-[1,3'-biindazol]-3(2H)-one (2j):** Brown solid (34.8 mg, 74%); M.p. 183-184 °C;  $R_f = 0.50$  (PE : EA = 75 : 25);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.06 (d,  $J = 7.6$  Hz, 1H), 7.72 (d,  $J = 8.8$  Hz, 1H), 7.68-7.64 (m, 1H), 7.48-7.40 (m, 3H), 7.38-7.35 (m, 2H), 7.32-7.28 (m, 1H), 7.20 (d,  $J = 8.4$  Hz, 1H), 7.14-7.05 (m, 4H), 6.90-6.88 (m, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  161.6, 149.4, 148.4, 139.3, 135.3, 135.2, 134.7, 134.2, 130.1, 129.9, 129.7, 129.2, 128.1, 127.8, 125.6, 125.3, 125.2, 124.7, 124.6, 123.4, 122.9, 119.0, 118.4, 118.3, 118.0, 112.3; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{26}\text{H}_{17}\text{Cl}_2\text{N}_4\text{O}]^+$ : 471.0774; found: 471.0776.

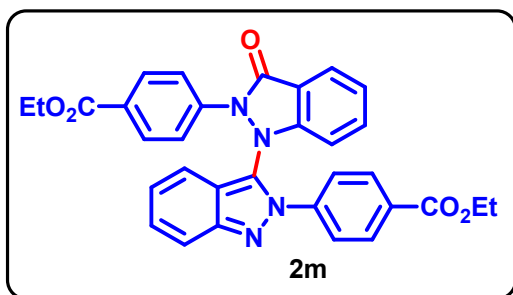


**2,2'-Bis(3-bromophenyl)-2'H-[1,3'-biindazol]-3(2H)-one (2k):** Black solid (38.6 mg, 69%); M.p. 192-193 °C;  $R_f = 0.55$  (PE : EA = 75 : 25);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.06 (d,  $J = 7.6$  Hz, 1H), 7.72 (d,  $J = 8.8$  Hz, 1H), 7.68-7.64 (m, 1H), 7.63-7.60 (m, 1H), 7.49 (d,  $J = 2.0$  Hz, 1H), 7.42 (t,  $J = 7.6$  Hz, 1H), 7.36-7.28 (m, 4H), 7.21 (d,  $J = 8.8$  Hz, 1H), 7.14-7.10 (m, 2H), 7.04-7.00 (m, 2H), 6.94 (d,  $J = 8.0$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  161.6, 149.5, 148.5, 139.4, 135.4, 134.2, 132.7, 131.0, 130.4, 130.2, 129.2, 128.5, 128.1, 127.8, 125.2, 124.75, 124.71, 124.0, 123.3, 123.1, 122.5, 119.0, 118.4, 118.3, 118.0, 112.3; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{26}\text{H}_{17}\text{Br}_2\text{N}_4\text{O}]^+$ : 558.9764; found: 558.9767.

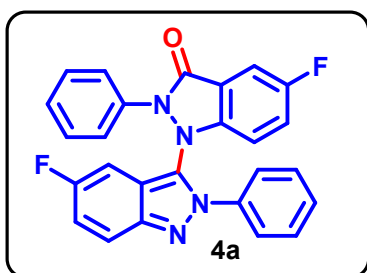


**2,2'-Bis(3-chloro-4-fluorophenyl)-2'H-[1,3'-biindazol]-3(2H)-one (2l):** Brown solid (32.9 mg, 65%); M.p. 143-144 °C;  $R_f = 0.45$  (PE : EA = 85 : 15);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.06 (d,  $J = 8.0$  Hz, 1H), 7.72 (d,  $J = 8.8$  Hz, 1H), 7.70-7.65 (m, 1H), 7.46-7.42 (m, 2H), 7.37-7.33 (m, 1H), 7.32-7.28 (m, 1H), 7.25-7.20 (m, 1H), 7.13-7.11 (m, 3H), 6.97-6.91 (m, 2H), 6.89-6.85 (m, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  161.9, 158.5 ( $J_{\text{C-F}} = 252$  Hz), 155.3 ( $J_{\text{C-F}} = 206$  Hz), 149.5, 148.5, 134.9, 134.4, 130.9, 129.2, 128.3 ( $J_{\text{C-F}} = 10$  Hz), 128.07, 128.04, 127.7, 125.8 ( $J_{\text{C-F}} = 8$  Hz), 125.3, 124.7 ( $J_{\text{C-F}} = 22$  Hz), 124.5 ( $J_{\text{C-F}} = 8$  Hz), 122.4 ( $J_{\text{C-F}} = 20$  Hz), 119.1, 118.4, 118.2, 117.9, 117.2, 117.0 ( $J_{\text{C-F}} = 9$  Hz), 116.8, 112.3;  $^{19}\text{F NMR}$  (376 MHz,  $\text{CDCl}_3$ ):  $\delta$  -112.5, -114.2; Anal. Calcd for  $\text{C}_{26}\text{H}_{14}\text{Cl}_2\text{F}_2\text{N}_4\text{O}$ : C, 61.56; H, 2.78; N, 11.04%; Found C, 61.77; H, 2.72; N, 10.96%.

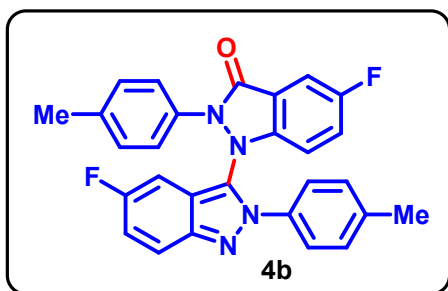




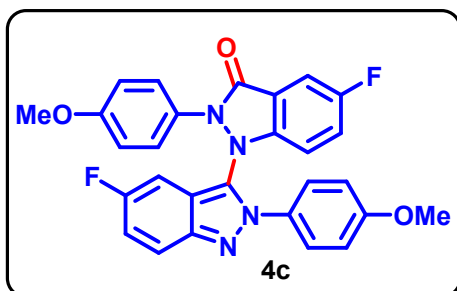
**Diethyl 4,4'-(3-oxo-2'*H*-[1,3'-biindazole]-2,2'(3*H*)-diyl)dibenzoate (2m):** Brown gummy mass (36.6 mg, 67%);  $R_f = 0.50$  (PE : EA = 75 : 25);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.12 (d,  $J = 8.8$  Hz, 2H), 8.07 (d,  $J = 8.0$  Hz, 1H), 7.78 (d,  $J = 8.4$  Hz, 2H), 7.71-7.64 (m, 2H), 7.47-7.41 (m, 3H), 7.37-7.32 (m, 2H), 7.17-7.12 (m, 2H), 7.07 (d,  $J = 8.4$  Hz, 2H), 4.43 (q,  $J = 7.2$  Hz, 2H), 4.30 (d,  $J = 7.2$  Hz, 2H), 1.44 (t,  $J = 7.2$  Hz, 3H), 1.33 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  165.7, 165.5, 161.2, 149.3, 148.5, 142.0, 137.9, 134.3, 131.2, 130.7, 130.4, 129.3, 128.8, 128.0, 125.3, 124.8, 124.4, 123.4, 119.0, 118.8, 118.7, 118.3, 118.0, 112.2, 61.7, 61.2, 14.4, 14.3; Anal. Calcd for  $\text{C}_{32}\text{H}_{26}\text{N}_4\text{O}_5$ : C, 70.32; H, 4.79; N, 10.25%; Found C, 70.15; H, 4.82; N, 10.31%.



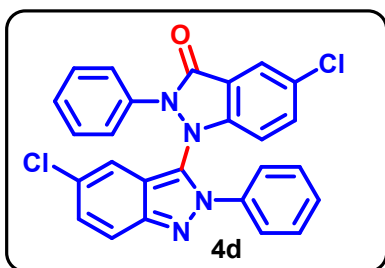
**5,5'-Difluoro-2,2'-diphenyl-2'*H*-[1,3'-biindazol]-3(2*H*)-one (4a):** Reddish solid (31.5 mg, 72%); M.p. 148-149 °C;  $R_f = 0.55$  (PE : EA = 80 : 20);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.76-7.72 (m, 2H), 7.52-7.49 (m, 1H), 7.46-7.39 (m, 3H), 7.29-7.25 (m, 2H), 7.19-7.10 (m, 5H), 6.94-6.86 (m, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  161.0, 159.6 ( $J_{\text{C-F}} = 222$  Hz), 159.4 ( $J_{\text{C-F}} = 225$  Hz), 145.5, 145.1, 138.3, 133.8, 129.6, 129.2, 129.0 ( $J_{\text{C-F}} = 10$  Hz), 128.9, 128.2, 125.5, 124.9, 122.2 ( $J_{\text{C-F}} = 26$  Hz), 121.4 ( $J_{\text{C-F}} = 10$  Hz), 119.6 ( $J_{\text{C-F}} = 22$  Hz), 119.2, 118.0, 113.6 ( $J_{\text{C-F}} = 7$  Hz), 110.5 ( $J_{\text{C-F}} = 26$  Hz), 100.7 ( $J_{\text{C-F}} = 25$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ):  $\delta$  -114.8, -117.3; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{26}\text{H}_{17}\text{F}_2\text{N}_4\text{O}]^+$ : 439.1365; found: 439.1370.



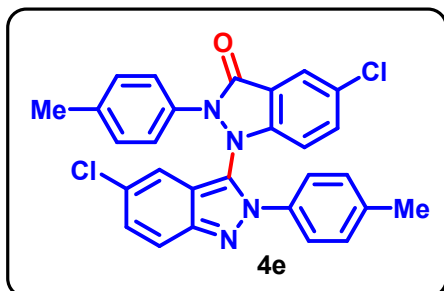
**5,5'-Difluoro-2,2'-di-*p*-tolyl-2'*H*-[1,3'-biindazol]-3(2*H*)-one (4b):** Brown solid (35.9 mg, 77%); M.p 190-191 °C;  $R_f = 0.50$  (PE : EA = 78 : 22);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.71-7.67 (m, 2H), 7.38-7.33 (m, 1H), 7.19 (d,  $J = 8.0$  Hz, 2H), 7.14-7.09 (m, 3H), 7.06-7.03 (m, 1H), 6.93 (d,  $J = 8.0$  Hz, 2H), 6.84-6.81 (m, 1H), 6.79 (d,  $J = 8.4$  Hz, 2H), 2.42 (s, 3H), 2.24 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  160.9, 159.6 ( $J_{\text{C-F}} = 225$  Hz), 159.4 ( $J_{\text{C-F}} = 232$  Hz), 145.4, 145.0, 139.8, 138.4, 136.0, 131.2, 129.76, 129.73, 125.7, 124.7, 122.1, 121.8, 121.3 ( $J_{\text{C-F}} = 10$  Hz), 119.2, 119.0, 118.2 ( $J_{\text{C-F}} = 12$  Hz), 113.5 ( $J_{\text{C-F}} = 8$  Hz), 110.4 ( $J_{\text{C-F}} = 25$  Hz), 100.7 ( $J_{\text{C-F}} = 25$  Hz), 21.3, 21.2;  $^{19}\text{F NMR}$  (376 MHz,  $\text{CDCl}_3$ ):  $\delta$  -115.2, -117.7; Anal. Calcd for  $\text{C}_{28}\text{H}_{20}\text{F}_2\text{N}_4\text{O}$ : C, 72.09; H, 4.32; N, 12.01%; Found C, 71.91; H, 4.37; N, 11.94%.



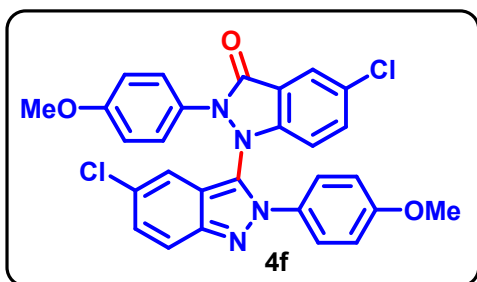
**5,5'-Difluoro-2,2'-bis(4-methoxyphenyl)-2'*H*-[1,3'-biindazol]-3(2*H*)-oneonate (4c):** Brown solid (39.8 mg, 80%); M.p 161-162 °C;  $R_f = 0.40$  (PE : EA = 70 : 30);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.71-7.67 (m, 2H), 7.37-7.32 (m, 1H), 7.15 (d,  $J = 9.2$  Hz, 2H), 7.12-7.09 (m, 1H), 7.05-7.01 (m, 1H), 6.88 (d,  $J = 8.8$  Hz, 2H), 6.79-6.74 (m, 3H), 6.64 (d,  $J = 8.8$  Hz, 2H), 3.85 (s, 3H), 3.71 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  160.3, 159.6, 159.5 ( $J_{\text{C-F}} = 234$  Hz), 159.4 ( $J_{\text{C-F}} = 243$  Hz), 145.3, 144.7, 131.3, 128.4 ( $J_{\text{C-F}} = 9$  Hz), 128.0, 126.3 ( $J_{\text{C-F}} = 20$  Hz), 122.0, 121.8, 121.3, 121.2, 119.5 ( $J_{\text{C-F}} = 9$  Hz), 119.1, 118.8, 118.0 ( $J_{\text{C-F}} = 9$  Hz), 114.3 ( $J_{\text{C-F}} = 16$  Hz), 113.3 ( $J_{\text{C-F}} = 8$  Hz), 110.4 ( $J_{\text{C-F}} = 24$  Hz), 100.6 ( $J_{\text{C-F}} = 25$  Hz), 55.7, 55.5;  $^{19}\text{F NMR}$  (376 MHz,  $\text{CDCl}_3$ ):  $\delta$  -115.1, -117.7; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{Na}]^+$  Calcd for  $[\text{C}_{28}\text{H}_{20}\text{F}_2\text{N}_4\text{NaO}_3]^+$ : 521.1396; found: 521.1379.



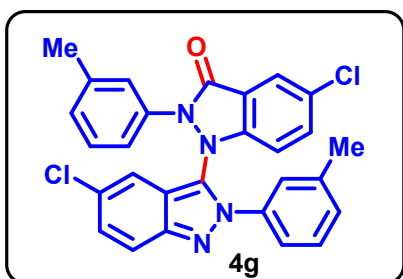
**5,5'-Dichloro-2,2'-diphenyl-2'*H*-[1,3'-biindazol]-3(2*H*)-one (4d):** Brown solid (35.3 mg, 75%); M.p 193-194 °C;  $R_f = 0.50$  (PE : EA = 80 : 20);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.99 (d,  $J = 2.0$  Hz, 1H), 7.63 (d,  $J = 9.6$  Hz, 1H), 7.57-7.55 (m, 1H), 7.46-7.42 (m, 1H), 7.39-7.35 (m, 2H), 7.25-7.22 (m, 2H), 7.19-7.16 (m, 2H), 7.13-7.07 (m, 3H), 7.03 (d,  $J = 8.8$  Hz, 1H), 6.83-6.81 (m, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  160.1, 146.9, 146.5, 138.1, 134.2, 133.7, 130.3, 130.1, 129.7, 129.3, 129.17, 129.16, 128.3, 127.8, 125.6, 124.8, 124.7, 120.7, 119.7, 119.0, 116.5, 113.2; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{26}\text{H}_{17}\text{Cl}_2\text{N}_4\text{O}]^+$ : 471.0774; found: 471.0761.



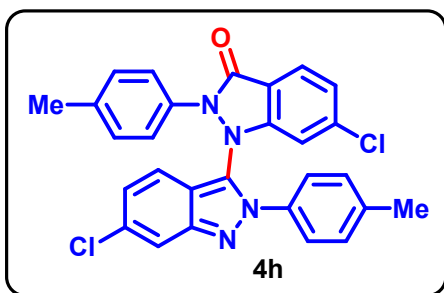
**5,5'-Dichloro-2,2'-di-*p*-tolyl-2'*H*-[1,3'-biindazol]-3(2*H*)-one (4e):** Yellow solid (38.9 mg, 78%); M.p 209-210 °C;  $R_f = 0.45$  (PE : EA = 80 : 20);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.01 (d,  $J = 2.0$  Hz, 1H), 7.67-7.65 (m, 1H), 7.58-7.56 (m, 1H), 7.28-7.25 (m, 2H), 7.20 (d,  $J = 8.0$  Hz, 2H), 7.10 (d,  $J = 8.4$  Hz, 2H), 7.02 (d,  $J = 8.8$  Hz, 1H), 6.92 (d,  $J = 8.4$  Hz, 2H), 6.76 (d,  $J = 8.4$  Hz, 2H), 2.43 (s, 3H), 2.24 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  160.1, 146.7, 146.3, 140.0, 138.6, 135.8, 134.0, 131.0, 130.2, 130.0, 129.9, 129.8, 129.7, 128.9, 127.6, 125.7, 124.6, 120.6, 119.7, 119.0, 116.5, 113.1, 21.3, 21.2; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{28}\text{H}_{21}\text{Cl}_2\text{N}_4\text{O}]^+$ : 499.1087; found: 499.1092.



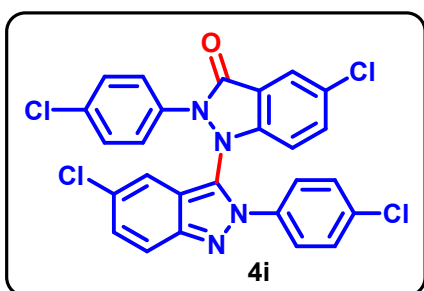
**5,5'-Dichloro-2,2'-bis(4-methoxyphenyl)-2'*H*-[1,3'-biindazol]-3(2*H*)-one (4f):** Brown solid (43.0 mg, 81%); M.p. 168-169 °C;  $R_f = 0.45$  (PE : EA = 75 : 25);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.00 (s, 1H), 7.65 (d,  $J = 9.2$  Hz, 1H), 7.56 (d,  $J = 8.4$  Hz, 1H), 7.26-7.24 (m, 1H), 7.18 (s, 1H), 7.13 (d,  $J = 8.8$  Hz, 2H), 7.05 (d,  $J = 8.8$  Hz, 1H), 6.87 (d,  $J = 8.8$  Hz, 2H), 6.75 (d,  $J = 8.8$  Hz, 2H), 6.63 (d,  $J = 8.8$  Hz, 2H), 3.84 (s, 3H), 3.71 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  160.4, 160.3, 159.7, 146.5, 146.2, 133.9, 131.1, 130.1, 129.8, 128.8, 128.1, 127.3, 126.2, 126.1, 124.6, 120.6, 119.7, 118.9, 116.5, 114.4, 114.3, 113.0, 55.7, 55.5; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{28}\text{H}_{21}\text{Cl}_2\text{N}_4\text{O}_3]^+$ : 531.0985; found: 531.0992.



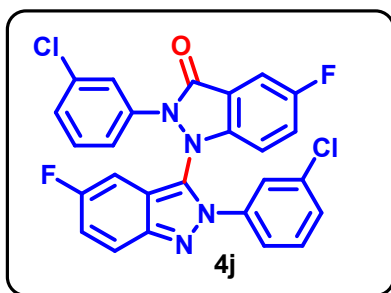
**5,5'-Dichloro-2,2'-di-*m*-tolyl-2'*H*-[1,3'-biindazol]-3(2*H*)-one (4g):** Reddish solid (35.9 mg, 72%); M.p. 159-160 °C;  $R_f = 0.5$  (PE : EA = 80 : 20);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.01 (d,  $J = 2.0$  Hz, 1H), 7.66 (d,  $J = 9.2$  Hz, 1H), 7.60-7.58 (m, 1H), 7.29-7.24 (m, 4H), 7.06-7.04 (m, 2H), 7.02-6.96 (m, 3H), 6.70 (d,  $J = 7.6$  Hz, 1H), 6.65 (s, 1H), 2.34 (s, 3H), 2.10 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  160.1, 147.0, 146.5, 139.5, 139.1, 138.2, 134.1, 133.6, 130.4, 130.2, 130.1, 129.2, 129.0, 128.9, 128.8, 127.9, 126.3, 125.7, 124.6, 122.8, 121.8, 120.6, 119.9, 119.0, 116.6, 113.3, 21.3, 21.2; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{28}\text{H}_{21}\text{Cl}_2\text{N}_4\text{O}]^+$ : 499.1087; found: 499.1092.



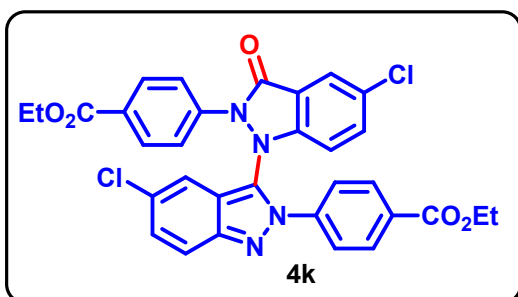
**6,6'-Dichloro-2,2'-di-*p*-tolyl-2'*H*-[1,3'-biindazol]-3(2*H*)-one (4h):** Yellow solid (36.4 mg, 73%); M.p. 208-209 °C;  $R_f = 0.50$  (PE : EA = 85 : 15);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.09 (d,  $J = 8.4$  Hz, 1H), 7.86 (s, 1H), 7.47 (d,  $J = 8.4$  Hz, 1H), 7.40-7.33 (m, 4H), 7.25-7.23 (m, 2H), 7.19 (s, 1H), 7.07 (d,  $J = 7.2$  Hz, 2H), 6.88 (d,  $J = 6.8$  Hz, 2H), 2.56 (s, 3H), 2.38 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  160.6, 149.0, 148.2, 140.1, 140.0, 138.6, 135.7, 133.4, 131.1, 130.7, 129.8, 129.7, 126.1, 126.0, 125.8, 125.0, 124.6, 119.2, 118.0, 117.1, 117.0, 111.9, 21.3, 21.2; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{28}\text{H}_{21}\text{Cl}_2\text{N}_4\text{O}]^+$ : 499.1087; found: 499.1094.



**5,5'-Dichloro-2,2'-bis(4-chlorophenyl)-2'*H*-[1,3'-biindazol]-3(2*H*)-one (4i):** Yellow solid (38.3 mg, 71%); M.p. 186-187 °C;  $R_f = 0.45$  (PE : EA = 82 : 18);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.03 (d,  $J = 2.0$  Hz, 1H), 7.67 (d,  $J = 9.2$  Hz, 1H), 7.63-7.61 (m, 1H), 7.43-7.39 (m, 2H), 7.30-7.27 (m, 1H), 7.24-7.21 (m, 3H), 7.12-7.10 (m, 2H), 7.06 (d,  $J = 8.4$  Hz, 1H), 6.83-6.80 (m, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  160.2, 146.9, 146.7, 136.6, 135.9, 134.6, 134.3, 132.2, 130.8, 130.6, 129.6, 129.5, 129.4, 127.7, 126.6, 125.8, 124.9, 120.8, 119.6, 118.8, 116.3, 113.3; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{26}\text{H}_{15}\text{Cl}_4\text{N}_4\text{O}]^+$ : 538.9994; found: 538.9996.



**2,2'-Bis(3-chlorophenyl)-5,5'-difluoro-2'H-[1,3'-biindazol]-3(2H)-one (4j):** Yellow solid (35.5 mg, 70%); M.p. 177-178 °C;  $R_f = 0.5$  (PE : EA = 80 : 20);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.73-7.70 (m, 2H), 7.50-7.48 (m, 1H), 7.44-7.37 (m, 2H), 7.31-7.30 (m, 1H), 7.24-7.23 (m, 1H), 7.17-7.08 (m, 4H), 6.89-6.86 (m, 2H), 6.77-6.74 (m, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  160.9, 160.0 ( $J_{\text{C-F}} = 245$  Hz), 159.6 ( $J_{\text{C-F}} = 219$  Hz), 145.8, 145.5, 139.1, 135.4, 135.0, 134.9, 130.3, 130.0 ( $J_{\text{C-F}} = 10$  Hz), 129.3, 128.5, 125.5, 125.4, 123.5, 122.8, 122.6, 121.6 ( $J_{\text{C-F}} = 10$  Hz), 120.0, 119.6 ( $J_{\text{C-F}} = 9$  Hz), 117.9, 117.8, 113.8 ( $J_{\text{C-F}} = 8$  Hz), 110.8 ( $J_{\text{C-F}} = 24$  Hz), 100.5 ( $J_{\text{C-F}} = 25$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ):  $\delta$  -113.7, -116.3; HRMS (ESI-TOF) m/z:  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{26}\text{H}_{15}\text{Cl}_2\text{F}_2\text{N}_4\text{O}]^+$ : 507.0585; found:507.0562.



**Diethyl 4,4'-(5,5'-dichloro-3-oxo-2'H-[1,3'-biindazole]-2,2'(3H)-diyl)dibenzoate (4k):** Black solid (38.1 mg, 62%); M.p. 185-186 °C;  $R_f = 0.45$  (PE : EA = 80 : 20);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.13 (d,  $J = 8.8$  Hz, 2H), 8.04 (d,  $J = 2.0$  Hz, 1H), 7.81 (d,  $J = 8.8$  Hz, 2H), 7.67-7.62 (m, 2H), 7.39 (d,  $J = 8.4$  Hz, 2H), 7.34 (d,  $J = 1.2$  Hz, 1H), 7.30-7.27 (m, 1H), 7.10 (d,  $J = 8.4$  Hz, 1H), 7.02 (d,  $J = 8.4$  Hz, 2H), 4.44 (q,  $J = 7.2$  Hz, 2H), 4.31 (q,  $J = 7.2$  Hz, 2H), 1.44 (t,  $J = 7.2$  Hz, 3H), 1.34 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  165.5, 165.3, 159.8, 147.1, 146.8, 141.5, 137.4, 134.8, 131.7, 131.0, 130.8, 130.5, 129.7, 129.4, 128.1, 126.2, 125.0, 124.3, 123.6, 120.8, 119.6, 119.1, 116.3, 113.4, 61.8, 61.4, 14.4, 14.3; HRMS (ESI-TOF) m/z:  $[\text{M} + \text{H}]^+$  Calcd for  $[\text{C}_{32}\text{H}_{25}\text{Cl}_2\text{N}_4\text{O}_5]^+$ : 615.1197; found:615.1201.

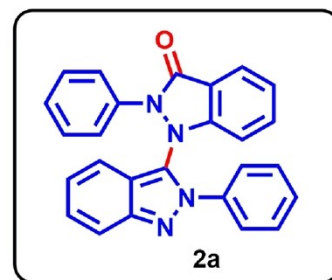
## 6. References:

1. a) M. R. Kumar, A. Park, N. Park and S. Lee, *Org. Lett.*, 2011, **13**, 3542; b) D. Maiti, K. Mahanty and S. D. Sarkar, *Org. Lett.*, 2021, **23**, 1742; c) G. Bogonda, H. Y. Kim and K. Oh, *Org. Lett.*, 2018, **20**, 2711.

## **7. NMR spectra [ $^1\text{H}$ , $^{13}\text{C}\{^1\text{H}\}$ and $^{19}\text{F}$ ] of synthesized products**



8.068  
8.048  
7.738  
7.716  
7.648  
7.646  
7.628  
7.609  
7.607  
7.474  
7.472  
7.463  
7.456  
7.450  
7.438  
7.419  
7.407  
7.403  
7.399  
7.389  
7.382  
7.379  
7.370  
7.356  
7.355  
7.338  
7.335  
7.332  
7.318  
7.316  
7.316  
7.293  
7.275  
7.272  
7.260  
7.260  
7.139  
7.117  
7.106  
7.098  
7.088  
7.082  
7.075  
6.914  
6.907  
6.904  
6.887  
6.883



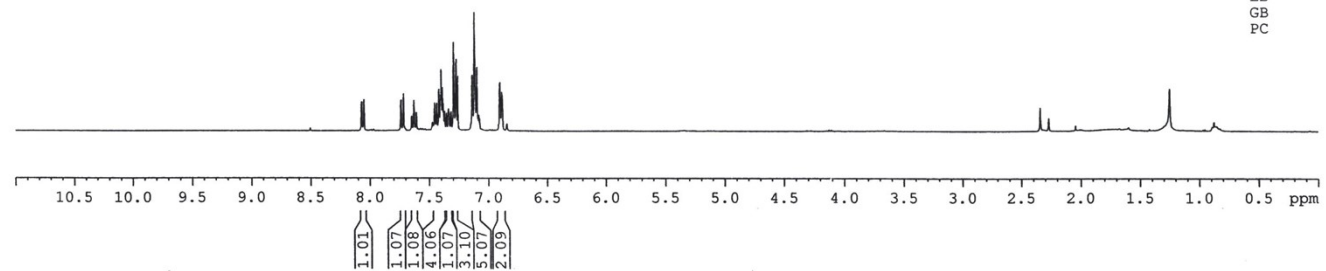
**<sup>1</sup>H NMR: 400 MHz**  
**Solvent: CDCl<sub>3</sub>**

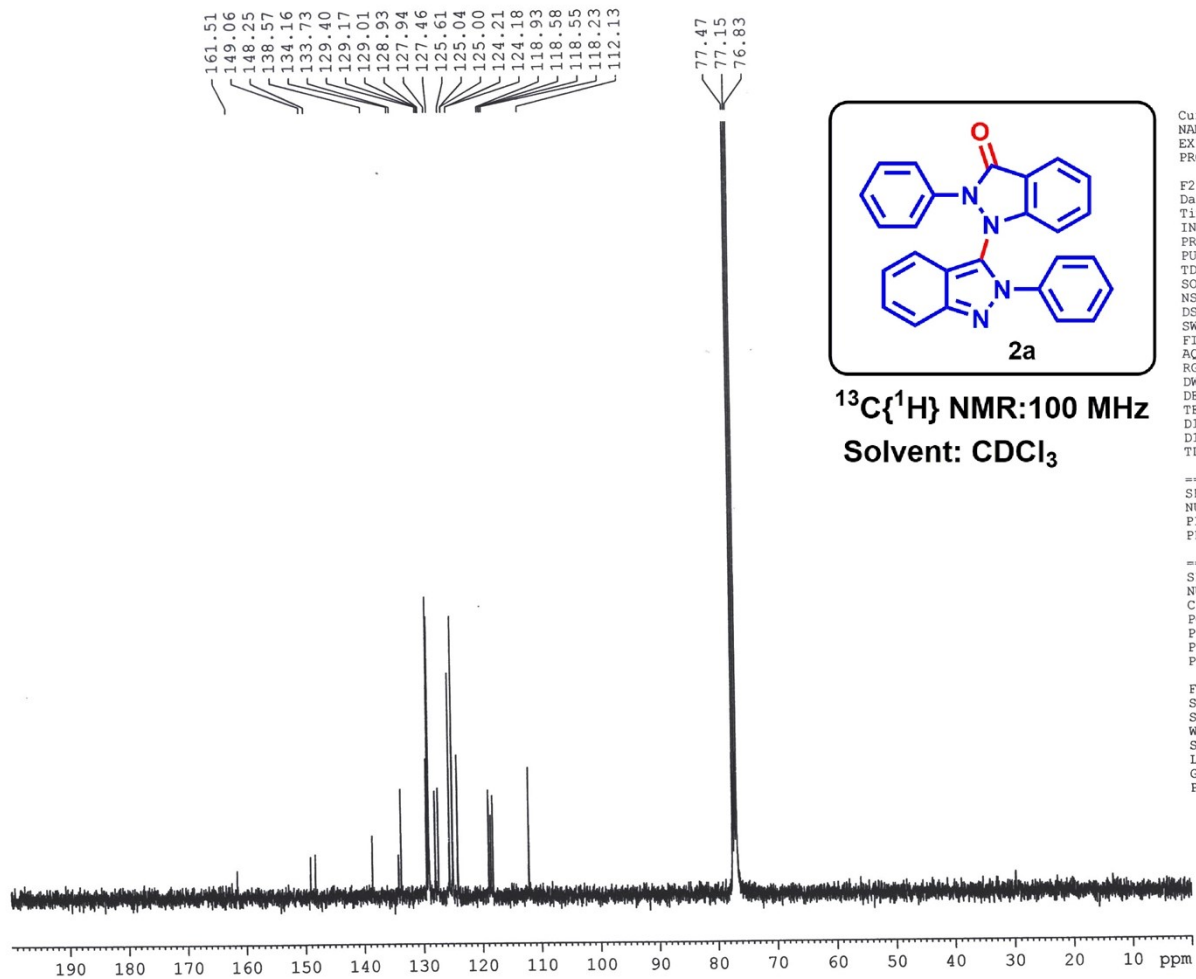
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EXPNO     108
PROCNO    1

F2 - Acquisition Parameters
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PULPROG   zg30
TD        32768
SOLVENT   CDCl3
NS        8
DS        2
SWH       8223.685 Hz
FIDRES    0.250967 Hz
AQ        1.9922944 sec
RG        135.7
DW        60.800 usec
DE        6.50 usec
TE        290.2 K
D1        1.00000000 sec
TDO       1

===== CHANNEL f1 =====
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NUC1      1H
P1        14.75 usec
PLW1      12.00000000 W

F2 - Processing parameters
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WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
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Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 43  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220213  
Time\_ 20.53  
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 135.7  
DW 20.800 usec  
DE 6.50 usec  
TE 293.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

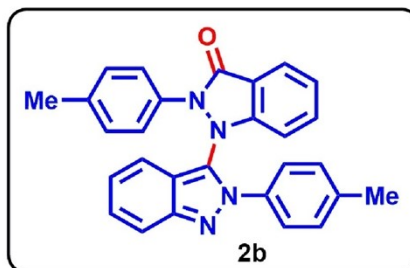
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NUC1 13C  
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PLW1 54.00000000 W

===== 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

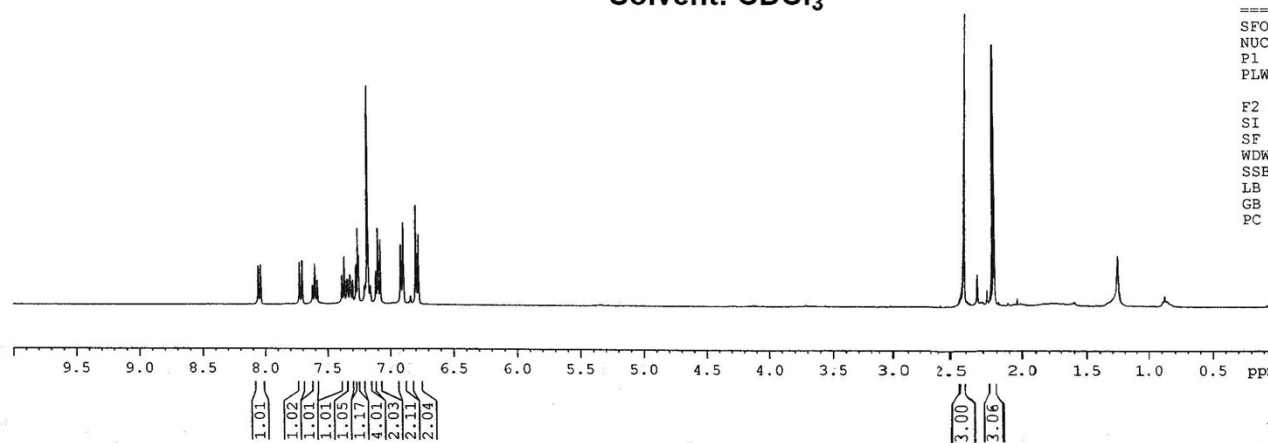
F2 - Processing parameters  
SI 16384  
SF 100.6177872 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

8.055  
7.723  
7.702  
7.623  
7.620  
7.601  
7.583  
7.581  
7.583  
7.365  
7.346  
7.338  
7.336  
7.319  
7.299  
7.297  
7.272  
7.259  
7.251  
7.205  
7.181  
7.178  
7.163  
7.156  
7.115  
7.099  
7.079  
6.918  
6.897  
6.798  
6.777

2.417  
2.223



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

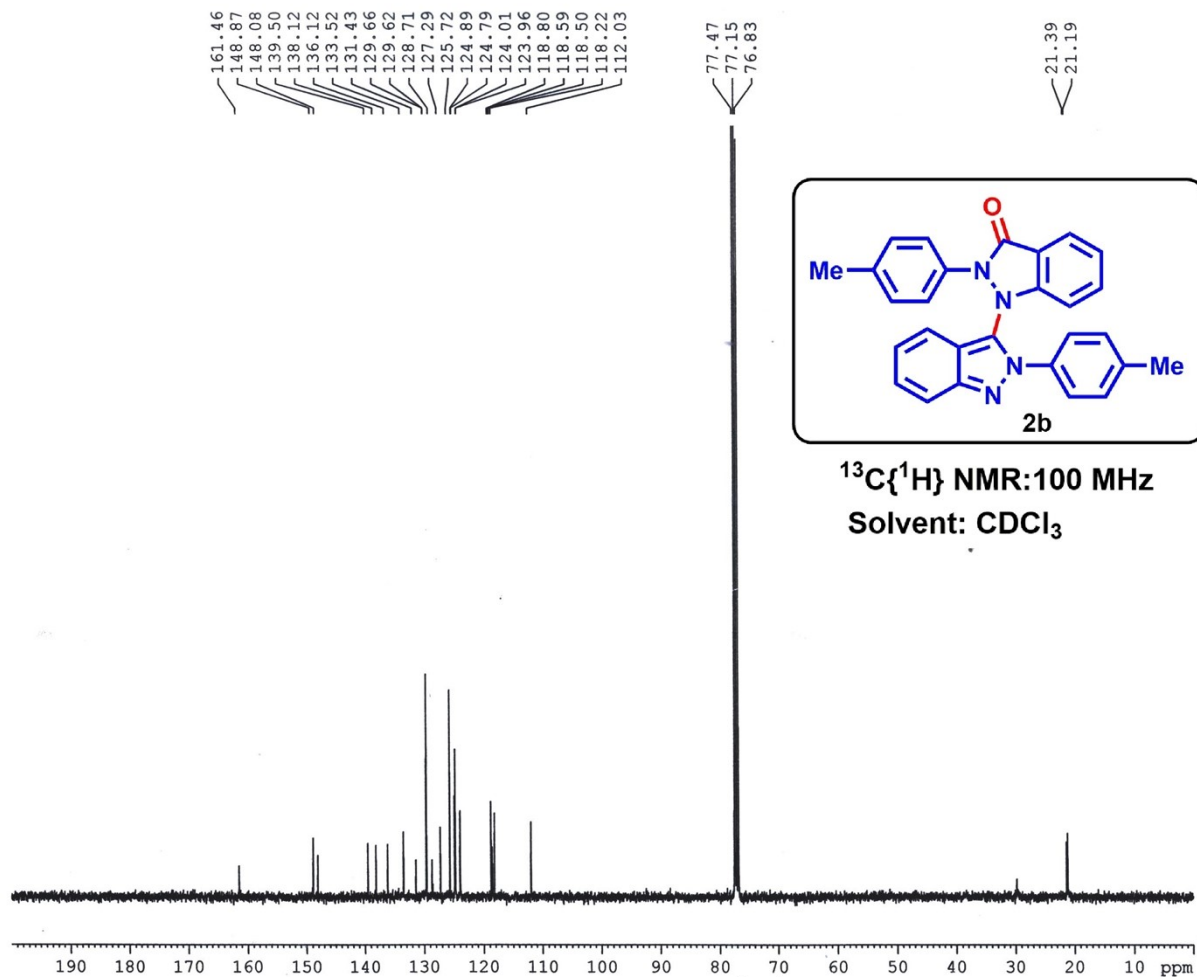


Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 89  
PROCNO 1

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INSTRUM spect  
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PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 120.16  
DW 60.800 usec  
DE 6.50 usec  
TE 288.5 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
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NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
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WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



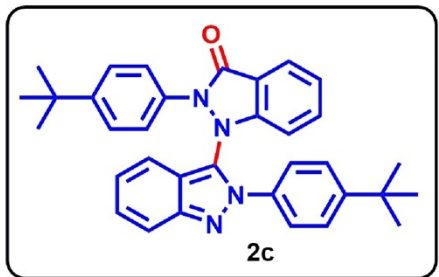
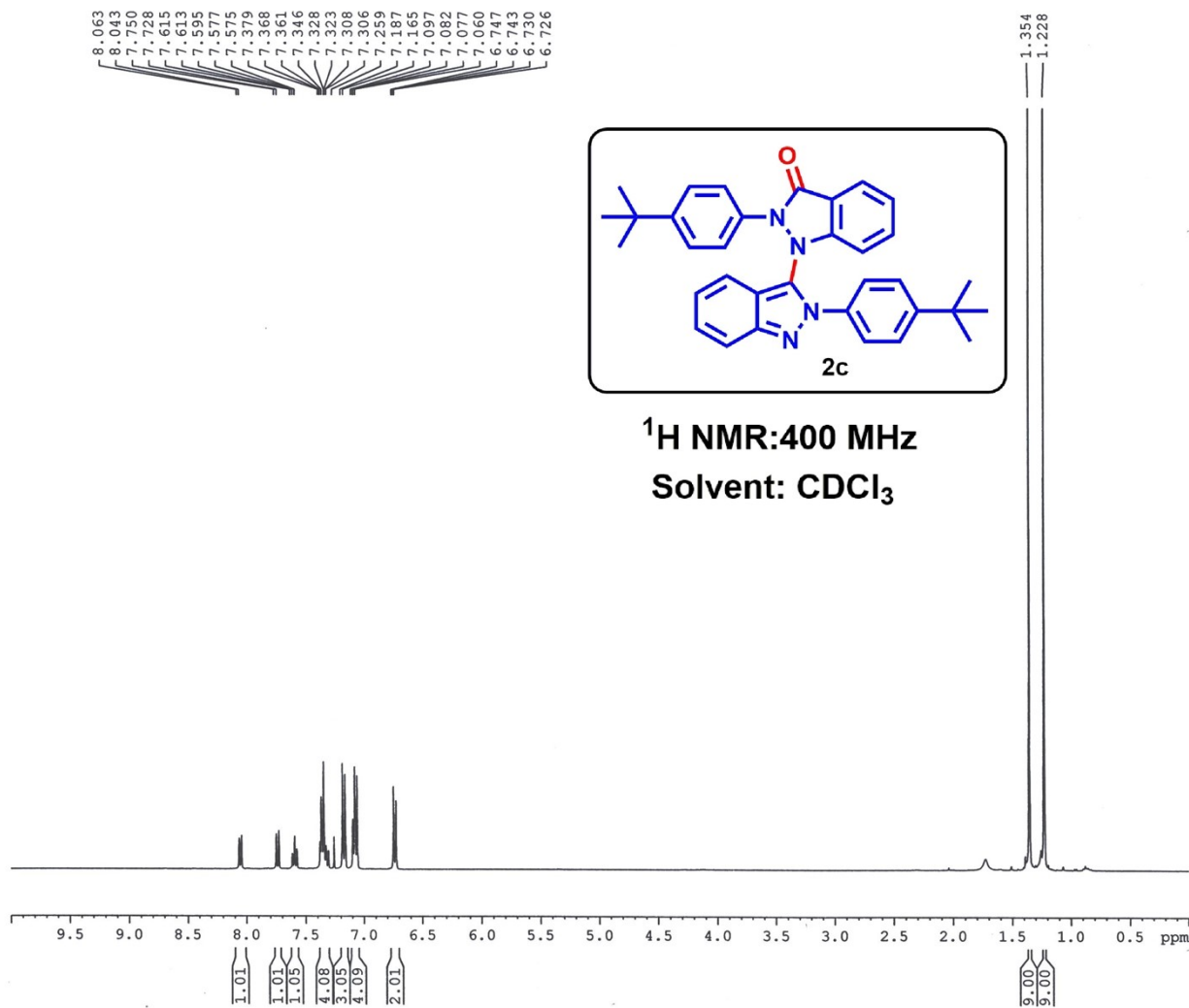
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NAME Dr. A HAJRA-2022-13C  
EXPNO 35  
PROCNO 1

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Time 12.59  
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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 289.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

----- CHANNEL f1 -----  
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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

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WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



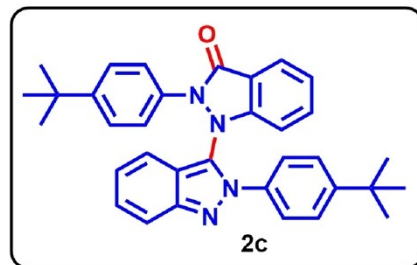
**<sup>1</sup>H NMR:400 MHz**  
**Solvent: CDCl<sub>3</sub>**

Current Data Parameters  
 NAME Dr. A HAJRA 2022 1H  
 EXPNO 525  
 PROCNO 1

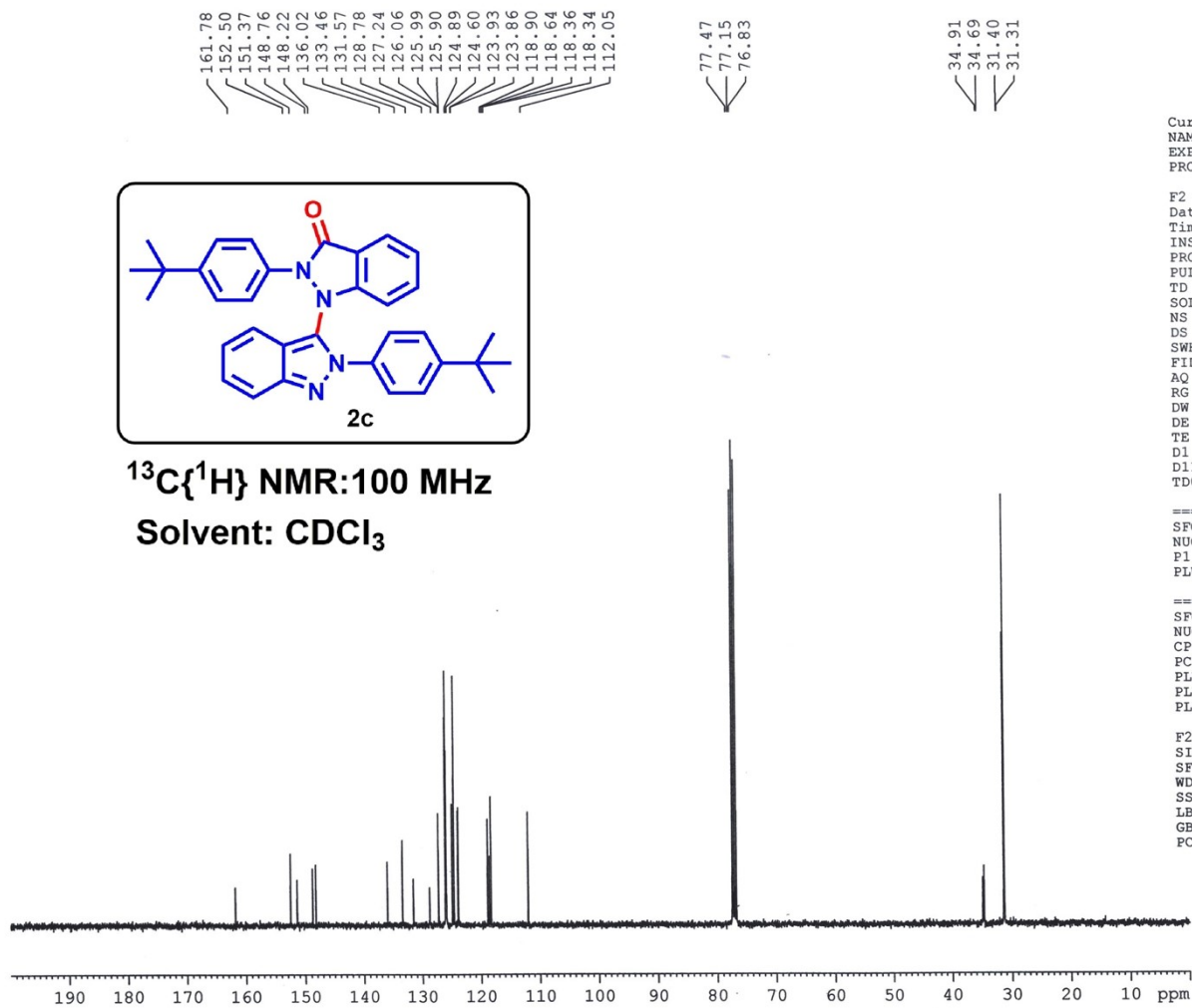
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 Time 10.29  
 INSTRUM spect  
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 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9922944 sec  
 RG 87.66  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 299.7 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 16384  
 SF 400.1500091 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



**$^{13}\text{C}\{^1\text{H}\}$  NMR: 100 MHz**  
**Solvent:  $\text{CDCl}_3$**



161.78  
152.50  
151.37  
148.76  
148.22  
136.02  
133.46  
131.57  
128.78  
127.24  
126.06  
125.99  
125.90  
124.89  
124.60  
123.93  
123.86  
118.90  
118.64  
118.36  
118.34  
112.05

77.47  
77.15  
76.83

34.91  
34.69  
31.40  
31.31

Current Data Parameters  
 NAME Dr. A HAJRA-2022-13C  
 EXPNO 208  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220522  
 Time 11.02  
 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 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.9 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 =====  
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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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 SF 100.6177859 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 1.40

8.056  
8.037  
7.731  
7.709  
7.616  
7.614  
7.605  
7.596  
7.583  
7.577  
7.575  
7.379  
7.360  
7.341  
7.324  
7.322  
7.320  
7.317  
7.303  
7.301  
7.259  
7.218  
7.209  
7.204  
7.192  
7.187  
7.180  
7.106  
7.089  
7.080  
7.068  
7.060  
6.894  
6.886  
6.881  
6.869  
6.864  
6.856  
6.806  
6.798  
6.793  
6.781  
6.775  
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6.636  
6.630  
6.618  
6.613  
6.605  
3.848  
3.710

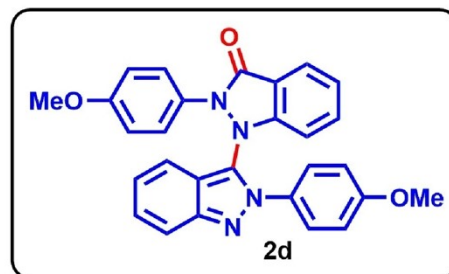


Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 396  
PROCNO 1

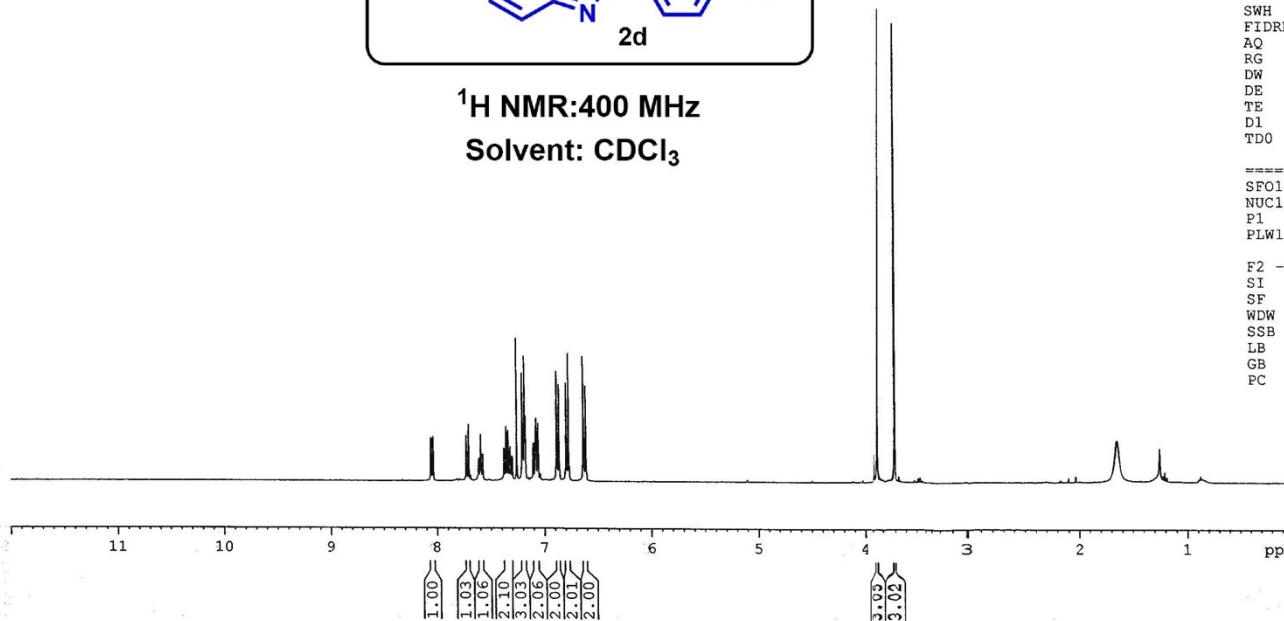
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PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 186.42  
DW 60.800 usec  
DE 6.50 usec  
TE 297.9 K  
D1 1.00000000 sec  
TD0 1

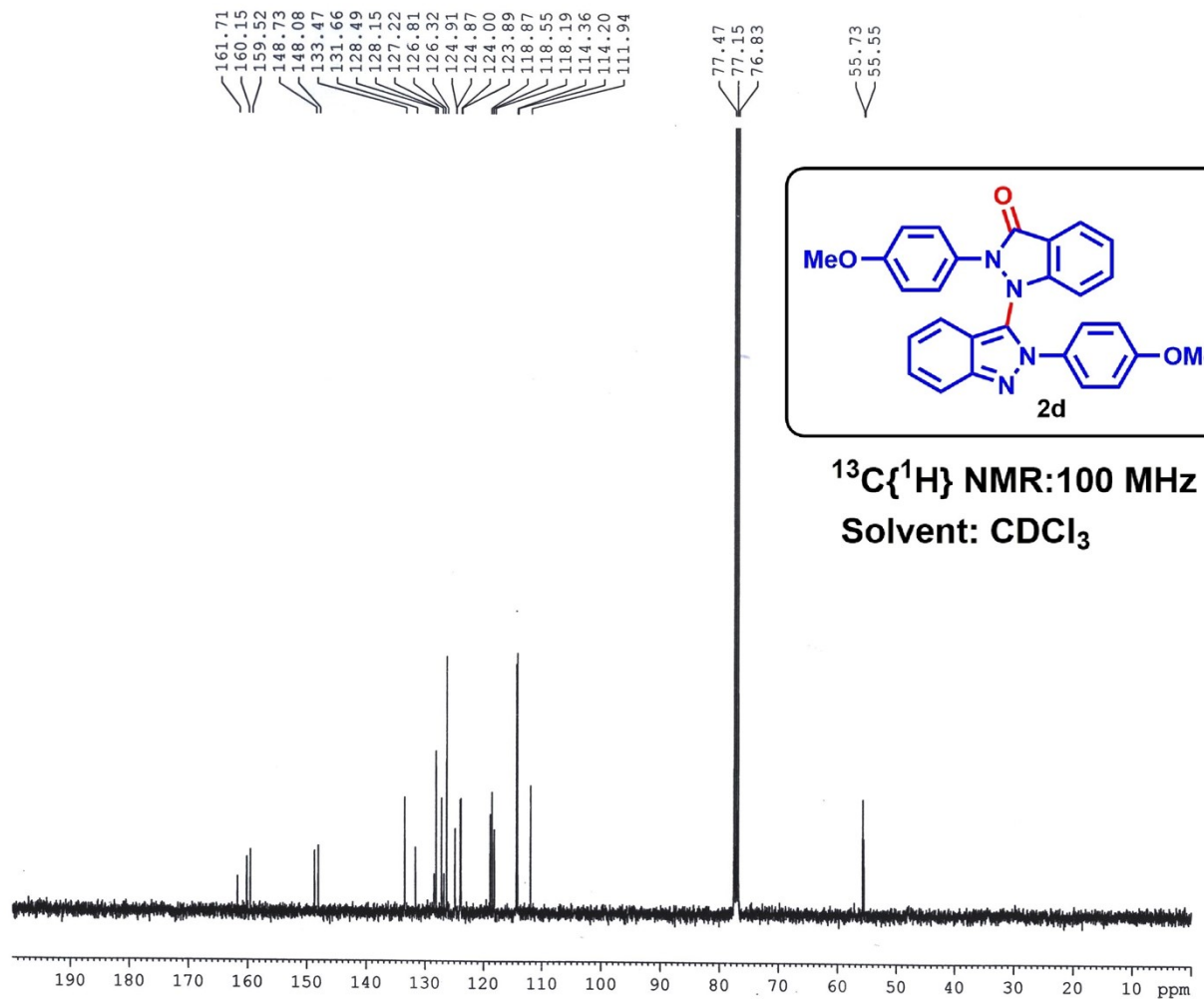
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P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
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SF 400.1500092 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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





Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 157  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220410  
Time 11.28  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 720  
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 298.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

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P1 8.90 usec  
PLW1 54.00000000 W

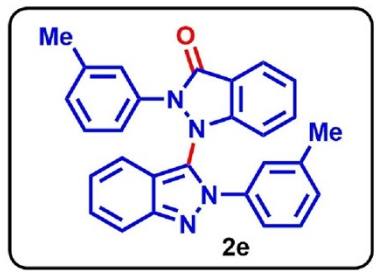
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PLW12 0.32231000 W  
PLW13 0.16212000 W

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SSB 0  
LB 1.00 Hz  
GB 0  
FC 1.40

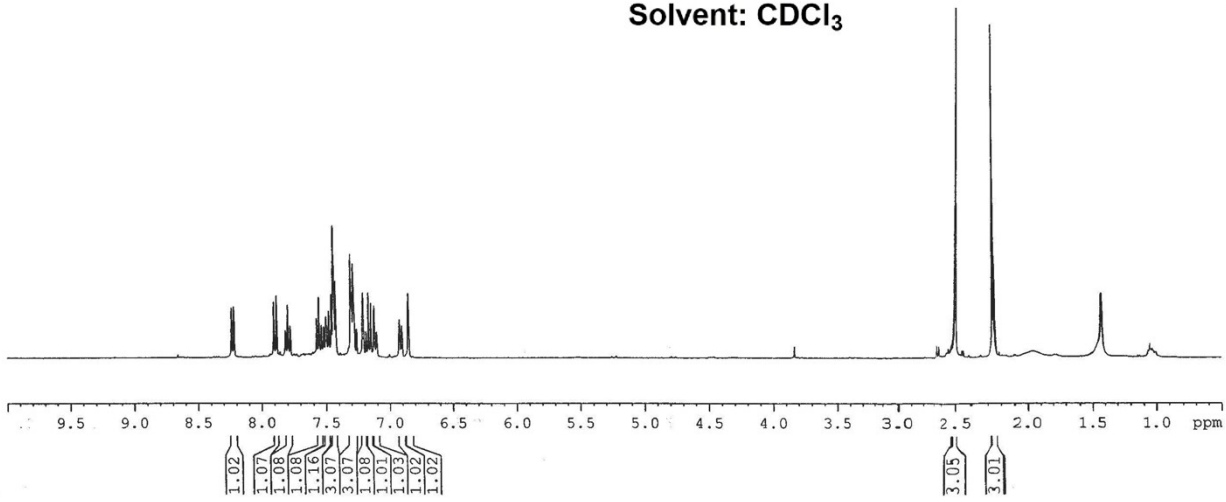


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7.880  
7.814  
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7.793  
7.775  
7.773  
7.572  
7.553  
7.534  
7.516  
7.499  
7.496  
7.494  
7.477  
7.457  
7.439  
7.434  
7.423  
7.305  
7.298  
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7.277  
7.260  
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7.186  
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7.147  
7.121  
7.102  
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6.851

2.505  
2.255



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

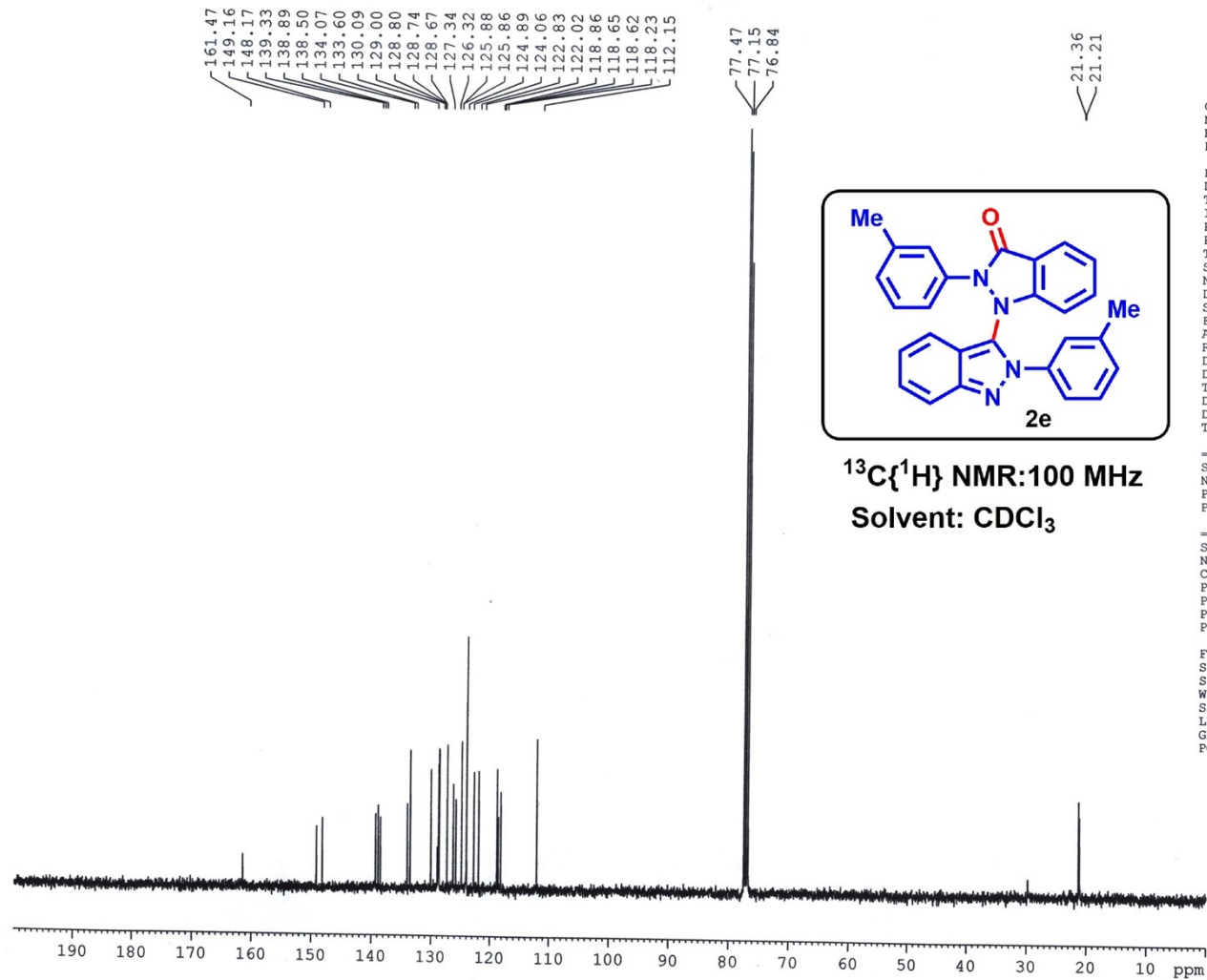


Current Data Parameters  
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EXPNO 179  
PROCNO 1

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PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 87.66  
DW 60.800 usec  
DE 6.50 usec  
TE 291.9 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
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NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
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SF 400.1499392 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
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PC 1.00



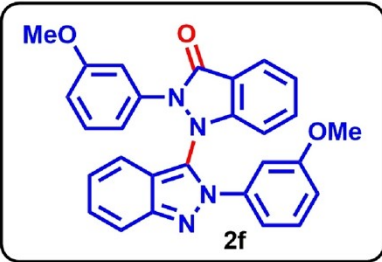
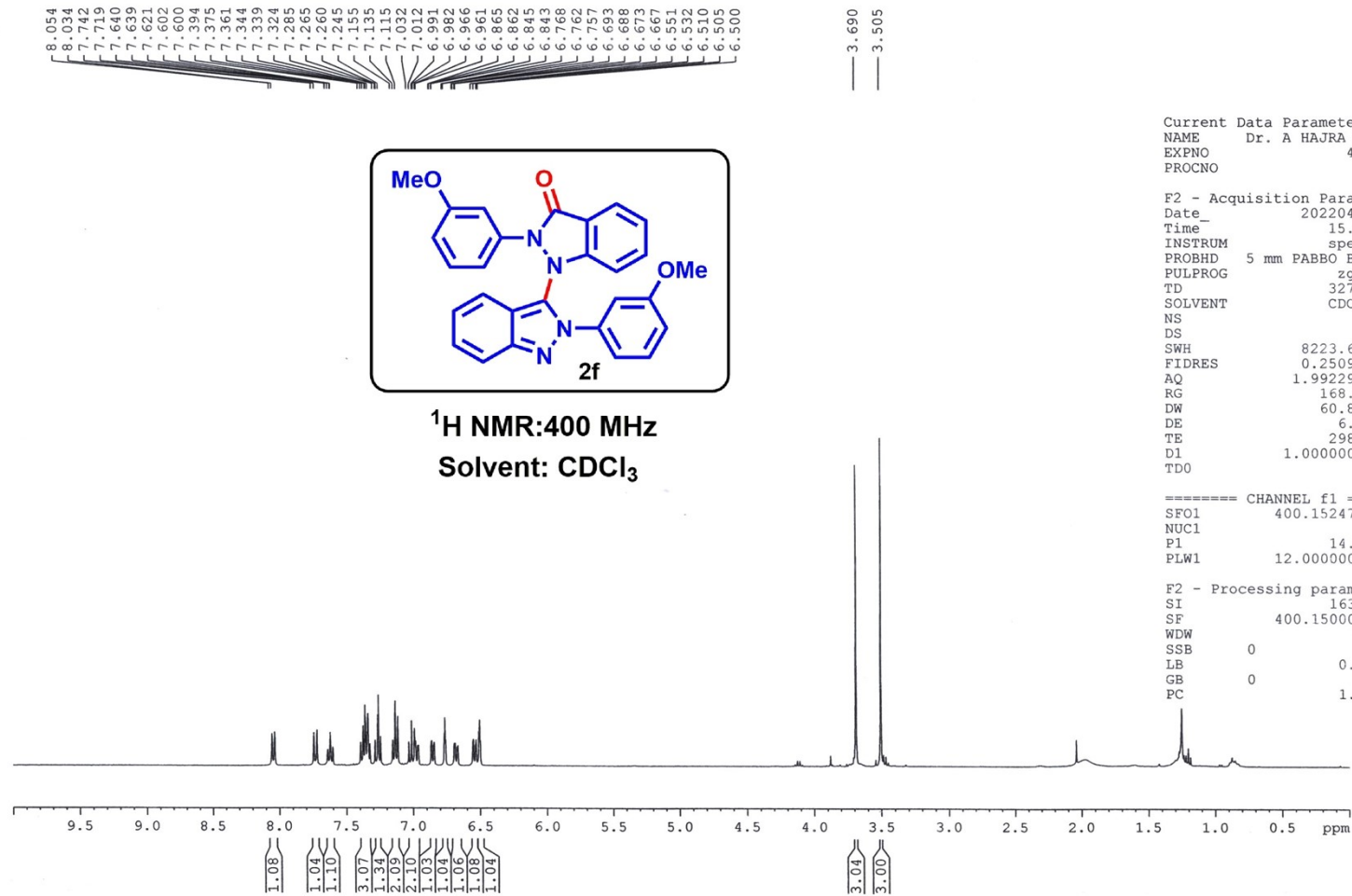
Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 84  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220303  
Time\_ 10.40  
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 186.42  
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  
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



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

Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 439  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220417  
Time\_ 15.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 168.31  
DW 60.800 usec  
DE 6.50 usec  
TE 298.4 K  
D1 1.00000000 sec  
TD0 1

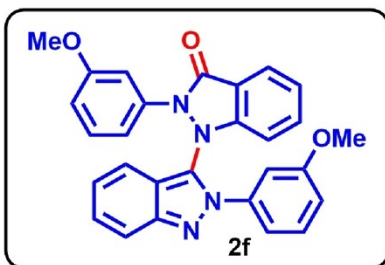
===== CHANNEL f1 =====  
SF01 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500087 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

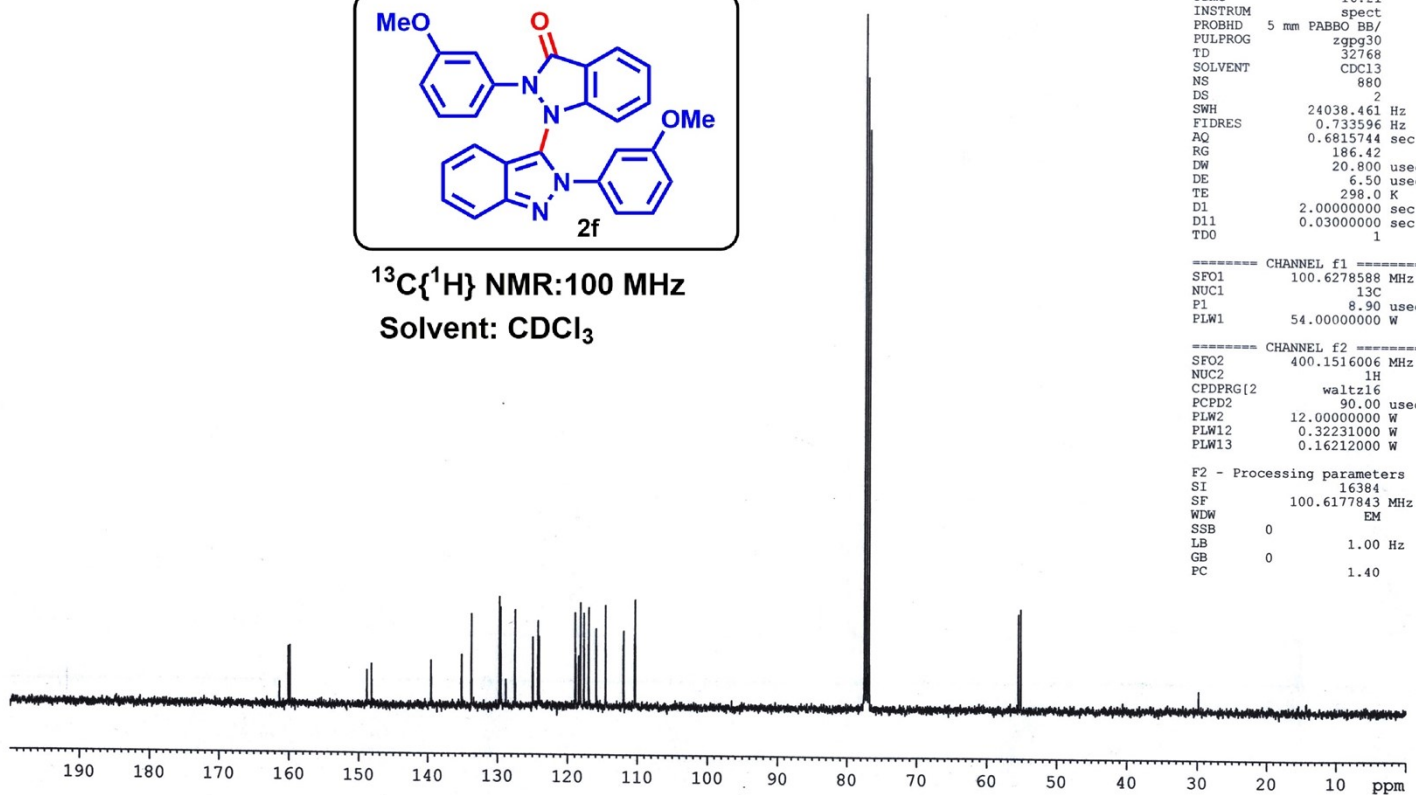
161.37  
160.11  
159.89  
148.85  
148.18  
139.53  
135.14  
133.76  
129.78  
129.60  
128.86  
127.52  
125.01  
124.28  
124.11  
118.96  
118.87  
118.48  
118.21  
117.71  
117.02  
115.95  
114.61  
112.01  
110.40  
110.35

77.47  
77.16  
76.84

55.51  
55.19



$^{13}\text{C}\{^1\text{H}\}$  NMR: 100 MHz  
Solvent:  $\text{CDCl}_3$



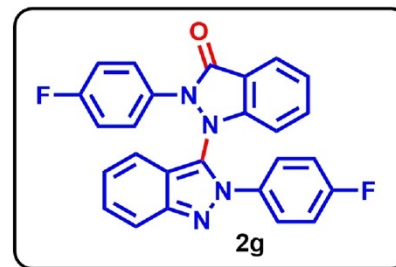
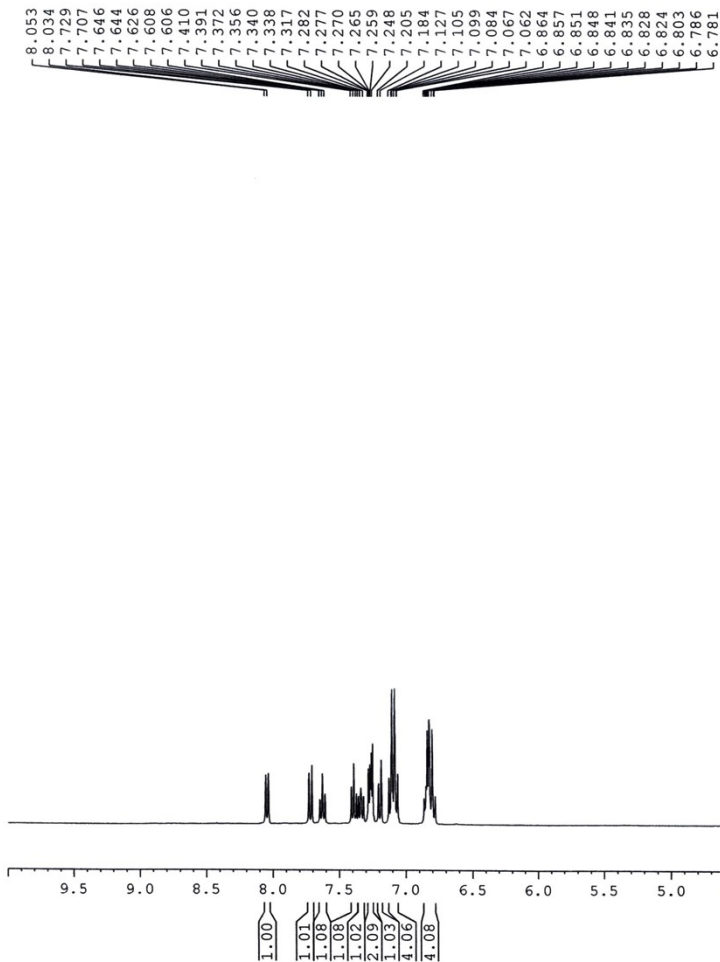
Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 170  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220417  
Time 16.21  
INSTRUM spect  
PROBHD 5 mm PABBO 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 298.0 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 100.6177843 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



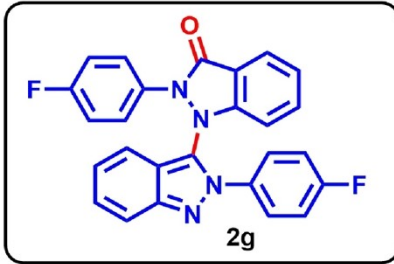
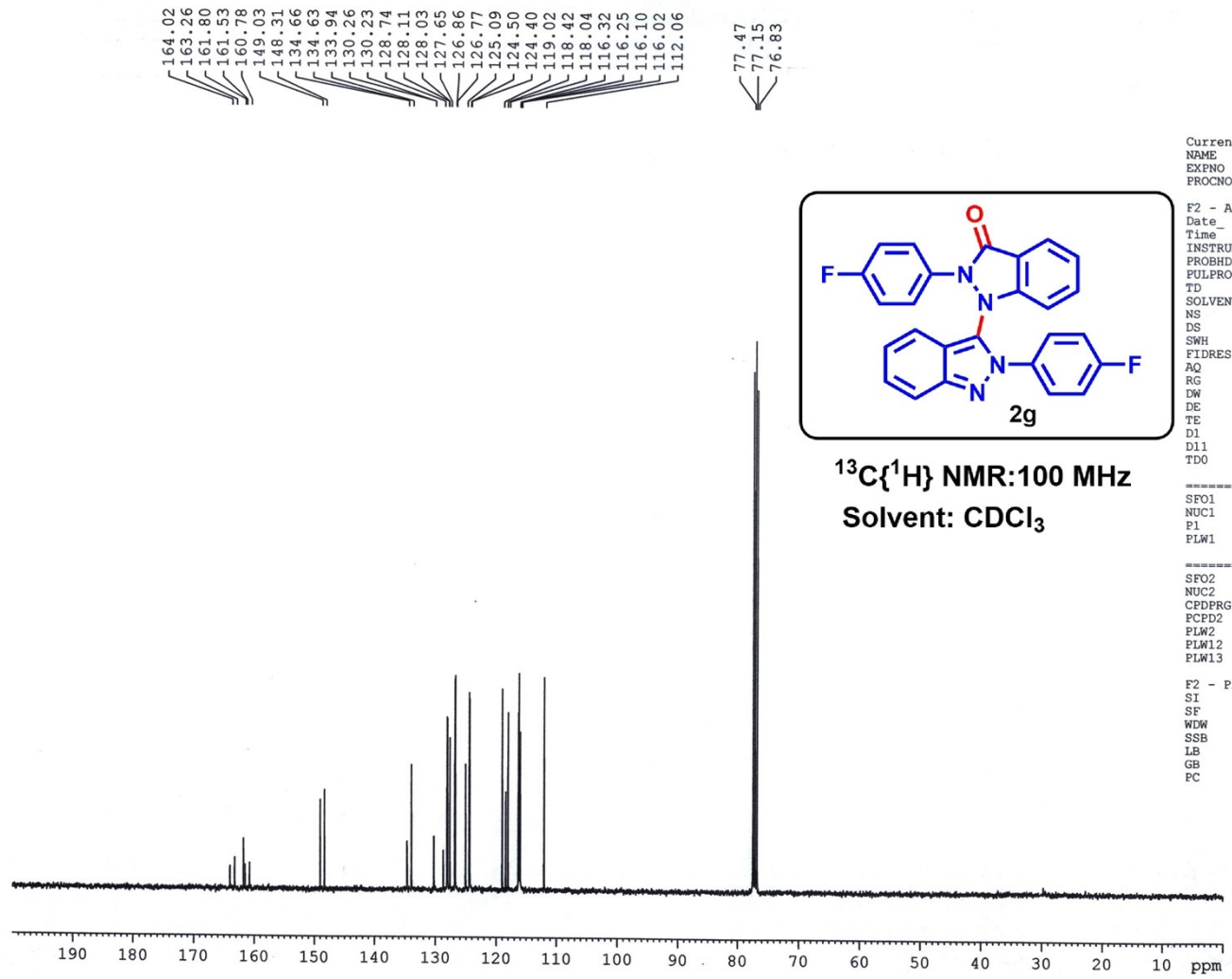
<sup>1</sup>H NMR:400 MHz  
Solvent: CDCl<sub>3</sub>

Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 397  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220410  
Time 11.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 106.66  
DW 60.800 usec  
DE 6.50 usec  
TE 297.9 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500129 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C{<sup>1</sup>H} NMR: 100 MHz  
Solvent: CDCl<sub>3</sub>

Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 158  
PROCNO 1

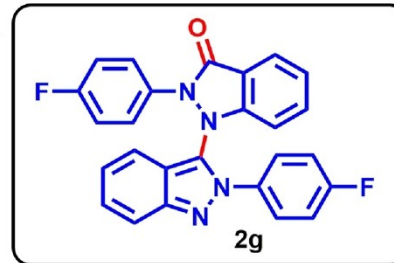
F2 - Acquisition Parameters  
Date\_ 20220410  
Time 12.29  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 1024  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 186.42  
DW 20.800 usec  
DE 6.50 usec  
TE 298.5 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

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

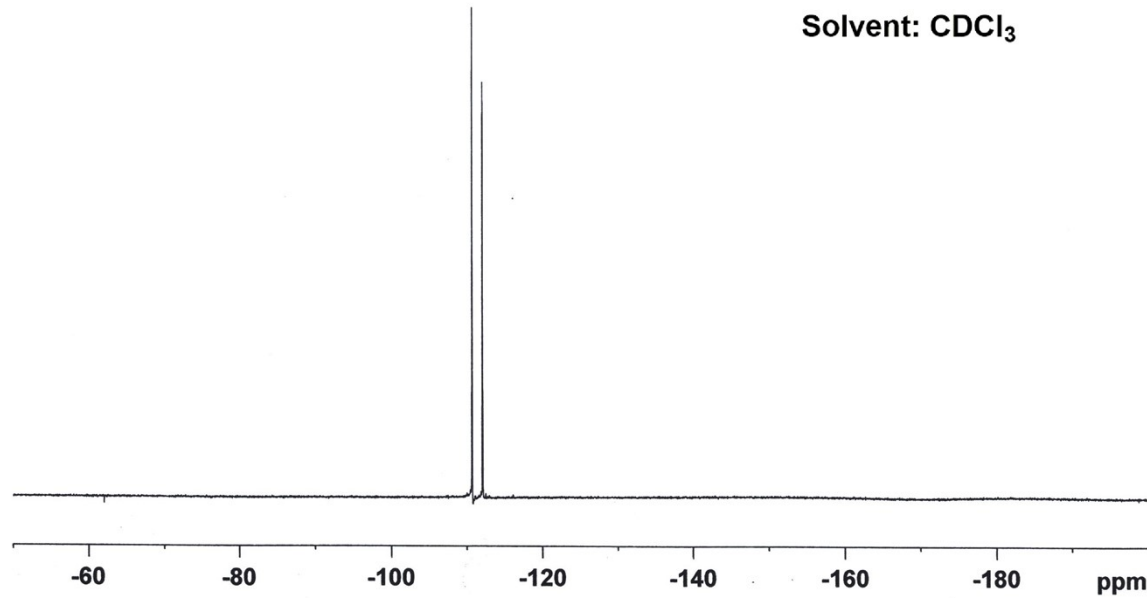
===== CHANNEL f2 =====  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

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

-110.72  
-112.08



<sup>19</sup>F NMR: 376 MHz  
Solvent: CDCl<sub>3</sub>

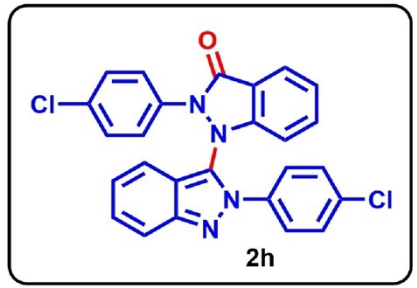
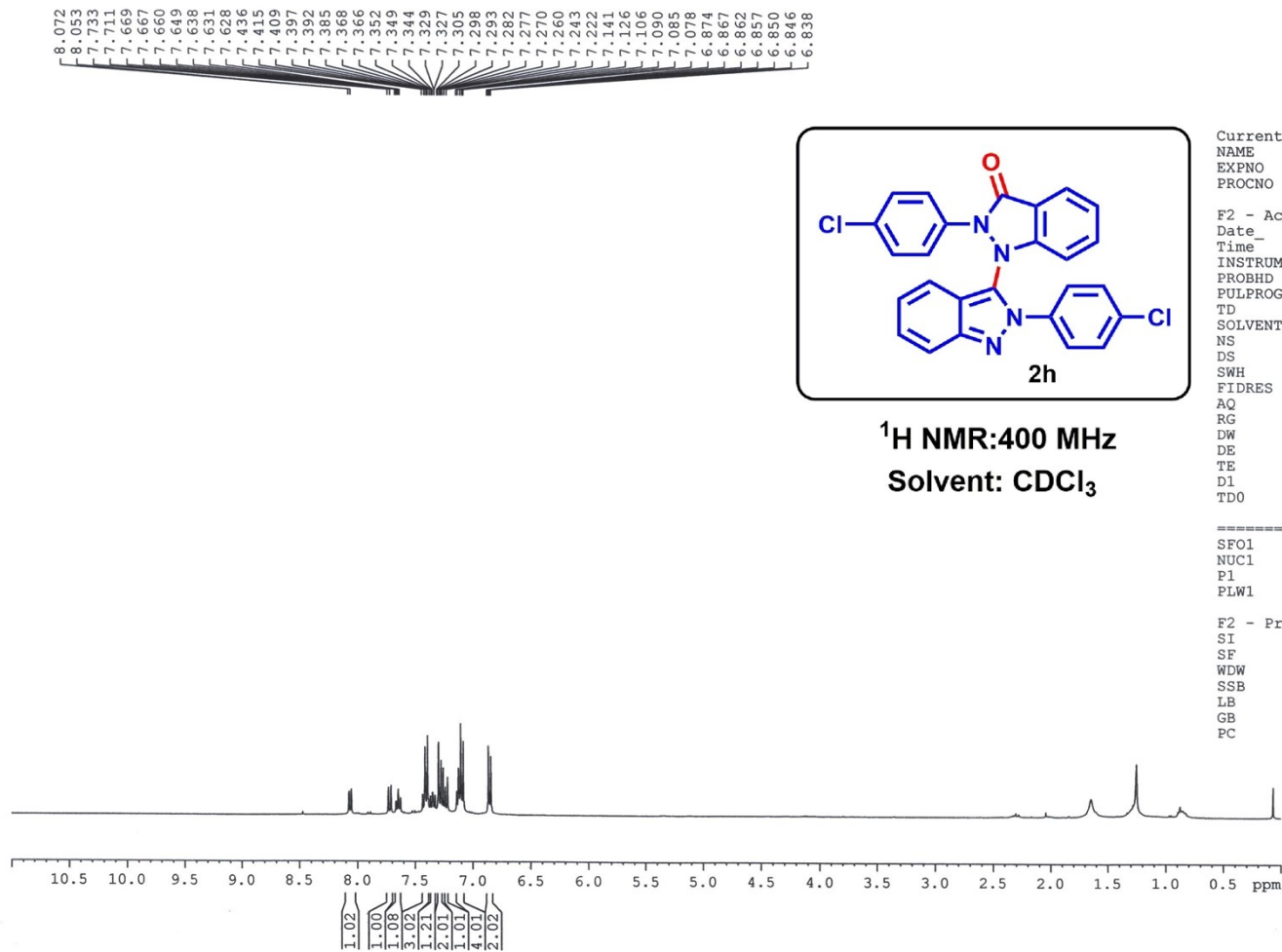


Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 398  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220410  
Time 11.39  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 89285.711 Hz  
FIDRES 2.724784 Hz  
AQ 0.1835008 sec  
RG 186.42  
DW 5.600 usec  
DE 6.50 usec  
TE 297.9 K  
D1 1.0000000 sec  
TDO 1

===== CHANNEL f1 =====  
SF01 376.4795333 MHz  
NUC1 19F  
P1 12.50 usec  
PLW1 20.0000000 W

F2 - Processing parameters  
SI 16384  
SF 376.5171850 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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

```

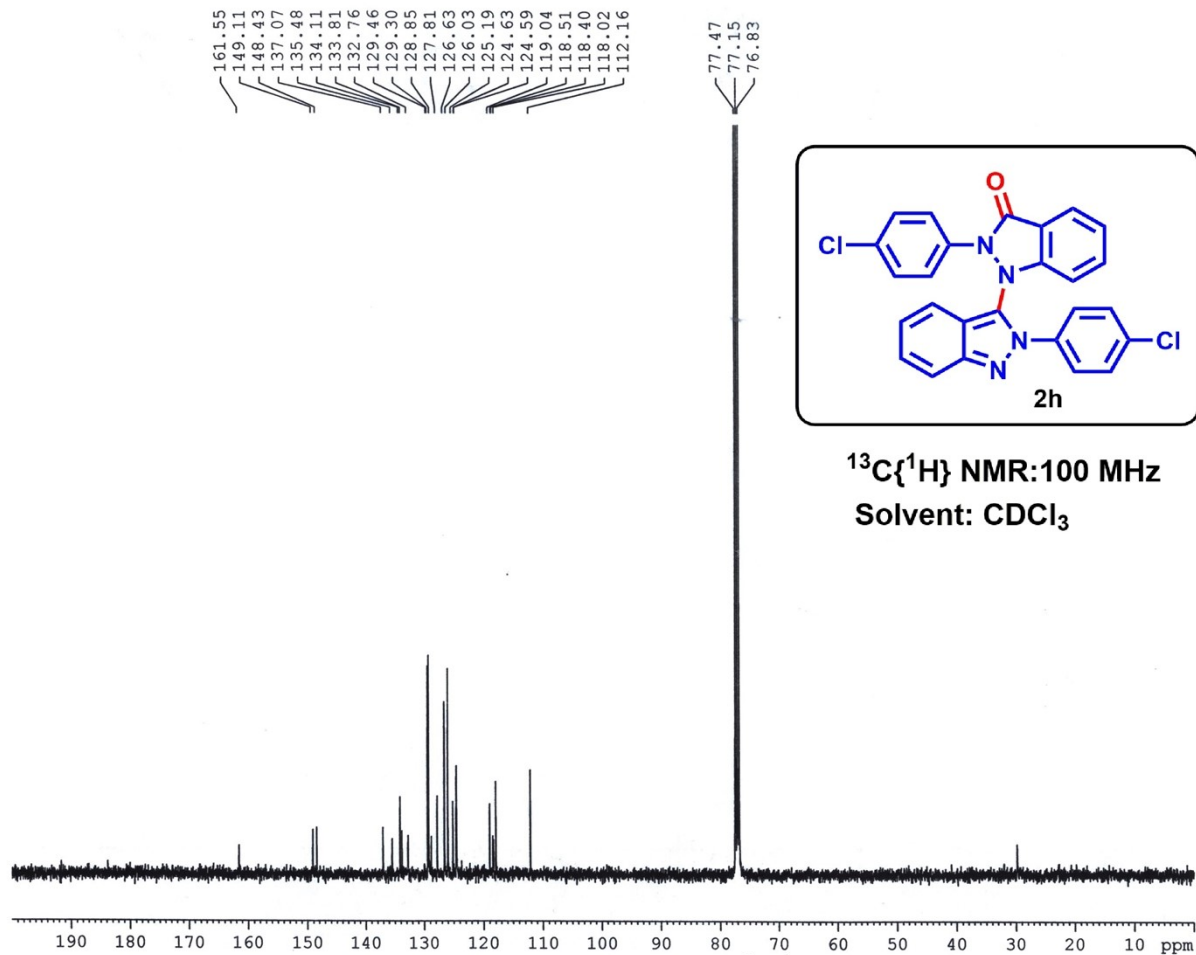
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO     164
PROCNO    1

F2 - Acquisition Parameters
Date_     20220223
Time      18.56
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         8
DS         2
SWH        8223.685 Hz
FIDRES     0.250967 Hz
AQ         1.9922944 sec
RG         186.42
DW         60.800 usec
DE         6.50 usec
TE         294.0 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      400.1524711 MHz
NUC1       1H
P1         14.75 usec
PLW1      12.00000000 W

F2 - Processing parameters
SI         16384
SF         400.1500088 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```





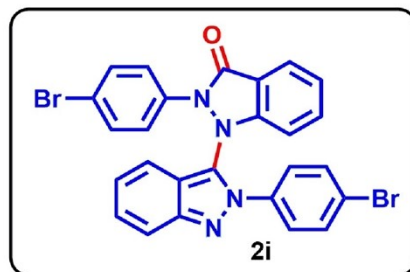
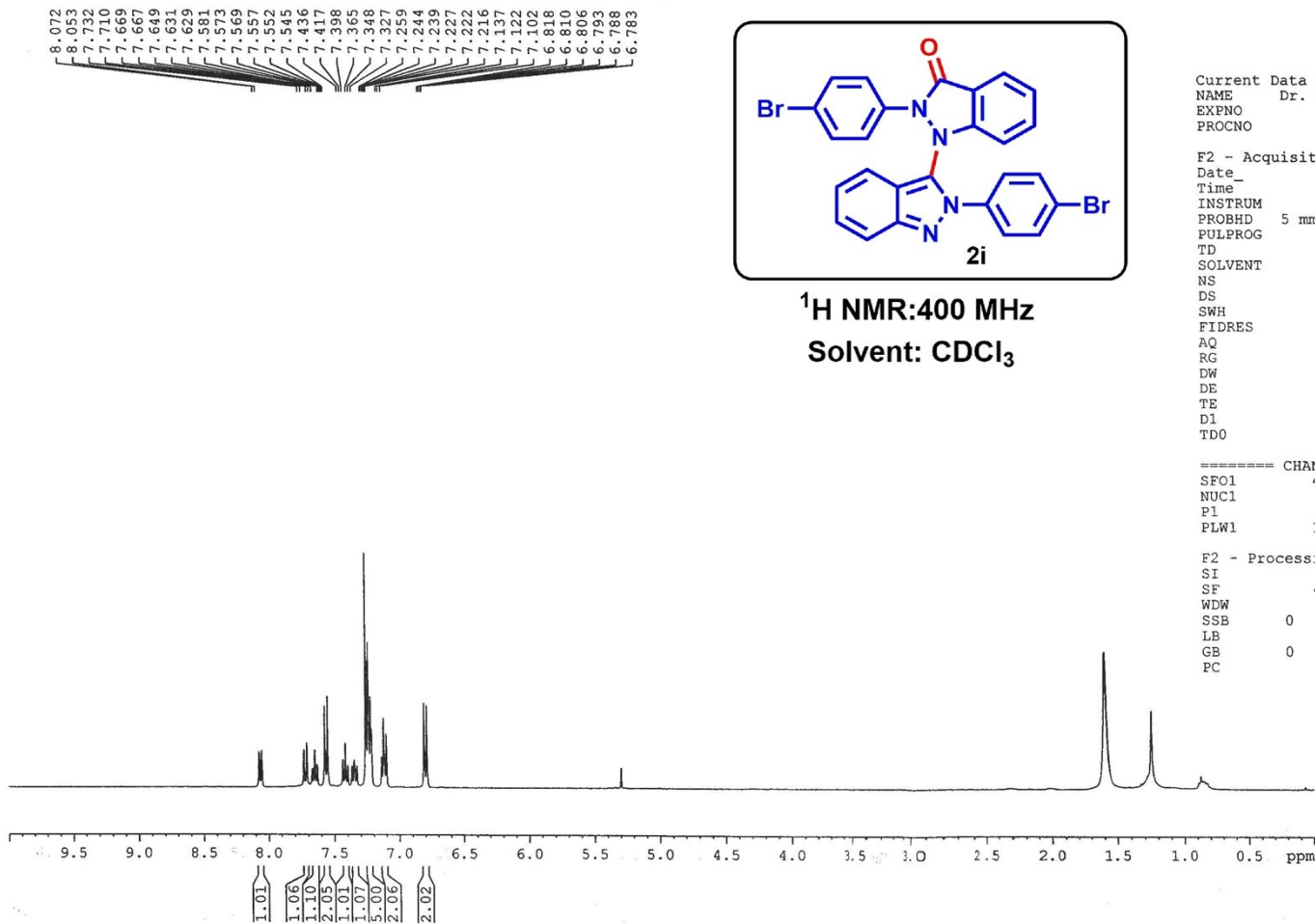
Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 60  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220223  
Time 19.34  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT  $\text{CDCl}_3$   
NS 720  
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 294.4 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 100.6177858 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>

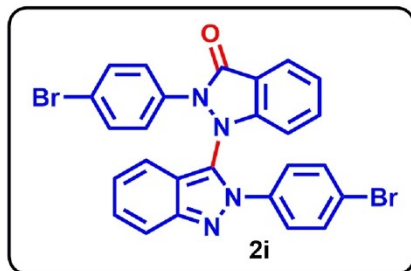
Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 891  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221017  
Time\_ 10.31  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 186.42  
DW 60.800 usec  
DE 6.50 usec  
TE 295.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500086 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

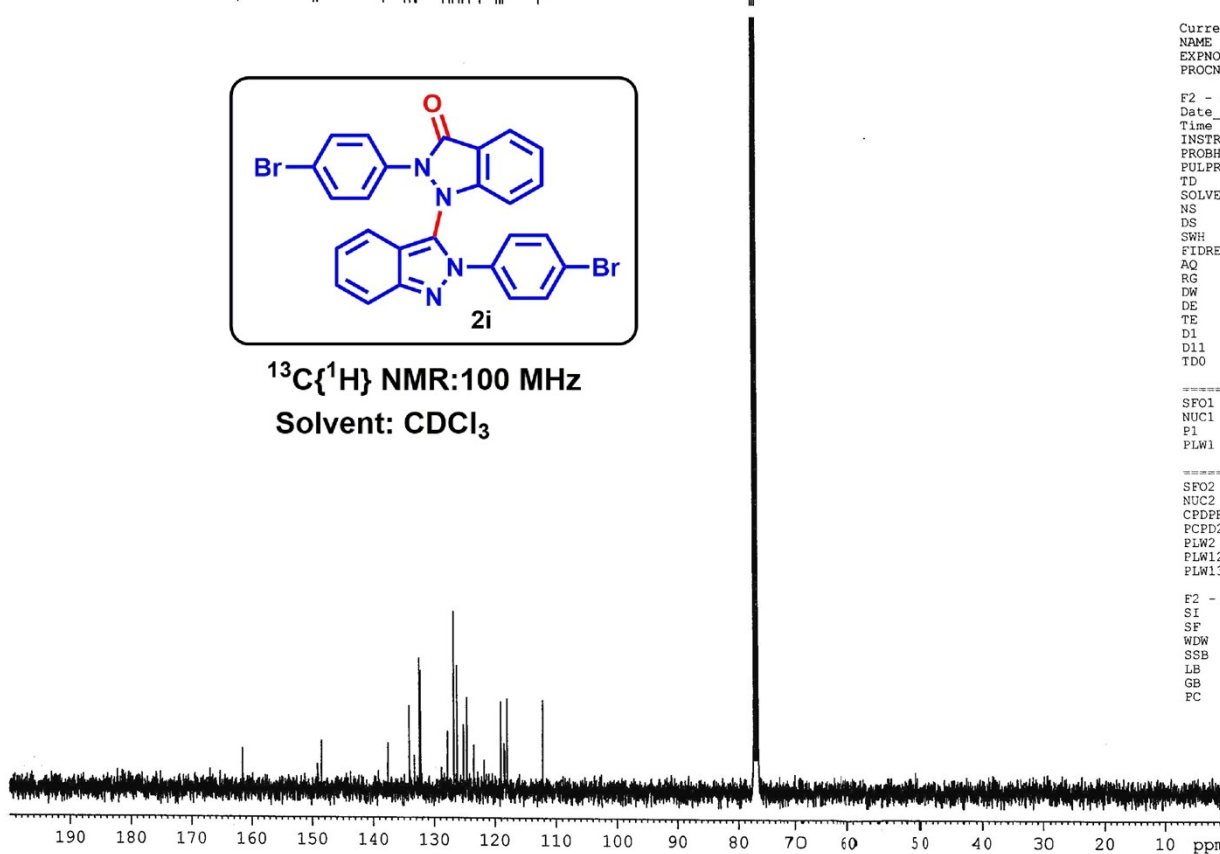
161.54  
149.09  
148.47  
137.59  
134.15  
133.32  
132.47  
132.28  
132.20  
127.85  
126.82  
126.27  
125.22  
124.66  
124.62  
123.49  
121.81  
119.06  
118.52  
118.42  
118.03  
112.19



$^{13}\text{C}\{^1\text{H}\}$  NMR: 100 MHz

Solvent:  $\text{CDCl}_3$

77.47  
77.15  
76.83



Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 364  
PROCNO 1

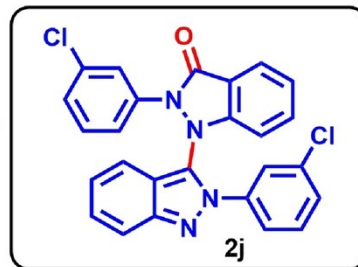
F2 - Acquisition Parameters  
Date\_ 20221017  
Time 11.21  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 1024  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 186.42  
DW 20.800 usec  
DE 6.50 usec  
TE 295.6 K  
D1 2.0000000 sec  
D11 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 100.6177844 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

8.075  
8.056  
7.734  
7.712  
7.686  
7.684  
7.665  
7.647  
7.646  
7.686  
7.484  
7.464  
7.447  
7.428  
7.409  
7.402  
7.382  
7.362  
7.356  
7.350  
7.326  
7.304  
7.286  
7.284  
7.260  
7.217  
7.196  
7.147  
7.136  
7.126  
7.100  
7.080  
7.059  
6.905  
6.902  
6.897  
6.892  
6.888



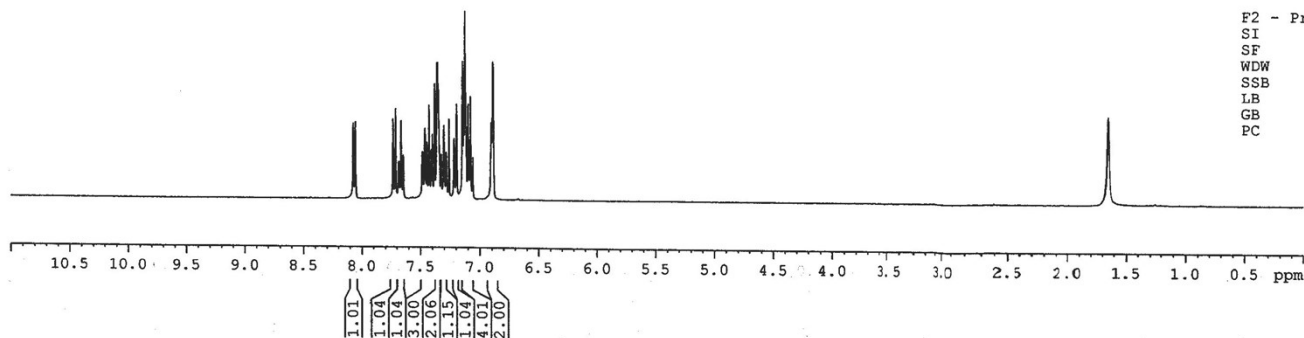
<sup>1</sup>H NMR:400 MHz  
Solvent: CDCl<sub>3</sub>

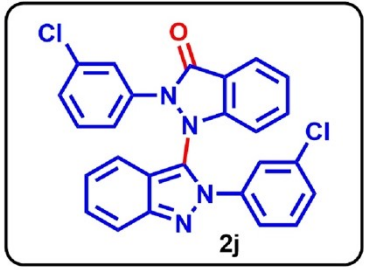
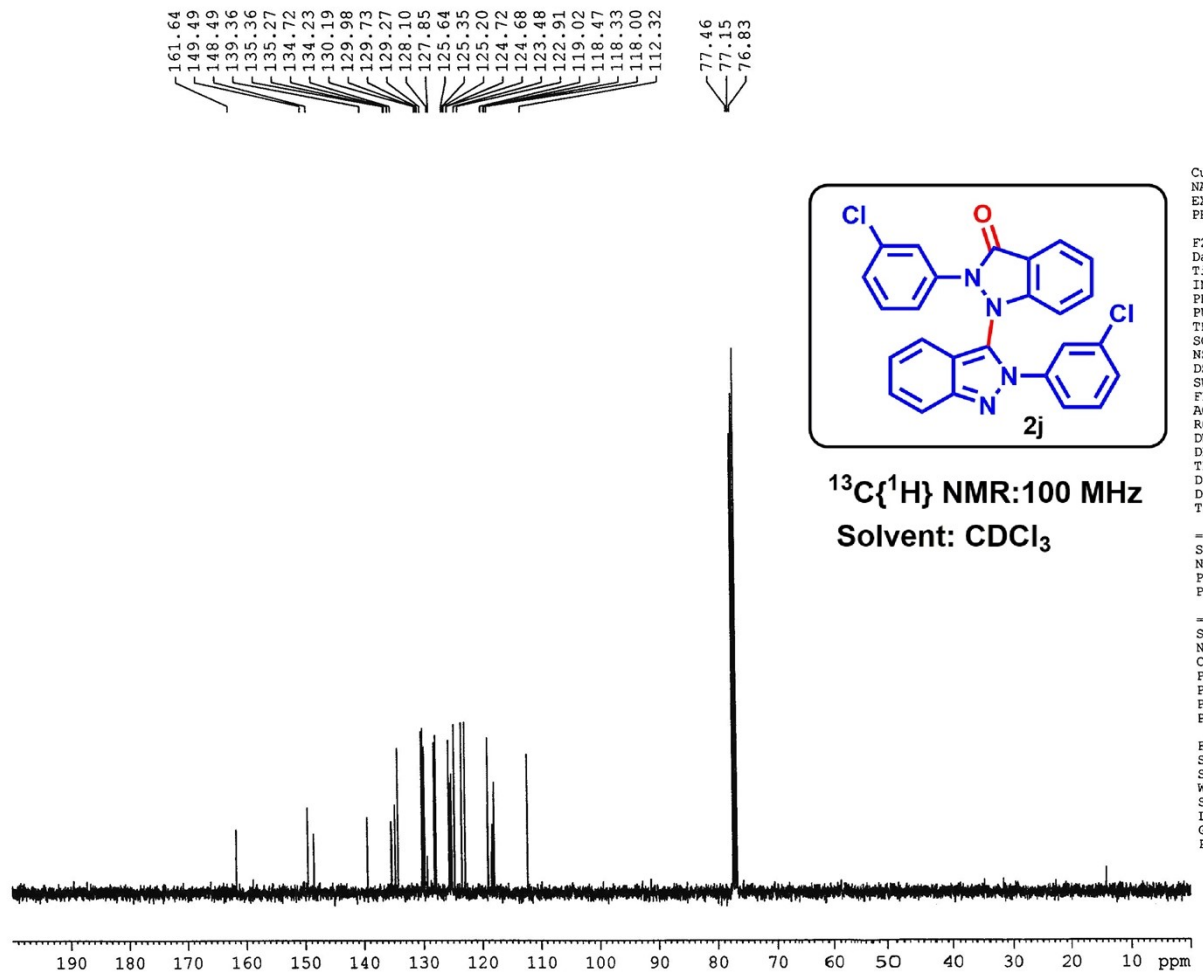
Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 908  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221019  
Time\_ 10.15  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 148.91  
DW 60.800 usec  
DE 6.50 usec  
TE 294.6 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500084 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





<sup>13</sup>C{<sup>1</sup>H} NMR: 100 MHz  
Solvent: CDCl<sub>3</sub>

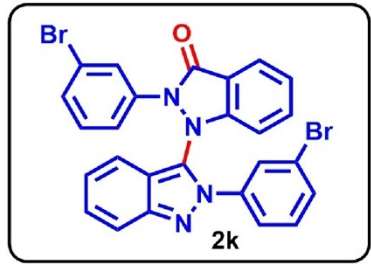
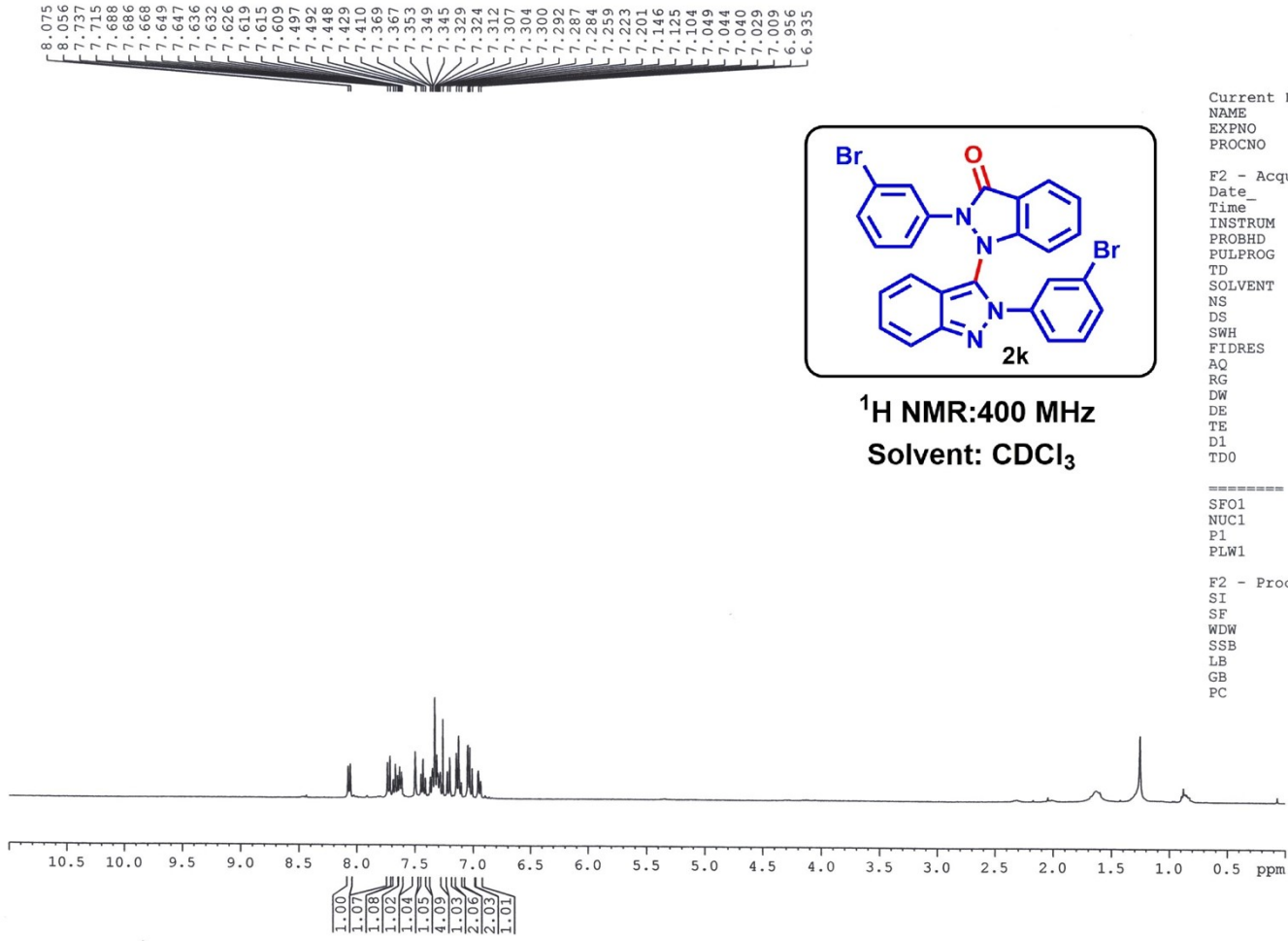
Current Data Parameters  
 NAME Dr. A HAJRA-2022-13C  
 EXPNO 366  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20221017  
 Time 19.28  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 105  
 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 296.7 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  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177887 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 2022 1H  
 EXPNO 232  
 PROCNO 1

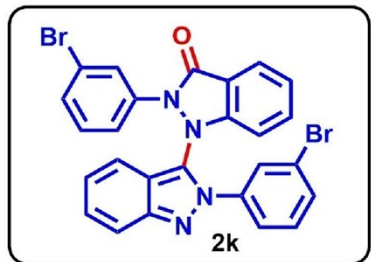
F2 - Acquisition Parameters  
 Date\_ 20220306  
 Time\_ 16.50  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9922944 sec  
 RG 168.31  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 293.5 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 12.00000000 W

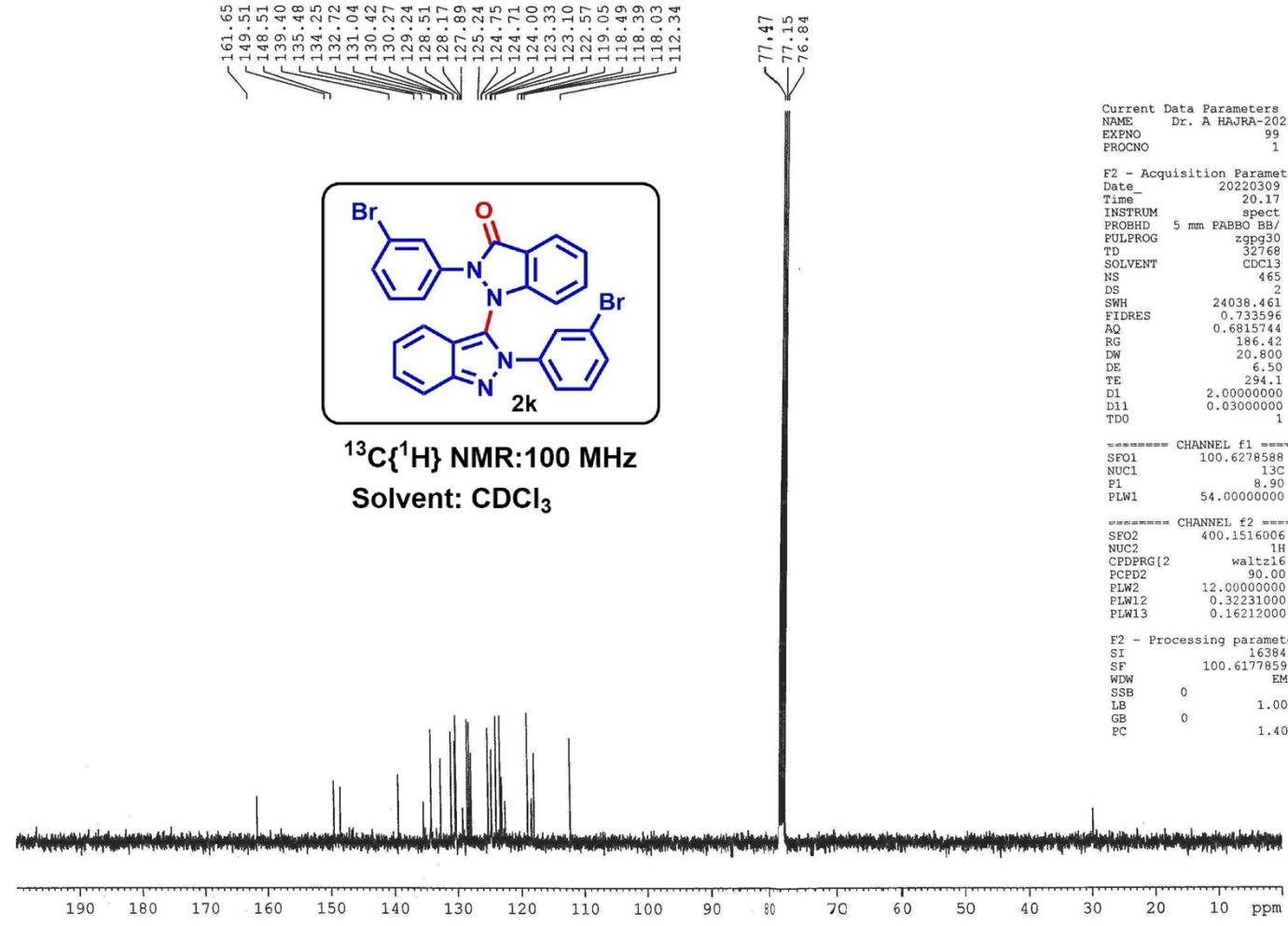
F2 - Processing parameters  
 SI 16384  
 SF 400.1500087 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

161.65  
149.51  
148.51  
139.40  
135.48  
134.25  
132.72  
131.04  
130.42  
130.27  
129.24  
128.51  
128.17  
127.89  
125.24  
124.75  
124.71  
124.00  
123.33  
123.10  
122.57  
119.05  
118.49  
118.39  
118.03  
112.34

77.47  
77.15  
76.84



$^{13}\text{C}\{^1\text{H}\}$  NMR: 100 MHz  
Solvent:  $\text{CDCl}_3$



```

Current Data Parameters
NAME      Dr. A HAJRA-2022-13C
EXPNO     99
PROCNO    1

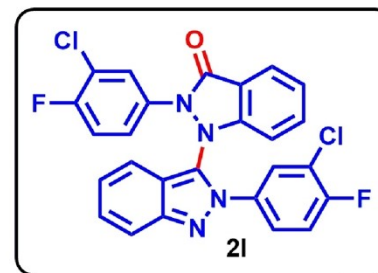
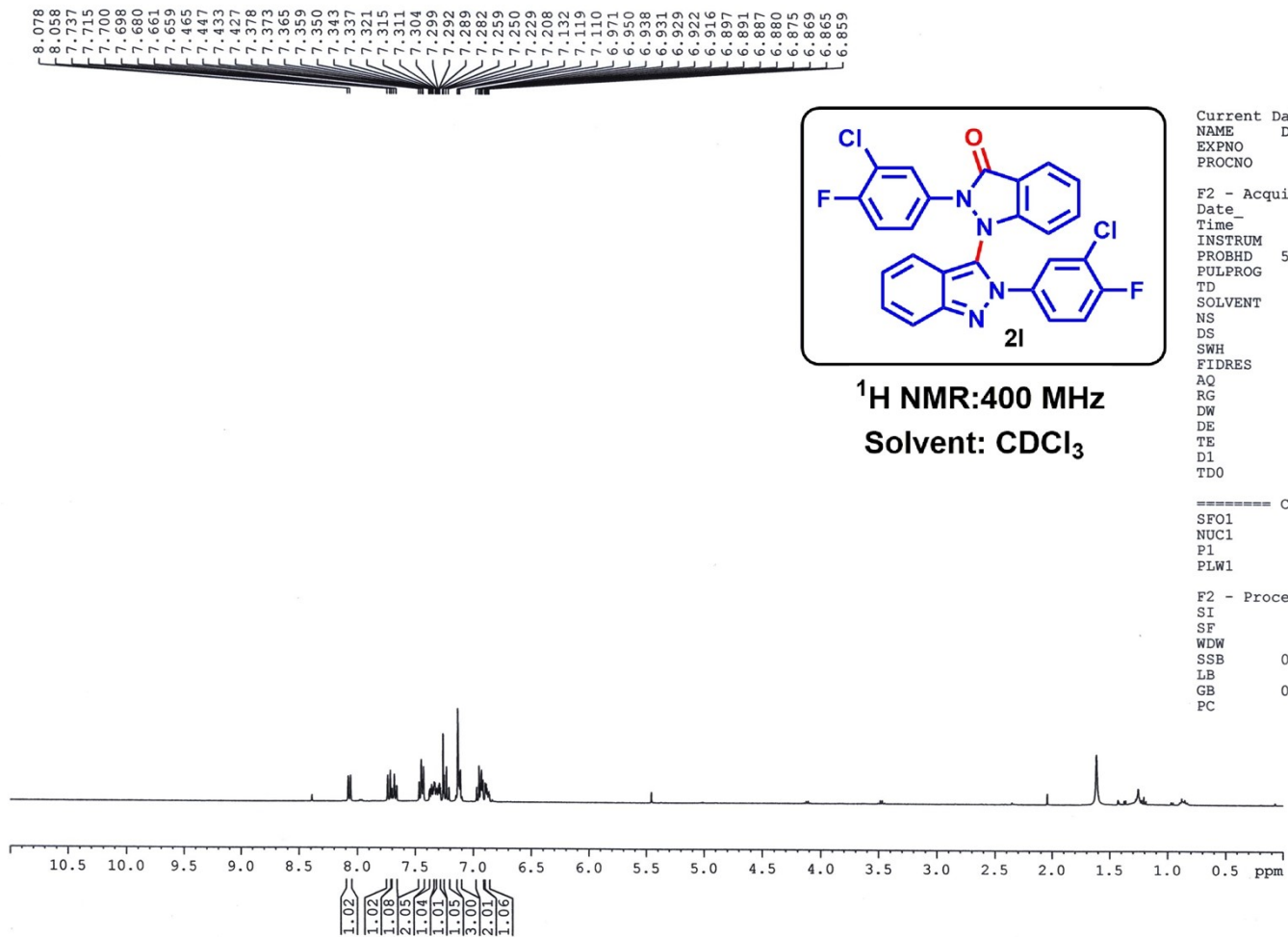
F2 - Acquisition Parameters
Date_     20220309
Time      20.17
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         465
DS         2
SWH        24038.461 Hz
FIDRES     0.733596 Hz
AQ         0.6815744 sec
RG         186.42
DW         20.800 usec
DE         6.50 usec
TE         294.1 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

```



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

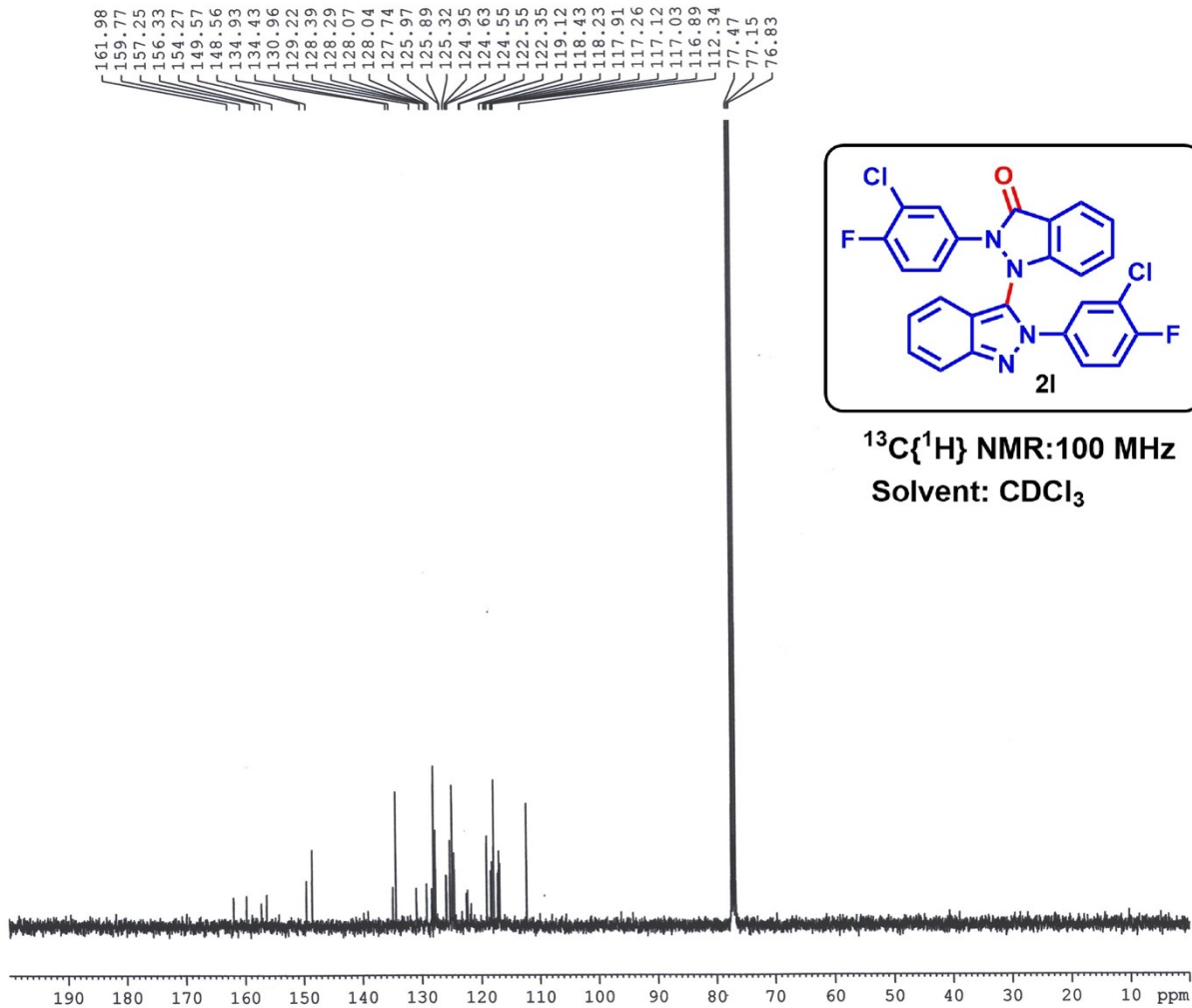
Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 422  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220414  
Time 20.19  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 148.91  
DW 60.800 usec  
DE 6.50 usec  
TE 296.5 K  
D1 1.00000000 sec  
TDO 1

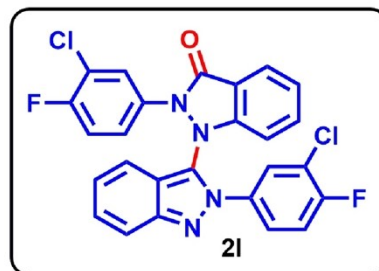
===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500090 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



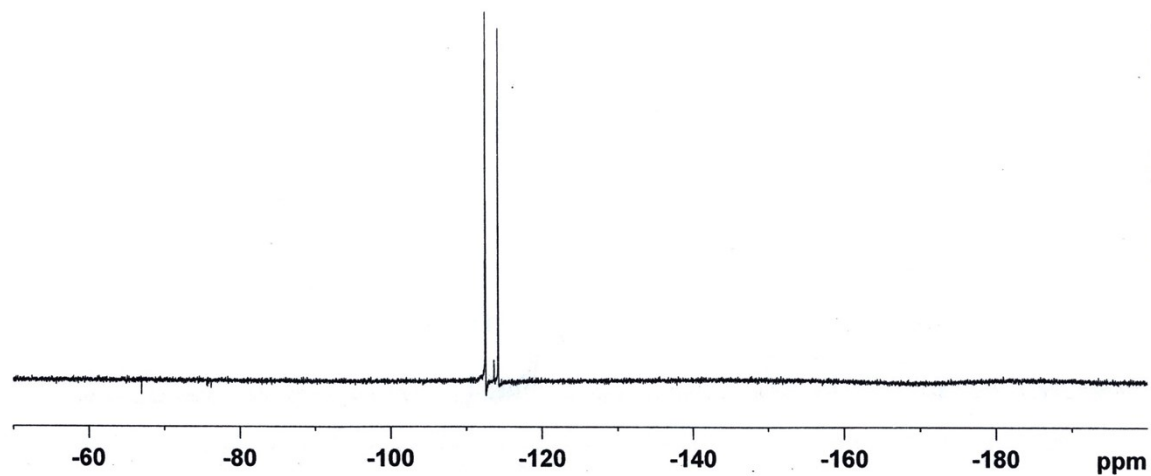


-112.53  
-114.20



**<sup>19</sup>F NMR: 376 MHz**

**Solvent: CDCl<sub>3</sub>**



Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 423  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220414  
Time\_ 20.26  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgflqn  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 89285.711 Hz  
FIDRES 2.724784 Hz  
AQ 0.1835008 sec  
RG 186.42  
DW 5.600 usec  
DE 6.50 usec  
TE 296.5 K  
D1 1.00000000 sec  
TDO 1

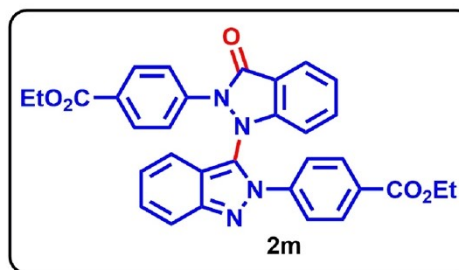
===== CHANNEL f1 =====  
SFO1 376.4795333 MHz  
NUC1 19F  
P1 12.50 usec  
PLW1 20.00000000 W

F2 - Processing parameters  
SI 16384  
SF 376.5171850 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

8.137  
8.115  
8.080  
8.060  
7.800  
7.779  
7.715  
7.693  
7.667  
7.648  
7.479  
7.457  
7.432  
7.413  
7.378  
7.357  
7.347  
7.325  
7.260  
7.171  
7.150  
7.128  
7.083  
7.062

4.458  
4.441  
4.423  
4.405  
4.328  
4.311  
4.293  
4.275

1.458  
1.441  
1.423  
1.349  
1.331  
1.313



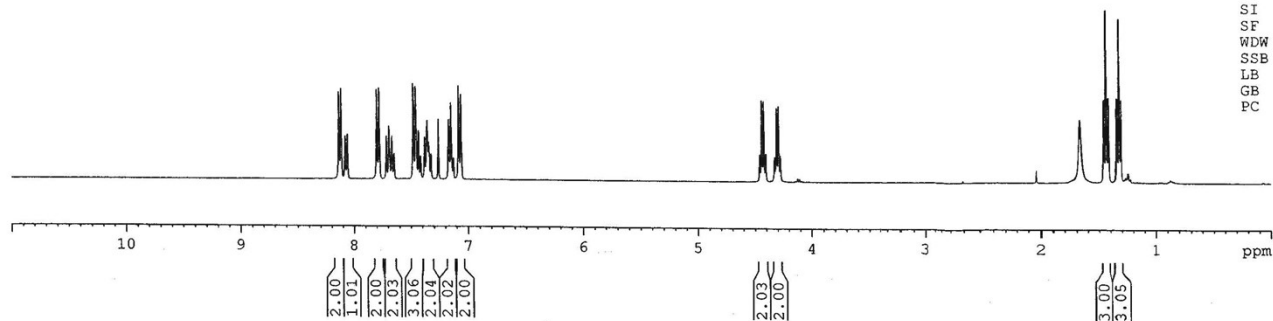
<sup>1</sup>H NMR: 400 MHz  
Solvent: CDCl<sub>3</sub>

Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 923  
PROCNO 1

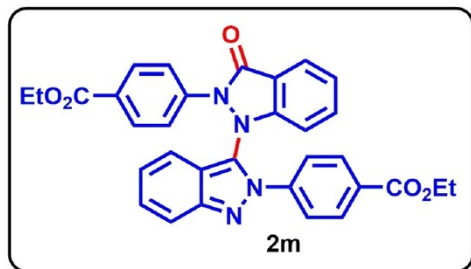
F2 - Acquisition Parameters  
Date\_ 20221021  
Time 10.19  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 120.16  
DW 60.800 usec  
DE 6.50 usec  
TE 294.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

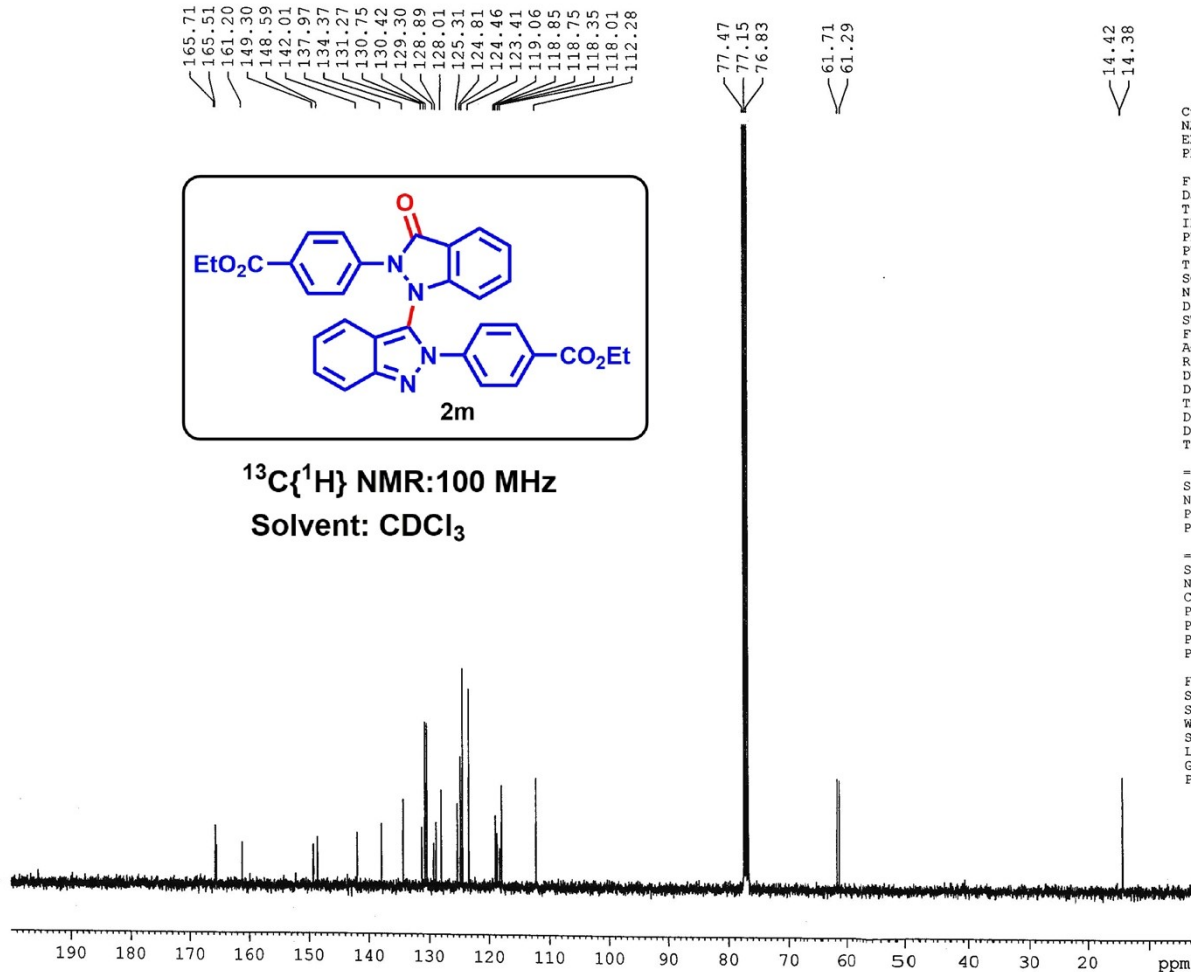
F2 - Processing parameters  
SI 16384  
SF 400.1500077 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



165.71  
165.51  
161.20  
149.30  
148.59  
142.01  
137.97  
134.37  
131.27  
130.75  
130.42  
129.30  
128.89  
128.01  
125.31  
124.81  
124.46  
123.41  
119.06  
118.85  
118.75  
118.35  
118.01  
112.28



<sup>13</sup>C{<sup>1</sup>H} NMR: 100 MHz  
Solvent: CDCl<sub>3</sub>



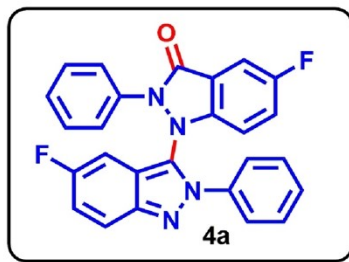
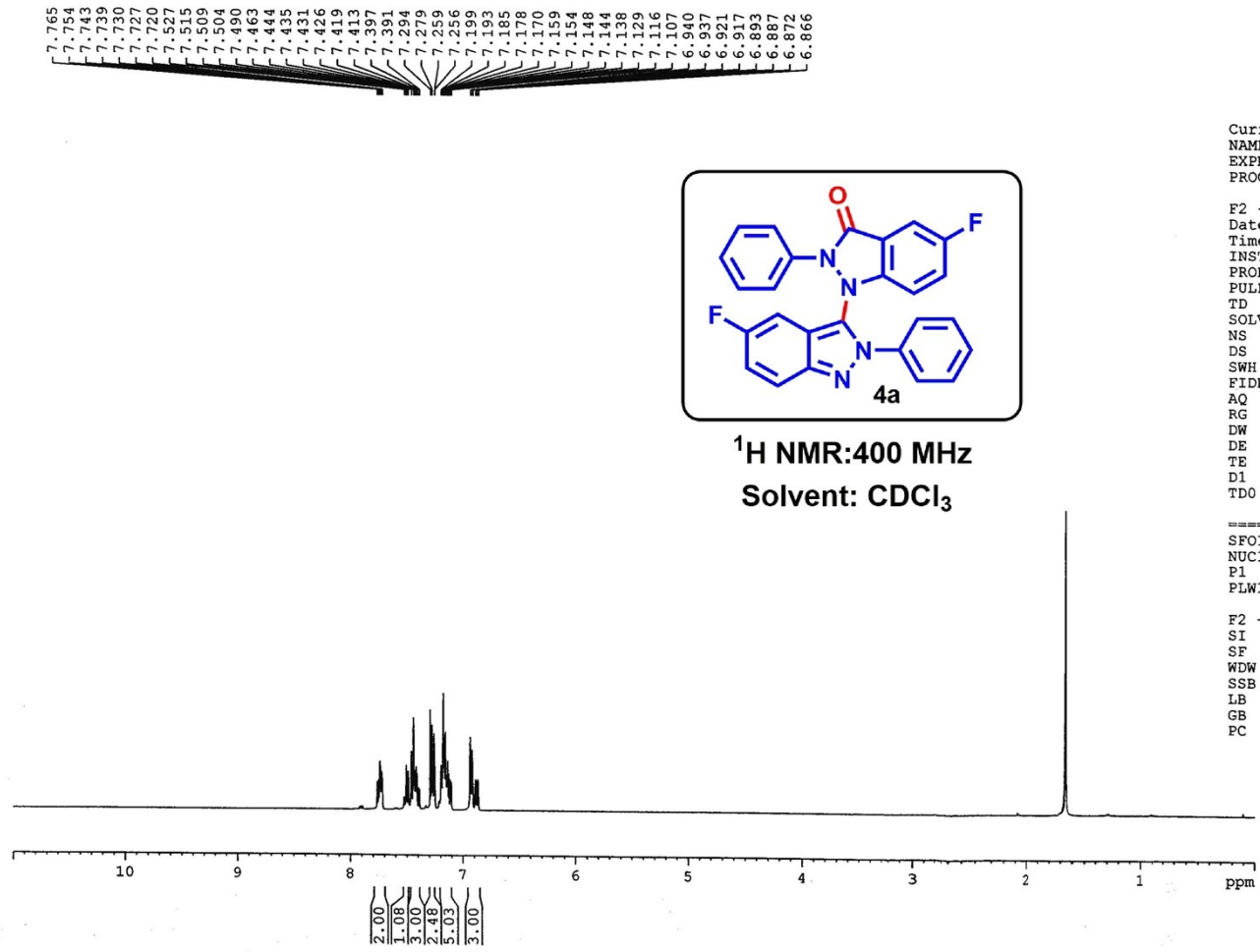
Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXNO 375  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221021  
Time 10.58  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 720  
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 294.8 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  
CPDPRG12 waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

F2 - Processing parameters  
SI 16384  
SF 100.6177857 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



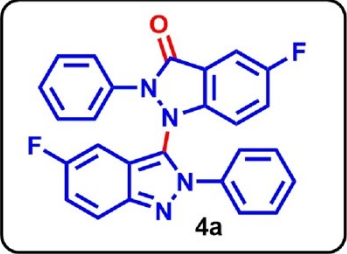
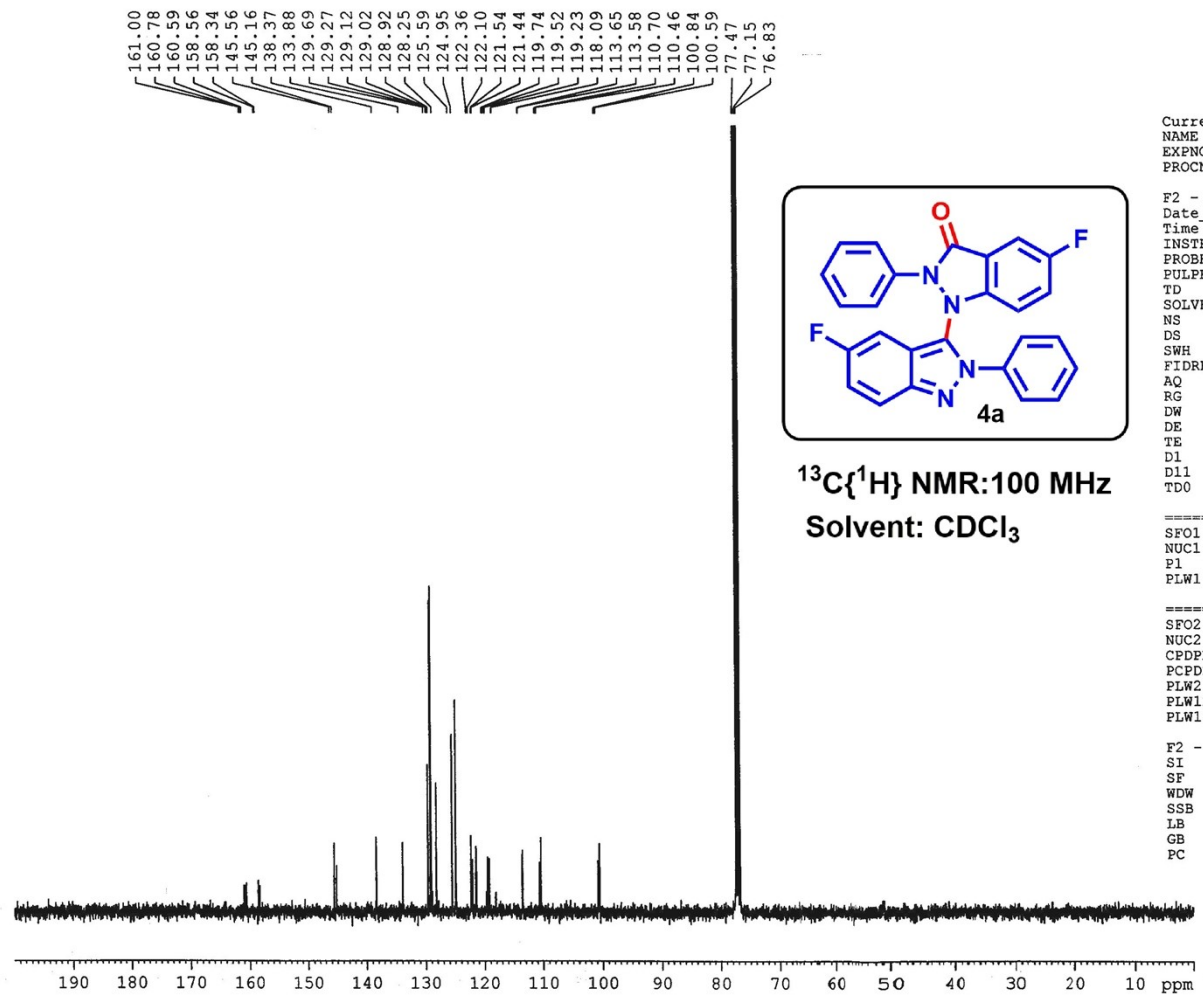
<sup>1</sup>H NMR:400 MHz  
Solvent: CDCl<sub>3</sub>

Current Data Parameters  
 NAME Dr. A HAJRA 2022 1H  
 EXPNO 909  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20221019  
 Time 10.21  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9922944 sec  
 RG 148.91  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 294.5 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SF01 400.1524711 MHz  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 16384  
 SF 400.1499947 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



<sup>13</sup>C{<sup>1</sup>H} NMR: 100 MHz  
Solvent: CDCl<sub>3</sub>

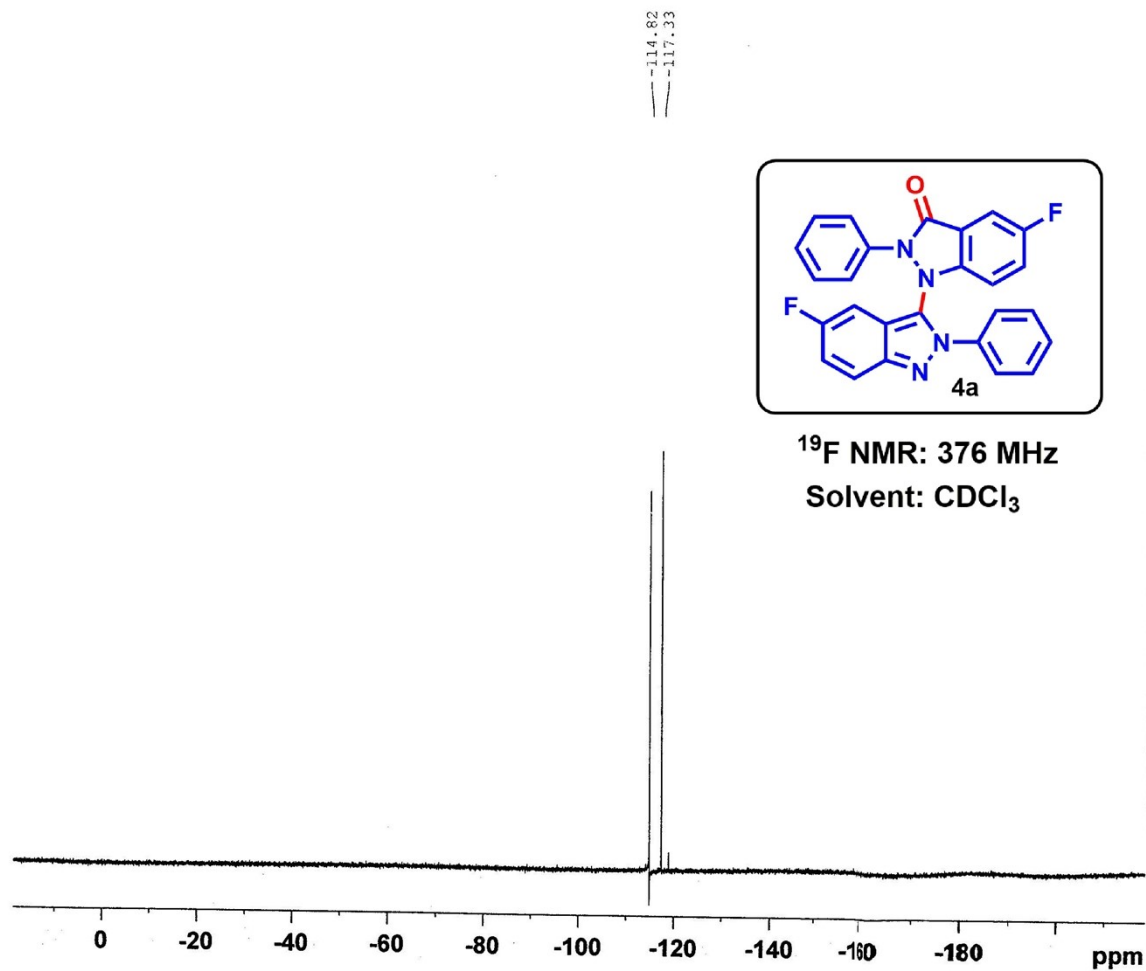
Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 372  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221019  
Time 11.16  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 1024  
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 295.2 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

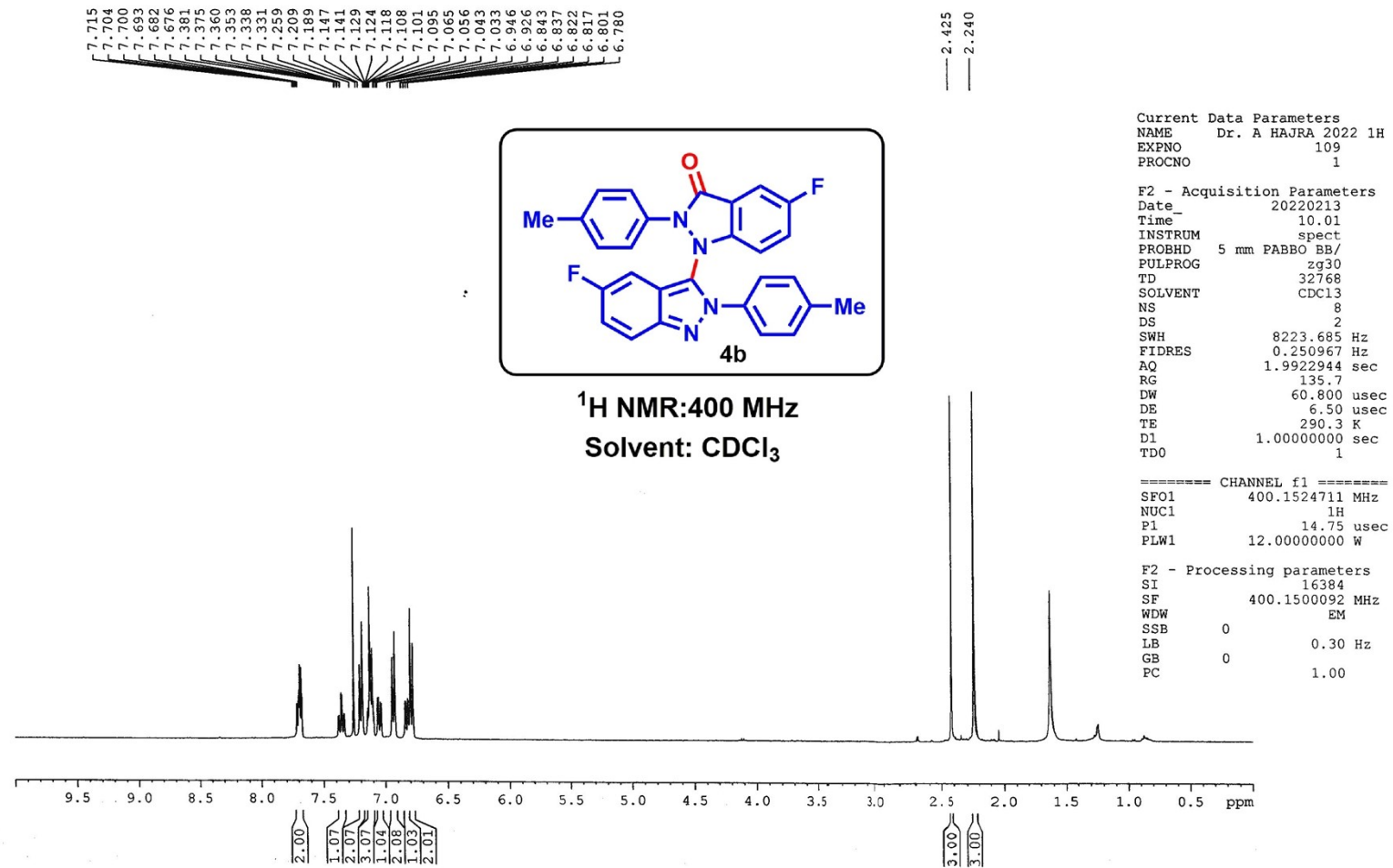


Current Data Parameters  
 NAME Dr. A HAJRA 2022 1H  
 EXPNO 910  
 PROCNO 1

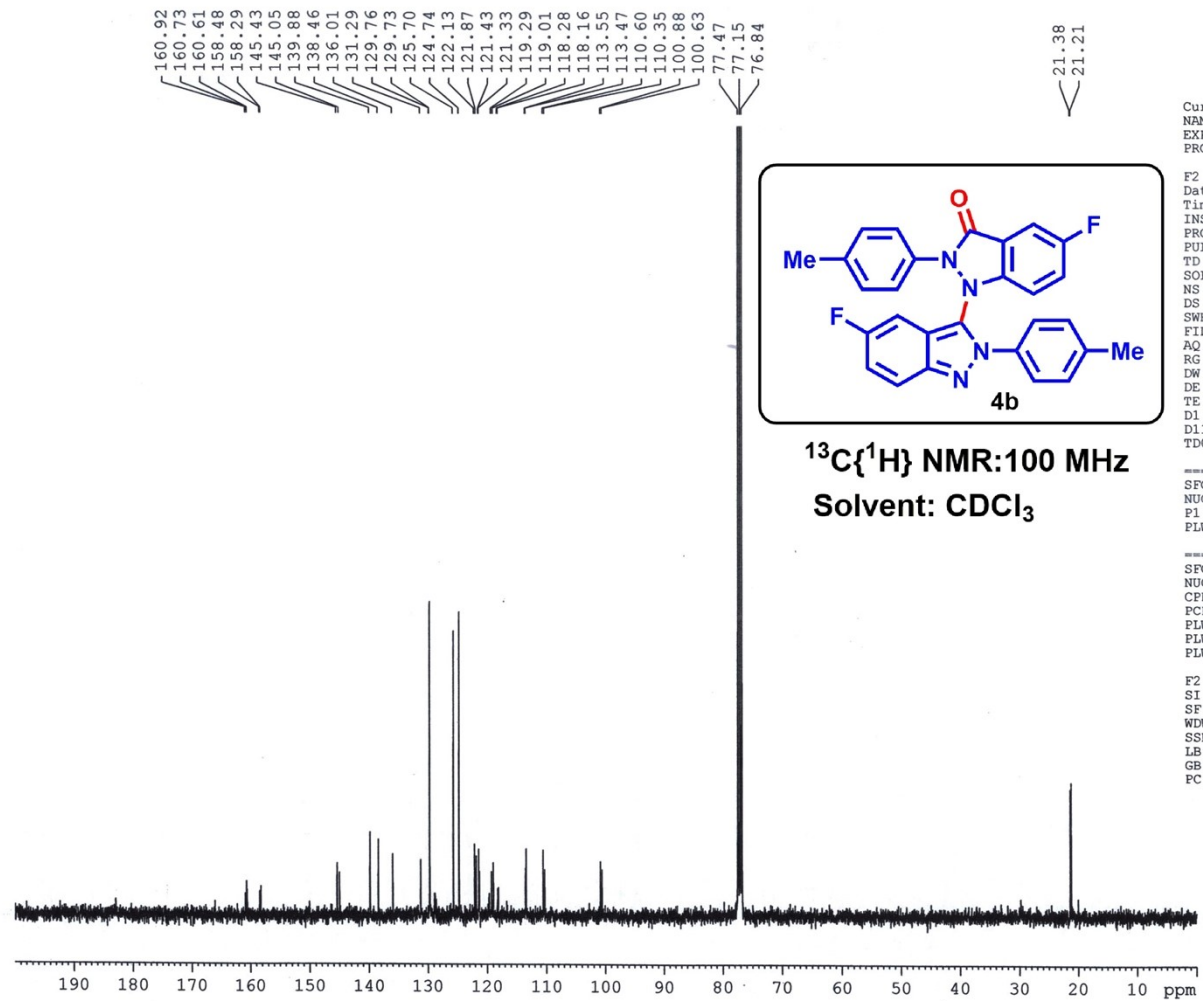
F2 - Acquisition Parameters  
 Date\_ 20221019  
 Time\_ 10.25  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgfg1qn  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 89285.711 Hz  
 FIDRES 2.724784 Hz  
 AQ 0.1835008 sec  
 RG 186.42  
 DW 5.600 usec  
 DE 6.50 usec  
 TE 294.5 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SF01 376.4795333 MHz  
 NUC1 19F  
 P1 12.50 usec  
 PLW1 20.00000000 W

F2 - Processing parameters  
 SI 16384  
 SF 376.5171850 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00







Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXNO 166  
PROCNO 1

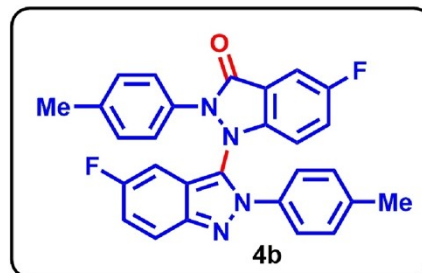
F2 - Acquisition Parameters  
Date\_ 20220415  
Time\_ 20.17  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 1500  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 186.42  
DW 20.800 usec  
DE 6.50 usec  
TE 299.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

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

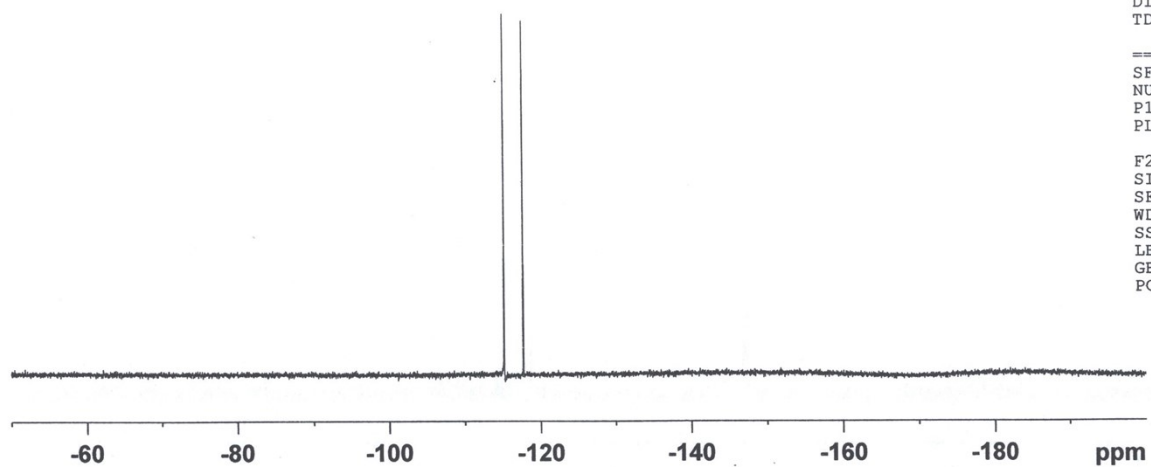
----- CHANNEL f2 -----  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

F2 - Processing parameters  
SI 16384  
SF 100.6177836 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

----- -115.21  
----- -117.73



**<sup>19</sup>F NMR: 376 MHz**  
**Solvent: CDCl<sub>3</sub>**

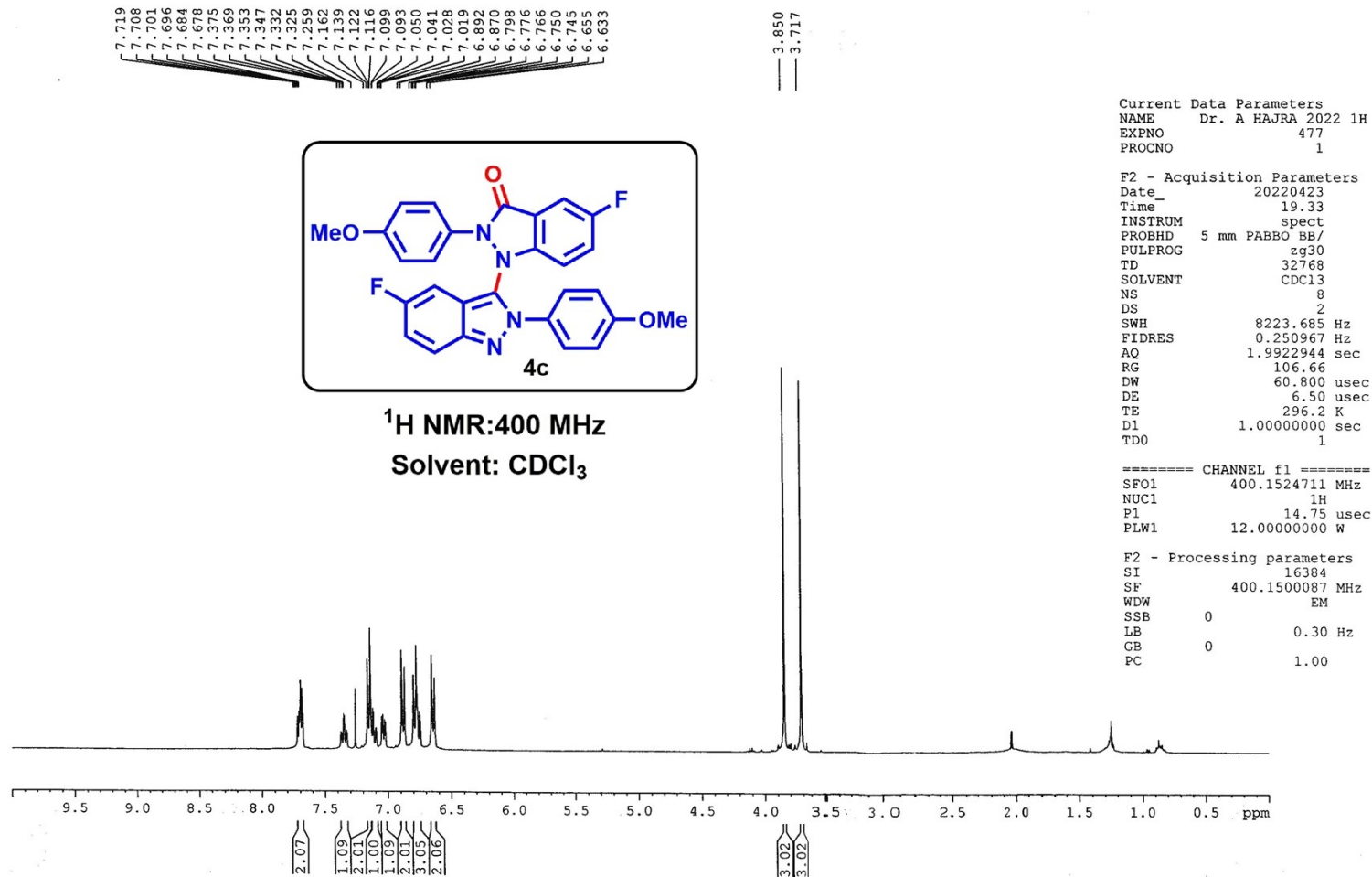


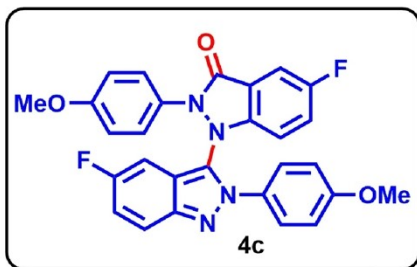
Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 428  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220415  
Time\_ 19.05  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgflqn  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 89285.711 Hz  
FIDRES 2.724784 Hz  
AQ 0.1835008 sec  
RG 186.42  
DW 5.600 usec  
DE 6.50 usec  
TE 298.7 K  
D1 1.00000000 sec  
TDO 1

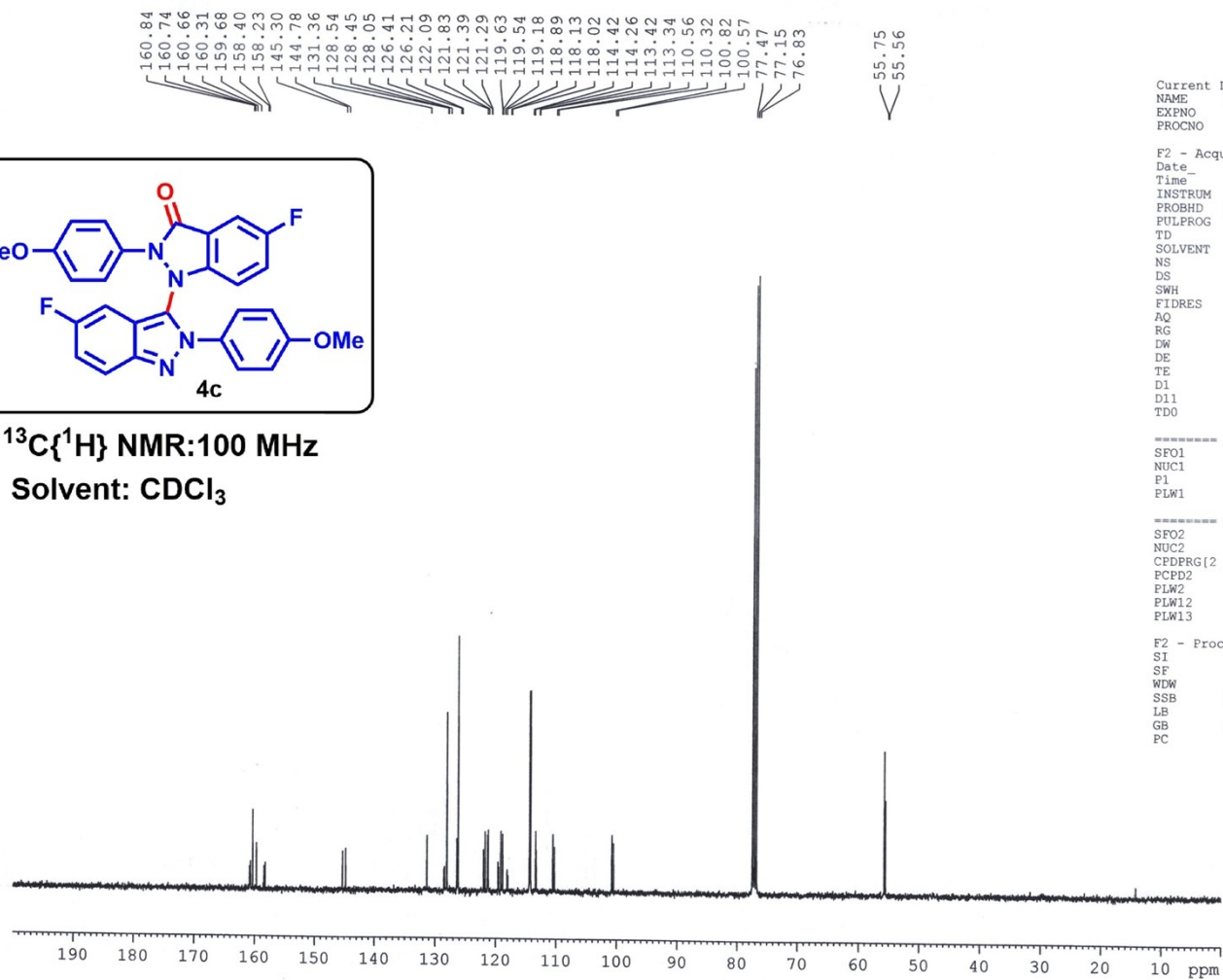
==== CHANNEL f1 =====  
SFO1 376.4795333 MHz  
NUC1 19F  
P1 12.50 usec  
PLW1 20.00000000 W

F2 - Processing parameters  
SI 16384  
SF 376.5171850 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





$^{13}\text{C}\{^1\text{H}\}$  NMR: 100 MHz  
Solvent:  $\text{CDCl}_3$



Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 185  
PROCNO 1

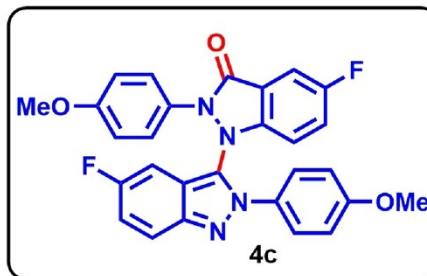
F2 - Acquisition Parameters  
Date\_ 20220423  
Time 20.12  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 745  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 106.66  
DW 20.800 usec  
DE 6.50 usec  
TE 296.5 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

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

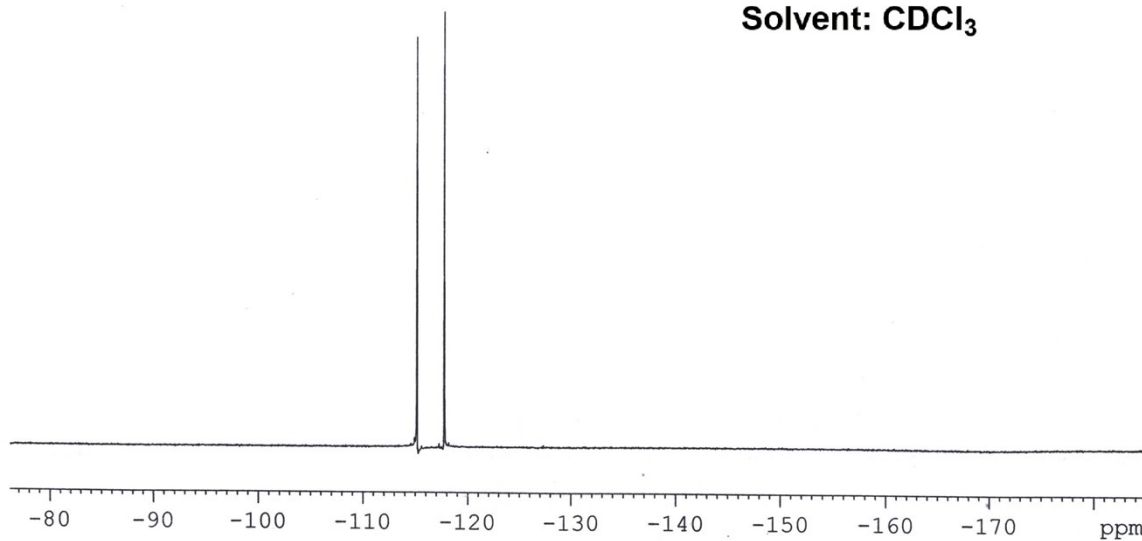
===== CHANNEL f2 =====  
SFO2 400.1516006 MHz  
NUC2 1H  
CFDPRG{2 waltz16  
PCPD2 90.00 usec  
PLW2 12.0000000 W  
PLW12 0.3223100 W  
PLW13 0.1621200 W

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

---115.18  
---117.76



**<sup>19</sup>F NMR: 376 MHz**  
**Solvent: CDCl<sub>3</sub>**

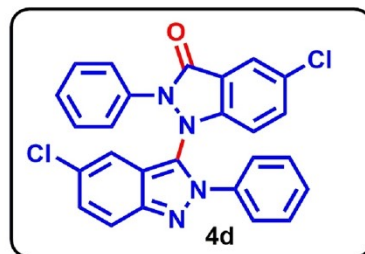
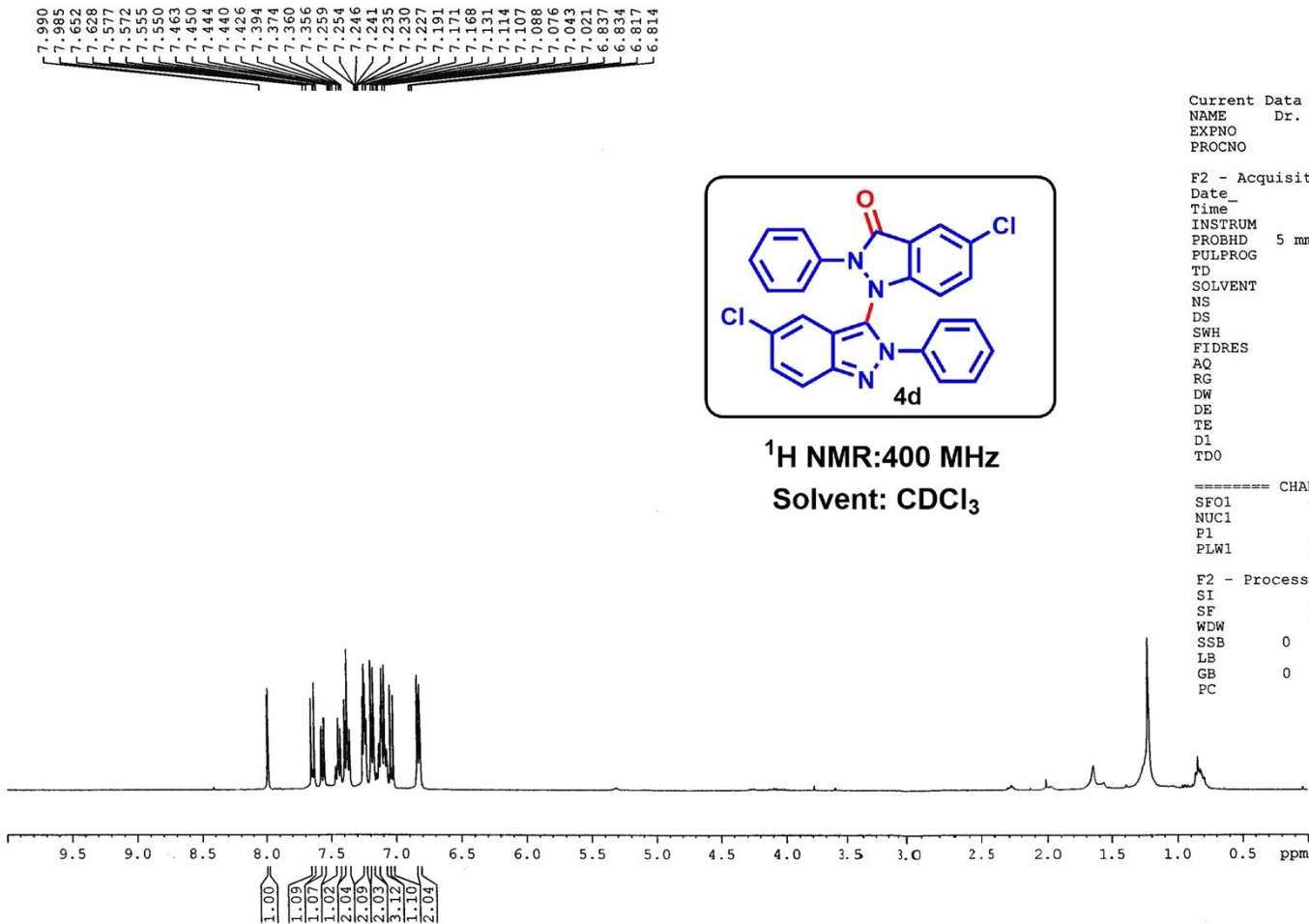


Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 478  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220423  
Time\_ 19.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgfg  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 89285.711 Hz  
FIDRES 2.724784 Hz  
AQ 0.1835008 sec  
RG 106.66  
DW 5.600 usec  
DE 6.50 usec  
TE 296.2 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SF01 376.4795333 MHz  
NUC1 19F  
P1 12.50 usec  
PLW1 20.00000000 W

F2 - Processing parameters  
SI 16384  
SF 376.5171850 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



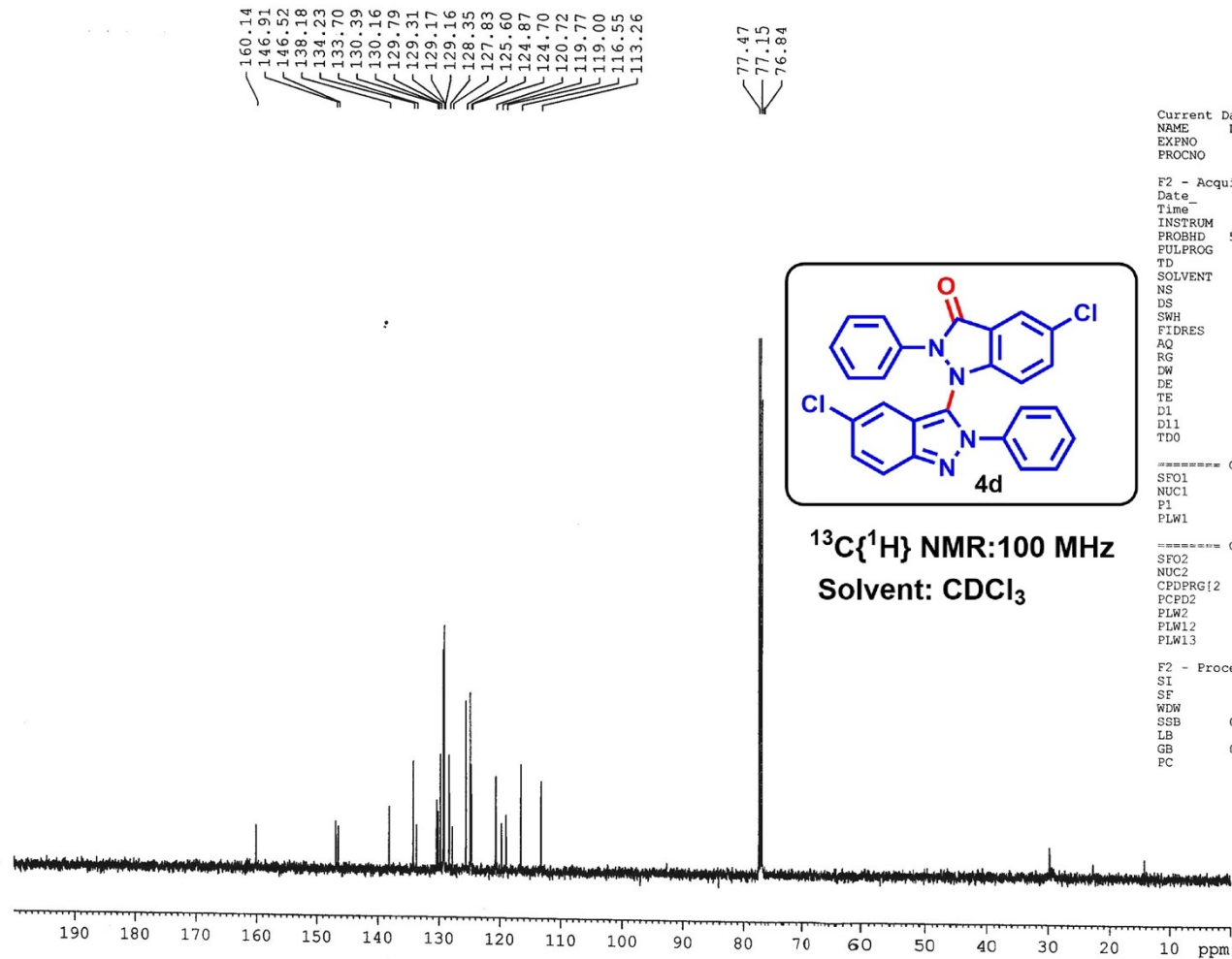
<sup>1</sup>H NMR: 400 MHz  
Solvent: CDCl<sub>3</sub>

Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 237  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220309  
Time 14.28  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 120.16  
DW 60.800 usec  
DE 6.50 usec  
TE 292.9 K  
D1 1.00000000 sec  
TDO 1

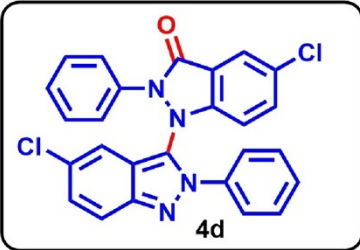
===== CHANNEL f1 =====  
SF01 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500219 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
 NAME Dr. A HAJRA-2022-13C  
 EXPNO 96  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220309  
 Time 14.43  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 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 293.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1



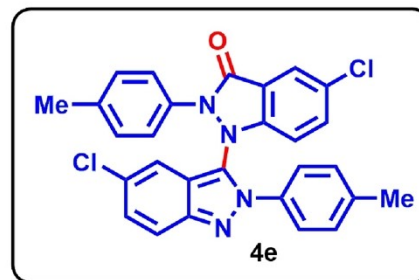
<sup>13</sup>C{<sup>1</sup>H} NMR: 100 MHz  
 Solvent: CDCl<sub>3</sub>

===== 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

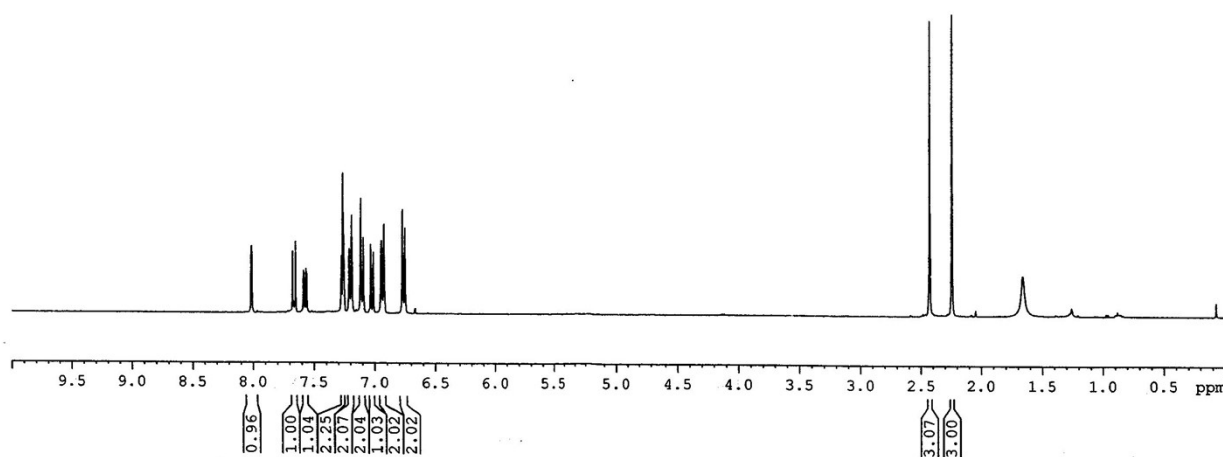
F2 - Processing parameters  
 SI 16384  
 SF 100.6177873 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 1.40

8.017  
8.012  
7.676  
7.668  
7.660  
7.652  
7.588  
7.583  
7.566  
7.561  
7.280  
7.275  
7.265  
7.259  
7.256  
7.252  
7.212  
7.192  
7.117  
7.096  
7.036  
7.014  
6.950  
6.929  
6.776  
6.755

2.430  
2.245



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



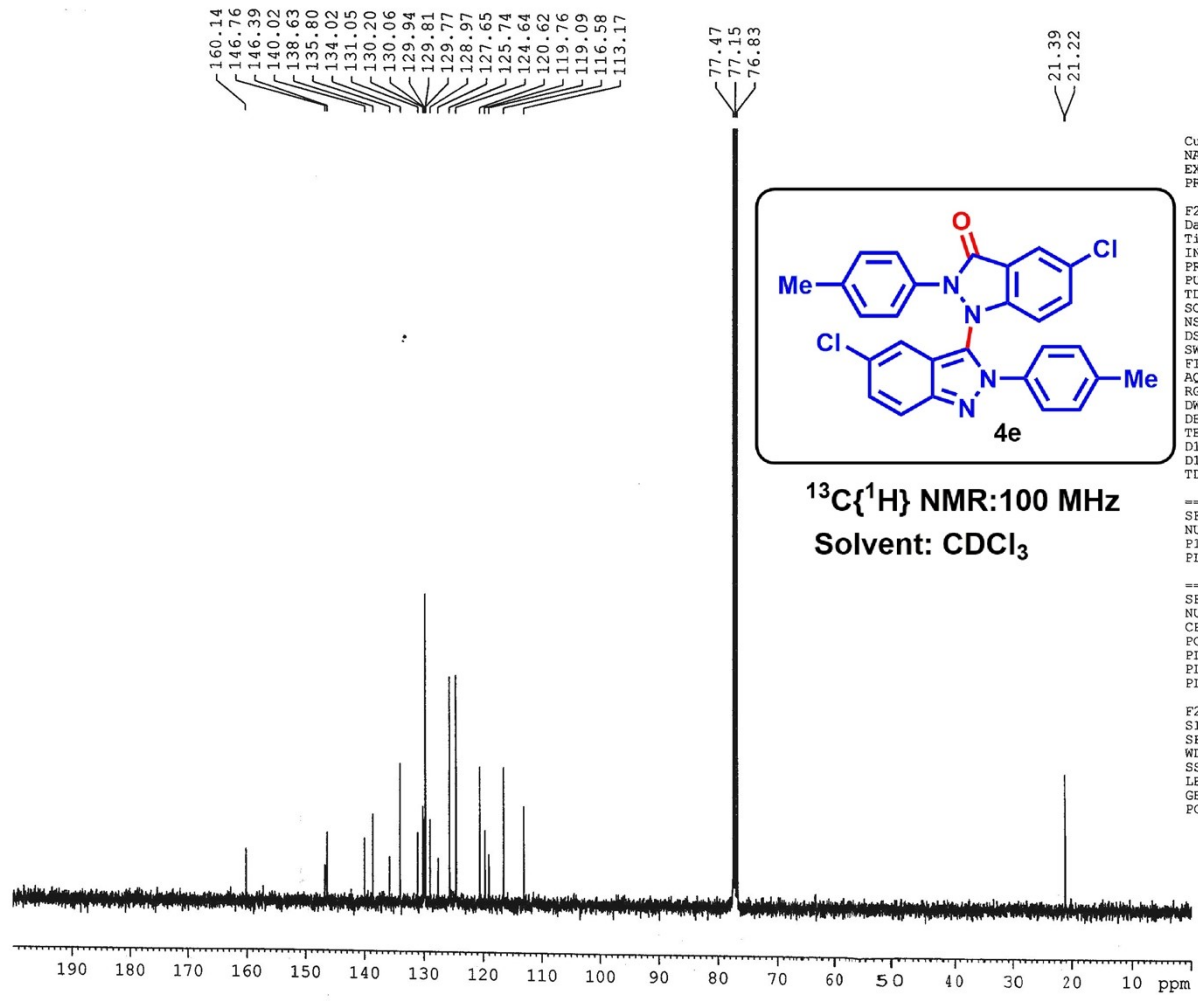
Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 876  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221015  
Time 20.56  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 148.91  
DW 60.800 usec  
DE 6.50 usec  
TE 295.3 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500067 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





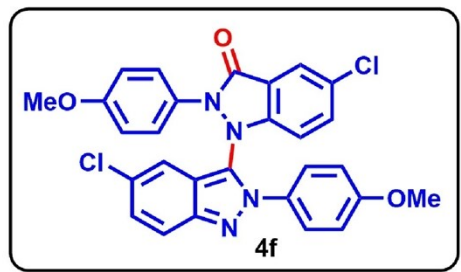
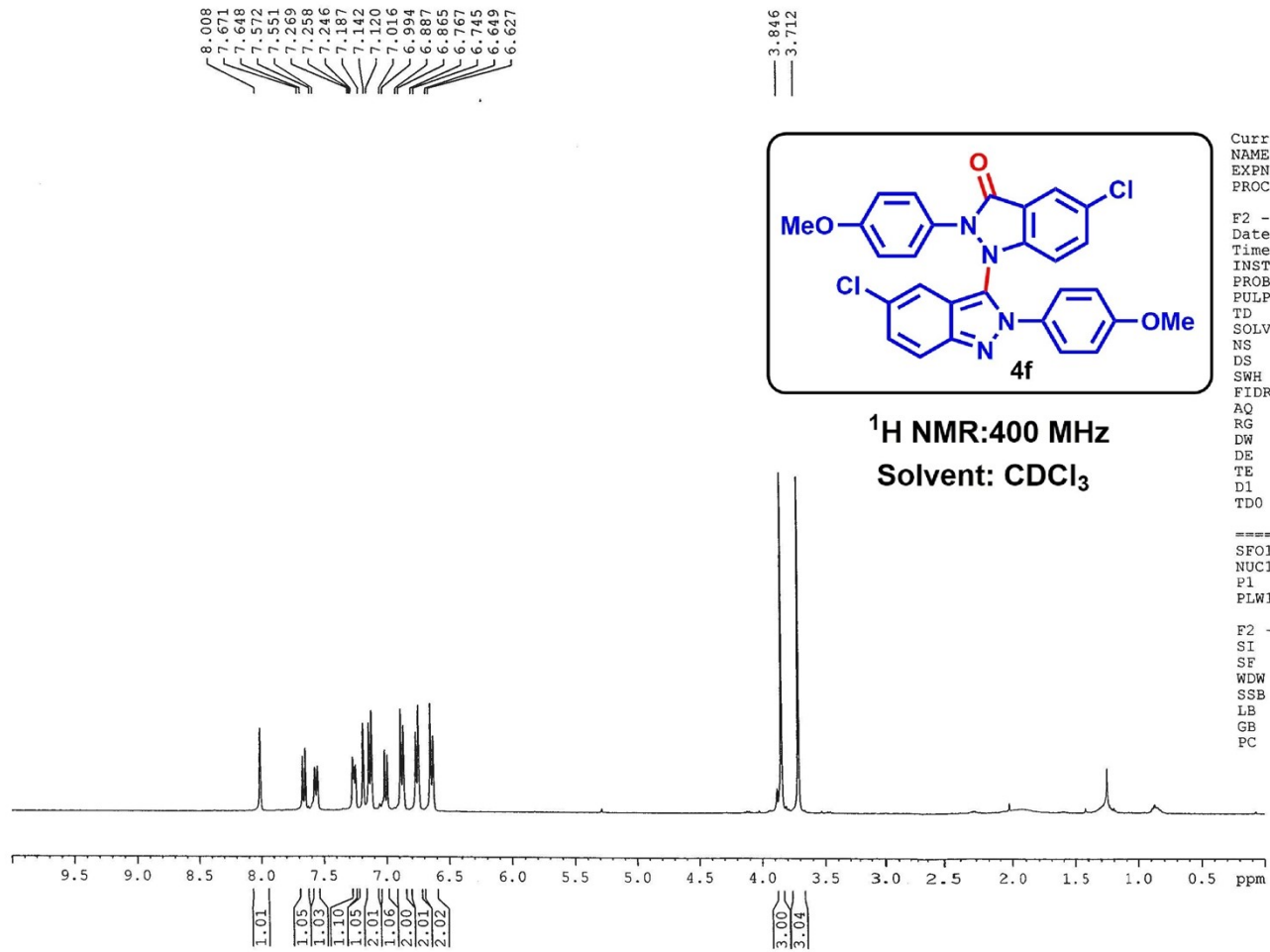
Current Data Parameters  
 NAME Dr. A HAJRA-2022-13C  
 EXPNO 358  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20221015  
 Time 21.30  
 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 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.9 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  
 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 100.6177857 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



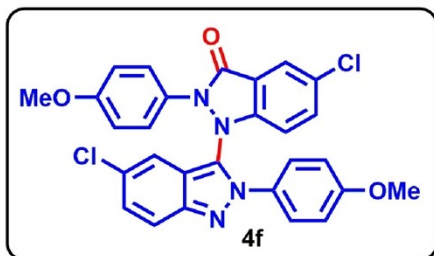
**<sup>1</sup>H NMR: 400 MHz**  
**Solvent: CDCl<sub>3</sub>**

Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 461  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220420  
Time\_ 19.06  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 93.46  
DW 60.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1

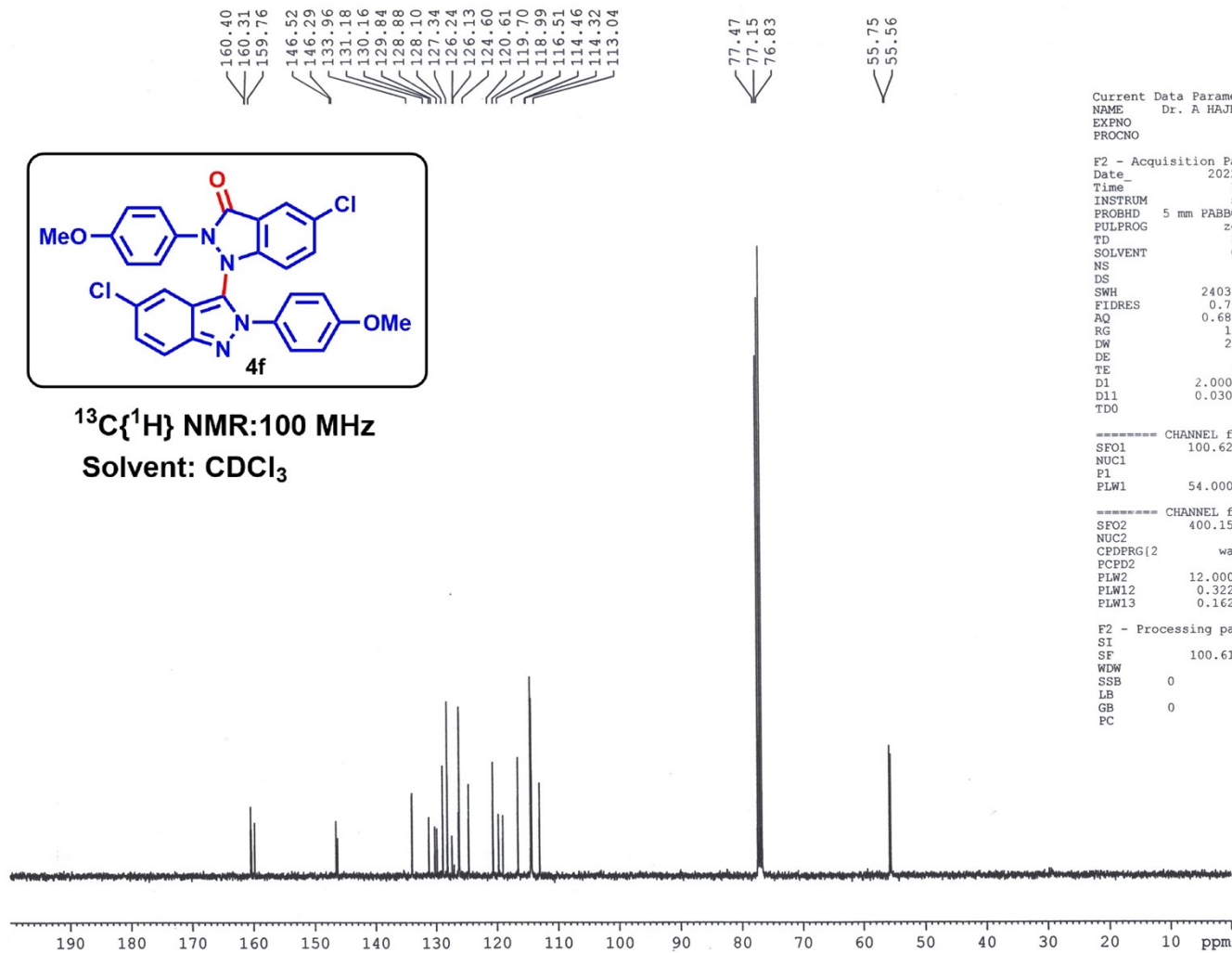
----- CHANNEL f1 -----  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500089 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



$^{13}\text{C}\{^1\text{H}\}$  NMR: 100 MHz

Solvent:  $\text{CDCl}_3$



Current Data Parameters  
 NAME Dr. A HAJRA-2022-13C  
 EXPNO 179  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220420  
 Time\_ 19.34  
 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 298.3 K  
 DI 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

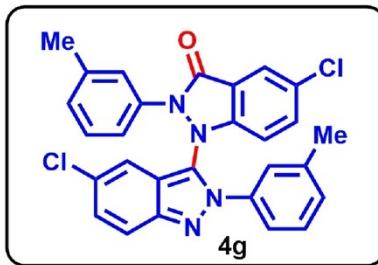
===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

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

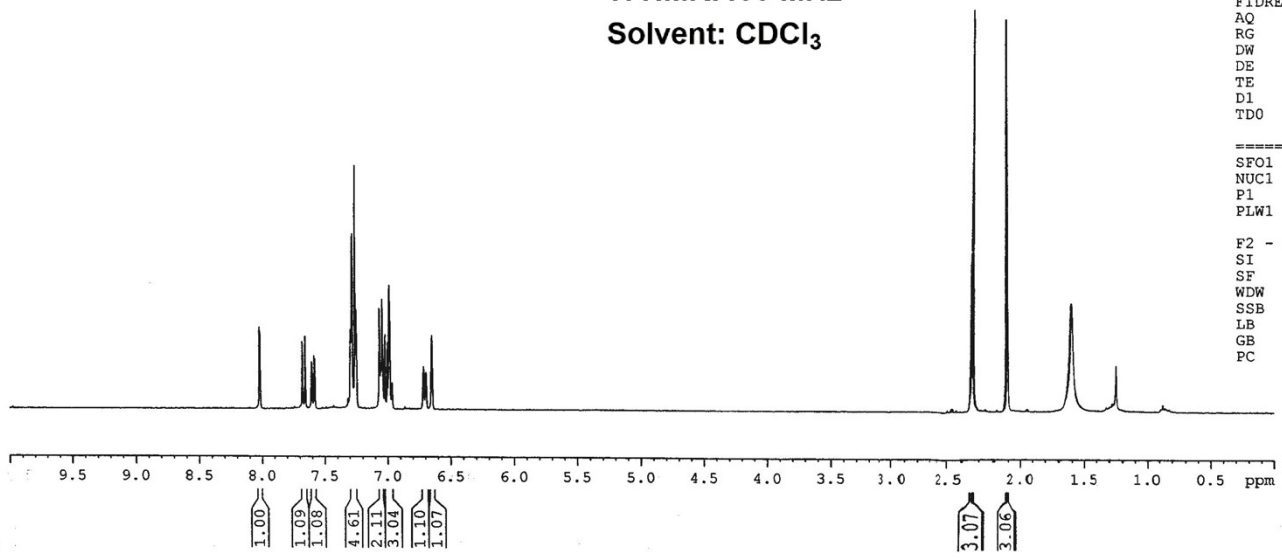
F2 - Processing parameters  
 SI 16384  
 SF 100.6177871 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

8.021  
8.016  
7.678  
7.658  
7.606  
7.601  
7.585  
7.580  
7.295  
7.280  
7.259  
7.249  
7.066  
7.055  
7.050  
7.044  
7.021  
7.002  
6.985  
6.965  
6.716  
6.697  
6.651

2.342  
2.105



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

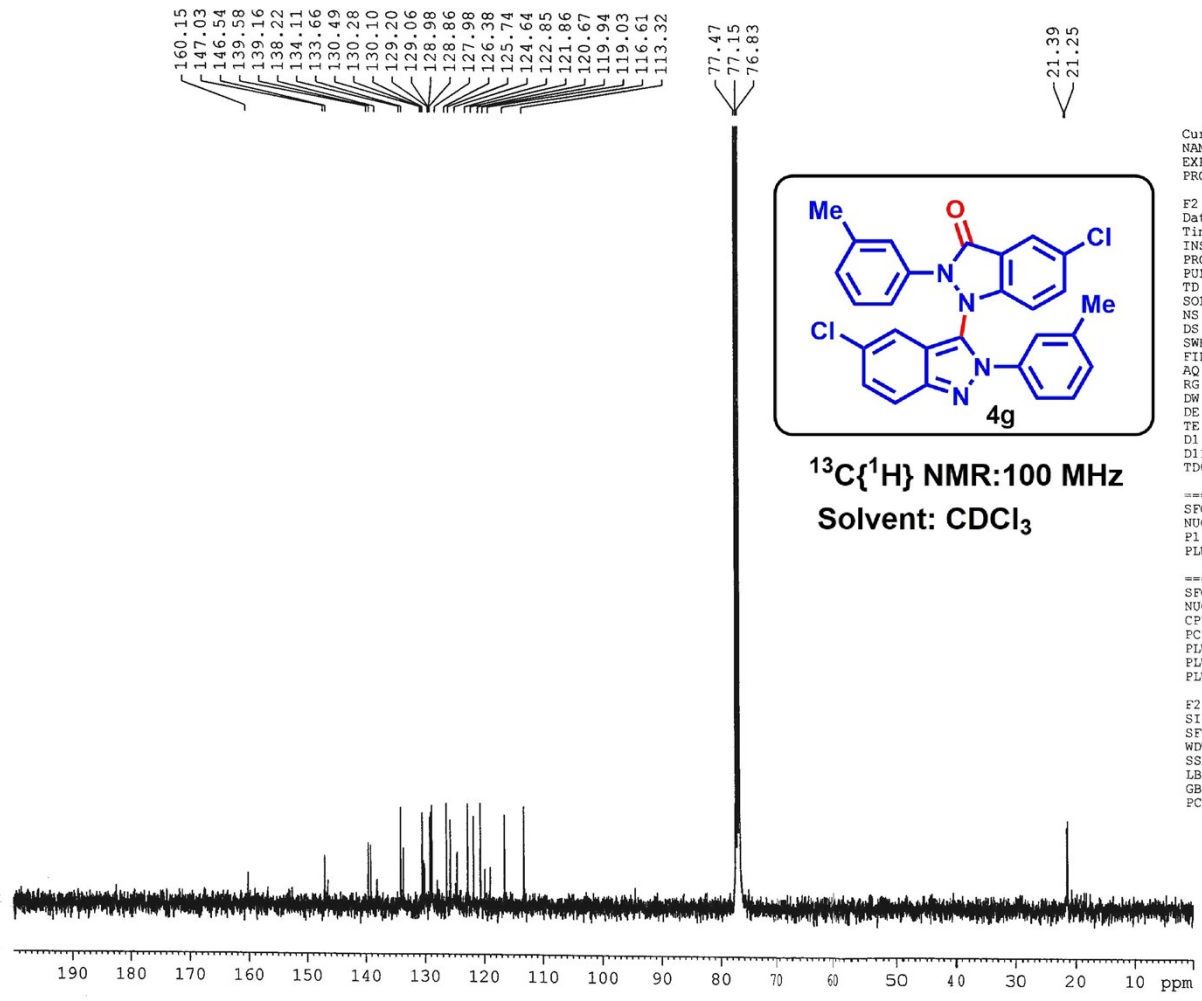


```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO    884
PROCNO   1

F2 - Acquisition Parameters
Date_    20221016
Time     20.09
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       32768
SOLVENT  CDCl3
NS       8
DS       2
SWH      8223.685 Hz
FIDRES   0.250967 Hz
AQ       1.9922944 sec
RG       168.31
DW       60.800 usec
DE       6.50 usec
TE       295.0 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1    400.1524711 MHz
NUC1     1H
P1       14.75 usec
PLW1    12.00000000 W

F2 - Processing parameters
SI      16384
SF      400.1500087 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
```



Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 363  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221017  
Time 4.51  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 1024  
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 297.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

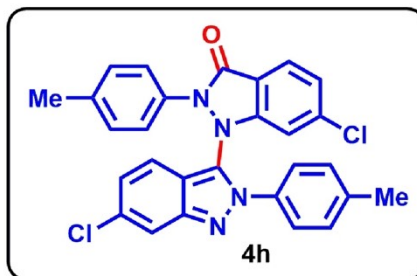
===== CHANNEL f1 =====  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W

===== 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 100.6177842 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

8.106  
8.085  
7.867  
7.486  
7.465  
7.404  
7.378  
7.353  
7.335  
7.259  
7.238  
7.193  
7.081  
7.063  
6.896  
6.879

2.569  
2.386



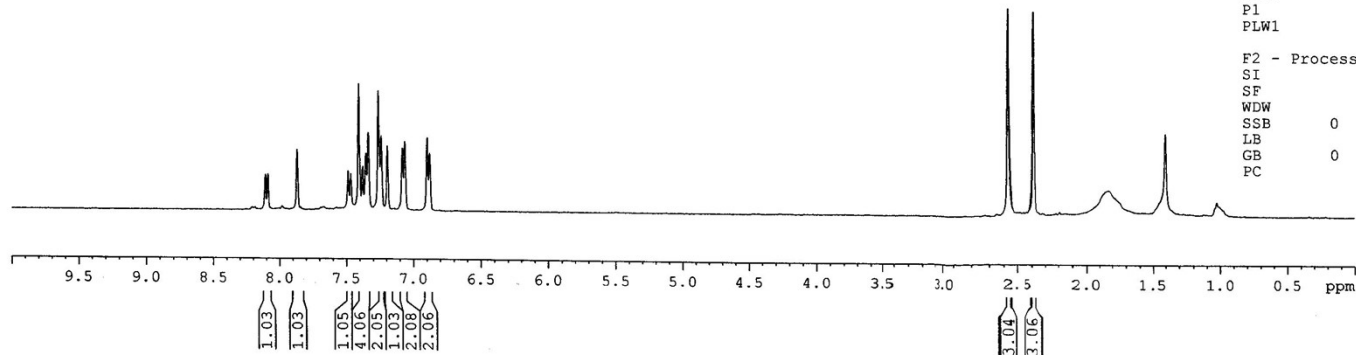
<sup>1</sup>H NMR: 400 MHz  
Solvent: CDCl<sub>3</sub>

Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 520  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220521  
Time\_ 4.16  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 148.91  
DW 60.800 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

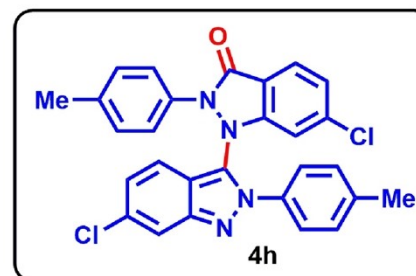
F2 - Processing parameters  
SI 16384  
SF 400.1499495 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



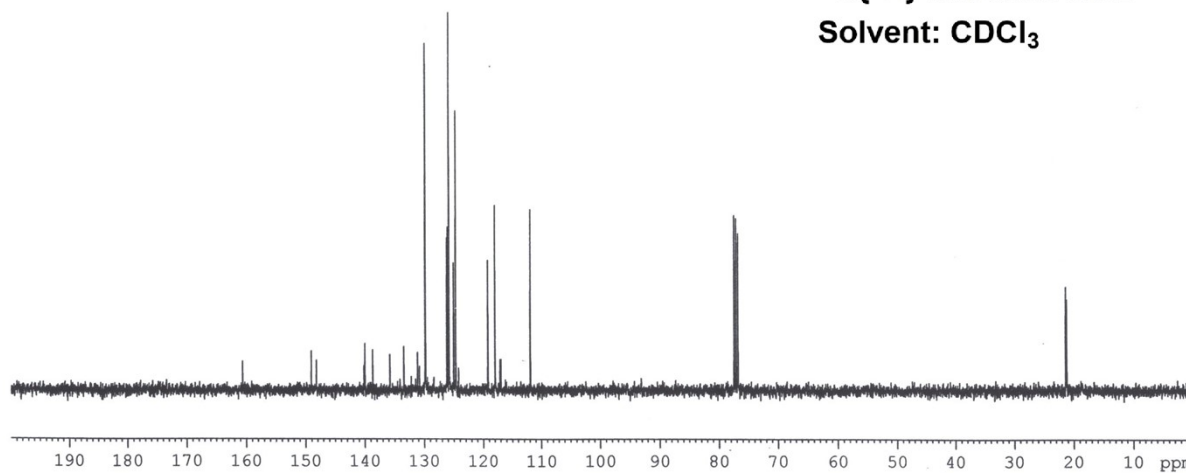
160.64  
149.06  
148.20  
140.14  
140.00  
138.67  
135.77  
133.43  
131.14  
130.79  
129.82  
129.78  
126.17  
126.02  
125.81  
125.03  
124.67  
119.26  
118.01  
117.17  
111.93

77.48  
77.16  
76.84

21.38  
21.21



**$^{13}\text{C}\{^1\text{H}\}$  NMR: 100 MHz**  
**Solvent:  $\text{CDCl}_3$**



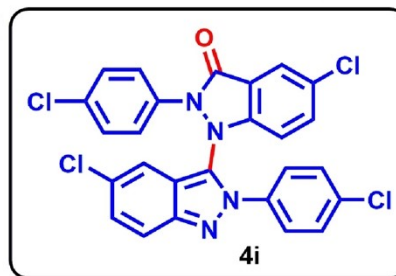
Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 210  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220522  
Time 14.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgdc  
TD 32768  
SOLVENT CDC13  
NS 200  
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 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

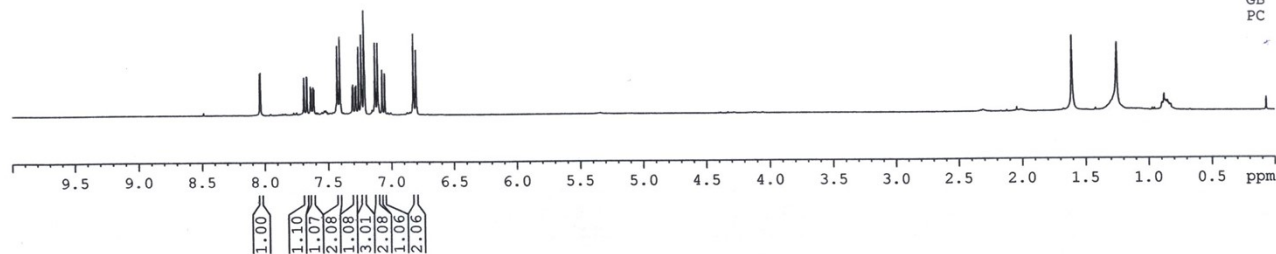
----- CHANNEL f1 -----  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W  
  
----- CHANNEL f2 -----  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W

F2 - Processing parameters  
SI 16384  
SF 100.6177841 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.00

8.037  
8.032  
7.689  
7.686  
7.686  
7.633  
7.616  
7.611  
7.434  
7.427  
7.422  
7.410  
7.405  
7.398  
7.307  
7.303  
7.284  
7.279  
7.259  
7.243  
7.236  
7.232  
7.214  
7.129  
7.124  
7.111  
7.107  
7.100  
7.072  
7.051  
6.830  
6.823  
6.818  
6.806  
6.801  
6.794



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



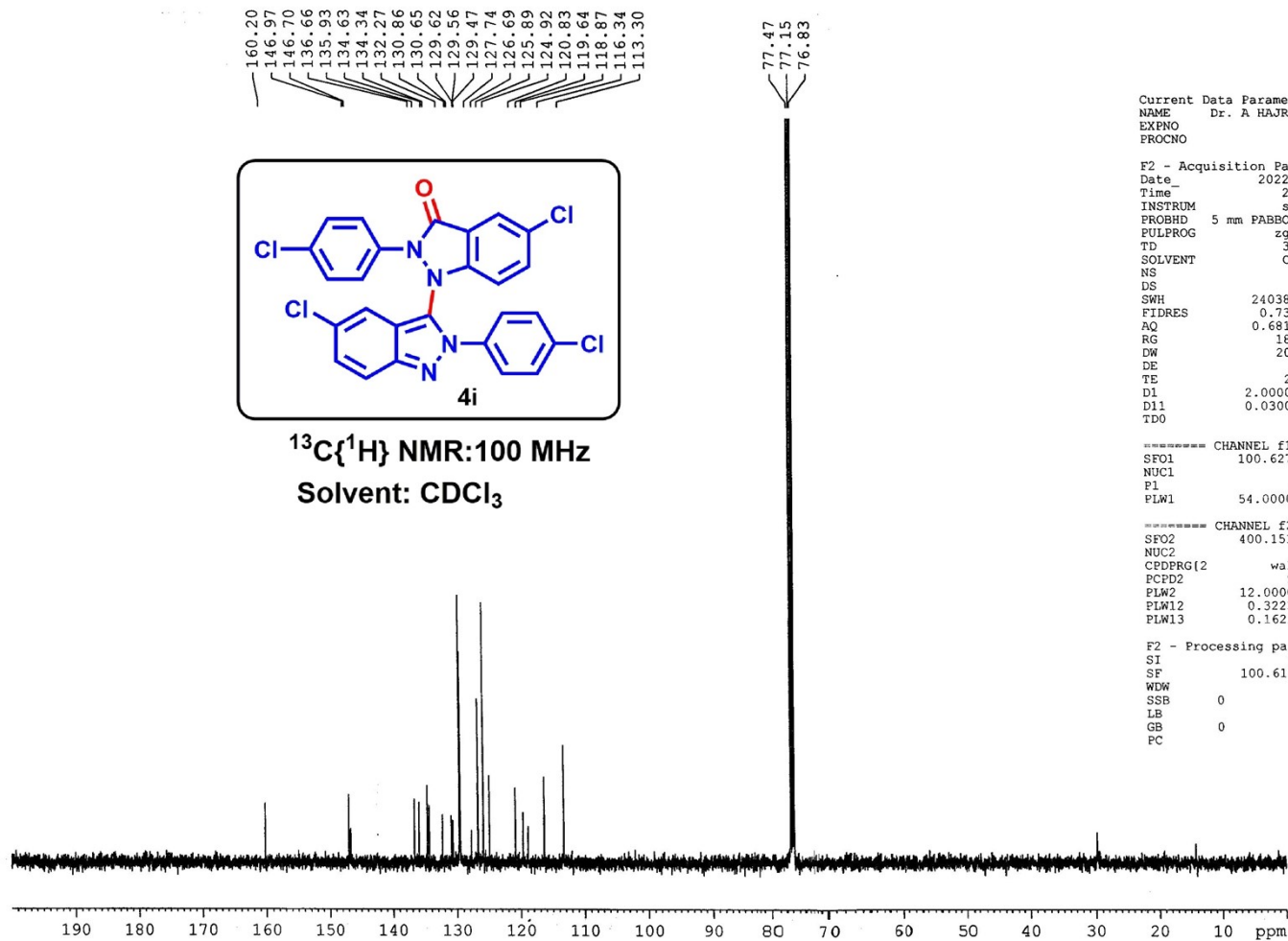
Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 214  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220303  
Time 20.36  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 186.42  
DW 60.800 usec  
DE 6.50 usec  
TE 294.9 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500088 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
 NAME Dr. A HAJRA-2022-13C  
 EXPNO 88  
 PROCNO 1

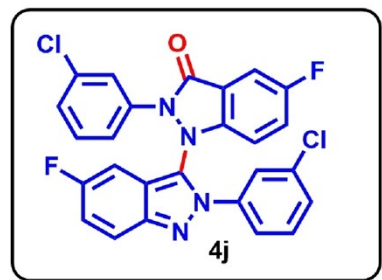
F2 - Acquisition Parameters  
 Date\_ 20220303  
 Time 21.15  
 INSTRUM spect  
 FROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 760  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

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

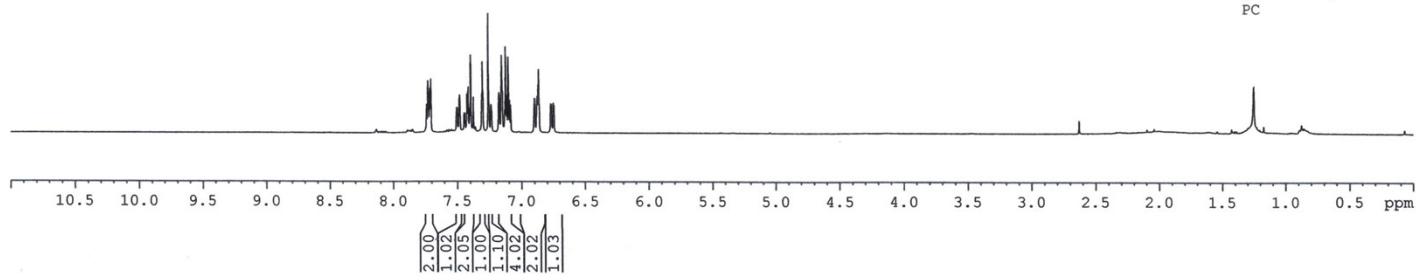
----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

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

7.739  
7.729  
7.724  
7.714  
7.705  
7.504  
7.502  
7.499  
7.483  
7.482  
7.448  
7.441  
7.426  
7.419  
7.416  
7.404  
7.396  
7.376  
7.311  
7.306  
7.301  
7.260  
7.240  
7.238  
7.236  
7.178  
7.173  
7.160  
7.156  
7.132  
7.125  
7.116  
7.105  
7.094  
7.085  
6.898  
6.895  
6.878  
6.875  
6.870  
6.866  
6.862  
6.771  
6.766  
6.751  
6.745



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

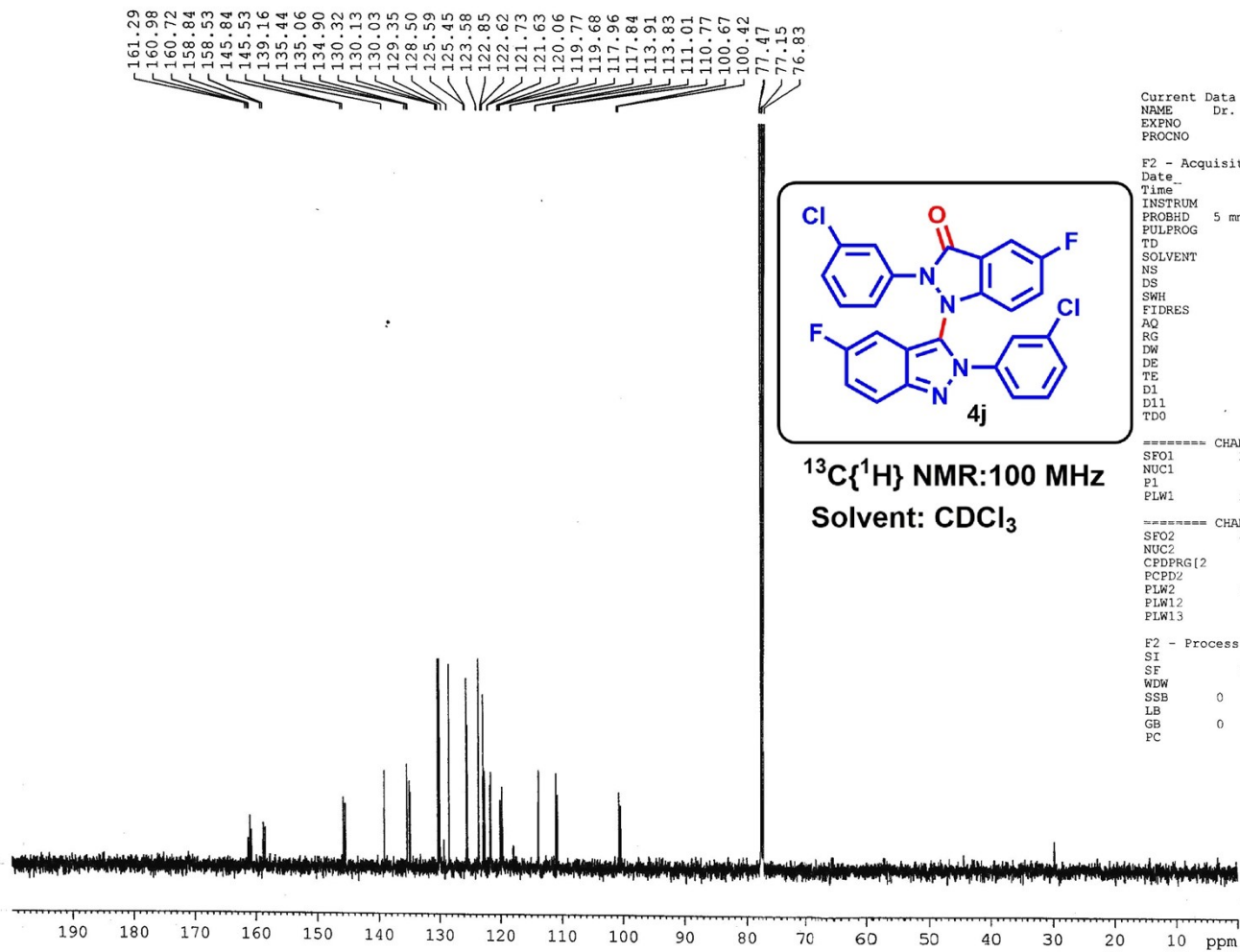


Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 454  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220419  
Time 18.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 186.42  
DW 60.800 usec  
DE 6.50 usec  
TE 298.4 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.0000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500087 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 176  
PROCNO 1

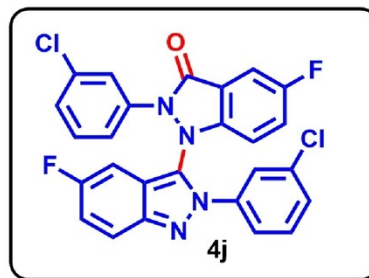
F2 - Acquisition Parameters  
Date\_ 20220419  
Time 19.20  
INSTRUM spect  
PROBHD 5 mm FAPBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 795  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 186.42  
DW 20.800 usec  
DE 6.50 usec  
TE 298.5 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
TDO 1

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

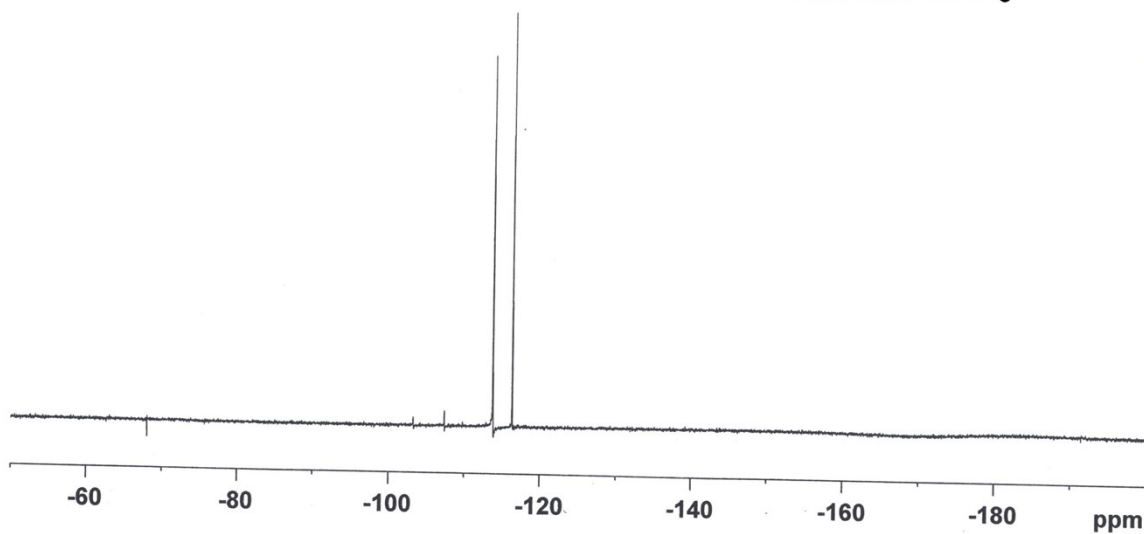
===== CHANNEL f2 =====  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW3 0.32231000 W  
PLW4 0.16212000 W

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

--- -113.79  
--- -116.35



<sup>19</sup>F NMR: 376 MHz  
Solvent: CDCl<sub>3</sub>



Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 455  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220419  
Time\_ 18.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgflqn  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 89285.711 Hz  
FIDRES 2.724784 Hz  
AQ 0.1835008 sec  
RG 186.42  
DW 5.600 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

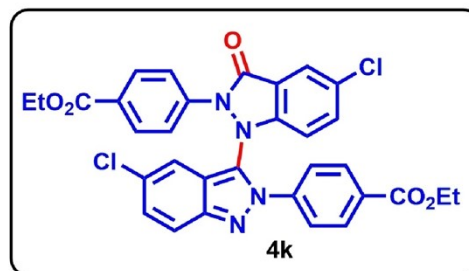
=====  
CHANNEL f1  
SFO1 376.4795333 MHz  
NUC1 19F  
P1 12.50 usec  
PLW1 20.00000000 W

F2 - Processing parameters  
SI 16384  
SF 376.5171850 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

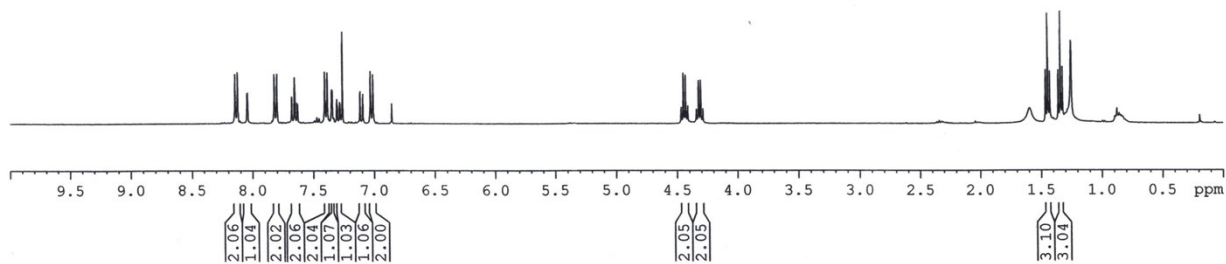
8.145  
8.123  
8.045  
8.040  
7.821  
7.799  
7.676  
7.654  
7.633  
7.628  
7.405  
7.384  
7.347  
7.344  
7.306  
7.301  
7.283  
7.278  
7.260  
7.115  
7.094  
7.031  
7.010

4.467  
4.449  
4.431  
4.413  
4.341  
4.324  
4.306  
4.288

1.464  
1.446  
1.429  
1.359  
1.341  
1.323



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

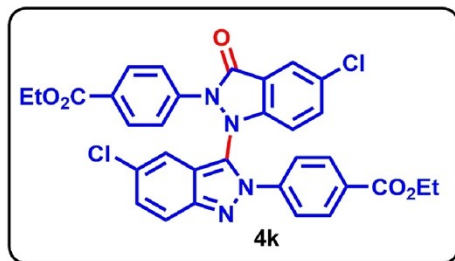


Current Data Parameters  
NAME Dr. A HAJRA 2022 1H  
EXPNO 485  
PROCNO 1

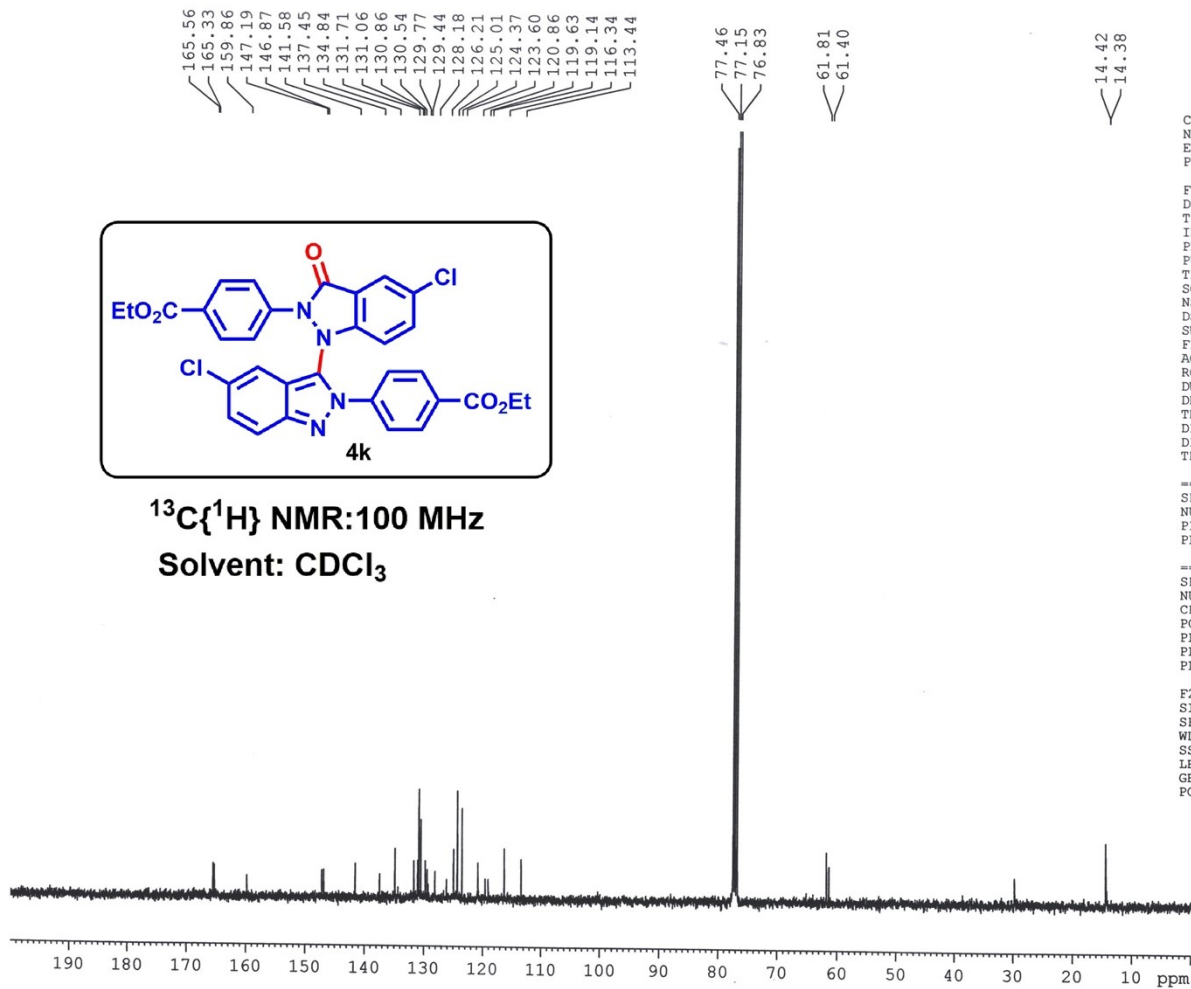
F2 - Acquisition Parameters  
Date\_ 20220425  
Time 15.03  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 186.42  
DW 60.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SF01 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500087 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C{<sup>1</sup>H} NMR: 100 MHz  
Solvent: CDCl<sub>3</sub>



Current Data Parameters  
NAME Dr. A HAJRA-2022-13C  
EXPNO 189  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220425  
Time 15.58  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 1024  
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 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6278588 MHz  
NUC1 <sup>13</sup>C  
P1 8.90 usec  
PLW1 54.00000000 W

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

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