

## Supporting Information

### Visible Light-Induced Photocatalytic C-H Ethoxycarbonylmethylation of Imidazoheterocycles with Ethyl Diazoacetate

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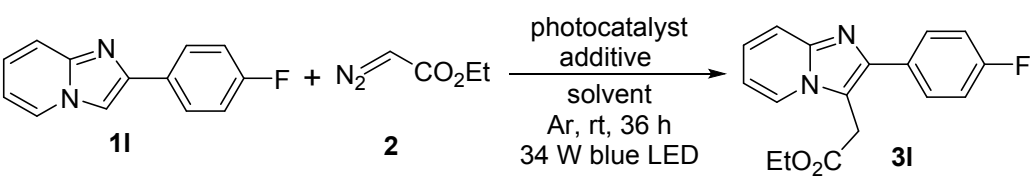
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**1. General Information:** All reagents were bought from commercial sources and used as received without further purification. All reactions involving moisture sensitive reactants were executed using oven dried glassware. All commercially available solvents were used after distillation.  $^1\text{H}$  NMR spectra were determined on 400 MHz spectrometer as solutions in  $\text{CDCl}_3$  and  $^{13}\text{C}\{^1\text{H}\}$  spectra were recorded at 100 MHz spectrometer in  $\text{CDCl}_3$  solution. Chemical shifts ( $\delta$ ) are expressed in parts per million (ppm) and coupling constants ( $J$ ) are given in Hz. 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. NMR spectra use the following abbreviations to describe the multiplicity: s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet). The progress of reaction was checked by TLC plates (silica gel coated glass slide) and the spots were visualized under UV light. Melting points (M.p.) were determined after recrystallization of solid compounds from a solution of dichloromethane/petroleum ether (1:3).

**Table S1. Optimization of the Reaction Conditions<sup>a</sup>**



Entry	Photocatalyst (0.2 mol %)	Additive (10 mol %)	Solvent	Yield (%)
1	$\text{Ru}(\text{bpy})_3\text{Cl}_2$	-	$\text{MeOH}:\text{H}_2\text{O}$ (2:1)	trace
2	$\text{Ru}(\text{bpy})_3\text{Cl}_2$	aniline	$\text{MeOH}:\text{H}_2\text{O}$ (2:1)	42
3	$\text{Ru}(\text{bpy})_3\text{Cl}_2$	DBU	$\text{MeOH}:\text{H}_2\text{O}$ (2:1)	11
4	$\text{Ru}(\text{bpy})_3\text{Cl}_2$	TEA	$\text{MeOH}:\text{H}_2\text{O}$ (2:1)	38
5	$\text{Ru}(\text{bpy})_3\text{Cl}_2$	<i>N,N</i> -dimethyl aniline	$\text{MeOH}:\text{H}_2\text{O}$ (2:1)	78
<b>6</b>	<b><math>\text{Ru}(\text{bpy})_3\text{Cl}_2</math></b>	<b><i>N,N</i>-dimethyl <i>m</i>-toluidine</b>	<b><math>\text{MeOH}:\text{H}_2\text{O}</math> (2:1)</b>	<b>92</b>
7	$\text{Ru}(\text{bpy})_3\text{Cl}_2$	DABCO	$\text{MeOH}:\text{H}_2\text{O}$ (2:1)	24

<sup>a</sup>Reaction conditions: 0.25 mmol of **11**, 0.5 mmol of **2** in presence of 0.2 mol% of  $\text{Ru}(\text{bpy})_3\text{Cl}_2$  and 10 mol% of additive in 2.0 mL of  $\text{MeOH}:\text{H}_2\text{O}$  (2:1) at room temperature under 34 W blue LED and argon atmosphere for 36 h.

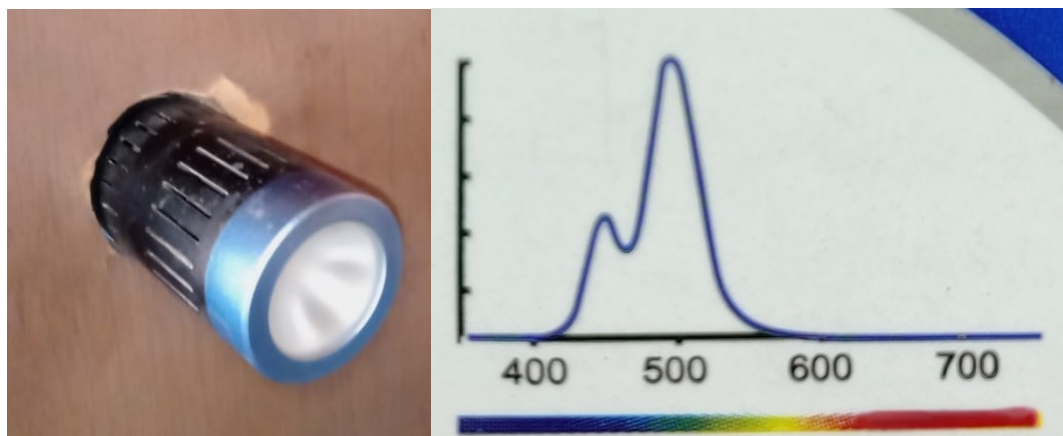
## 2. Reaction setup

The reaction was irradiated with Kessil 34 W blue LED (Model No: H150-Blue). The LED light was positioned 7 cm away from the reaction vessel. The description of this light is given below:



**Figure S1.** Milligram scale reaction set up

### Description for Kessil (34 W) Blue LED



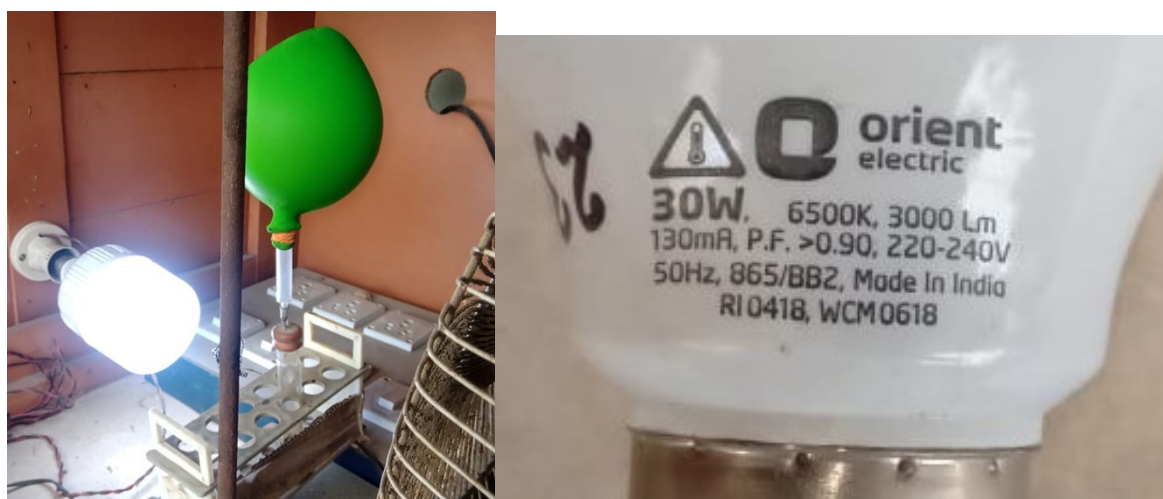
**Figure S2.** Kessil H150 Blue LED **Figure S3.** Emission spectrum of 34 W blue LED

	<b>Specification</b>
Power	34 W
Voltage	1.5 A
Wavelength	~ 450, 495 nm (max)

**Figure S4.** Description for 34 W blue LED light

For optimizing the reaction conditions, photo-induced reaction was also checked with commercially available 30 W white LED light, which was positioned 7 cm away from the reaction vessel but no desired product was produced. The description of this light is given below. The reaction is not significantly affected by temperature. The fan was used to maintain temperature of the reactor (20 ~ 30 °C). There is no spectral description.

#### Description for 30 W white LED light



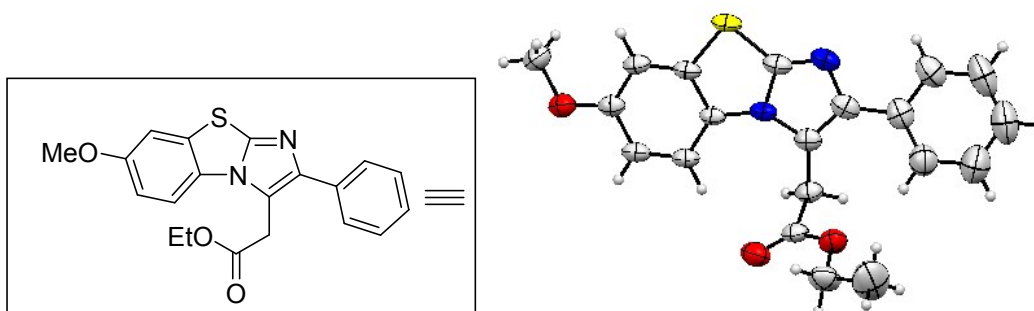
**Figure S5.** Set up of 30 W white LED

	<b>Specification</b>
Power	30 W
Voltage	130 mA

**Figure S6.** Description for 30 W white LED

### 3. Structure determination (X-ray crystallographic data for 5c):

The white crystal of **5c** was obtained by crystallization from a solution in dichloromethane/petroleum ether after purification by column chromatography. Chemical formula  $C_{20}H_{18}N_2O_3S$ .



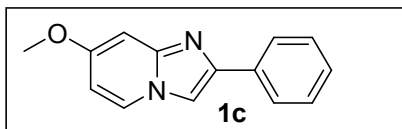
ORTEP (with 50% probability) diagram for the structure ethyl 2-(7-methoxy-2-phenylbenzo[d]imidazo[2,1-b]thiazol-3-yl)acetate (**5c**).

<b>Wavelength</b>	0.71073 Å	
<b>Formula</b>	$C_{20}H_{18}N_2O_3S$	
<b>Crystal system</b>	orthorhombic	
<b>Space group</b>	P c a 21	
<b>Unit cell dimensions</b>	$a = 7.0148(14)\text{Å}$	$\alpha = 90^\circ$
	$b = 17.582(4)\text{Å}$	$\beta = 90^\circ$
	$c = 14.402(3)\text{Å}$	$\gamma = 90^\circ$
<b>Volume</b>	$1776.2(6)\text{Å}^3$	
<b>Z</b>	4	
<b>R-factor (%)</b>	4.16	

The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication with a CCDC reference number CCDC **1976157**.

#### 4. Characterization data for the synthesized compounds (1c):

**Starting Materials:** All the imidazoheterocycles were prepared by our reported method.<sup>13</sup>



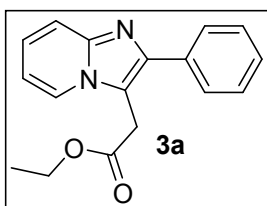
**7-Methoxy-2-phenylimidazo[1,2-*a*]pyridine (1c):**<sup>13</sup> Yellow solid (3.0 mmol, 88%, 592 mg);

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz):  $\delta$  7.90-7.86 (m, 3H), 7.65 (s, 1H), 7.40 (t,  $J = 7.6$  Hz, 2H), 7.29 (t,  $J = 7.6$  Hz, 1H), 6.89 (s, 1H), 6.48-6.45 (m, 1H), 3.83 (s, 3H); <sup>13</sup>C {<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 100 MHz):  $\delta$  158.0, 147.2, 145.4, 133.9, 128.7, 127.7, 126.0, 125.8, 107.6, 106.9, 94.7, 55.5.

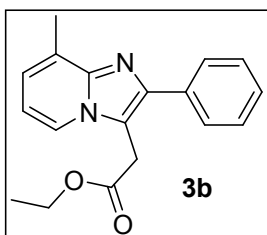
#### 5. General experimental procedure for the synthesized compounds (3a-5f):

A mixture of 2-phenylimidazo[1,2-*a*]pyridine (**1a**, 0.25 mmol, 48.5 mg), ethyl diazoacetate (**2**, 0.5 mmol, 40  $\mu$ L, containing ~15% of toluene as a stabilizer) and 0.2 mol % Ru(bpy)<sub>3</sub>Cl<sub>2</sub> (0.2 mol %, 0.3 mg) were taken in an oven-dried reaction vessel equipped with a magnetic stir bar under argon atmosphere. Then (2:1) solvent mixture MeOH:H<sub>2</sub>O (2.0 mL) was added to the reaction. After that the reaction mixture was stirred under the irradiation of 34 W blue LED (Kessil 34 W) at room temperature for 36 h. The progress of the reaction was monitored by TLC. After completion, the reaction mixture was evaporated and quenched with 10 mL water/ethyl acetate (1:3). Then the reaction mixture was extracted with ethyl acetate and the organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The crude residue was obtained after evaporating the solvent in vacuum and was purified by column chromatography on silica gel (100-200 mesh) using a mixture of petroleum ether and ethyl acetate as an eluting solvent to afford the pure product.

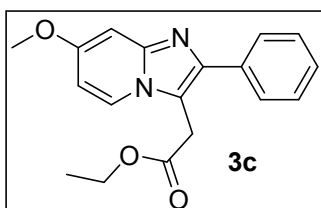
## 6. Characterization data for the synthesized compounds (3a-8a):



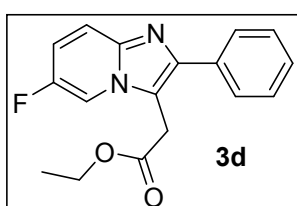
**Ethyl 2-(2-phenylimidazo[1,2-*a*]pyridin-3-yl)acetate (3a):**<sup>11c</sup> Yellow solid (62 mg, 89%); M.p. 127-128 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.12 (d, *J* = 6.8 Hz, 1H), 7.83 (d, *J* = 7.2 Hz, 2H), 7.67 (d, *J* = 8.8 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.25-7.21 (m, 1H), 6.87 (t, *J* = 6.8 Hz, 1H), 4.22 (q, *J* = 7.2 Hz, 2H), 4.04 (s, 2H), 1.27 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 100 MHz): δ 169.5, 145.1, 144.7, 134.1, 128.7, 128.0, 124.6, 123.8, 118.0, 117.7, 113.1, 112.5, 61.7, 30.9, 14.2.



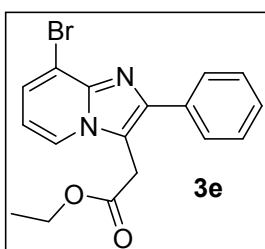
**Ethyl 2-(8-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)acetate (3b):**<sup>2b</sup> Yellow solid (61 mg, 83%); M.p. 85-86 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.98 (d, *J* = 6.8 Hz, 1H), 7.84-7.82 (m, 2H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.39-7.35 (m, 1H), 7.03-7.01 (m, 1H), 6.78 (t, *J* = 6.8 Hz, 1H), 4.21 (q, *J* = 7.2 Hz, 2H), 4.01 (s, 2H), 2.67 (s, 3H), 1.27 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 100 MHz): δ 169.6, 145.5, 144.3, 134.4, 128.9, 128.7, 127.9, 127.7, 123.4, 121.6, 113.4, 112.5, 61.7, 31.0, 17.2, 14.3.



**Ethyl 2-(7-methoxy-2-phenylimidazo[1,2-*a*]pyridin-3-yl)acetate (3c):** Yellow gummy mass (67 mg, 87%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.96 (d,  $J = 7.6$  Hz, 1H), 7.82-7.80 (m, 2H), 7.46 (t,  $J = 7.6$  Hz, 2H), 7.36 (t,  $J = 7.6$  Hz, 1H), 6.93 (d,  $J = 2.4$  Hz, 1H), 6.59-6.56 (m, 1H), 4.21 (q,  $J = 7.2$  Hz, 2H), 3.98 (s, 2H), 3.86 (s, 3H), 1.27 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.6, 158.2, 146.4, 143.7, 133.9, 128.7, 128.4, 127.9, 124.4, 111.8, 107.6, 94.7, 61.7, 55.7, 30.8, 14.2; Anal. Calcd for  $\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_3$ : C, 69.66; H, 5.85; N, 9.03%; Found C, 69.49; H, 5.80; N, 9.10%.



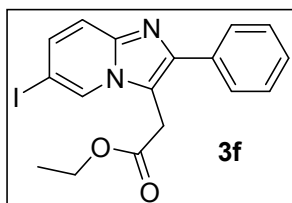
**Ethyl 2-(6-fluoro-2-phenylimidazo[1,2-*a*]pyridin-3-yl)acetate (3d):**<sup>2b</sup> Yellow gummy mass (53 mg, 71%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.10-8.08 (m, 1H), 7.81-7.79 (m, 2H), 7.68-7.64 (m, 1H), 7.48 (t,  $J = 7.6$  Hz, 2H), 7.43-7.34 (m, 1H), 7.18-7.13 (m, 1H), 4.24 (q,  $J = 7.2$  Hz, 2H), 4.01 (s, 2H), 1.29 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.1, 153.4 ( $J_{\text{C-F}} = 236.0$  Hz), 146.0, 142.8, 133.8, 128.7 ( $J_{\text{C-F}} = 18.0$  Hz), 128.2, 126.1, 118.1 ( $J_{\text{C-F}} = 10.0$  Hz), 116.5 ( $J_{\text{C-F}} = 26.0$  Hz), 114.5, 110.6 ( $J_{\text{C-F}} = 41.0$  Hz), 61.8, 31.0, 14.2.



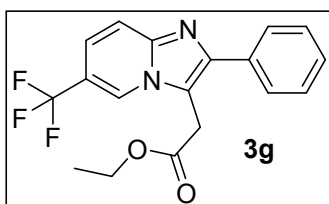
**Ethyl 2-(8-bromo-2-phenylimidazo[1,2-*a*]pyridin-3-yl)acetate (3e):** Yellow gummy mass (60 mg, 67%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.11-8.09 (m, 1H), 7.84-7.82 (m, 2H), 7.49-7.45 (m, 3H), 7.41-7.36 (m, 1H), 6.75-6.72 (m, 1H), 4.21 (q,  $J = 7.2$  Hz, 2H), 4.01 (s, 2H), 1.26 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.2, 145.5, 143.0, 133.6,



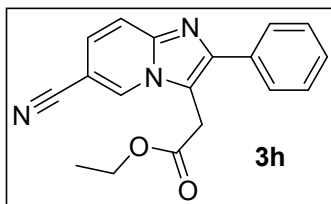
129.0, 128.7, 128.2, 127.0, 123.2, 114.9, 112.5, 111.8, 61.8, 31.1, 14.2; Anal. Calcd for  $C_{17}H_{15}BrN_2O_2$ : C, 56.84; H, 4.21; N, 7.80%; Found C, 56.70; H, 4.25; N, 7.88%.



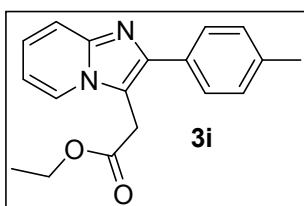
**Ethyl 2-(6-iodo-2-phenylimidazo[1,2-*a*]pyridin-3-yl)acetate (3f):** Yellow solid (73 mg, 72%); M.p. 98-99 °C;  $^1H$  NMR ( $CDCl_3$ , 400 MHz):  $\delta$  8.42 (s, 1H), 7.81 (d,  $J = 7.2$  Hz, 2H), 7.56 (d,  $J = 9.6$  Hz, 1H), 7.53-7.39 (m, 4H), 4.25 (q,  $J = 7.2$  Hz, 2H), 4.03 (s, 2H), 1.31 (t,  $J = 7.2$  Hz, 3H);  $^{13}C\{^1H\}$  NMR ( $CDCl_3$ , 100 MHz):  $\delta$  169.1, 145.2, 143.7, 133.6, 132.5, 129.0, 128.8, 128.7, 128.3, 126.3, 118.7, 113.1, 61.9, 30.9, 14.3; Anal. Calcd for  $C_{17}H_{15}IN_2O_2$ : C, 50.26; H, 3.72; N, 6.90%; Found C, 50.43; H, 3.78; N, 6.79%.



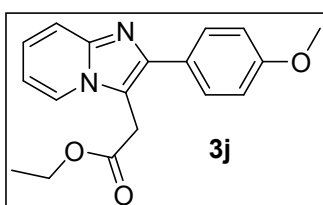
**Ethyl 2-(2-phenyl-6-(trifluoromethyl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3g):** Yellow solid (78 mg, 90%); M.p. 82-83 °C;  $^1H$  NMR ( $CDCl_3$ , 400 MHz):  $\delta$  8.54 (s, 1H), 7.82 (d,  $J = 7.2$  Hz, 2H), 7.74 (d,  $J = 9.6$  Hz, 1H), 7.49 (t,  $J = 7.6$  Hz, 2H), 7.42-7.36 (m, 2H), 4.24 (q,  $J = 7.2$  Hz, 2H), 4.07 (s, 2H), 1.29 (t,  $J = 7.2$  Hz, 3H);  $^{13}C\{^1H\}$  NMR ( $CDCl_3$ , 100 MHz):  $\delta$  168.9, 145.7 ( $J_{C-F} = 175.0$  Hz), 133.3, 128.8 ( $J_{C-F} = 12.0$  Hz), 128.5, 125.1, 119.8 (q,  $J_{C-F} = 263.0$  Hz), 123.2 (q,  $J_{C-F} = 6.0$  Hz), 122.4, 120.4, 118.3, 117.3 (q,  $J_{C-F} = 34.0$  Hz), 114.5, 62.0, 30.8, 14.1; Anal. Calcd for  $C_{18}H_{15}F_3N_2O_2$ : C, 62.07; H, 4.34; N, 8.04%; Found C, 62.22; H, 4.39; N, 7.91%.



**Ethyl 2-(6-cyano-2-phenylimidazo[1,2-*a*]pyridin-3-yl)acetate (3h):** Yellow gummy mass (62 mg, 82%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.62 (s, 1H), 7.82-7.80 (m, 2H), 7.73 (d,  $J = 9.6$  Hz, 1H), 7.51 (t,  $J = 7.6$  Hz, 2H), 7.43 (t,  $J = 7.6$  Hz, 1H), 7.35-7.32 (m, 1H), 4.26 (q,  $J = 7.2$  Hz, 2H), 4.08 (s, 2H), 1.32 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  168.8, 144.3, 132.9, 132.8, 130.3, 129.0, 128.89, 128.81, 124.4, 118.6, 116.9, 114.5, 98.7, 62.2, 30.7, 14.3; Anal. Calcd for  $\text{C}_{18}\text{H}_{15}\text{N}_3\text{O}_2$ : C, 70.81; H, 4.95; N, 13.76%; Found C, 71.01; H, 5.01; N, 13.66%.

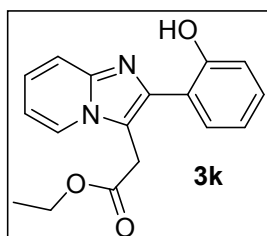


**Ethyl 2-(2-(*p*-tolyl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3i):**<sup>2b</sup> Yellow gummy mass (59 mg, 81%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.12 (d,  $J = 6.8$  Hz, 1H), 7.74-7.72 (m, 2H), 7.68-7.65 (m, 1H), 7.29 (d,  $J = 8.0$  Hz, 2H), 7.24-7.20 (m, 1H), 6.88-6.84 (m, 1H), 4.22 (q,  $J = 7.2$  Hz, 2H), 4.03 (s, 2H), 2.41 (s, 3H), 1.27 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.6, 145.0, 144.7, 137.9, 131.2, 129.5, 128.6, 124.5, 123.8, 117.6, 112.8, 112.4, 61.7, 31.0, 21.4, 14.3.

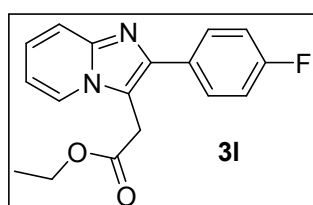


**Ethyl 2-(2-(4-methoxyphenyl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3j):**<sup>2b</sup> Yellow gummy mass (57.5 mg, 74%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.09 (d,  $J = 6.8$  Hz, 1H), 7.77-7.75 (m,

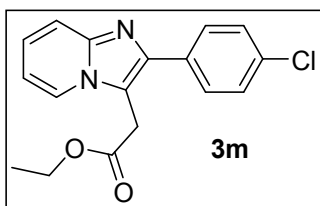
2H), 7.64-7.61 (m, 1H), 7.21-7.17 (m, 1H), 7.00 (d,  $J = 8.8$  Hz, 2H), 6.85-6.81 (m, 1H), 4.20 (q,  $J = 7.2$  Hz, 2H), 3.99 (s, 2H), 3.83 (s, 3H), 1.25 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.5, 159.6, 144.9, 144.4, 130.3, 129.8, 126.5, 124.5, 123.7, 117.3, 114.1, 112.3, 61.6, 55.3, 30.9, 14.2.



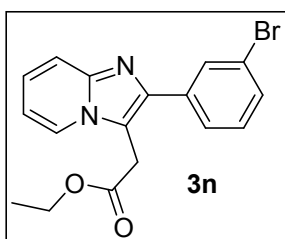
**Ethyl 2-(2-(2-hydroxyphenyl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3k):** Yellow gummy mass (48 mg, 65%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.20 (d,  $J = 7.2$  Hz, 1H), 7.73-7.71 (m, 1H), 7.62 (d,  $J = 9.2$  Hz, 1H), 7.32-7.28 (m, 2H), 7.08-7.06 (m, 1H), 6.97-6.95 (m, 2H), 4.24 (q,  $J = 7.2$  Hz, 2H), 4.13 (s, 2H), 1.28 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.2, 157.5, 143.3, 142.4, 129.9, 127.5, 125.4, 123.6, 119.3, 117.6, 117.2, 116.9, 113.2, 112.6, 61.9, 31.2, 14.2; Anal. Calcd for  $\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_3$ : C, 68.91; H, 5.44; N, 9.45%; Found: C, 68.67; H, 5.38; N, 9.57%.



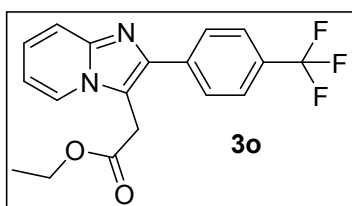
**Ethyl 2-(2-(4-fluorophenyl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3l):** Yellow solid (68 mg, 92%); M.p. 92-93 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.11 (d,  $J = 6.8$  Hz, 1H), 7.83-7.78 (m, 2H), 7.63 (d,  $J = 9.2$  Hz, 1H), 7.23-7.12 (m, 3H), 6.85 (t,  $J = 6.8$  Hz, 1H), 4.20 (q,  $J = 7.2$  Hz, 2H), 3.99 (s, 2H), 1.26 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.4, 162.8 ( $J_{\text{C-F}} = 245.0$  Hz), 145.0, 143.8, 130.3 ( $J_{\text{C-F}} = 8.0$  Hz), 130.3, 130.2, 124.7, 123.8, 117.6, 115.6 ( $J_{\text{C-F}} = 21.0$  Hz), 112.7 ( $J_{\text{C-F}} = 30.0$  Hz), 61.7, 30.8, 14.2; Anal. Calcd for  $\text{C}_{17}\text{H}_{15}\text{FN}_2\text{O}_2$ : C, 68.45; H, 5.07; N, 9.39%; Found C, 68.24; H, 5.10; N, 9.29%.



**Ethyl 2-(2-(4-chlorophenyl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3m):**<sup>2b</sup> Yellow gummy mass (67 mg, 86%); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.12 (d, *J* = 7.2 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 9.2 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.24-7.20 (m, 1H), 6.86 (t, *J* = 7.2 Hz, 1H), 4.20 (q, *J* = 7.2 Hz, 2H), 3.99 (s, 2H), 1.26 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 100 MHz): δ 169.3, 145.1, 143.5, 134.0, 132.6, 129.8, 128.9, 124.8, 123.8, 117.6, 113.1, 112.6, 61.8, 30.9, 14.2; HRMS (ESI-TOF) *m/z*: [M + H<sup>+</sup>] Calcd for C<sub>17</sub>H<sub>16</sub>ClN<sub>2</sub>O<sub>2</sub>: 315.0895; Found 315.0894.

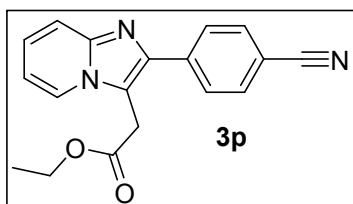


**Ethyl 2-(2-(3-bromophenyl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3n):**<sup>11c</sup> Yellow gummy mass (79 mg, 88%); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.13 (d, *J* = 7.2 Hz, 1H), 8.04 (s, 1H), 7.76 (d, *J* = 7.6 Hz, 1H), 7.63 (d, *J* = 8.2 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.32 (t, *J* = 8.4 Hz, 1H), 7.24-7.20 (m, 1H), 6.88-6.84 (m, 1H), 4.21 (q, *J* = 7.2 Hz, 2H), 4.00 (s, 2H), 1.28 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 100 MHz): δ 169.2, 145.1, 143.1, 136.2, 131.5, 130.9, 130.2, 127.1, 124.9, 123.8, 122.8, 117.7, 113.4, 112.7, 61.8, 30.8, 14.2.

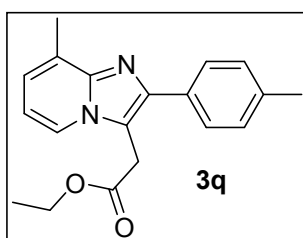


**Ethyl 2-(2-(4-(trifluoromethyl)phenyl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3o):** Yellow solid (59 mg, 68%); M.p. 88-89 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.16 (d, *J* = 6.8 Hz, 1H),

7.99 (d,  $J = 8.0$  Hz, 2H), 7.73 (d,  $J = 8.0$  Hz, 2H), 7.67 (d,  $J = 9.2$  Hz, 1H), 7.29-7.25 (m, 1H), 6.92-6.89 (m, 1H), 4.23 (q,  $J = 7.2$  Hz, 2H), 4.04 (s, 2H), 1.29 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.2, 145.3, 143.2, 137.7, 129.4, 128.8, 125.5 (q,  $J_{\text{C-F}} = 4.0$  Hz), 125.1, 124.7, 123.9, 119.6 (q,  $J_{\text{C-F}} = 258.0$  Hz), 117.9, 112.9, 61.9, 30.9, 14.2; Anal. Calcd for  $\text{C}_{18}\text{H}_{15}\text{F}_3\text{N}_2\text{O}_2$ : C, 62.07; H, 4.34; N, 8.04%; Found C, 62.27; H, 4.30; N, 8.13%.

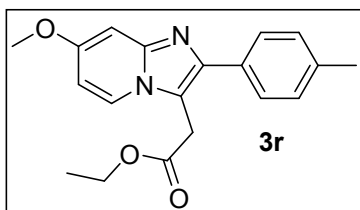


**Ethyl 2-(2-(4-cyanophenyl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3p)**: Yellow gummy mass (48 mg, 63%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.16 (d,  $J = 6.8$  Hz, 1H), 7.99 (d,  $J = 8.4$  Hz, 2H), 7.78-7.74 (m, 2H), 7.66 (d,  $J = 8.8$  Hz, 1H), 7.29-7.25 (m, 1H), 6.93-6.90 (m, 1H), 4.23 (q,  $J = 7.2$  Hz, 2H), 4.03 (s, 2H), 1.28 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.0, 145.4, 142.6, 138.8, 132.5, 129.0, 125.4, 123.9, 119.0, 117.9, 114.2, 113.0, 111.4, 62.0, 30.9, 14.2; Anal. Calcd for  $\text{C}_{18}\text{H}_{15}\text{N}_3\text{O}_2$ : C, 70.81; H, 4.95; N, 13.76%; Found: C, 70.65; H, 4.88; N, 13.84%.

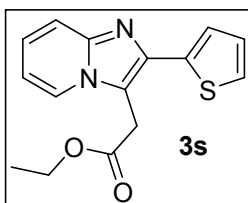


**Ethyl 2-(8-methyl-2-(*p*-tolyl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3q)**: Brown gummy mass (70 mg, 91%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.95 (d,  $J = 7.2$  Hz, 1H), 7.72 (d,  $J = 8.0$  Hz, 2H), 7.28 (d,  $J = 8.0$  Hz, 2H), 7.00-6.98 (m, 1H), 6.75 (t,  $J = 6.8$  Hz, 1H), 4.19 (q,  $J = 7.2$  Hz, 2H), 3.99 (s, 2H), 2.65 (s, 3H), 2.40 (s, 3H), 1.25 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.6, 145.4, 144.2, 137.5, 131.4, 129.3, 128.7, 127.4, 123.2, 121.5, 113.1,

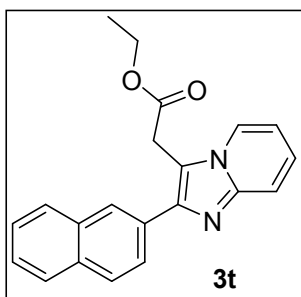
112.3, 61.5, 30.9, 21.3, 17.2, 14.2; HRMS (ESI-TOF)  $m/z$ :  $[M + H^+]$  Calcd for  $C_{19}H_{21}N_2O_2$ : 309.1598; Found 309.1603.



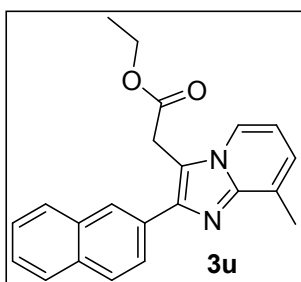
**Ethyl 2-(7-methoxy-2-(*p*-tolyl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3r):** Yellow gummy mass (64 mg, 79%);  $^1H$  NMR ( $CDCl_3$ , 400 MHz):  $\delta$  7.96 (d,  $J = 7.6$  Hz, 1H), 7.70 (d,  $J = 8.0$  Hz, 2H), 7.27 (d,  $J = 7.6$  Hz, 2H), 6.98 (d,  $J = 2.4$  Hz, 1H), 6.60-6.58 (m, 1H), 4.21 (q,  $J = 7.2$  Hz, 2H), 3.97 (s, 2H), 3.87 (s, 3H), 2.40 (s, 3H), 1.27 (t,  $J = 7.2$  Hz, 3H);  $^{13}C\{^1H\}$  NMR ( $CDCl_3$ , 100 MHz):  $\delta$  169.6, 158.3, 146.2, 143.5, 137.8, 130.9, 129.4, 128.8, 124.4, 111.6, 107.6, 94.7, 61.7, 55.7, 30.9, 21.4, 14.2; Anal. Calcd for  $C_{19}H_{20}N_2O_3$ : C, 70.35; H, 6.21; N, 8.64%; Found: C, 70.56; H, 6.27; N, 8.52%.



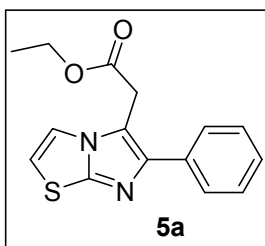
**Ethyl 2-(2-(thiophen-2-yl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3s):**<sup>2b</sup> Yellow gummy mass (41.5 mg, 58%);  $^1H$  NMR ( $CDCl_3$ , 400 MHz):  $\delta$  8.11 (d,  $J = 7.2$  Hz, 1H), 7.64 (d,  $J = 7.2$  Hz, 1H), 7.53-7.52 (m, 1H), 7.41-7.38 (m, 1H), 7.24-7.20 (m, 1H), 7.15-7.13 (m, 1H), 6.90-6.81 (m, 1H), 4.19 (q,  $J = 7.2$  Hz, 2H), 4.11 (s, 2H), 1.25 (t,  $J = 7.2$  Hz, 3H);  $^{13}C\{^1H\}$  NMR ( $CDCl_3$ , 100 MHz):  $\delta$  169.1, 145.1, 137.2, 127.9, 126.5, 126.1, 125.4, 124.9, 123.7, 117.5, 112.6, 112.4, 61.8, 30.9, 14.2.



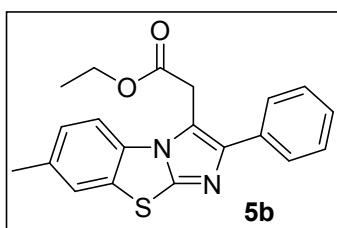
**Ethyl 2-(2-(naphthalen-2-yl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3t):** Yellow gummy mass (66 mg, 80%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.33 (s, 1H), 8.17 (d,  $J = 6.8$  Hz, 1H), 8.02-8.00 (m, 1H), 7.96-7.86 (m, 3H), 7.70 (d,  $J = 9.2$  Hz, 1H), 7.51-7.48 (m, 2H), 7.26-7.22 (m, 1H), 6.89-6.86 (m, 1H), 4.25 (q,  $J = 7.2$  Hz, 2H), 4.10 (s, 2H), 1.32 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.5, 145.2, 144.6, 133.5, 133.0, 131.5, 128.45, 128.40, 127.8, 127.7, 126.6, 126.3, 126.2, 124.7, 123.8, 117.6, 113.3, 112.5, 61.8, 31.0, 14.3; Anal. Calcd for  $\text{C}_{21}\text{H}_{18}\text{N}_2\text{O}_2$ : C, 76.34; H, 5.49; N, 8.48%; Found: C, 76.52; H, 5.43; N, 8.59%.



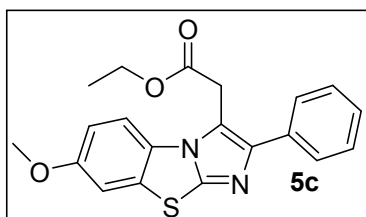
**Ethyl 2-(8-methyl-2-(naphthalen-2-yl)imidazo[1,2-*a*]pyridin-3-yl)acetate (3u):** Yellow gummy mass (61 mg, 71%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.31 (s, 1H), 8.04-8.00 (m, 2H), 7.96-7.91 (m, 2H), 7.89-7.86 (m, 1H), 7.51-7.49 (m, 2H), 7.05 (d,  $J = 6.8$  Hz, 1H), 6.81 (t,  $J = 6.8$  Hz, 1H), 4.25 (q,  $J = 7.2$  Hz, 2H); 4.08 (s, 2H), 2.70 (s, 3H), 1.32 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.6, 145.8, 144.2, 133.6, 133.0, 131.8, 128.5, 128.3, 127.88, 127.84, 127.7, 126.9, 126.2, 126.1, 123.5, 121.7, 113.8, 112.6, 61.7, 31.2, 17.3, 14.3; HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}^+]$  Calcd for  $\text{C}_{22}\text{H}_{21}\text{N}_2\text{O}_2$ : 345.1598; Found 345.1598.



**Ethyl 2-(6-phenylimidazo[2,1-*b*]thiazol-5-yl)acetate (5a):**<sup>2b</sup> Yellow gummy mass (47 mg, 66%); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.73-7.71 (m, 2H), 7.49 (d, *J* = 4.4 Hz, 1H), 7.45-7.41 (m, 2H), 7.32 (t, *J* = 7.2 Hz, 1H), 6.82 (d, *J* = 4.4 Hz, 1H), 4.20 (q, *J* = 8.0 Hz, 2H), 3.92 (s, 2H), 1.27 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 100 MHz): δ 169.5, 149.2, 145.5, 134.2, 128.6, 127.9, 127.5, 118.0, 114.5, 112.3, 61.7, 31.6, 14.2.

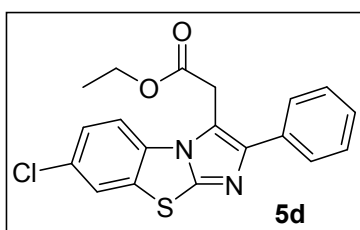


**Ethyl 2-(7-methyl-2-phenylbenzo[*d*]imidazo[2,1-*b*]thiazol-3-yl)acetate (5b):** Yellow solid (64 mg, 73%); M.p. 137-138 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.73 (d, *J* = 7.2 Hz, 2H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.50 (s, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 7.2 Hz, 1H), 7.21 (d, *J* = 8.4 Hz, 1H), 4.25 (q, *J* = 7.2 Hz, 2H), 4.18 (s, 2H), 2.45 (s, 3H), 1.27 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 100 MHz): δ 170.1, 147.5, 145.9, 134.8, 134.1, 131.1, 130.6, 128.7, 128.1, 127.7, 127.1, 124.6, 116.8, 112.7, 61.8, 31.9, 21.3, 14.3; HRMS (ESI-TOF) *m/z*: [M + H<sup>+</sup>] Calcd for C<sub>20</sub>H<sub>19</sub>N<sub>2</sub>O<sub>2</sub>S: 351.1162; Found 351.1163.

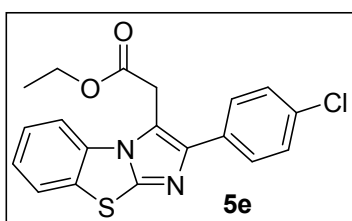




**Ethyl 2-(7-methoxy-2-phenylbenzo[d]imidazo[2,1-b]thiazol-3-yl)acetate (5c):** White solid (71 mg, 78%); M.p. 140-141 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.73 (d, *J* = 7.2 Hz, 2H), 7.67 (d, *J* = 8.8 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 2H), 7.36-7.32 (m, 1H), 7.19 (d, *J* = 2.8 Hz, 1H), 6.97-6.95 (m, 1H), 4.25 (q, *J* = 7.2 Hz, 2H), 4.15 (s, 2H), 3.85 (s, 3H), 1.26 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 100 MHz): δ 170.0, 156.9, 146.9, 145.6, 134.1, 131.8, 128.6, 128.0, 127.6, 127.3, 116.7, 113.6, 113.1, 108.8, 61.8, 55.9, 31.7, 14.2; HRMS (ESI-TOF) *m/z*: [M + H<sup>+</sup>] Calcd for C<sub>20</sub>H<sub>19</sub>N<sub>2</sub>O<sub>3</sub>S: 367.1110; Found 367.1110.

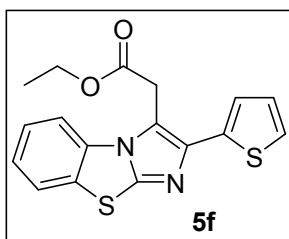


**Ethyl 2-(7-chloro-2-phenylbenzo[d]imidazo[2,1-b]thiazol-3-yl)acetate (5d):** Yellow solid (65 mg, 71%); M.p. 141-142 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.73 (d, *J* = 8.4 Hz, 3H), 7.69 (d, *J* = 2.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 2H), 7.41-7.35 (m, 2H), 4.26 (q, *J* = 7.2 Hz, 2H), 4.17 (s, 2H), 1.28 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 100 MHz): δ 169.8, 147.3, 146.5, 133.7, 132.1, 131.7, 130.2, 128.7, 128.1, 127.9, 126.4, 124.2, 117.0, 113.8, 62.0, 31.7, 14.3; Anal. Calcd for C<sub>19</sub>H<sub>15</sub>ClN<sub>2</sub>O<sub>2</sub>S: C, 61.54; H, 4.08; N, 7.55%; Found C, 61.36; H, 4.01; N, 7.63%.

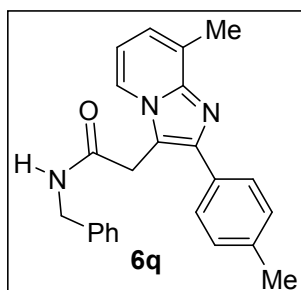


**Ethyl 2-(2-(4-chlorophenyl)benzo[d]imidazo[2,1-b]thiazol-3-yl)acetate (5e):** Yellow solid (67 mg, 72%); M.p. 90-91 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.81 (d, *J* = 8.0 Hz, 1H), 7.72-7.68 (m, 3H), 7.45-7.41 (m, 3H), 7.36-7.32 (m, 1H), 4.26 (q, *J* = 7.2 Hz, 2H), 4.16 (s, 2H), 1.27 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 100 MHz): δ 169.8, 147.7, 145.1, 133.7,

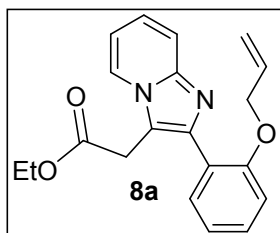
133.1, 132.5, 130.5, 129.3, 128.9, 126.2, 124.8, 124.5, 117.1, 113.1, 62.0, 31.8, 14.2; Anal. Calcd for C<sub>19</sub>H<sub>15</sub>ClN<sub>2</sub>O<sub>2</sub>S: C, 61.54; H, 4.08; N, 7.55%; Found C, 61.74; H, 4.04; N, 7.64%.



**Ethyl 2-(2-(thiophen-2-yl)benzo[d]imidazo[2,1-b]thiazol-3-yl)acetate (5f):** Yellow solid (67 mg, 79%); M.p. 91-92 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.45-7.40 (m, 2H), 7.35-7.31 (m, 2H), 7.12-7.10 (m, 1H), 4.26-4.21 (m, 4H), 1.25 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 100 MHz): δ 169.5, 147.8, 140.5, 136.9, 133.0, 130.5, 127.7, 126.2, 125.4, 124.9, 124.8, 124.4, 116.3, 113.1, 61.9, 31.9, 14.2; Anal. Calcd for C<sub>17</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>: C, 59.63; H, 4.12; N, 8.18%; Found C, 59.47; H, 4.15; N, 8.07%.

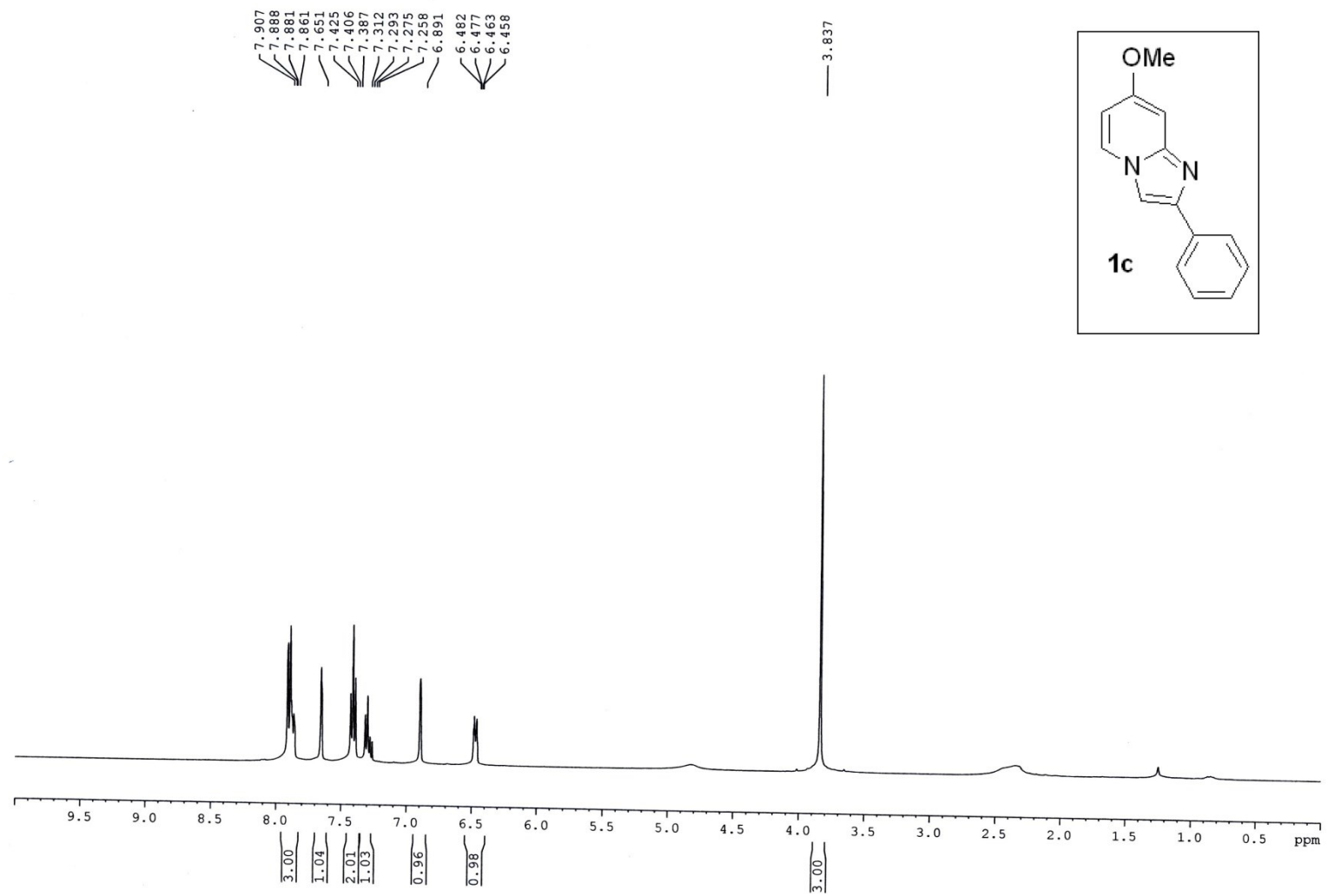


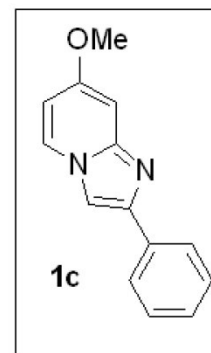
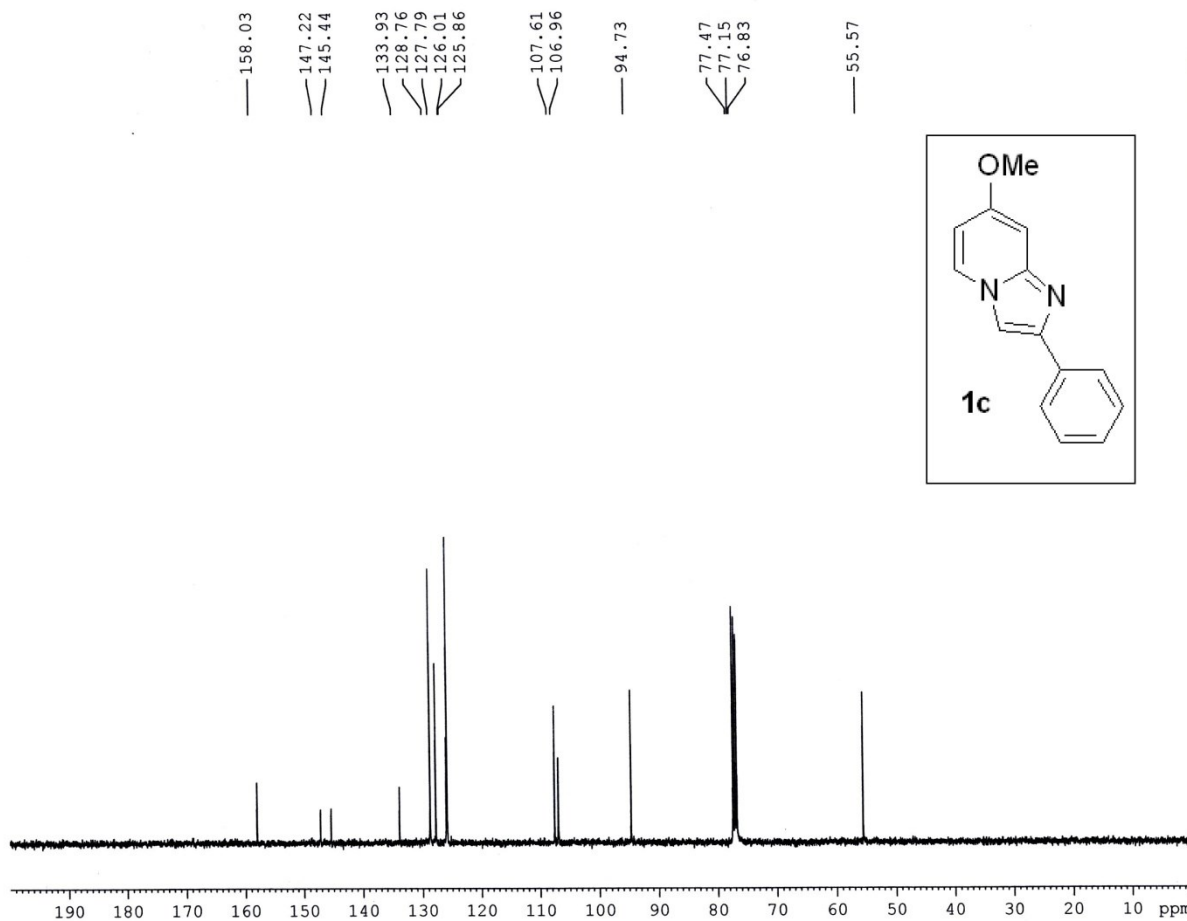
**N-Benzyl-2-(8-methyl-2-(*p*-tolyl)imidazo[1,2-*a*]pyridin-3-yl)acetamide (6q):** Brown gummy (52 mg, 56%); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.86 (d, *J* = 6.8 Hz, 1H), 7.62-7.59 (m, 2H), 7.24-7.19 (m, 4H), 7.08-7.03 (m, 4H), 6.78 (t, *J* = 6.8 Hz, 1H), 5.98 (s, 1H), 4.37 (d, *J* = 5.6 Hz, 2H), 4.03 (s, 2H), 2.65 (s, 3H), 2.39 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 100 MHz): δ 168.5, 145.4, 144.5, 138.1, 137.8, 130.9, 129.6, 128.7, 128.4, 127.7, 127.66, 127.60, 124.0, 121.2, 113.5, 113.0, 43.8, 32.8, 21.4, 17.2; Anal. Calcd for C<sub>24</sub>H<sub>23</sub>N<sub>3</sub>O: C, 78.02; H, 6.27; N, 11.37%; Found C, 78.21; H, 6.32; N, 11.30%.



**Ethyl 2-(2-(2-(allyloxy)phenyl)imidazo[1,2-*a*]pyridin-3-yl)acetate (8a):** Yellow Gummy (29 mg, 35%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.98 (d,  $J = 6.8$  Hz, 1H), 7.67-7.64 (m, 2H), 7.36-7.32 (m, 1H), 7.26-7.18 (m, 1H), 7.08 (t,  $J = 7.2$  Hz, 1H), 7.00-6.98 (m, 1H), 6.84 (t,  $J = 6.8$  Hz, 1H), 5.98-5.88 (m, 1H), 5.29-5.24 (m, 1H), 5.19-5.16 (m, 1H), 4.52 (d,  $J = 2.8$  Hz, 2H), 4.12 (q,  $J = 7.2$  Hz, 2H), 3.93 (s, 2H), 1.20 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.7, 155.8, 145.1, 141.4, 133.6, 132.5, 129.5, 140.0, 123.9, 123.6, 121.4, 117.7, 117.4, 115.1, 113.2, 112.1, 69.9, 61.3, 30.9, 14.2; Anal. Calcd for  $\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_3$ : C, 71.41; H, 5.99; N, 8.33%; Found C, 71.24; H, 6.03; N, 8.41%.

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





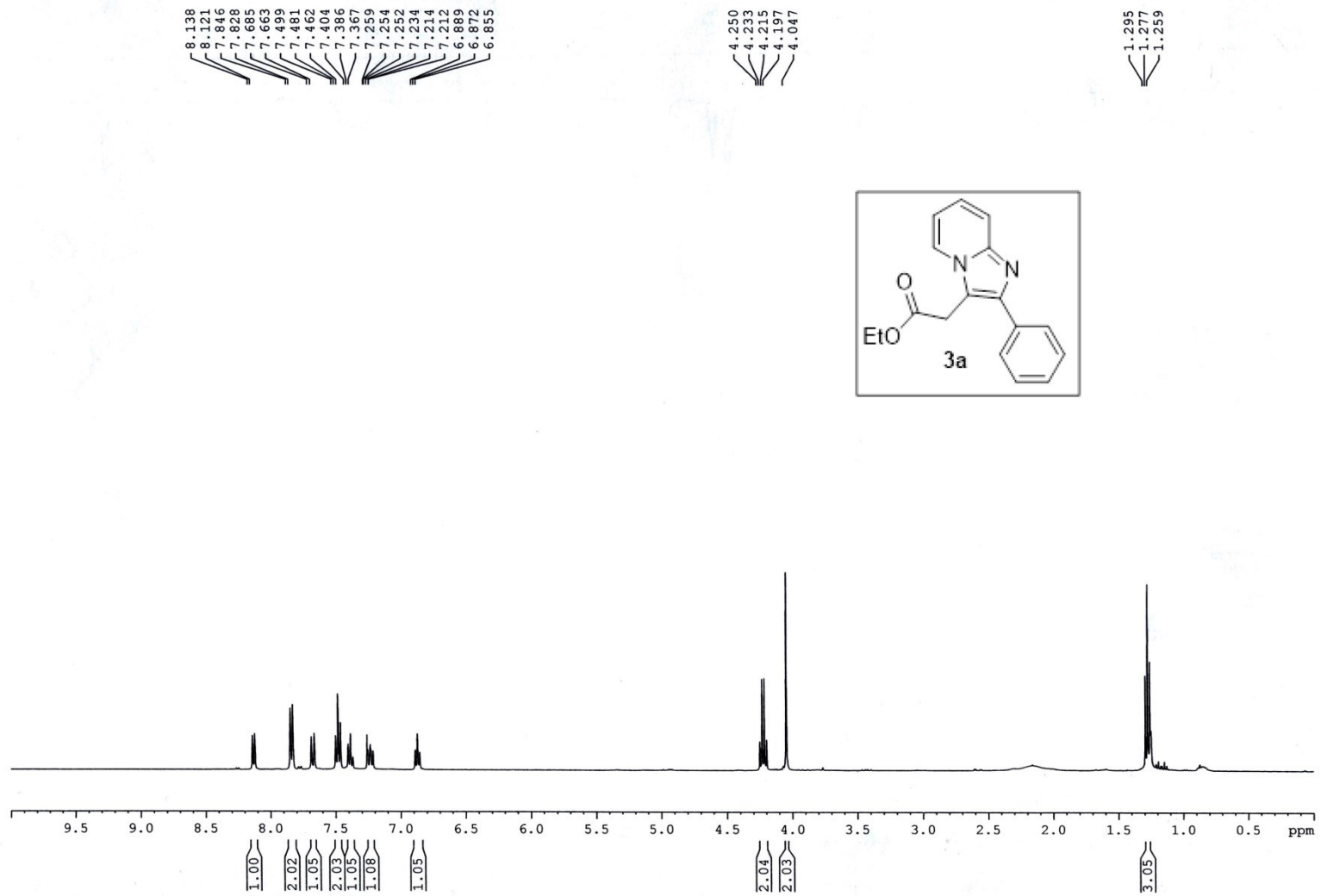
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NAME Dr. A HAJRA-2020-13C  
EXPNO 5  
PROCNO 1

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PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 250  
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 296.9 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

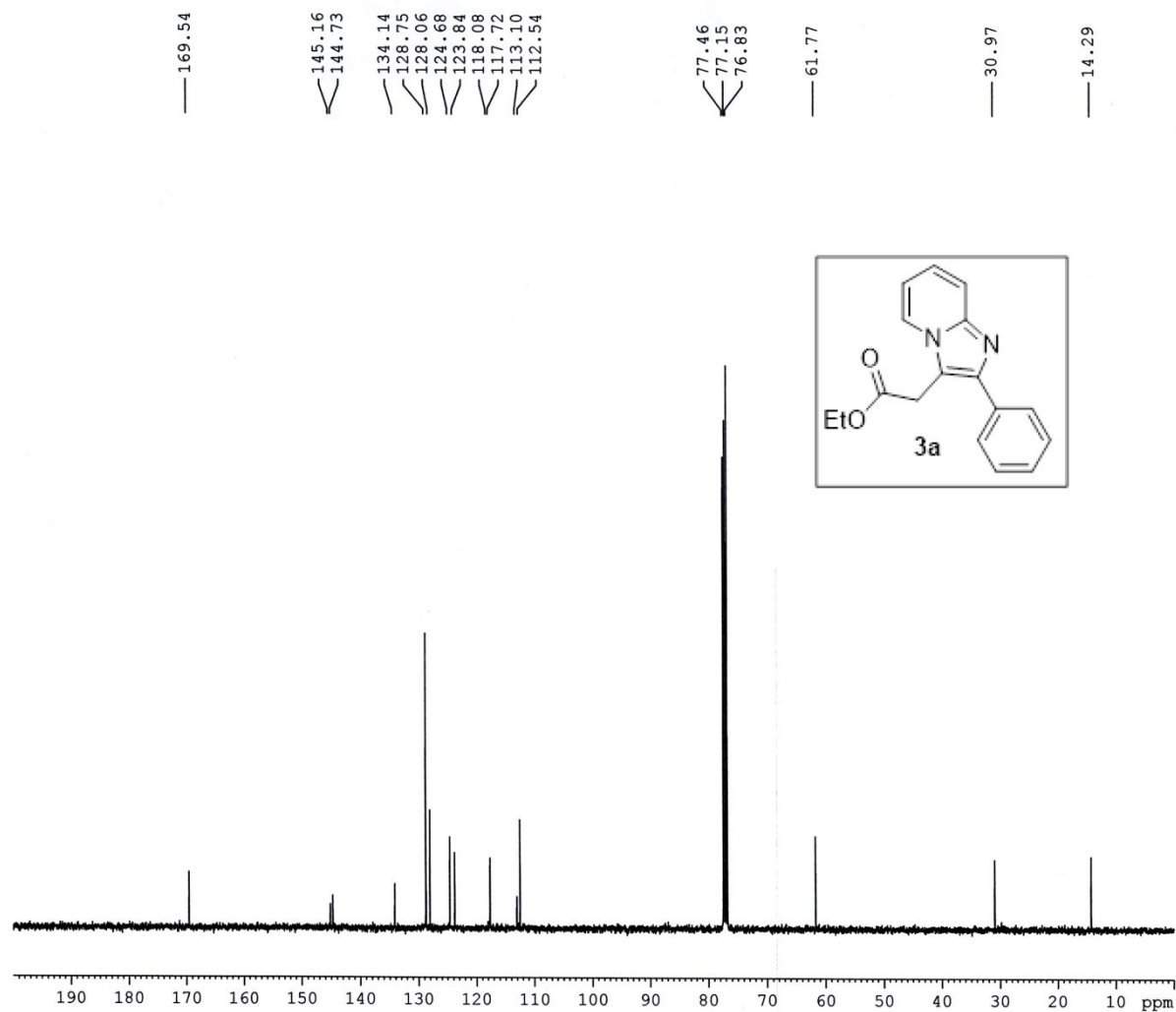
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P1 8.90 usec  
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NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.0000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

F2 - Processing parameters  
SI 16384  
SF 100.6177894 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



13C of VBSB 22/3



Current Data Parameters  
NAME Dr. A HAJRA-2019-13C  
EXPNO 360  
PROCNO 1

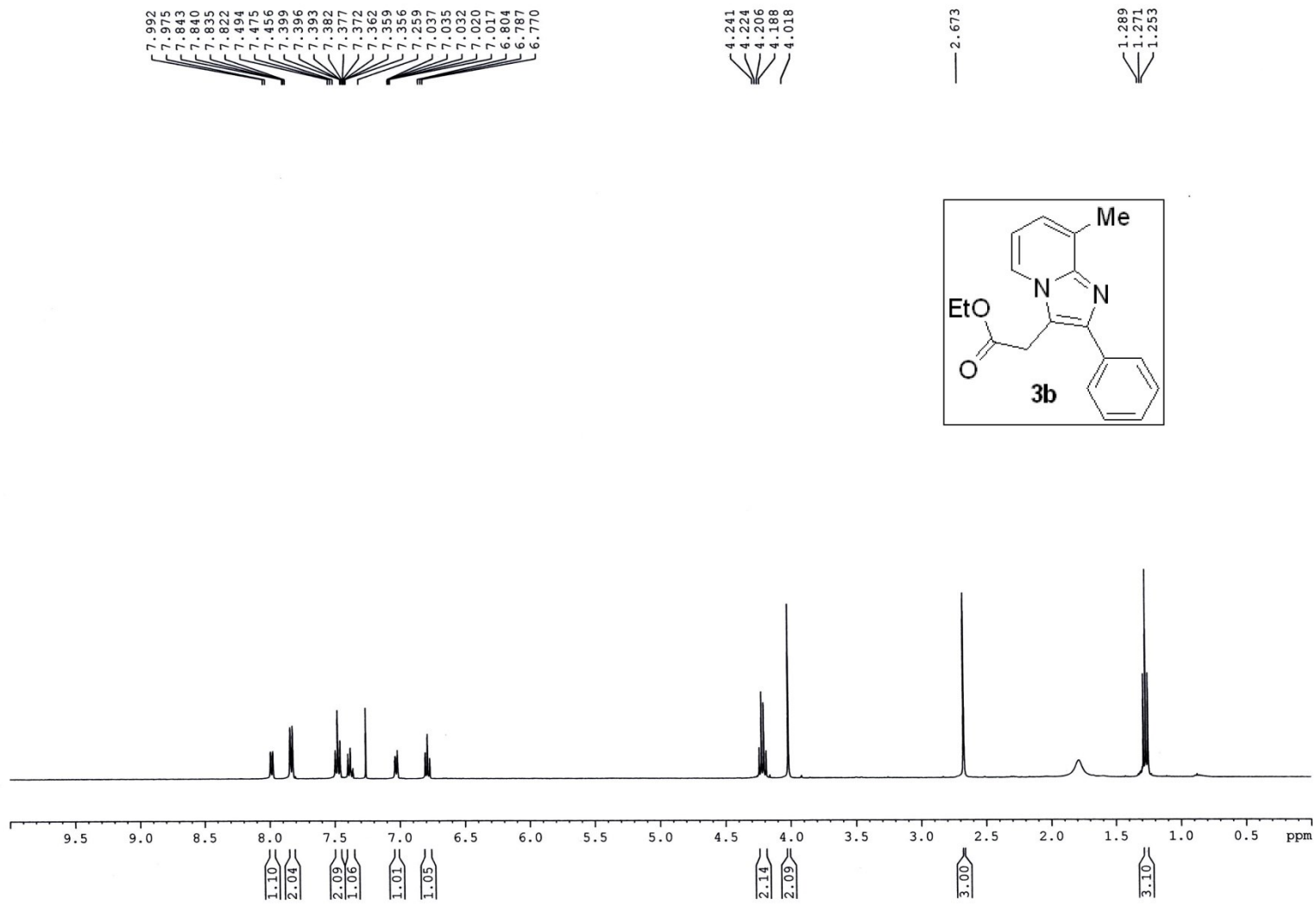
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PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 512  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 135.7  
DW 20.800 usec  
DE 6.50 usec  
TE 298.7 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

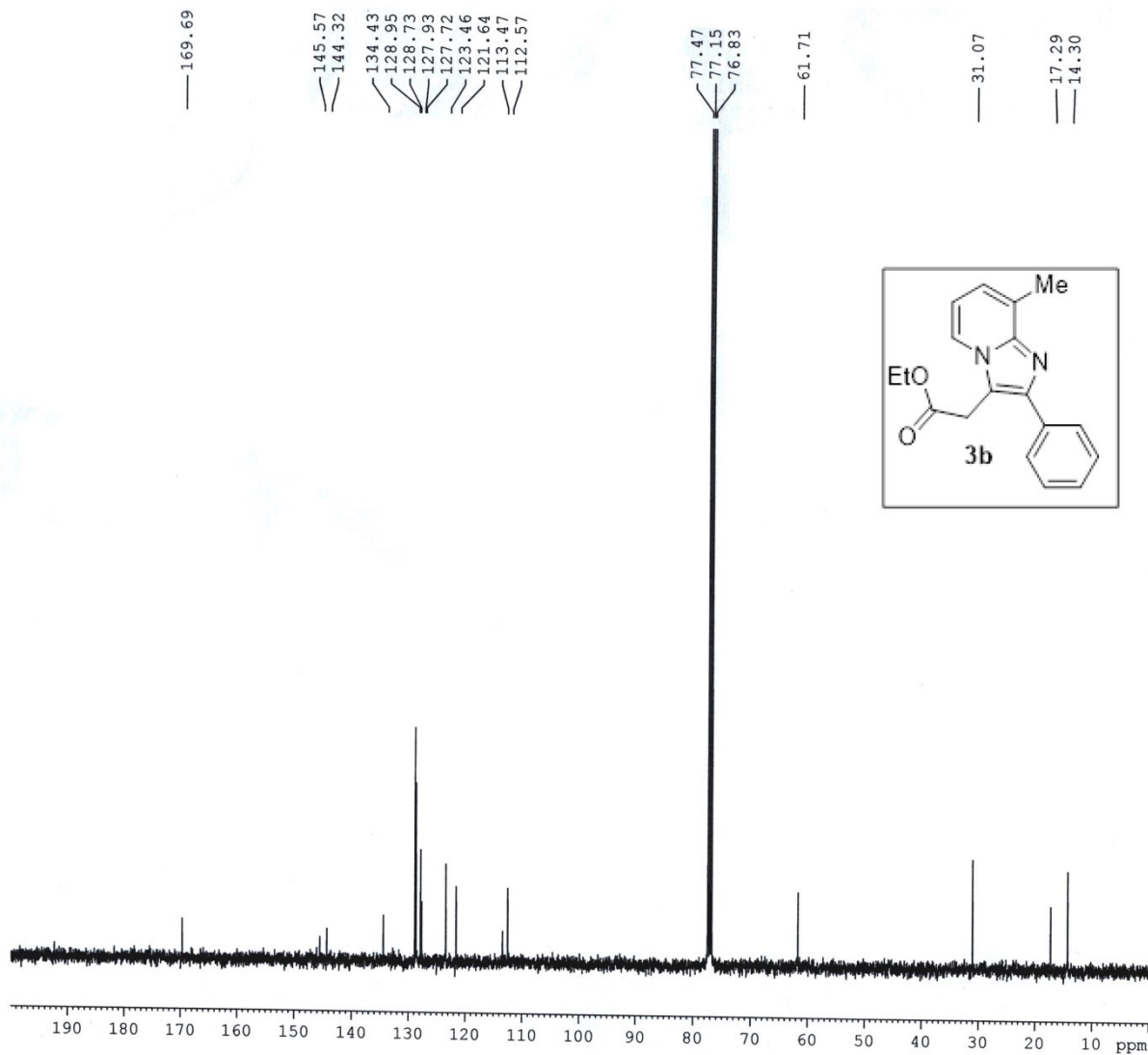
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NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

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







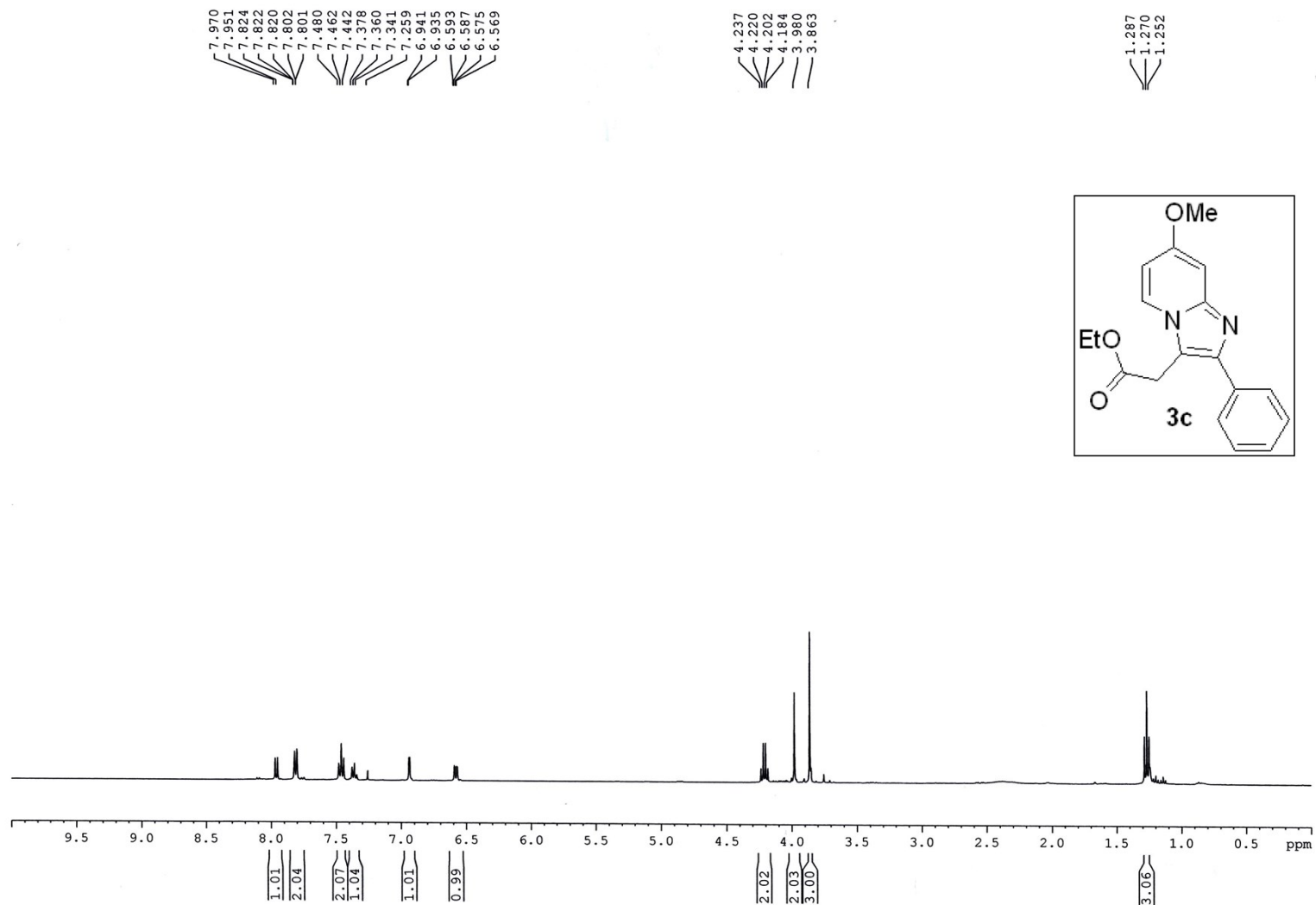
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 NAME Dr. A HAJRA-2019-13C  
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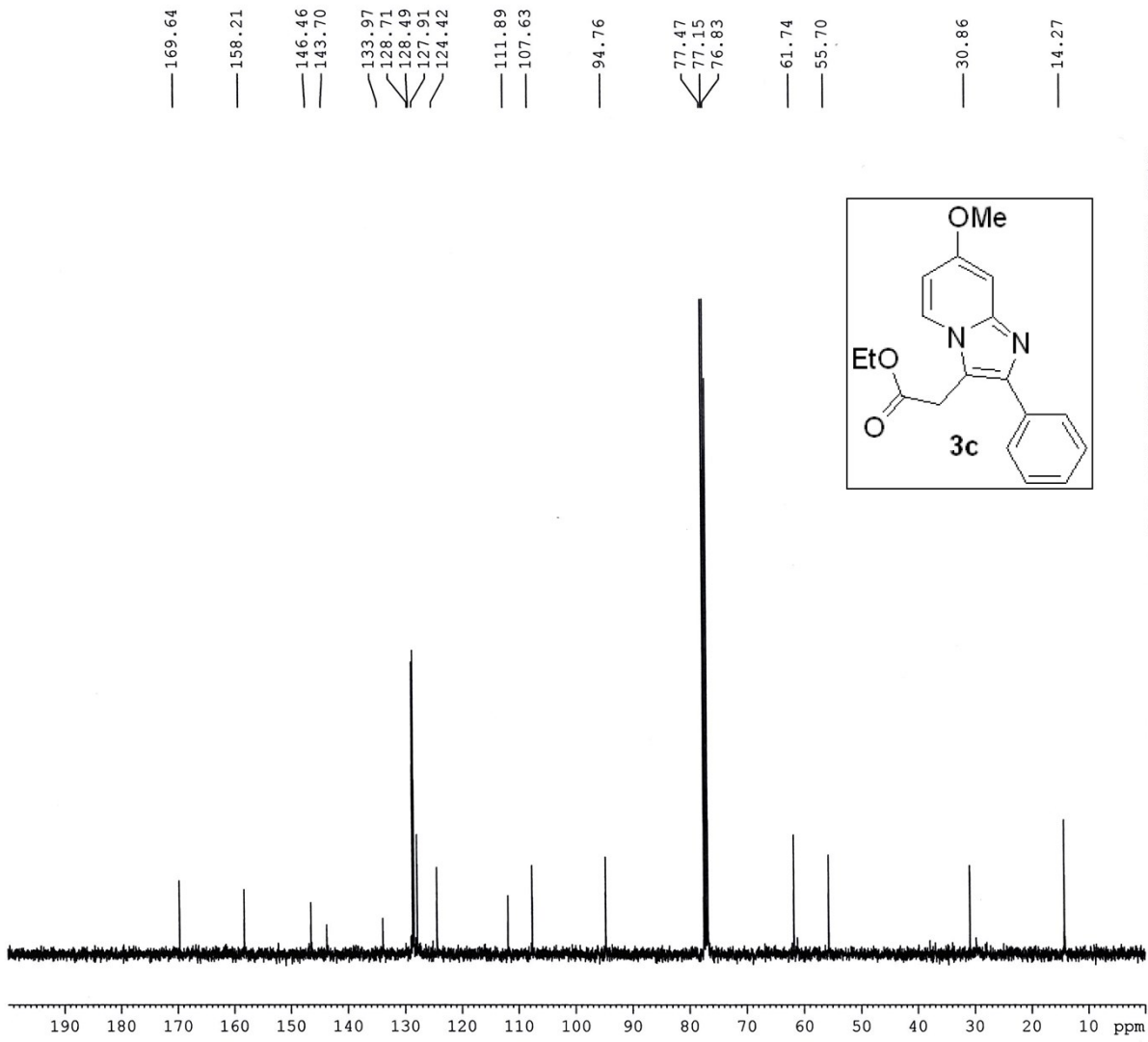
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 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 512  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 135.7  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

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

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

F2 - Processing parameters  
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 GB 0  
 PC 1.40





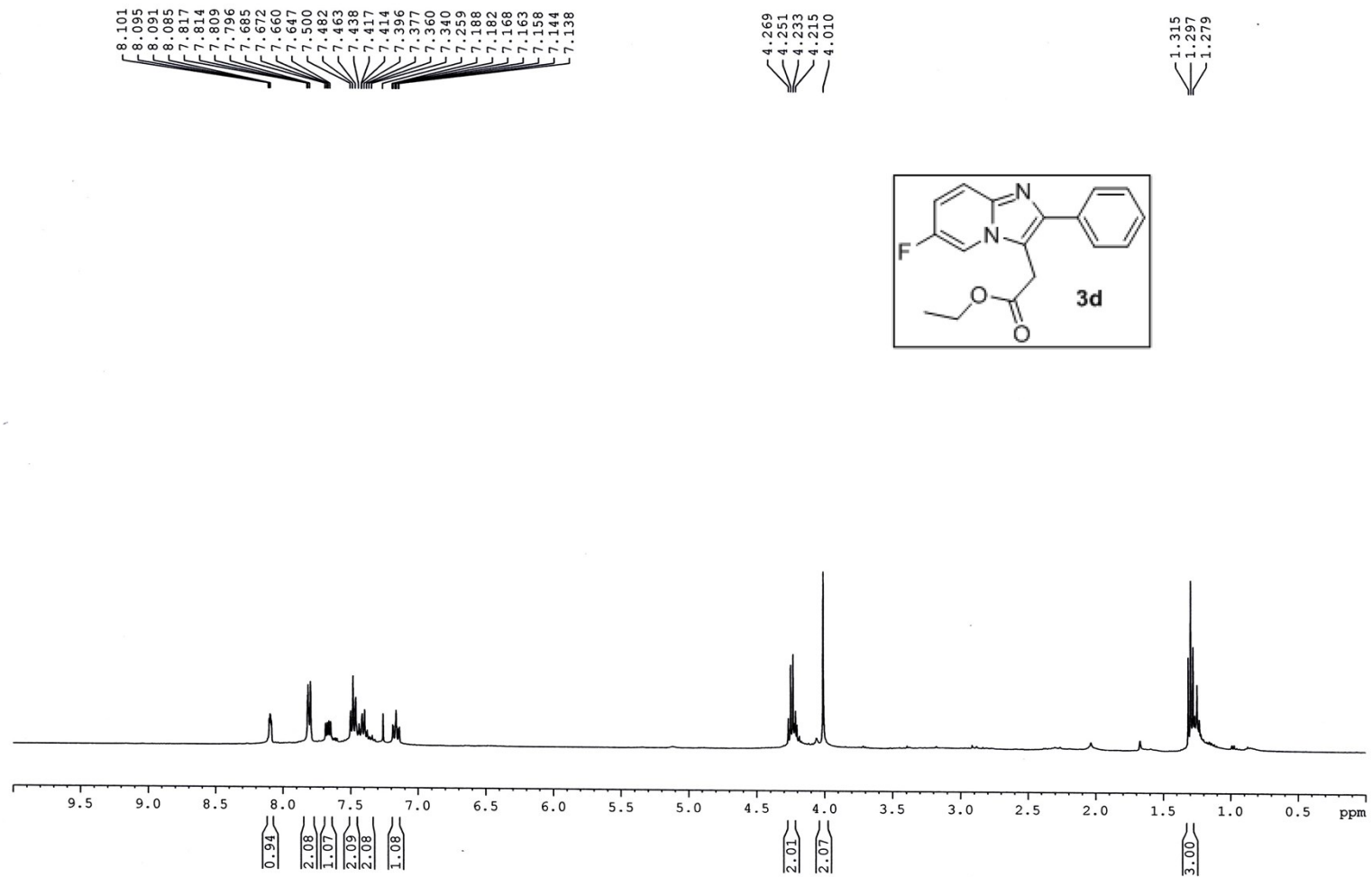
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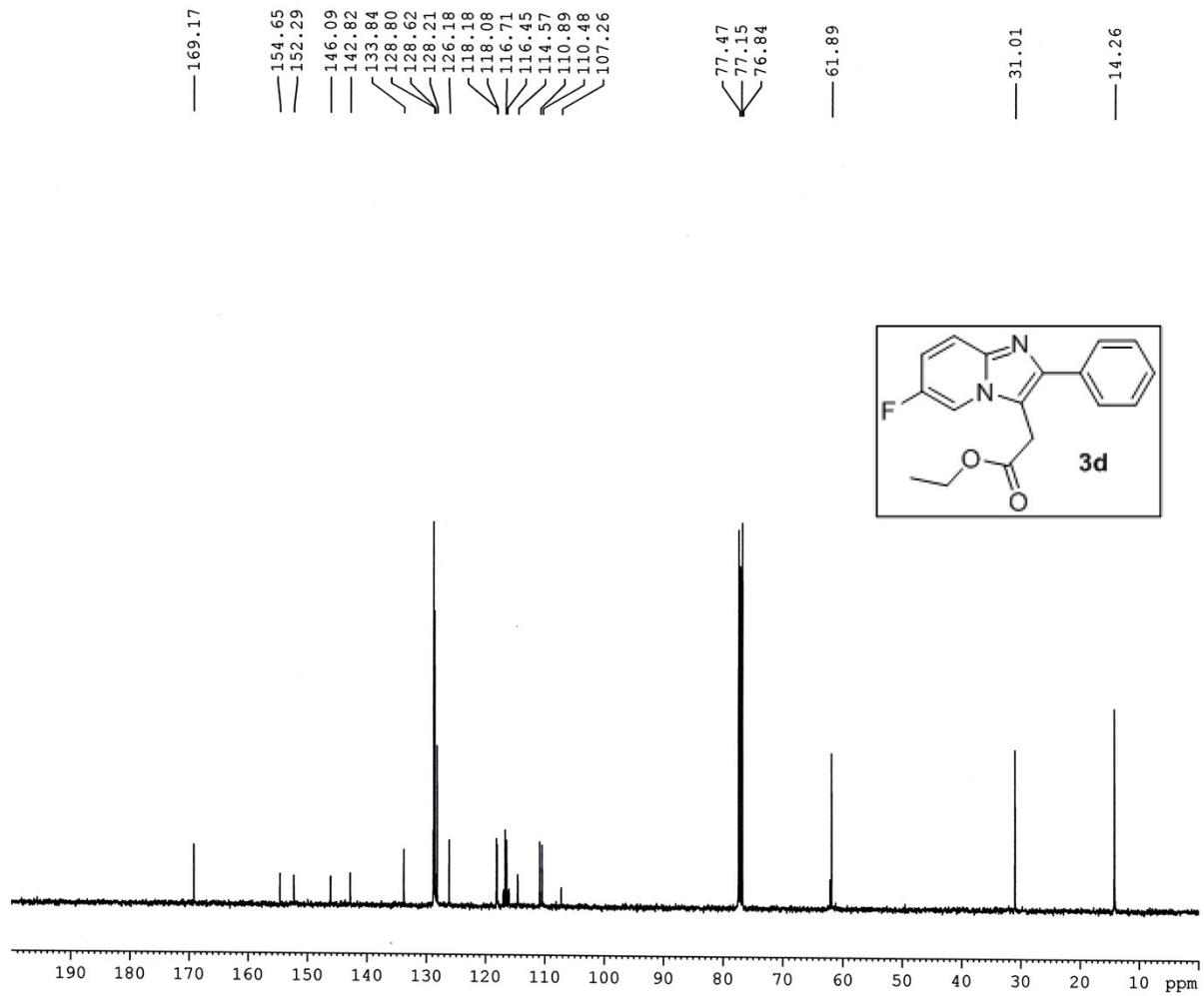
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 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 200  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.3 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TDO 1

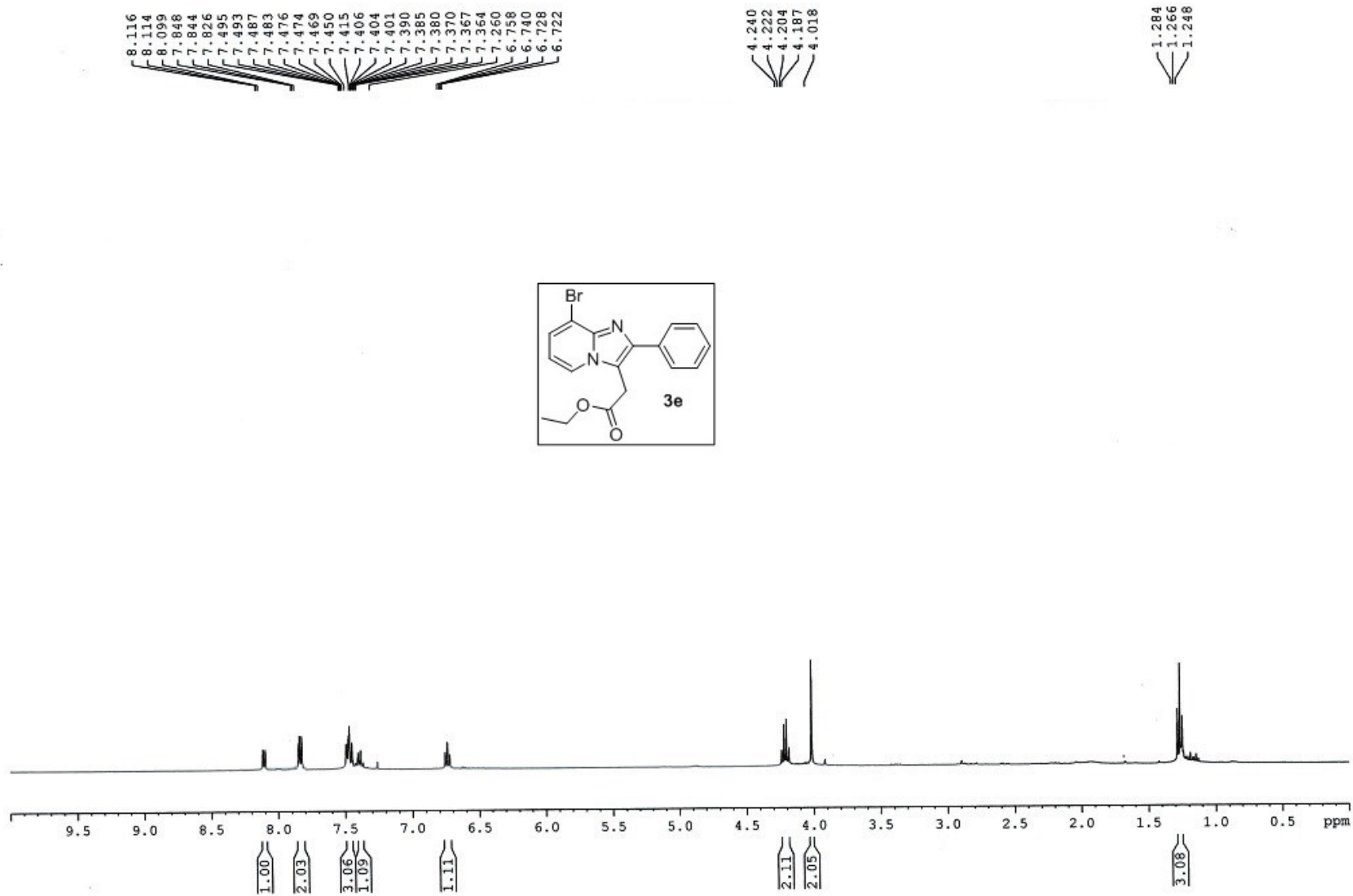
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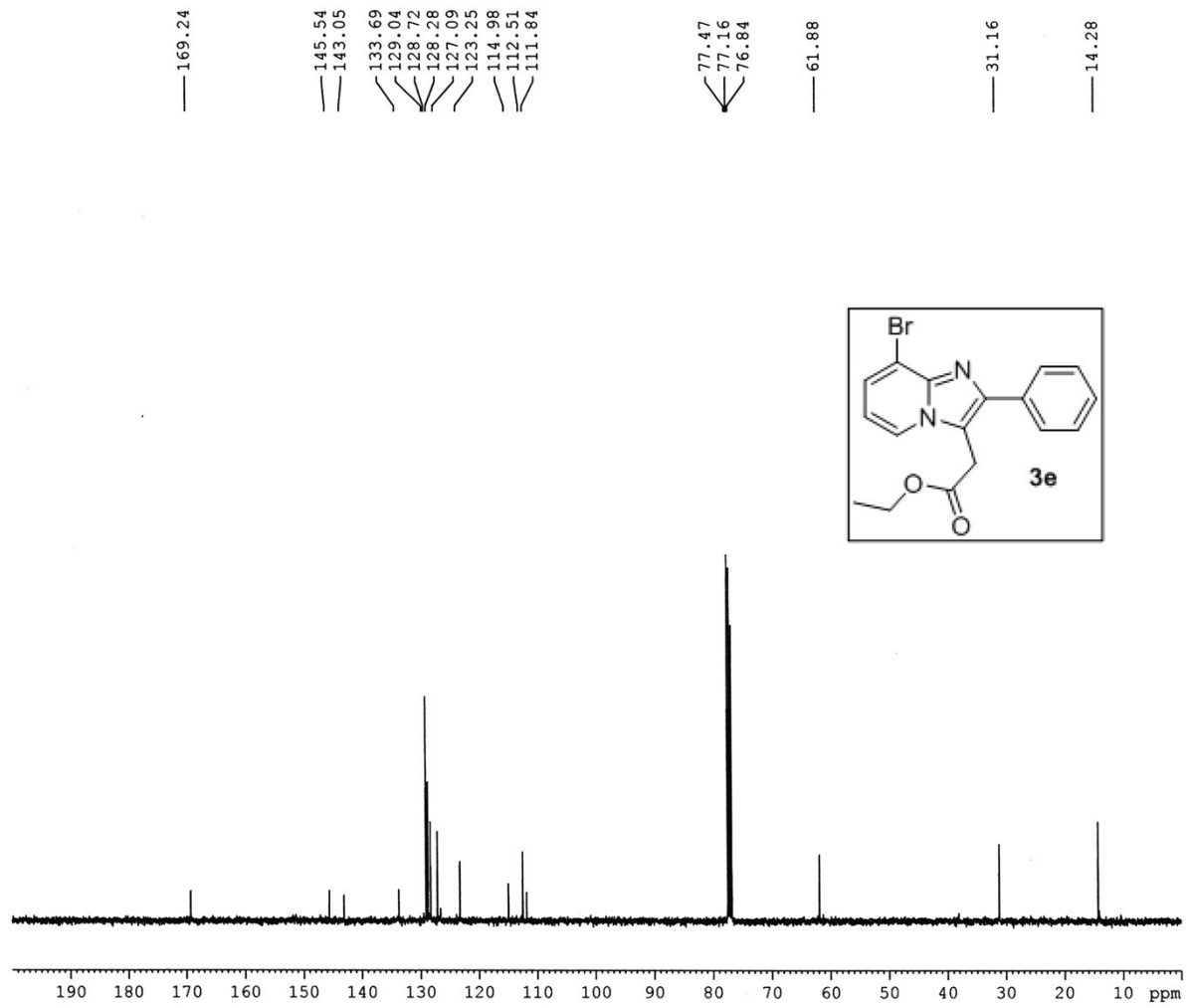
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 PLW2 12.0000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
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 SF 100.6177874 MHz  
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 PC 1.40

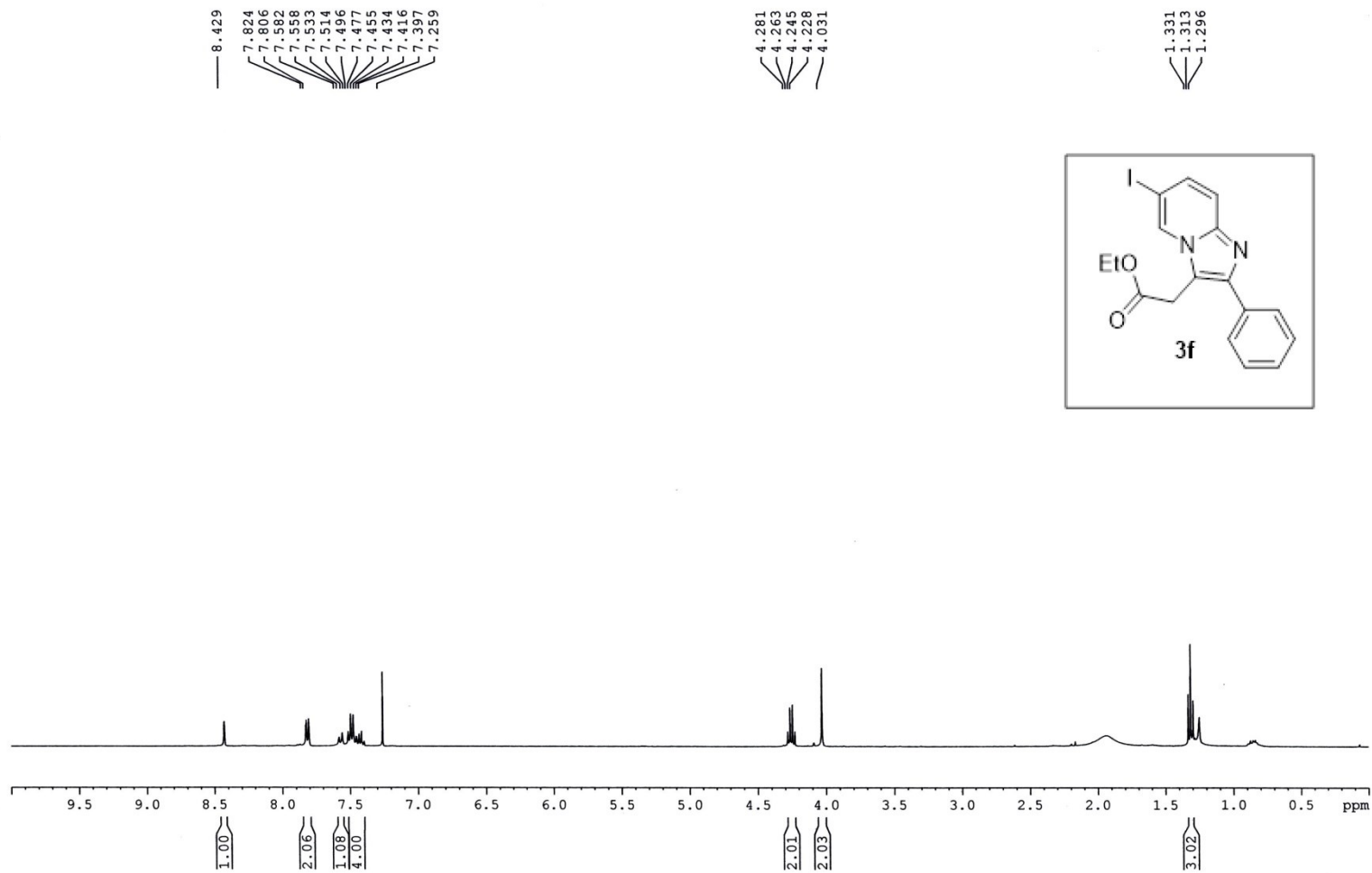


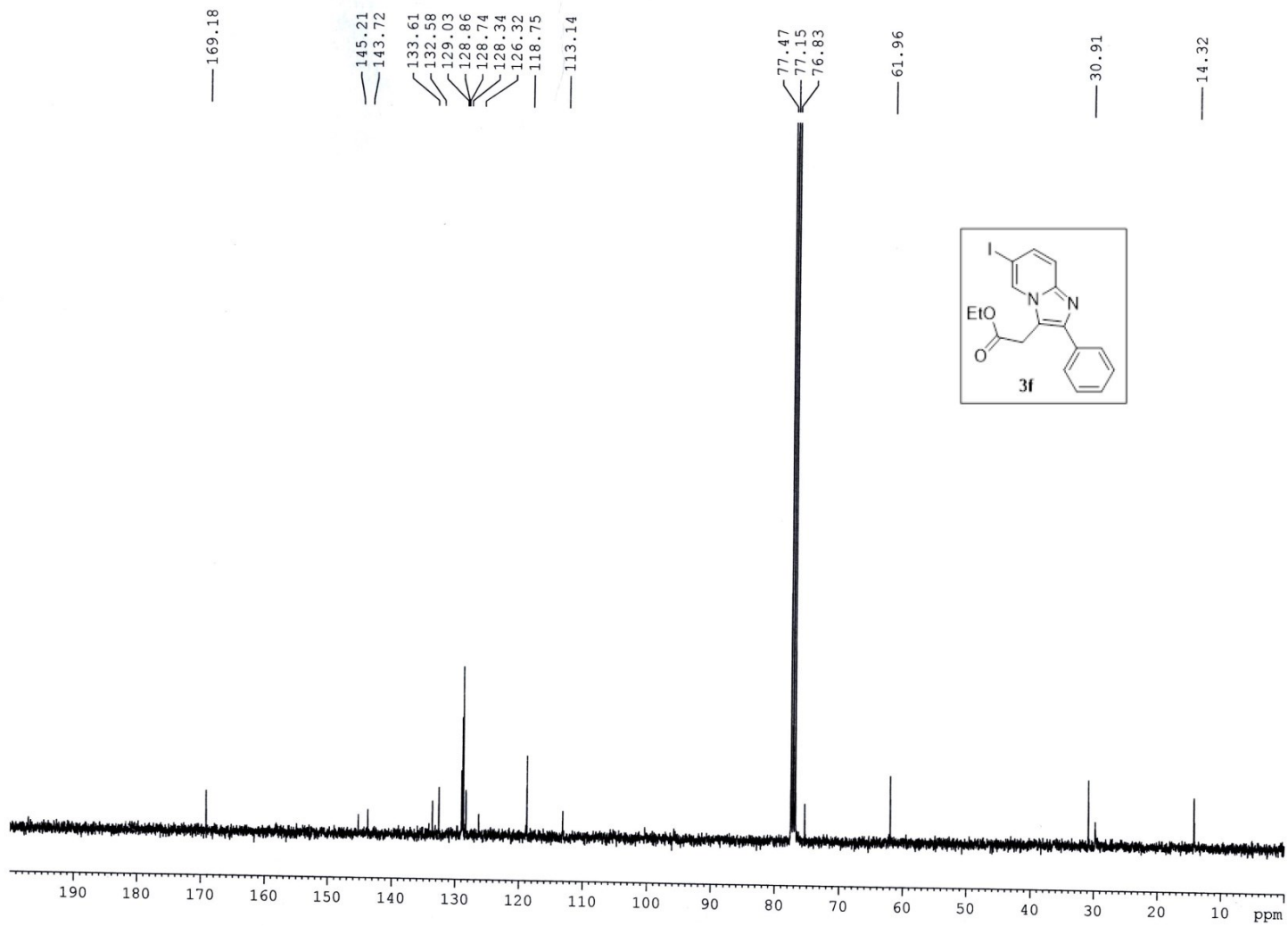


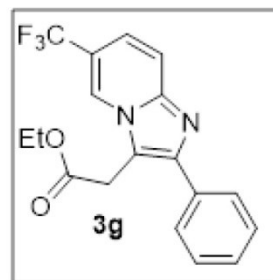
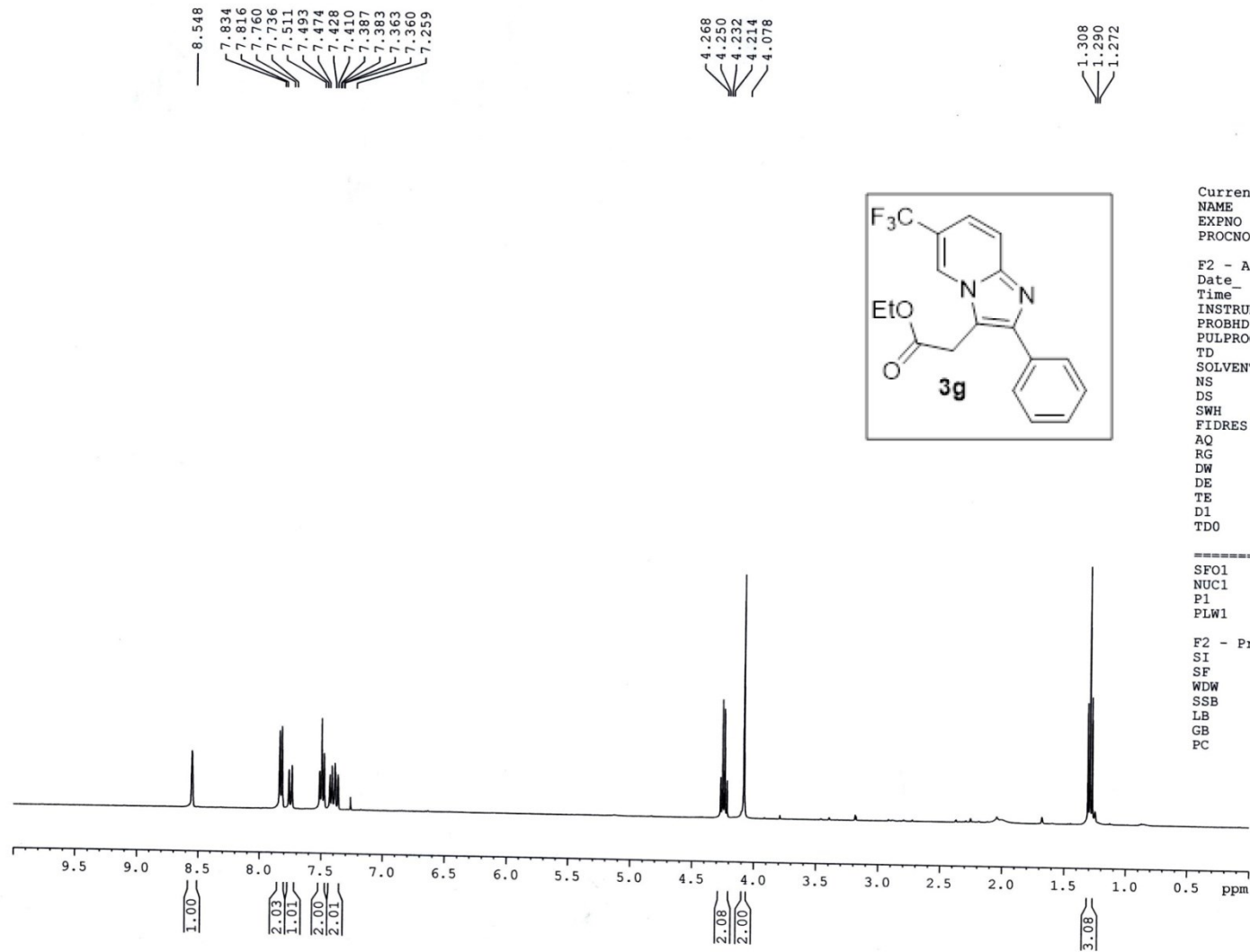










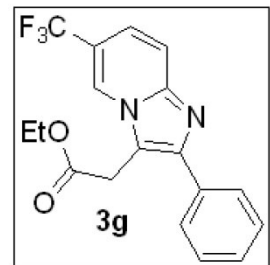
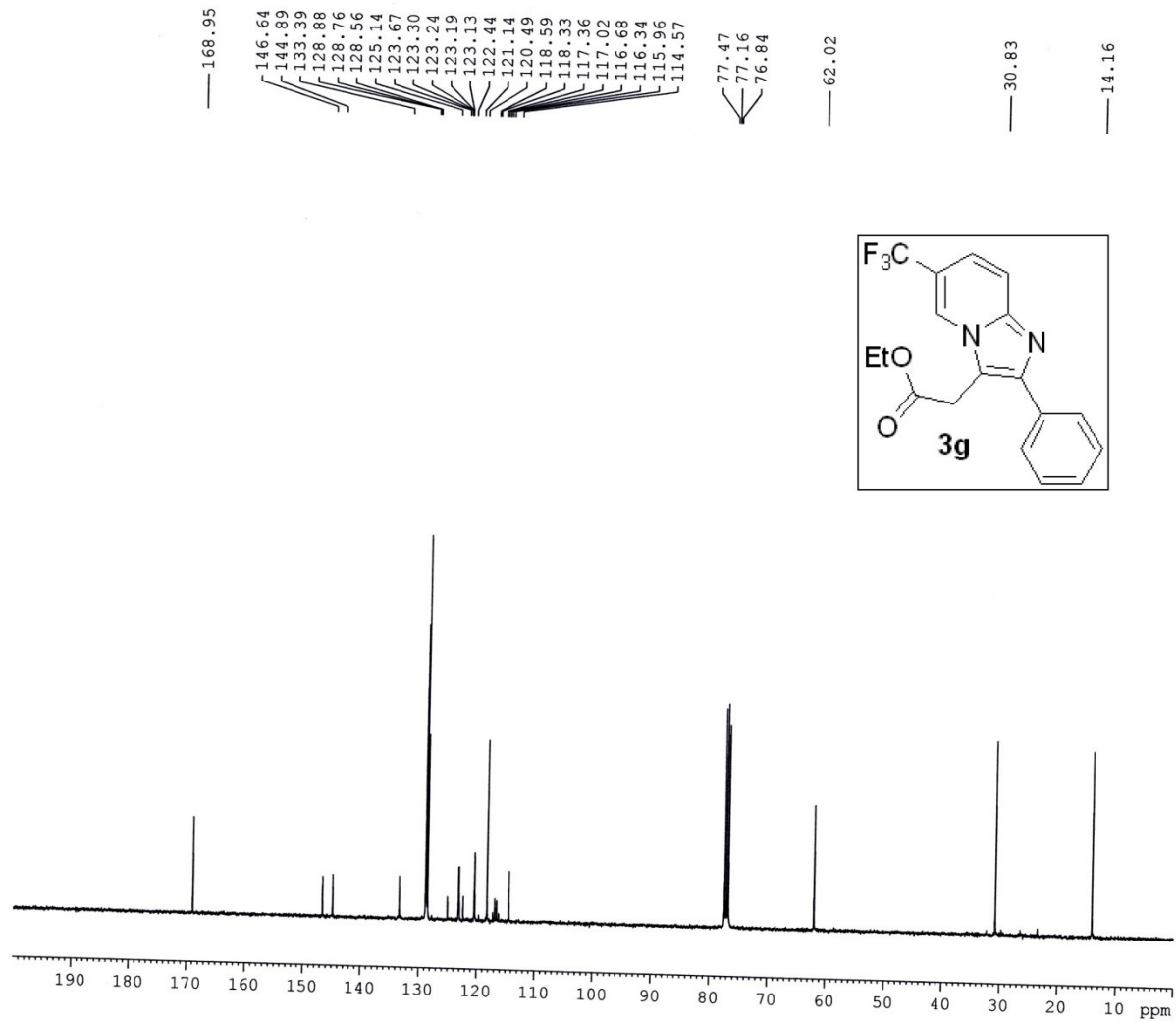


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 NAME Dr. A HAJRA 2019 1H  
 EXPNO 873  
 PROCNO 1

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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 67.81  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.4 K  
 D1 1.00000000 sec  
 TD0 1

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 NUC1 1H  
 P1 14.75 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
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 SSB 0  
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 GB 0  
 PC 2.00



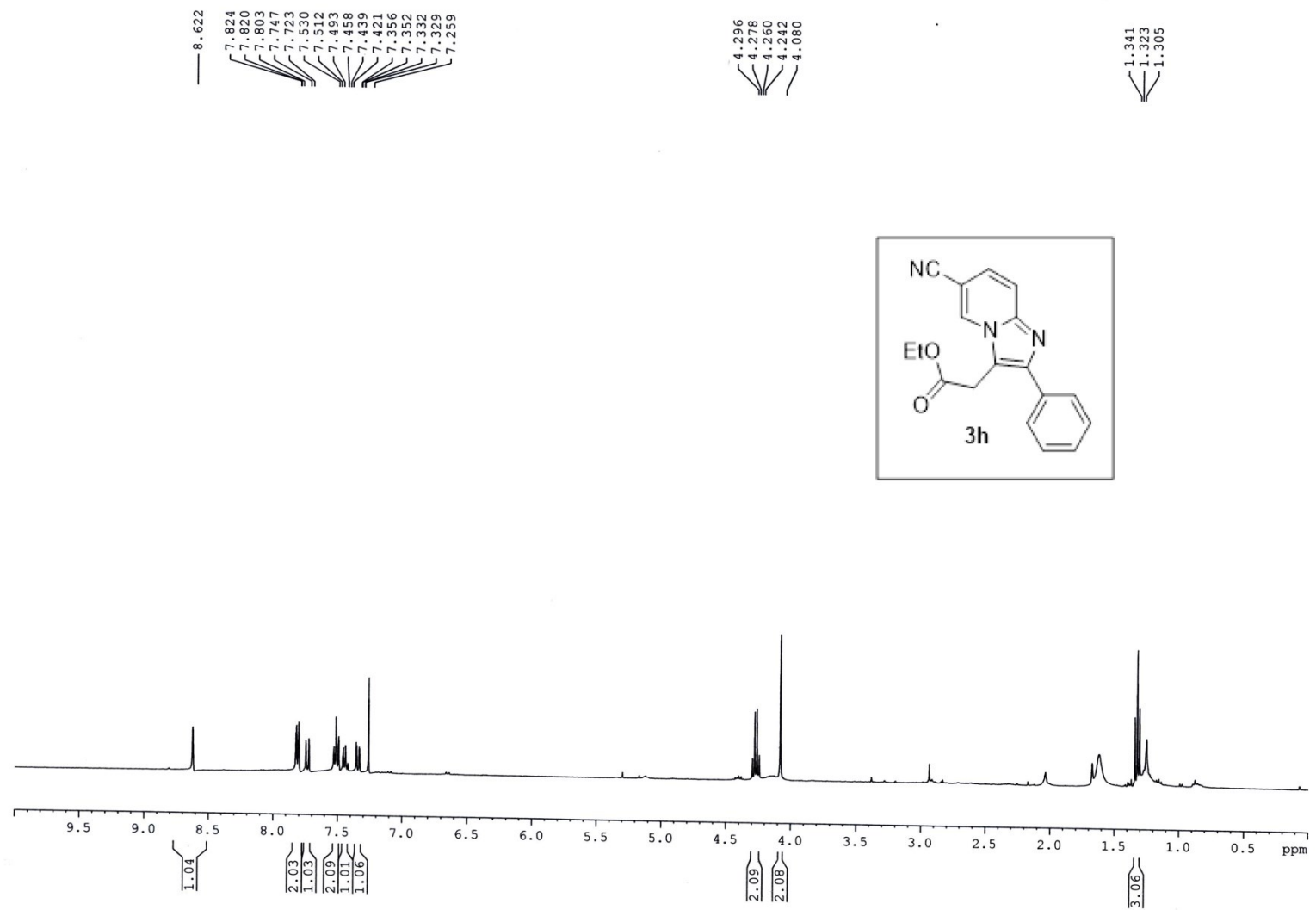
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 NAME Dr. A HAJRA-2019-13C  
 EXPNO 416  
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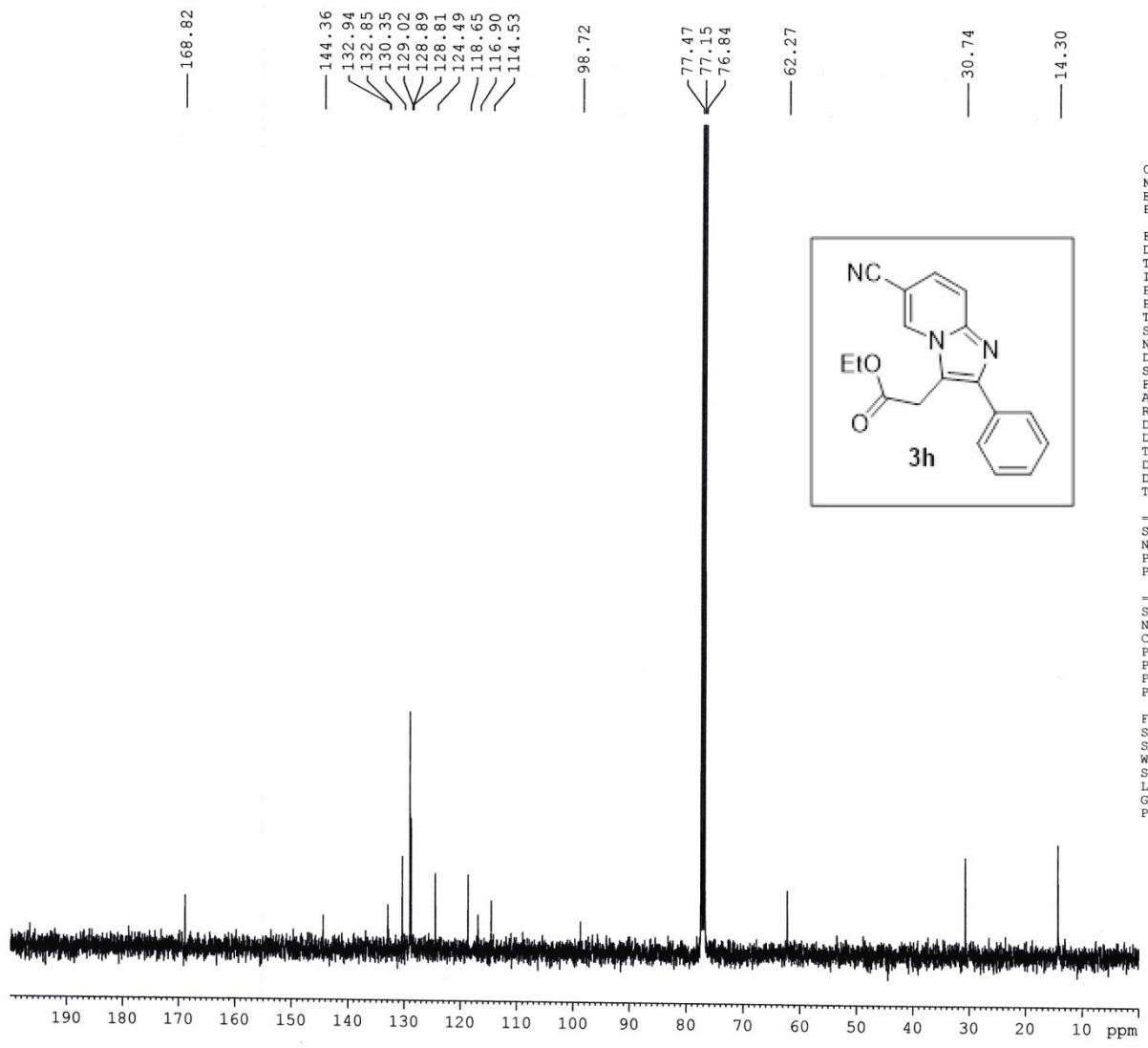
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 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 960  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 302.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== 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  
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 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
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 GB 0  
 PC 1.40





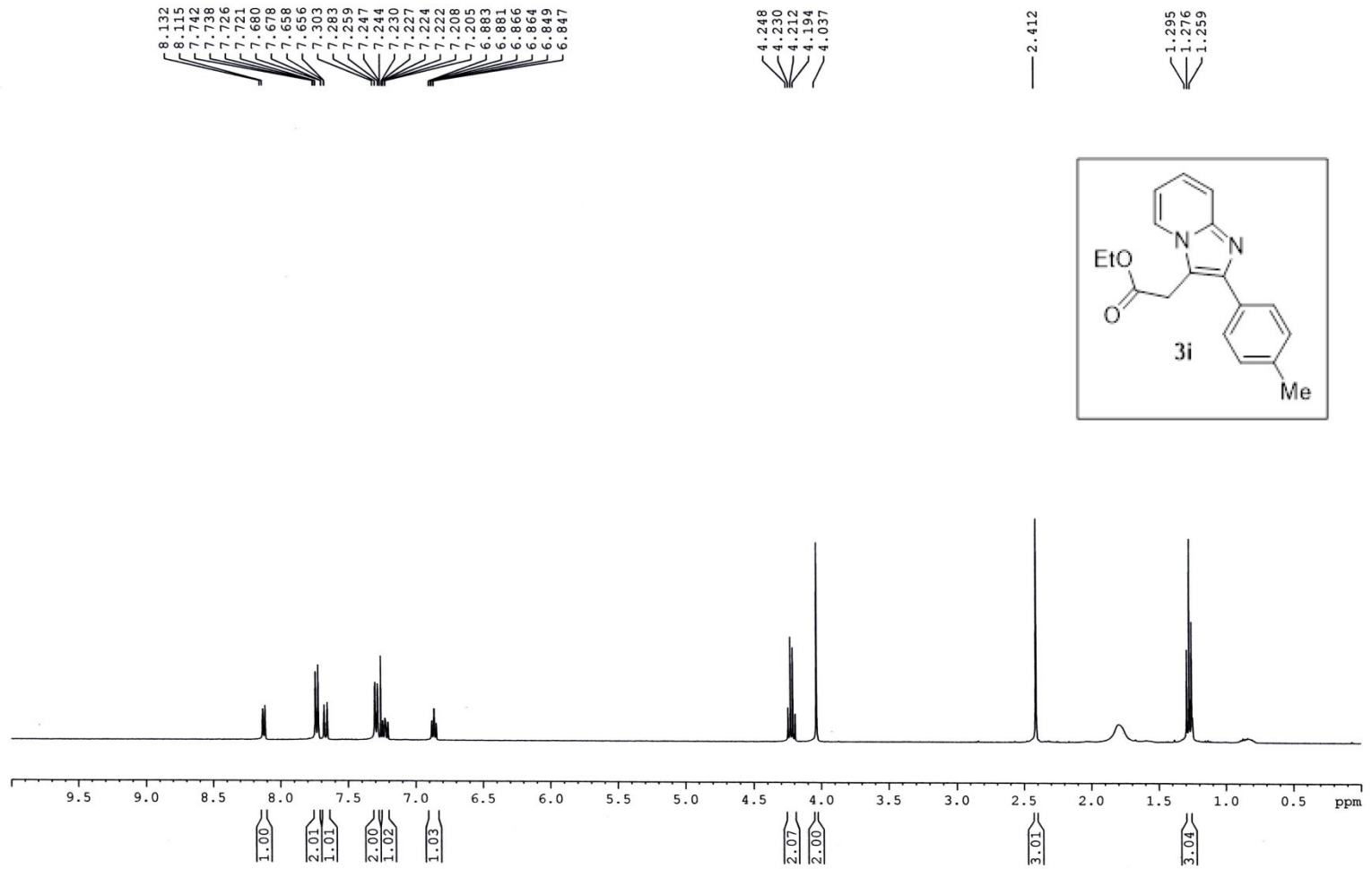
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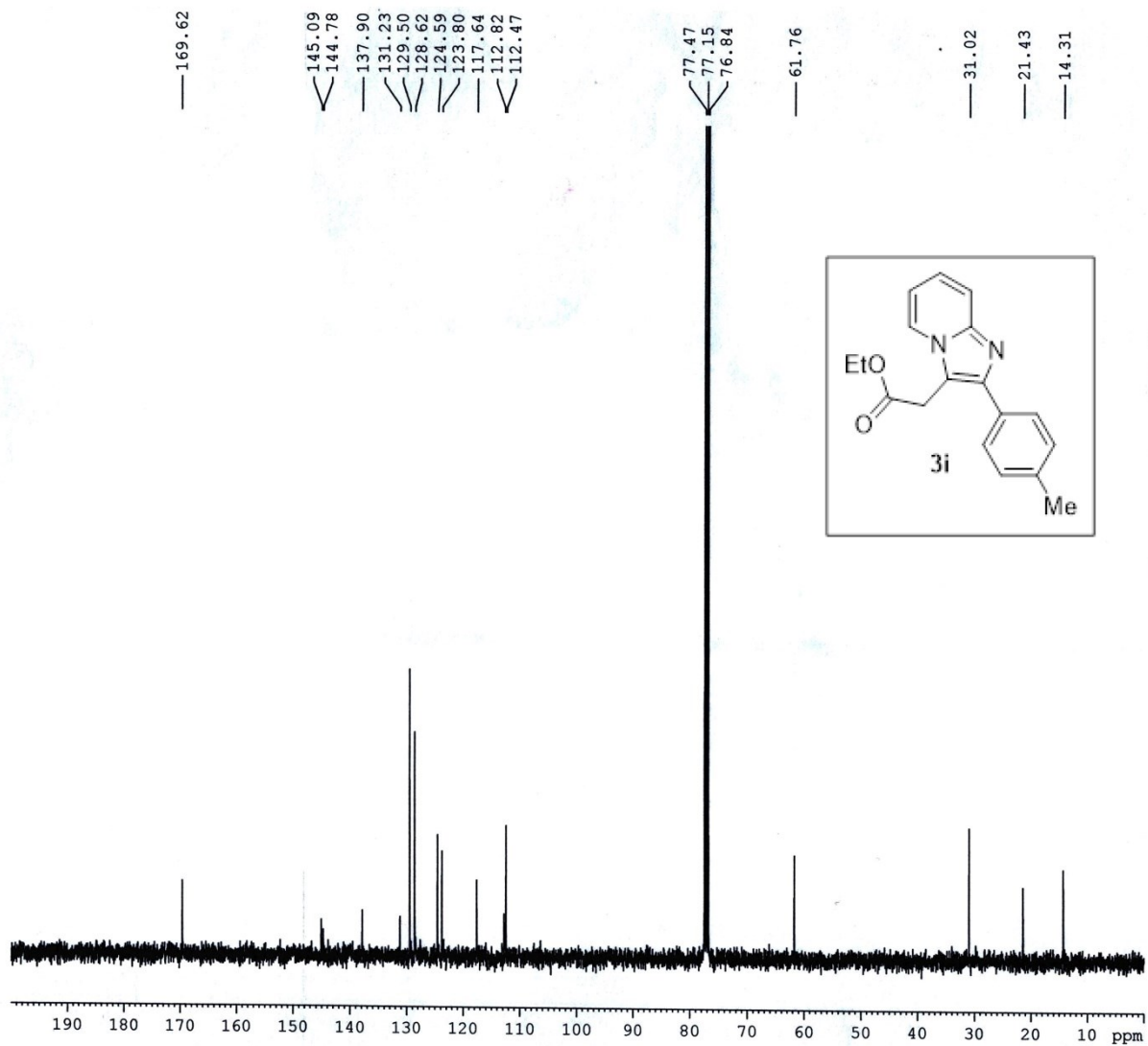
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 SOLVENT CDCl3  
 NS 640  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.3 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== 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 100.6177844 MHz  
 WDW EM  
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 GB 0  
 FC 1.40





Current Data Parameters  
 NAME Dr. A HAJRA-2019-13C  
 EXPNO 342  
 PROCNO 1

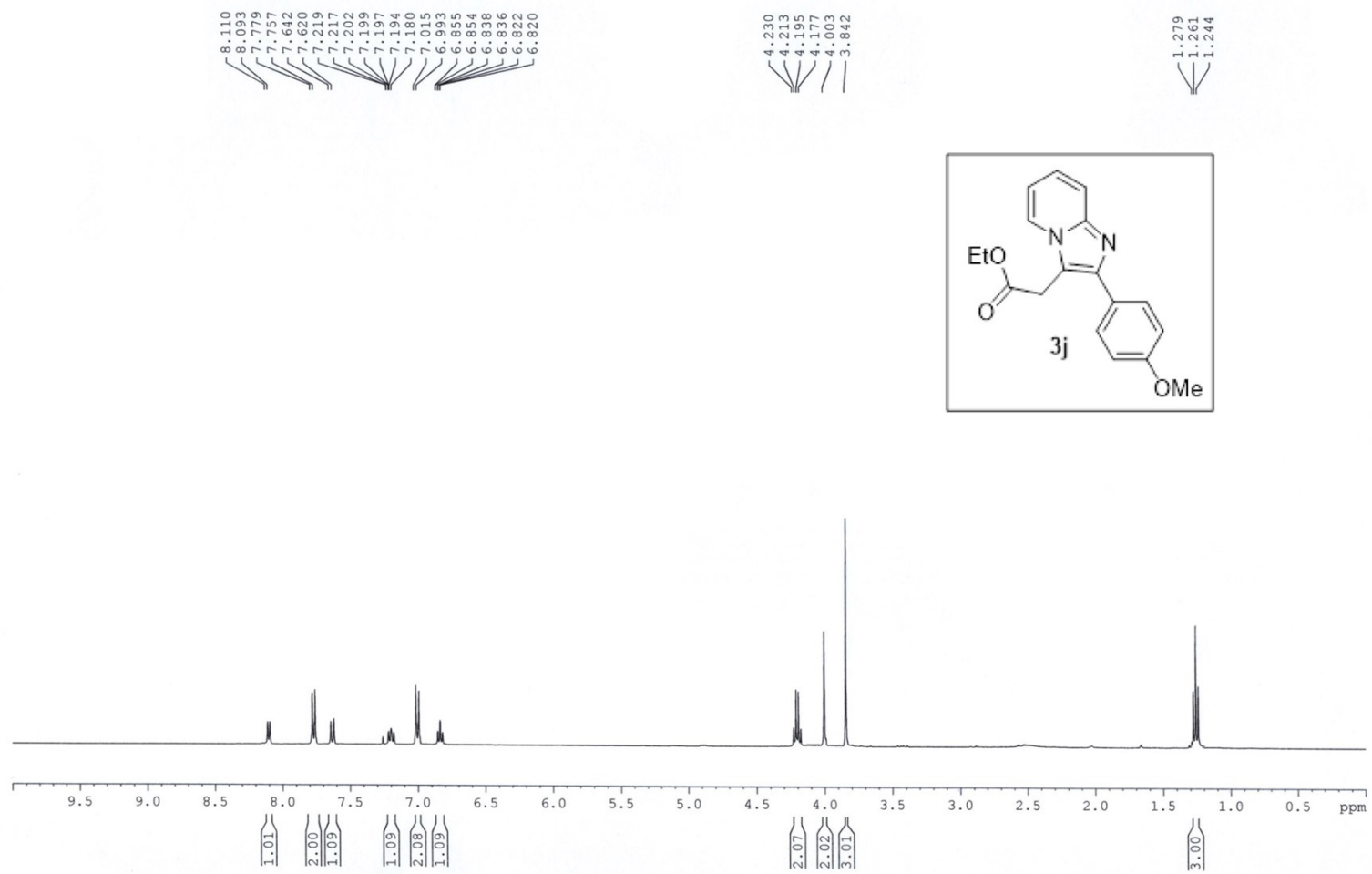
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 TD 32768  
 SOLVENT CDCl3  
 NS 410  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
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 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.7 K  
 D1 2.00000000 sec  
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 TD0 1

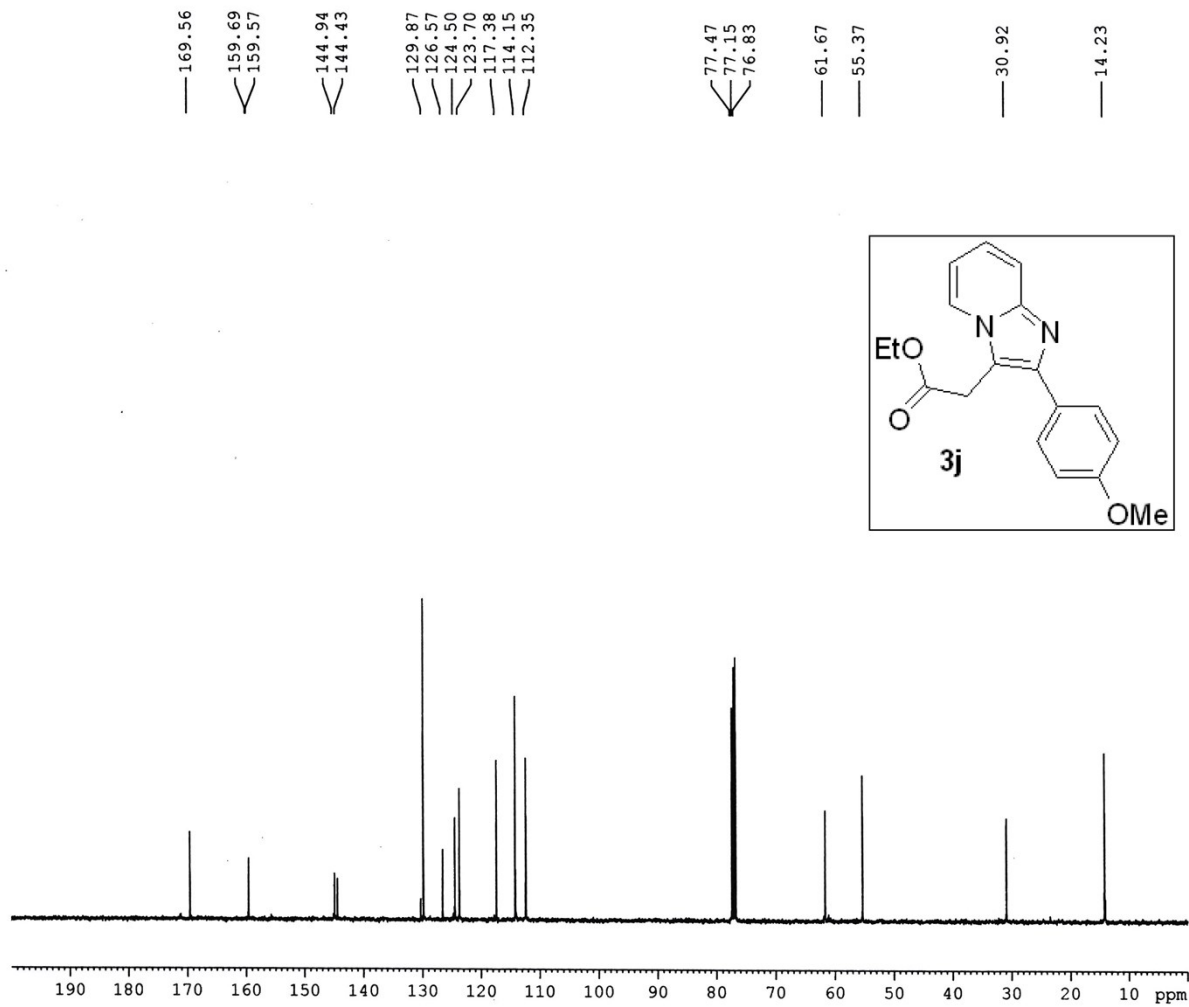
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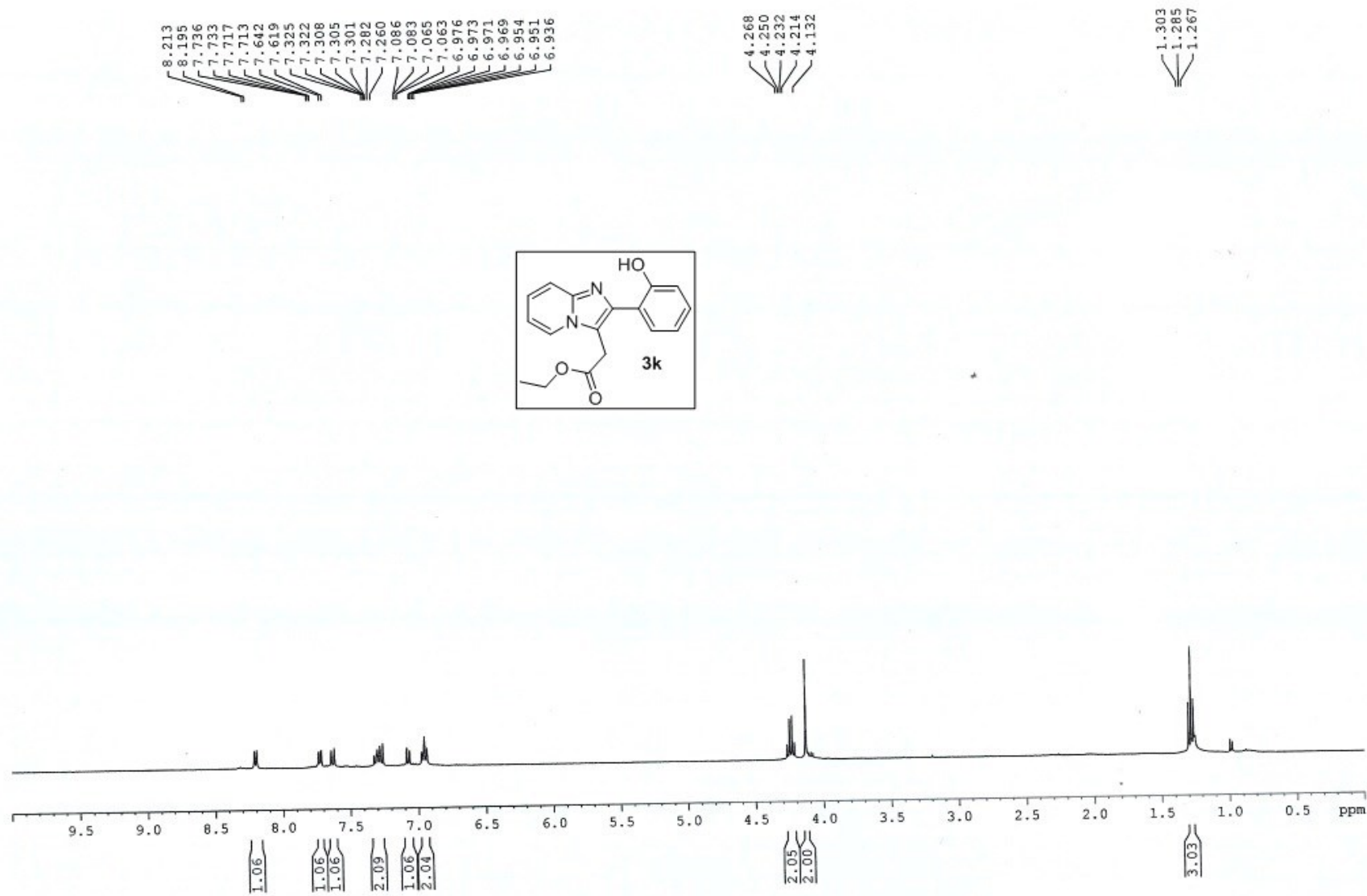
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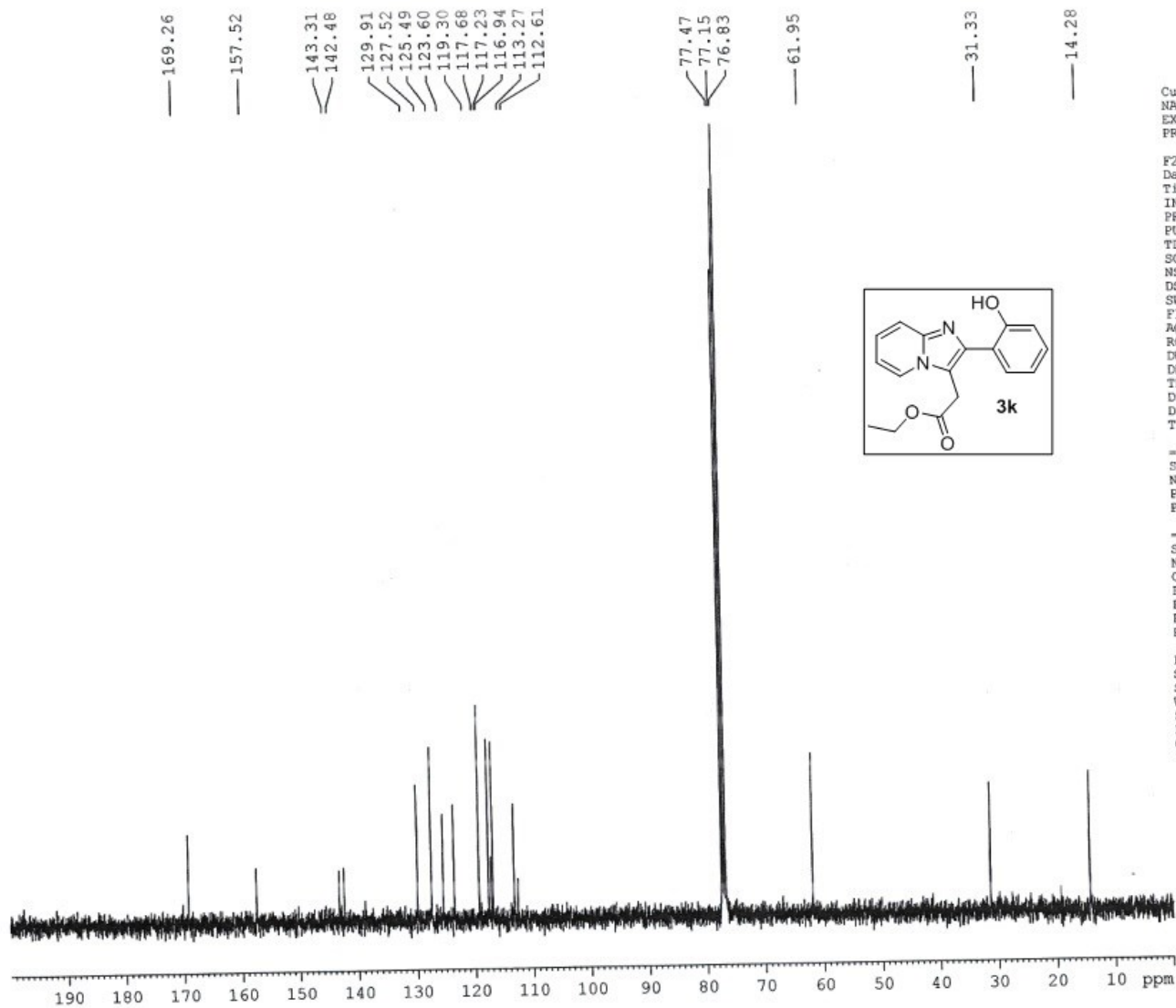
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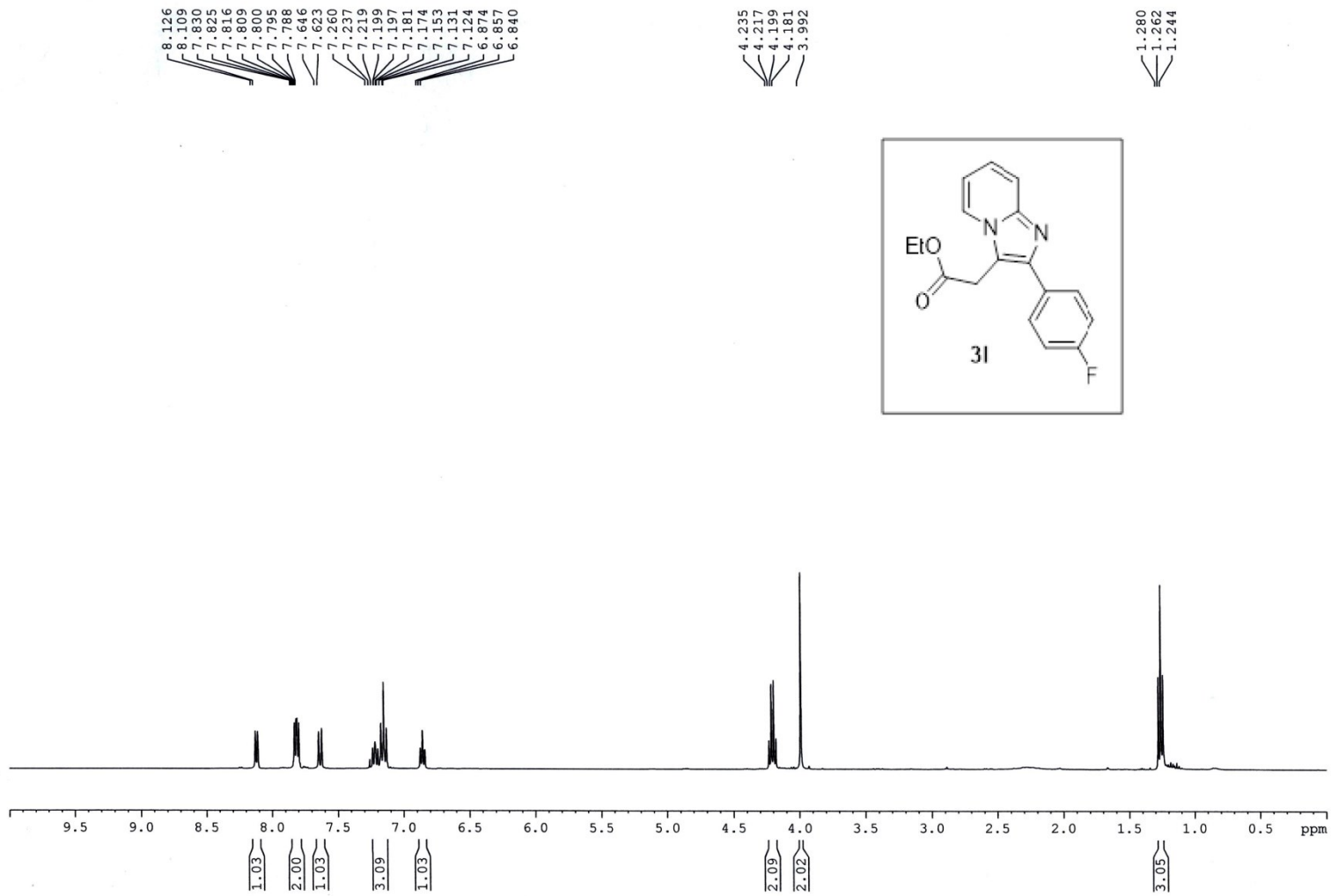
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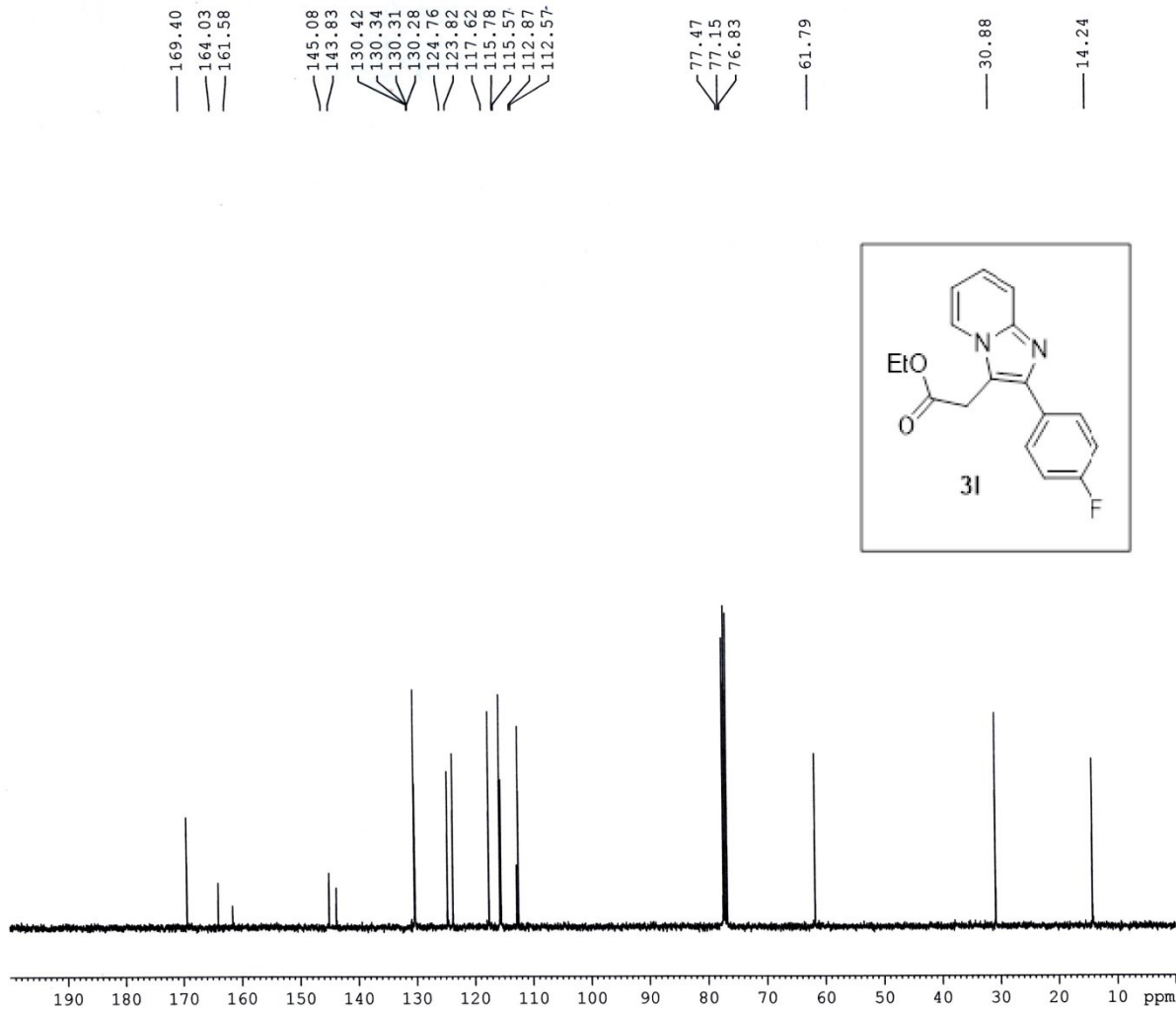
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 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 135.7  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

----- CHANNEL f1 -----  
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 NUC1 13C  
 F1 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 100.6177855 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





— 169.40  
— 164.03  
— 161.58

145.08  
143.83  
130.42  
130.34  
130.31  
130.28  
124.76  
123.82  
117.62  
115.78  
115.57  
112.87  
112.57

77.47  
77.15  
76.83

— 61.79

— 30.88

— 14.24



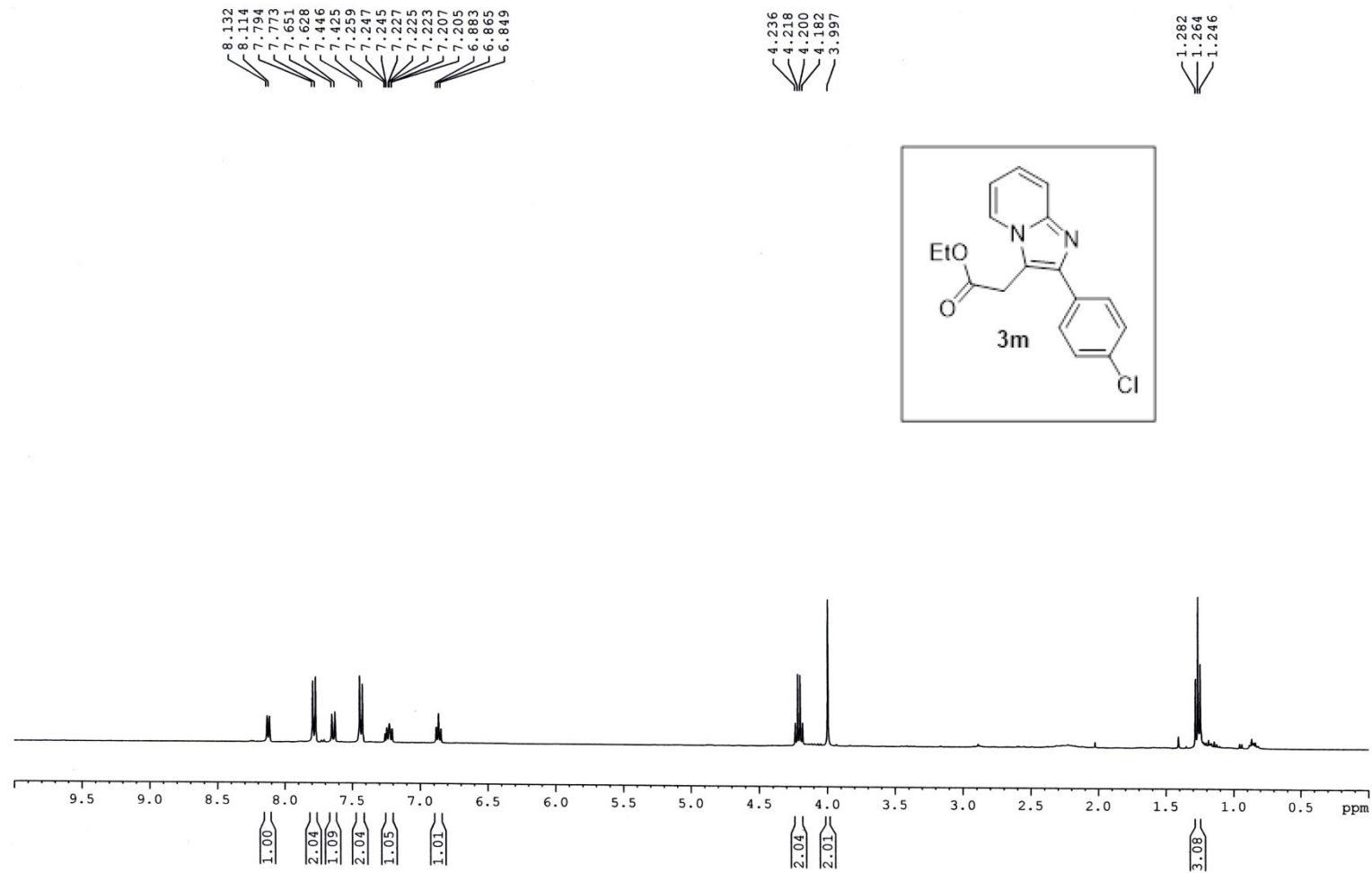
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NAME Dr. A HAJRA-2019-13C  
EXPNO 376  
PROCNO 1

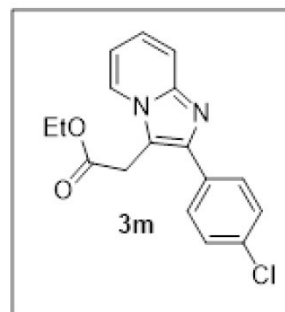
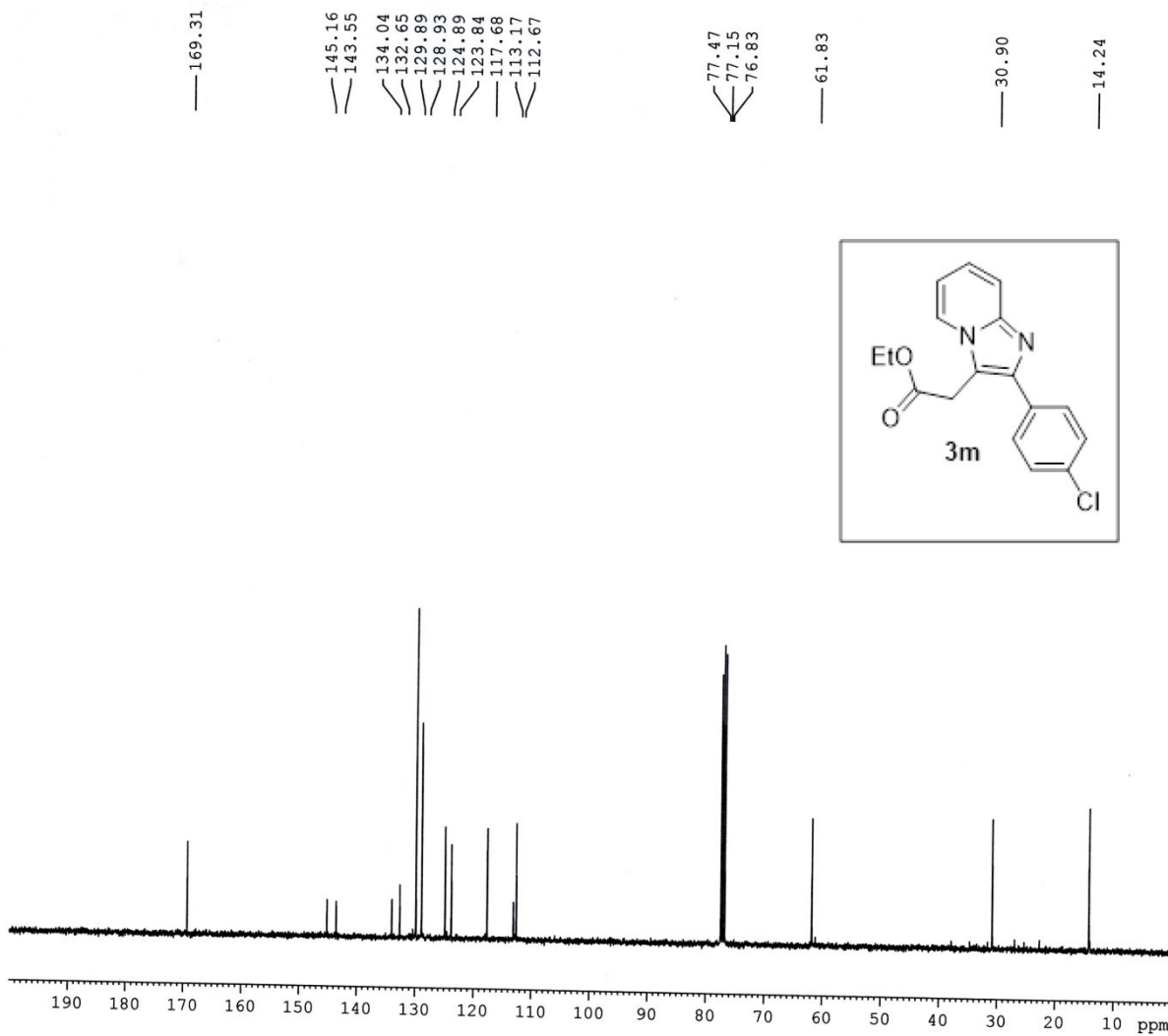
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PULPROG zgpg30  
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SOLVENT CDCl3  
NS 200  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 62.69  
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DE 6.50 usec  
TE 299.1 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  
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  
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SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
 NAME Dr. A HAJRA-2019-13C  
 EXPNO 384  
 PROCNO 1

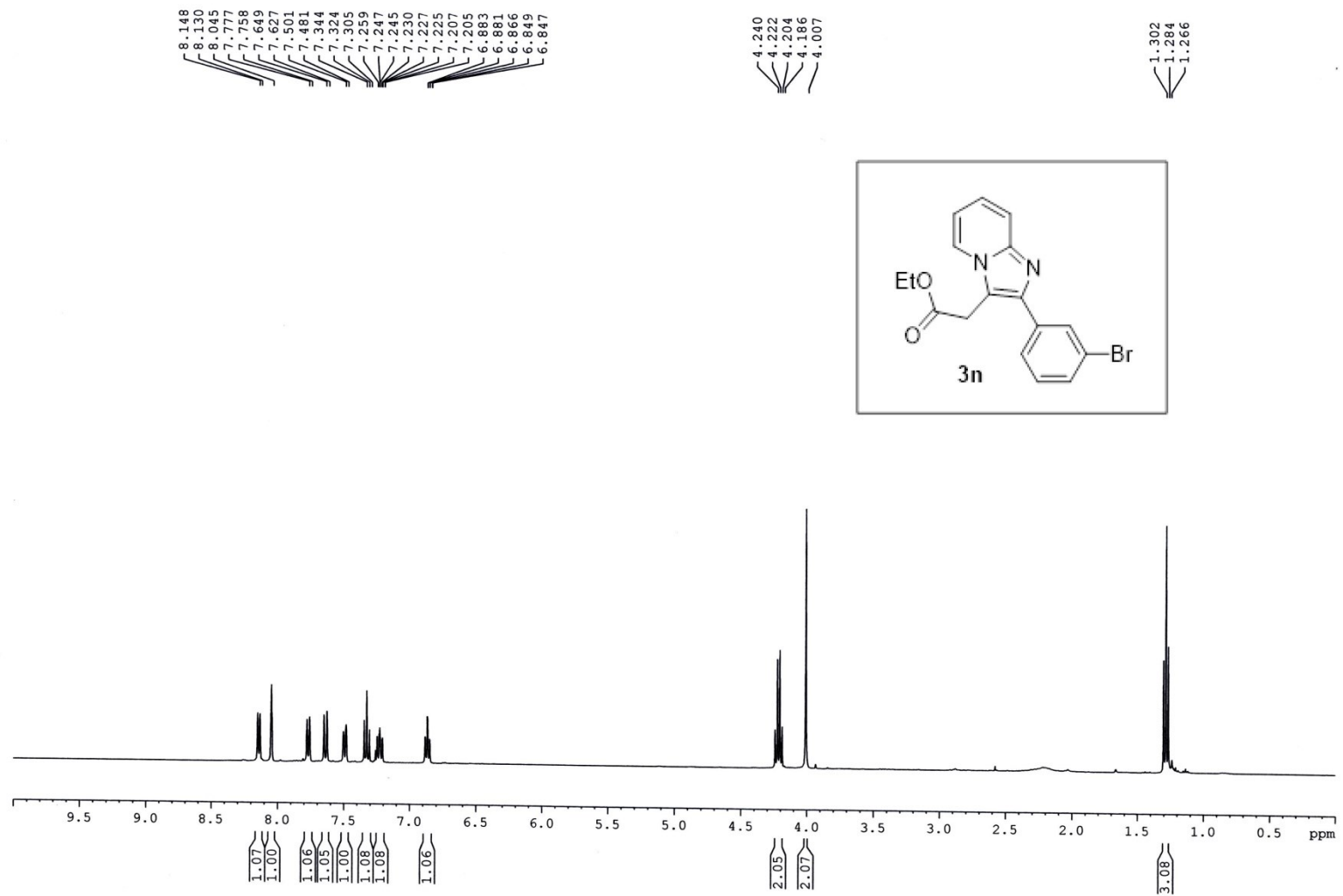
F2 - Acquisition Parameters  
 Date\_ 20190924  
 Time\_ 11.29  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDC13  
 NS 200  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 62.69  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

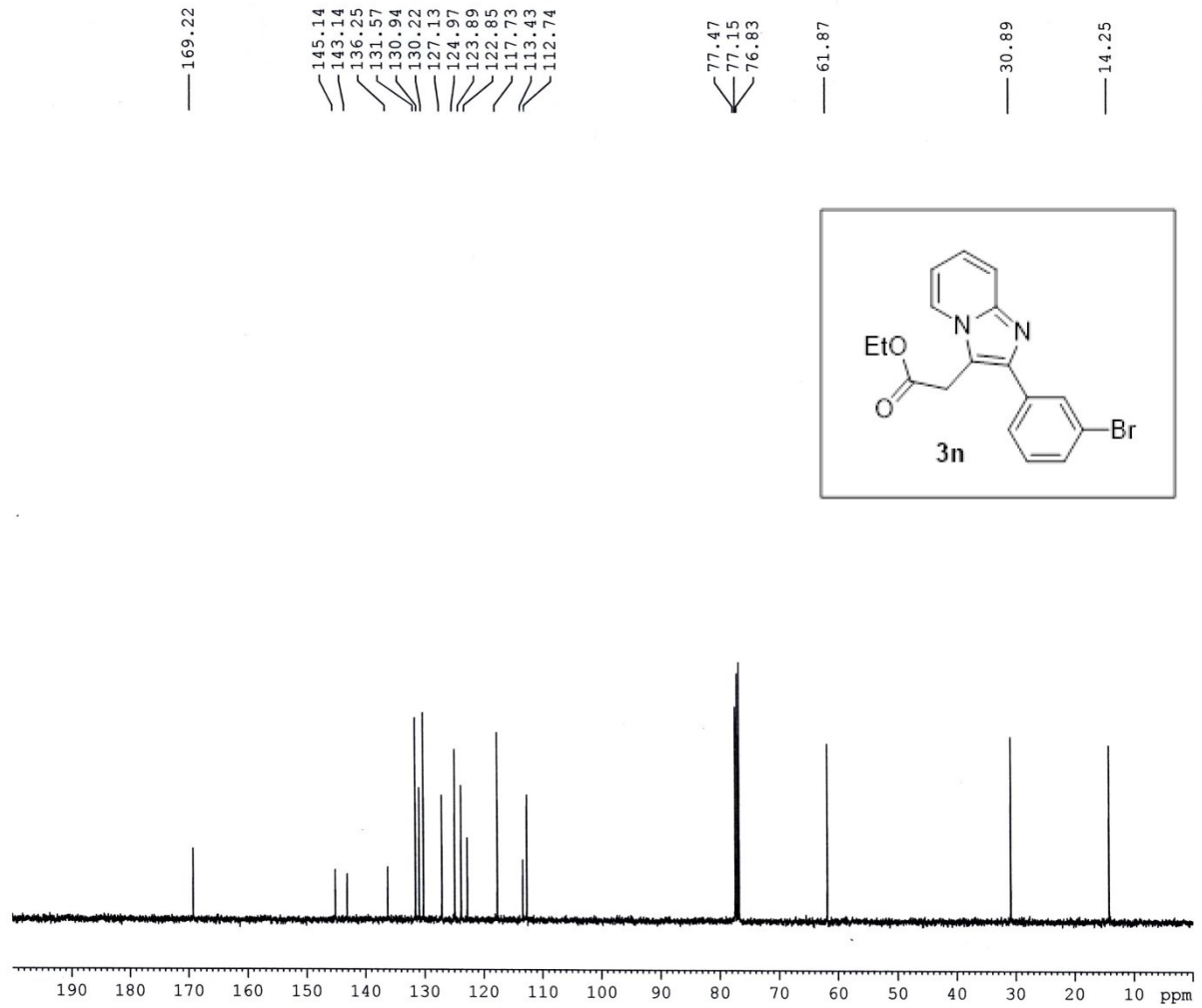
===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 F1 8.90 usec  
 PLW1 54.0000000 W

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

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







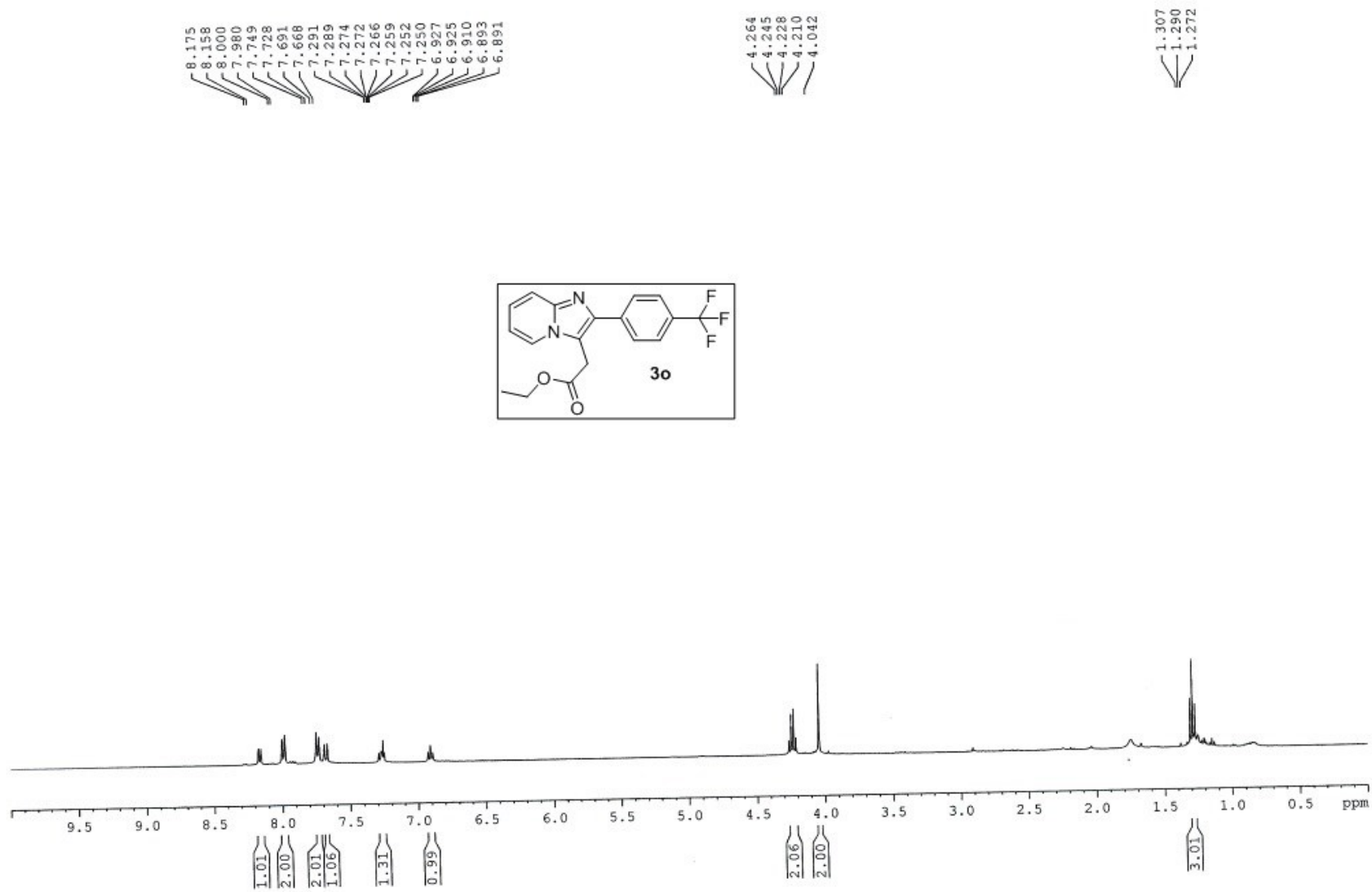
Current Data Parameters  
 NAME Dr. A HAJRA-2019-13C  
 EXPNO 397  
 PROCNO 1

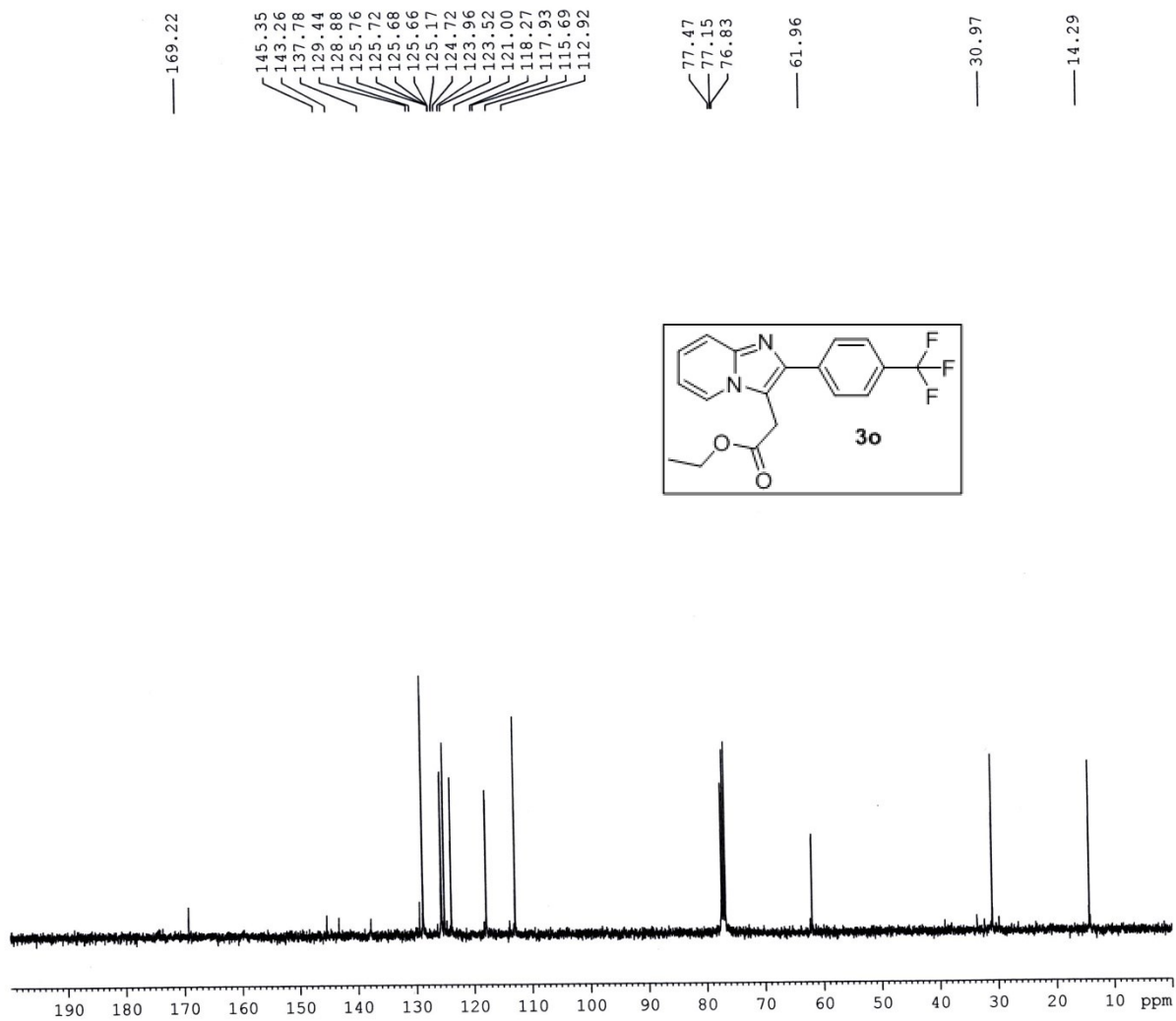
F2 - Acquisition Parameters  
 Date\_ 20191002  
 Time 10.54  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 120  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

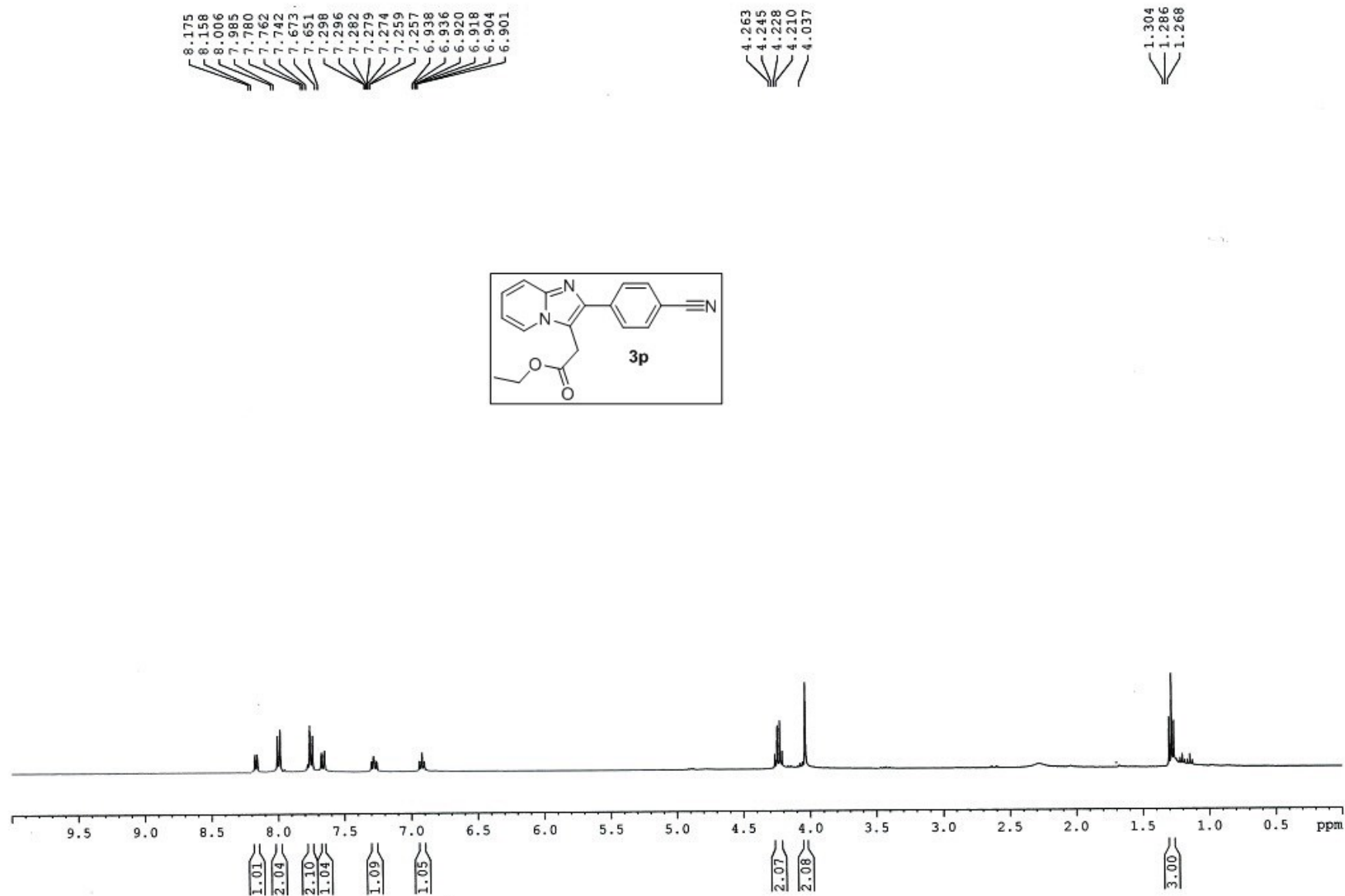
----- CHANNEL f1 -----  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

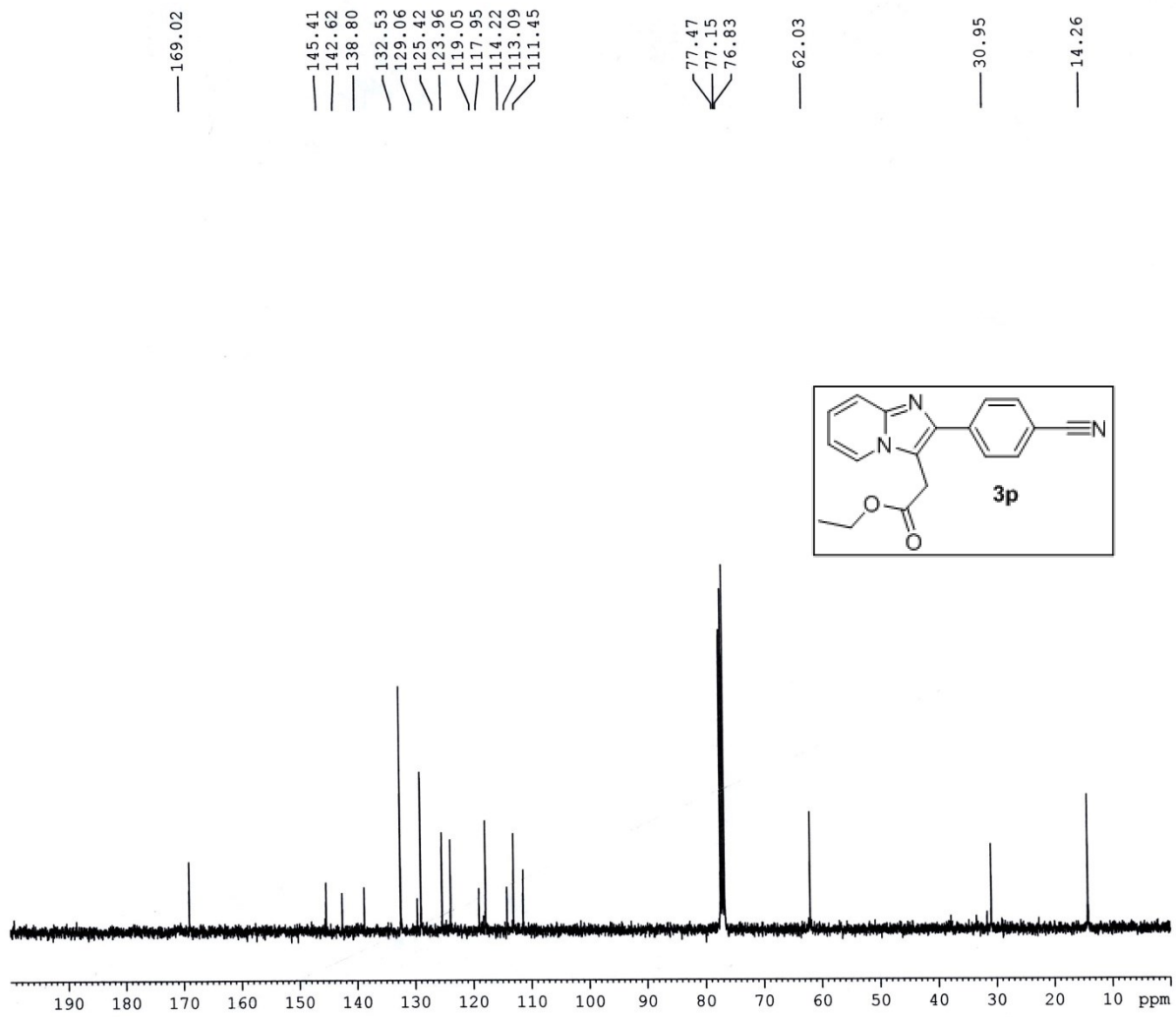
----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 FCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

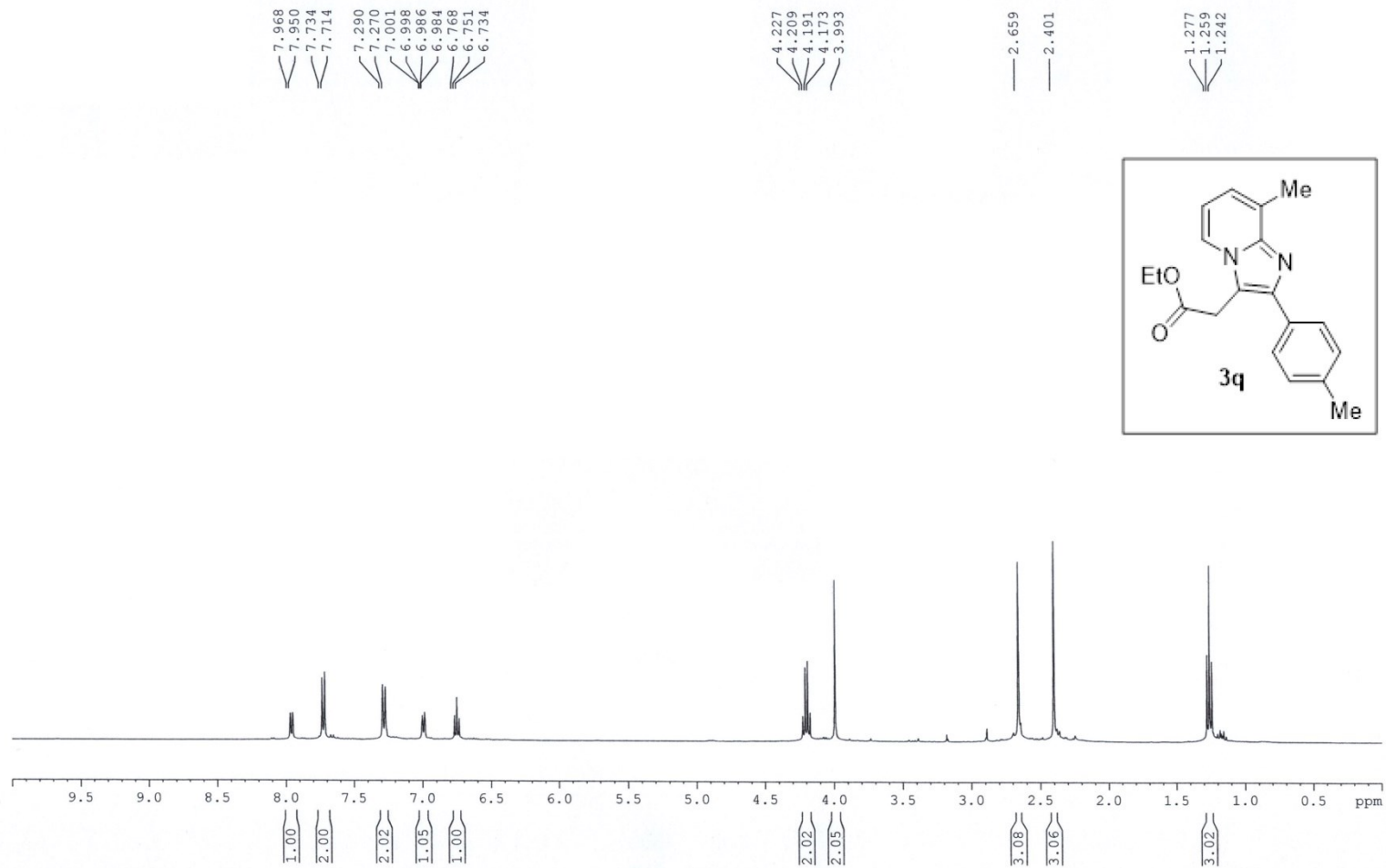
F2 - Processing parameters  
 SI 16384  
 SF 100.6177902 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

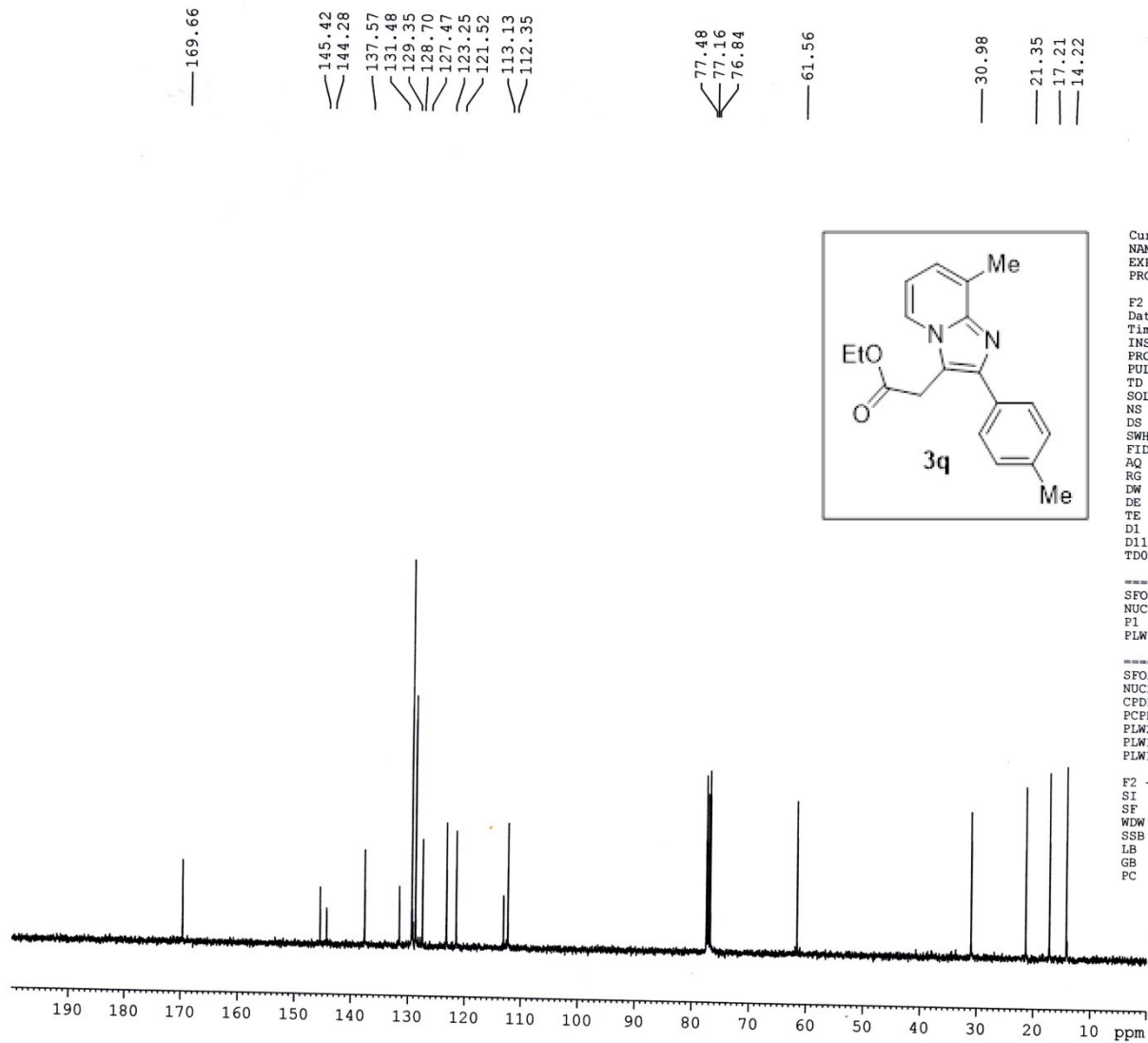












Current Data Parameters  
 NAME Dr. A HAJRA-2019-13C  
 EXNO 428  
 PROCNO 1

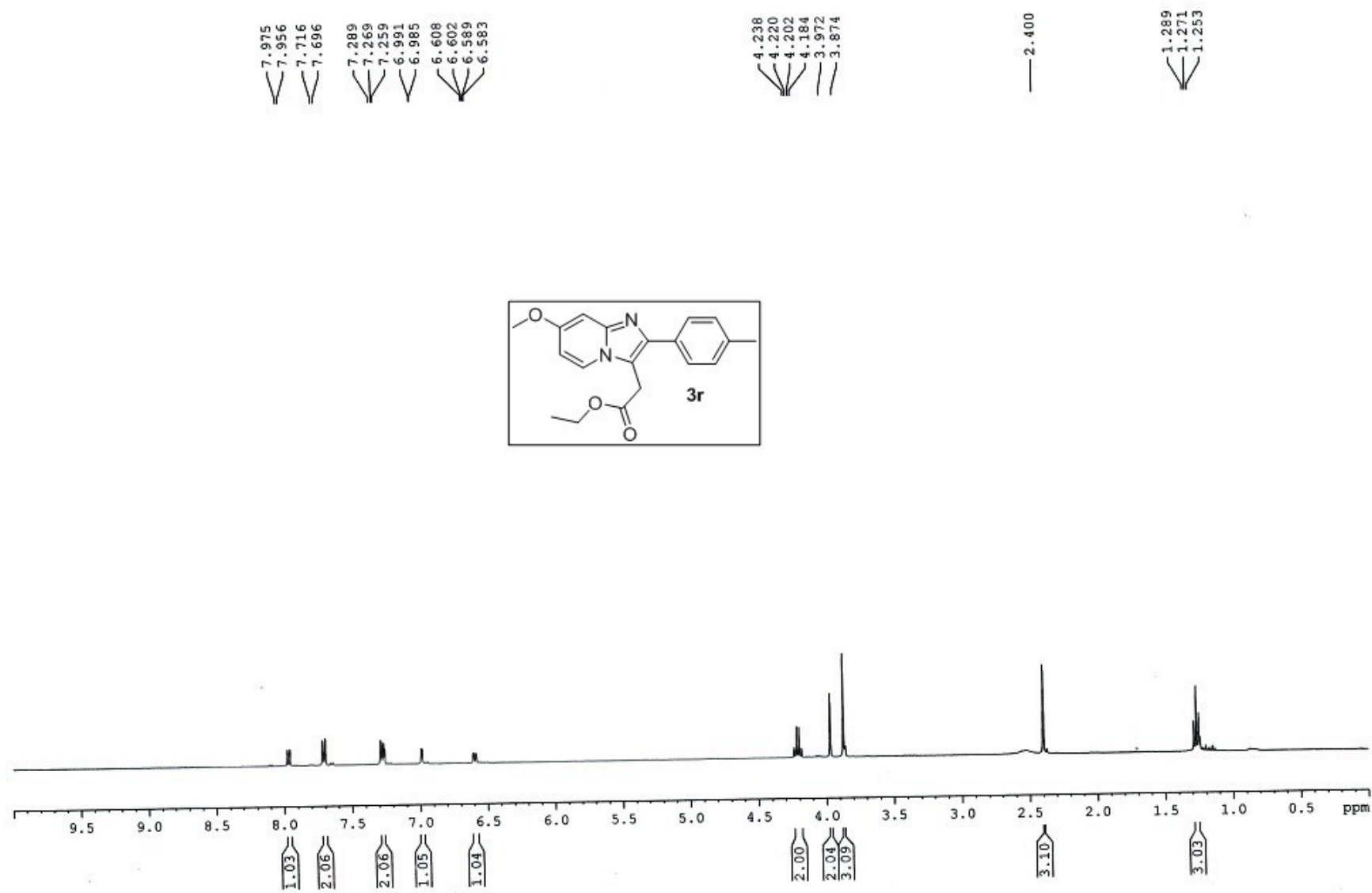
F2 - Acquisition Parameters  
 Date\_ 20191019  
 Time\_ 10.48  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 120  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

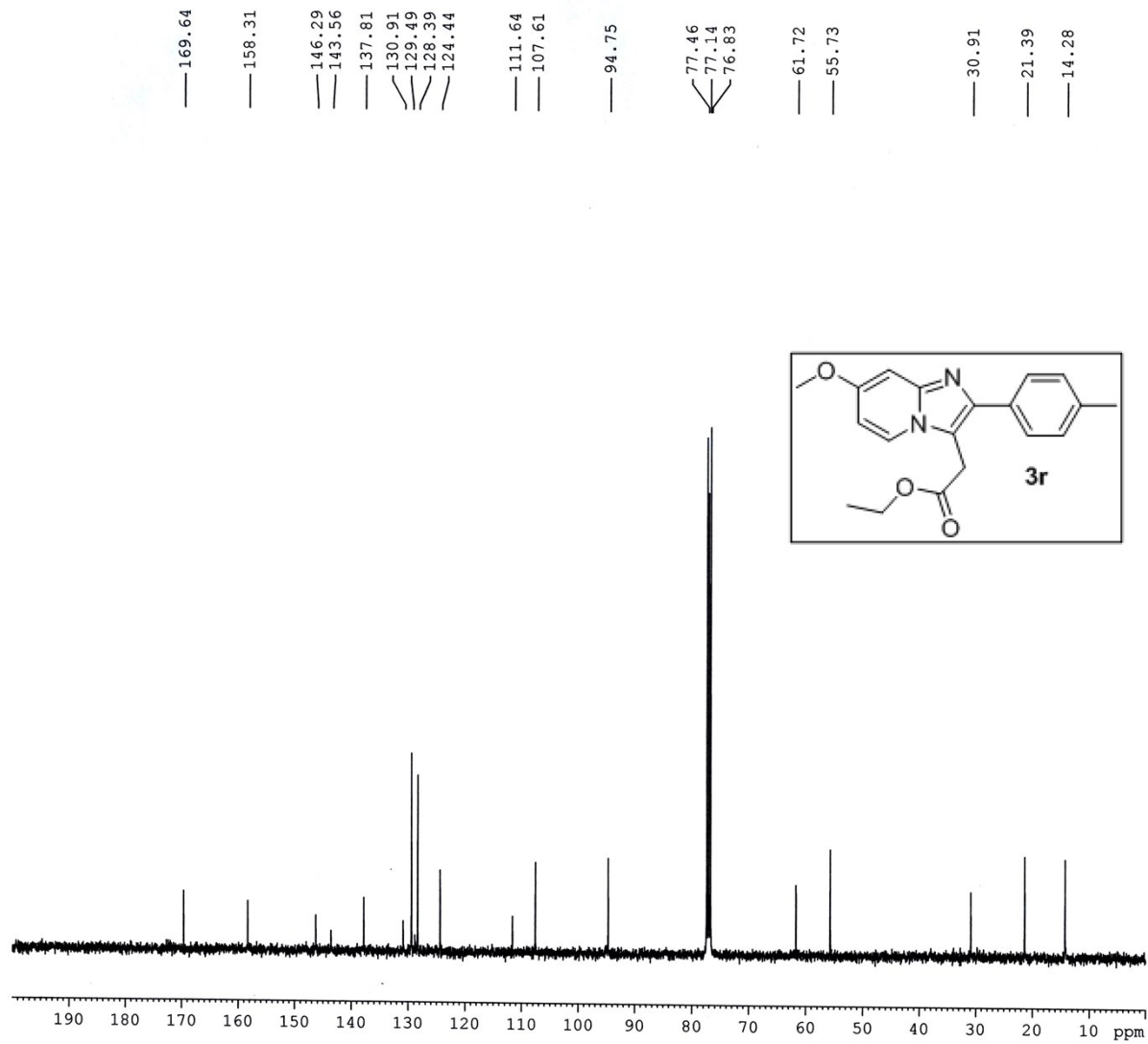
----- CHANNEL f1 -----  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

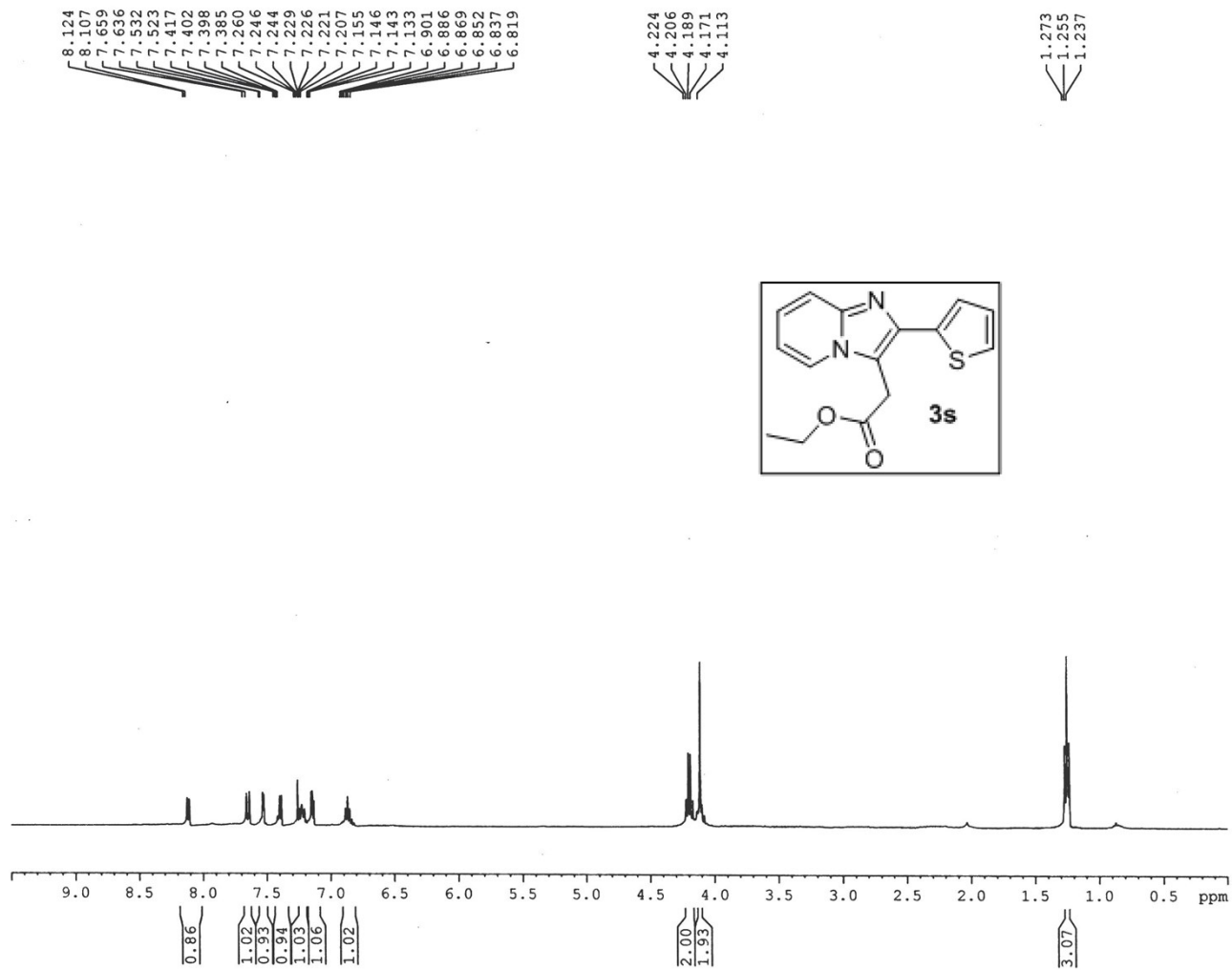
----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPDZ 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

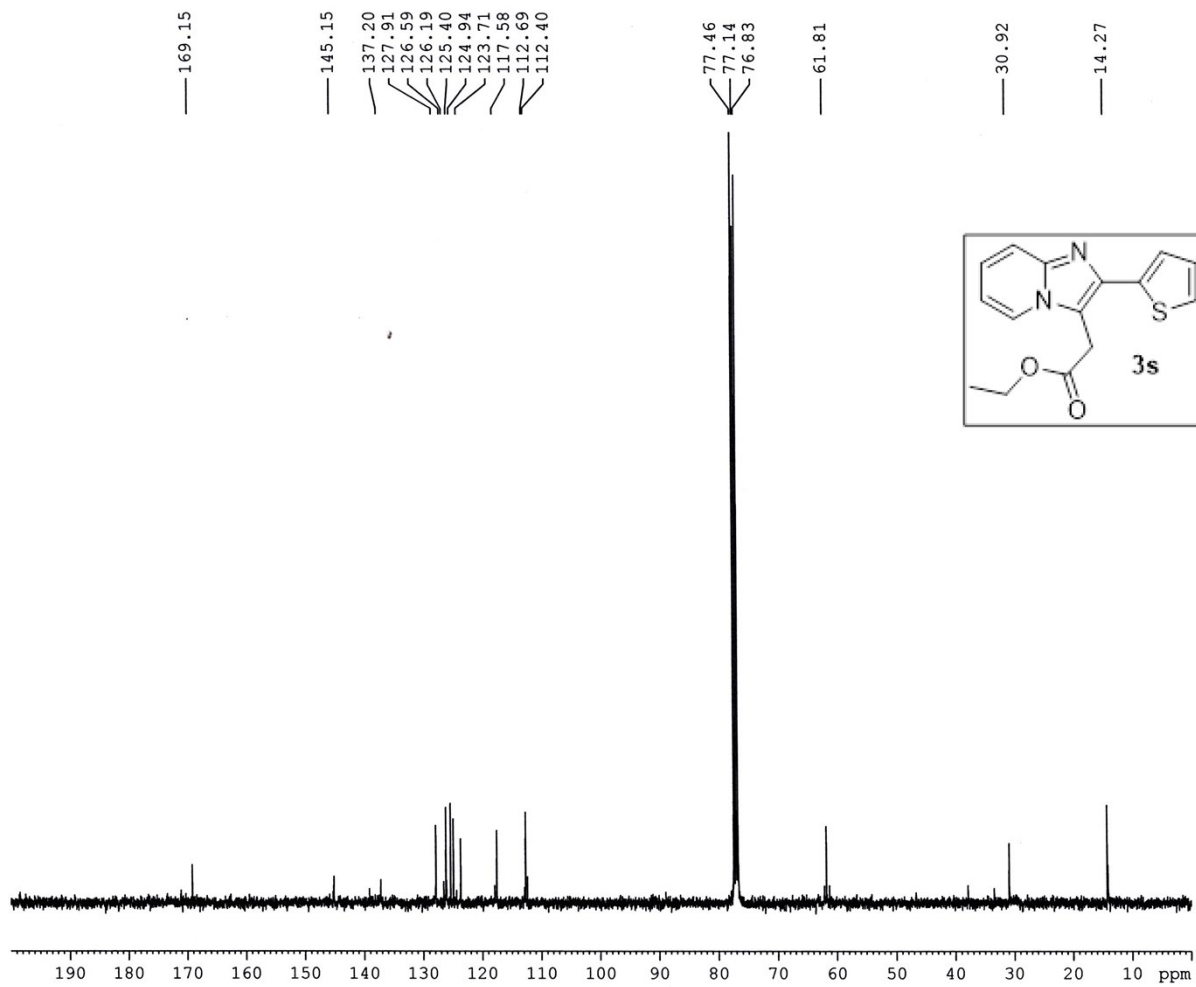
F2 - Processing parameters  
 SI 16384  
 SF 100.6177932 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

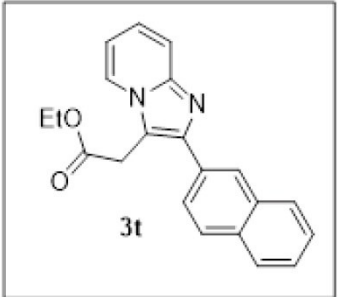
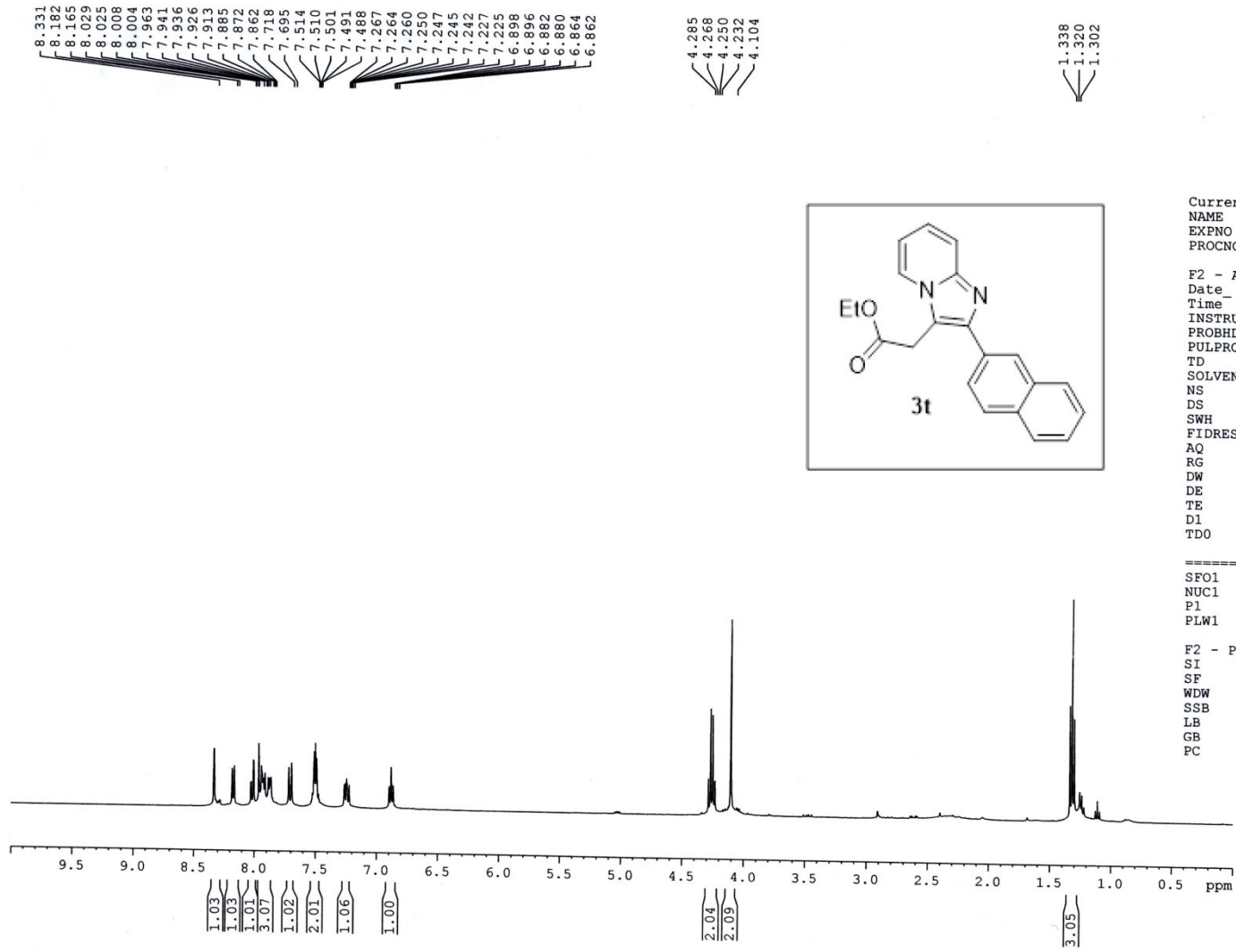










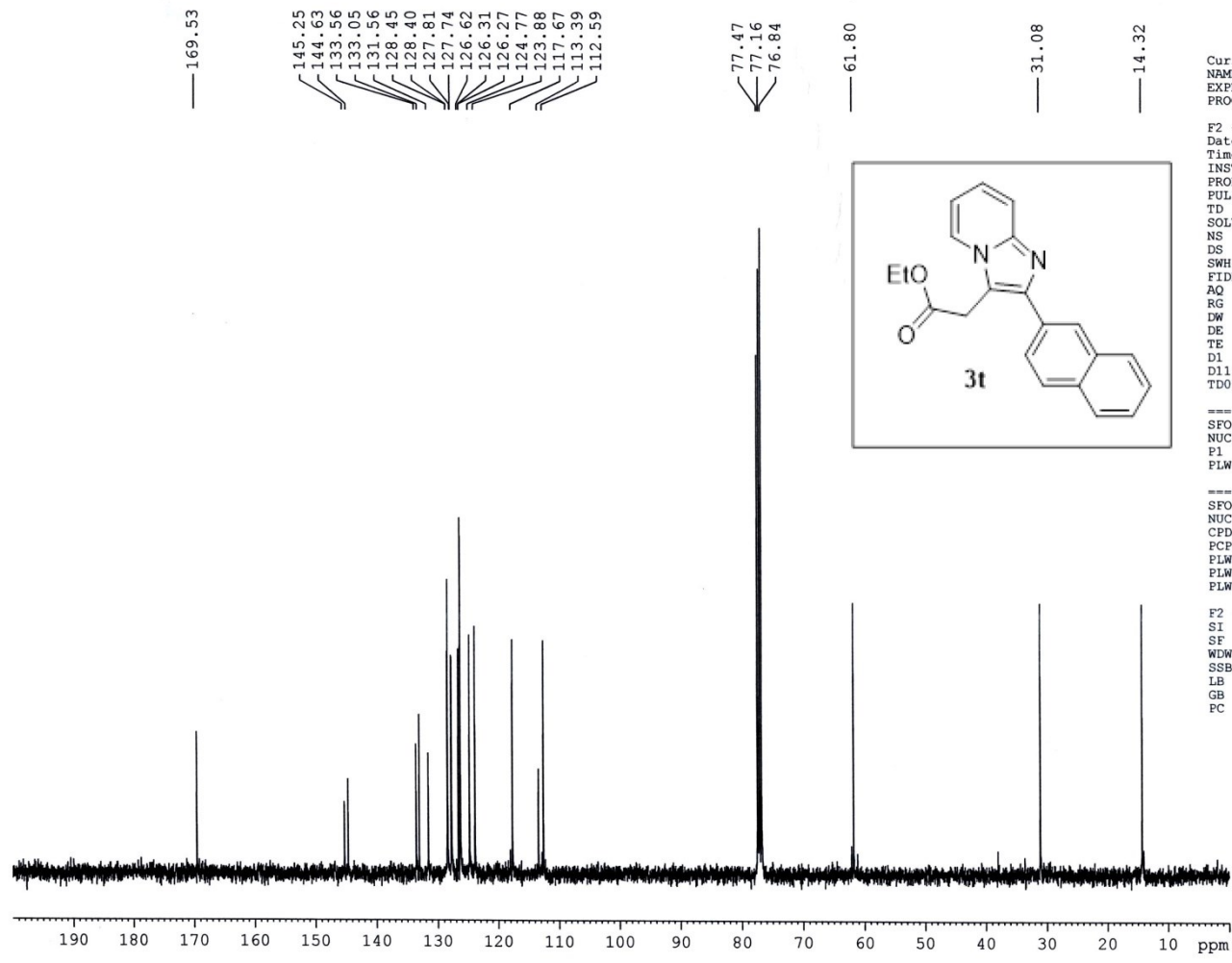


Current Data Parameters  
 NAME Dr. A HAJRA 2019 1H  
 EXPNO 874  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20191017  
 Time\_ 17.25  
 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 67.81  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.1 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 400.1500092 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00



169.53  
 145.25  
 144.63  
 133.56  
 133.05  
 131.56  
 128.45  
 128.40  
 127.81  
 127.74  
 126.62  
 126.31  
 126.27  
 124.77  
 123.88  
 117.67  
 113.39  
 112.59  
 77.47  
 77.16  
 76.84  
 61.80  
 31.08  
 14.32



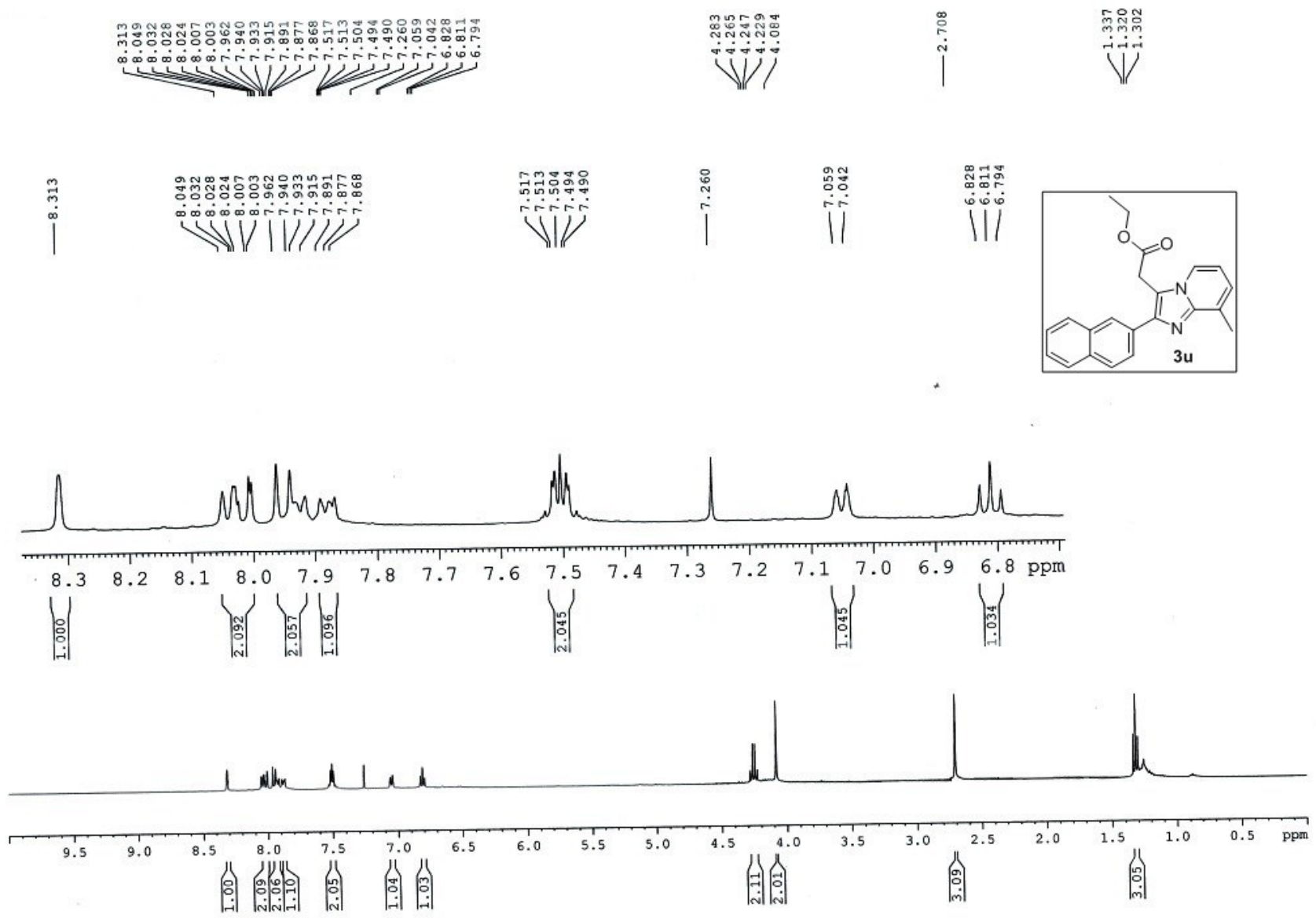
Current Data Parameters  
 NAME Dr. A HAJRA-2019-130  
 EXPNO 417  
 PROCNO 1

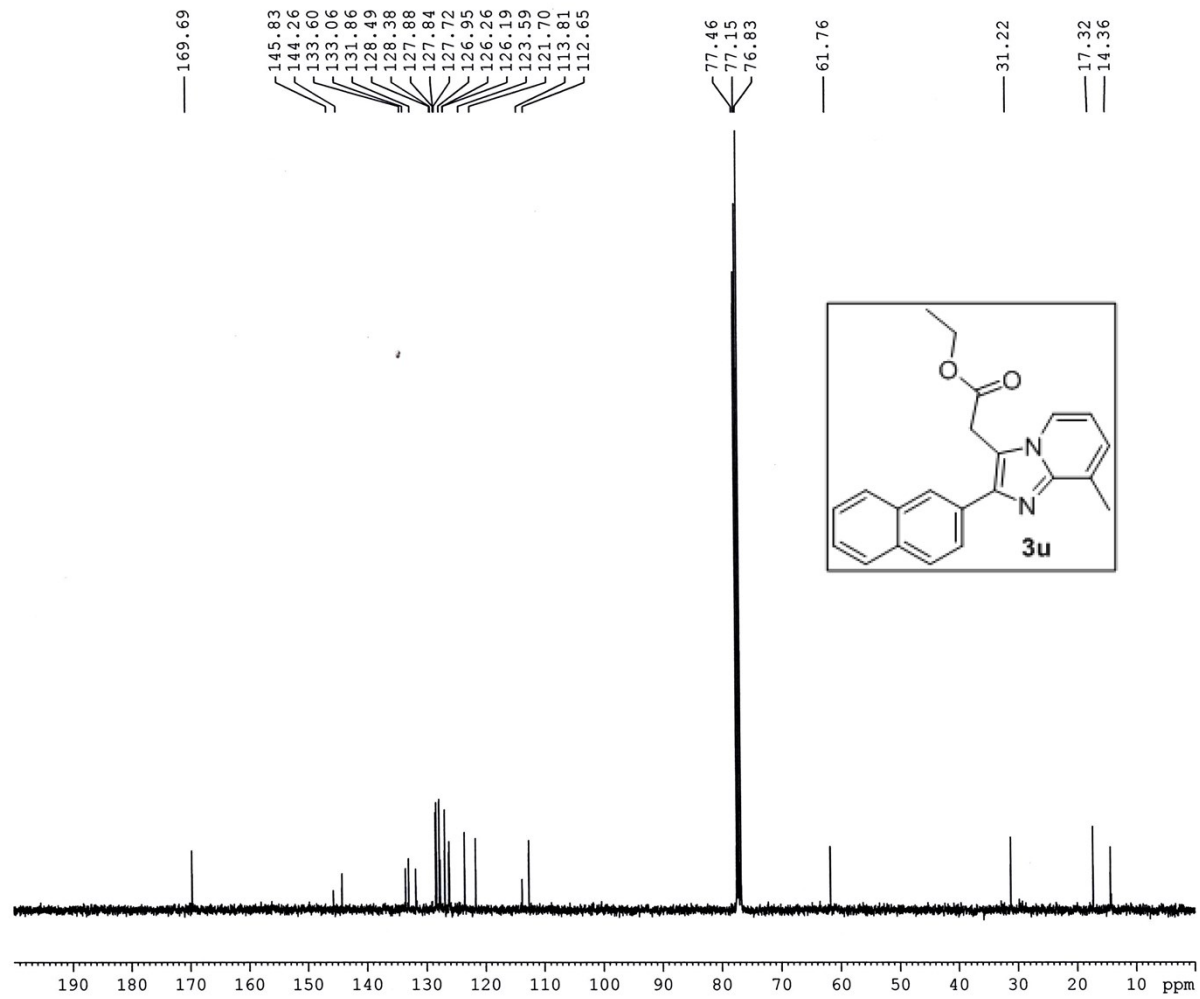
F2 - Acquisition Parameters  
 Date\_ 20191017  
 Time 17.38  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 240  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 9.90 usec  
 PLW1 54.00000000 W

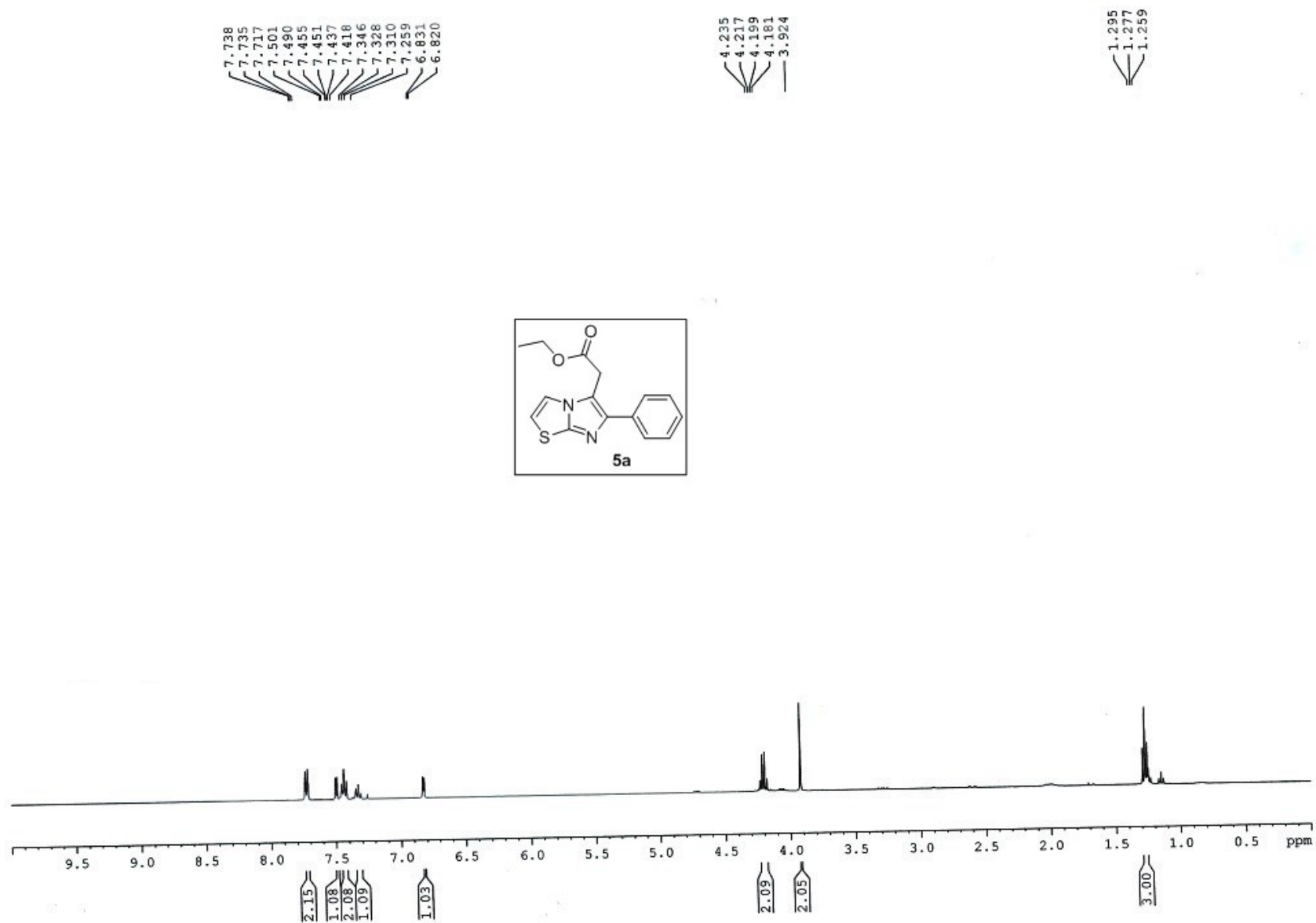
===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

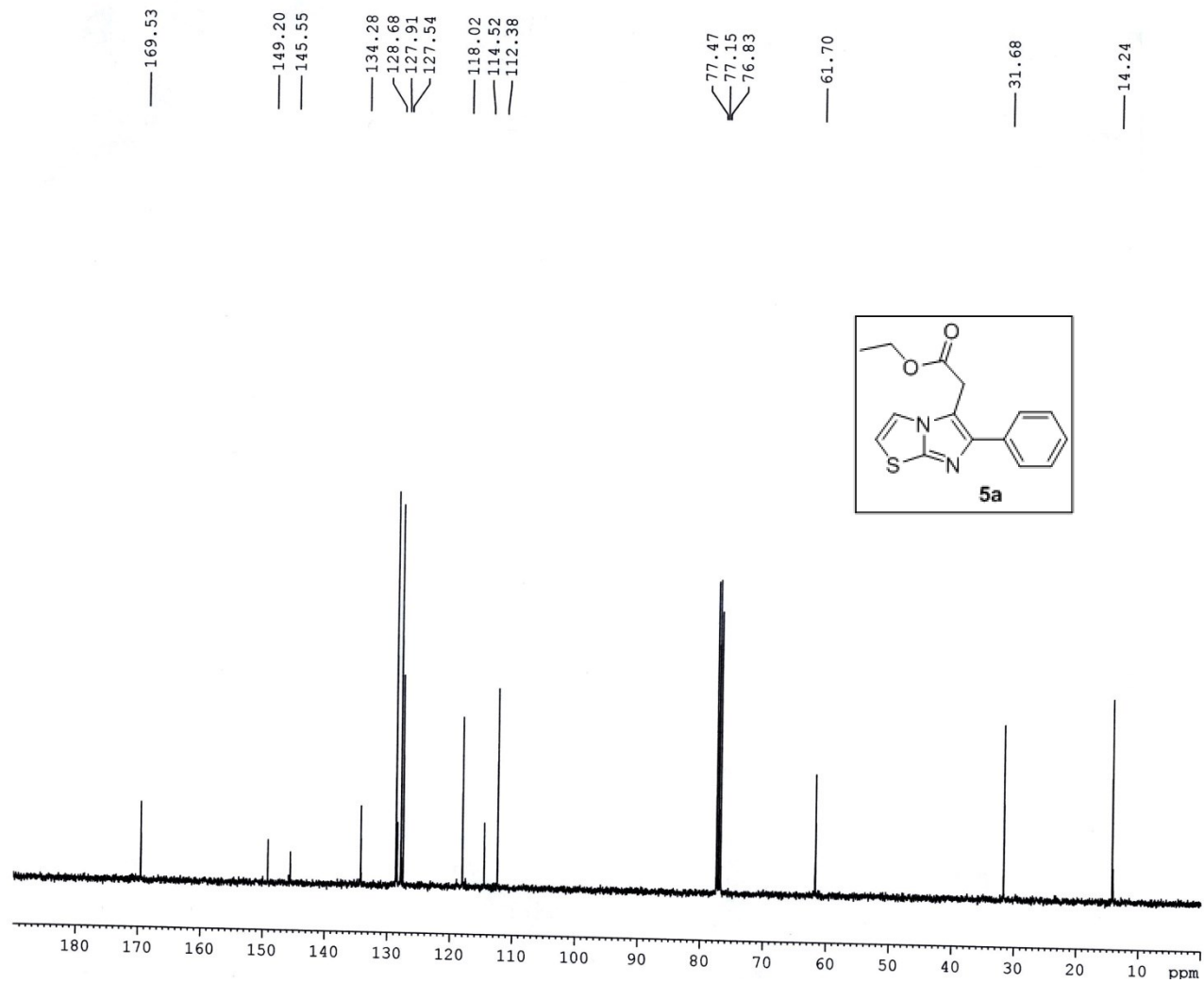
F2 - Processing parameters  
 SI 16384  
 SF 100.6177897 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

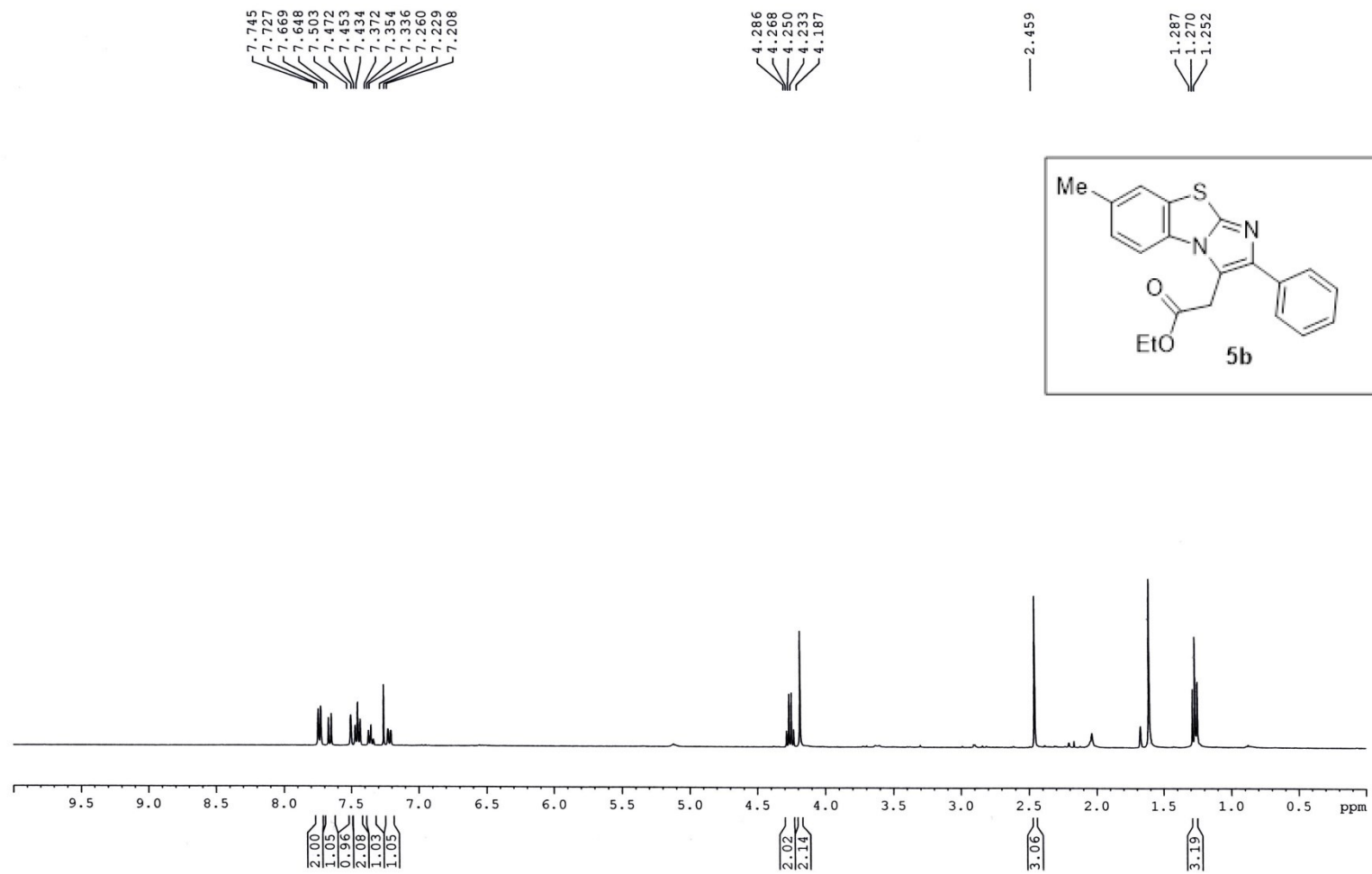


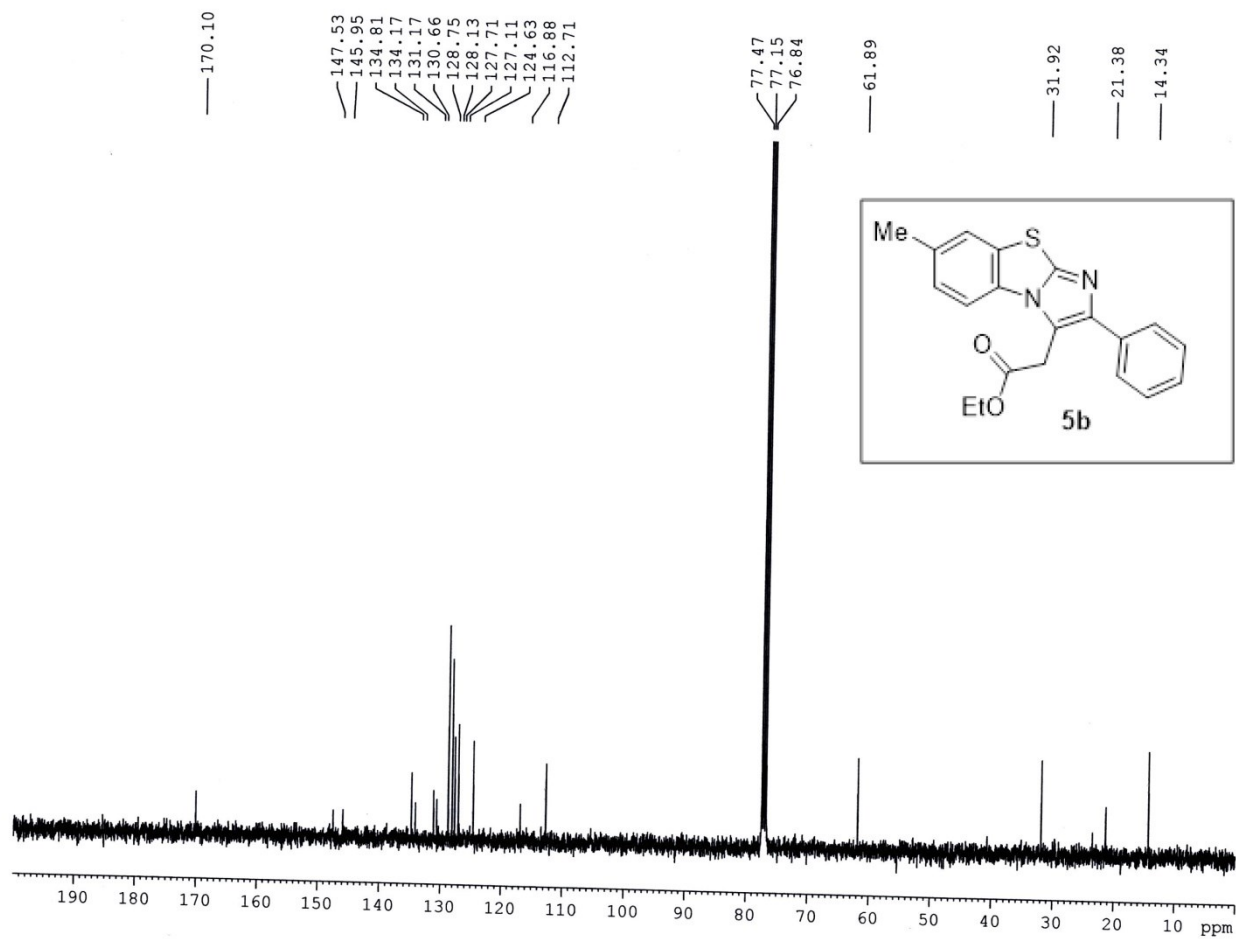












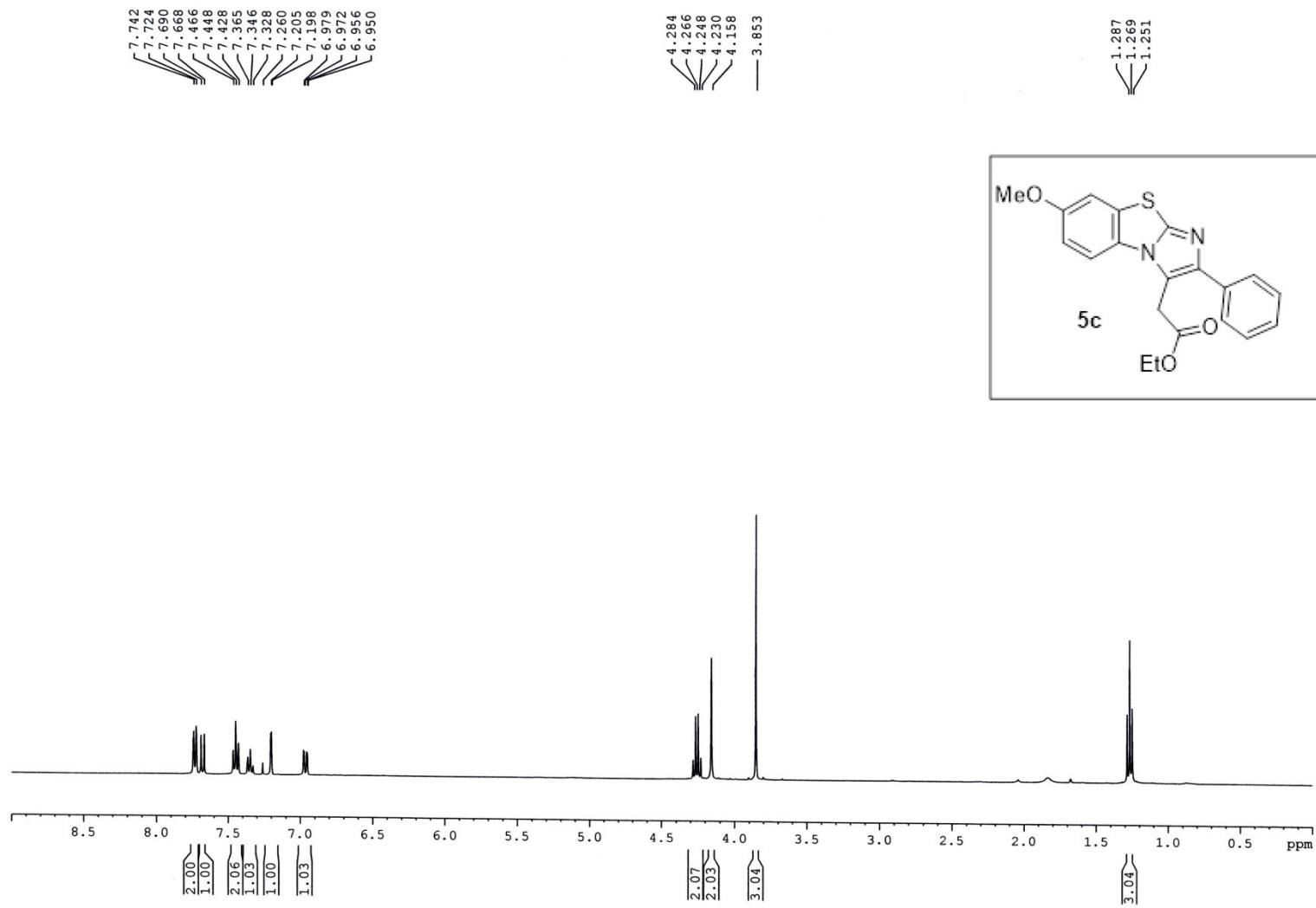
Current Data Parameters  
 NAME Dr. A HAJRA-2019-13C  
 EXPNO 484  
 PROCNO 1

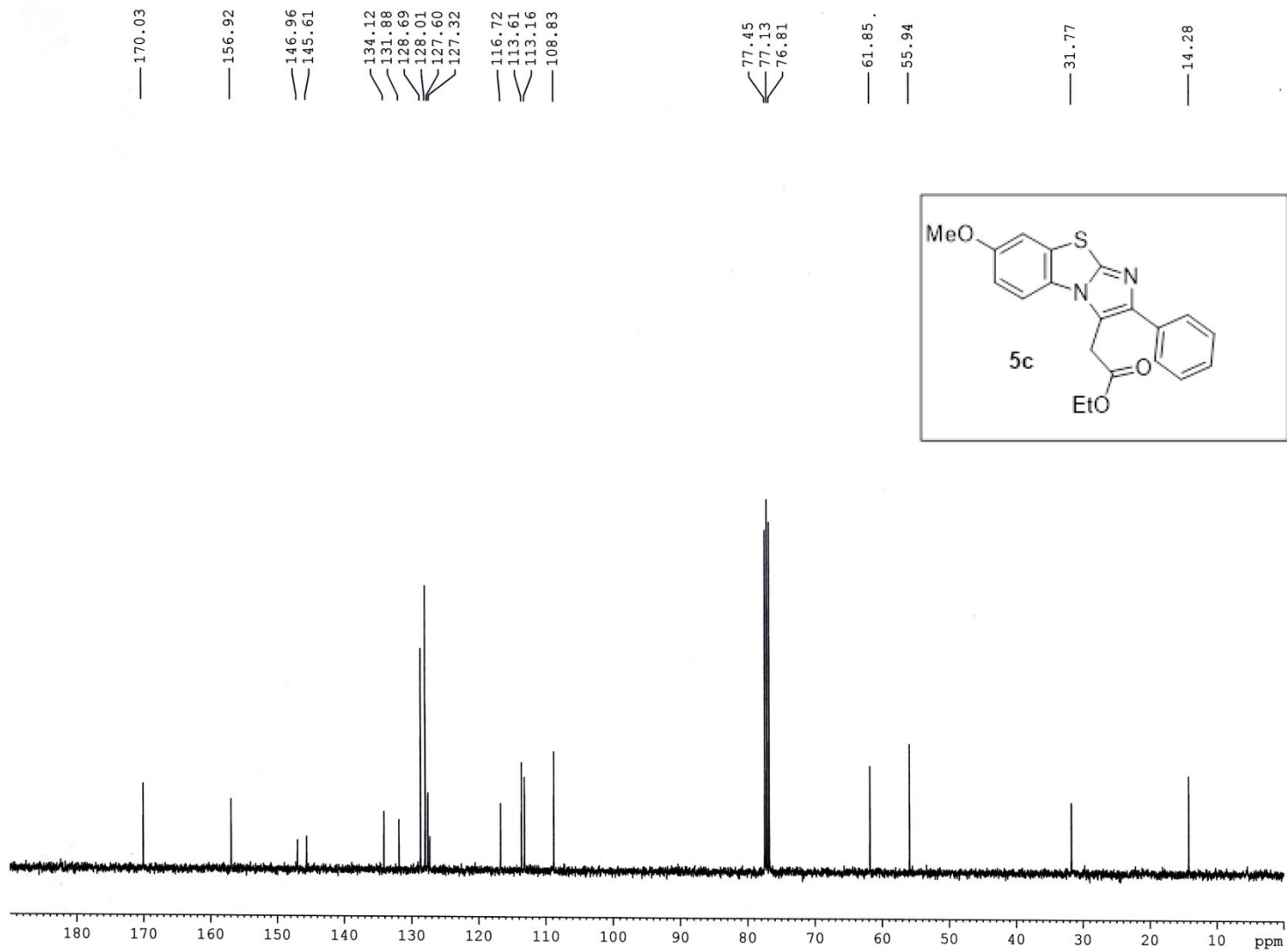
F2 - Acquisition Parameters  
 Date\_ 20191031  
 Time 21.26  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDC13  
 NS 640  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

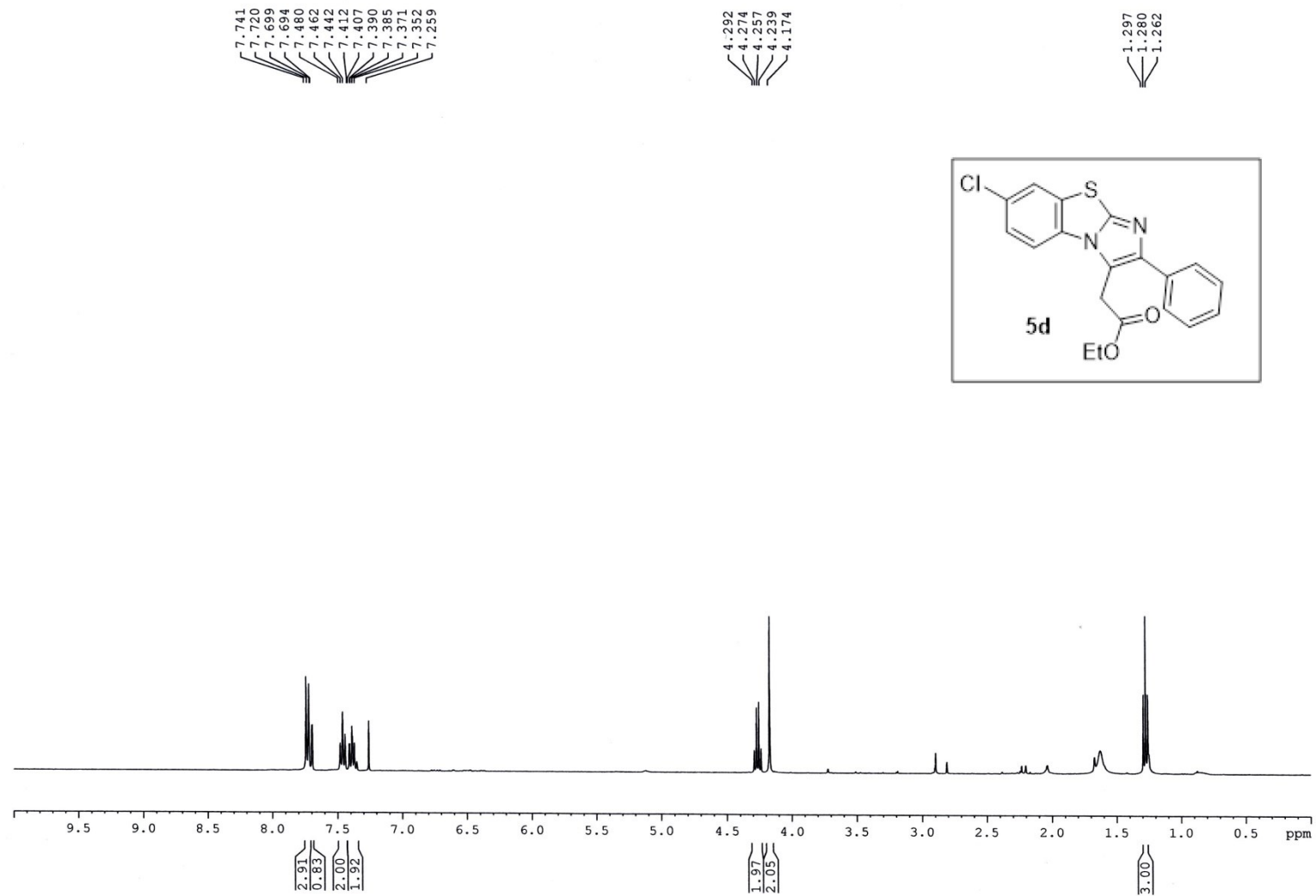
----- CHANNEL f1 -----  
 SFO1 100.6278588 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W

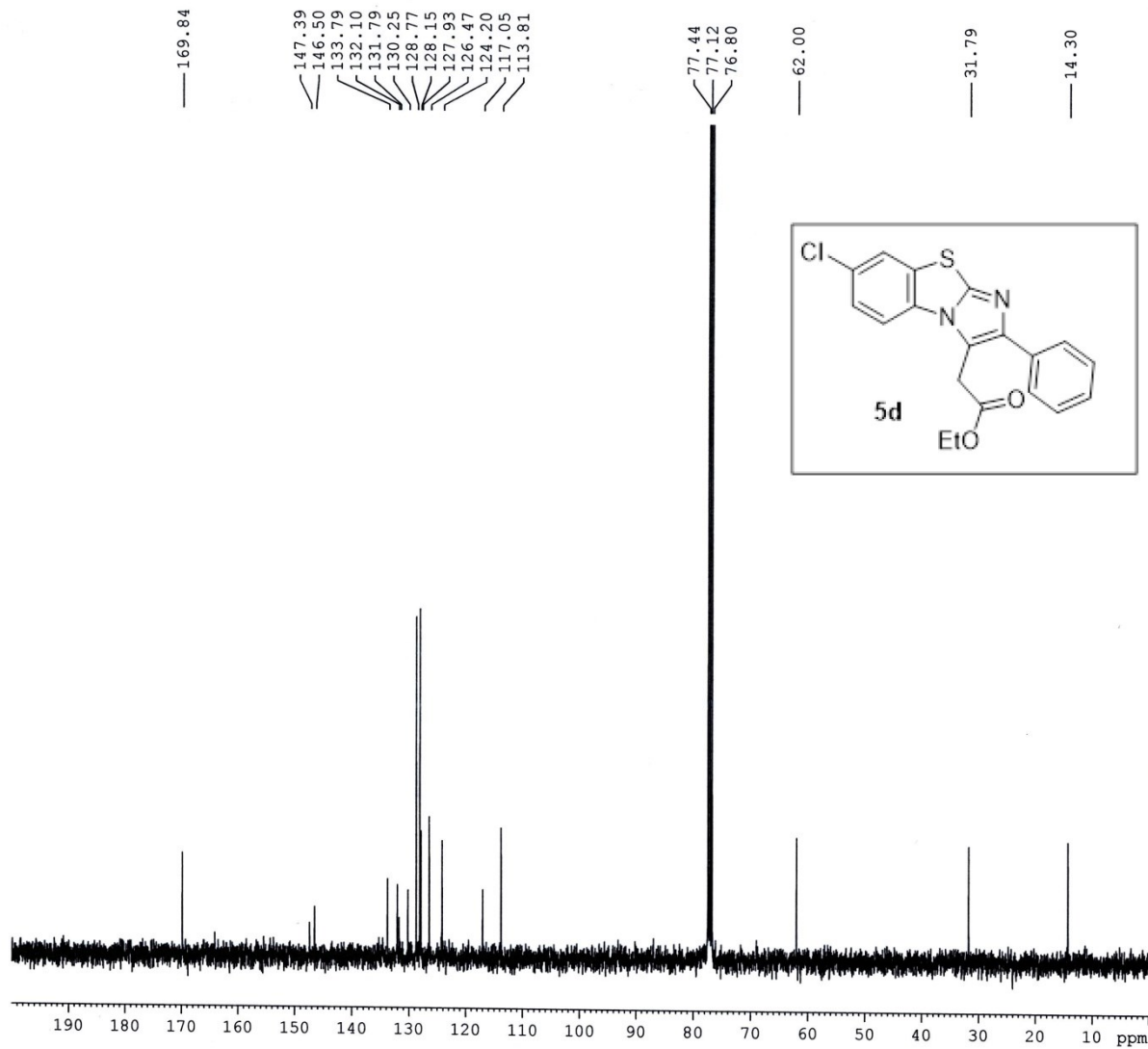
----- CHANNEL f2 -----  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177841 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40









Current Data Parameters  
 NAME Dr. A HAJRA-2019-13C  
 EXPNO 437  
 PROCNO 1

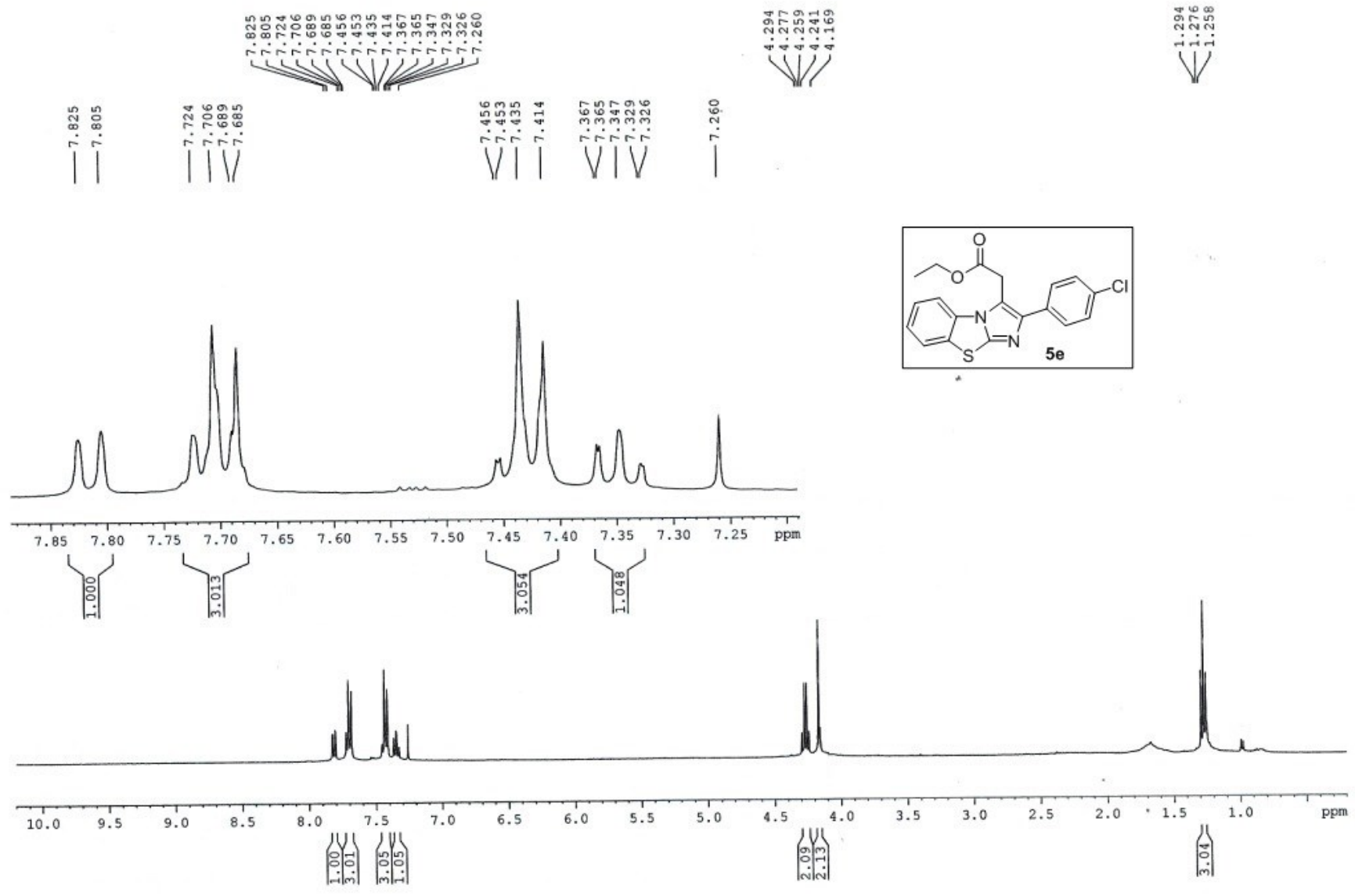
F2 - Acquisition Parameters  
 Date\_ 20191021  
 Time 18.18  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 420  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.5 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

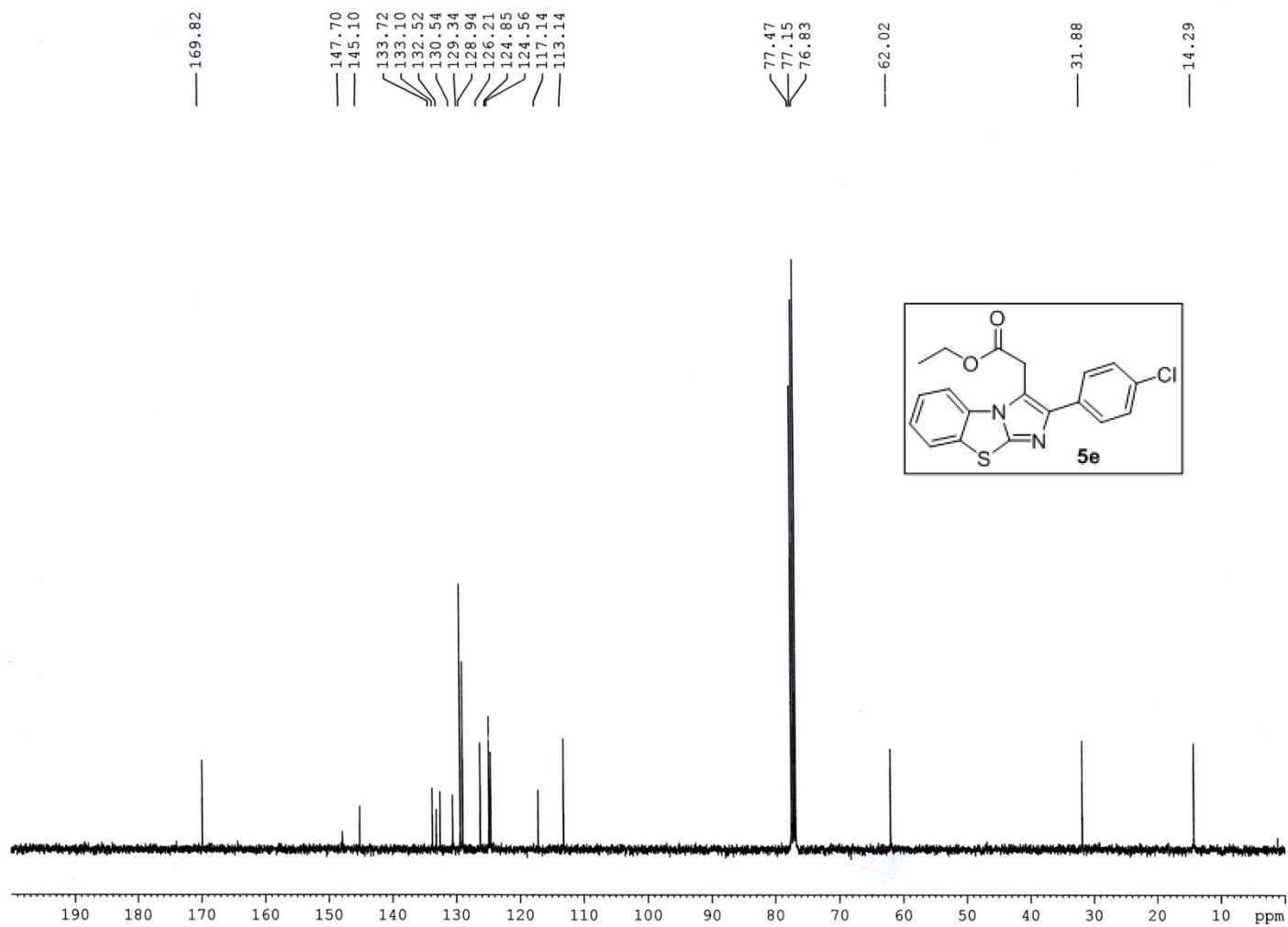
===== CHANNEL f1 =====  
 SFO1 100.6278588 MHz  
 NUC1 13c  
 P1 8.90 usec  
 PLW1 54.0000000 W

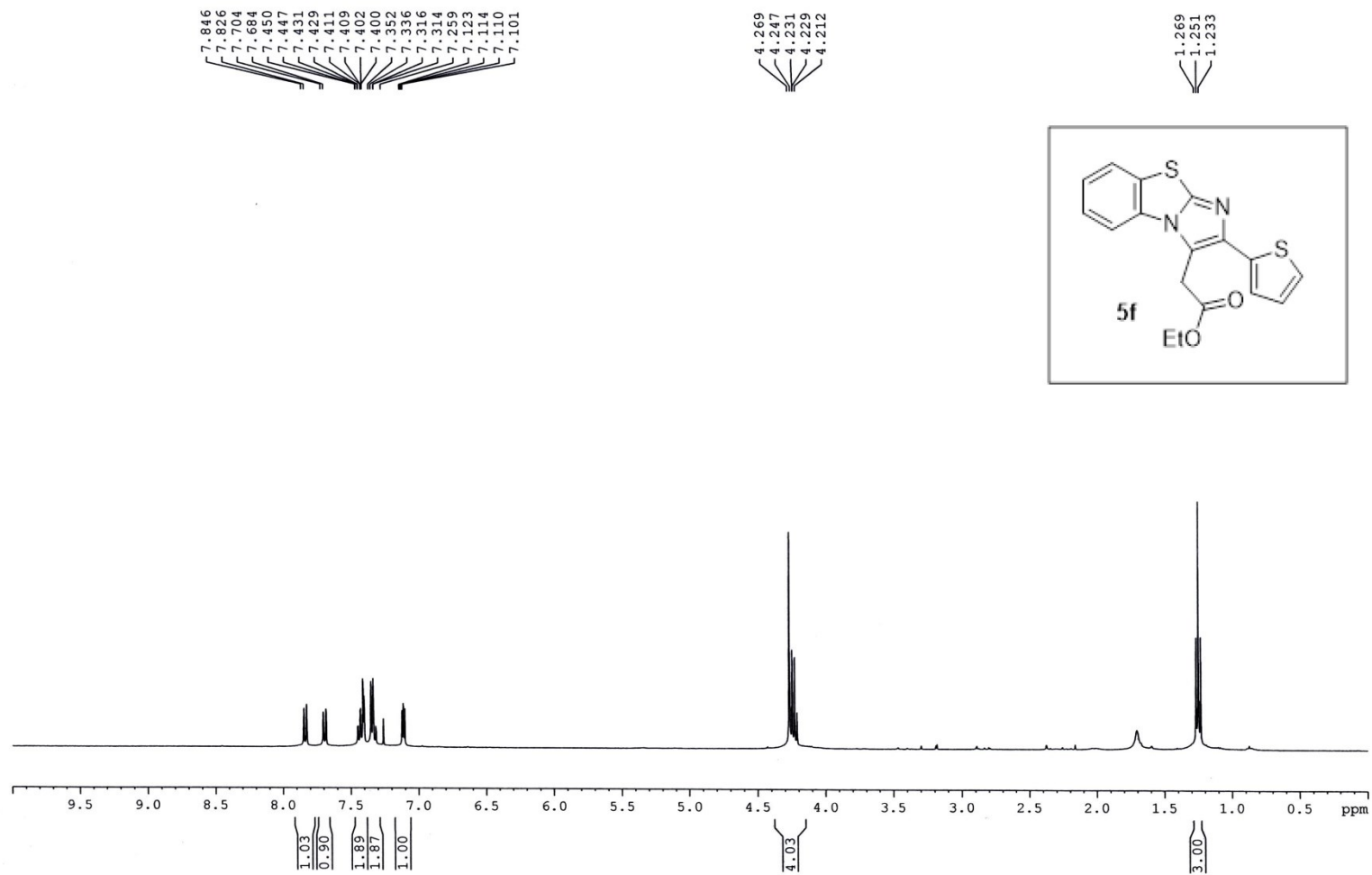
===== CHANNEL f2 =====  
 SFO2 400.1516006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

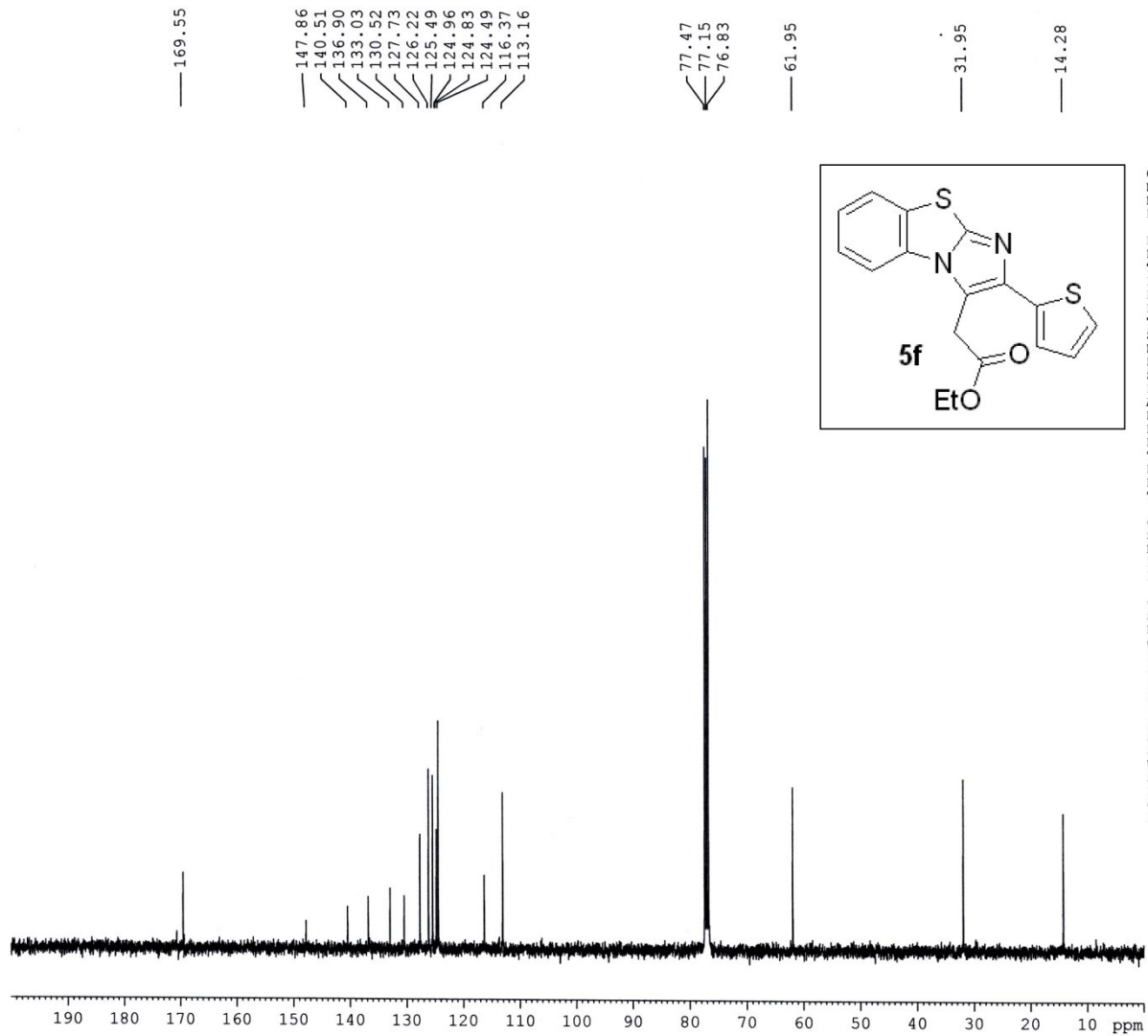
F2 - Processing parameters  
 SI 16384  
 SF 100.6177873 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40











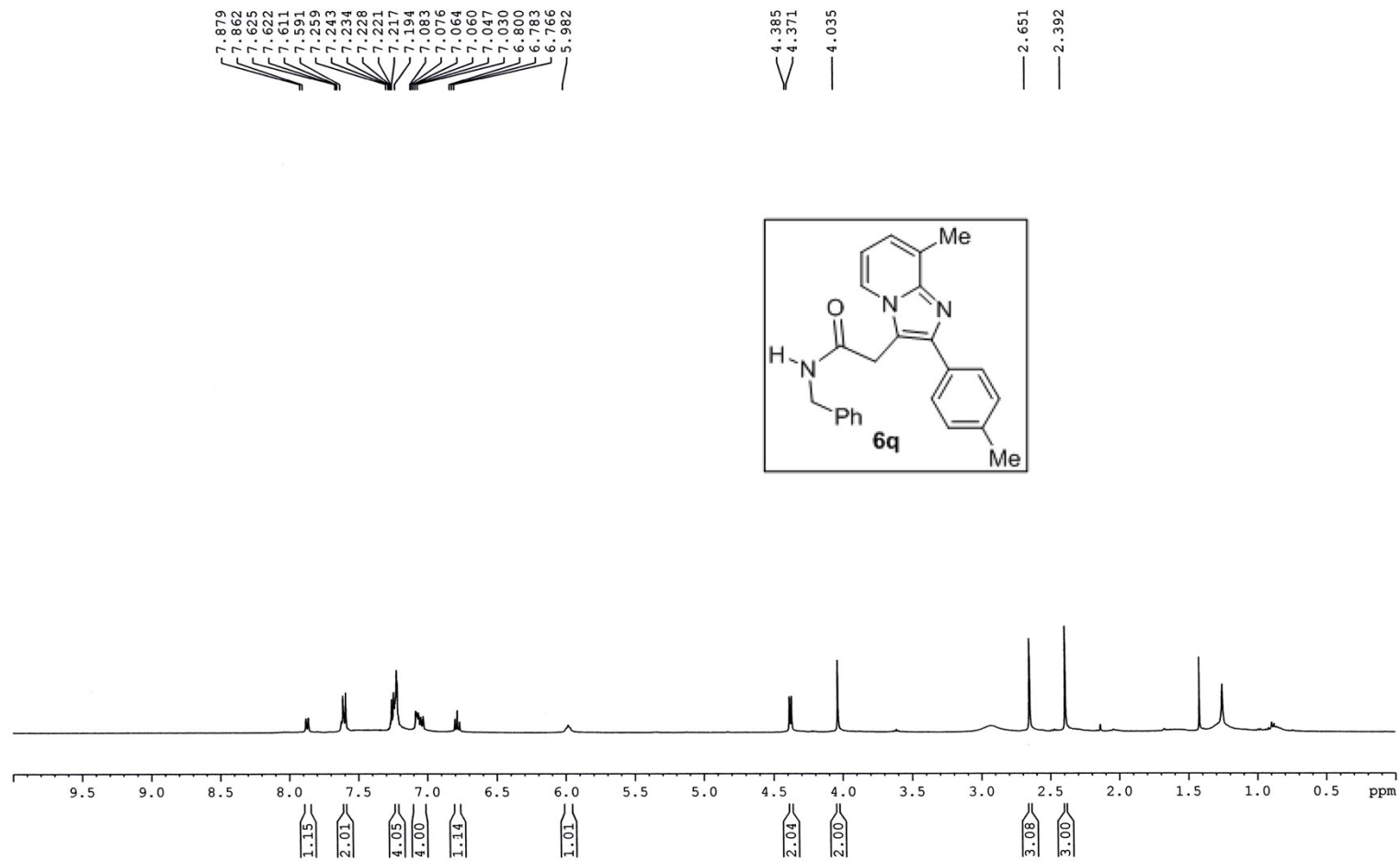
Current Data Parameters  
NAME Dr. A HAJRA-2019-13C  
EXPNO 464  
PROCNO 1

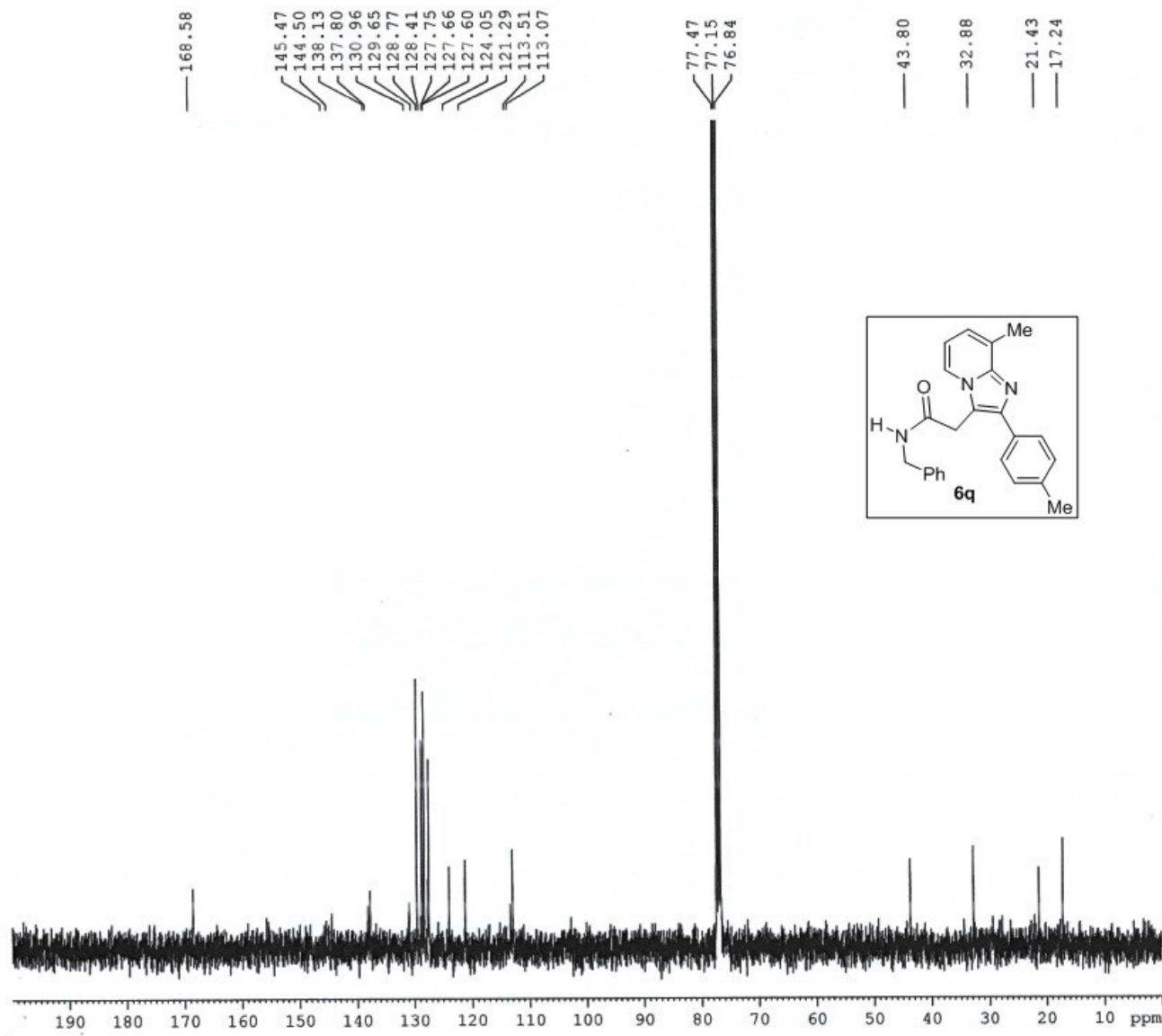
F2 - Acquisition Parameters  
Date 20191026  
Time 20.43  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 285  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 93.46  
DW 20.800 usec  
DE 6.50 usec  
TE 297.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

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

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

F2 - Processing parameters  
SI 16384  
SF 100.6177870 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





— 168.58

145.47  
144.50  
138.13  
137.80  
130.96  
129.65  
128.77  
128.41  
127.75  
127.66  
127.60  
124.05  
121.29  
113.51  
113.07

77.47  
77.15  
76.84

— 43.80

— 32.88

— 21.43

— 17.24



Current Data Parameters  
NAME Dr. A HAJRA-2020-13C  
EXPNO 109  
PROCNO 1

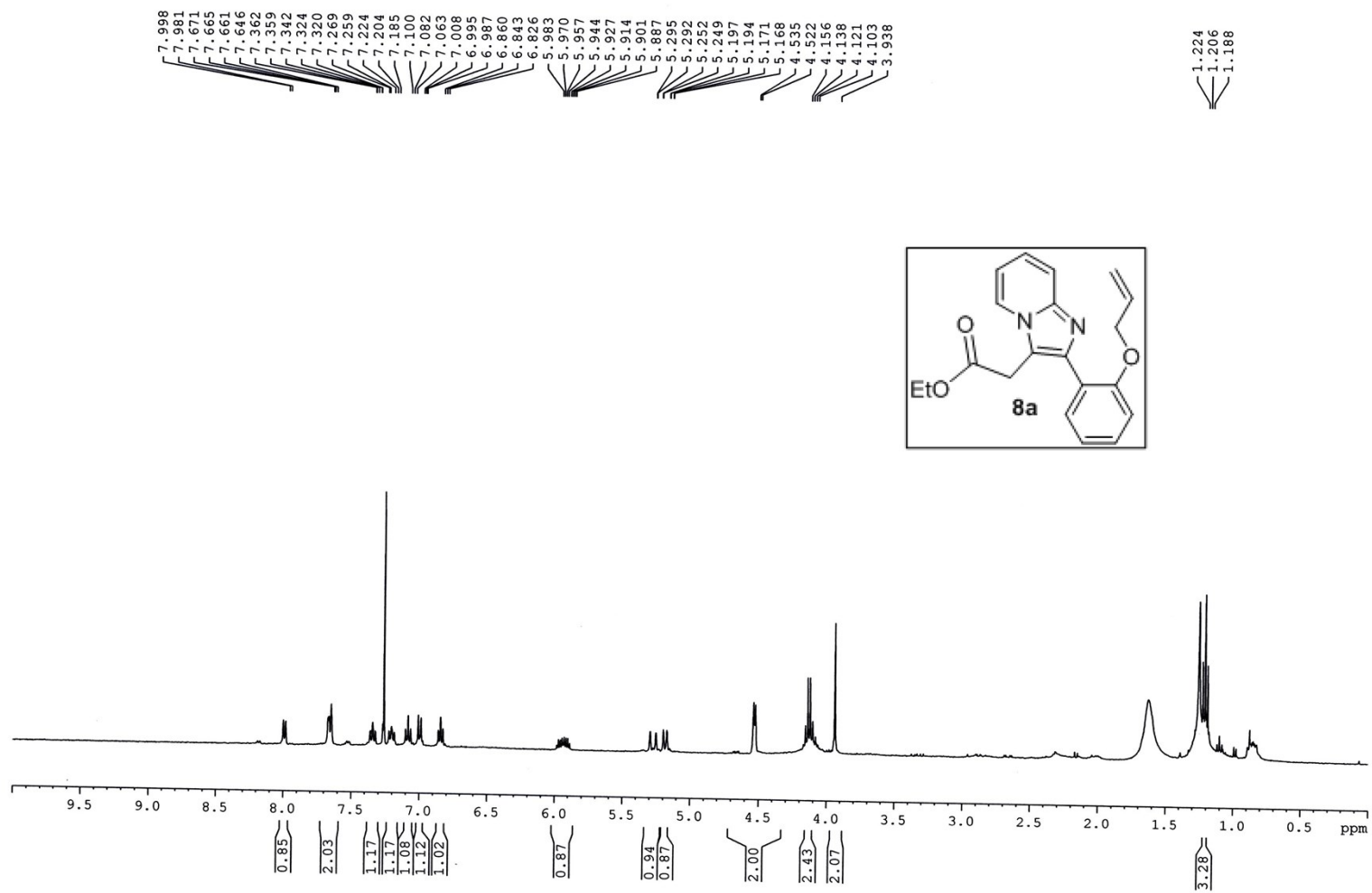
F2 - Acquisition Parameters  
Date 20200617  
Time 12.03  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 270  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 186.42  
DW 20.800 usec  
DE 6.50 usec  
TE 298.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

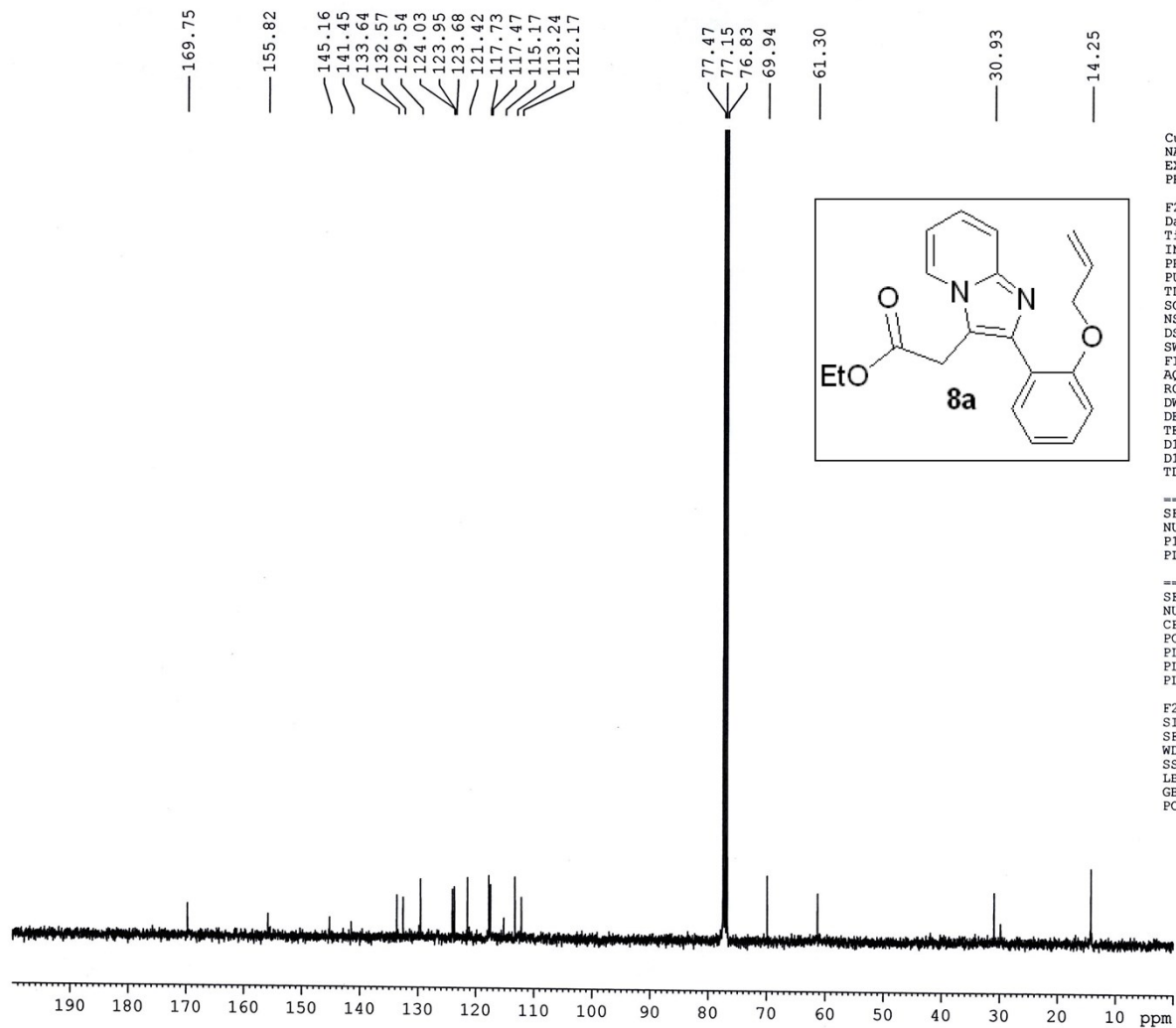
----- CHANNEL f1 -----  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W

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

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

<sup>1</sup>H of VBSB-22/REV-dwn





Current Data Parameters  
 NAME Dr. A HAJRA-2020-13C  
 EXPNO 92  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200311  
 Time 19.19  
 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 148.91  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.5 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  
 CPDPRG12 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 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