

## Supporting Information

### Catalyst-free selenylation of imidazoheterocycles

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## 1. Experimental Section

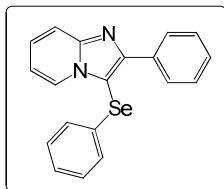
### A. General:

$^1\text{H}$  NMR spectra were determined on a Bruker 400 (400 MHz) spectrometer as solutions in  $\text{CDCl}_3$ . Chemical shifts are expressed in parts per million ( $\delta$ ) and the signals were reported as s (singlet), d (doublet), t (triplet), m (multiplet) and coupling constants  $J$  were given in Hz.  $^{13}\text{C}$  NMR spectra were recorded at 100 MHz in  $\text{CDCl}_3$  solution. Chemical shifts are expressed in parts per million ( $\delta$ ) and are referenced to  $\text{CDCl}_3$  ( $\delta = 7.16$  for  $^1\text{H}$  and  $\delta = 77.16$  for  $^{13}\text{C}$  NMR) as internal standard. TLC was done on silica gel coated glass slide (Merck, Silica gel G for TLC). All solvents were dried and distilled before use. Commercially available substrates were freshly distilled before the reaction. Solvents, reagents and chemicals were purchased from Aldrich, Fluka, Merck, SRL, Spectrochem and Process Chemicals. All reactions involving moisture sensitive reactants were executed using oven dried glassware. All the imidazoheterocycles were prepared by our reported methods.<sup>1,2</sup>

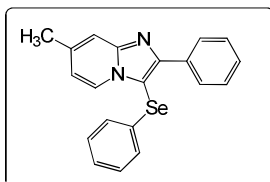
### B. Typical Experimental Procedure:

A 1:3 mixture of polyethylene glycol (PEG 400) and water ( $\text{H}_2\text{O}$ ) (2 mL) was added to a mixture of 2-phenylimidazo[1,2-*a*]pyridine (39 mg, 0.2 mmol), and phenylselenenyl bromide (52 mg, 0.22 mmol) and the mixture was stirred at room temperature for 3 h. Then the reaction mixture was extracted with ethyl acetate. After evaporation of solvent under reduced pressure the crude residue was obtained which was purified by column chromatography on silica gel (60-120 mesh) using petroleum ether:ethylacetate = 9:1 as an eluent to afford the pure product (**3a**) (66 mg, 95%) as a light yellow solid, mp: 48-49 °C.

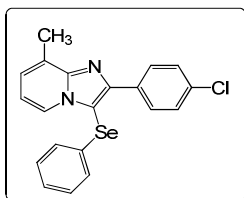
### C. Characterization Data of the synthesized compounds:



**2-Phenyl-3-(phenylselenenyl)imidazo[1,2-*a*]pyridine (3a):** Yellow solid (66 mg, 95%), mp: 48-49 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.25 (d,  $J$  = 8.4 Hz, 1H), 8.08-8.05 (m, 2H), 7.64 (d,  $J$  = 9.2 Hz, 1H), 7.37-7.33 (m, 2H), 7.30-7.26 (m, 1H), 7.23-7.19 (m, 1H), 7.09-7.05 (m, 3H), 7.02-7.00 (m, 2H), 6.77-6.73 (m, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  151.7, 147.7, 133.7, 130.9, 129.7, 128.8, 128.6, 128.4, 128.3, 126.8, 126.6, 125.7, 117.5, 113.1, 103.0; Anal. Calcd for  $\text{C}_{19}\text{H}_{14}\text{N}_2\text{Se}$ : C, 65.33; H, 4.04; N, 8.02%. Found C, 65.14; H, 3.87; N, 7.86%.

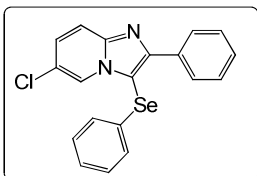


**7-Methyl-2-phenyl-3-(phenylselenenyl)imidazo[1,2-*a*]pyridine (3b):** Yellow solid (68 mg, 93%), mp: 99-101 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.11-8.04 (m, 3H), 7.38-7.24 (m, 4H), 7.08-6.98 (m, 5H), 6.57-6.55 (m, 1H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  151.7, 148.1, 137.7, 133.9, 131.2, 129.7, 128.7, 128.4, 128.3, 128.2, 126.6, 124.8, 116.0, 115.7, 102.0, 21.4; Anal. Calcd for  $\text{C}_{20}\text{H}_{16}\text{N}_2\text{Se}$ : C, 66.12; H, 4.44; N, 7.71%. Found C, 66.04; H, 4.30; N, 7.54%.

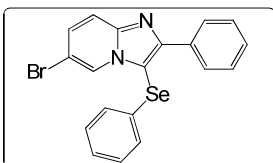


**2-(4-Chlorophenyl)-8-methyl-3-(phenylselenenyl)imidazo[1,2-*a*]pyridine (3c):** White solid (76 mg, 96%), mp: 82-83 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.12 (d,  $J$  = 6.8 Hz, 1H), 8.01 (d,  $J$  = 8.4 Hz, 2H), 7.30 (d,  $J$  = 8.4 Hz, 2H), 7.09-7.05 (m, 3H), 7.03-6.97 (m, 3H), 6.68 (t,  $J$  = 6.8 Hz, 1H), 2.61 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  150.0, 147.9, 134.4, 132.3,

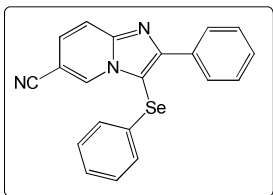
130.8, 130.2, 129.8, 128.5, 128.3, 127.6, 126.8, 125.8, 123.5, 113.3, 103.5, 17.0; Anal. Calcd for C<sub>20</sub>H<sub>15</sub>ClN<sub>2</sub>Se: C, 60.39; H, 3.80; N, 7.04%. Found C, 60.24; H, 3.69; N, 6.89%.



**6-Chloro-2-phenyl-3-(phenylselenenyl)imidazo[1,2-*a*]pyridine (3d):** Yellow solid (67 mg, 87%), mp: 89-91 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.32 (s, 1H), 8.07-8.05 (m, 2H), 7.59 (d, *J* = 9.6 Hz, 1H), 7.38-7.34 (m, 2H), 7.32-7.30 (m, 1H), 7.20 (s, 1H), 7.13-7.09 (m, 3H), 7.04-7.01 (m, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 152.5, 146.0, 133.3, 130.4, 129.9, 128.8, 128.8, 128.5, 128.0, 127.9, 127.1, 123.7, 121.6, 117.9, 103.9; Anal. Calcd for C<sub>19</sub>H<sub>13</sub>ClN<sub>2</sub>Se: C, 59.47; H, 3.41; N, 7.30%. Found C, 59.34; H, 3.22; N, 7.14%.

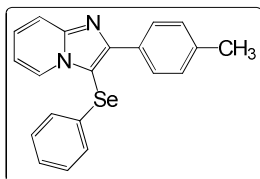


**6-Bromo-2-phenyl-3-(phenylselenenyl)imidazo[1,2-*a*]pyridine (3e):** Brown solid (76 mg, 89%), mp: 118-120 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.42 (s, 1H), 8.06 (d, *J* = 7.6 Hz, 2H), 7.53 (d, *J* = 9.2 Hz, 1H), 7.37-7.27 (m, 4H), 7.18-7.10 (m, 3H), 7.03-7.01 (m, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 152.2, 146.1, 133.2, 131.0, 130.4, 130.2, 129.9, 128.9, 128.8, 128.5, 127.1, 125.9, 118.2, 108.1, 103.7; Anal. Calcd for C<sub>19</sub>H<sub>13</sub>BrN<sub>2</sub>Se: C, 53.30; H, 3.06; N, 6.54%. Found C, 53.12; H, 2.94; N, 6.39%.

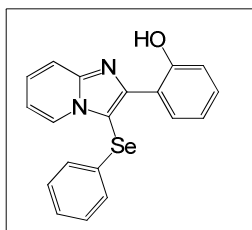


**2-Phenyl-3-(phenylselenenyl)imidazo[1,2-*a*]pyridine-6-carbonitrile (3f):** Orange solid (69 mg, 93%), mp: 114-115 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.70 (s, 1H), 8.12-8.10 (m, 2H), 7.72 (d, *J* = 9.2 Hz, 1H), 7.41-7.32 (m, 4H), 7.15-7.13 (m, 3H), 7.06-7.03 (m, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 153.6, 146.9, 132.5, 131.8, 130.1, 129.4, 128.9, 128.8, 128.6, 128.5,

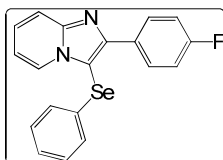
127.6, 126.5, 118.5, 116.5, 105.4, 99.4; Anal. Calcd for C<sub>20</sub>H<sub>13</sub>N<sub>3</sub>Se: C, 64.18; H, 3.50; N, 11.23%. Found C, 65.08; H, 3.34; N, 11.09%.



**3-(Phenylselenenyl)-2-(p-tolyl)imidazo[1,2-a]pyridine (3g):** Orange solid (65 mg, 89%), mp: 66-68 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.22 (d, *J* = 6.80 Hz, 1H), 7.95 (d, *J* = 8.00 Hz, 2H), 7.64 (d, *J* = 8.80 Hz, 1H), 7.20-7.14 (m, 3H), 7.07-6.98 (m, 3H), 6.99 (t, *J* = 5.20 Hz, 2H), 6.73-6.70 (m, 1H), 2.28 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 151.8, 147.6, 138.4, 130.9, 130.7, 129.7, 129.1, 128.7, 128.2, 126.7, 126.6, 125.6, 117.4, 113.0, 102.6, 21.4; Anal. Calcd for C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>Se: C, 66.12; H, 4.44; N, 7.71%. Found C, 66.03; H, 4.29; N, 7.59%.

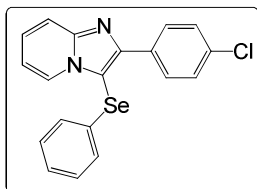


**2-(3-(phenylselenenyl)imidazo[1,2-a]pyridin-2-yl)phenol (3h):** Brown solid (63 mg, 86%), mp: 64-66 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 12.91 (brs, 1H), 8.54 (d, *J* = 7.6 Hz, 1H), 8.34 (d, *J* = 6.8 Hz, 1H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.27-7.23 (m, 1H), 7.21-7.15 (m, 1H), 7.10-7.00 (m, 5H), 6.97 (d, *J* = 8.0 Hz, 1H), 6.85-6.75 (m, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 158.5, 149.4, 145.4, 130.6, 130.4, 129.8, 128.5, 128.1, 127.3, 127.0, 125.4, 118.7, 117.8, 116.6, 116.5, 113.7, 101.8; Anal. Calcd for C<sub>19</sub>H<sub>14</sub>N<sub>2</sub>OSe: C, 62.47; H, 3.86; N, 7.67%. Found C, 62.34; H, 3.79; N, 7.50%.

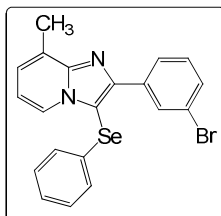


**2-(4-Fluorophenyl)-3-(phenylselenenyl)imidazo[1,2-a]pyridine (3i):** Yellow solid (67 mg, 91%), mp: 68-70 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.23 (d, *J* = 8.0 Hz, 1H), 8.06-8.01 (m, 2H), 7.62 (d, *J* = 9.2 Hz, 1H), 7.22-7.18 (m, 1H), 7.09-6.96 (m, 7H), 6.76-6.72 (m, 1H); <sup>13</sup>C

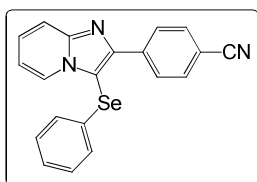
NMR (CDCl<sub>3</sub>, 100 MHz):  $\delta$  163.0 (d,  $J_{\text{C-F}} = 247$  Hz), 150.8, 147.7, 130.7, 130.6, 130.5, 129.8 (d,  $J_{\text{C-F}} = 3$  Hz), 129.8, 128.2, 126.8 (d,  $J_{\text{C-F}} = 8$  Hz), 125.6, 117.4, 115.3 (d,  $J_{\text{C-F}} = 22$  Hz), 113.2, 102.7; Anal. Calcd for C<sub>19</sub>H<sub>13</sub>FN<sub>2</sub>Se: C, 62.13; H, 3.57; N, 7.63%. Found C, 62.01; H, 3.41; N, 7.50%.



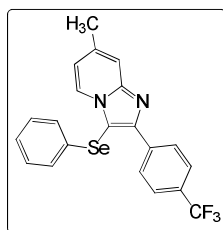
**2-(4-Chlorophenyl)-3-(phenylselenenyl)imidazo[1,2-*a*]pyridine (3j):** Yellow solid (74 mg, 97%), mp: 82-84 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz):  $\delta$  8.25-8.23 (m, 1H), 8.03-8.00 (m, 2H), 7.64-7.62 (m, 1H), 7.33-7.28 (m, 2H), 7.23-7.19 (m, 1H), 7.09-7.05 (m, 3H), 7.01-6.96 (m, 2H), 6.77-6.74 (m, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz):  $\delta$  150.4, 147.7, 134.5, 132.2, 130.6, 130.0, 129.8, 128.6, 128.3, 126.9, 126.8, 125.6, 117.5, 113.3, 103.1; Anal. Calcd for C<sub>19</sub>H<sub>13</sub>ClN<sub>2</sub>Se: C, 59.47; H, 3.41; N, 7.30%. Found C, 59.27; H, 3.30; N, 7.16%.



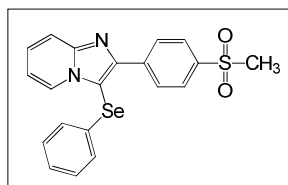
**2-(3-Bromophenyl)-8-methyl-3-(phenylselenenyl)imidazo[1,2-*a*]pyridine (3k):** Yellow solid (79 mg, 89%), mp: 67-69 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz):  $\delta$  8.25 (s, 1H), 8.14 (d,  $J = 6.8$  Hz, 1H), 8.02-8.00 (m, 1H), 7.41-7.38 (m, 1H), 7.22-7.17 (m, 1H), 7.09-7.03 (m, 3H), 7.02-6.99 (m, 3H), 6.69 (t,  $J = 6.8$  Hz, 1H), 2.62 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz):  $\delta$  149.6, 148.0, 136.2, 131.8, 131.3, 130.9, 129.8, 129.8, 128.5, 127.8, 127.4, 126.9, 125.6, 123.5, 122.5, 113.3, 103.9, 16.9; Anal. Calcd for C<sub>20</sub>H<sub>15</sub>BrN<sub>2</sub>Se: C, 54.32; H, 3.42; N, 6.33%. Found C, 54.15; H, 3.31; N, 6.18%.



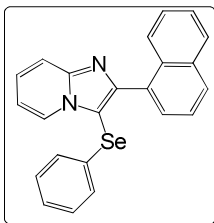
**4-(3-(Phenylselenyl)imidazo[1,2-*a*]pyridin-2-yl)benzonitrile (3l):** Yellow solid (70 mg, 93%), mp: 93-95 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.28-8.22 (m, 3H), 7.63-7.59 (m, 3H), 7.27-7.23 (m, 1H), 7.09-7.08 (m, 3H), 7.00-6.97 (m, 2H), 6.82-6.78 (m, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 149.2, 147.8, 138.3, 132.1, 130.2, 129.9, 129.0, 128.3, 127.2, 127.1, 125.7, 129.0, 117.8, 113.6, 111.7, 104.2; Anal. Calcd for C<sub>20</sub>H<sub>13</sub>N<sub>3</sub>Se: C, 64.18; H, 3.50; N, 11.23%. Found C, 64.05; H, 3.39; N, 11.14%.



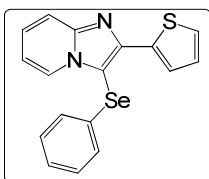
**7-Methyl-3-(phenylselenyl)-2-(4-(trifluoromethyl)phenyl)imidazo[1,2-*a*]pyridine (3m):** White solid (78 mg, 90%), mp: 78-80 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.19 (d, *J* = 8.4 Hz, 2H), 8.11 (d, *J* = 7.2 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.37 (s, 1H), 7.07-7.04 (m, 3H), 6.99-6.96 (m, 2H), 6.59-6.57 (m, 1H), 2.31 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 149.8, 148.1, 138.3, 137.4, 130.7, 130.1 (d, *J*<sub>C-F</sub> = 32 Hz), 129.8, 128.8, 128.2, 126.9, 125.2 (d, *J*<sub>C-F</sub> = 4 Hz), 124.8, 124.3 (d, *J*<sub>C-F</sub> = 267 Hz), 116.1, 116.1, 103.0, 21.4; Anal. Calcd for C<sub>21</sub>H<sub>15</sub>F<sub>3</sub>N<sub>2</sub>Se: C, 58.48; H, 3.51; N, 6.49%. Found C, 58.21; H, 3.39; N, 6.31%.



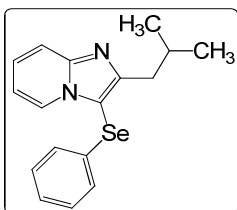
**2-(4-(Methylsulfonyl)phenyl)-3-(phenylselenyl)imidazo[1,2-*a*]pyridine (3n):** Yellow solid (67mg, 78%), mp: 68-70 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.34-8.30 (m, 3H), 7.92-7.90 (m, 2H), 7.66 (d, *J* = 9.2 Hz, 1H), 7.31-7.26 (m, 1H), 7.11-7.09 (m, 3H), 7.02-6.99 (m, 2H), 6.85-6.82 (m, 1H), 2.99 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 149.1, 147.8, 139.8, 139.1, 130.2, 129.9, 129.4, 128.4, 127.4, 127.3, 127.1, 125.8, 117.8, 113.7, 104.5, 44.6; Anal. Calcd for C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>SSe: C, 56.21; H, 3.77; N, 6.55%. Found C, 56.07; H, 3.55; N, 6.32%.



**2-(Naphthalen-1-yl)-3-(phenylselenenyl)imidazo[1,2-*a*]pyridine (3o):** Yellow solid (75 mg, 94%), mp: 84-86 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.56 (s, 1H), 8.25-8.22 (m, 2H), 7.79-7.77 (m, 2H), 7.73-7.70 (m, 1H), 7.64 (d,  $J$  = 8.8 Hz, 1H), 7.37-7.33 (m, 2H), 7.20-7.13 (m, 1H), 7.03 (s, 5H) 6.72-6.68 (m, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  151.4, 147.7, 133.3, 131.1, 130.9, 129.7, 128.7, 128.5, 128.4, 128.2, 127.9, 127.6, 126.8, 126.7, 126.4, 126.4, 126.1, 125.6, 117.4, 113.1, 103.5; Anal. Calcd for  $\text{C}_{23}\text{H}_{16}\text{N}_2\text{S}$ : C, 69.17; H, 4.04; N, 7.01%. Found C, 69.04; H, 3.89; N, 6.84%.



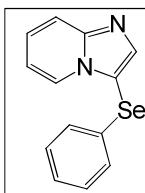
**3-(Phenylselenenyl)-2-(thiophen-2-yl)imidazo[1,2-*a*]pyridine (3p):** Yellow solid (46 mg, 64%), mp: 105-107 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.24 (d,  $J$  = 8.0 Hz, 1H), 7.95-7.94 (m, 1H), 7.60 (d,  $J$  = 8.8 Hz, 1H), 7.27 (dd,  $J$  = 4.8, 1.2 Hz, 1H), 7.22-7.18 (m, 1H), 7.07 (s, 5H), 7.04-7.00 (m, 1H), 6.77-6.73 (m, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  147.5, 146.8, 136.6, 130.4, 129.7, 128.7, 127.7, 127.0, 126.9, 126.8, 126.8, 125.5, 117.2, 113.2, 102.3; Anal. Calcd for  $\text{C}_{17}\text{H}_{12}\text{N}_2\text{SSe}$ : C, 57.46; H, 3.40; N, 7.88%. Found C, 57.33; H, 3.21; N, 7.71%.



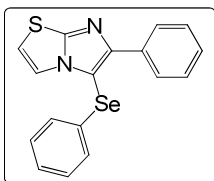
**2-Isobutyl-3-(phenylselenenyl)imidazo[1,2-*a*]pyridine (3q):** Yellow liquid, (48 mg, 73%);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.12-8.10 (m, 1H), 7.57-7.54 (m, 1H), 7.19-7.13 (m, 1H), 7.05 (t,  $J$  = 3.2 Hz, 3H), 6.96-6.94 (m, 2H), 6.71-6.68 (m, 1H), 2.75 (d,  $J$  = 7.2, 2H), 2.17-2.10 (m, 1H), 0.86 (d,  $J$  = 6.4 Hz, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  154.5, 147.5, 131.0, 129.5,



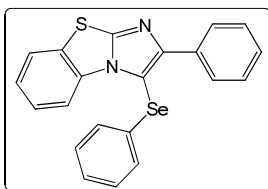
128.3, 126.6, 125.9, 125.3, 116.9, 112.6, 104.8, 37.6, 29.1, 22.6; Anal. Calcd for  $C_{17}H_{18}N_2Se$ : C, 62.01; H, 5.51; N, 8.51%. Found C, 61.87; H, 5.42; N, 8.39%.



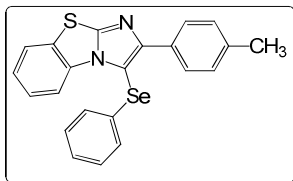
**2-(Phenylselenenyl)imidazo[1,2-*a*]pyridine (3r):** Yellow liquid, (43 mg, 78%);  $^1H$  NMR ( $CDCl_3$ , 400 MHz):  $\delta$  8.21 (d,  $J$  = 6.8 Hz, 1H), 7.91 (s, 1H), 7.65 (d,  $J$  = 9.2 Hz, 1H), 7.25-7.21 (m, 1H), 7.12-7.06 (m, 5H), 6.80 (t,  $J$  = 6.8 Hz, 1H);  $^{13}C$  NMR ( $CDCl_3$ , 100 MHz):  $\delta$  148.1, 142.6, 130.4, 129.6, 129.1, 127.0, 126.1, 125.3, 117.9, 113.3, 106.7; Anal. Calcd for  $C_{13}H_{10}N_2Se$ : C, 57.15; H, 3.69; N, 10.25%. Found C, 57.02; H, 3.51; N, 10.14%.



**6-Phenyl-5-(phenylselenenyl)imidazo[2,1-*b*]thiazole (5a):** Yellow solid (53 mg, 74%), mp: 67-69 °C;  $^1H$  NMR ( $CDCl_3$ , 400 MHz):  $\delta$  8.00-7.98 (m, 2H), 7.33-7.29 (m, 3H), 7.24-7.20 (m, 1H), 7.12-7.04 (m, 5H), 6.70 (d,  $J$  = 4.4 Hz, 1H);  $^{13}C$  NMR ( $CDCl_3$ , 100 MHz):  $\delta$  152.8, 151.6, 133.8, 131.4, 129.7, 128.5, 128.4, 128.1, 127.8, 126.8, 118.8, 112.6, 102.6; Anal. Calcd for  $C_{17}H_{12}N_2SSe$ : C, 57.46; H, 3.40; N, 7.88%. Found C, 57.32; H, 3.31; N, 7.71%.



**2-Phenyl-3-(phenylselenenyl)benzo[*d*]imidazo[2,1-*b*]thiazole (5b):** Orange solid (76 mg, 92%), mp: 87-89 °C;  $^1H$  NMR ( $CDCl_3$ , 400 MHz):  $\delta$  8.44-8.41 (m, 1H), 7.94 (d,  $J$  = 7.2 Hz, 2H), 7.58-7.56 (m, 1H), 7.32 (t,  $J$  = 7.2 Hz, 2H), 7.27-7.16 (m, 5H), 7.12-7.06 (m, 3H);  $^{13}C$  NMR ( $CDCl_3$ , 100 MHz):  $\delta$  154.2, 151.5, 133.9, 133.6, 132.5, 130.3, 129.9, 128.5, 128.3, 128.3, 128.2, 126.8, 126.2, 125.0, 124.0, 114.6, 104.2; Anal. Calcd for  $C_{21}H_{14}N_2SSe$ : C, 62.22; H, 3.48; N, 6.91%. Found C, 62.08; H, 3.31; N, 6.75%.



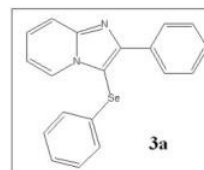
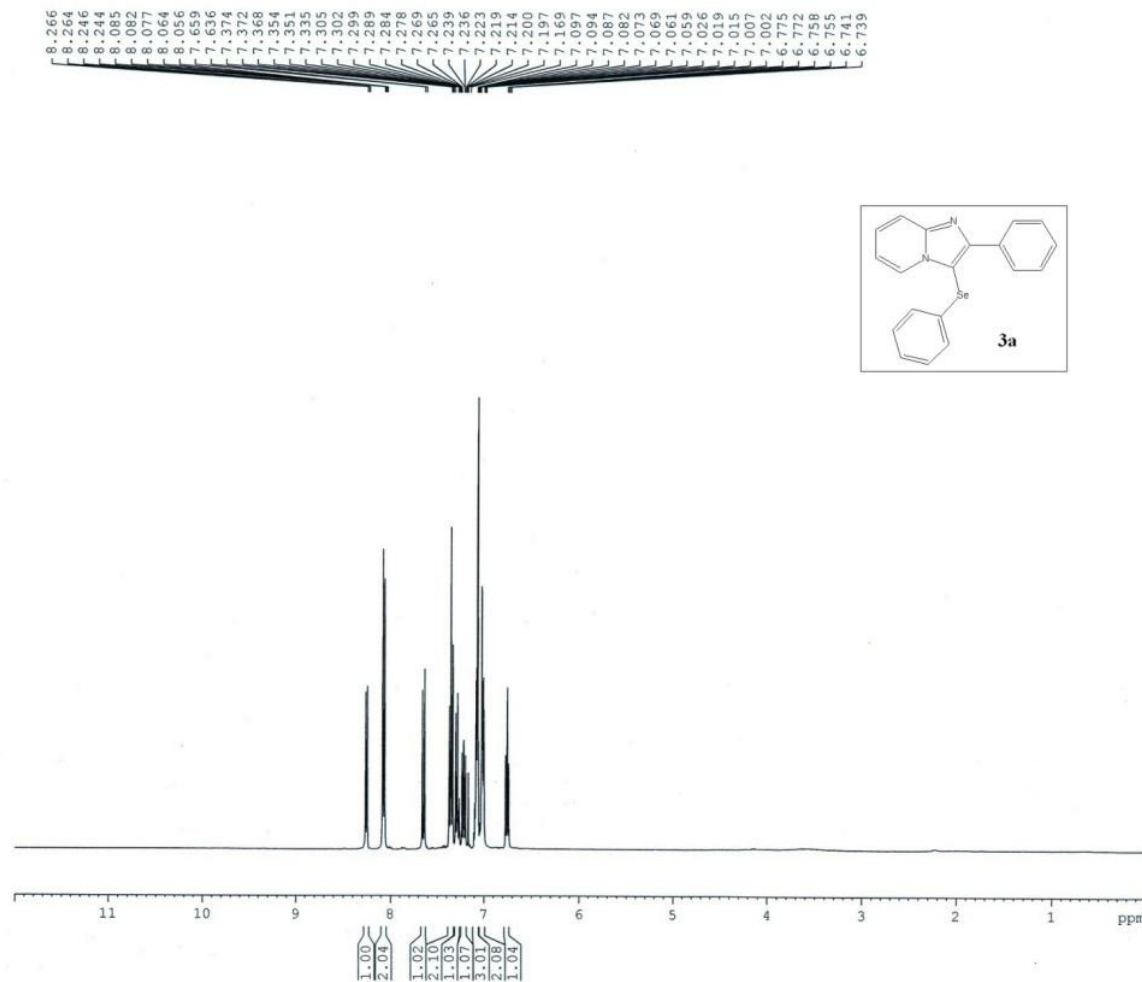
**3-(Phenylselenenyl)-2-(p-tolyl)benzo[d]imidazo[2,1-b]thiazole (5c):** Orange solid (70 mg, 84%), mp: 110-112 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.46-8.44 (m, 1H), 7.84 (d,  $J$  = 8.0 Hz, 2H), 7.62-7.59 (m, 1H), 7.28-7.21 (m, 2H), 7.19-7.08 (m, 7H), 2.30 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  154.0, 151.3, 138.3, 133.9, 132.5, 130.5, 130.3, 129.9, 129.1, 128.3, 128.2, 126.8, 126.2, 125.0, 124.1, 114.6, 104.0, 21.4; Anal. Calcd for  $\text{C}_{22}\text{H}_{16}\text{N}_2\text{SSe}$ : C, 63.00; H, 3.85; N, 6.68%. Found C, 62.85; H, 3.67; N, 6.51%.

### **References:**

1. (a) S. Santra, A. Majee and A. Hajra, *Tetrahedron Lett.*, 2011, **52**, 3825; (b) S. Das, M. Rahman, D. Kundu, A. Majee and A. Hajra, *Can. J. Chem.*, 2010, **88**, 150.
2. M. Mirza-Aghayan, A. Moradi, M. Bolourtchain and R. Boukherroub, *Synthetic Commun.*, 2010, **40**, 8.
3. B. Kaur and R. Kaur, *Arkivoc*, 2007, **xv**, 315.

## **$^1\text{H}$ and $^{13}\text{C}$ NMR spectra of Compounds**



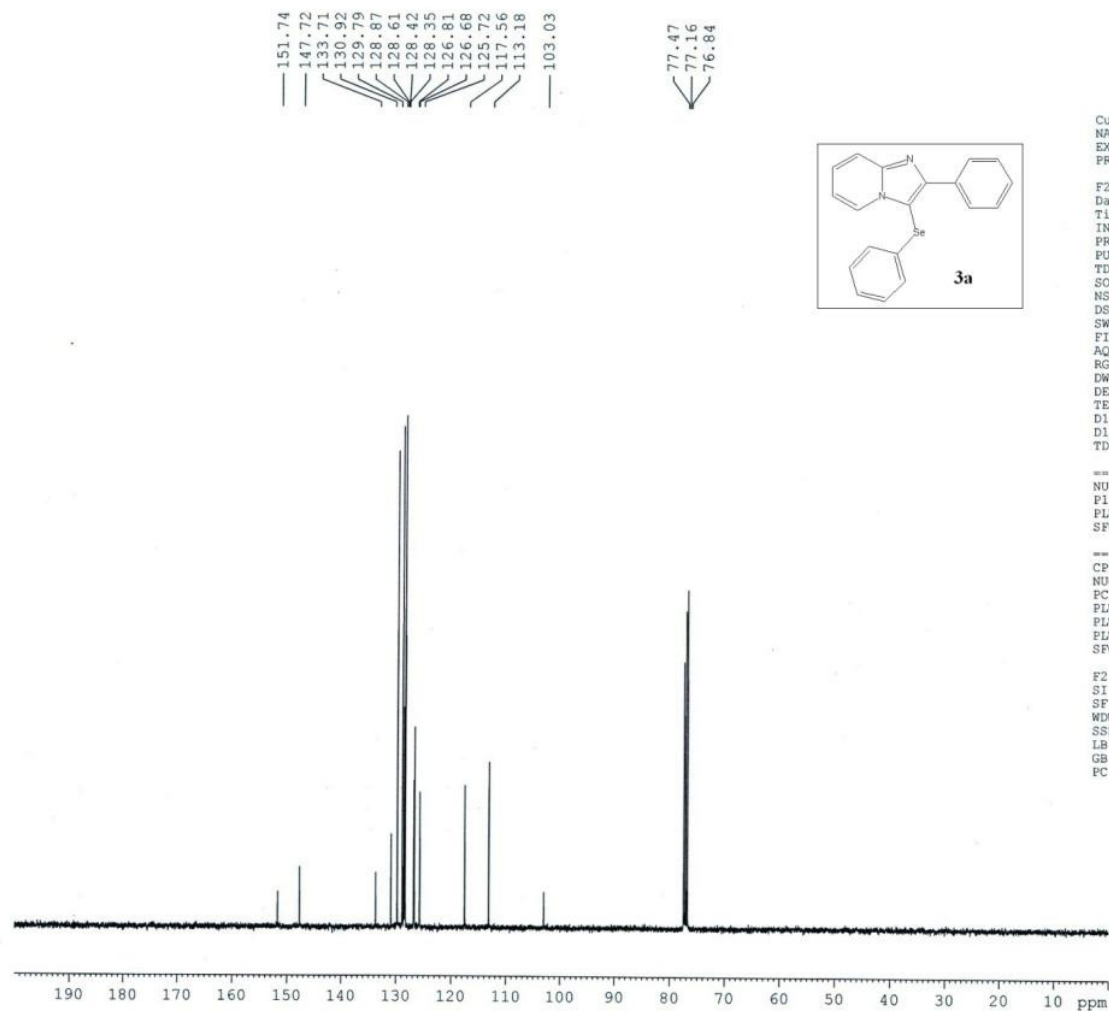


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 EXPNO 210  
 PROCNO 1

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 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 24  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 62.69  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SFO1 400.1524711 MHz

F2 - Processing parameters  
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 SF 400.1500455 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



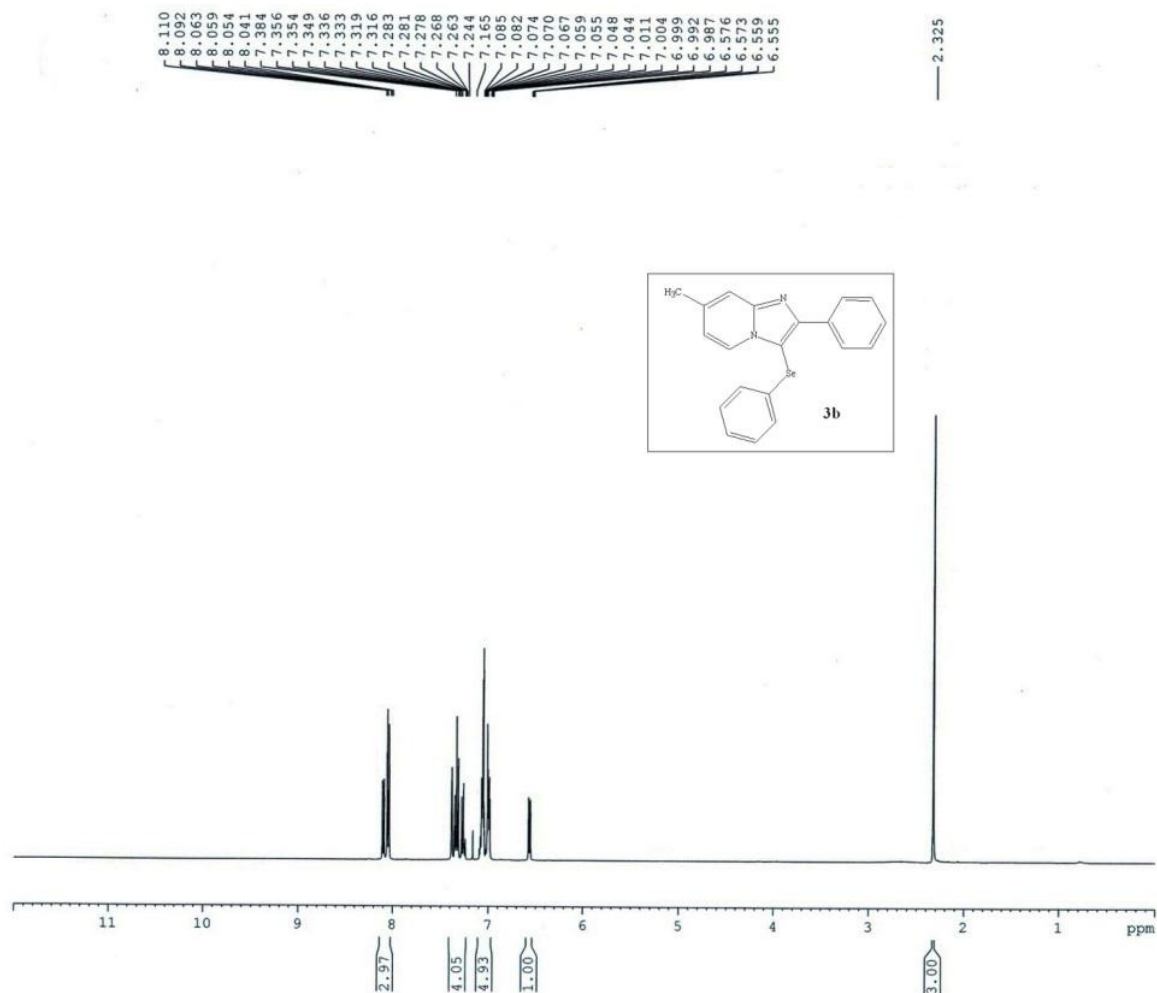
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EXPNO 211  
PROCNO 1

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PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 320  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6816244 sec  
RG 62.69  
DW 20.800 usec  
DE 6.50 usec  
TE 299.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 12.00000000 W  
PLW12 0.40792999 W  
PLW13 0.26107001 W  
SFO2 400.1516006 MHz

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

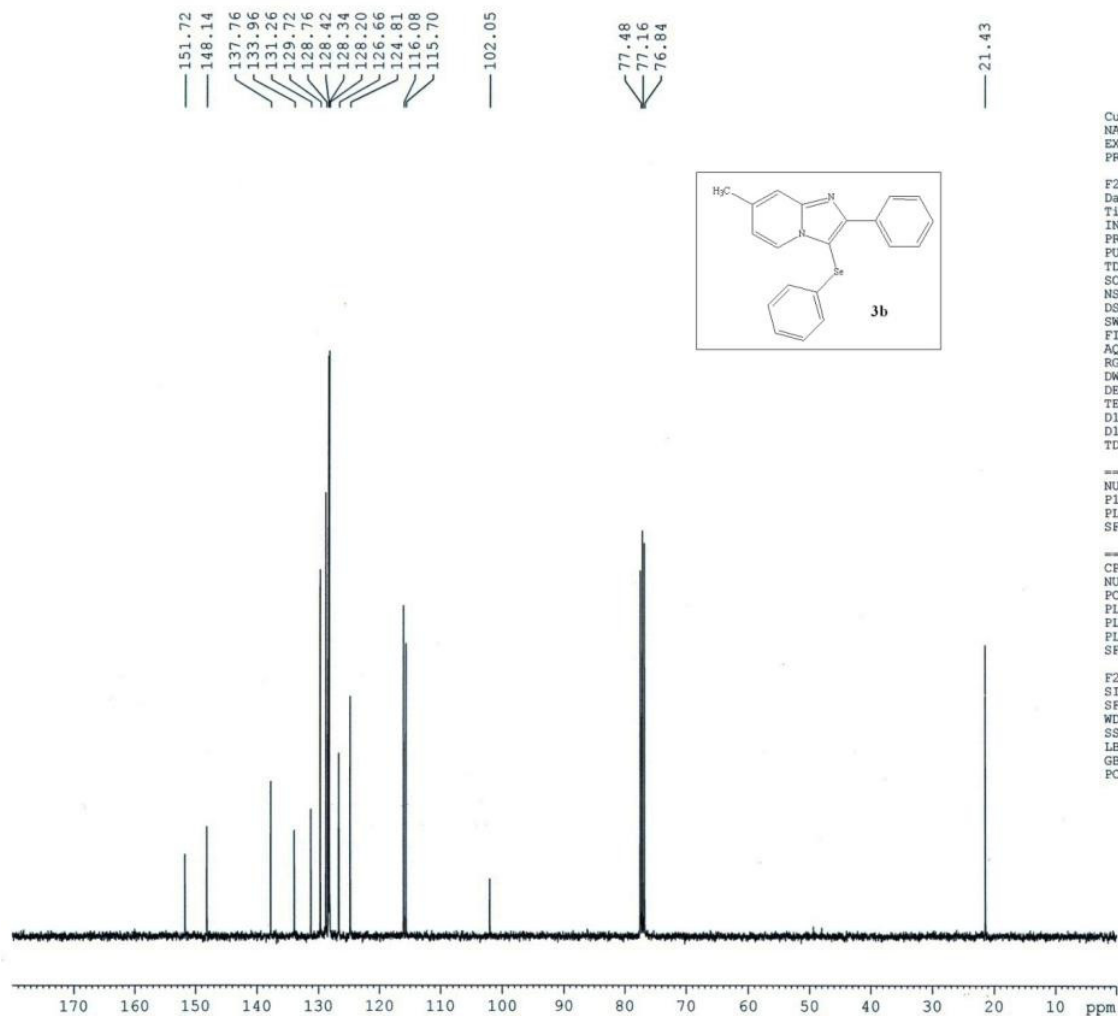


Current Data Parameters  
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 EXPNO 105  
 PROCNO 1

F2 - Acquisition Parameters  
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 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 24  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 40.87  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.1 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SFO1 400.1524711 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500472 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 109  
 PROCNO 1

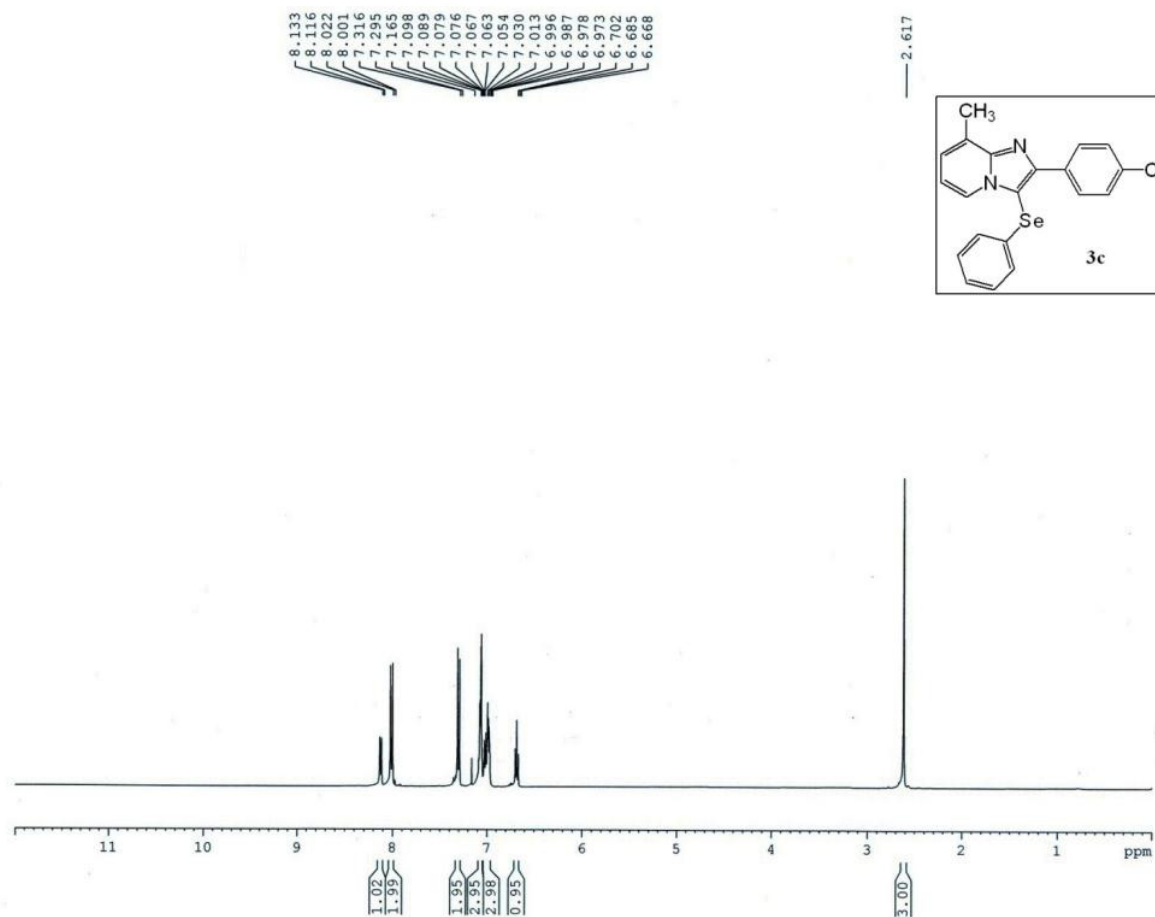
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 Time\_ 17.17  
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 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 245  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6816244 sec  
 RG 40.87  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

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

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.40792999 W  
 PLW13 0.26107001 W  
 SFO2 400.1516006 MHz

F2 - Processing parameters  
 SI 16384  
 SF 100.6177909 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



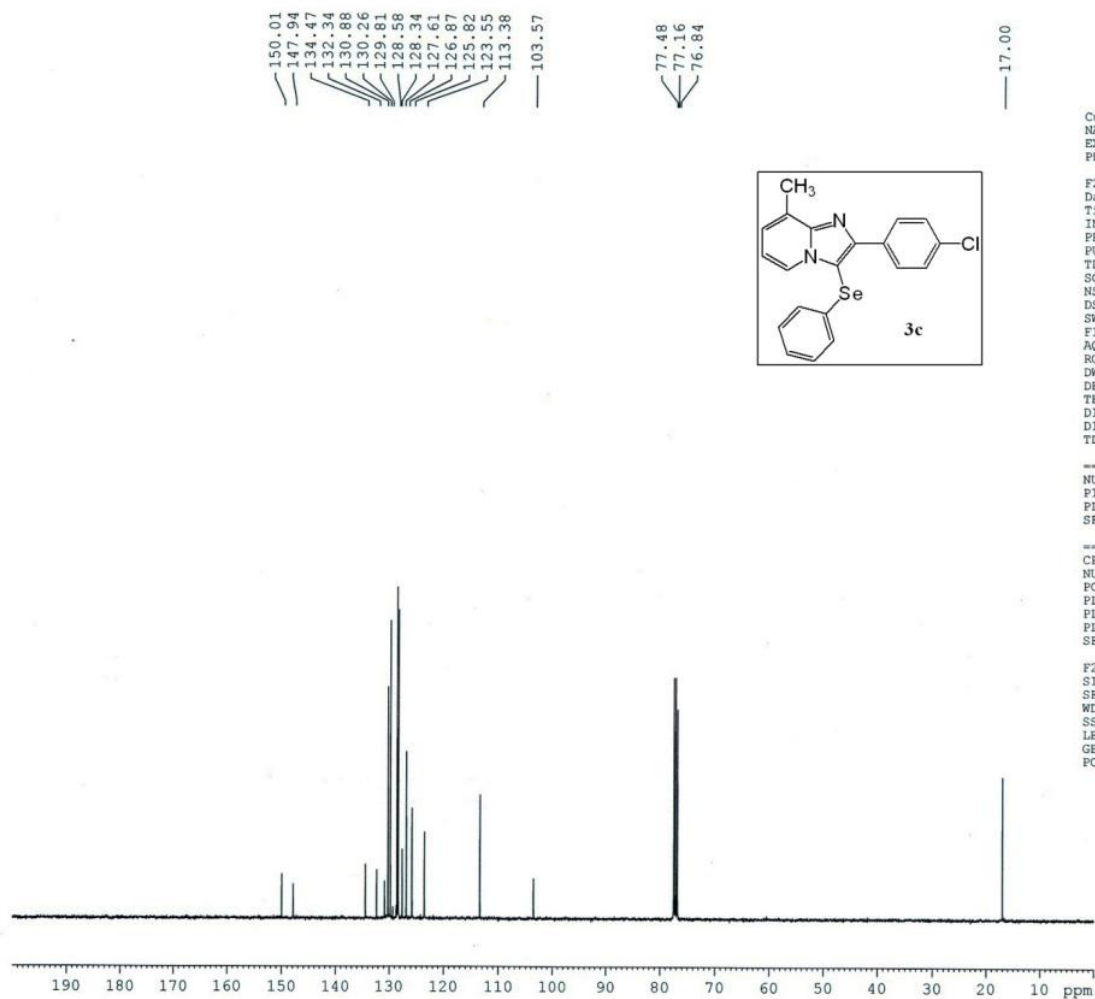


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EXPNO 39  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150218  
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PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 32  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9923444 sec  
RG 40.87  
DW 60.800 usec  
DE 6.50 usec  
TE 296.4 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.75 usec  
PLW1 11.99499989 W  
SF01 400.1524711 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1500471 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



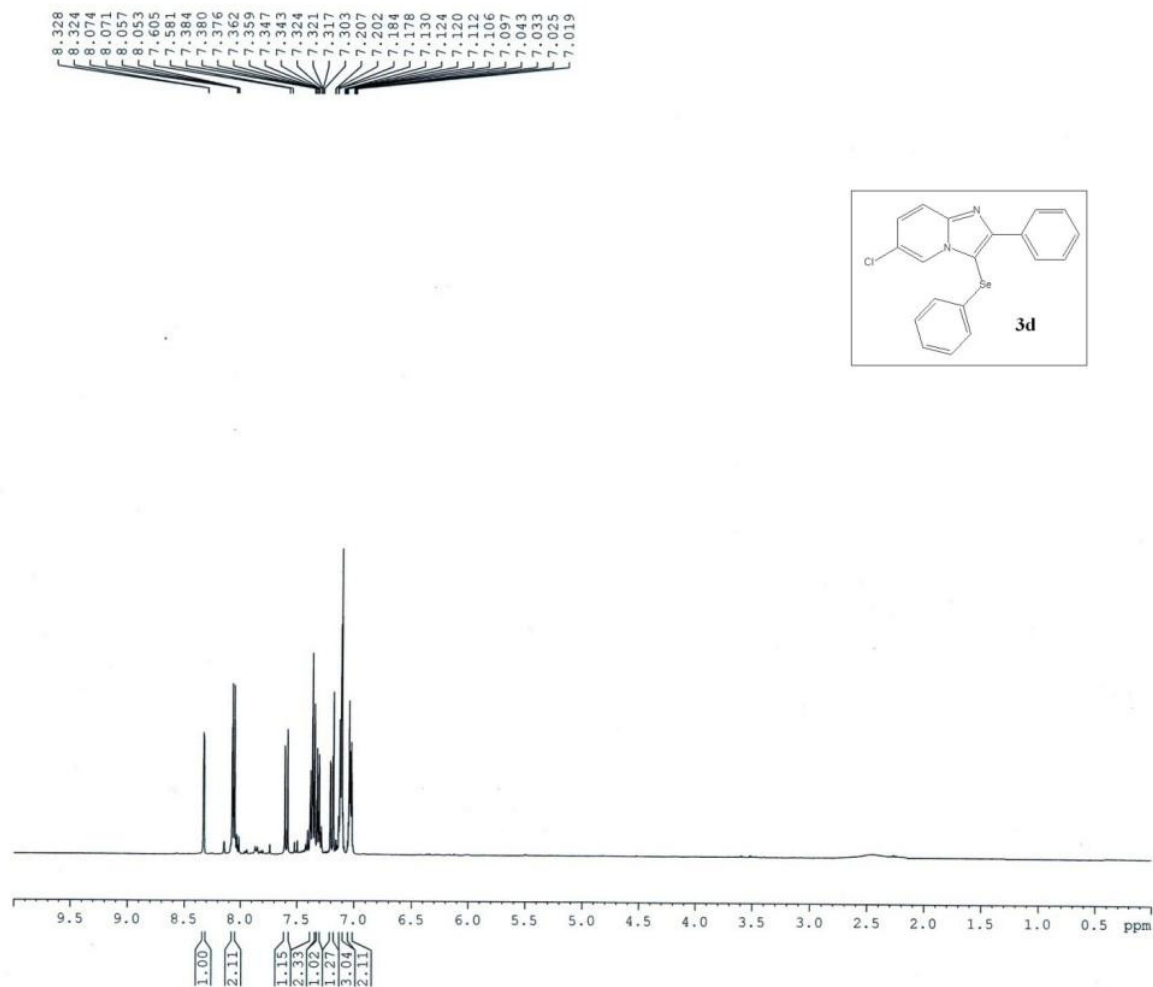
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 EXPNO 40  
 PROCNO 1

F2 - Acquisition Parameters  
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 Time 18.28  
 INSTRUM spect  
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 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 512  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6816244 sec  
 RG 40.87  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

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

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.40792999 W  
 PLW13 0.26107001 W  
 SFO2 400.1516006 MHz

F2 - Processing parameters  
 SI 16384  
 SF 100.6177895 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

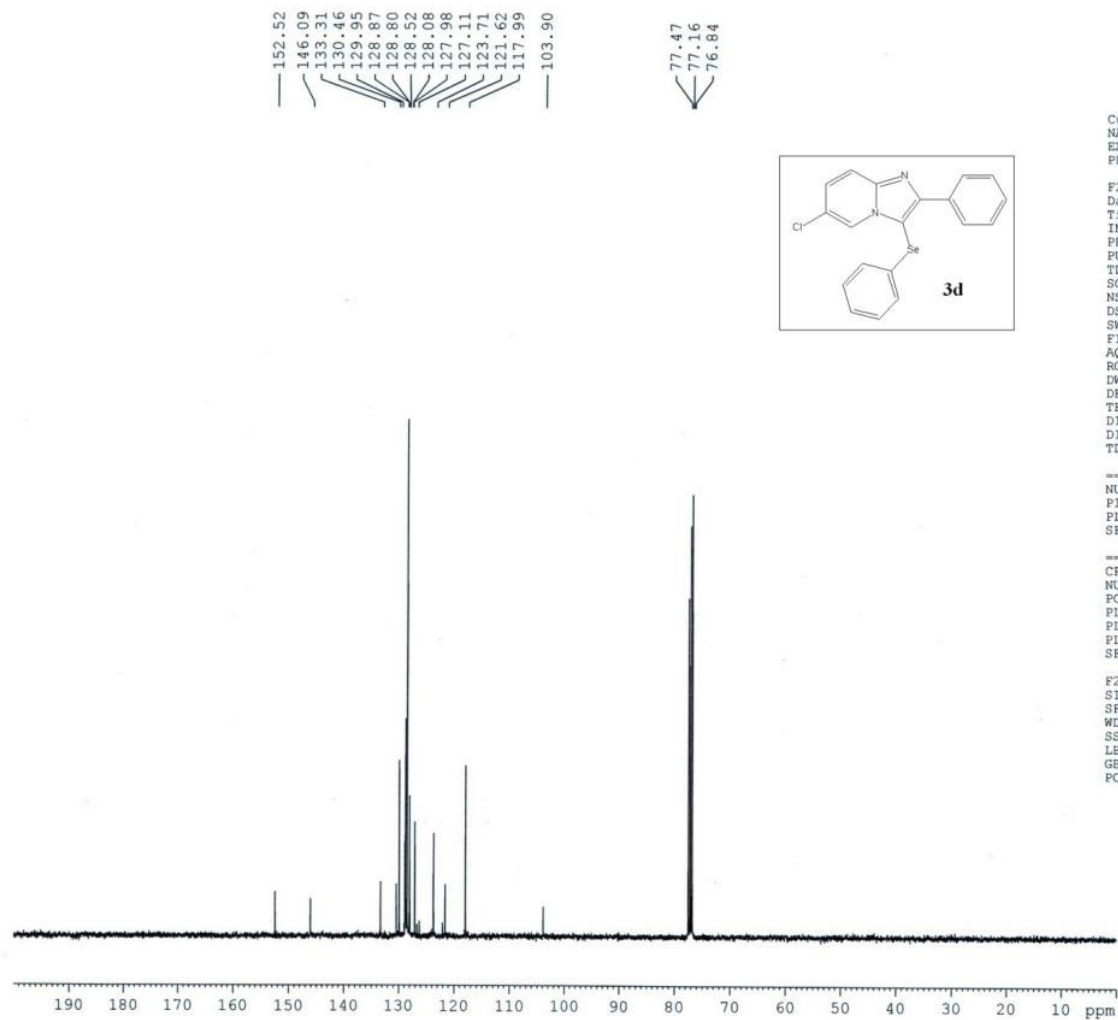


Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 130  
PROCNO 1

F2 - Acquisition Parameters  
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Time\_ 16.30  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 24  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9923444 sec  
RG 93.46  
DW 60.800 usec  
DE 6.50 usec  
TE 297.7 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.75 usec  
PLW1 11.99499989 W  
SFO1 400.1524711 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1500419 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



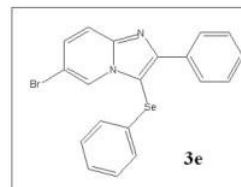
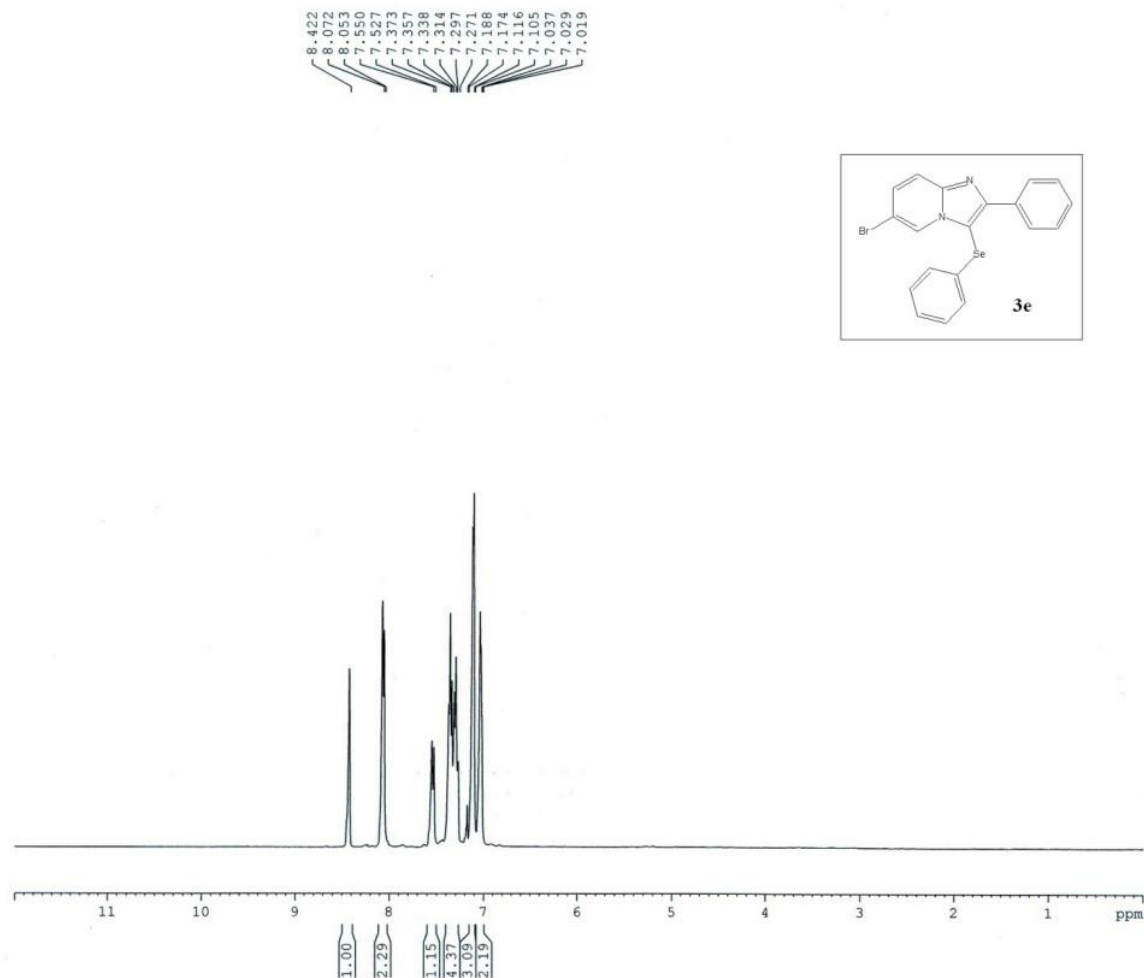
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 EXPNO 131  
 PROCNO 1

F2 - Acquisition Parameters  
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 PULPROG zgpg30  
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 SOLVENT CDCl3  
 NS 512  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6816244 sec  
 RG 87.66  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

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

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.40792999 W  
 PLW13 0.26107001 W  
 SFO2 400.1516006 MHz

F2 - Processing parameters  
 SI 16384  
 SF 100.6177865 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

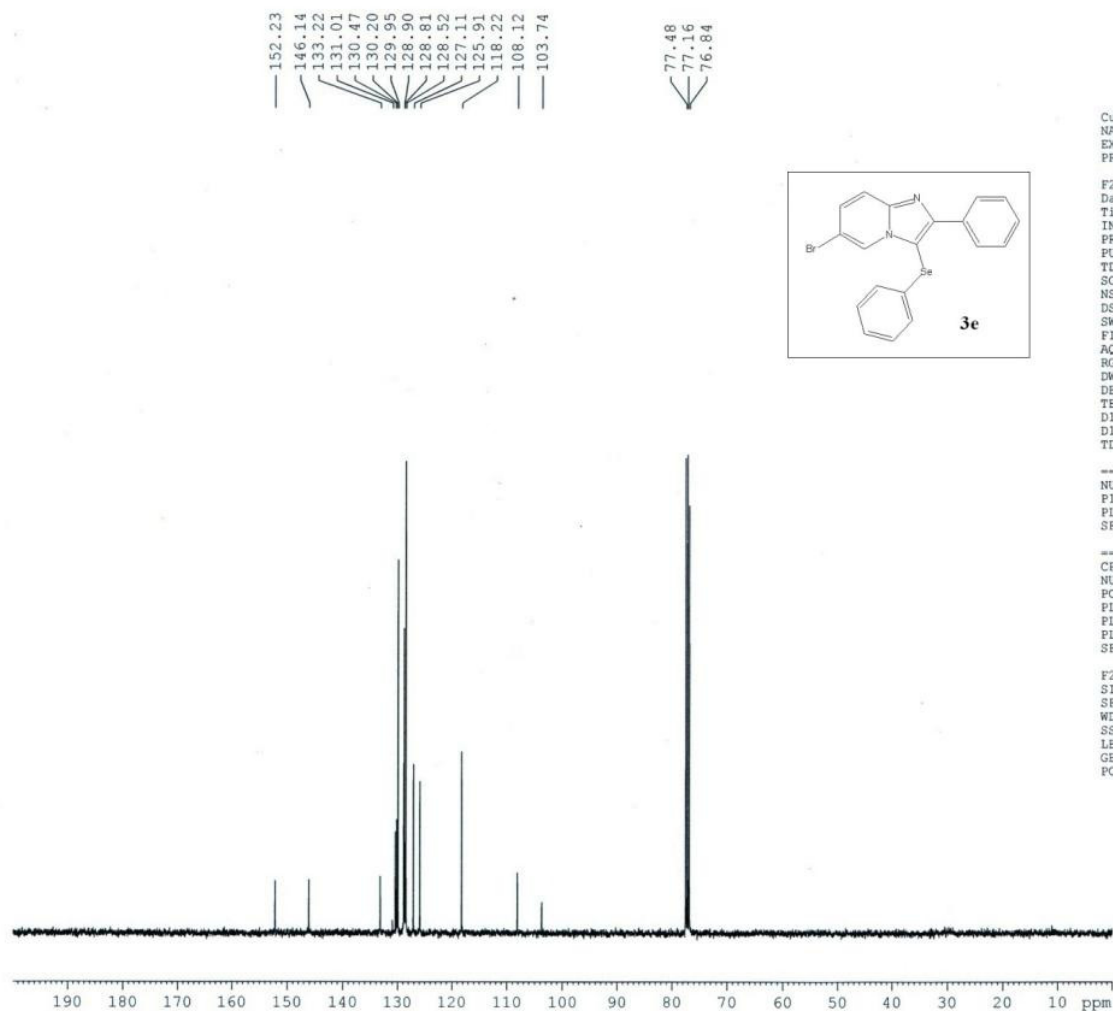


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 NAME Dr. A HAJRA 2015  
 EXPNO 172  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150430  
 Time 12.53  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 77.59  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.6 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SF01 400.1524711 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500432 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



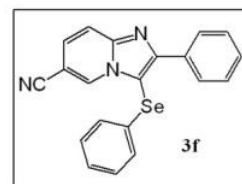
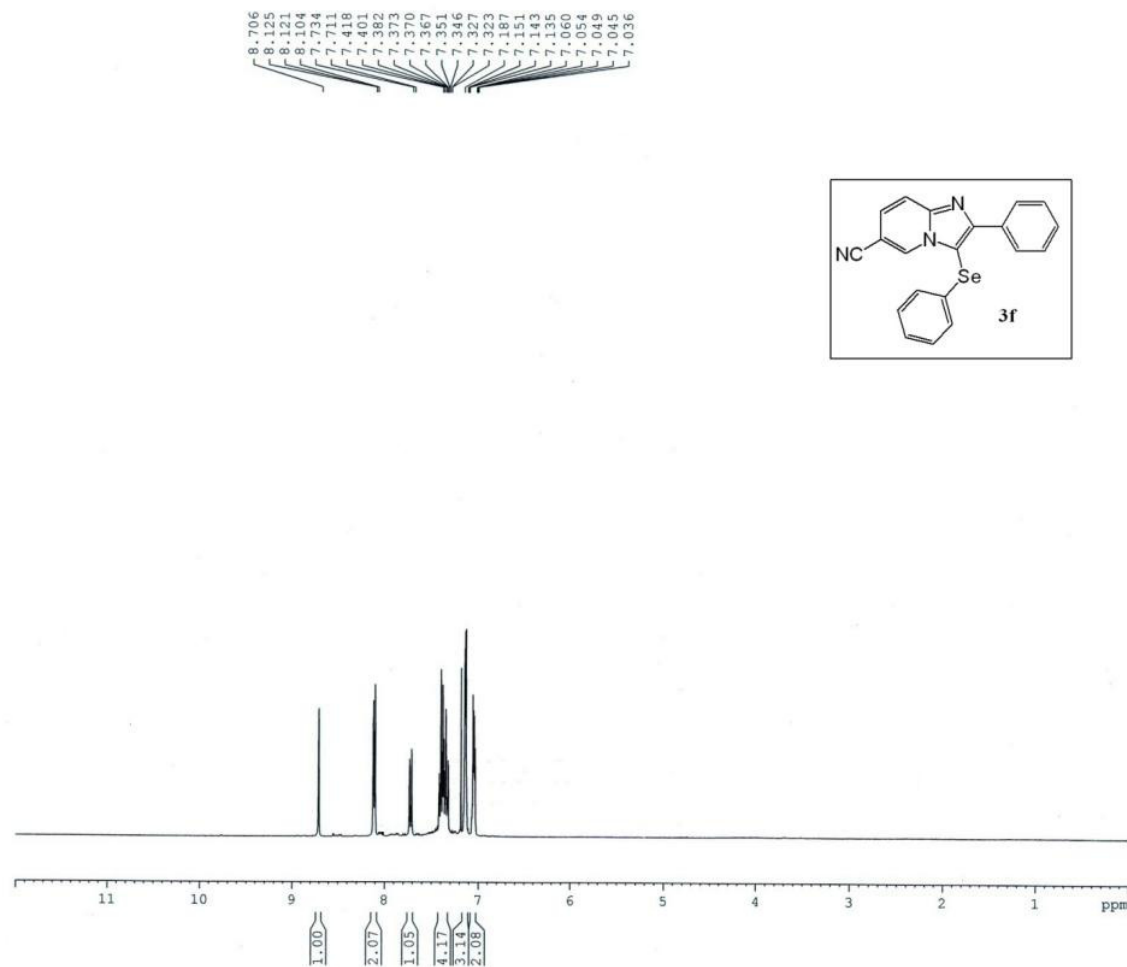
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 EXPNO 173  
 PROCNO 1

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 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 512  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6816244 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

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

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.40792999 W  
 PLW13 0.26107001 W  
 SFO2 400.1516006 MHz

F2 - Processing parameters  
 SI 16384  
 SF 100.6177880 MHz  
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 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

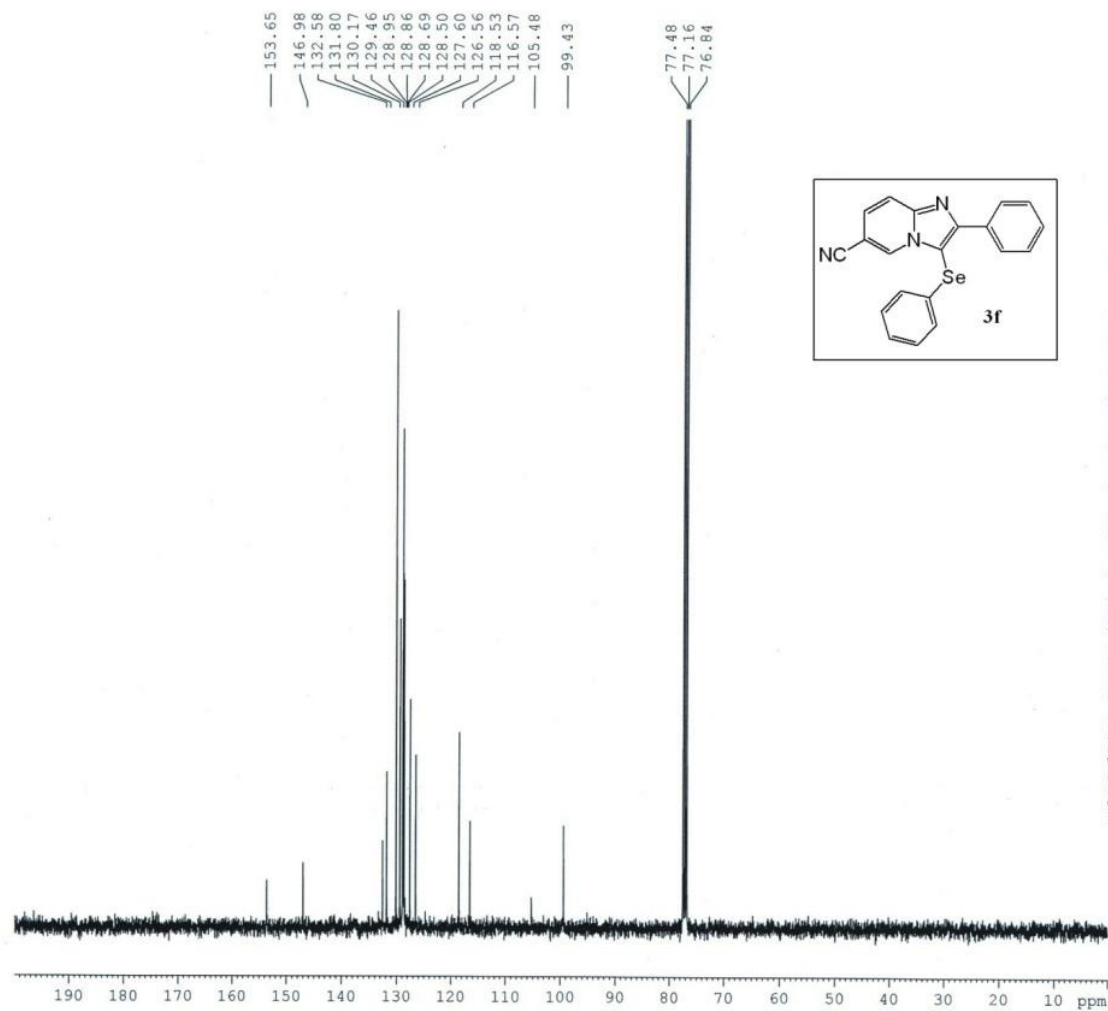


Current Data Parameters  
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 EXPNO 163  
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F2 - Acquisition Parameters  
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 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 93.46  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
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 P1 14.75 usec  
 PLW1 11.99499989 W  
 SFO1 400.1524711 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500382 MHz  
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 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 164  
 PROCNO 1

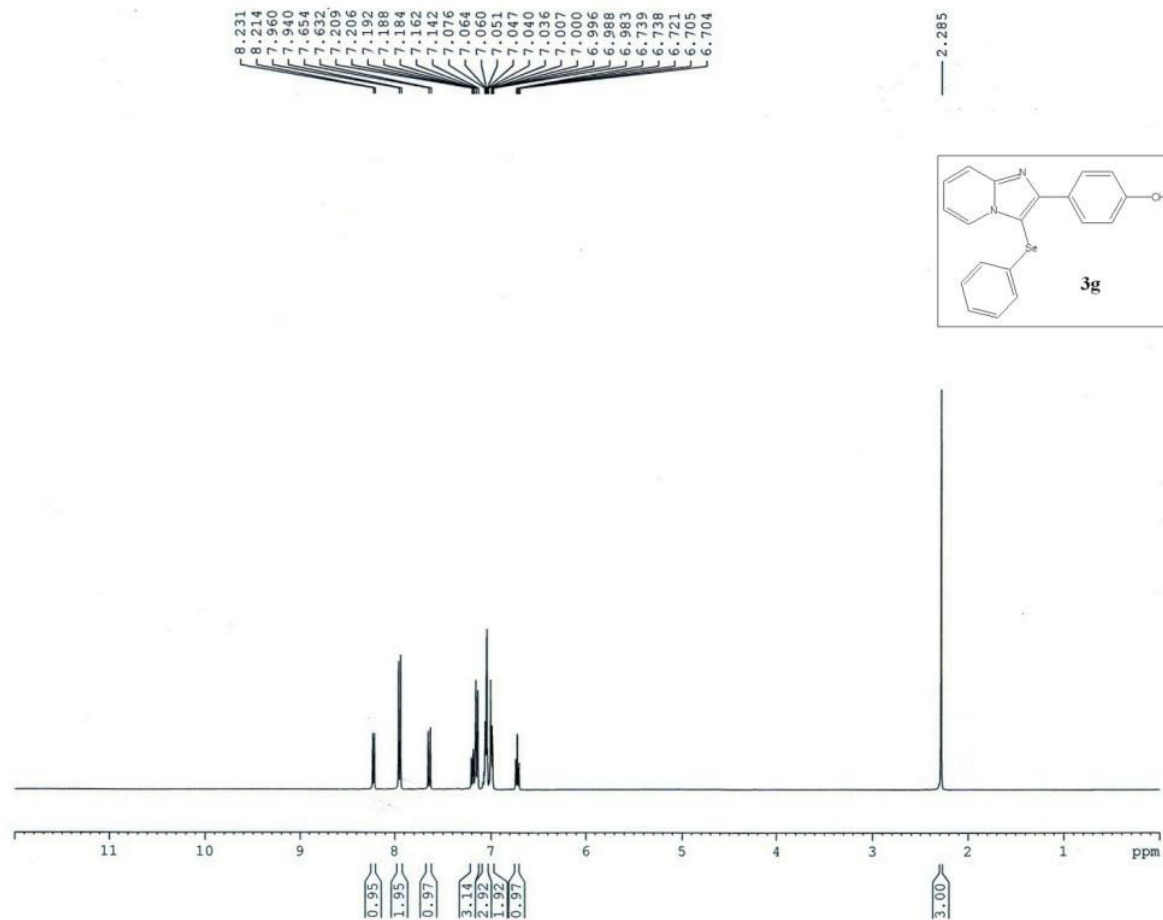
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 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 512  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6816244 sec  
 RG 93.46  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

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

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 80.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.40792999 W  
 PLW13 0.26107001 W  
 SFO2 400.1516006 MHz

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



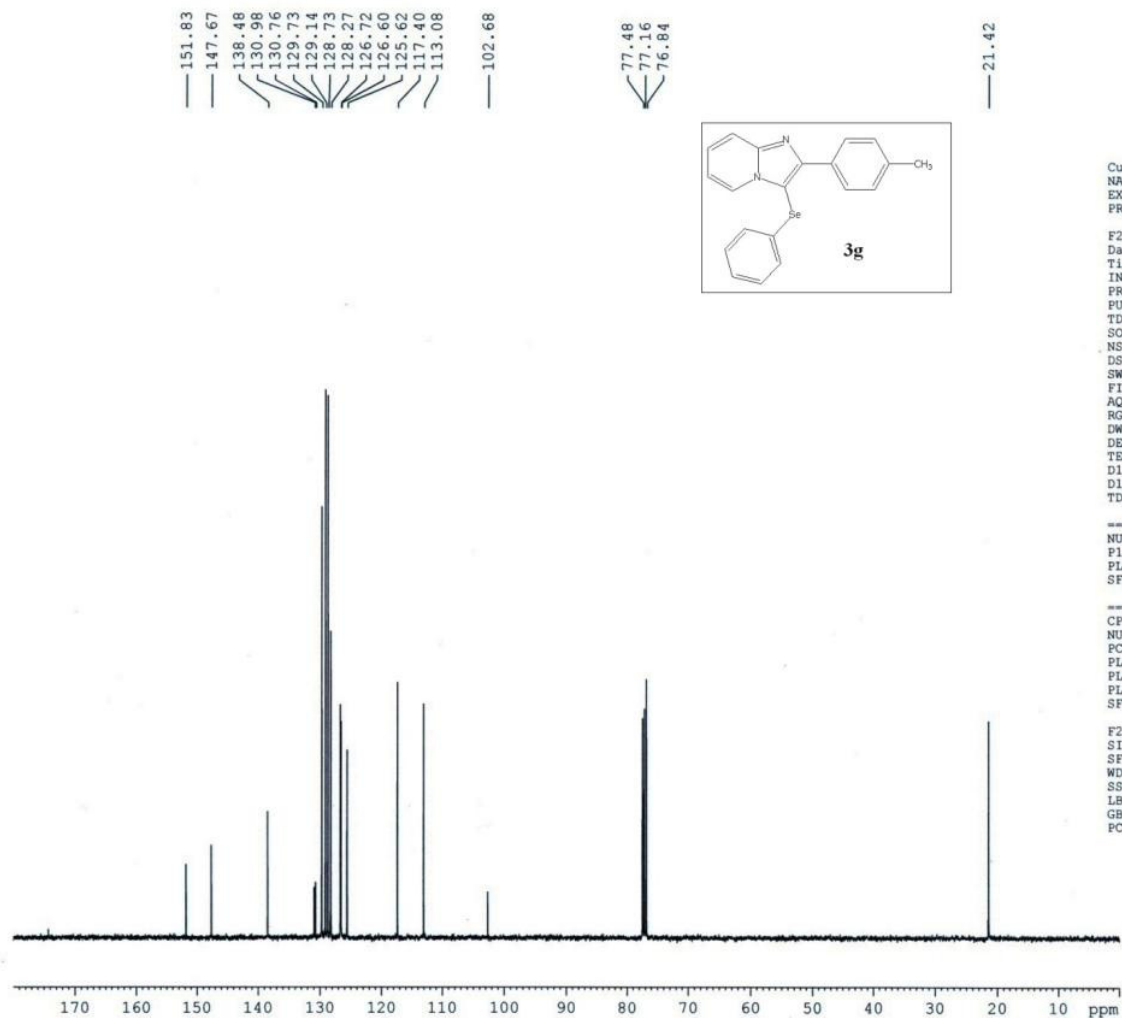


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 EXPNO 100  
 PROCNO 1

F2 - Acquisition Parameters  
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 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 2  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 40.87  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.6 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SFO1 400.1524711 MHz

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



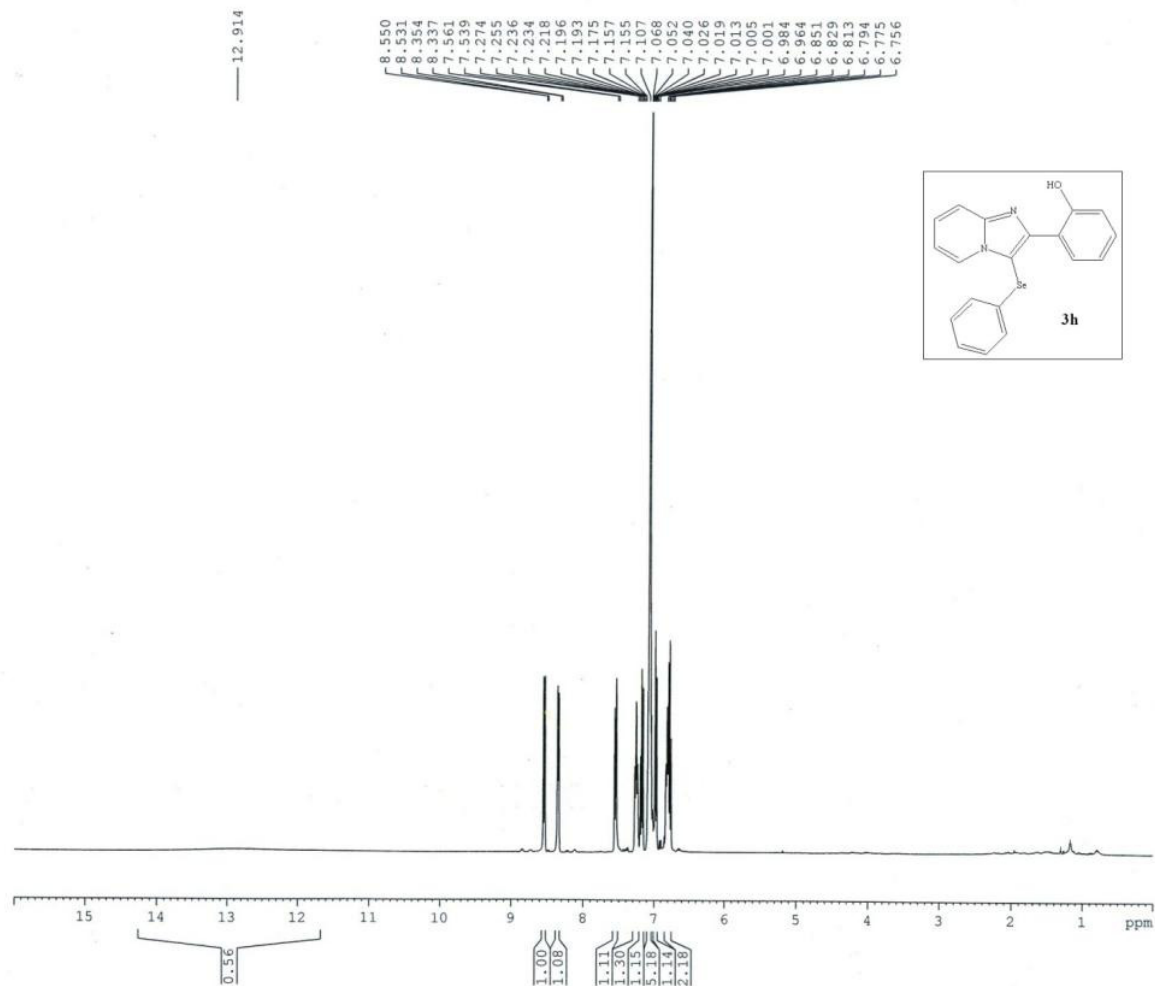
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EXPNO 103  
PROCNO 1

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PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 240  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6816244 sec  
RG 40.87  
DW 20.800 usec  
DE 6.50 usec  
TE 296.8 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 12.00000000 W  
PLW12 0.40792999 W  
PLW13 0.26107001 W  
SFO2 400.1516006 MHz

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

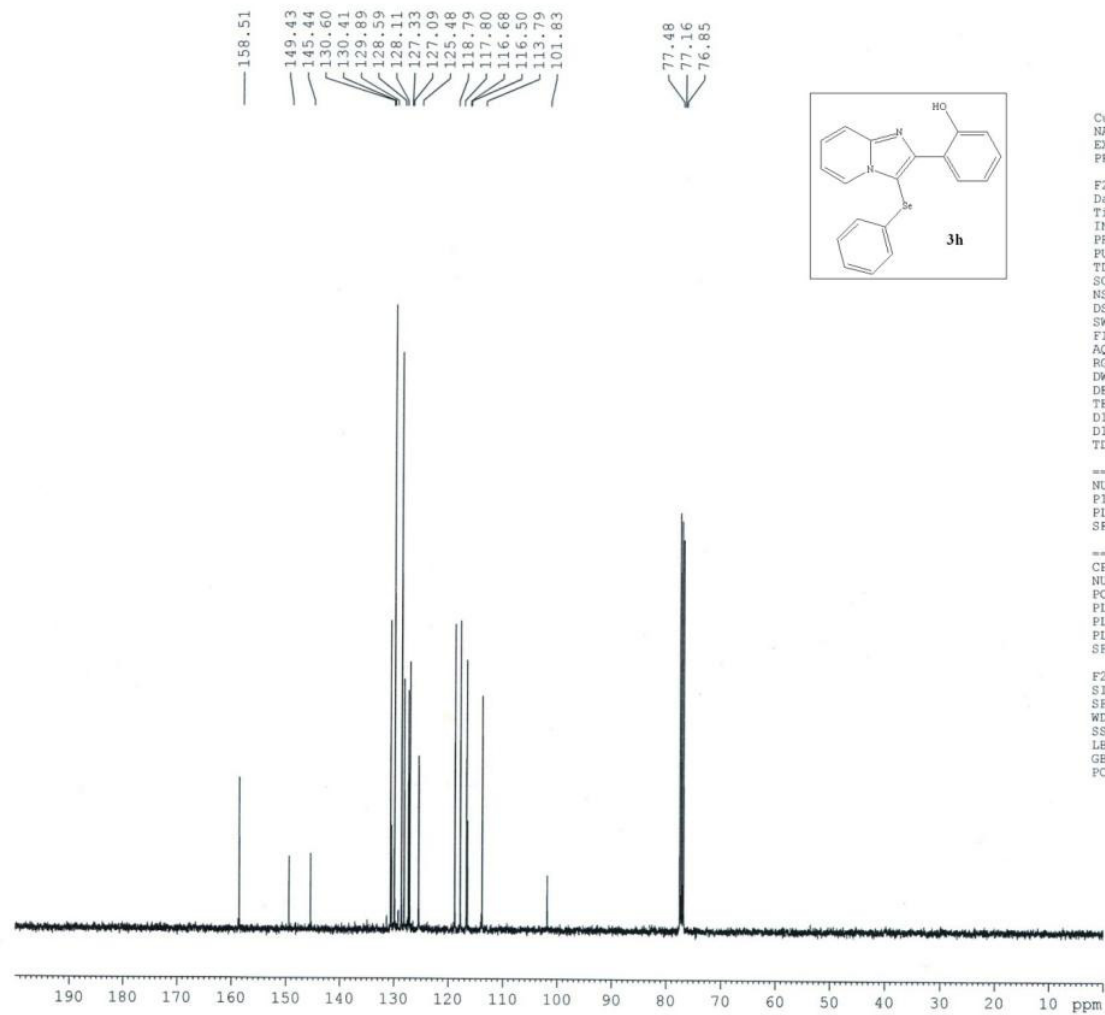


Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 385  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20150716  
 Time 17.43  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 1  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 67.81  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1

CHANNEL f1  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SFO1 400.1524711 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500511 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



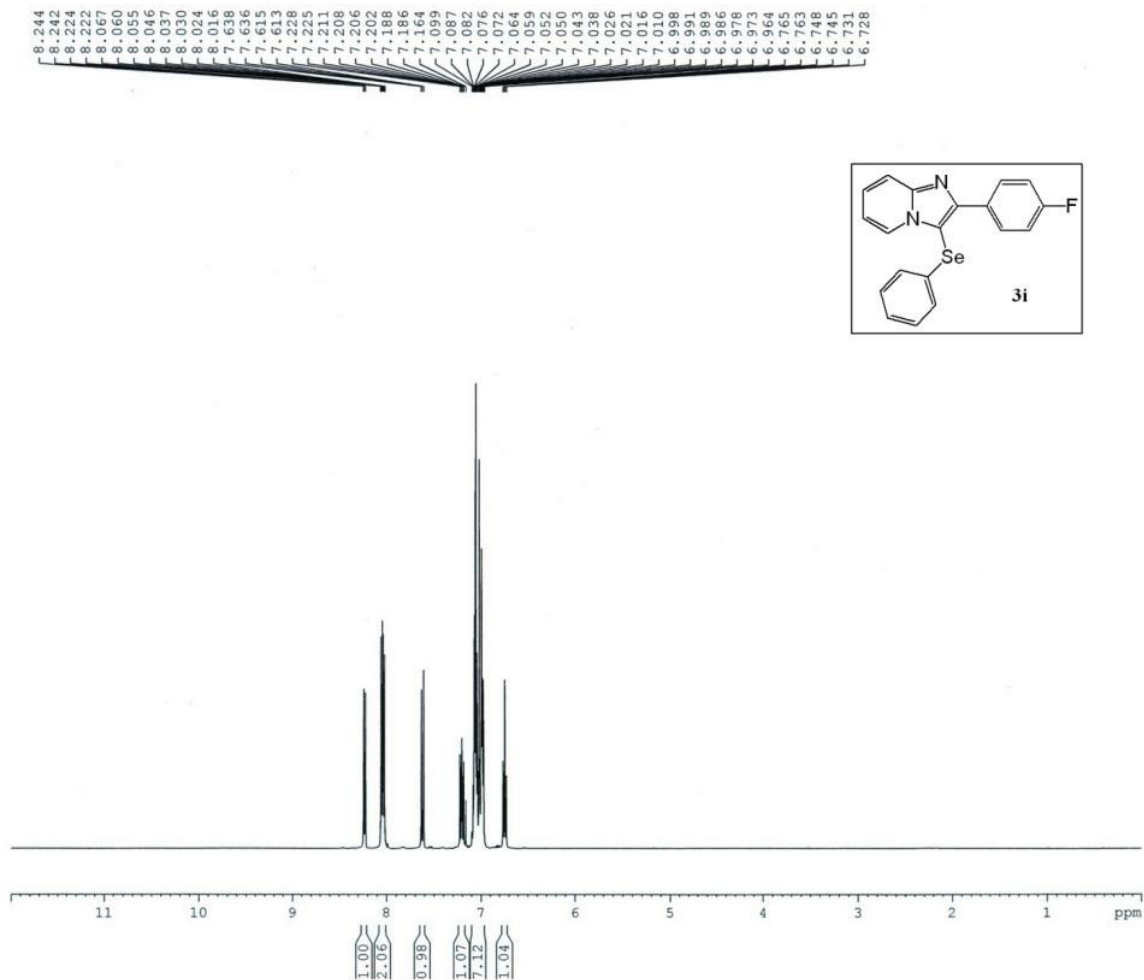
Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 386  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20150716  
 Time 18.13  
 INSTRUM spect  
 PROBRD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 512  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6816244 sec  
 RG 47.25  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 54.00000000 W  
 SFO1 100.6278586 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.40792999 W  
 PLW13 0.26107001 W  
 SFO2 400.1516006 MHz

F2 - Processing parameters  
 SI 16384  
 SF 100.6177880 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

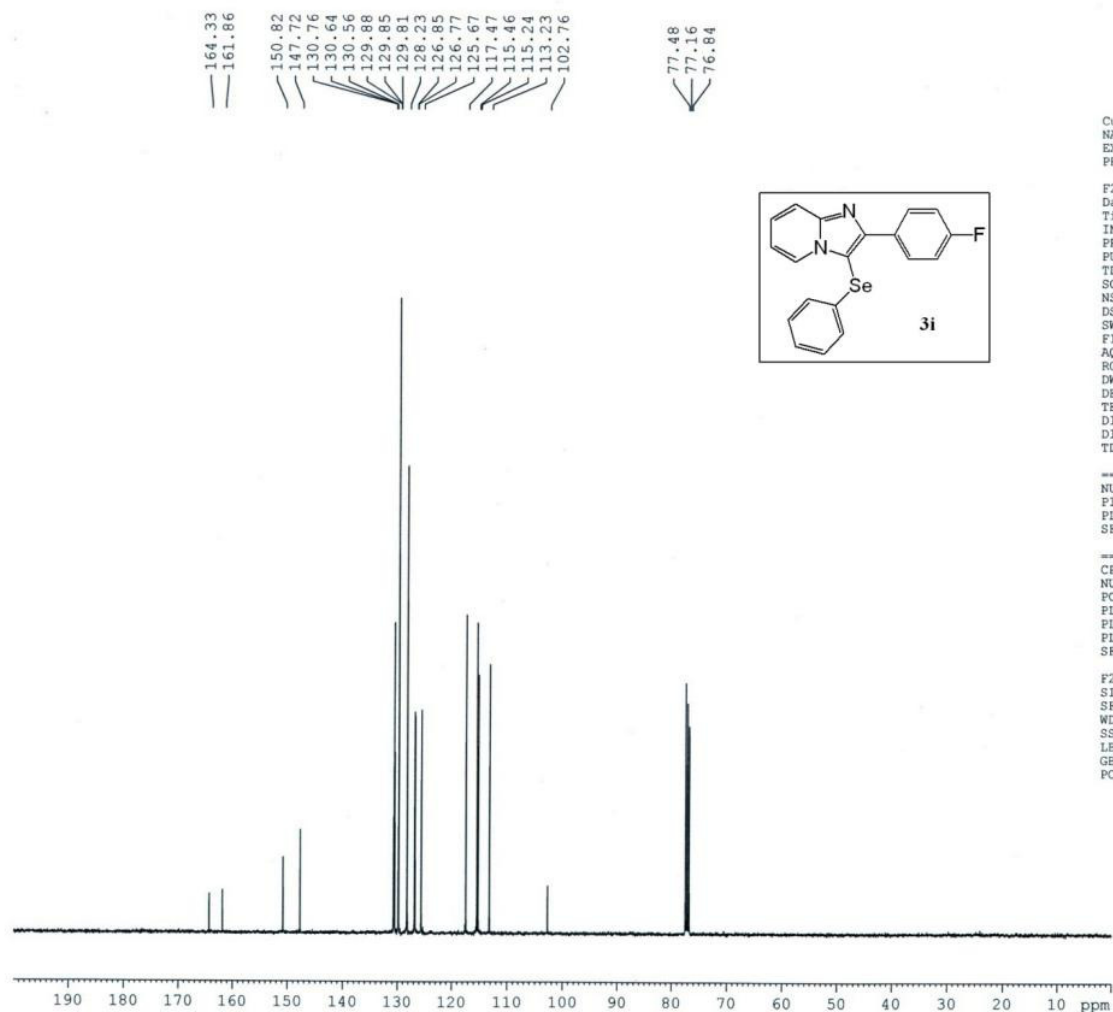


Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 107  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150411  
 Time\_ 16.03  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 24  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 40.87  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.1 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SF01 400.1524711 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500473 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



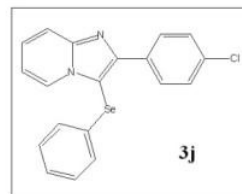
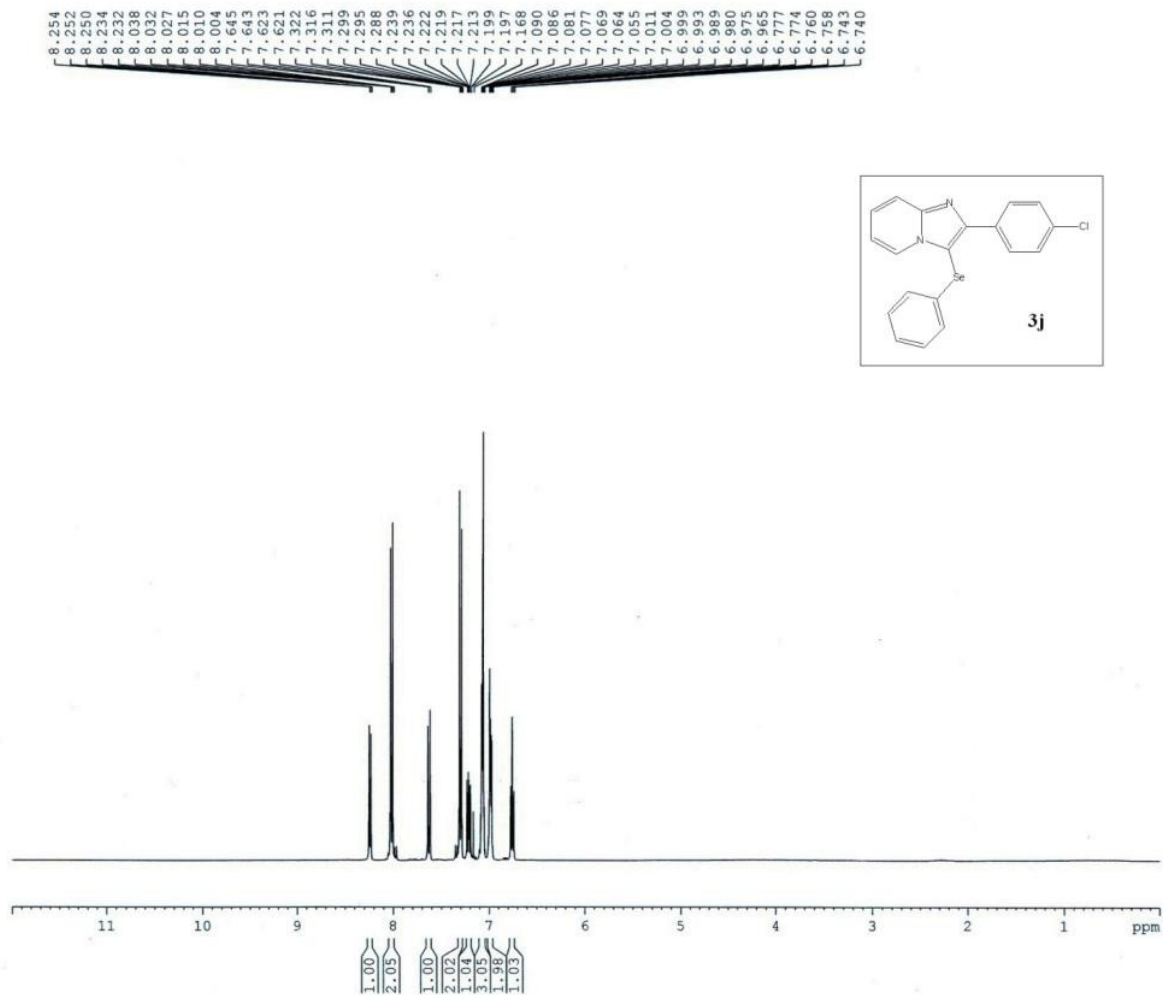
Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 114  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150412  
Time 12.28  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 512  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6816244 sec  
RG 87.66  
DW 20.800 usec  
DE 6.50 usec  
TE 296.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 6.90 usec  
PLW1 54.00000000 W  
SFO1 100.6278588 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 12.00000000 W  
PLW12 0.40792999 W  
PLW13 0.26107001 W  
SFO2 400.1516006 MHz

F2 - Processing parameters  
SI 16384  
SF 100.6177930 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

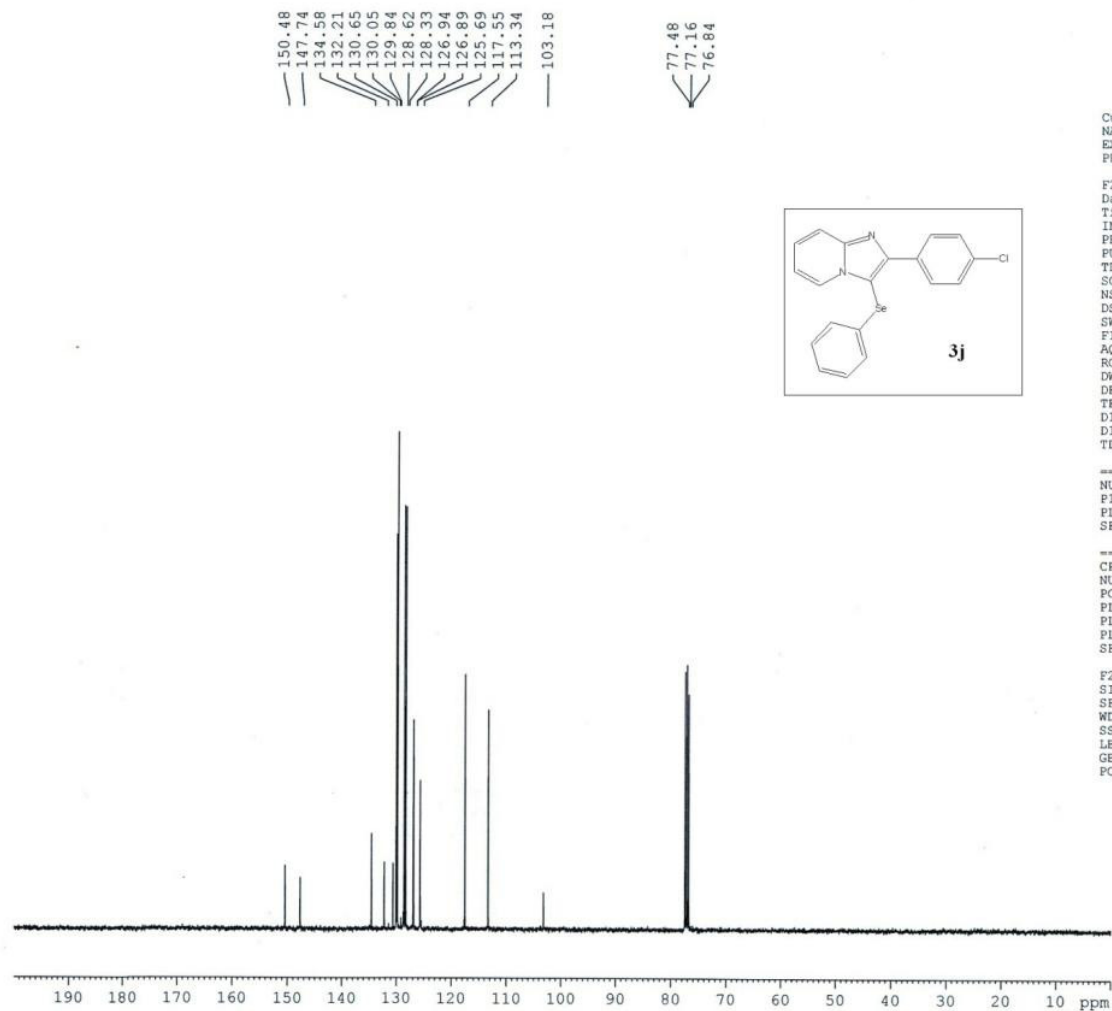


Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 106  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150411  
Time 15.56  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 24  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9923444 sec  
RG 40.87  
DW 60.800 usec  
DE 6.50 usec  
TE 296.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.75 usec  
PLW1 11.99499989 W  
SF01 400.1524711 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1500458 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 111  
PROCNO 1

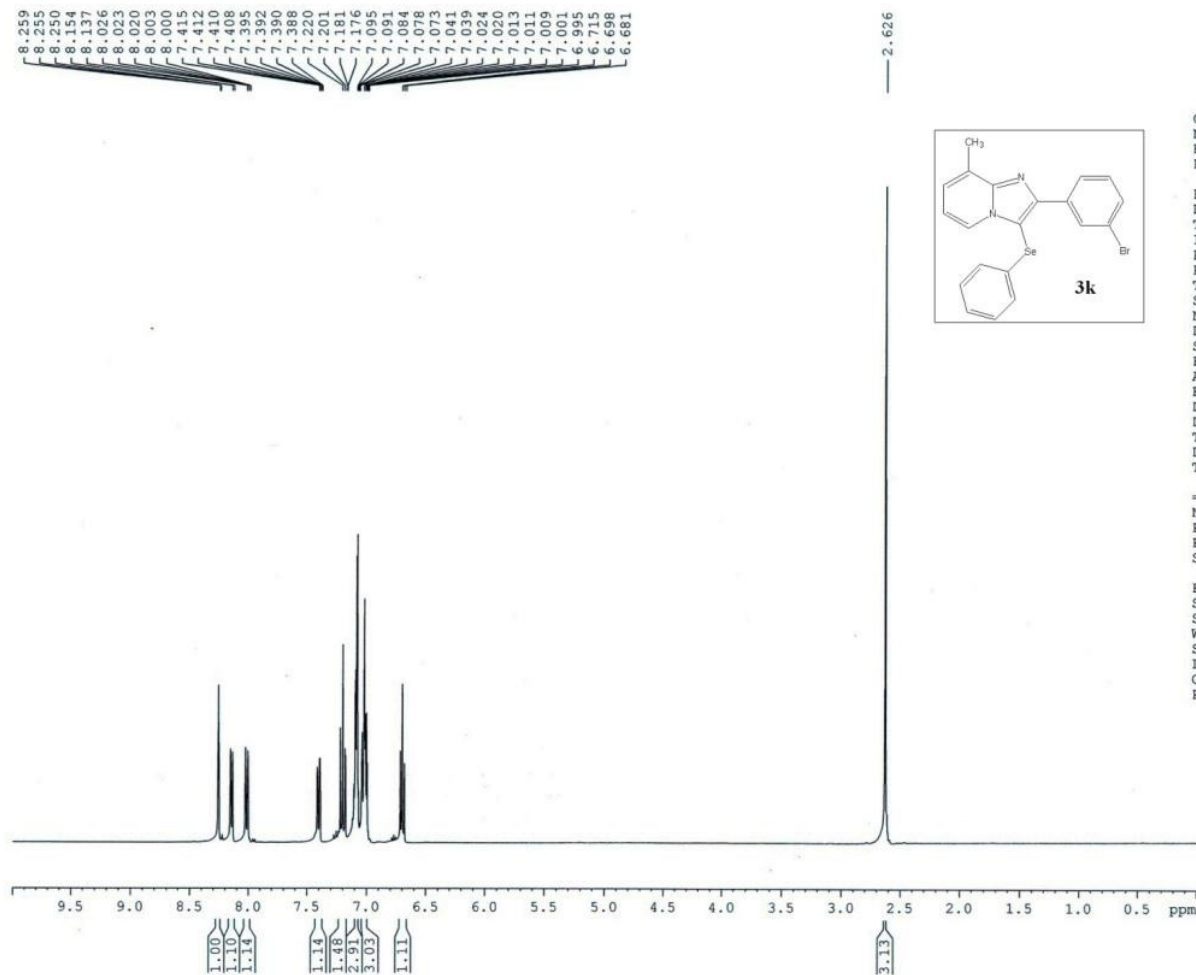
F2 - Acquisition Parameters  
Date\_ 20150411  
Time 17.51  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 320  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6816244 sec  
RG 40.87  
DW 20.800 usec  
DE 6.50 usec  
TE 297.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 12.00000000 W  
PLW12 0.40792999 W  
PLW13 0.26107001 W  
SFO2 400.1516006 MHz

F2 - Processing parameters  
SI 16384  
SF 100.6177909 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



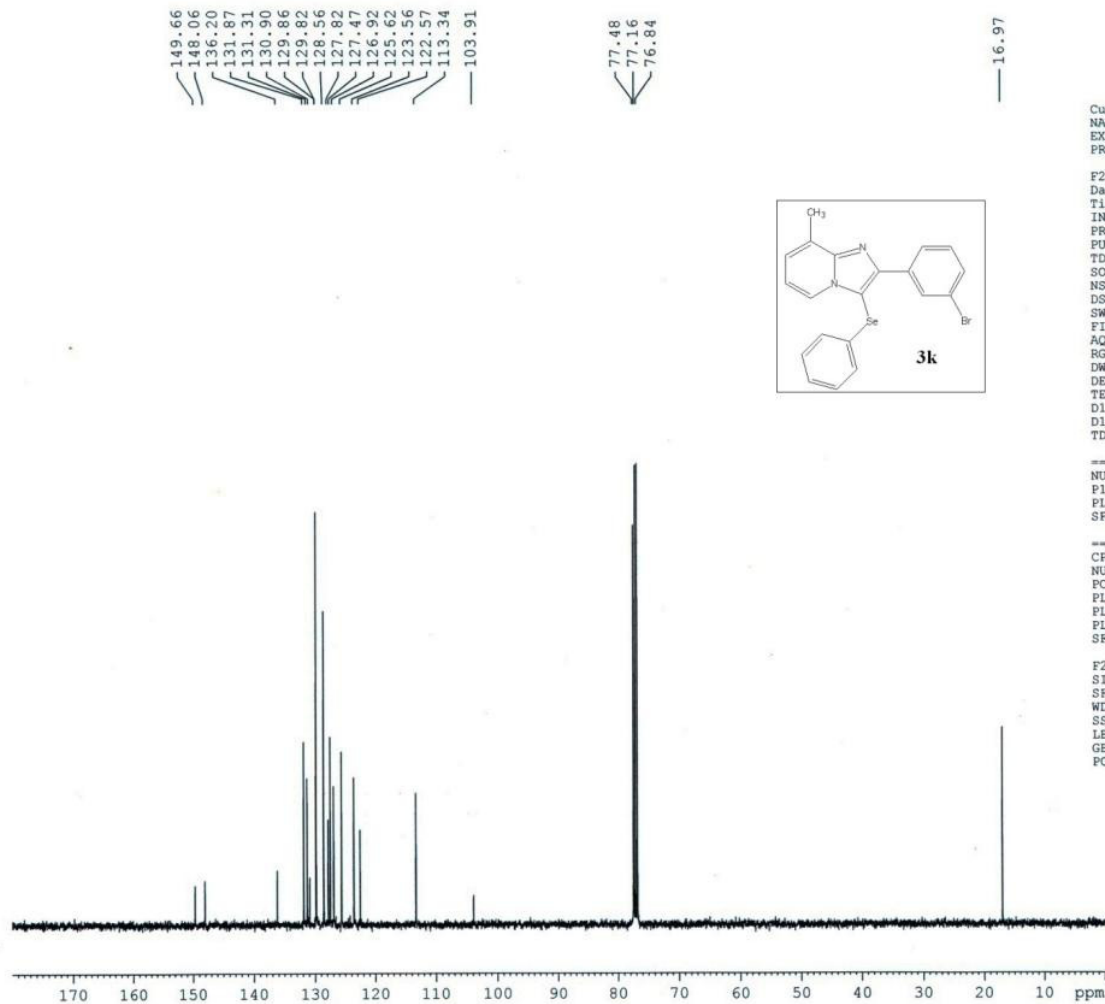


Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 61  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150225  
Time\_ 18.02  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 24  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9923444 sec  
RG 87.66  
DW 60.800 usec  
DE 6.50 usec  
TE 296.7 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.75 usec  
PLW1 11.99499989 W  
SFO1 400.1524711 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1500423 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



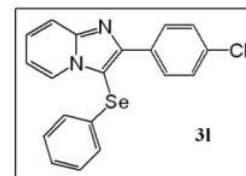
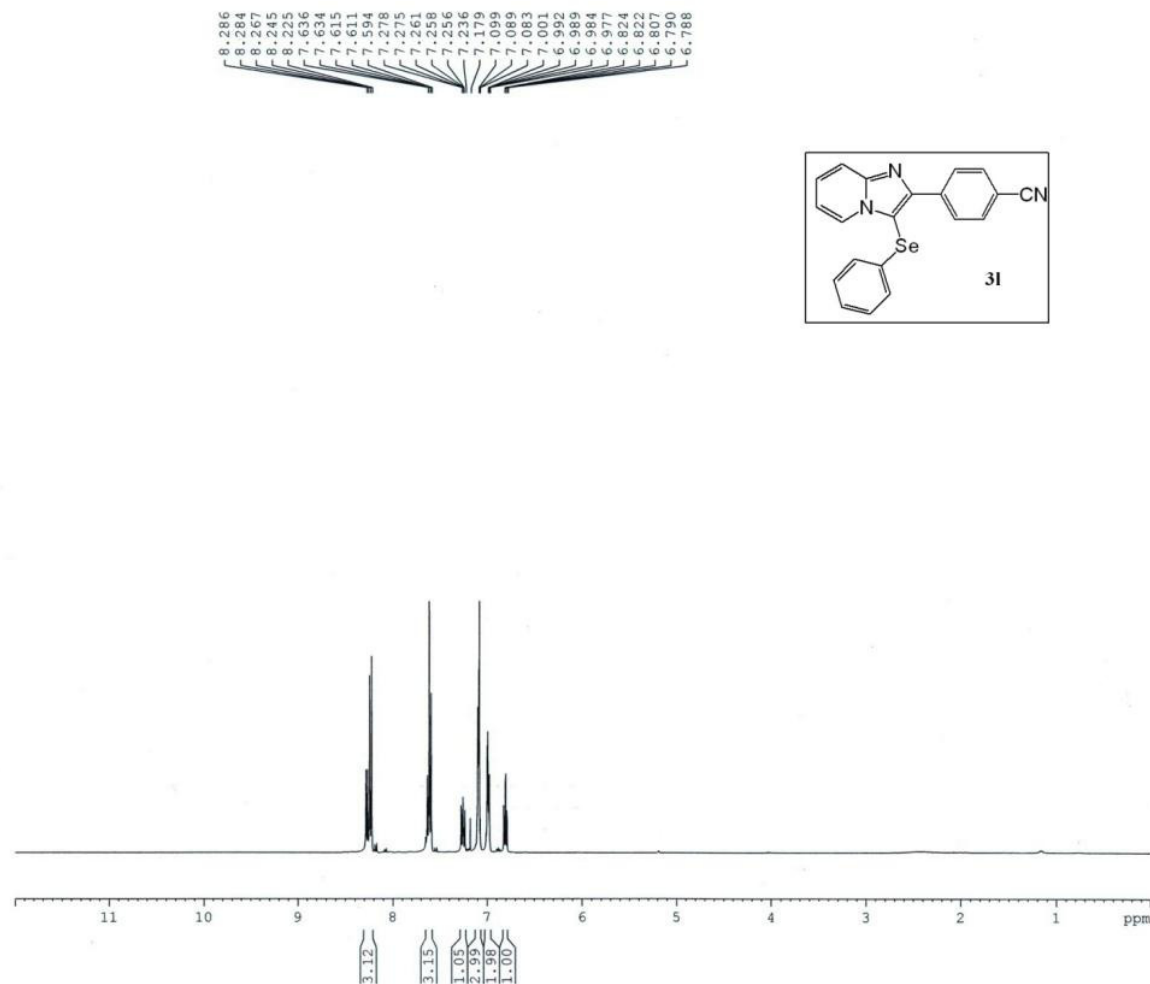
Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 63  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150225  
Time 18.30  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 400  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6816244 sec  
RG 77.59  
DW 20.800 usec  
DE 6.50 usec  
TE 297.8 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 12.00000000 W  
PLW12 0.40792999 W  
PLW13 0.26107001 W  
SFO2 400.1516006 MHz

F2 - Processing parameters  
SI 16384  
SF 100.6177865 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

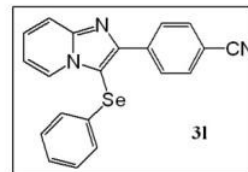
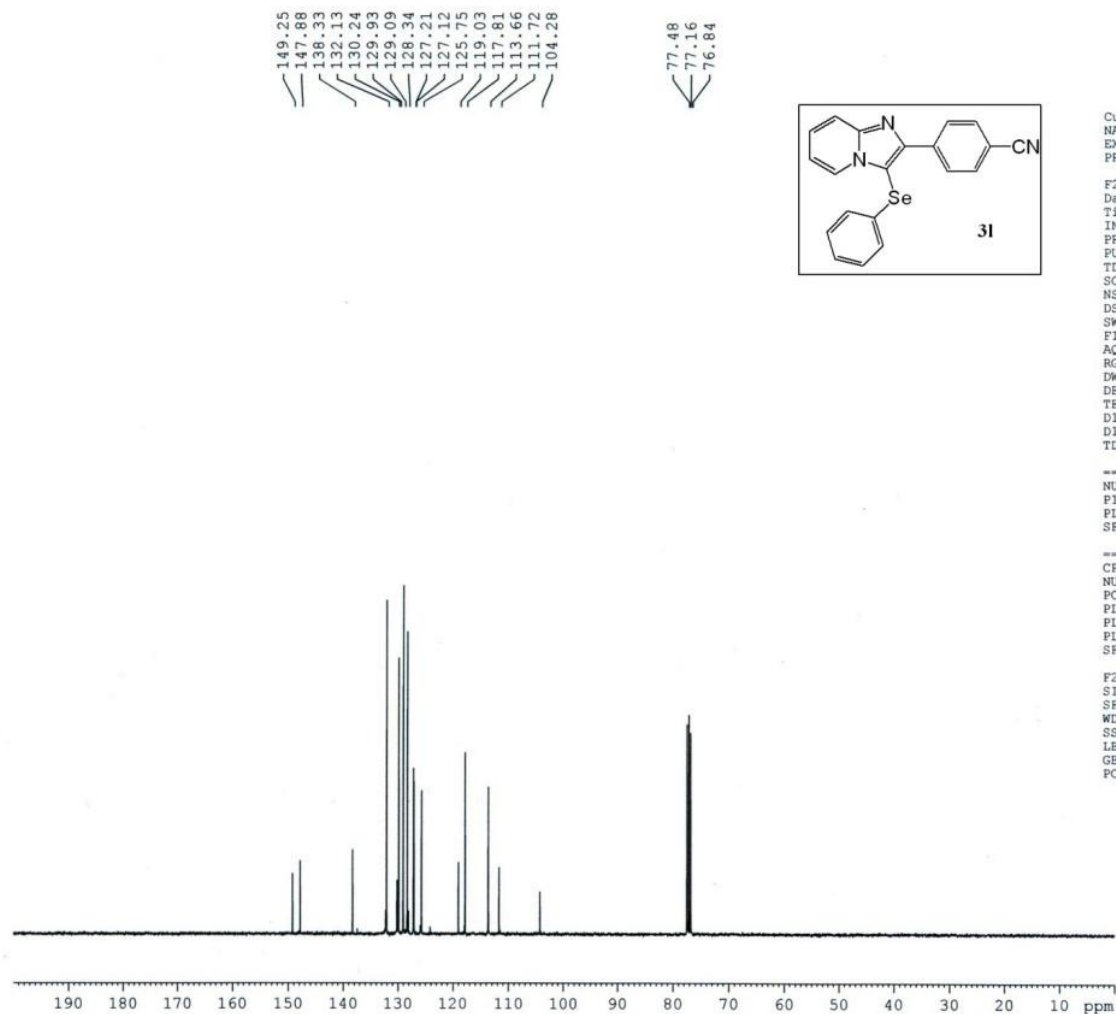


Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 125  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150417  
 Time 11.46  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 40.87  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.2 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SFO1 400.1524711 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500413 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



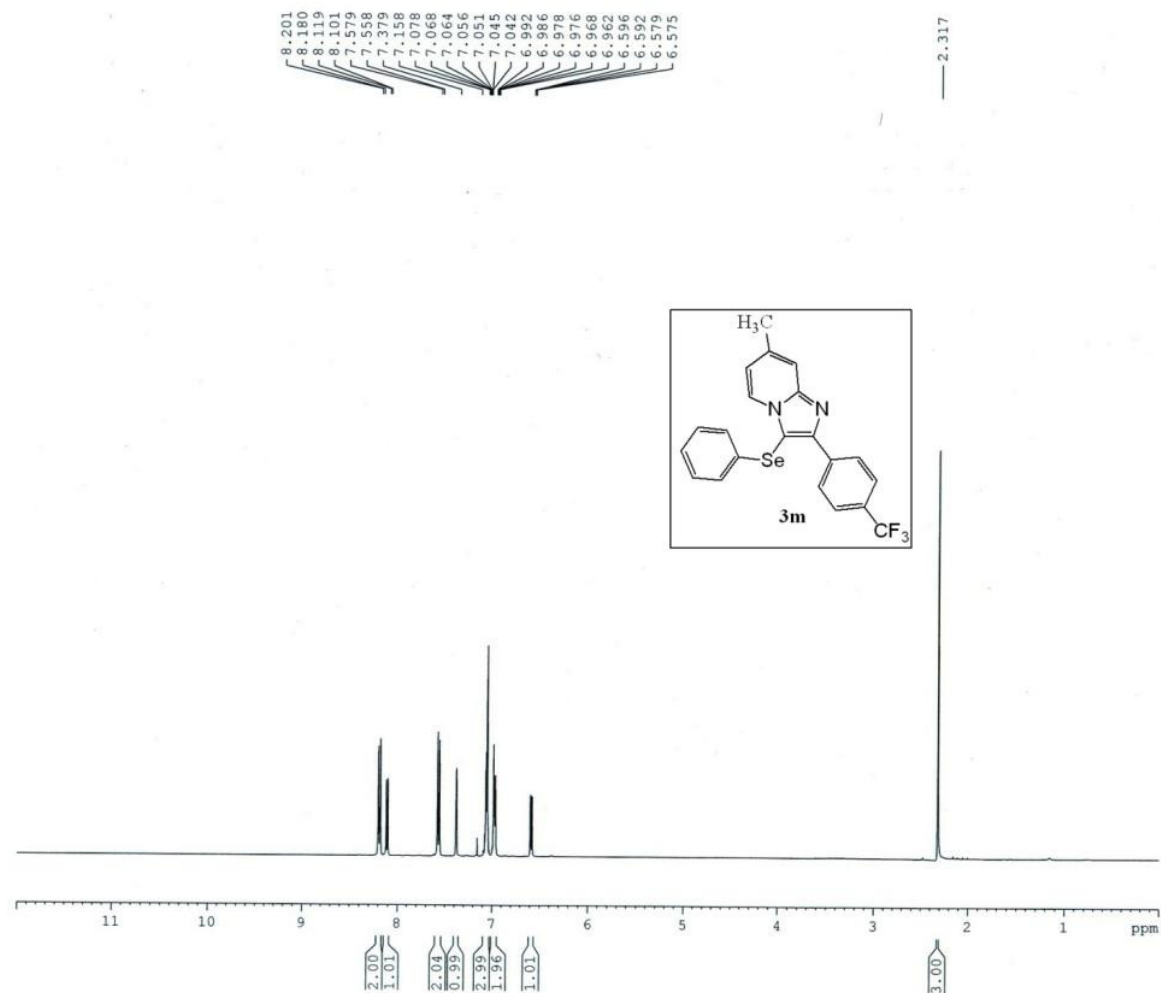
Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 126  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150417  
Time\_ 12.12  
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 0.6816244 sec  
RG 40.87  
DW 20.800 usec  
DE 6.50 usec  
TE 297.5 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 12.00000000 W  
PLW12 0.40792999 W  
PLW13 0.26107001 W  
SFO2 400.1516006 MHz

F2 - Processing parameters  
SI 16384  
SF 100.6177939 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

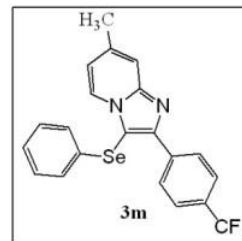
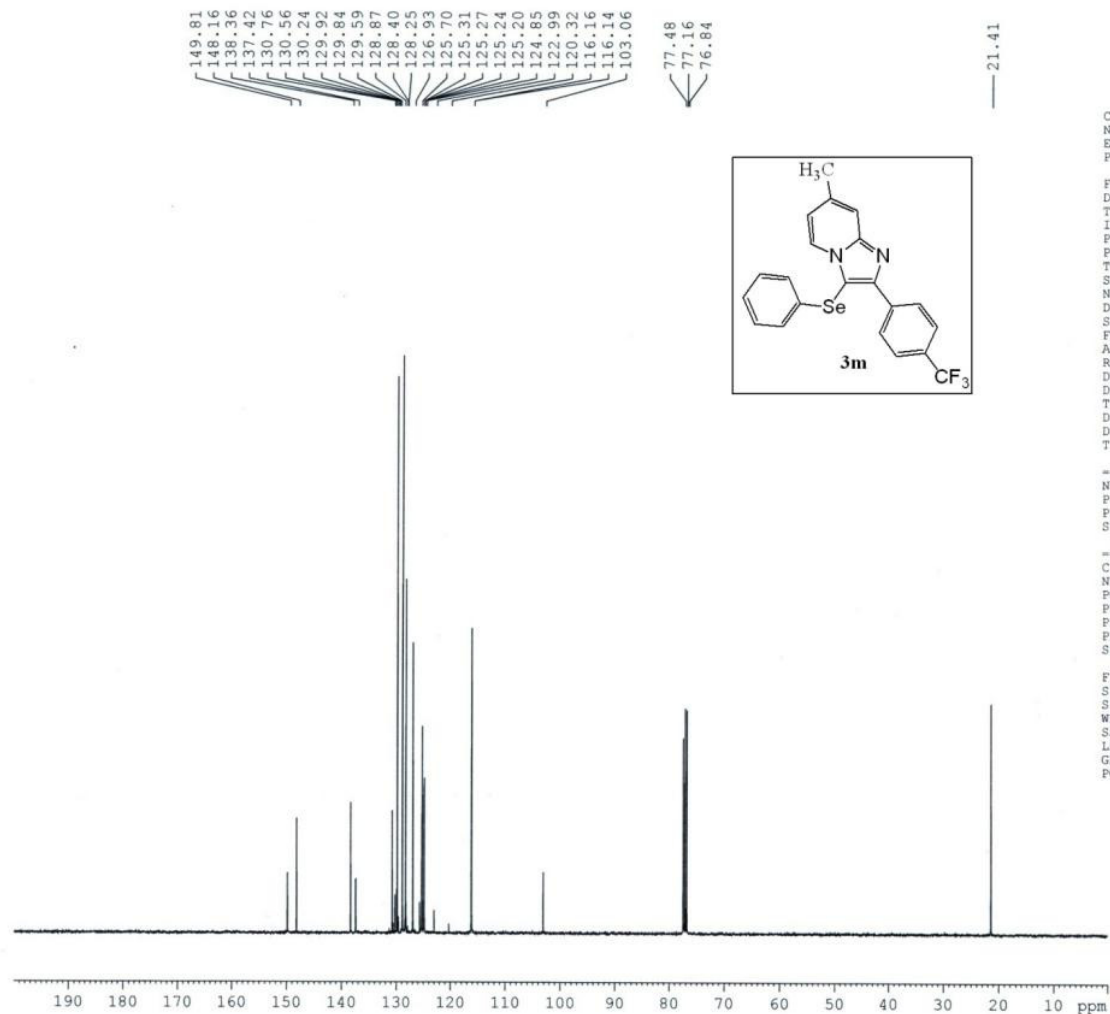


Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 170  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150430  
 Time 12.08  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 40.87  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.3 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SFO1 400.1524711 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500497 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



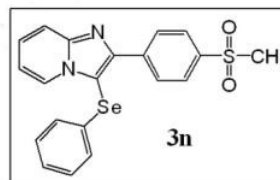
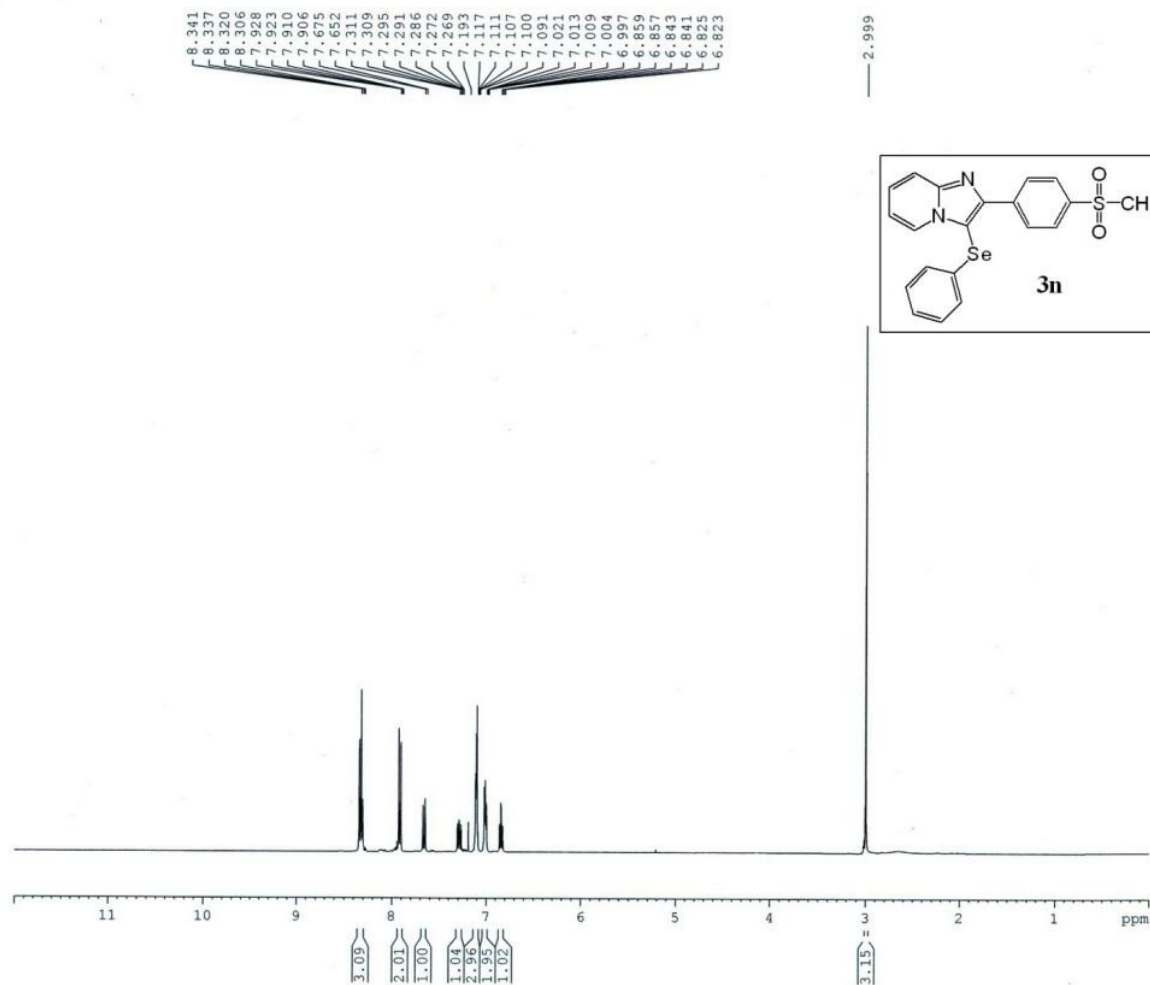
Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 171  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150430  
Time 12.37  
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 0.6816244 sec  
RG 47.25  
DW 20.800 usec  
DE 6.50 usec  
TE 297.6 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 12.00000000 W  
PLW12 0.40792999 W  
PLW13 0.26107001 W  
SFO2 400.1516006 MHz

F2 - Processing parameters  
SI 16384  
SF 100.6177909 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

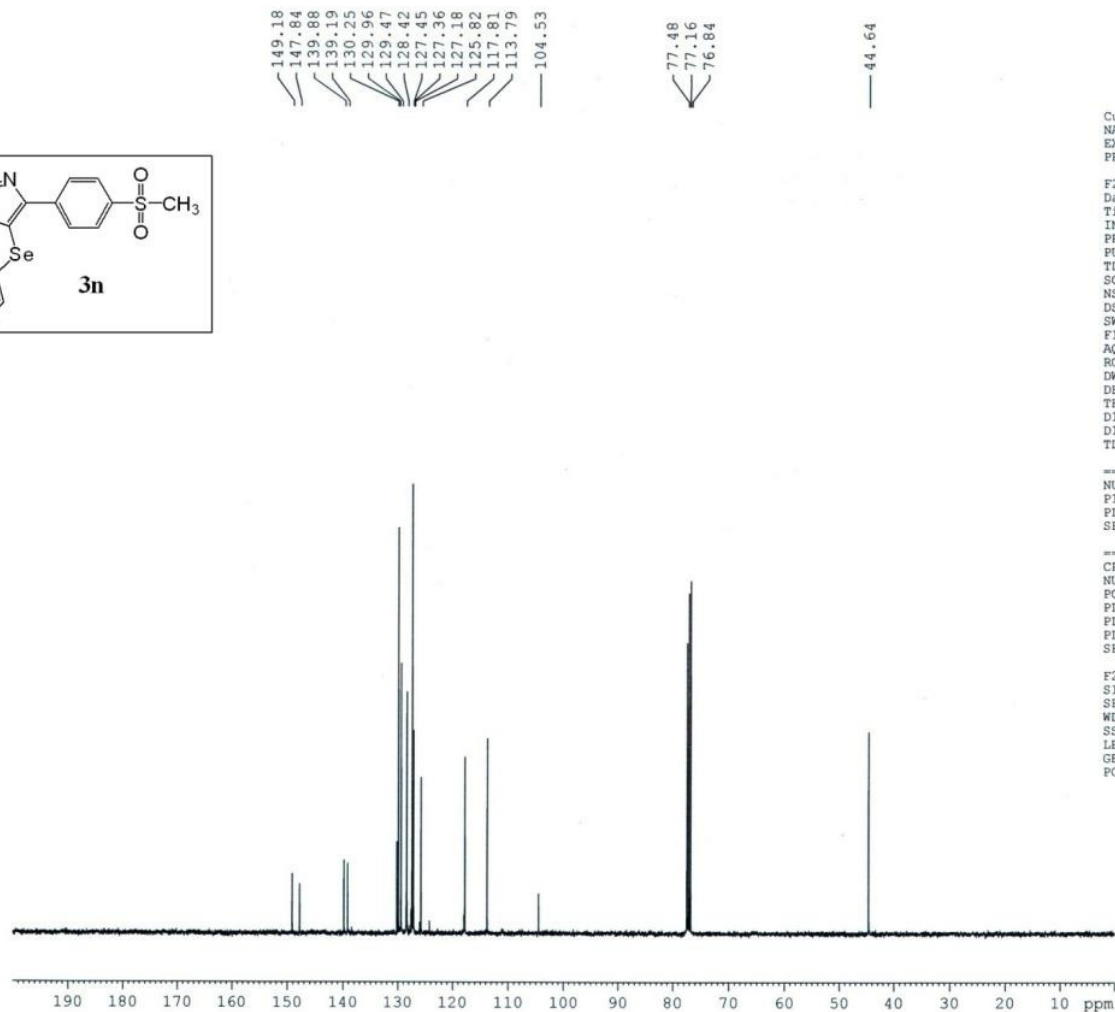
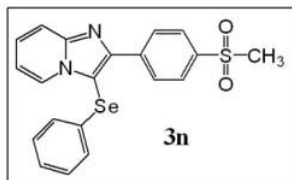


Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 184  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150503  
Time 11.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 24  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9923444 sec  
RG 62.69  
DW 60.800 usec  
DE 6.50 usec  
TE 294.8 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.75 usec  
PLW1 11.99499989 W  
SFO1 400.1524711 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1500358 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 185  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150503  
Time 12.07  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 512  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6816244 sec  
RG 62.69  
DW 20.800 usec  
DE 6.50 usec  
TE 295.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

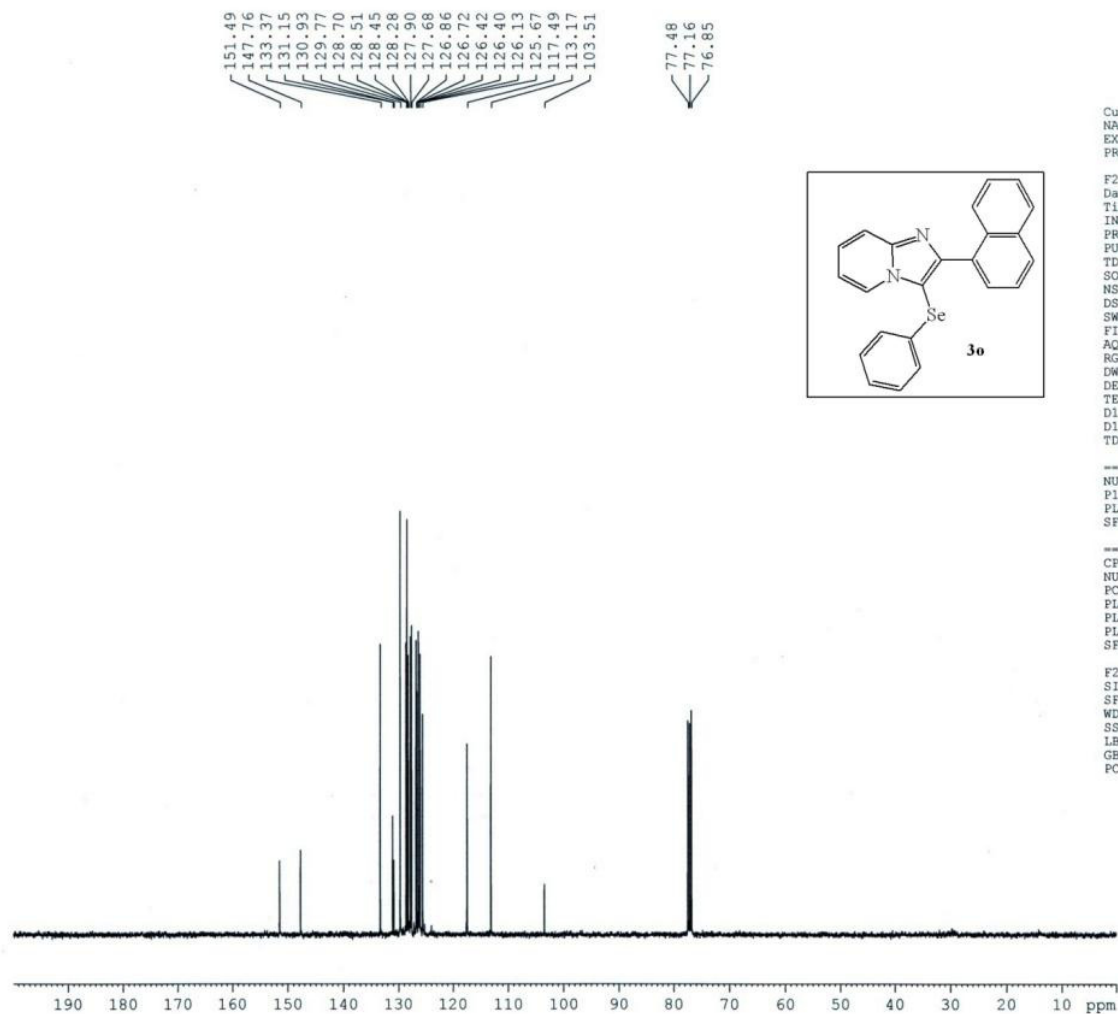
===== CHANNEL f1 =====  
NUC1 13C  
P1 8.90 usec  
PLW1 54.00000000 W  
SFO1 100.6278588 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 12.00000000 W  
PLW12 0.40792999 W  
PLW13 0.26107001 W  
SFO2 400.1516006 MHz

F2 - Processing parameters  
SI 16384  
SF 100.6177910 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40







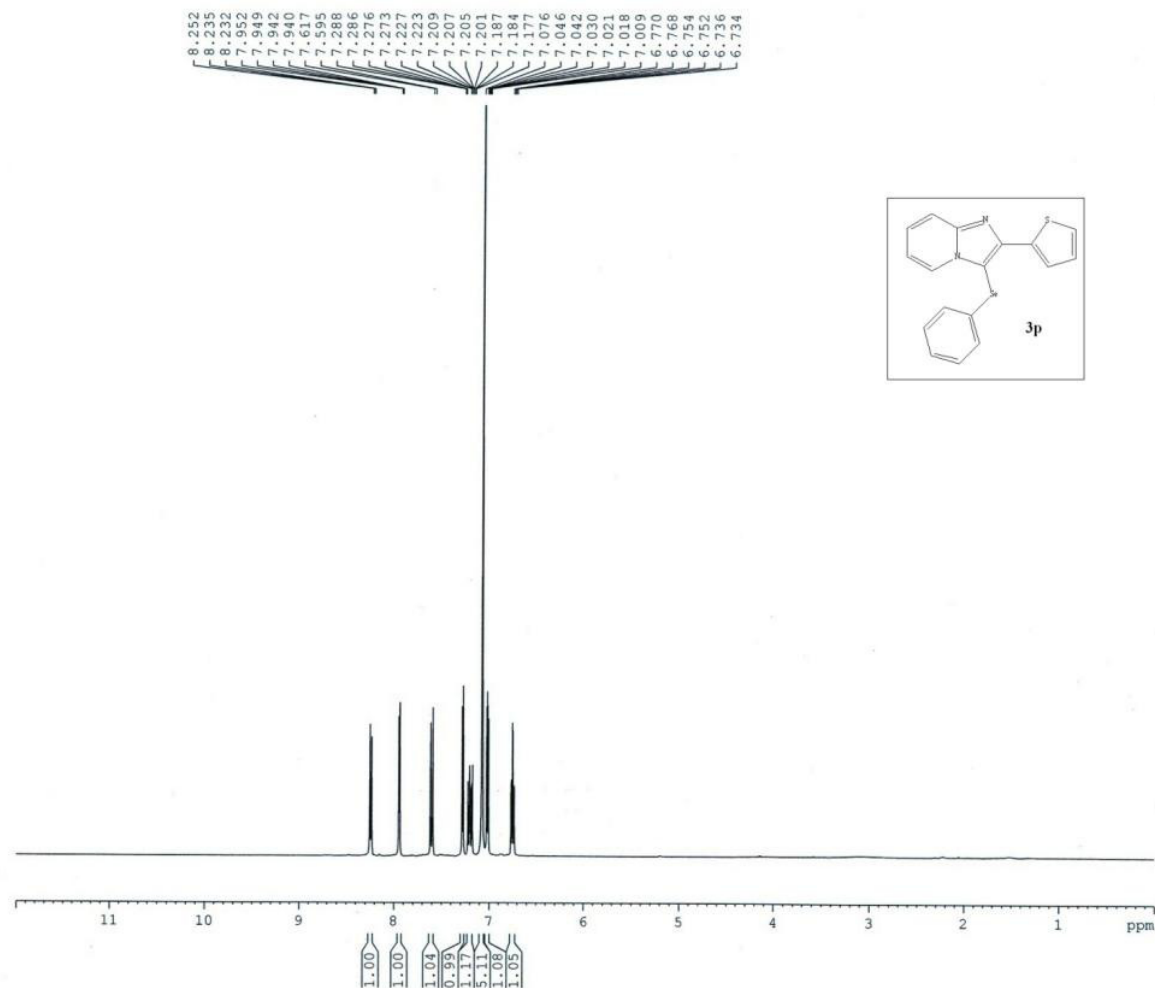
Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 159  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150428  
Time\_ 16.31  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 320  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6816244 sec  
RG 40.87  
DW 20.800 usec  
DE 6.50 usec  
TE 299.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

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

----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 12.00000000 W  
PLW12 0.40792999 W  
PLW13 0.26107001 W  
SFO2 400.1516006 MHz

F2 - Processing parameters  
SI 16384  
SF 100.6177946 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

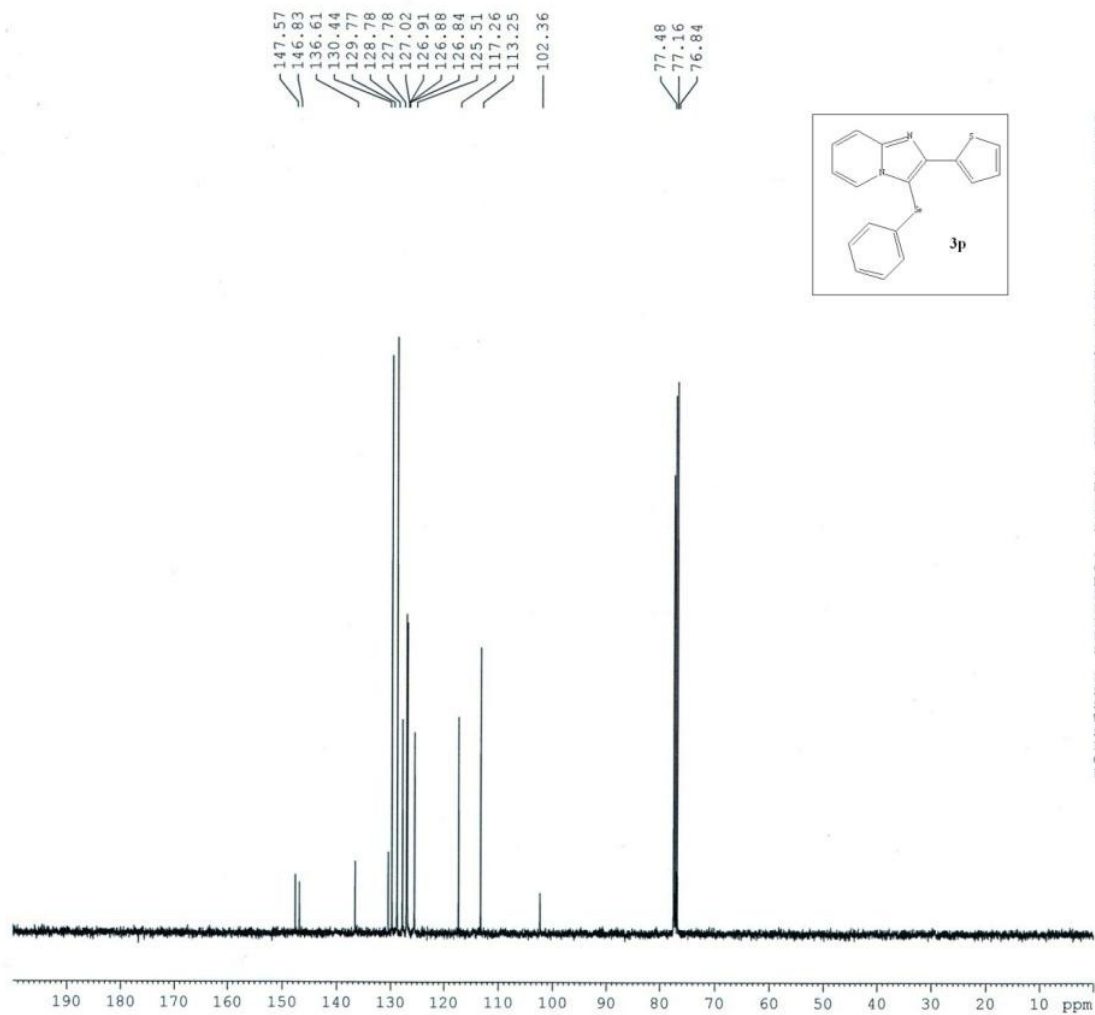


Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 189  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20150504  
 Time 17.37  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDC13  
 NS 24  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 77.59  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.1 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SF01 400.1524711 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500423 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



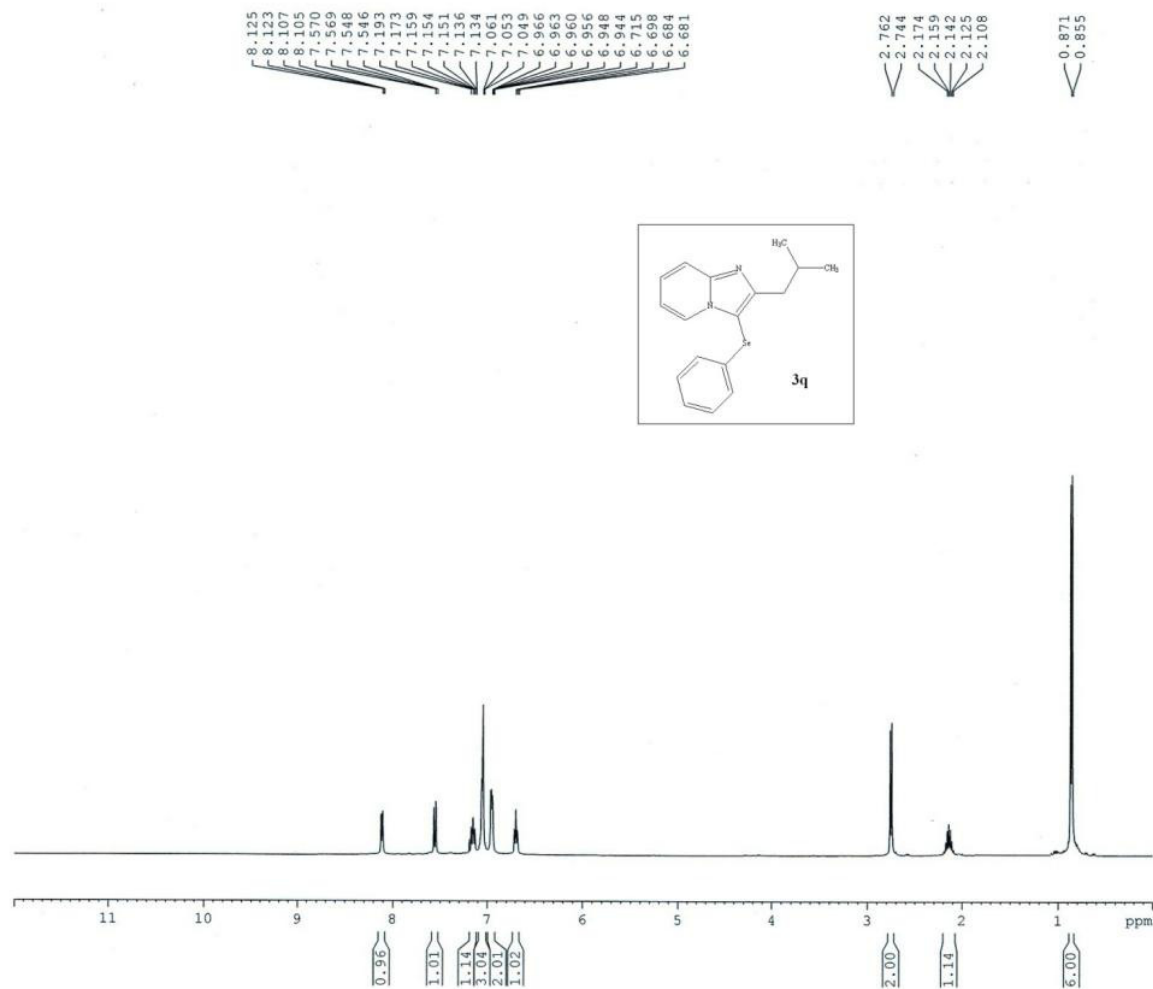
Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 190  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150504  
Time 18.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 320  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6816244 sec  
RG 77.59  
DW 20.800 usec  
DE 6.50 usec  
TE 297.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 12.00000000 W  
PLW12 0.40792999 W  
PLW13 0.26107001 W  
SFO2 400.1516006 MHz

F2 - Processing parameters  
SI 16384  
SF 100.6177895 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

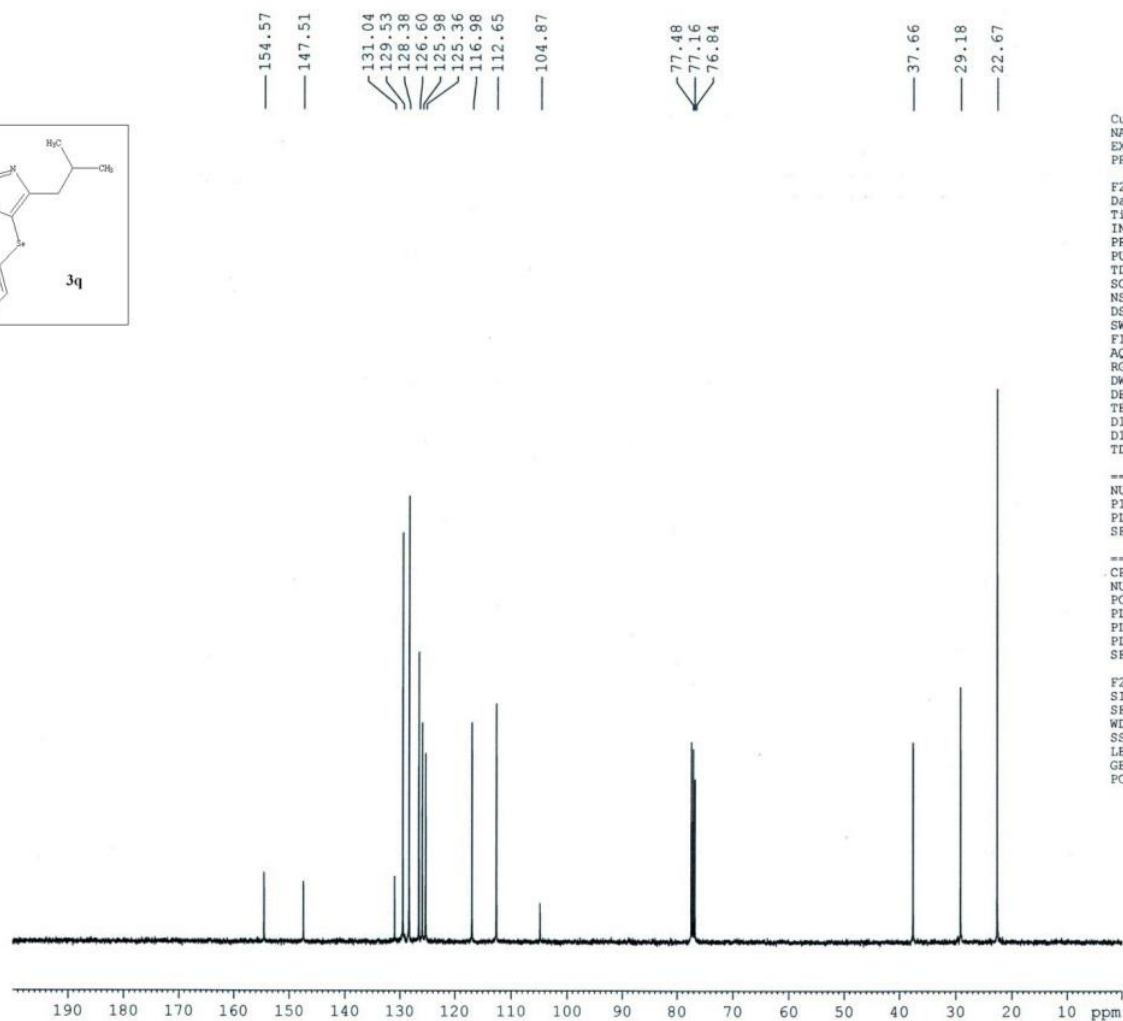
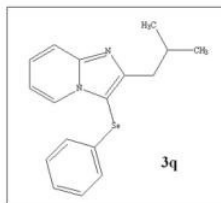


Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 156  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150427  
 Time 12.47  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl<sub>3</sub>  
 NS 24  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 40.87  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.4 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SFO1 400.1524711 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500362 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



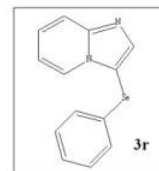
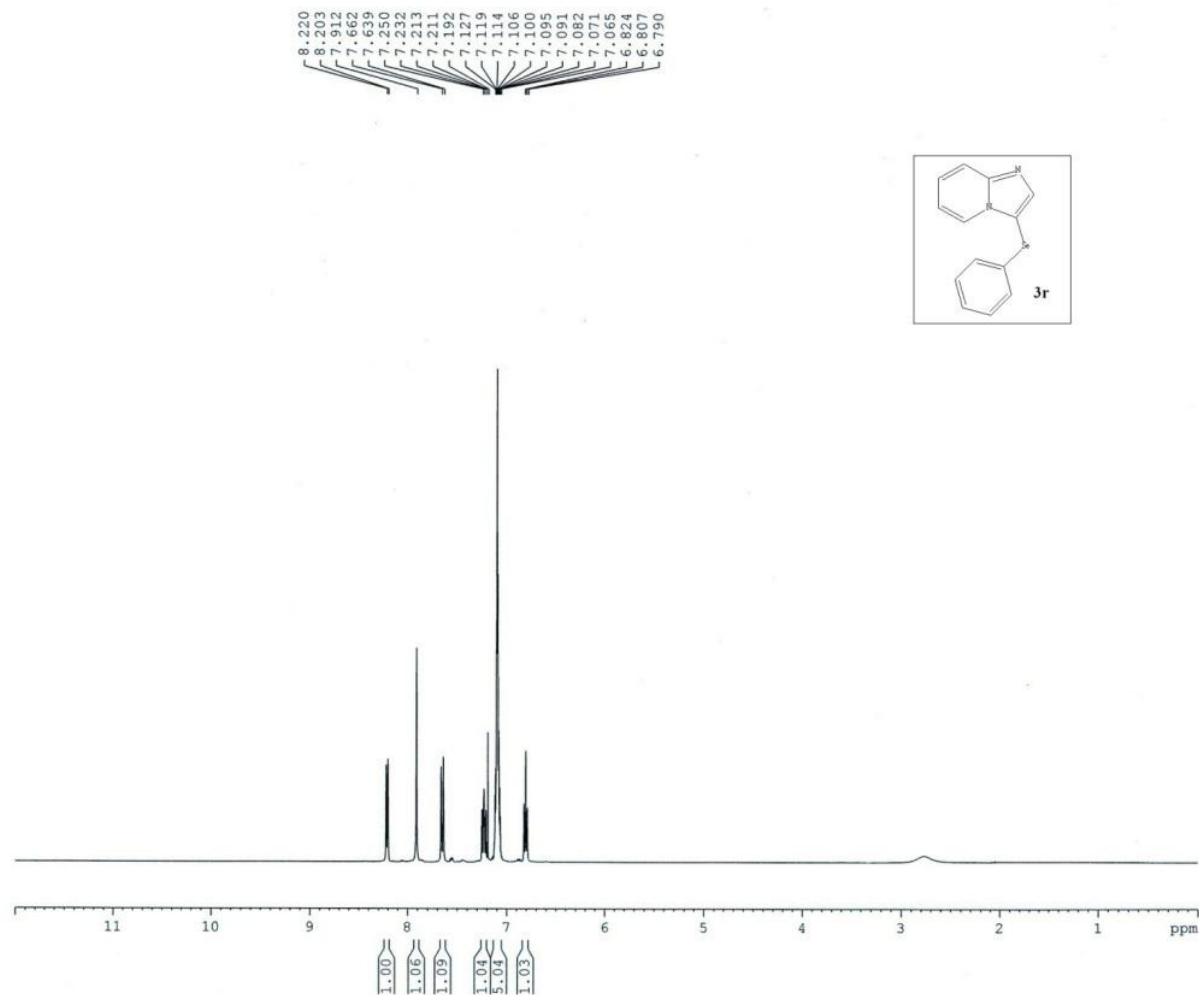
Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 157  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150427  
 Time 13.05  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDC13  
 NS 320  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6816244 sec  
 RG 40.87  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 300.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

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

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.40792999 W  
 PLW13 0.26107001 W  
 SFO2 400.1516006 MHz

F2 - Processing parameters  
 SI 16384  
 SF 100.6177927 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

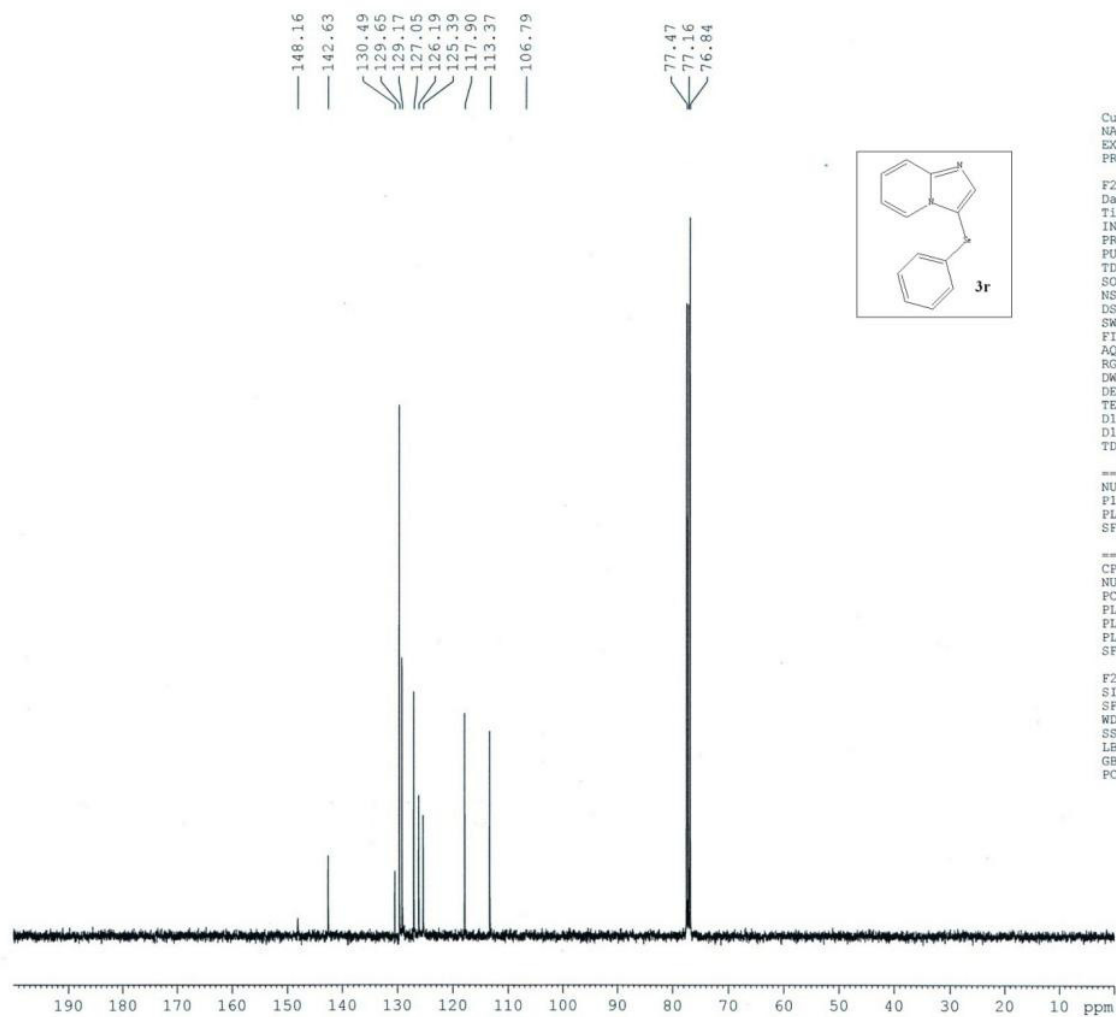


Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 199  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150506  
 Time 11.03  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 24  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 106.66  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 295.6 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SFO1 400.1524711 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500362 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 200  
PROCNO 1

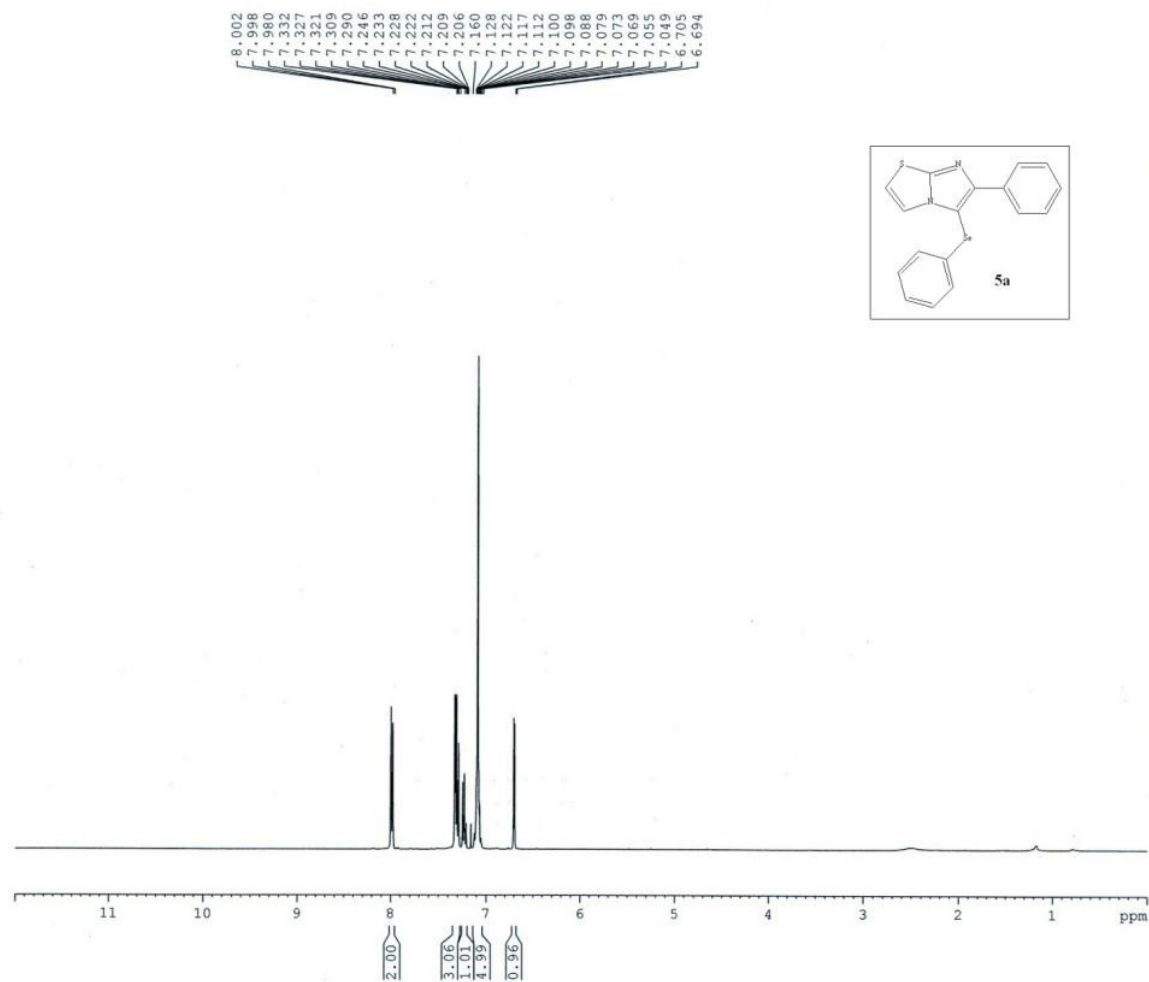
F2 - Acquisition Parameters  
Date\_ 20150506  
Time 11.29  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 512  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6816244 sec  
RG 47.25  
DW 20.800 usec  
DE 6.50 usec  
TE 297.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 12.00000000 W  
PLW12 0.40792999 W  
PLW13 0.26107001 W  
SF02 400.1516006 MHz

F2 - Processing parameters  
SI 16384  
SF 100.6177865 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



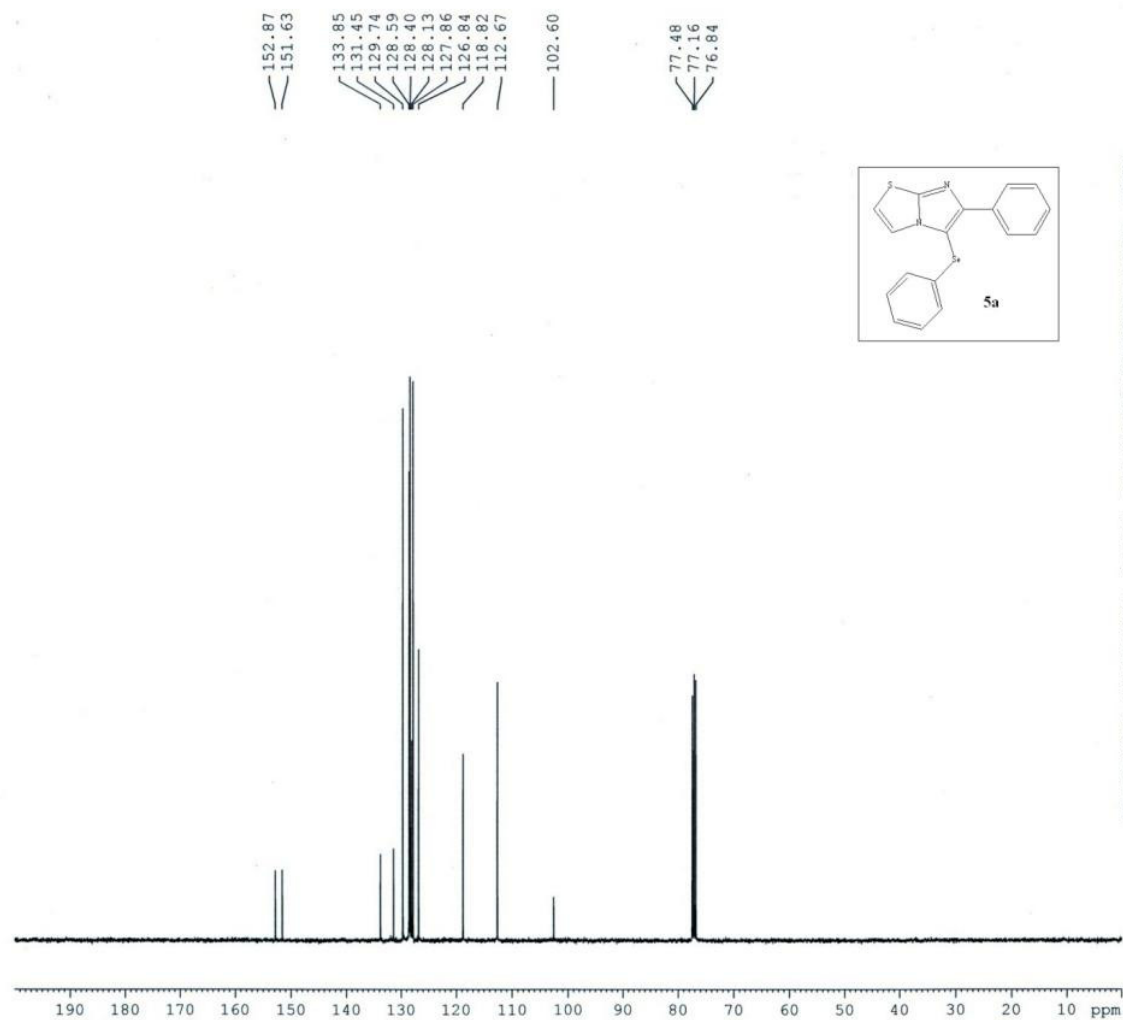


Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 180  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150502  
Time\_ 9.57  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 24  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9923444 sec  
RG 40.87  
DW 60.800 usec  
DE 6.50 usec  
TE 295.7 K  
D1 1.00000000 sec  
TD0 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 14.75 usec  
PLW1 11.99499989 W  
SFO1 400.1524711 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1500492 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



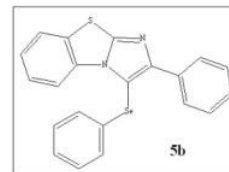
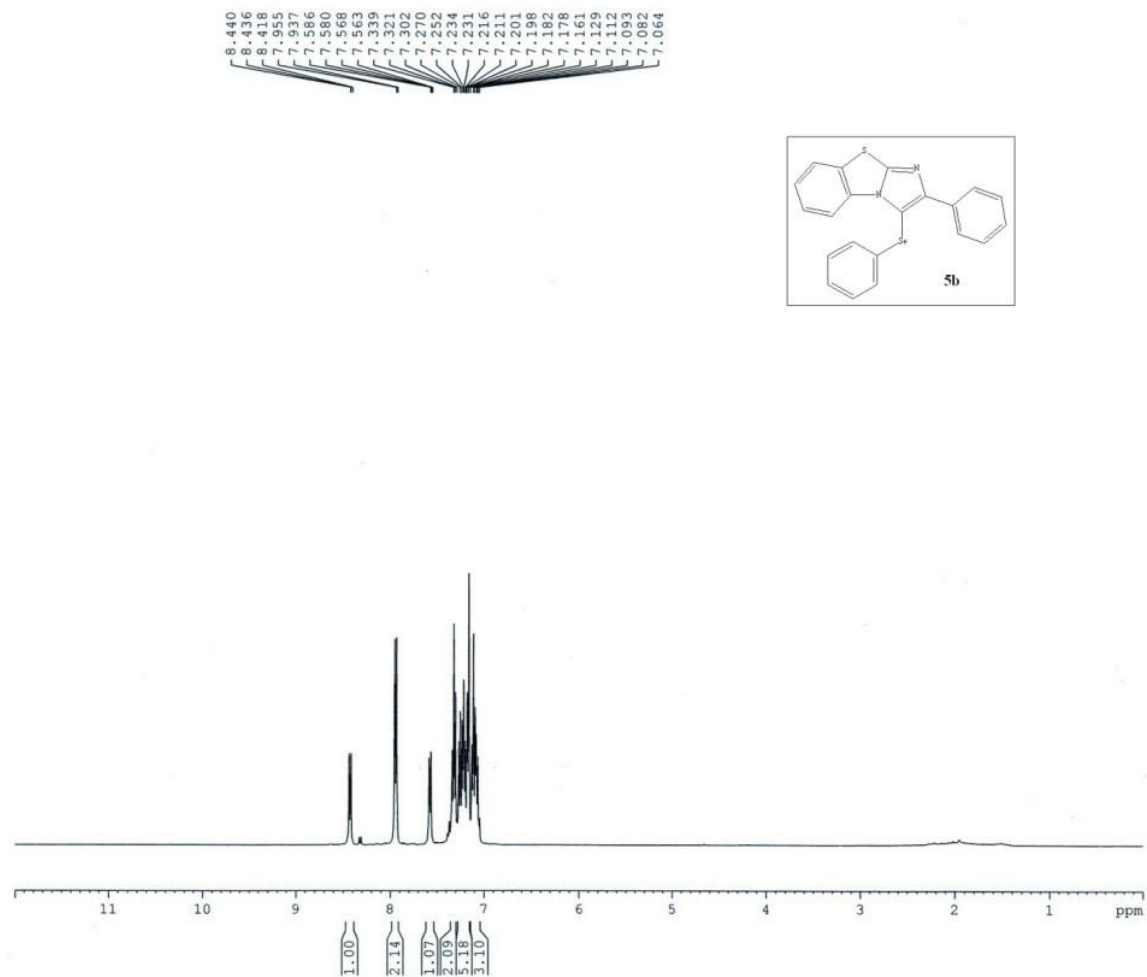
Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 181  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20150502  
 Time 10.22  
 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 0.6816244 sec  
 RG 40.87  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

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

----- CHANNEL f2 -----  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.40792999 W  
 PLW13 0.26107001 W  
 SFO2 400.1516006 MHz

F2 - Processing parameters  
 SI 16384  
 SF 100.6177924 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

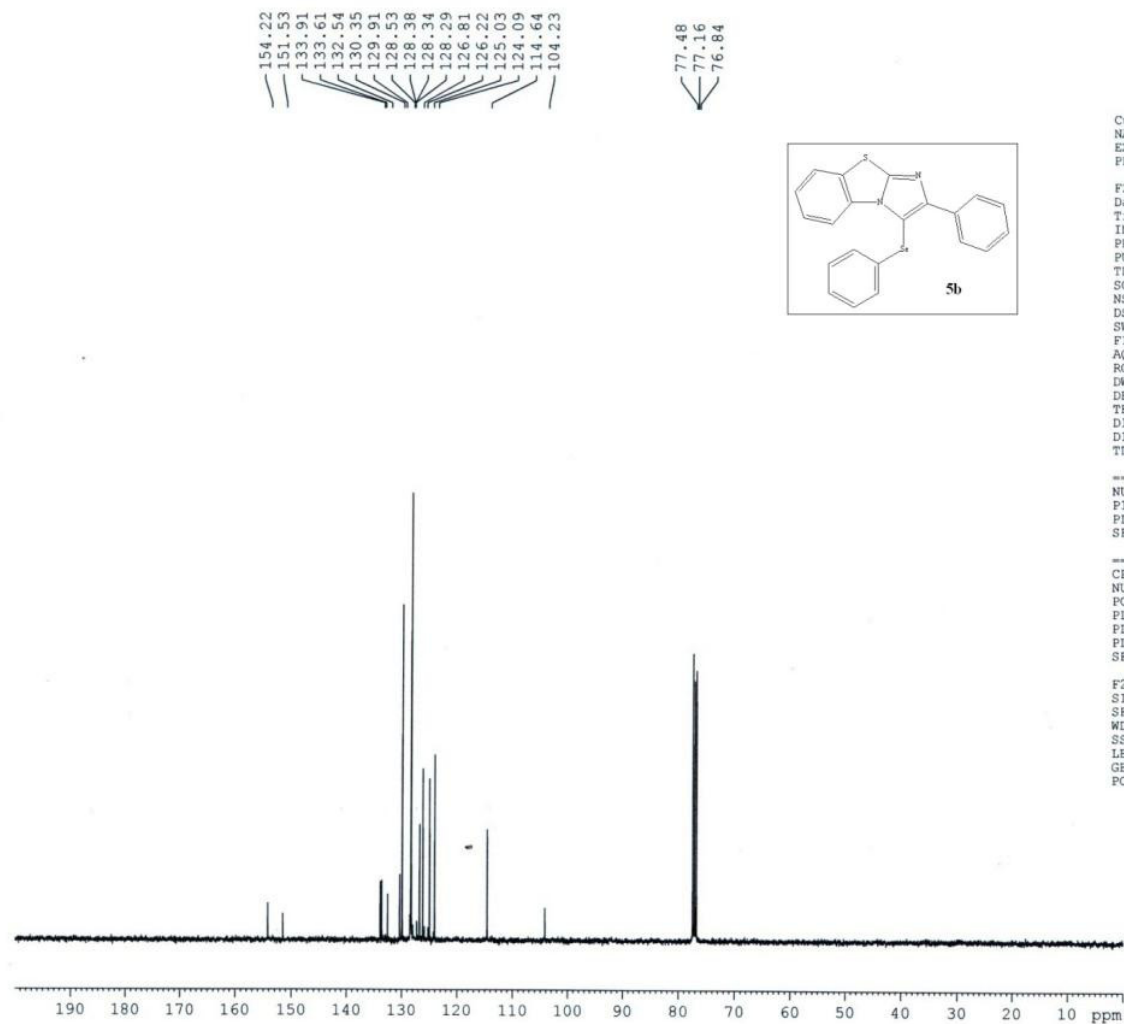


Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 112  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150412  
 Time 11.31  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 67.81  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 294.7 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SFO1 400.1524711 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500487 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



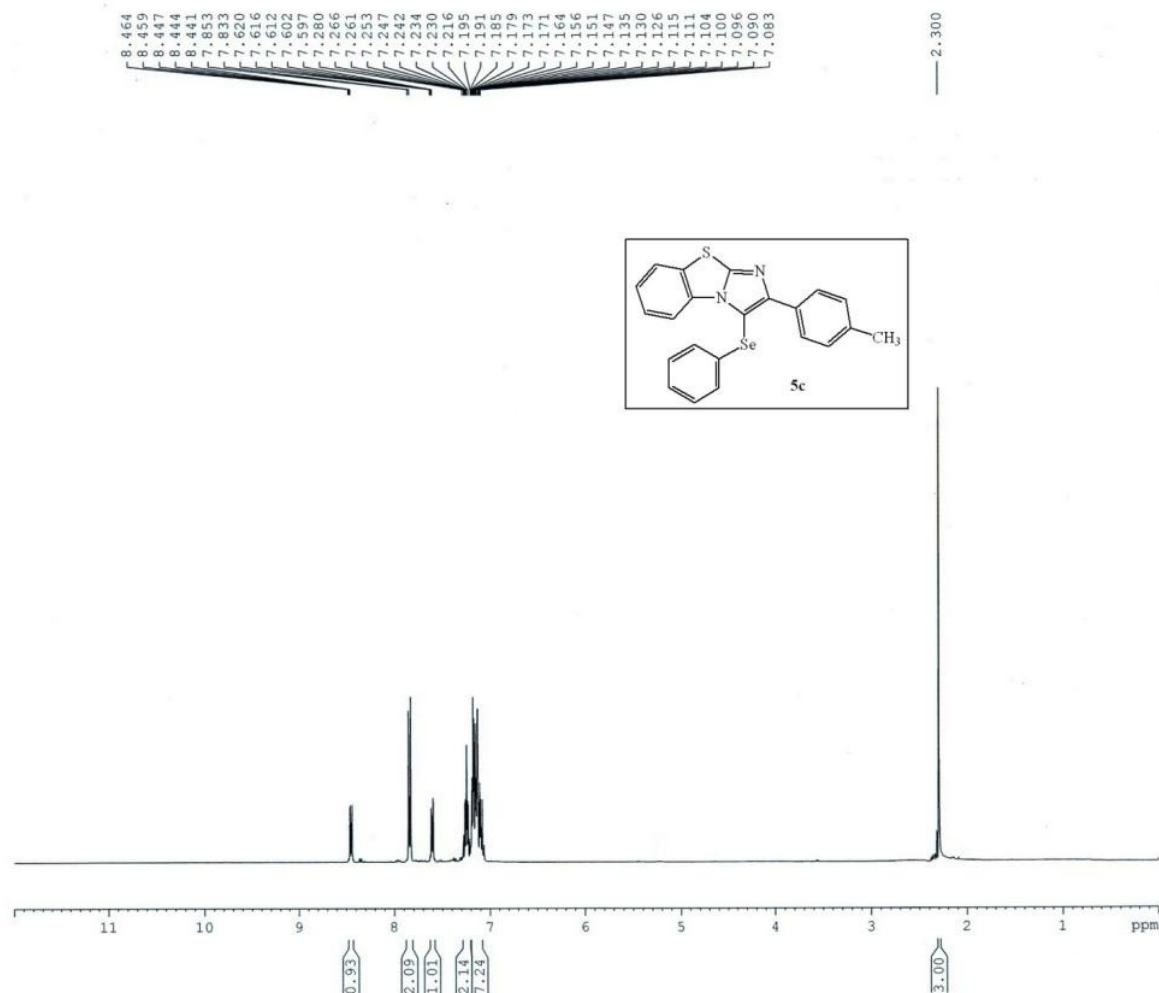
Current Data Parameters  
NAME Dr. A HAJRA 2015  
EXPNO 113  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150412  
Time\_ 11.48  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 320  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6816244 sec  
RG 62.69  
LW 20.800 usec  
DE 6.50 usec  
TE 295.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 12.00000000 W  
PLW12 0.40792999 W  
PLW13 0.26107001 W  
SFO2 400.1516006 MHz

F2 - Processing parameters  
SI 16384  
SF 100.6177901 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

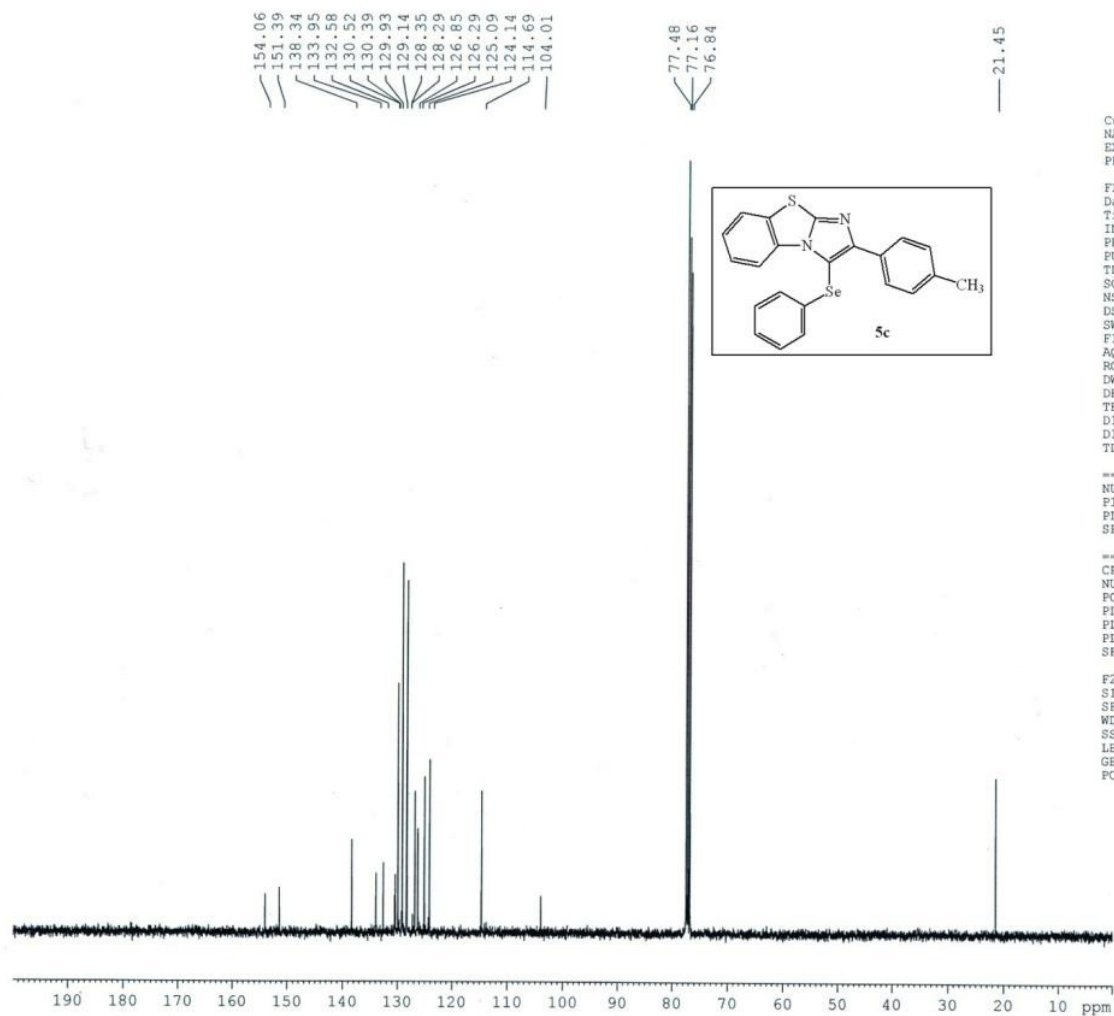


Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 175  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150501  
 Time 10.43  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9923444 sec  
 RG 93.46  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 295.3 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 11.99499989 W  
 SFO1 400.1524711 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500412 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME Dr. A HAJRA 2015  
 EXPNO 182  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150502  
 Time 12.57  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 512  
 DS 2  
 SWH 24036.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6816244 sec  
 RG 93.46  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

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

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.40792999 W  
 PLW13 0.26107001 W  
 SFO2 400.1516006 MHz

F2 - Processing parameters  
 SI 16384  
 SF 100.6177856 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40