

*Supporting Information*

**A new approach to pyridines through the reactions of  
methyl ketones with 1,2,4-triazines**

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## General

All reagents and solvents were obtained from commercial suppliers and used without further purification. All reagents were weighed and handled in air at room temperature. Melting points were recorded on a RY-1 microscopic melting apparatus and uncorrected.  $^1\text{H}$  NMR spectra were recorded on 500 MHz and  $^{13}\text{C}$  NMR spectra were recorded on 125 MHz by using a Bruker Avance 500 spectrometer. Chemical shifts were reported in parts per million ( $\delta$ ) relative to tetramethylsilane (TMS). IR spectra were recorded on a Nicolet iS10 FT-IR spectrometer and only major peaks were reported in  $\text{cm}^{-1}$ . Mass spectra were performed on an Ultima Global spectrometer with an ESI source. The X-ray single-crystal diffraction was performed on Saturn 724+ instrument.

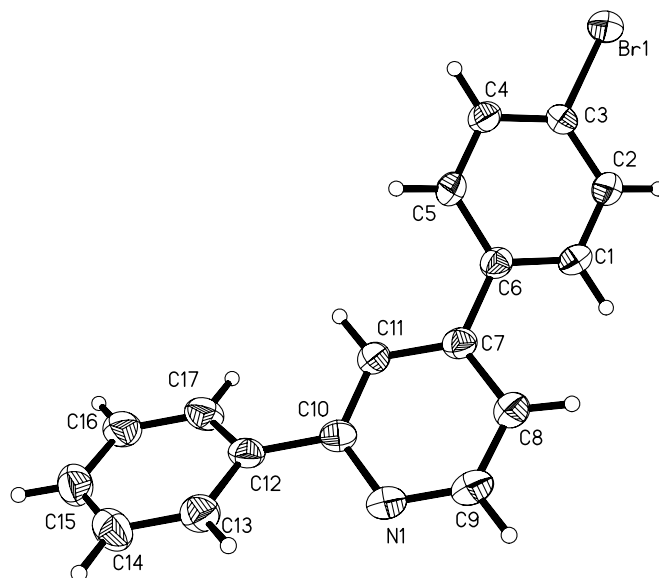
### General procedure for the preparation of 5-aryl-1,2,4-triazine 2a-c (2a for example)

3-hydrazino-5-phenyl-1,2,4-triazine (4.0 mmol), synthesized according to the literature,<sup>1</sup> EtONa (6.0 mmol) and 10 mL ethanol were added to 25 mL flask. The mixture was heated under refluxing for about 6 h. Then 2 M aqueous HCl was added and the mixture was extracted with  $\text{Et}_2\text{O}$  (10 mL  $\times$  3). The organic phase was combined and dried over anhydrous  $\text{Na}_2\text{SO}_4$ . Evaporation of the solvent followed by purification on silica gel (petroleum ether/EtOAc = 4:1, v/v) provided 5-phenyl-1,2,4-triazine (**2a**) as a yellow solid in 75 % yield, which was superior to the literature.<sup>2</sup>

### General procedure for the preparation of pyridine derivatives 3/4 , or 6 (3a/4a for example)

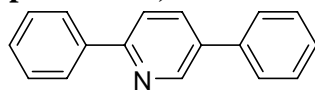
NaOH (2.0 mmol) was added to the mixture of acetophenone **1a** (1.0 mmol) and 5-phenyl-1,2,4-triazine **2a** (1.0 mmol) in 5 mL of ethanol. Then the mixture was stirred at reflux until completion of the reaction. Afterwards, 2 M aqueous HCl was added and the mixture was extracted with  $\text{Et}_2\text{O}$  (5 mL  $\times$  3). The organic phase was combined and dried over anhydrous  $\text{Na}_2\text{SO}_4$ . Evaporation of the solvent followed by purification on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) provided the pure products **3a/4a**.

**4-(4-Bromophenyl)-2-phenylpyridine (4d) (CCDC 955651)**



**Figure S1.** X- Ray Structure of **4d**

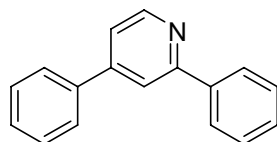
### Characterization data of compounds 3/4, and 6



**3a**

#### 2,5-Diphenylpyridine (3a)

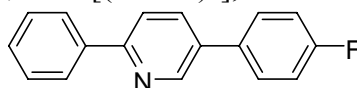
White solid; yield 25 %; mp 169–170 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3062, 3037, 1586, 1556, 1471, 1453, 752, 691;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.95 (d,  $J$  = 2.2 Hz, 1H, N=CH), 8.07 (d,  $J$  = 1.3 Hz, 1H, ArH), 8.05 (s, 1H, ArH), 7.97 (dd,  $J$  = 2.5, 8.2 Hz, 1H, ArH), 7.82 (d,  $J$  = 8.2 Hz, 1H, ArH), 7.66 (d,  $J$  = 1.7 Hz, 1H, ArH), 7.64 (s, 1H, ArH), 7.51 (t,  $J$  = 7.5 Hz, 4H, ArH), 7.41–7.45 (m, 2H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 156.2, 148.1, 139.0, 137.7, 135.0, 134.9, 129.0, 128.9, 128.8, 128.0, 127.0, 126.9, 120.0; HRMS (ESI-TOF $^+$ ):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{14}\text{N}$  [(M + H) $^+$ ], 232.1126; found, 232.1135.



**4a**

#### 2,4-Diphenylpyridine (4a)

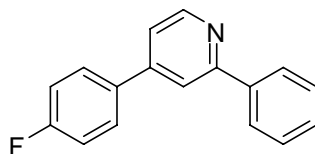
White solid; yield 60 %; mp 70–71 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3060, 3029, 1605, 1594, 1580, 1542, 1471, 1445, 760, 694;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.73 (d,  $J$  = 5.9 Hz, 1H, N=CH), 8.05 (d,  $J$  = 7.4 Hz, 2H, ArH), 7.92 (s, 1H, ArH), 7.69 (d,  $J$  = 7.6 Hz, 2H, ArH), 7.41–7.45 (m, 7H, ArH);  $^{13}\text{C}$  NMR ( $\text{DMSO}-d_6$ , 125 MHz):  $\delta$  = 158.1, 150.1, 149.3, 139.5, 138.6, 129.1, 129.0, 128.8, 127.1, 127.0, 120.3, 118.8; HRMS (ESI-TOF $^+$ ):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{14}\text{N}$  [(M + H) $^+$ ], 232.1126; found, 232.1120.



**3b**

#### 5-(4-Fluorophenyl)-2-phenylpyridine (3b)

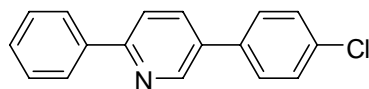
Yellow solid; yield 20 %; mp 182–183 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3050, 1599, 1556, 1519, 1473, 1445, 1239, 829, 757, 692  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.90 (d,  $J$  = 2.3 Hz, 1H, N=CH), 8.04–8.06 (m, 2H, ArH), 7.91 (dd,  $J$  = 2.3, 8.3 Hz, 1H, ArH), 7.81 (d,  $J$  = 8.3 Hz, 1H, ArH), 7.59–7.62 (m, 2H, ArH), 7.51 (d,  $J$  = 7.4, 2H, ArH), 7.44 (d,  $J$  = 7.5 Hz, 1H, ArH), 7.19 (d,  $J$  = 8.6 Hz, 2H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 162.8 (d,  $J_{\text{CF}}^1$  = 247.6 Hz), 156.2, 147.9, 138.9, 134.9, 134.0, 133.8, 129.0, 128.8, 128.6 (d,  $J_{\text{CF}}^3$  = 7.8 Hz), 126.8, 120.3, 116.1 (d,  $J_{\text{CF}}^2$  = 21.5 Hz); HRMS (ESI-TOF $^+$ ):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{13}\text{NF}$  [(M + H) $^+$ ], 250.1032; found, 250.1039.



**4b**

#### 4-(4-Fluorophenyl)-2-phenylpyridine (4b)

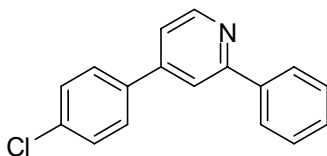
Yellow oil; yield 59 %; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3060, 1606, 1580, 1544, 1513, 14732, 1446, 12392, 827, 775, 695;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.71 (d,  $J$  = 5.1 Hz, 1H, N=CH), 8.03 (d,  $J$  = 7.5 Hz, 2H, ArH), 7.86 (s, 1H, ArH), 7.63–7.66 (m, 2H, ArH), 7.49 (t,  $J$  = 7.6 Hz, 2H, ArH), 7.43 (d,  $J$  = 7.2, 1H, ArH), 7.37 (d,  $J$  = 5.0 Hz, 1H, ArH), 7.16 (d,  $J$  = 8.3 Hz, 2H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 166.0 (d,  $J_{\text{CF}}^1$  = 251.3 Hz), 160.7, 152.7, 150.8, 141.9, 137.2, 131.7, 131.4, 129.6, 122.6, 121.1, 118.7 (d,  $J_{\text{CF}}^2$  = 21.6 Hz); HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{13}\text{NF}$  [(M + H)<sup>+</sup>], 250.1032; found, 250.1039.



3c

#### 5-(4-Chlorophenyl)-2-phenylpyridine (3c)

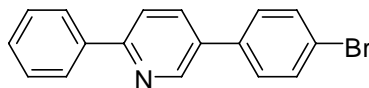
White solid; yield 20 %; mp 193–194 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3059, 1596, 1589, 1551, 1497, 1471, 1447, 824, 737, 691;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.90 (d,  $J$  = 2.2 Hz, 1H, N=CH), 8.04 (d,  $J$  = 7.5 Hz, 2H, ArH), 7.92 (dd,  $J$  = 2.2, 8.3 Hz, 1H, ArH), 7.81 (d,  $J$  = 8.3 Hz, 1H, ArH), 7.57 (d,  $J$  = 8.3 Hz, 2H, ArH), 7.42–7.52 (m, 5H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 156.5, 147.9, 138.8, 136.1, 134.9, 134.3, 133.7, 129.3, 129.1, 128.8, 128.2, 126.8, 120.3; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{13}\text{NCl}$  [(M + H)<sup>+</sup>], 266.0737; found, 266.0745.



4c

#### 4-(4-Chlorophenyl)-2-phenylpyridine (4c)

White solid; yield 61 %; mp 79–81 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3086, 3060, 3029, 1602, 1579, 1541, 1496, 1470, 1445, 821, 776, 697;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.75 (d,  $J$  = 5.3 Hz, 1H, N=CH), 8.05 (d,  $J$  = 7.3 Hz, 2H, ArH), 7.89 (s, 1H, ArH), 7.63 (d,  $J$  = 8.0 Hz, 2H, ArH), 7.44–7.52 (m, 5H, ArH); 7.41 (dd,  $J$  = 1.5, 5.1 Hz, 1H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 158.3, 150.2, 148.0, 139.3, 137.0, 135.3, 129.3, 129.1, 128.8, 128.3, 127.0, 120.0, 118.4; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{13}\text{NCl}$  [(M + H)<sup>+</sup>], 266.0737; found, 266.0725.

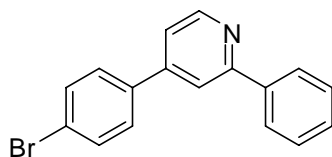


3d

#### 5-(4-Bromophenyl)-2-phenylpyridine (3d)

White solid; yield 21 %; mp 202–204 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3062, 3037, 1630, 1588, 1551, 1470, 1447, 822, 758, 691;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.90 (d,  $J$  = 2.2 Hz, 1H, N=CH), 8.05 (d,  $J$  = 7.6 Hz, 2H, ArH), 7.93 (dd,  $J$  = 2.2, 8.3 Hz, 1H, ArH), 7.82 (d,  $J$  = 8.3 Hz, 1H, ArH), 7.63 (d,  $J$  = 8.3 Hz, 2H, ArH), 7.43–7.52 (m, 5H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 156.5, 147.8, 138.9, 136.6, 134.9, 133.8, 132.3, 129.2,

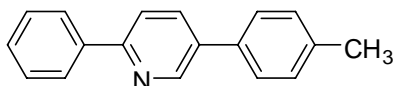
128.9, 128.5, 126.9, 122.5, 120.5; HRMS (ESI-TOF<sup>+</sup>): *m/z* calcd for C<sub>17</sub>H<sub>13</sub>NBr [(M + H)<sup>+</sup>], 310.0231; found, 310.0231.



**4d**

#### 4-(4-Bromophenyl)-2-phenylpyridine (4d)

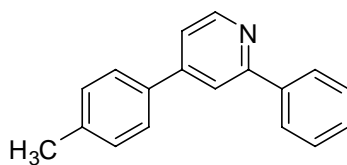
Pale yellow solid; yield 62 %; mp 68–70 °C; IR (KBr)  $\nu_{\text{max}}/\text{cm}^{-1}$ : 3058, 3029, 1598, 1579, 1541, 1496, 1471, 1445, 819, 775, 694; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz):  $\delta$  = 8.75 (d, *J* = 5.3 Hz, 1H, N=CH), 8.05 (t, *J* = 2.0 Hz, 1H, ArH), 8.03 (s, 1H, ArH), 7.89 (d, *J* = 1.4 Hz, 1H, ArH), 7.44–7.466 (m, 7H, ArH), 7.42 (dd, *J* = 1.9, 5.2, 1H, ArH); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz):  $\delta$  = 158.3, 150.2, 148.1, 139.3, 137.5, 132.3, 129.1, 128.8, 128.6, 127.0, 123.5, 119.9, 118.4; HRMS (ESI-TOF<sup>+</sup>): *m/z* calcd for C<sub>17</sub>H<sub>13</sub>NBr [(M + H)<sup>+</sup>], 310.0231; found, 310.0238.



**3e**

#### 2-Phenyl-5-*p*-tolylpyridine (3e)

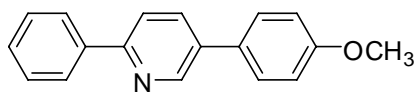
Yellow solid; yield 35 %; mp 148–149 °C; IR (KBr)  $\nu_{\text{max}}/\text{cm}^{-1}$ : 3086, 3027, 2916, 2854, 1615, 1588, 1576, 1473, 1445, 1373, 816, 779, 690; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz):  $\delta$  = 8.93 (d, *J* = 2.2 Hz, 1H, N=CH), 8.05 (d, *J* = 7.6 Hz, 2H, ArH), 7.95 (dd, *J* = 2.4, 8.5, 1H, ArH), 7.80 (d, *J* = 8.3 Hz, 1H, ArH), 7.55 (d, *J* = 8.0 Hz, 2H, ArH), 7.50 (t, *J* = 7.7 Hz, 2H, ArH), 7.43 (t, *J* = 7.6 Hz, 1H, ArH), 7.31 (d, *J* = 7.8 Hz, 2H, ArH), 2.43 (s, 1H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz):  $\delta$  = 155.9, 147.9, 139.1, 138.0, 134.7, 129.8, 129.1, 128.9, 128.8, 128.0, 127.0, 126.8, 120.3, 21.2; HRMS (ESI-TOF<sup>+</sup>): *m/z* calcd for C<sub>18</sub>H<sub>16</sub>N [(M + H)<sup>+</sup>], 246.1283; found, 246.1275.



**4e**

#### 2-Phenyl-4-*p*-tolylpyridine (4e)

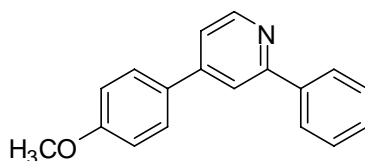
Yellow solid; yield 53 %; mp 89–91 °C; IR (KBr)  $\nu_{\text{max}}/\text{cm}^{-1}$ : 3029, 2918, 2852, 1594, 1578, 1541, 1518, 1471, 1445, 1384, 813, 776, 697; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz):  $\delta$  = 8.73 (d, *J* = 5.1 Hz, 1H, N=CH), 8.06 (d, *J* = 7.6 Hz, 2H, ArH), 7.93 (s, 1H, ArH), 7.61 (d, *J* = 8.0 Hz, 2H, ArH), 7.51 (d, *J* = 7.6 Hz, 2H, ArH), 7.44–7.49 (m, 2H, ArH), 7.32 (d, *J* = 8.0 Hz, 2H, ArH), 2.44 (s, 1H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz):  $\delta$  = 158.1, 150.1, 149.2, 139.6, 139.2, 135.6, 129.8, 129.0, 128.7, 127.0, 126.9, 120.0, 118.5, 21.2; HRMS (ESI-TOF<sup>+</sup>): *m/z* calcd for C<sub>18</sub>H<sub>16</sub>N [(M + H)<sup>+</sup>], 246.1283; found, 246.1276.



**3f**

**5-(4-Methoxyphenyl)-2-phenylpyridine (3f)**

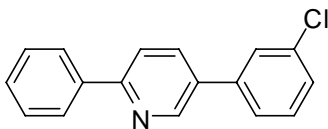
White solid; yield 35 %; mp 159–160 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3059, 2994, 2961, 2836, 1606, 1554, 1520, 1498, 1472, 1372, 1250, 829, 738, 692;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.91 (s, 1H, N=CH), 8.04 (d,  $J$  = 8.1 Hz, 2H, ArH), 7.91 (d,  $J$  = 8.1, 1H, ArH), 7.78 (d,  $J$  = 8.0 Hz, 1H, ArH), 7.58 (d,  $J$  = 8.1 Hz, 2H, ArH), 7.50 (t,  $J$  = 7.5 Hz, 2H, ArH), 7.42 (t,  $J$  = 7.5 Hz, 1H, ArH), 7.03 (d,  $J$  = 8.1 Hz, 2H, ArH), 3.88 (s, 1H,  $\text{OCH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 159.7, 155.5, 147.7, 139.1, 134.5, 130.0, 128.8, 128.1, 126.8, 120.3, 114.6, 55.2; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{18}\text{H}_{16}\text{NO}$  [(M + H)<sup>+</sup>], 262.1232; found, 262.1239.



**4f**

**4-(4-Methoxyphenyl)-2-phenylpyridine (4f)**

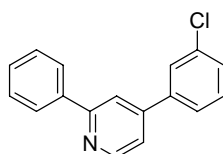
White solid; yield 52 %; mp 72–73 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3036, 2932, 2839, 1594, 1577, 1542, 1517, 1497, 1445, 1260, 823, 776, 691;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.70 (d,  $J$  = 5.2 Hz, 1H, N=CH), 8.05 (d,  $J$  = 1.6 Hz, 1H, ArH), 8.03 (s, 1H, ArH), 7.89 (d,  $J$  = 1.4 Hz, 1H, ArH), 7.66 (d,  $J$  = 8.9 Hz, 2H, ArH), 7.50 (t,  $J$  = 7.5 Hz, 2H, ArH), 7.44 (t,  $J$  = 7.4 Hz, 1H, ArH), 7.41 (dd,  $J$  = 1.7, 5.0 Hz, 1H, ArH), 7.03 (d,  $J$  = 8.9 Hz, 2H, ArH), 3.88 (s, 1H,  $\text{OCH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 160.5, 158.0, 150.0, 148.8, 139.6, 130.8, 128.9, 128.7, 128.2, 127.0, 119.7, 118.2, 114.5, 55.4; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{18}\text{H}_{16}\text{NO}$  [(M + H)<sup>+</sup>], 262.1232; found, 262.1242.



**3g**

**5-(3-Chlorophenyl)-2-phenylpyridine (3g)**

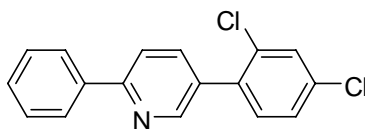
White solid; yield 19 %; mp 189–190 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3086, 3059, 1650, 1588, 1551, 1471, 1447, 1102, 824, 737, 691;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.89 (d,  $J$  = 2.2 Hz, 1H, N=CH), 8.04 (d,  $J$  = 7.5 Hz, 2H, ArH), 7.90 (dd,  $J$  = 2.2, 8.2 Hz, 1H, ArH), 7.80 (d,  $J$  = 8.2 Hz, 1H, ArH), 7.55 (d,  $J$  = 8.5 Hz, 2H, ArH), 7.42–7.51 (m, 5H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 156.5, 147.9, 138.8, 136.1, 134.9, 134.3, 133.7, 129.3, 129.2, 128.8, 128.2, 126.9, 120.4; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{13}\text{NCl}$  [(M + H)<sup>+</sup>], 266.0737; found, 266.0736.



**4g**

**4-(3-Chlorophenyl)-2-phenylpyridine (4g)**

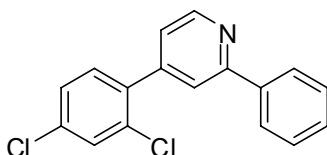
White solid; yield 56 %; mp 80–81 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3060, 3030, 1602, 1581, 1542, 1497, 1466, 1378, 1094, 821, 774, 693;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.89 (d,  $J$  = 5.2 Hz, 1H, N=CH), 8.01 (d,  $J$  = 7.3 Hz, 2H, ArH), 7.81 (s, 1H, ArH), 7.54 (d,  $J$  = 8.0 Hz, 2H, ArH), 7.39–7.48 (m, 5H, ArH), 7.31 (d,  $J$  = 5.2 Hz, 1H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.2, 159.2, 156.9, 148.3, 145.9, 144.3, 138.3, 138.1, 137.8, 137.3, 136.0, 128.9, 127.4; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{13}\text{NCl}$  [(M + H)<sup>+</sup>], 266.0737; found, 266.0742.



**3h**

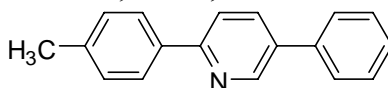
**5-(2,4-Dichlorophenyl)-2-phenylpyridine (3h)**

White solid; yield 18 %; mp 111–112.5 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3077, 3057, 1653, 1585, 1559, 1544, 1487, 1445, 1104, 737, 686;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.74 (d,  $J$  = 1.5 Hz, 1H, N=CH), 8.05 (d,  $J$  = 7.3 Hz, 2 H, ArH), 7.80–7.86 (m, 2 H, ArH), 7.43–7.55 (m, 4 H, ArH), 7.32–7.37 (m, 2 H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 156.8, 149.7, 138.8, 137.5, 135.4, 134.6, 133.6, 132.4, 131.9, 129.2, 128.8, 127.5, 126.9, 119.6; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{12}\text{NCl}_2$ [(M + H)<sup>+</sup>], 300.0347; found, 300.0352.



**4-(2,4-Dichlorophenyl)-2-phenylpyridine (4h)**

White solid; yield 57 %; mp 82–83 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3077, 3060, 1603, 1581, 1561, 1486, 1464, 1104, 770, 687;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.74 (d,  $J$  = 4.6 Hz, 1H, N=CH), 8.02 (d,  $J$  = 7.2 Hz, 2 H, ArH), 7.77 (s, 1 H, ArH), 7.25–7.54 (m, 7 H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 157.7, 149.7, 146.7, 139.1, 136.7, 135.1, 133.1, 130.1, 129.2, 128.8, 127.5, 127.0, 122.4, 121.0; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{12}\text{NCl}_2$ [(M + H)<sup>+</sup>], 300.0347; found, 300.0349.



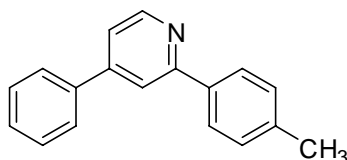
**3i**

**5-Phenyl-2-p-tolylpyridine (3i)**

White solid; yield 25 %; mp 143–144 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3053, 3025, 2915, 2854, 1611, 1590, 1556, 1471, 1447, 1373, 822, 771, 697;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  =



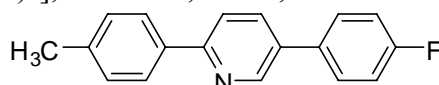
8.92 (d,  $J = 2.3$  Hz, 1H, N=CH), 7.92–7.96 (m, 3H, ArH), 7.78 (d,  $J = 8.5$ , 1H, ArH), 7.62–7.64 (m, 2 H, ArH), 7.48–7.51 (m, 2H, ArH), 7.39–7.42 (m, 1 H, ArH), 7.30 (d,  $J = 8.2$  Hz, 2H, ArH), 2.42 (s, 1H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz):  $\delta = 158.7$ , 150.5, 141.6, 140.30, 138.7, 137.6, 137.1, 132.1, 131.6, 130.5, 129.5, 129.2, 122.6, 23.8; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for C<sub>18</sub>H<sub>16</sub>N [(M + H)<sup>+</sup>], 246.1283; found, 246.1289.



**4i**

#### 4-Phenyl-2-*p*-tolylpyridine (4i)

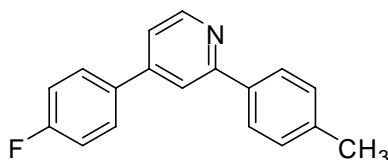
Pale yellow; solid yield 58 %; mp 57–58 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3057, 3029, 2919, 2859, 1595, 1574, 1541, 1516, 1497, 1469, 1448, 1375, 821, 779, 696; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz):  $\delta = 8.72$  (d,  $J = 5.2$  Hz, 1H, N=CH), 7.95 (d,  $J = 7.9$  Hz, 2 H, ArH), 7.90 (s, 1 H, ArH) 7.68–7.70 (m, 2H, ArH), 7.49–7.52 (m, 2H, ArH), 7.44–7.47 (m, 1 H, ArH), 7.42 (dd,  $J = 1.7, 5.3$  Hz, 1 H, ArH), 7.30 (d,  $J = 8.1$  Hz, 2 H, ArH), 2.41 (s, 1H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125MHz):  $\delta = 158.1$ , 150.1, 149.3, 139.1, 138.7, 136.7, 129.6, 129.2, 129.1, 127.2, 127.0, 120.1, 118.5, 21.4; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for C<sub>18</sub>H<sub>16</sub>N [(M + H)<sup>+</sup>], 246.1283; found, 246.1286.



**3j**

#### 5-(4-Fluorophenyl)-2-*p*-tolylpyridine (3j)

White solid; solid yield 18 %; mp 185–186 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3018, 2921, 1600, 1552, 1514, 1473, 1373, 1224, 818; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz):  $\delta = 8.86$  (d,  $J = 2.3$  Hz, 1H, N=CH), 7.94 (d,  $J = 8.0$  Hz, 2 H, ArH), 7.88 (dd,  $J = 2.3, 8.2$  Hz, 1H, ArH), 7.77 (d,  $J = 8.2$  Hz, 1 H, ArH), 7.57–7.60 (m, 2H, ArH), 7.30 (d,  $J = 8.0$  Hz, 2 H, ArH), 7.18 (t,  $J = 8.5$  Hz, 2 H, ArH), 2.42 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz):  $\delta = 162.9$  (d,  $J_{\text{CF}}^1 = 247.6$  Hz), 156.3, 147.8, 139.1, 136.1, 134.9, 133.9, 133.7, 129.5, 128.6 (d,  $J_{\text{CF}}^3 = 7.1$  Hz), 126.7, 120.0, 116.1 (d,  $J_{\text{CF}}^2 = 21.6$  Hz), 21.3; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for C<sub>18</sub>H<sub>15</sub>NF [(M + H)<sup>+</sup>], 264.1189; found, 264.1192.

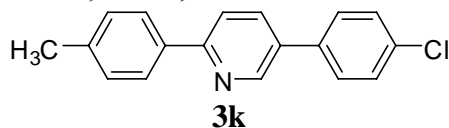


**4j**

#### 4-(4-Fluorophenyl)-2-*p*-tolylpyridine (4j)

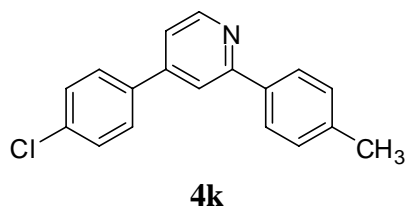
Yellow solid; yield 57 %; mp 72–73 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3030, 2920, 1599, 1541, 1511, 1471, 1382, 1222, 819 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz):  $\delta = 8.71$  (d,  $J = 5.1$  Hz, 1H, N=CH), 7.95 (d,  $J = 8.0$  Hz, 2 H, ArH), 7.85 (s, 1H, ArH), 7.64–7.67 (m, 2H, ArH), 7.37 (d,  $J = 5.2$  Hz, 1 H, ArH), 7.30 (d,  $J = 8.0$  Hz, 2 H, ArH), 7.19 (t,  $J = 8.5$

Hz, 2 H, ArH), 2.42 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): δ = 163.4 (d, *J*<sub>CF</sub><sup>1</sup> = 249.0 Hz), 158.1, 150.0, 148.1, 139.1, 136.5, 134.7, 129.5, 128.8 (d, *J*<sub>CF</sub><sup>3</sup> = 7.3 Hz), 126.8, 119.7, 118.2, 116.0 (d, *J*<sub>CF</sub><sup>2</sup> = 21.6 Hz), 21.3; HRMS (ESI-TOF<sup>+</sup>): *m/z* calcd for C<sub>18</sub>H<sub>15</sub>NF [(M + H)<sup>+</sup>], 264.1189; found, 264.1185.



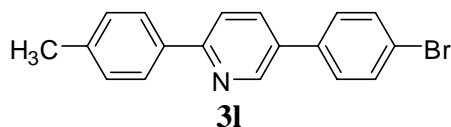
#### 5-(4-Chlorophenyl)-2-*p*-tolylpyridine (3k)

White solid; yield 19 %; mp 218–219 °C; IR (KBr) *v*<sub>max</sub>/cm<sup>-1</sup>: 3031, 2916, 2852, 1587, 1546, 1511, 1466, 1411, 817; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz): δ = 8.87 (s, 1H, N=CH), 7.94 (d, *J* = 8.0 Hz, 2 H, ArH), 7.88 (dd, *J* = 2.1, 8.0 Hz, 1 H, ArH), 7.77 (d, *J* = 8.0 Hz, 1 H, ArH), 7.55 (d, *J* = 8.0 Hz, 2 H, ArH), 7.45 (d, *J* = 8.0 Hz, 2 H, ArH), 7.30 (d, *J* = 8.0 Hz, 2 H, ArH), 2.43 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): δ = 159.0, 150.3, 141.7, 138.7, 138.5, 137.4, 136.7, 136.0, 132.1, 131.8, 130.7, 129.3, 122.6, 23.8; HRMS (ESI-TOF<sup>+</sup>): *m/z* calcd for C<sub>18</sub>H<sub>15</sub>NCl [(M + H)<sup>+</sup>], 280.0893; found, 280.0896.



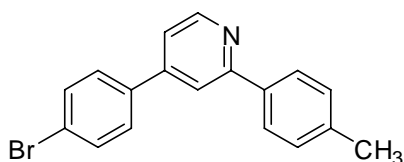
#### 4-(4-Chlorophenyl)-2-*p*-tolylpyridine (4k)

White solid; yield 57 %; mp 107–108 °C; IR (KBr) *v*<sub>max</sub>/cm<sup>-1</sup>: 3020, 2918, 1598, 1577, 1541, 1514, 1496, 1466, 1380, 814; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz): δ = 8.72 (d, *J* = 5.3 Hz, 1H, N=CH), 7.94 (d, *J* = 8.0 Hz, 2 H, ArH), 7.86 (d, *J* = 1.3 Hz, 1 H, ArH), 7.61–7.64 (m, 2H, ArH), 7.47–7.49 (m, 2H, ArH), 7.38 (dd, *J* = 1.6, 5.3 Hz, 1 H, ArH), 7.31 (d, *J* = 8.0 Hz, 2 H, ArH), 2.42 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): δ = 160.8, 152.7, 150.5, 141.7, 139.6, 139.0, 137.8, 132.1, 131.9, 130.9, 129.4, 122.2, 120.7, 23.8; HRMS (ESI-TOF<sup>+</sup>): *m/z* calcd for C<sub>18</sub>H<sub>15</sub>NCl [(M + H)<sup>+</sup>], 280.0893; found, 280.0886.



#### 5-(4-Bromophenyl)-2-*p*-tolylpyridine (3l)

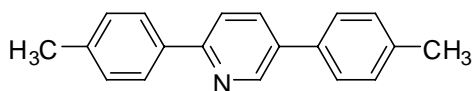
White solid; yield 20 %; mp 221–222 °C; IR (KBr) *v*<sub>max</sub>/cm<sup>-1</sup>: 3029, 2917, 2852, 1624, 1586, 1507, 1467, 816; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz): δ = 8.87 (d, *J* = 2.3 Hz, 1H, N=CH), 7.94 (d, *J* = 8.0 Hz, 2 H, ArH), 7.89 (dd, *J* = 2.3, 8.4 Hz, 1 H, ArH), 7.78 (d, *J* = 8.4 Hz, 1 H, ArH), 7.61 (d, *J* = 8.4 Hz, 2 H, ArH), 7.49 (d, *J* = 8.4 Hz, 2 H, ArH), 7.30 (d, *J* = 8.0 Hz, 2 H, ArH), 2.42 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): δ = 156.6, 147.7, 139.2, 136.7, 136.0, 134.8, 133.4, 132.2, 129.6, 128.5, 126.7, 122.3, 120.1, 21.3; HRMS (ESI-TOF<sup>+</sup>): *m/z* calcd for C<sub>18</sub>H<sub>15</sub>NBr [(M + H)<sup>+</sup>], 324.0388; found, 324.0395.



**4l**

**4-(4-Bromophenyl)-2-*p*-tolylpyridine (4l)**

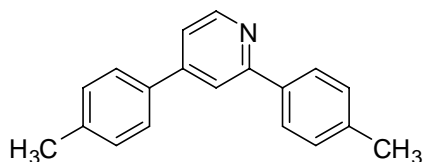
White solid; yield 58 %; mp 119–120 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3030, 2916, 2853, 1596, 1540, 1493, 1466, 1378, 812;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.72 (d,  $J$  = 5.1 Hz, 1H, N=CH), 7.94 (d,  $J$  = 8.0 Hz, 2 H, ArH), 7.85 (s, 1 H, ArH), 7.63 (d,  $J$  = 8.3 Hz, 2 H, ArH), 7.55 (d,  $J$  = 8.3 Hz, 2 H, ArH), 7.37 (d,  $J$  = 5.1 Hz, 1 H, ArH), 7.30 (d,  $J$  = 8.0 Hz, 2 H, ArH), 2.42 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 158.3, 150.2, 148.0, 139.2, 137.5, 136.5, 132.3, 129.5, 128.7, 126.9, 123.4, 119.7, 118.1, 21.3; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{18}\text{H}_{15}\text{NBr}$  [(M + H)<sup>+</sup>], 324.0388; found, 324.0376.



**3m**

**2,5-Dip-tolylpyridine (3m)**

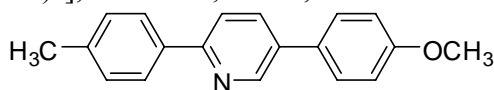
White solid; yield 34 %; mp 212–213 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3029, 2915, 1587, 1547, 1518, 1470, 1365, 815;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.90 (d,  $J$  = 2.3 Hz, 1H, N=CH), 7.94 (d,  $J$  = 8.0 Hz, 2H, ArH), 7.92 (dd,  $J$  = 2.3, 8.5 Hz, 1H, ArH), 7.77 (d,  $J$  = 8.5 Hz, 1 H, ArH), 7.53 (d,  $J$  = 8.0 Hz, 2 H, ArH), 7.30 (d,  $J$  = 8.0 Hz, 4 H, ArH), 2.42 (s, 6H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 155.9, 147.9, 138.9, 137.9, 136.3, 134.8, 134.5, 129.8, 129.5, 126.8, 126.7, 120.0, 21.3; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{19}\text{H}_{18}\text{N}$  [(M + H)<sup>+</sup>], 260.1439; found, 260.1443.



**4m**

**2,4-Dip-tolylpyridine (4m)**

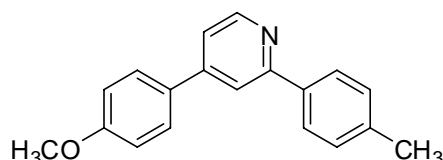
White solid; yield 52 %; mp 114–115 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3027, 2917, 1612, 1596, 1539, 1515, 1470, 1382, 809;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.69 (d,  $J$  = 5.1 Hz, 1H, N=CH), 7.94 (d,  $J$  = 8.0 Hz, 2 H, ArH), 7.89 (s, 1H, ArH), 7.60 (d,  $J$  = 8.0 Hz, 2 H, ArH), 7.41 (dd,  $J$  = 1.7, 5.1 Hz, 1H), 7.31 (t,  $J$  = 7.0 Hz, 4 H, ArH), 2.43 (s, 3H,  $\text{CH}_3$ ), 2.42 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 158.0, 150.0, 149.1, 139.1, 139.0, 136.8, 135.7, 129.8, 129.5, 126.9, 119.8, 118.2, 21.3; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{19}\text{H}_{18}\text{N}$  [(M + H)<sup>+</sup>], 260.1439; found, 260.1442.



**3n**

**5-(4-Methoxyphenyl)-2-*p*-tolylpyridine (3n)**

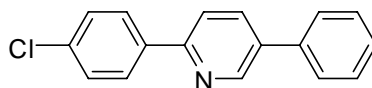
White solid; yield 35 %; mp 186–187 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3015, 2912, 2837, 1607, 1590, 1557, 1520, 1474, 1253, 818;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.88 (d,  $J$  = 2.0 Hz, 1H, N=CH), 7.93 (d,  $J$  = 8.0 Hz, 2 H, ArH), 7.88 (dd,  $J$  = 2.0, 8.2 Hz, 1 H, ArH), 7.75 (d,  $J$  = 8.2 Hz, 1 H, ArH), 7.57 (d,  $J$  = 8.6 Hz, 2 H, ArH), 7.29 (d,  $J$  = 8.0 Hz, 2 H, ArH), 7.02 (d,  $J$  = 8.6 Hz, 2 H, ArH), 3.87 (s, 3H, OCH<sub>3</sub>), 2.42 (s, 3H, CH<sub>3</sub>);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 159.7, 155.6, 147.6, 138.9, 136.3, 134.5, 134.3, 130.2, 129.5, 128.1, 126.6, 120.0, 114.6, 55.4, 21.3; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for C<sub>19</sub>H<sub>18</sub>N O[(M + H)<sup>+</sup>], 276.1388; found, 276.1395.



**4n**

#### 4-(4-Methoxyphenyl)-2-*p*-tolylpyridine (4n)

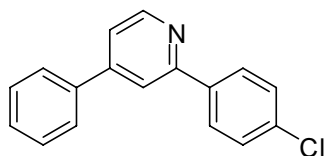
White solid; yield 52 %; mp 97–98 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3008, 2931, 2837, 1606, 1593, 1540, 1471, 1381, 818  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.87 (d,  $J$  = 5.1 Hz, 1H, N=CH), 7.94 (d,  $J$  = 8.0 Hz, 2 H, ArH), 7.87 (s, 1H, ArH), 7.64–7.66 (m, 2H, ArH), 7.38 (dd,  $J$  = 1.7, 5.1 Hz, 1 H, ArH), 7.30 (d,  $J$  = 8.0 Hz, 2 H, ArH), 7.02–7.04 (m, 2 H, ArH), 3.88 (s, 3H, OCH<sub>3</sub>), 2.42 (s, 3H, CH<sub>3</sub>);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 160.6, 158.1, 150.0, 148.8, 139.0, 136.9, 131.0, 129.5, 128.3, 127.0, 119.5, 117.9, 114.6, 55.5, 21.3; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for C<sub>19</sub>H<sub>18</sub>N O[(M + H)<sup>+</sup>], 276.1388; found, 276.1382.



**3o**

#### 2-(4-Chlorophenyl)-5-phenylpyridine (3o)

White solid; yield 25 %; mp 181–183 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3008, 1636, 1587, 1469, 1098, 827, 772, 692;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.92 (d,  $J$  = 2.0 Hz, 1H, N=CH), 7.99 (d,  $J$  = 8.5 Hz, 2 H, ArH), 7.95 (dd,  $J$  = 2.0, 8.2 Hz, 1 H, ArH), 7.77 (d,  $J$  = 8.2 Hz, 1 H, ArH), 7.63 (d,  $J$  = 7.7 Hz, 2 H, ArH), 7.41–7.51 (m, 5 H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 154.9, 148.2, 137.5, 137.4, 135.2, 135.1, 129.3, 129.1, 129.0, 128.1, 128.0, 127.0, 120.0; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for C<sub>17</sub>H<sub>13</sub>NCl [(M + H)<sup>+</sup>], 266.0737; found, 266.0742.

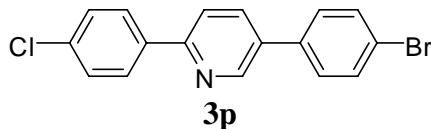


**4o**

#### 2-(4-Chlorophenyl)-4-phenylpyridine (4o)

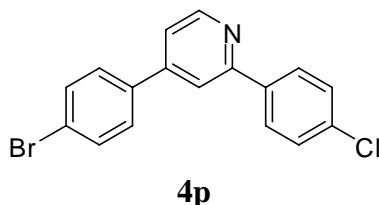
White solid; yield 59 %; mp 57–58 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3058, 3032, 1607, 1596, 1543, 1496, 1467, 1091, 832, 761, 697;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.70 (d,  $J$  = 5.1 Hz, 1H, N=CH), 7.98 (d,  $J$  = 8.5 Hz, 2 H, ArH), 7.86 (s, 1 H, ArH), 7.65 (d,  $J$  =

7.2 Hz, 2 H, ArH), 7.41–7.50 (m, 6 H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 156.7$ , 150.1, 149.7, 149.4, 138.3, 137.8, 136.7, 135.1, 129.1, 128.8, 128.2, 127.9, 127.0, 122.2, 120.4, 120.1, 118.3; HRMS (ESI-TOF $^+$ ):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{13}\text{NCl}[(\text{M} + \text{H})^+]$ , 266.0737; found, 266.0729.



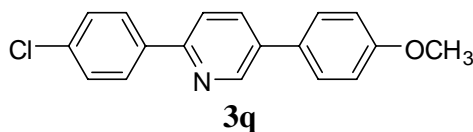
#### 5-(4-Bromophenyl)-2-(4-chlorophenyl)pyridine (3p)

White solid; yield 20 %; mp 239–241 °C; IR (KBr)  $\nu_{\text{max}}/\text{cm}^{-1}$ : 3083, 3014, 1577, 1548, 1464, 1102, 816;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 8.88$  (d,  $J = 2.2$  Hz, 1H, N=CH), 7.99 (d,  $J = 8.5$  Hz, 2H, ArH), 7.92 (dd,  $J = 2.2, 8.2$  Hz, 1H, ArH), 7.77 (d,  $J = 8.2$  Hz, 1H, ArH), 7.62 (d,  $J = 8.5$  Hz, 2H, ArH), 7.49 (d,  $J = 8.5$  Hz, 2H, ArH), 7.46 (d,  $J = 8.5$  Hz, 2H, ArH);  $^{13}\text{C}$  NMR ( $\text{DMSO-d}_6$ , 125 MHz):  $\delta = 164.4, 157.9, 147.3, 146.3, 145.5, 144.5, 143.6, 142.4, 139.2, 138.6, 132.2, 130.6$ ; HRMS (ESI-TOF $^+$ ):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{12}\text{BrClN}[(\text{M} + \text{H})^+]$ , 343.9842; found, 343.9836.



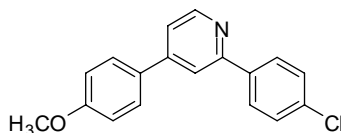
#### 4-(4-Bromophenyl)-2-(4-chlorophenyl)pyridine (4p)

White solid; yield 61 %; mp 118–119 °C; IR (KBr)  $\nu_{\text{max}}/\text{cm}^{-1}$ : 3083, 3014, 1577, 1548, 1464, 1102, 816;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 8.72$  (d,  $J = 5.1$  Hz, 1H, N=CH), 7.98 (d,  $J = 8.5$  Hz, 2H, ArH), 7.83 (s, 1H, ArH), 7.63 (d,  $J = 8.4$  Hz, 2H, ArH), 7.53 (d,  $J = 8.4$  Hz, 2H, ArH), 7.45 (d,  $J = 8.5$  Hz, 2H, ArH), 7.40 (d,  $J = 5.1$  Hz, 1H, ArH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 166.0, 159.3, 157.2, 146.7, 146.2, 144.3, 141.3, 138.0, 137.6, 137.3, 132.6, 129.1, 127.1$ ; HRMS (ESI-TOF $^+$ ):  $m/z$  calcd for  $\text{C}_{17}\text{H}_{12}\text{BrClN}[(\text{M} + \text{H})^+]$ , 343.9842; found, 343.9845.



#### 2-(4-Chlorophenyl)-5-(4-methoxyphenyl)pyridine (3q)

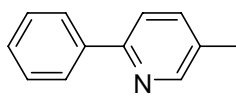
White solid; yield 34 %; mp 216–217 °C; IR (KBr)  $\nu_{\text{max}}/\text{cm}^{-1}$ : 3012, 2960, 2935, 1606, 1521, 1472, 1375, 1289, 1257, 821;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 8.88$  (d,  $J = 2.5$  Hz, 1H, N=CH), 7.98 (d,  $J = 8.5$  Hz, 2H, ArH), 7.90 (dd,  $J = 2.5, 8.2$  Hz, 1H, ArH), 7.74 (d,  $J = 8.2$  Hz, 1H, ArH), 7.56 (d,  $J = 8.5$  Hz, 2H, ArH), 7.48 (d,  $J = 8.5$  Hz, 2H, ArH), 7.03 (d,  $J = 8.5$  Hz, 2H, ArH), 3.87 (s, 3H,  $\text{OCH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 159.9, 154.3, 147.8, 137.5, 135.0, 134.9, 134.6, 129.9, 128.9, 128.1, 128.0, 120.0, 114.7, 55.4$ ; HRMS (ESI-TOF $^+$ ):  $m/z$  calcd for  $\text{C}_{18}\text{H}_{15}\text{ClNO}[(\text{M} + \text{H})^+]$ , 296.0842 found, 296.0846.



**4q**

**2-(4-Chlorophenyl)-4-(4-methoxyphenyl)pyridine (4q)**

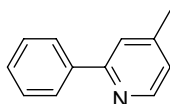
White solid; yield 52 %; mp 99–100 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3018, 2925, 2854, 1598, 1542, 1516, 1494, 1382, 1256, 1184, 821;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.68 (d,  $J$  = 5.1 Hz, 1H, N=CH), 7.99 (d,  $J$  = 8.6 Hz, 2H, ArH), 7.85 (s, 1H, ArH), 7.64 (d,  $J$  = 8.8 Hz, 2H, ArH), 7.45 (d,  $J$  = 8.6 Hz, 2H, ArH), 7.41 (dd,  $J$  = 1.6, 5.1 Hz, 1H, ArH), 7.03 (d,  $J$  = 8.8 Hz, 2H, ArH), 3.87 (s, 3H,  $\text{OCH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 160.6, 156.8, 150.1, 148.9, 138.0, 135.1, 130.6, 128.9, 128.3, 128.2, 120.0, 117.9, 114.6, 55.4; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{18}\text{H}_{15}\text{ClNO}$  [(M + H)<sup>+</sup>], 296.0842; found, 296.0847.



**3r**

**5-Methyl-2-phenylpyridine (3r)**

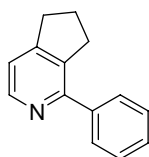
White solid; yield 42 %; mp 21.5–22 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3006, 2968, 2920, 1598, 1560, 1499, 1472, 743, 702;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.54 (s, 1H, N=CH), 7.98 (d,  $J$  = 7.5 Hz, 2H, ArH), 7.65 (d,  $J$  = 8.1 Hz, 1H, ArH), 7.57 (d,  $J$  = 8.1 Hz, 1H, ArH), 7.48 (t,  $J$  = 7.5 Hz, 2H, ArH), 7.41 (t,  $J$  = 7.5 Hz, 1H, ArH), 2.40 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 163.8, 159.1, 148.4, 146.3, 140.6, 137.7, 137.6, 135.7, 129.0, 27.2; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{12}\text{H}_{12}\text{N}$  [(M + H)<sup>+</sup>], 107.0970; found, 107.0971.



**4r**

**4-Methyl-2-phenylpyridine (4r)**

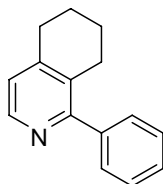
Colorless oil; yield 43 %; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3058, 2922, 2855, 1604, 1581, 1558, 1446, 776, 694;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.54 (d,  $J$  = 4.9 Hz, 1H, N=CH), 7.97 (d,  $J$  = 7.4 Hz, 2H, ArH), 7.65 (s, 1H, ArH), 7.46 (t,  $J$  = 7.3 Hz, 2H, ArH), 7.40 (t,  $J$  = 7.3 Hz, 1H, ArH), 7.05 (d,  $J$  = 4.9 Hz, 1H, ArH), 2.41 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 157.4, 149.4, 147.7, 139.5, 128.8, 128.7, 126.9, 123.1, 121.5, 21.2; HRMS (ESI-TOF<sup>+</sup>):  $m/z$  calcd for  $\text{C}_{12}\text{H}_{12}\text{N}$  [(M + H)<sup>+</sup>], 107.0970; found, 107.0975.



**6a**

### 1-Phenyl-6,7-dihydro-5H-cyclopenta[*c*]pyridine (6a)

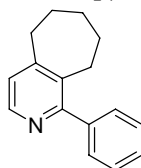
Yellow solid; yield: 92 %; mp 48–49 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3005, 2969, 2949, 1604, 1552, 1474, 1380, 780, 698;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.53 (s, 1H, N=CH), 7.94 (d,  $J$  = 7.0 Hz, 2H, ArH), 7.59 (s, 1H, ArH), 7.44 (t,  $J$  = 7.0 Hz, 2H, ArH), 7.37 (t,  $J$  = 7.5 Hz, 1H, ArH), 2.95 (t,  $J$  = 7.5 Hz, 4H,  $\text{CH}_2$ ), 2.10–2.16 (m, 2H,  $\text{CH}_2$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 155.4, 154.6, 145.4, 140.0, 138.7, 128.6, 128.4, 126.9, 116.8, 30.0, 25.1; HRMS (ESI-TOF+):  $m/z$  calcd for  $\text{C}_{14}\text{H}_{14}\text{N}$  [(M + H)<sup>+</sup>], 196.1126; found, 196.1135.



**6b**

### 1-Phenyl-5,6,7,8-tetrahydroisoquinoline (6b)

Yellow oil; yield: 90%; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3018, 2925, 2854, 1598, 1542, 1516, 1494, 1382, 1256, 1184, 821;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.40 (s, 1H, N=CH), 7.97 (d,  $J$  = 7.5 Hz, 2H, ArH), 7.47 (t,  $J$  = 7.5 Hz, 2H, ArH), 7.37–7.40 (m, 2H, ArH), 2.76–2.80 (m, 4H,  $\text{CH}_2$ ), 1.83–1.83 (m, 4H,  $\text{CH}_2$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 154.2, 150.1, 146.5, 139.6, 131.5, 128.4, 128.2, 126.5, 120.5, 28.8, 25.9, 22.5, 22.3; HRMS (ESI-TOF+):  $m/z$  calcd for  $\text{C}_{15}\text{H}_{16}\text{N}$  [(M + H)<sup>+</sup>], 210.1283; found, 210.1280.



**6c**

### 1-Phenyl-6,7,8,9-tetrahydro-5H-cyclohepta[*c*]pyridine (6c)

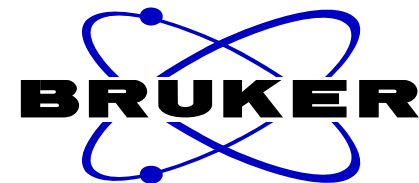
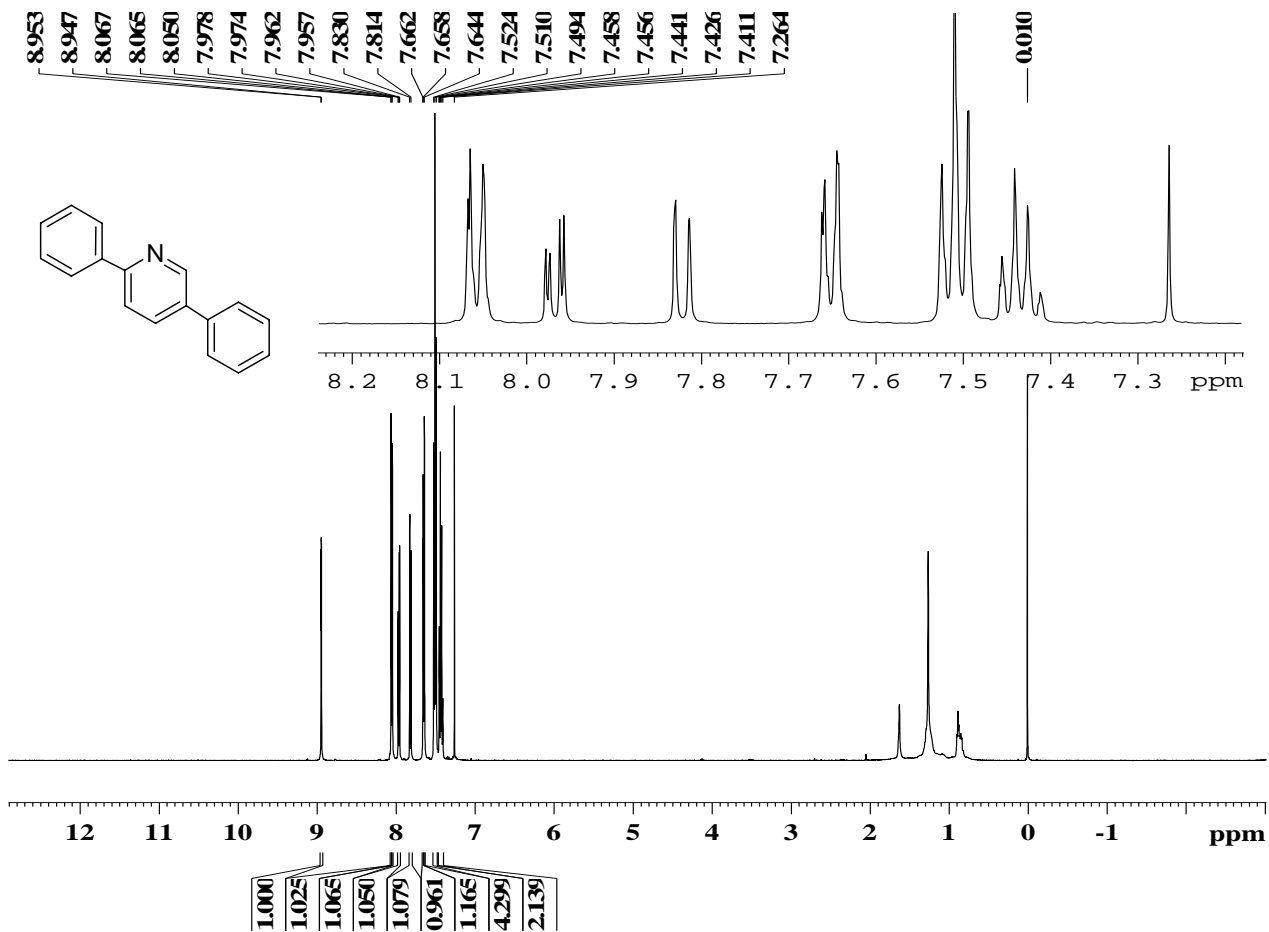
White solid; yield: 88 %; mp 59–60 °C; IR (KBr)  $\nu_{\max}/\text{cm}^{-1}$ : 3049, 2996, 2926, 2853, 1594, 1478, 1443, 756, 702;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.38 (s, 1H, N=CH), 7.96 (d,  $J$  = 7.5 Hz, 2H, ArH), 7.43–7.46 (m, 3H, ArH), 7.37 (t,  $J$  = 7.5 Hz, 1H, ArH), 2.80–2.84 (m, 4H,  $\text{CH}_2$ ), 1.87 (d,  $J$  = 5.0 Hz, 2H,  $\text{CH}_2$ ), 1.67 (d,  $J$  = 3.5 Hz, 4H,  $\text{CH}_2$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 155.6, 152.6, 149.2, 139.6, 137.2, 128.6, 128.4, 126.7, 120.7, 36.5, 33.0, 32.6, 28.1, 27.6; HRMS (ESI-TOF+):  $m/z$  calcd for  $\text{C}_{16}\text{H}_{18}\text{N}$  [(M + H)<sup>+</sup>], 224.1439; found, 224.1442.

## References

1. M. Ernd, M. Heuschmann, H. Zipse, *Helv. Chim. Acta*, 2005, **88**, 1491–1518.
2. W. P. Heilman, R. D. Heilman, J. A. Scozzie, R. J. Wayner, J. M. Gollo, Z. S. Ariyan, *J. Med. Chem.*, 1979, **22**, 671–677.

Compound 3a

WSW0610-1 1H 1D 2011 06 28

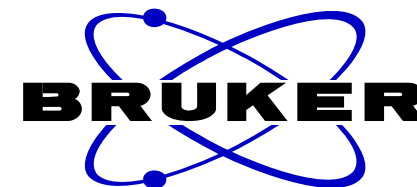
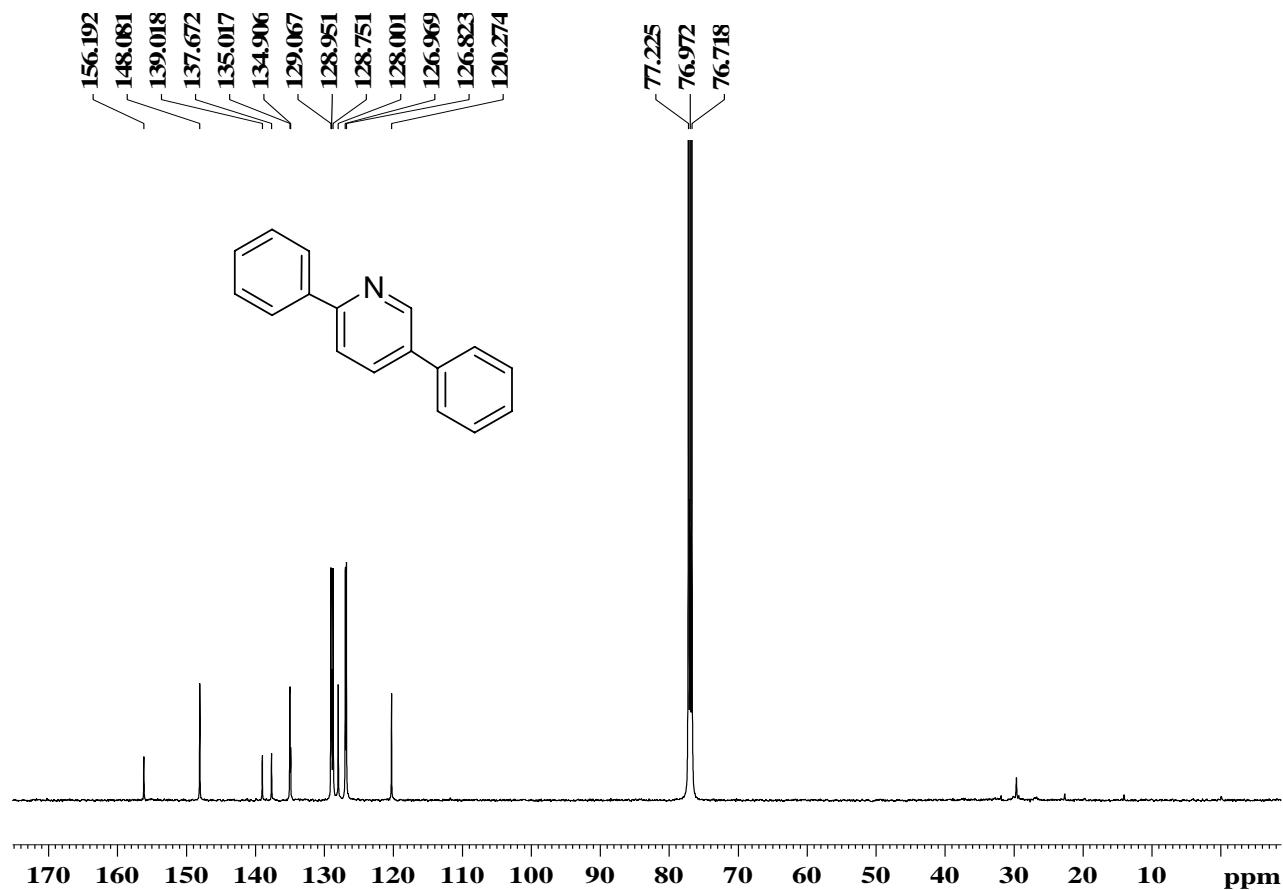


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WSW0610-1 13C 1D 2011 07 03



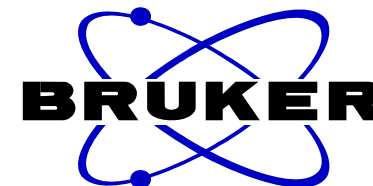
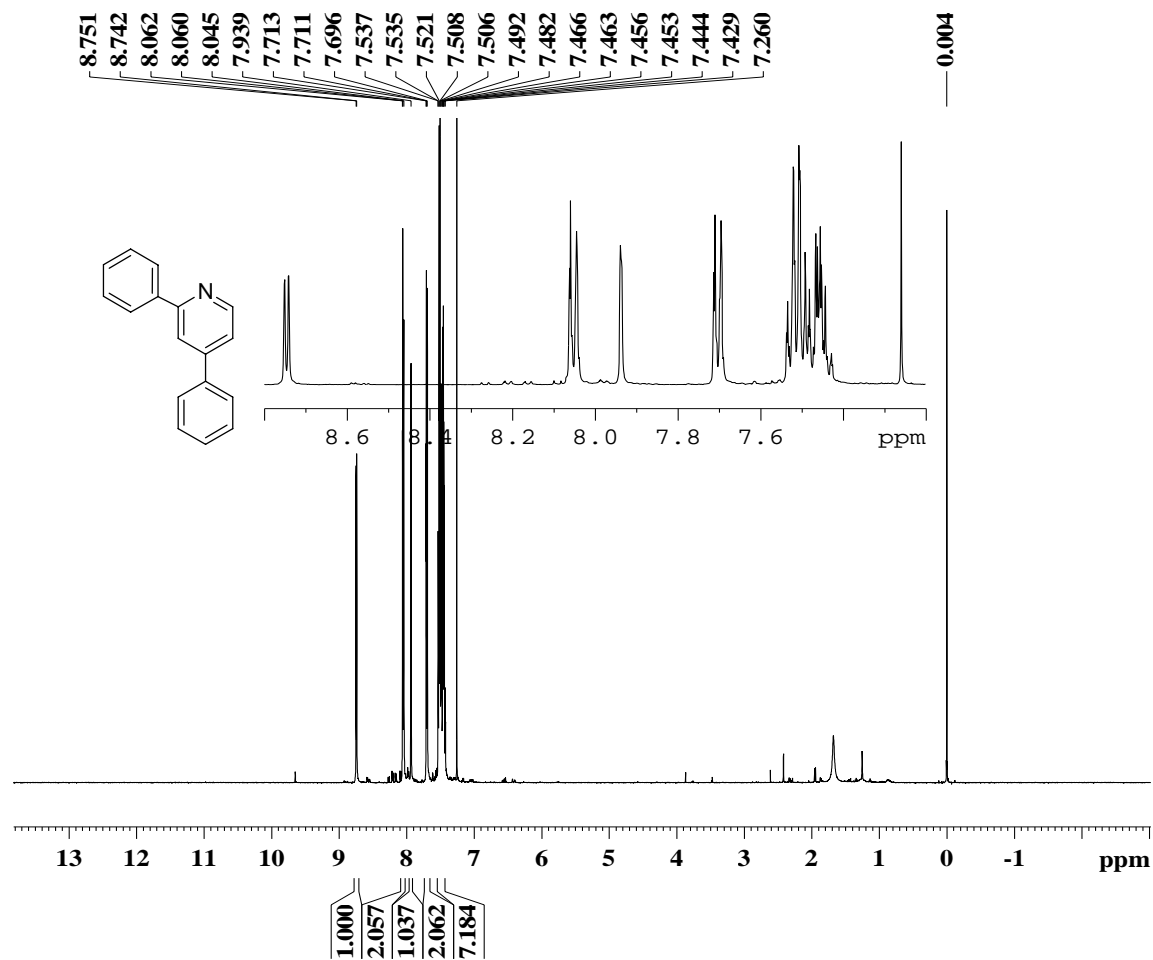
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WDW EM

Compound 4a

WSW1215-3 1H 2011 12 27

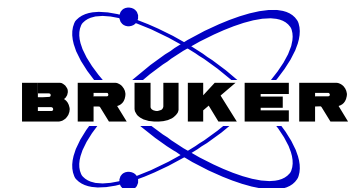
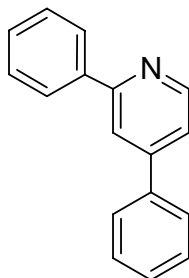


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WSW0610-2 13C 1D 2011 06 28

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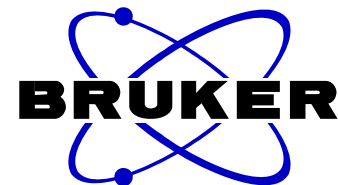
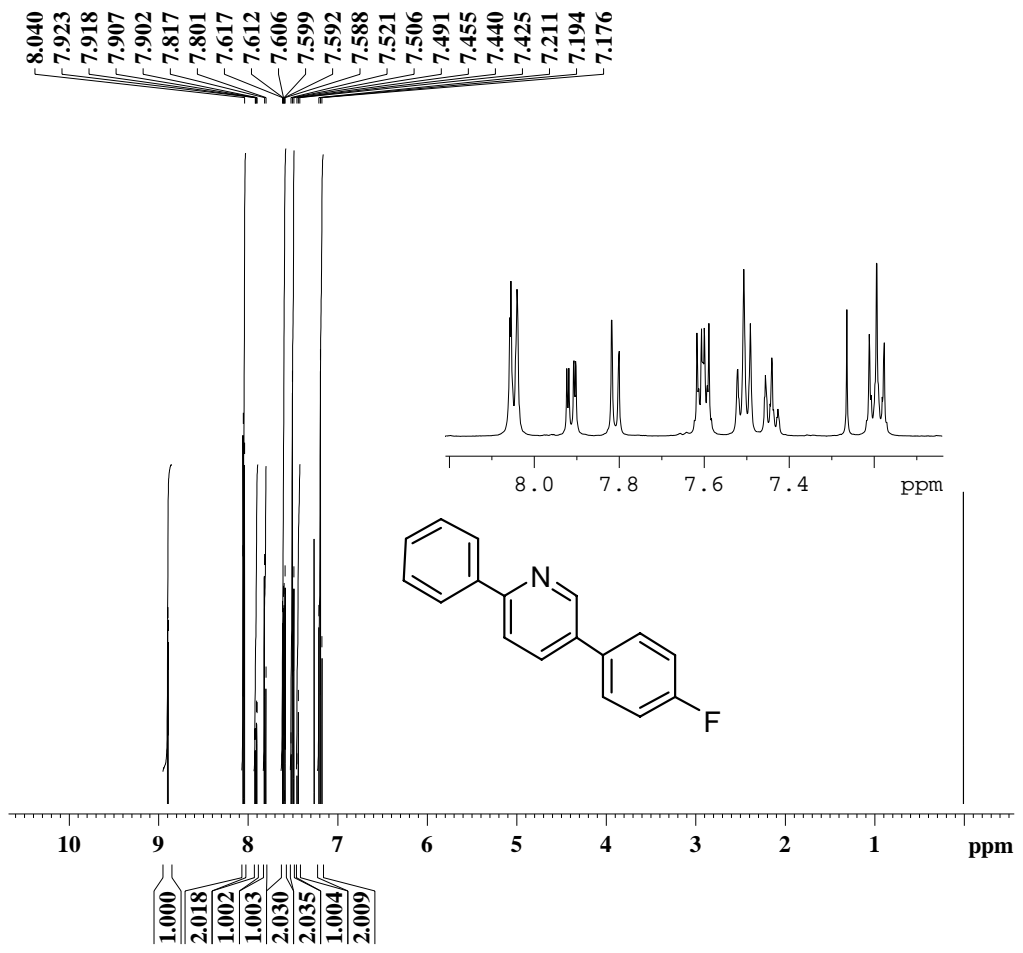
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Compound **3b**

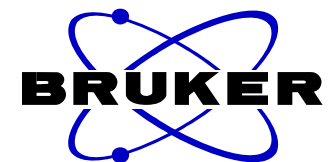
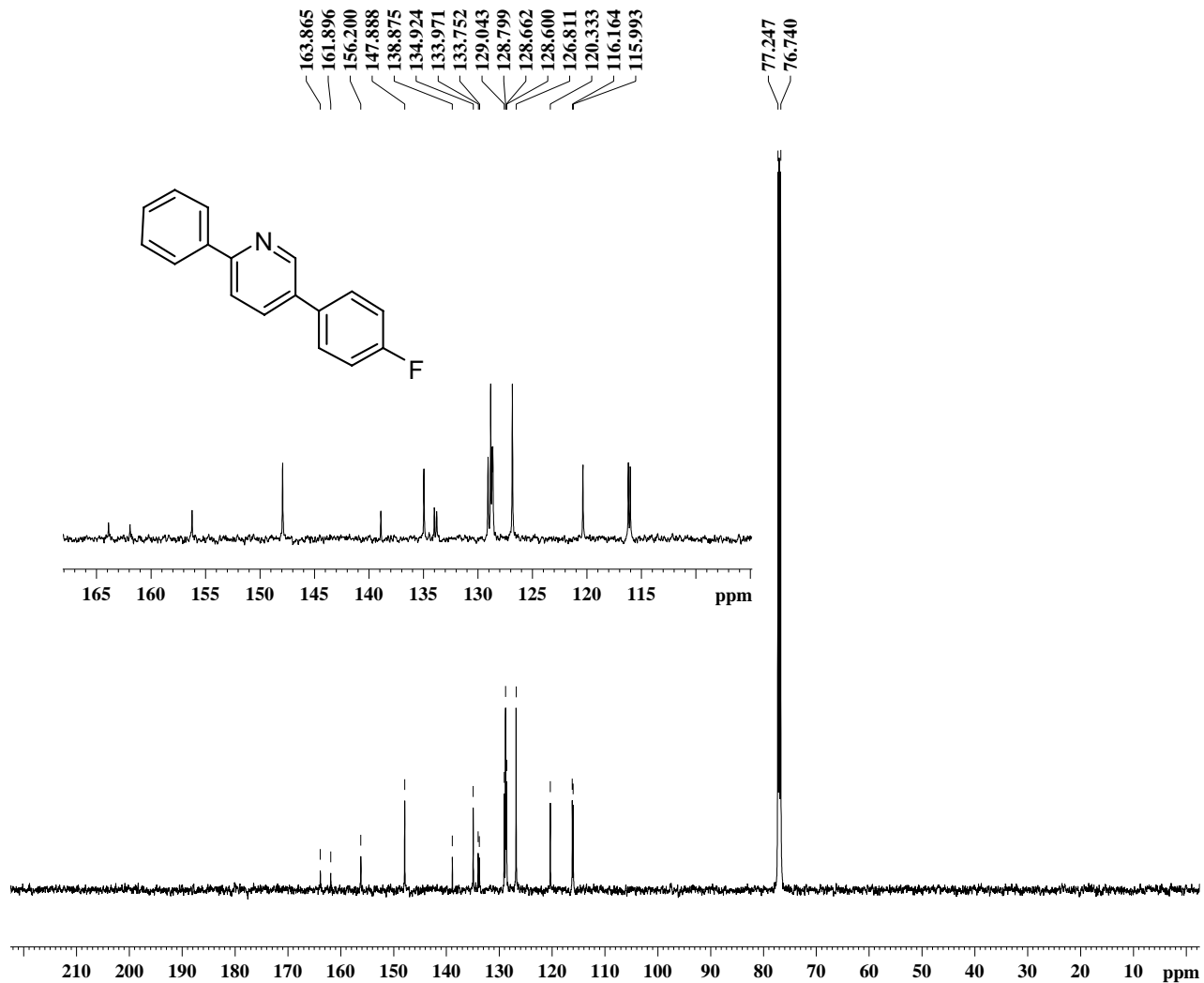
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 DS 1  
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 AQ 1.6385000 sec  
 RG 362  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 297.7 K  
 D1 2.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
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WSW0803-1 13C 1D 2011 08 18



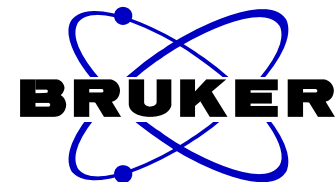
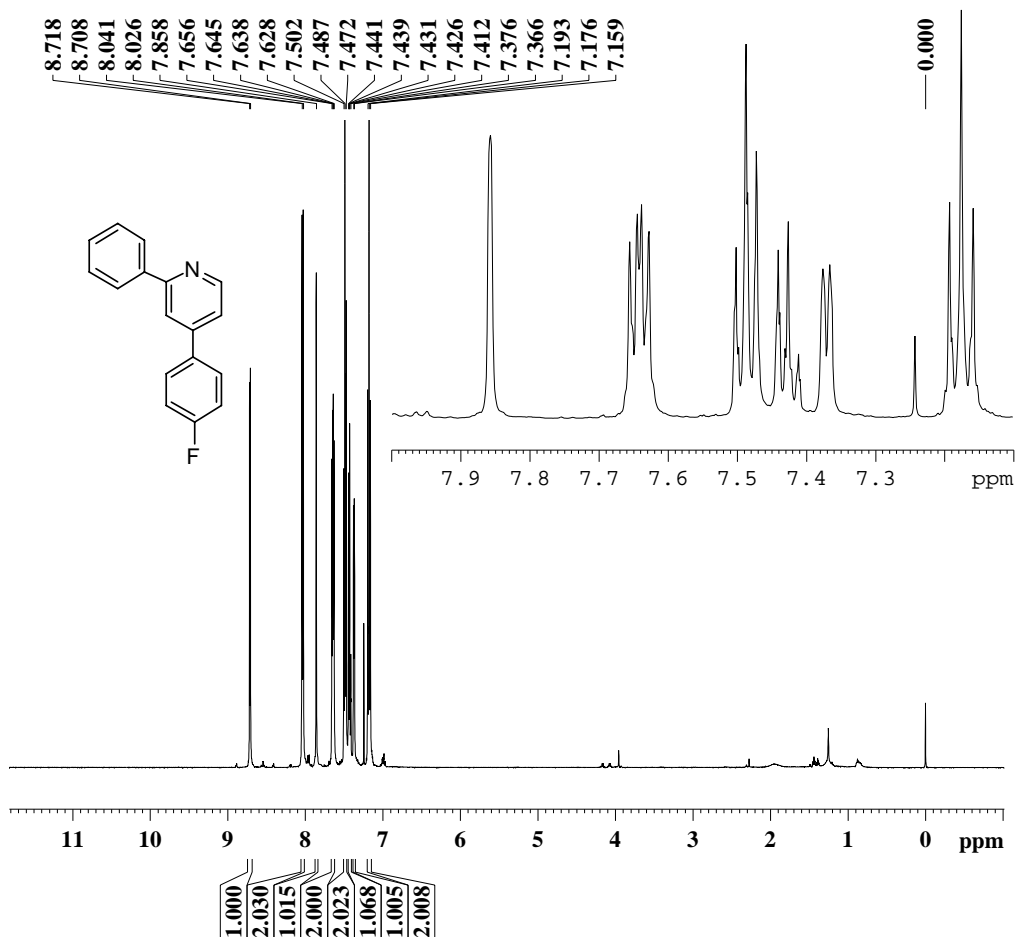
NAME WSW0803-1  
EXPNO 2  
PROCNO 1  
Date\_ 20110818  
Time 20.34  
INSTRUM av500  
PROBHD 5 mm PABBO B1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 15602  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 299.6 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 ==  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

==== CHANNEL f2 ==  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326470 MHz  
WDW EM  
SSB 0  
LB 6.00 Hz  
GB 0  
PC 2.00

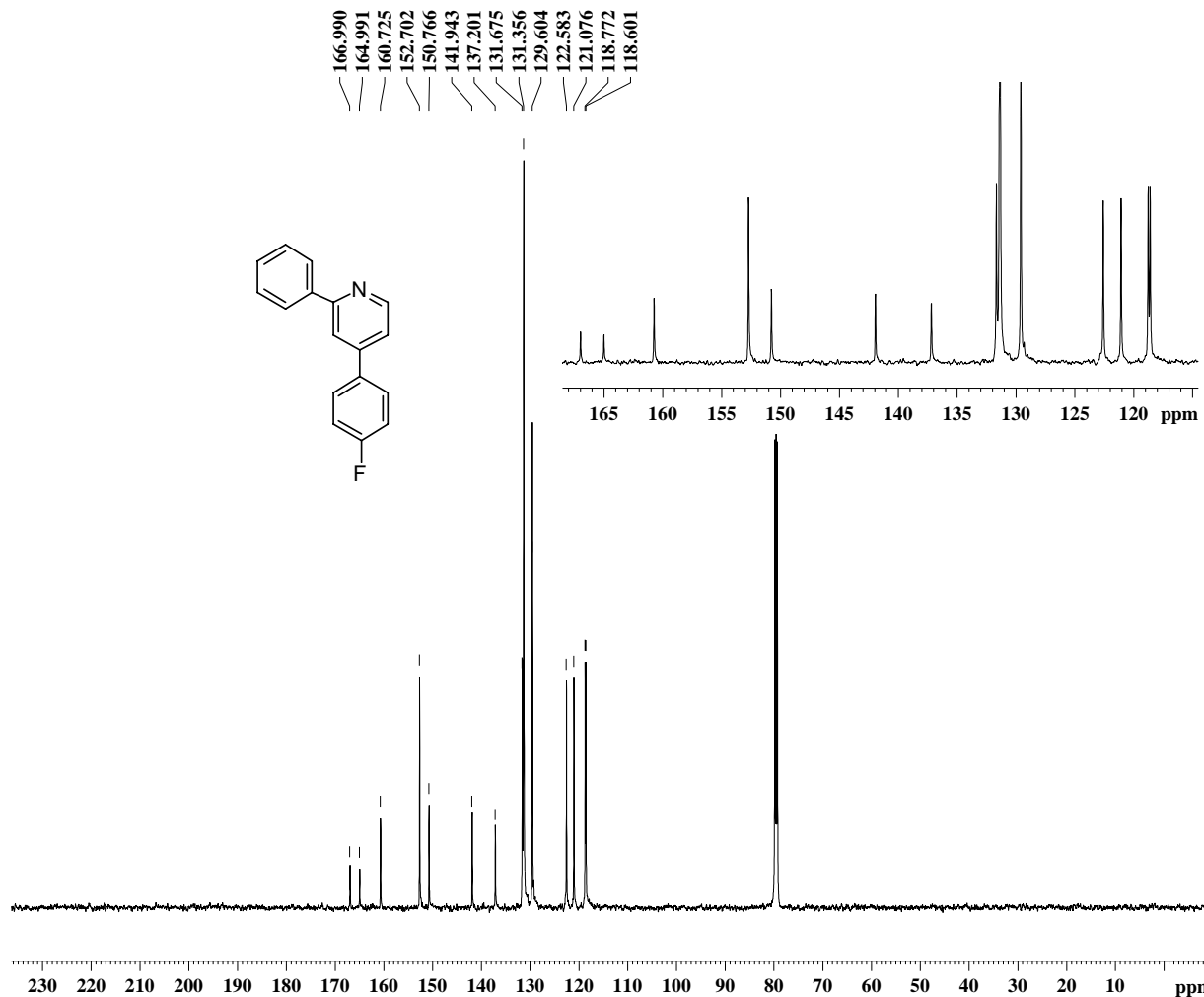
Compound **4b**

WSW0803-2 1H 2011 09 26



NAME WSW0803-2  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20110926  
 Time 20.16  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 144  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 297.1 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300186 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00



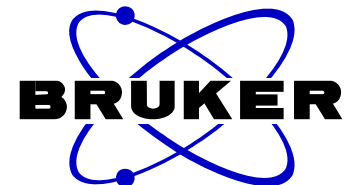
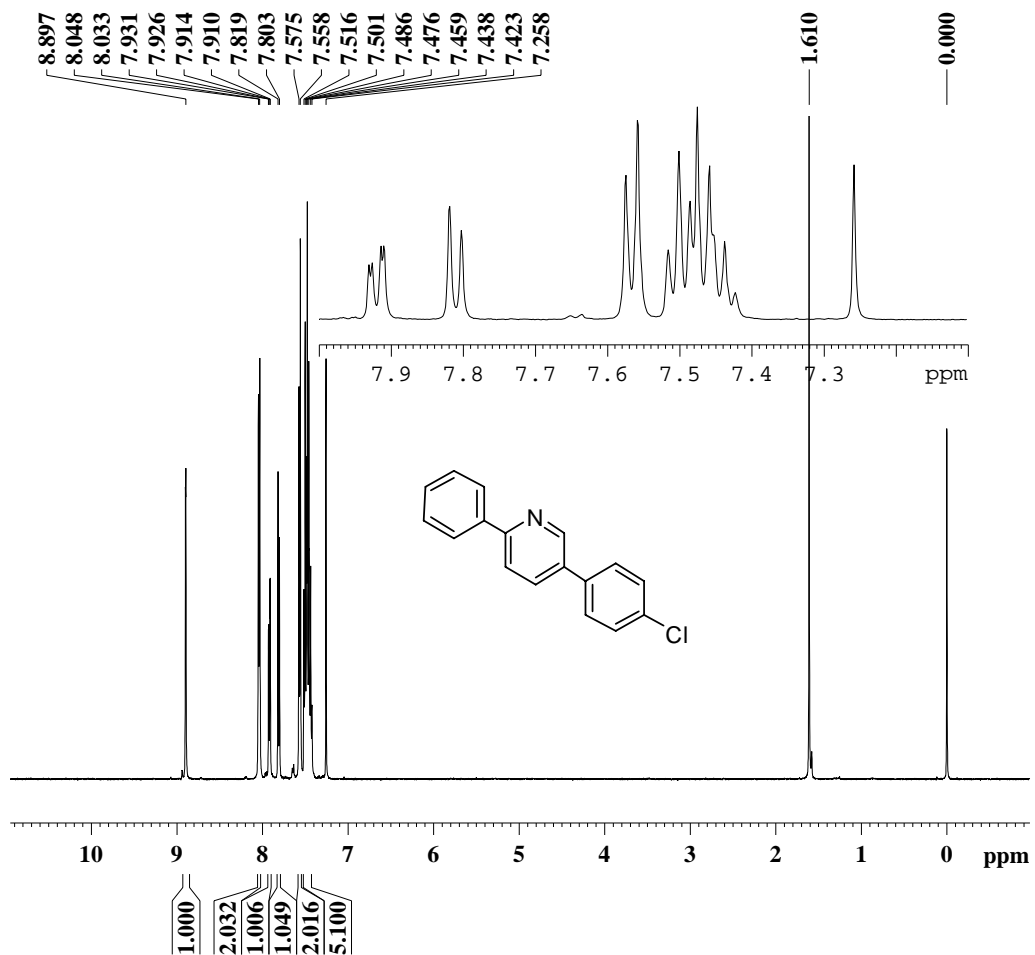
NAME WSW0803-2  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20110929  
 Time 10.15  
 INSTRUM av500  
 PROBHD 5 mm PABBO BE  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 452  
 DS 2  
 SWH 32679.738 Hz  
 FIDRES 0.498653 Hz  
 AQ 1.0027661 sec  
 RG 18400  
 DW 15.300 usec  
 DE 6.00 usec  
 TE 299.8 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

===== CHANNEL f1 ===  
 NUC1 13C  
 P1 9.60 usec  
 PL1 2.00 dB  
 SFO1 125.7464750 MHz

===== CHANNEL f2 ===  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 2.60 dB  
 PL12 17.66 dB  
 PL13 17.66 dB  
 SFO2 500.0355000 MHz  
 SI 32768  
 SF 125.7323258 MHz  
 WDW EM  
 SSB 0  
 LB 8.00 Hz  
 GB 0  
 PC 2.00

Compound 3c

WSW0721-1 1H 1D 2011 07 26

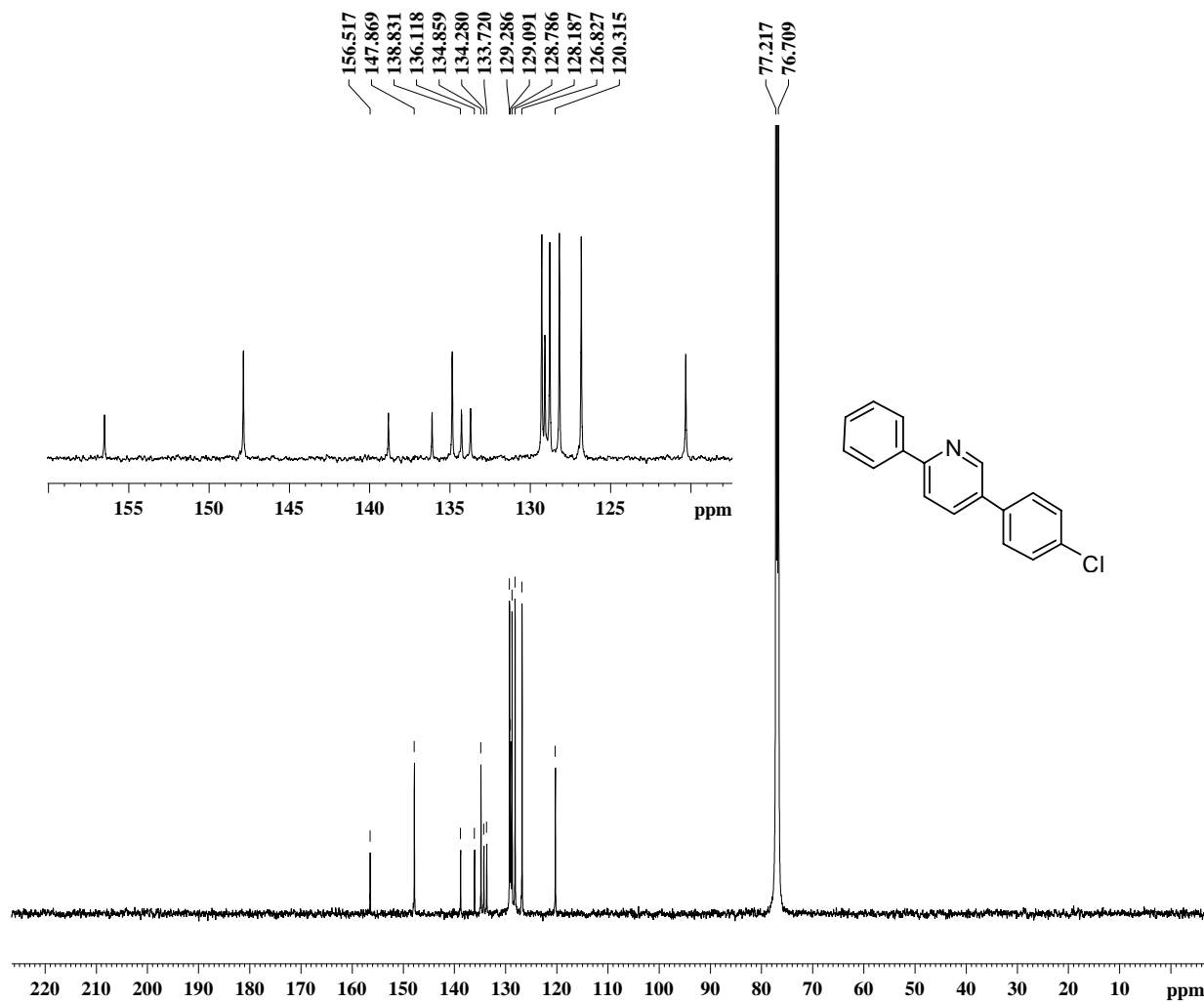


NAME WSW0721-1  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20110726  
 Time 9.49  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 575  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 296.8 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300110 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00



WSW0721-1 13C 1D 2011 07 26



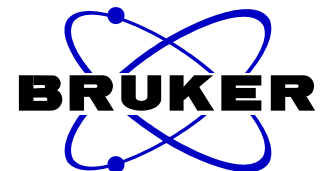
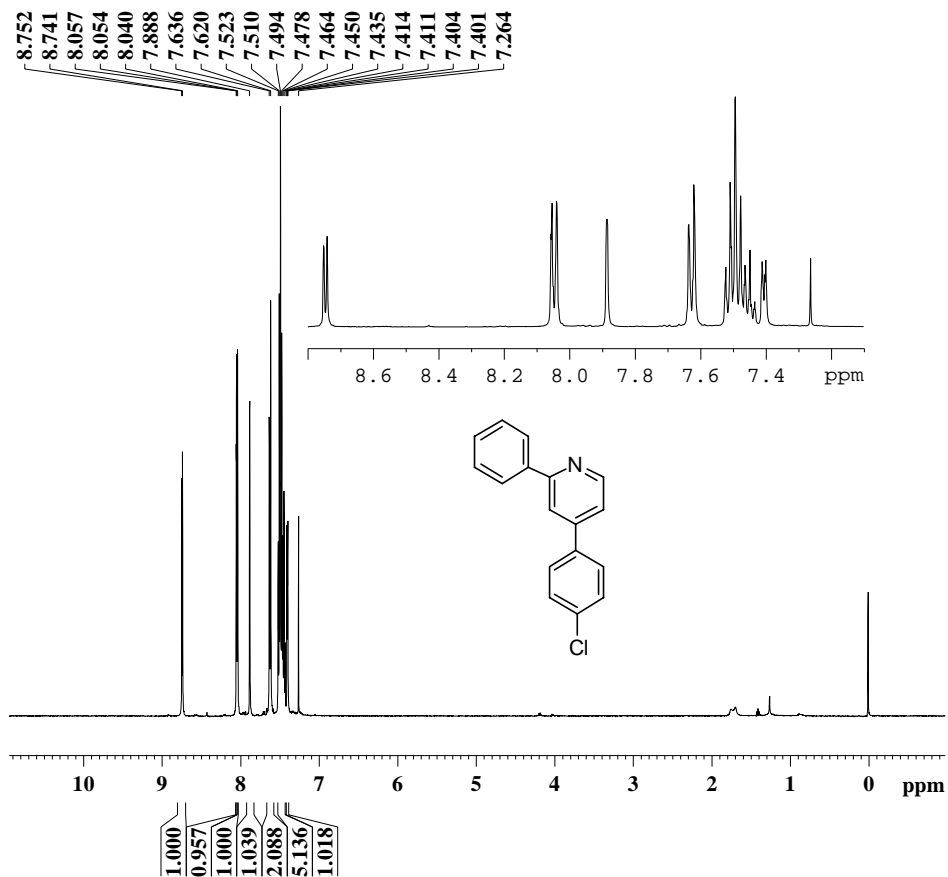
NAME WSW0721-1  
EXPNO 2  
PROCNO 1  
Date\_ 20110726  
Time 14.02  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 4758  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 300.3 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326470 MHz  
WDW EM  
SSB 0  
LB 6.00 Hz  
GB 0  
PC 2.00

Compound **4c**

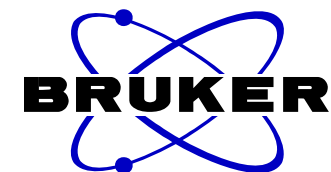
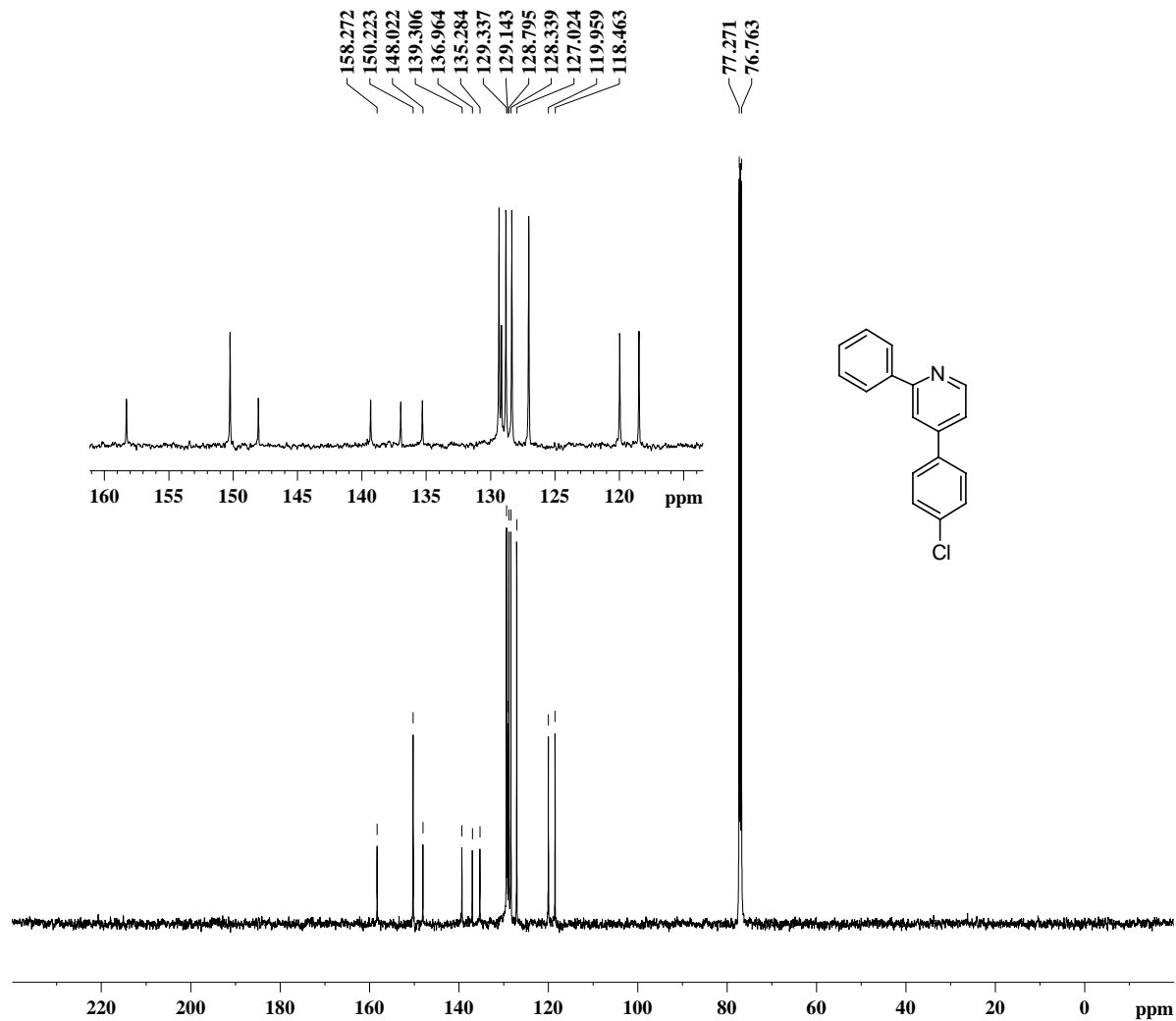
WSW0721-2 1H 1D 2011 08 16



NAME WSW0721-2  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20110816  
 Time 17.28  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 256  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 297.7 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300082 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW0721-2 13C 1D 2011 08 18



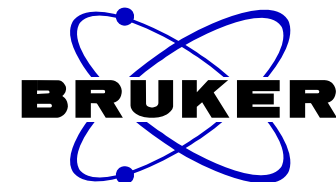
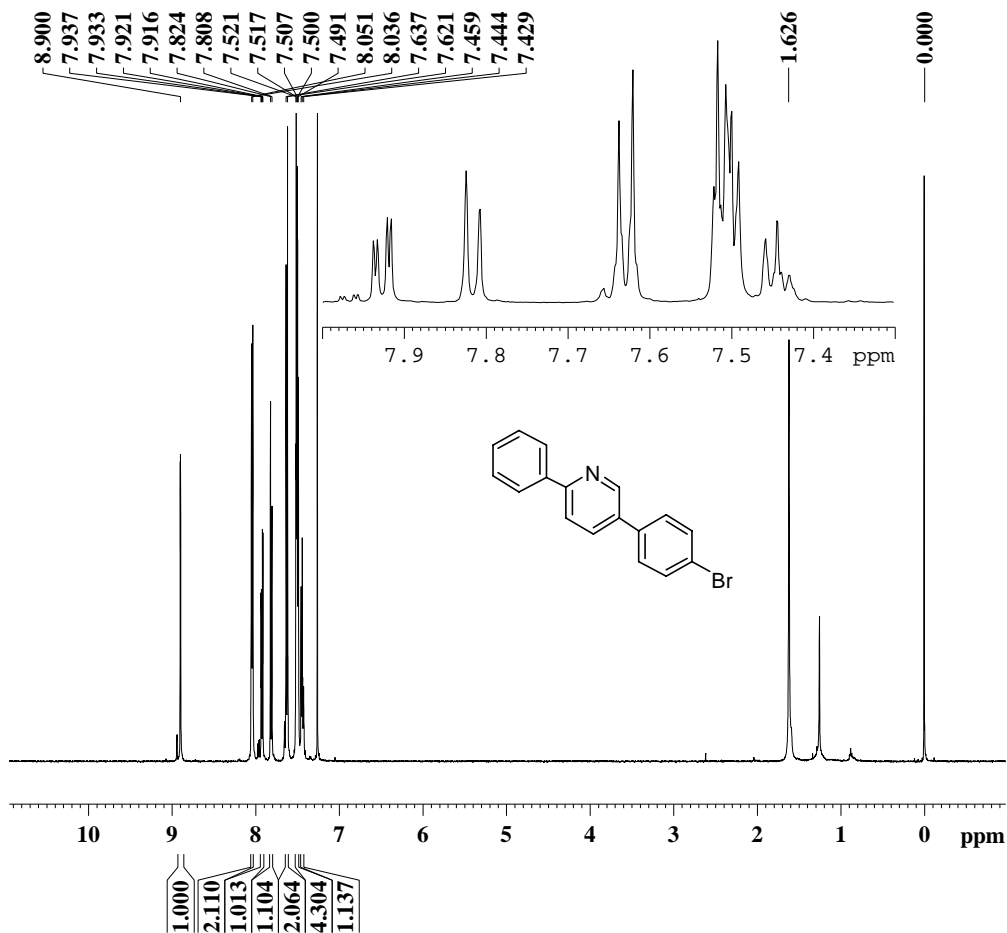
NAME WSW0721-2  
EXPNO 2  
PROCNO 1  
Date\_ 20110818  
Time 18.54  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 322  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 299.5 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326470 MHz  
WDW EM  
SSB 0  
LB 6.00 Hz  
GB 0  
PC 2.00

Compound **3d**

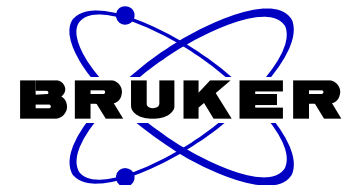
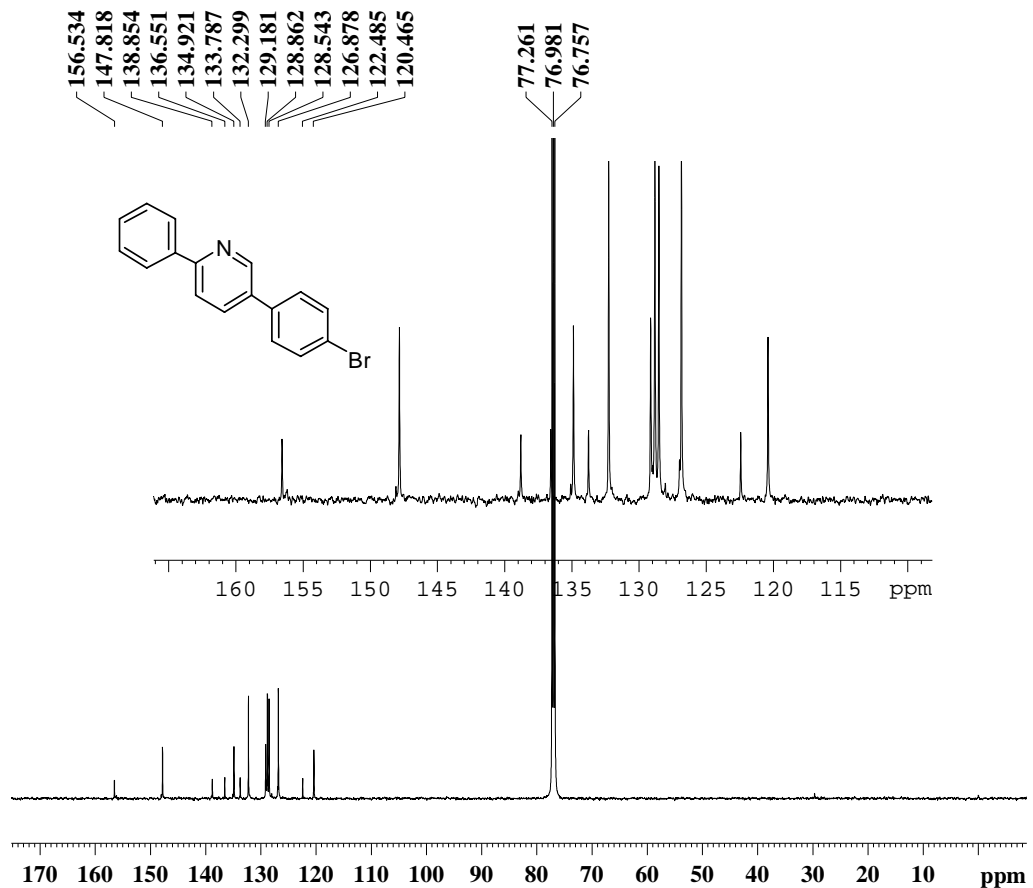
WSW0616-1 1H 1D 2011 07 05



NAME WSW0616-1  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20110705  
 Time 19.53  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 575  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 295.6 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300082 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW616-1 13C ID 2011 07 08



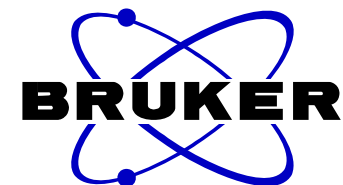
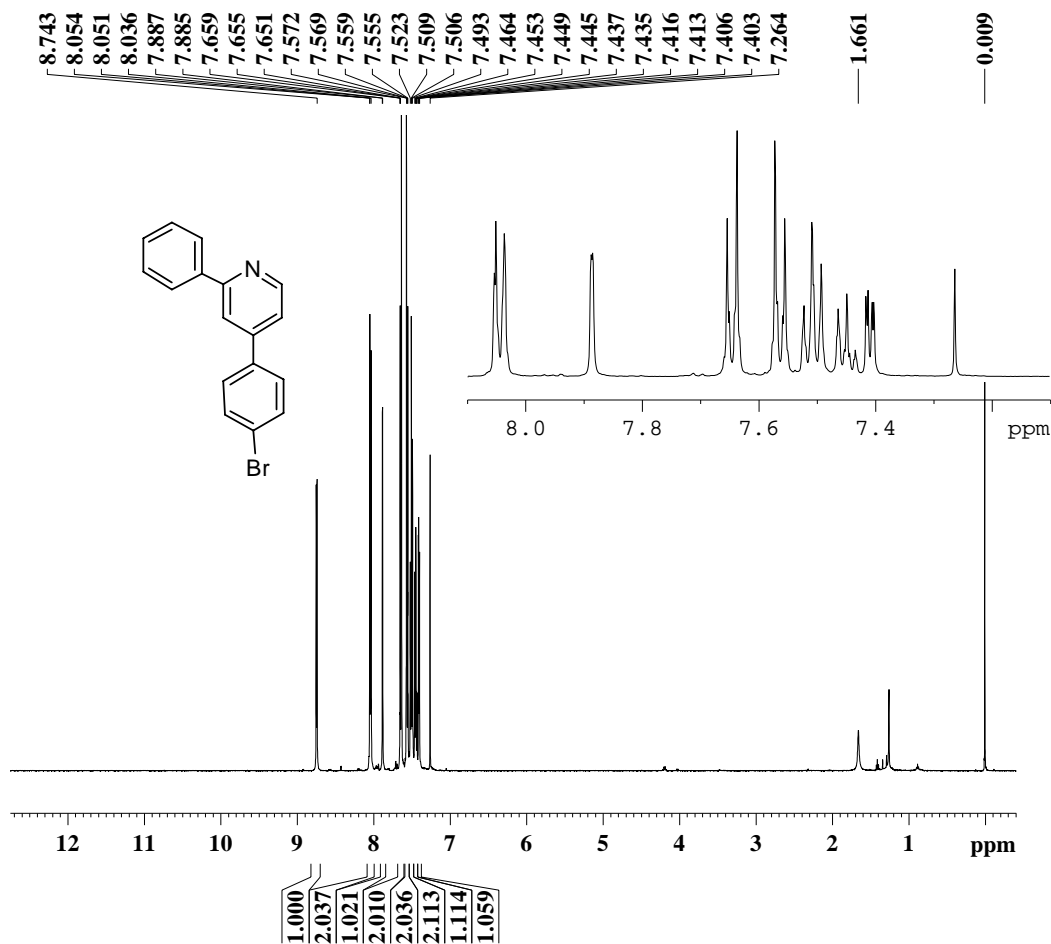
NAME WSW616-1  
EXPNO 2  
PROCNO 1  
Date\_ 20110708  
Time 10.32  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 4593  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 298.4 K  
D1 2.0000000 sec  
dL1 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326470 MHz  
WDW EM

Compound **4d**

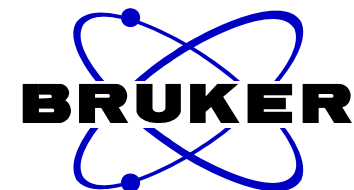
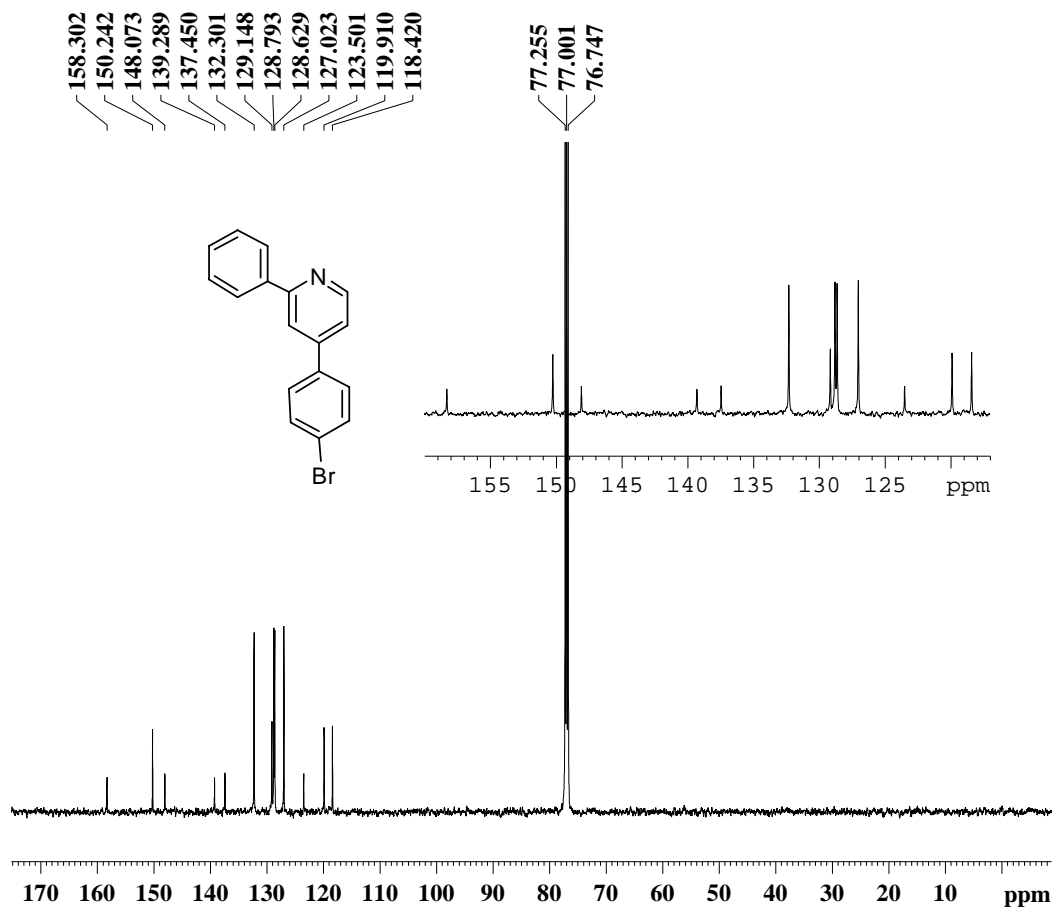
WSW0616-2 1H 1D 2011 08 16



NAME WSW0616-2  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20110816  
 Time 17.15  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 362  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 297.7 K  
 D1 2.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300082 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW0616-2 13C 1D 2011 08 18



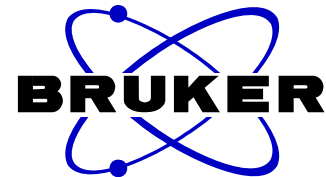
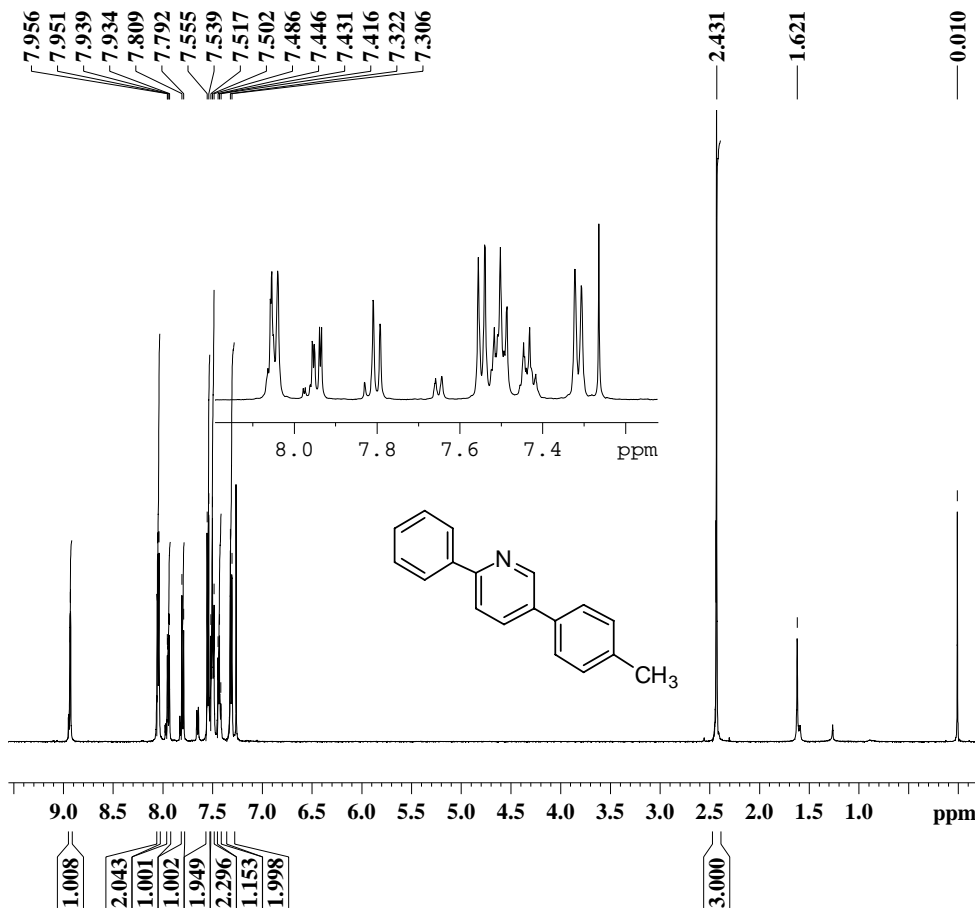
NAME WSW0616-2  
EXPNO 2  
PROCNO 1  
Date\_ 20110818  
Time 17.43  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 404  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 299.7 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326470 MHz  
WDW EM

Compound 3e

WSW0716-1 1H 1D 2011 08 16

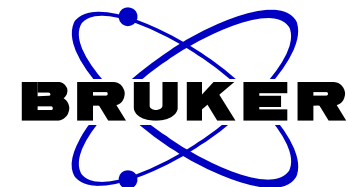
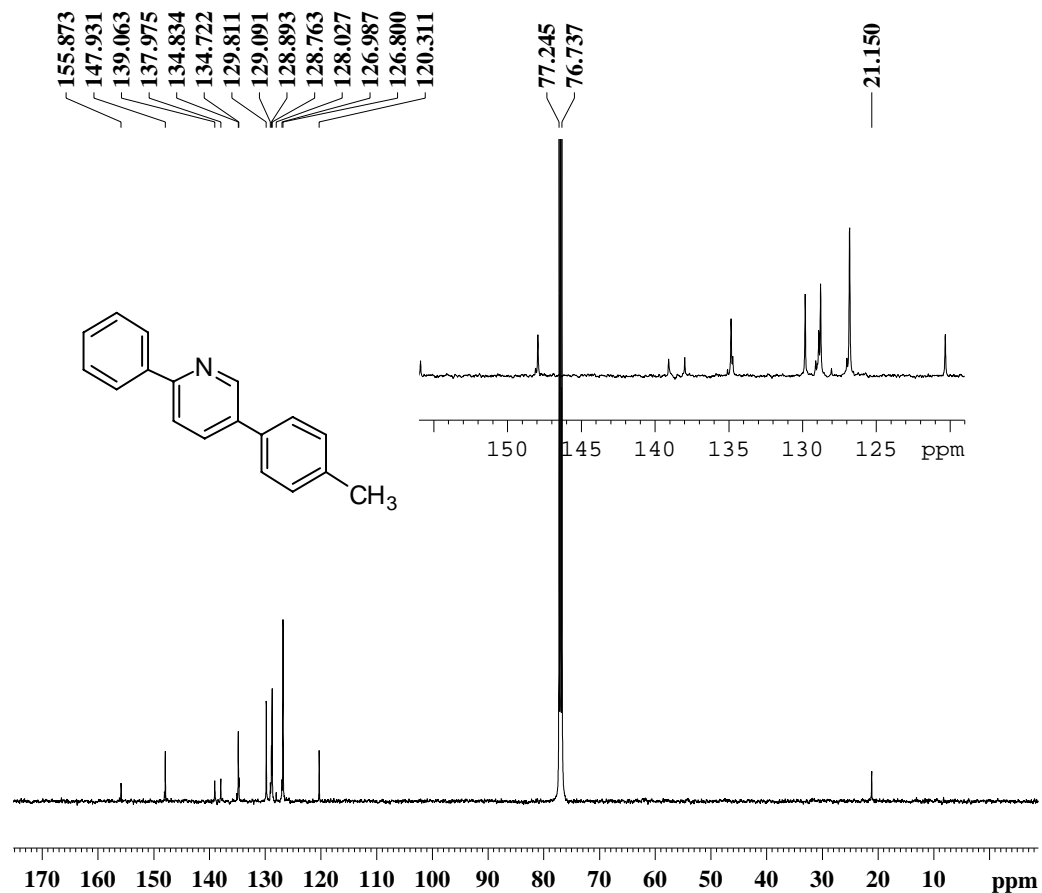


NAME WSW0716-1  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20110816  
 Time 17.32  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 456  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 297.7 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300082 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00



WSW0716-1 13C 1D 2011 08 18



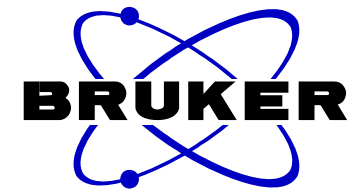
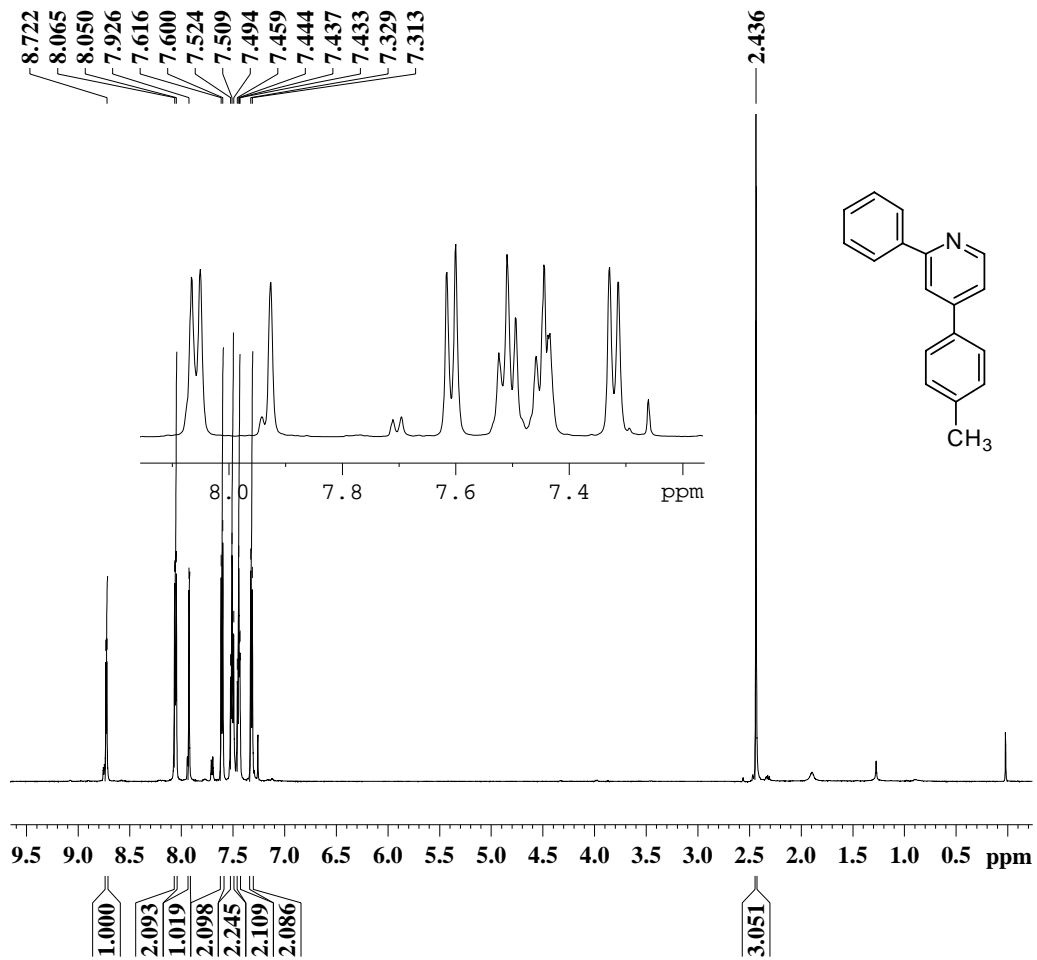
NAME WSW0716-1  
EXPNO 2  
PROCNO 1  
Date\_ 20110818  
Time 19.17  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1177  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 299.3 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326470 MHz  
WDW EM

Compound 4e

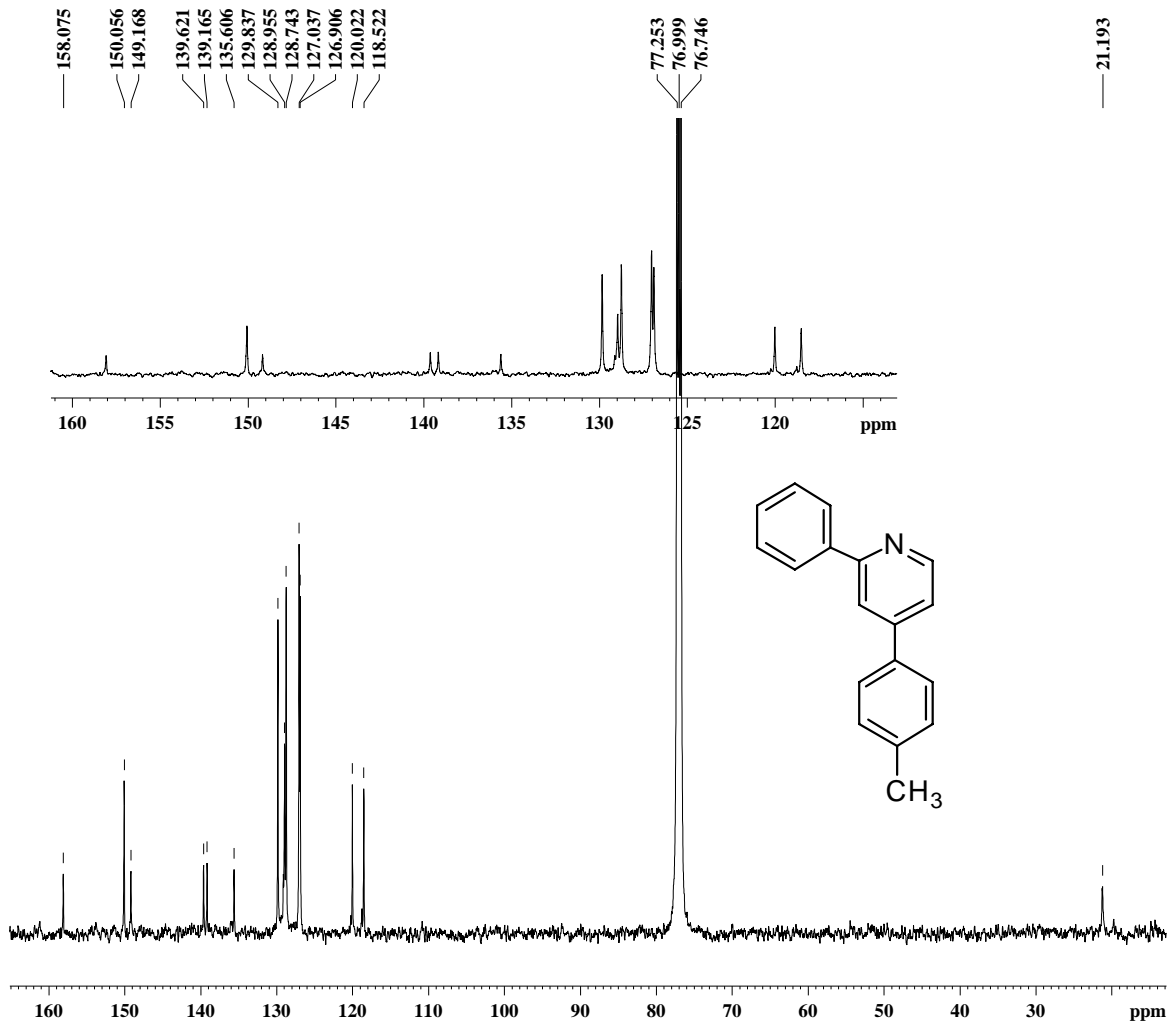
WSW0716-2 1H 2011 09 18



NAME WSW0716-2  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20110918  
 Time 19.36  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 144  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300101 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW0716-2 13C 1D 2011 09 27



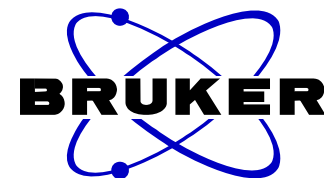
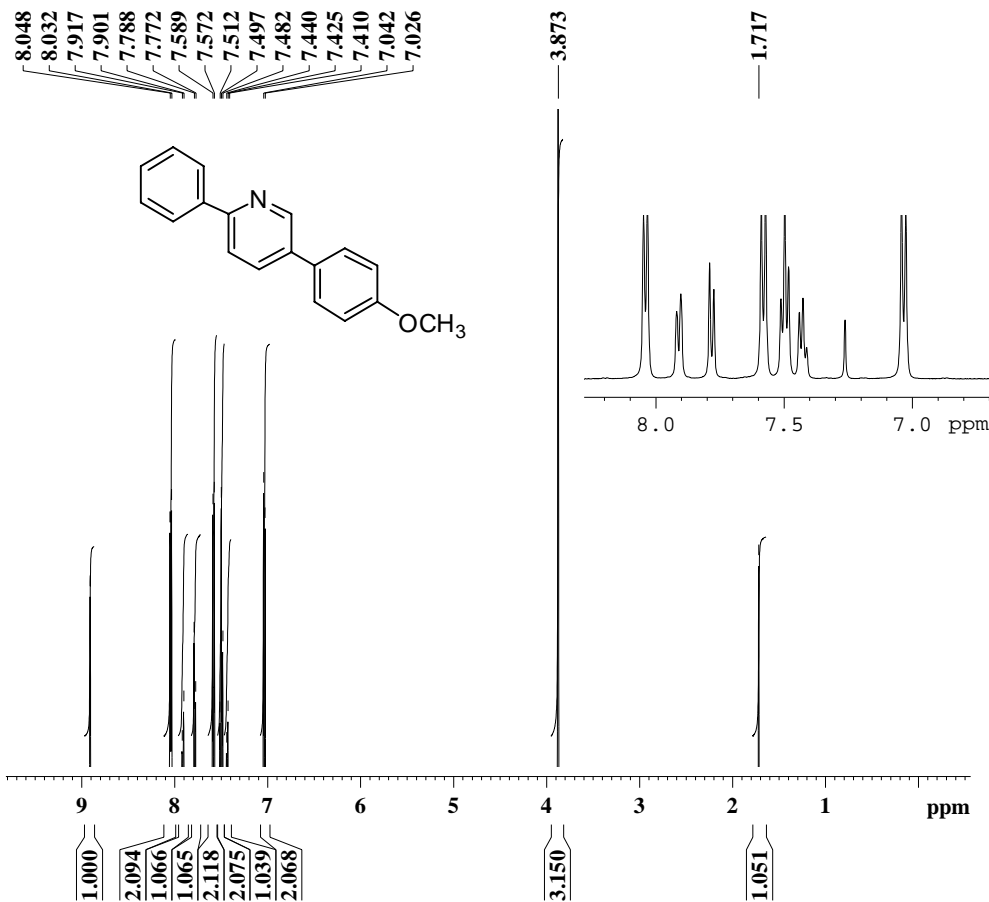
NAME WSW0716-2  
EXPNO 2  
PROCNO 1  
Date\_ 20110927  
Time 7.36  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT D2O  
NS 2514  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 299.6 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7323258 MHz  
WDW EM  
SSB 0  
LB 8.00 Hz  
GB 0  
PC 2.00

Compound 3f

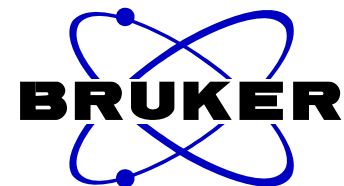
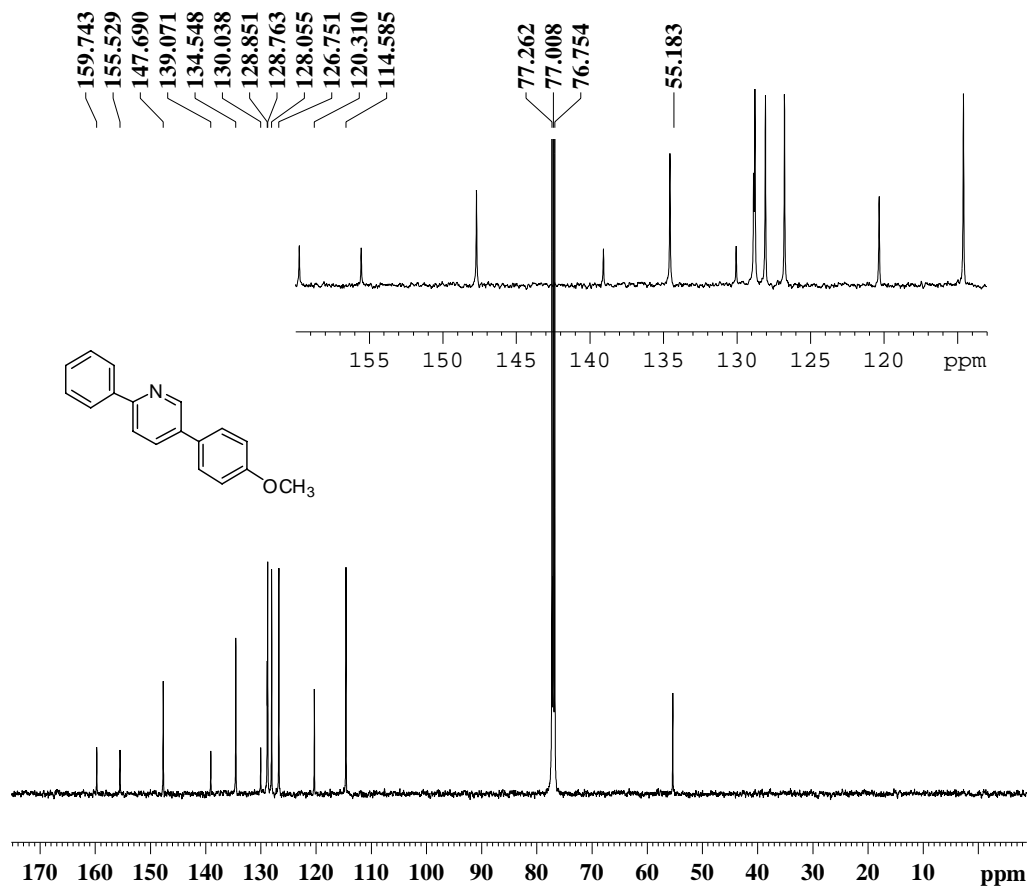
WSW0712-1 1H 1D 2011 07 22



NAME WSW0712-1  
EXPNO 1  
PROCNO 1  
Date\_ 20110722  
Time 15.29  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 4  
DS 1  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 1.6385000 sec  
RG 256  
DW 50.000 usec  
DE 6.00 usec  
TE 297.9 K  
D1 2.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 2.20 dB  
SFO1 500.0335010 MHz  
SI 16384  
SF 500.0300089 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 2.00

WSW0712-1 13C 1D 2011 07 22



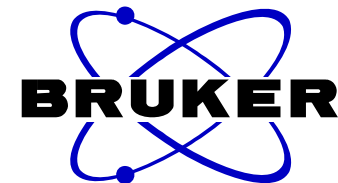
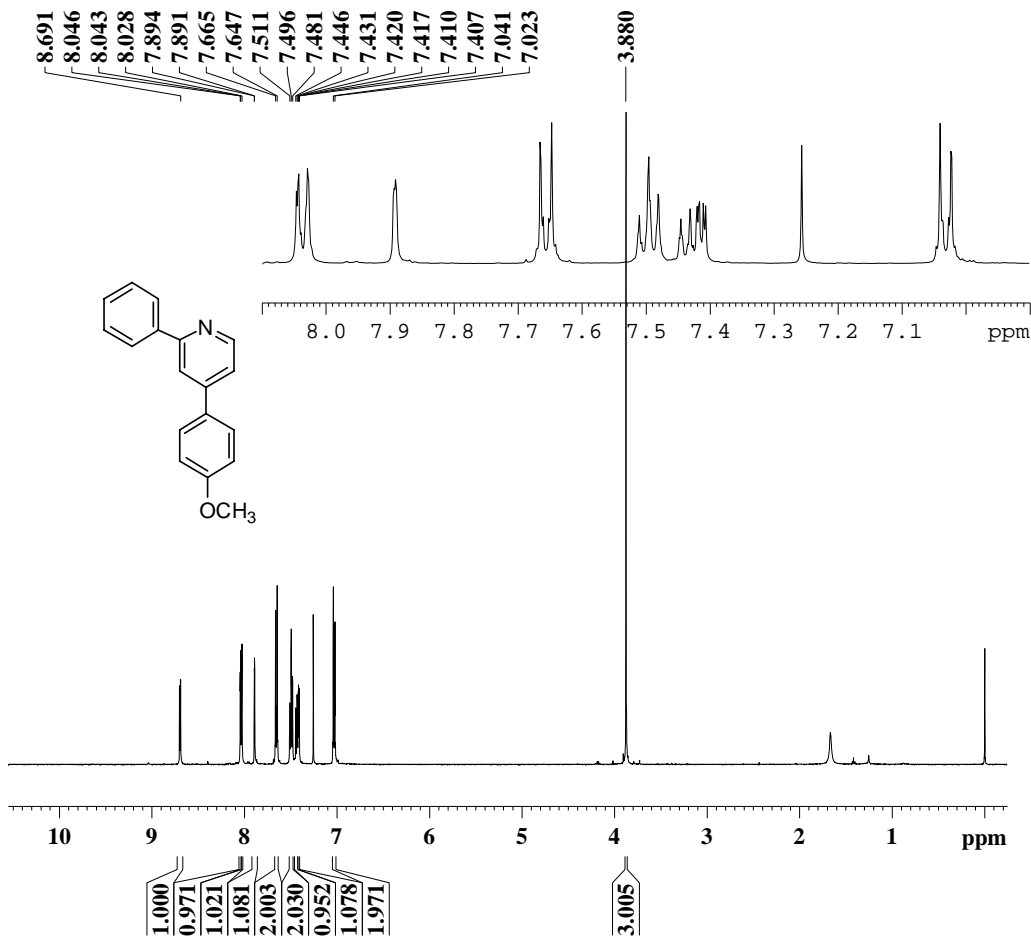
NAME WSW0712-1  
EXPNO 2  
PROCNO 1  
Date\_ 20110722  
Time 15.41  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 619  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 299.1 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326470 MHz  
WDW EM

Compound 4f

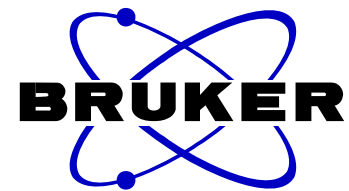
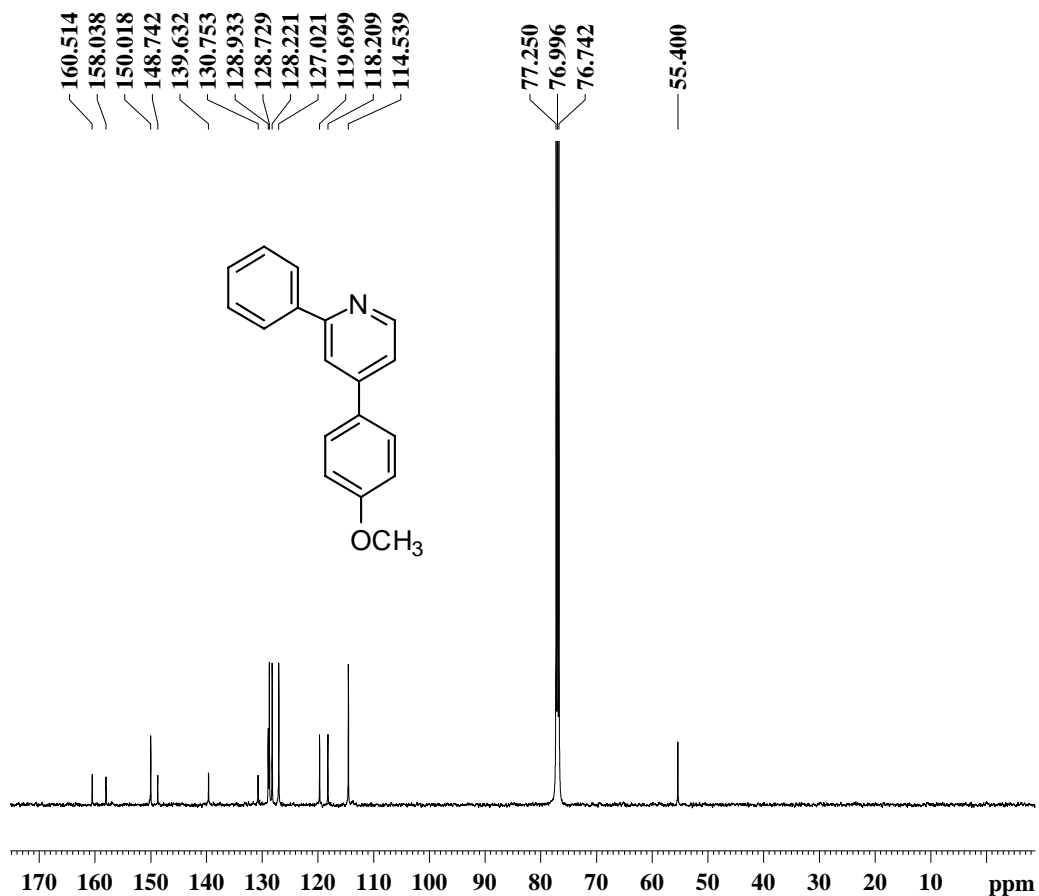
WSW0712-2 1H ID 2011 07 26



NAME WSW0712-2  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20110726  
 Time 9.55  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 575  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 296.9 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300119 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW0712-2 13C 1D 2011 07 26



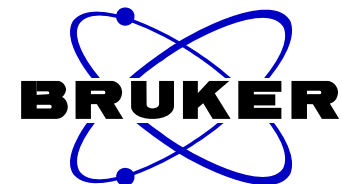
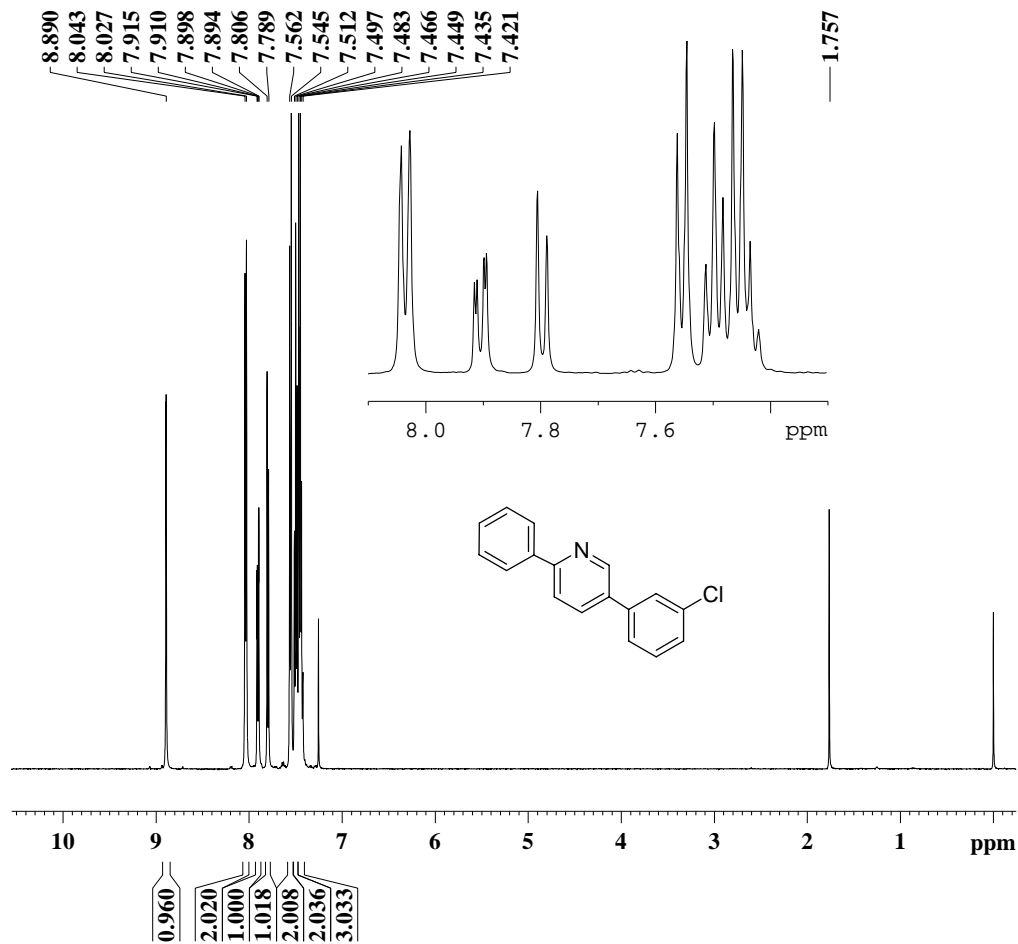
NAME WSW0712-2  
EXPNO 2  
PROCNO 1  
Date\_ 20110726  
Time 17.13  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2191  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 298.3 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326470 MHz  
WDW EM

Compound **3g**

WSW0518-1-(0601) 1H 2012 06 01

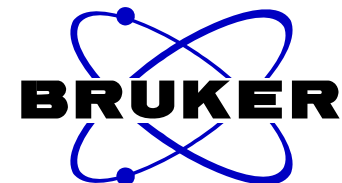
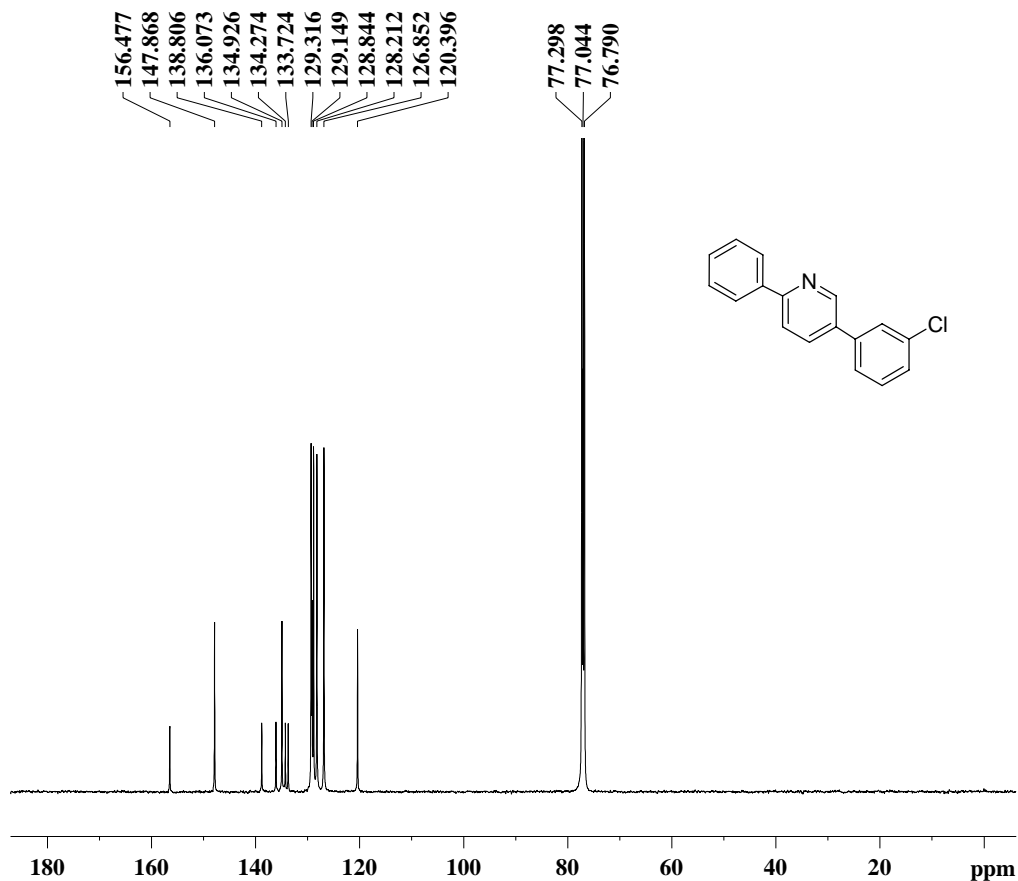


NAME WSW0518-1-(0601)  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20120601  
 Time 15.19  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 203  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 291.9 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300135 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00



WSW0518-1-(0601) 13C ID 2012 06 03



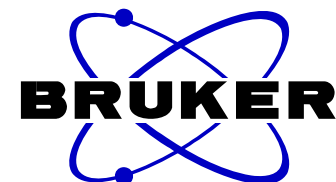
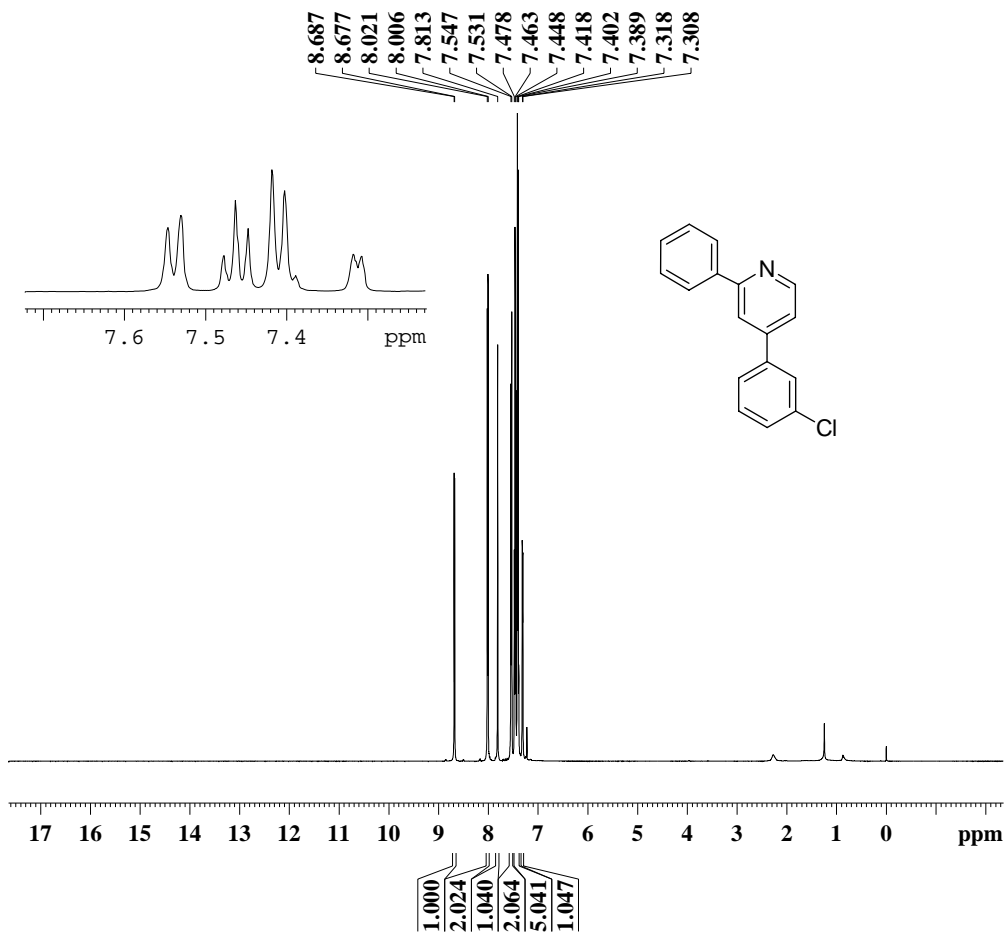
NAME WSW0518-1-(0601)  
EXPNO 2  
PROCNO 1  
Date\_ 20120604  
Time 14.29  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 3728  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 3250  
DW 15.300 usec  
DE 6.00 usec  
TE 295.8 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326455 MHz  
WDW EM

Compound **4g**

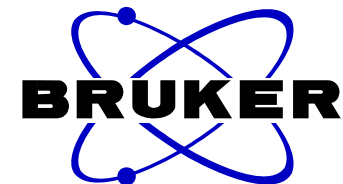
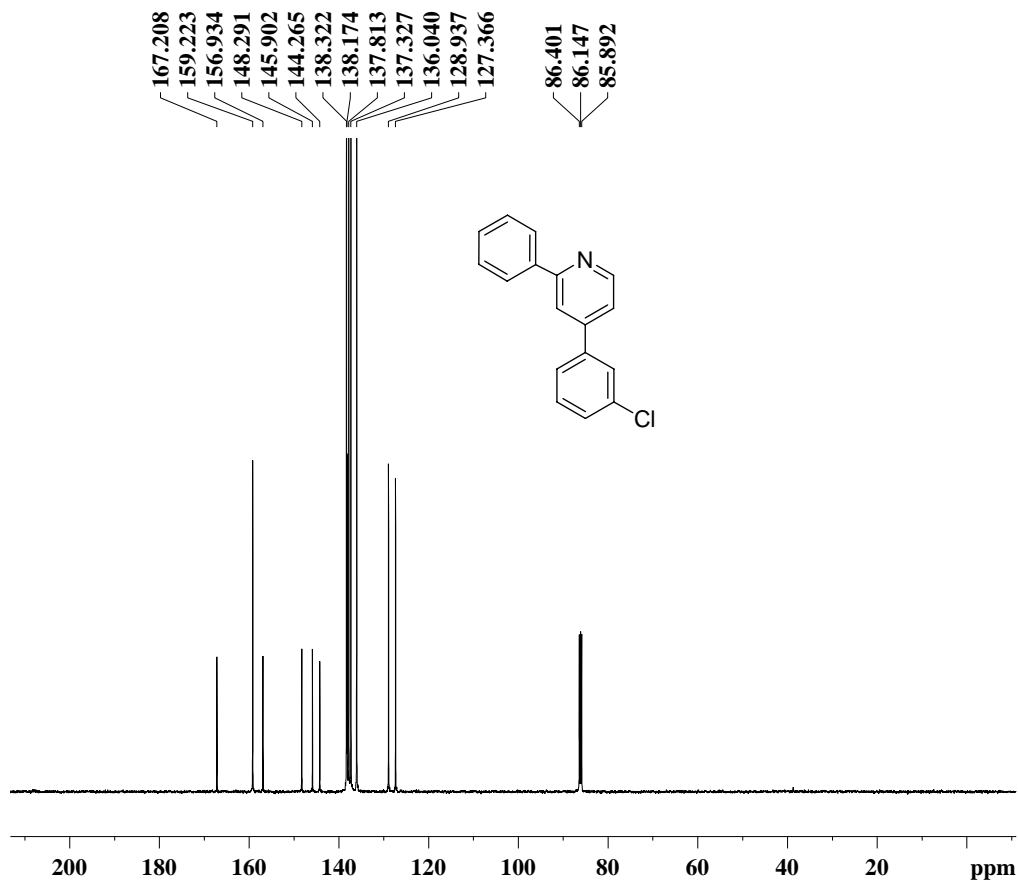
WSW0518-2 1H 1D 2012 09 10



NAME WSW0518-2  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20120910  
 Time 7.31  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 16384  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8193000 sec  
 RG 71.8  
 DW 50.000 usec  
 DE 8.00 usec  
 TE 296.9 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.00 usec  
 PL1 2.00 dB  
 SFO1 500.0338500 MHz  
 SI 16384  
 SF 500.0300269 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW0518-2 13C 1D 2012 09 13



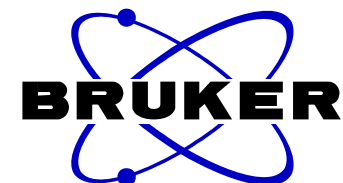
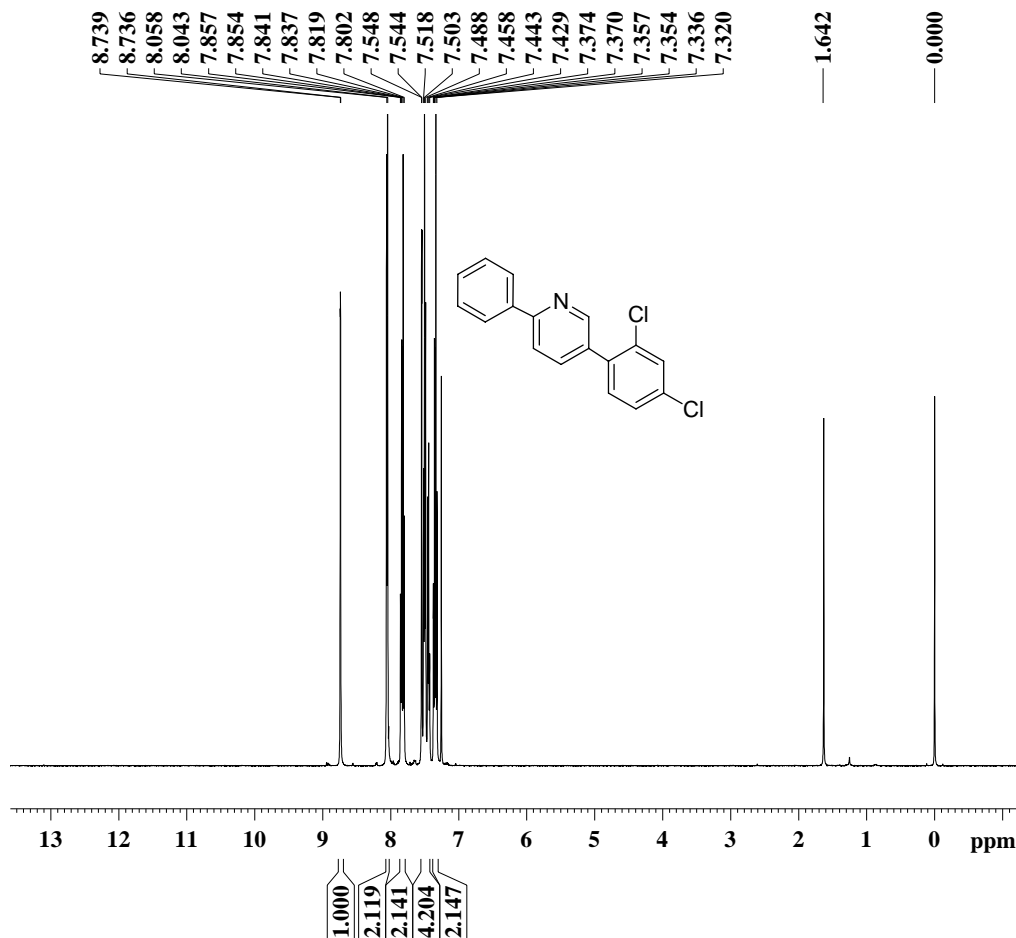
NAME WSW0518-2  
EXPNO 2  
PROCNO 1  
Date\_ 20120913  
Time 9.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 327  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 512  
DW 15.300 usec  
DE 6.00 usec  
TE 300.8 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 10

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.20 usec  
PL1 3.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 17.70 dB  
PL13 17.70 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7315152 MHz  
WDW EM

Compound **3h**

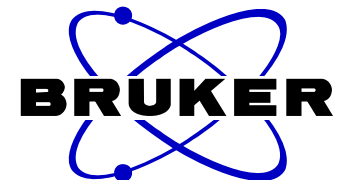
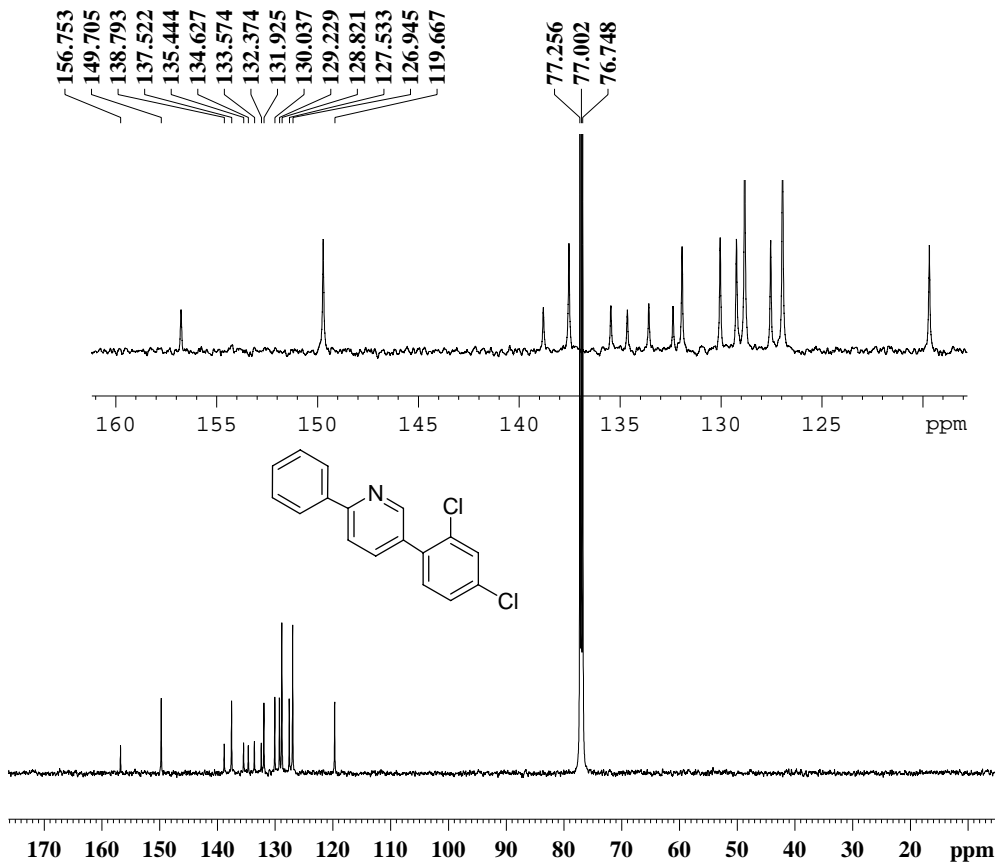
WSW0427-1 1H 2012 05 07



NAME WSW0427-1  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20120507  
 Time 22.07  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 456  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 295.4 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300124 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW0427-1 13C ID 2012 05 08



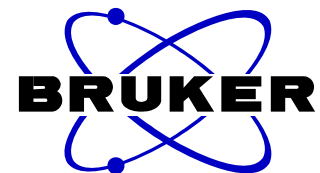
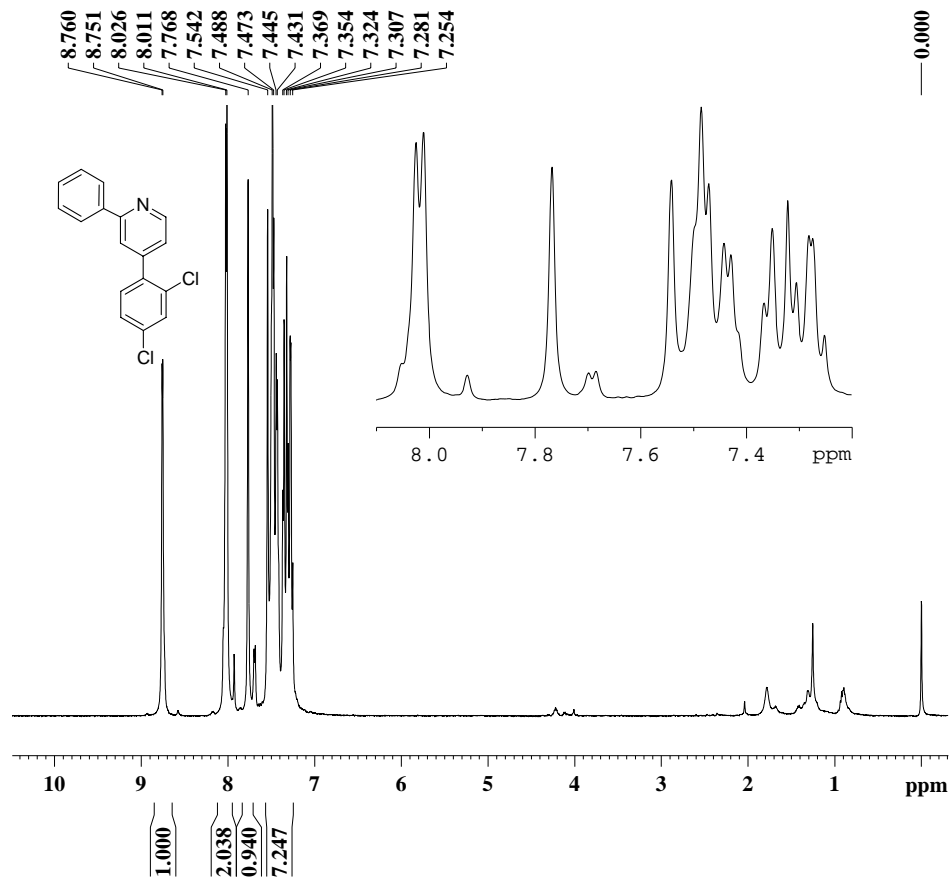
NAME WSW0427-1  
EXPNO 2  
PROCNO 11  
Date\_ 20120508  
Time 21.58  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 659  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 8200  
DW 15.300 usec  
DE 6.00 usec  
TE 299.5 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326463 MHz  
WDW EM

Compound **4h**

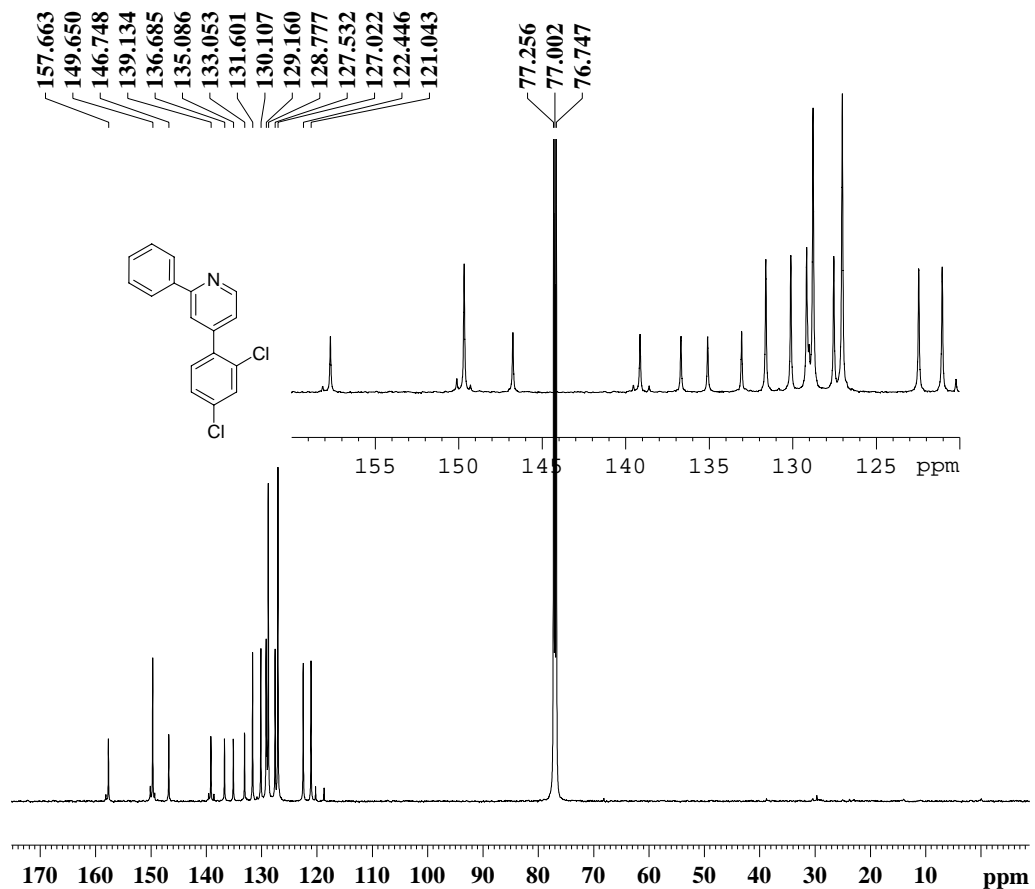
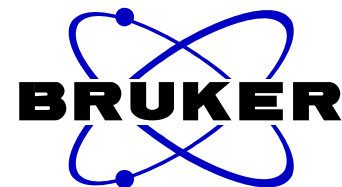
WSW0427-2 1H 2012 05 07



NAME WSW0427-2  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20120507  
 Time 22.11  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 256  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 295.4 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300152 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW0427-2 13C 1D 2012 05 08

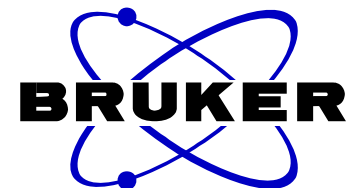
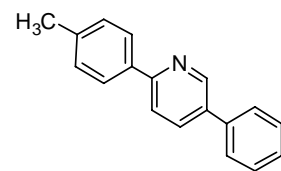
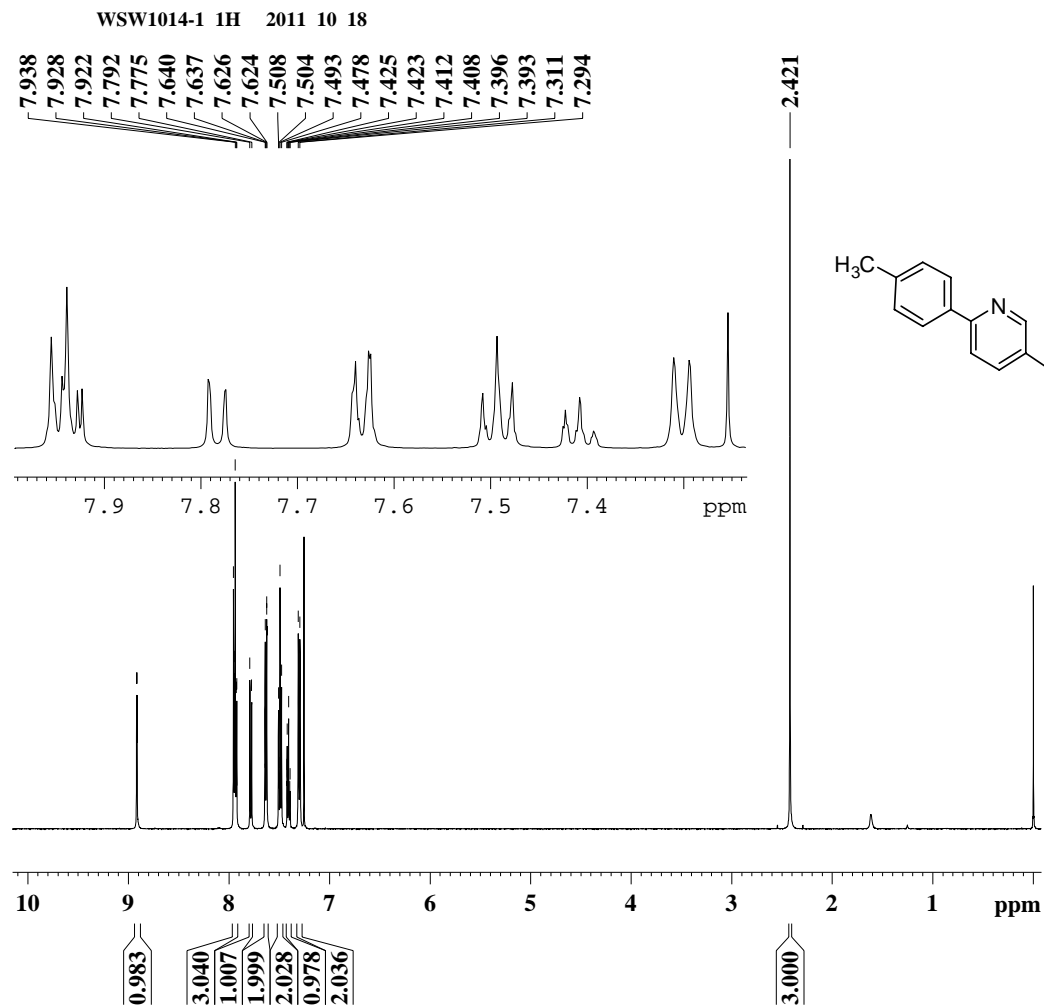


NAME WSW0427-2  
EXPNO 2  
PROCNO 11  
Date\_ 20120509  
Time 7.41  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 11316  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 3250  
DW 15.300 usec  
DE 6.00 usec  
TE 300.1 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326455 MHz  
WDW EM

Compound 3i

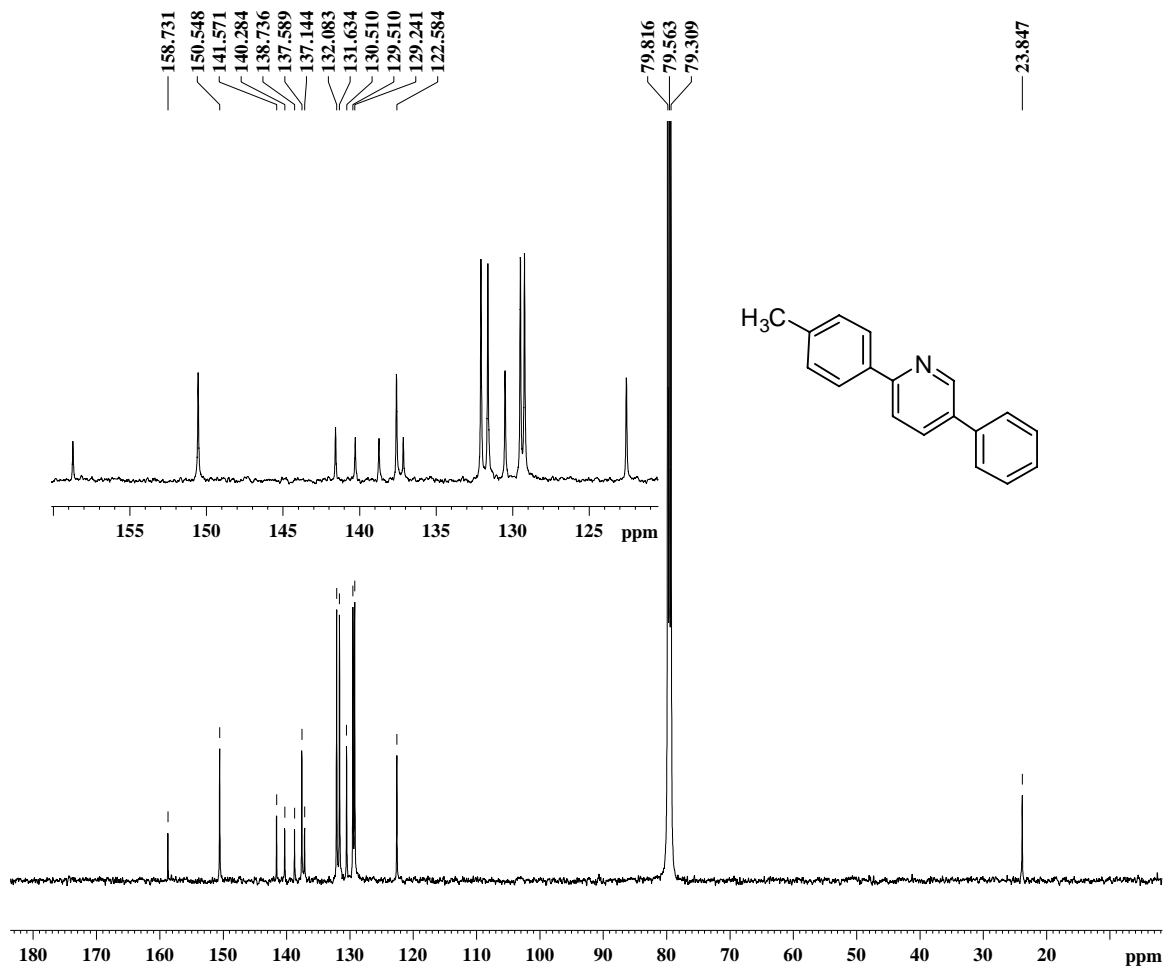
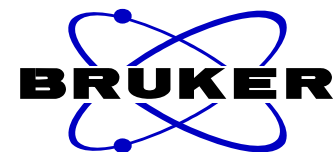


NAME WSW1014-1  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20111018  
 Time 15.55  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 362  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 296.1 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300131 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00



WSW1014-1 13C ID 2011 10 20



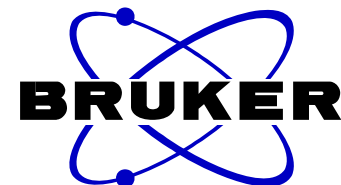
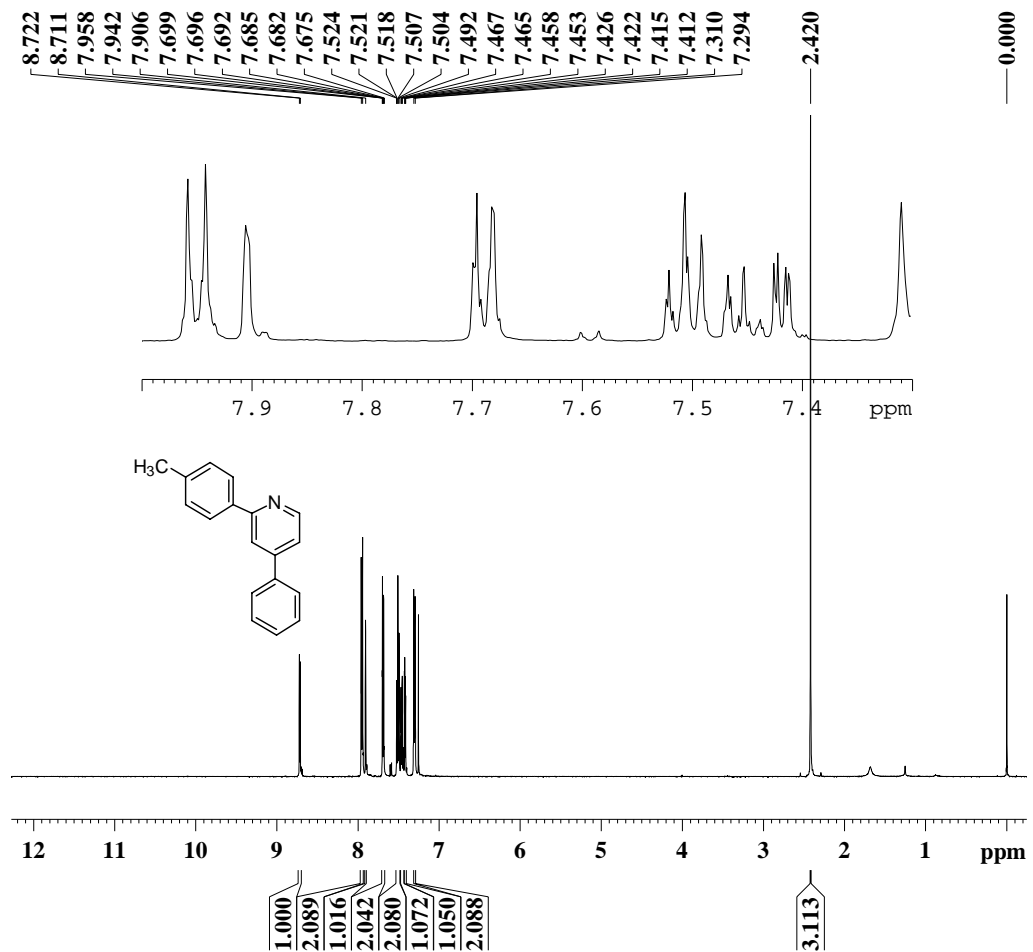
NAME WSW1014-1  
EXPNO 2  
PROCNO 1  
Date\_ 20111021  
Time 22.12  
INSTRUM av500  
PROBHD 5 mm PABBO BB  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2171  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 296.9 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

=====  
CHANNEL f1 ===  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

=====  
CHANNEL f2 ===  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7323258 MHz  
WDW EM  
SSB 0  
LB 8.00 Hz  
GB 0  
PC 2.00

Compound 4i

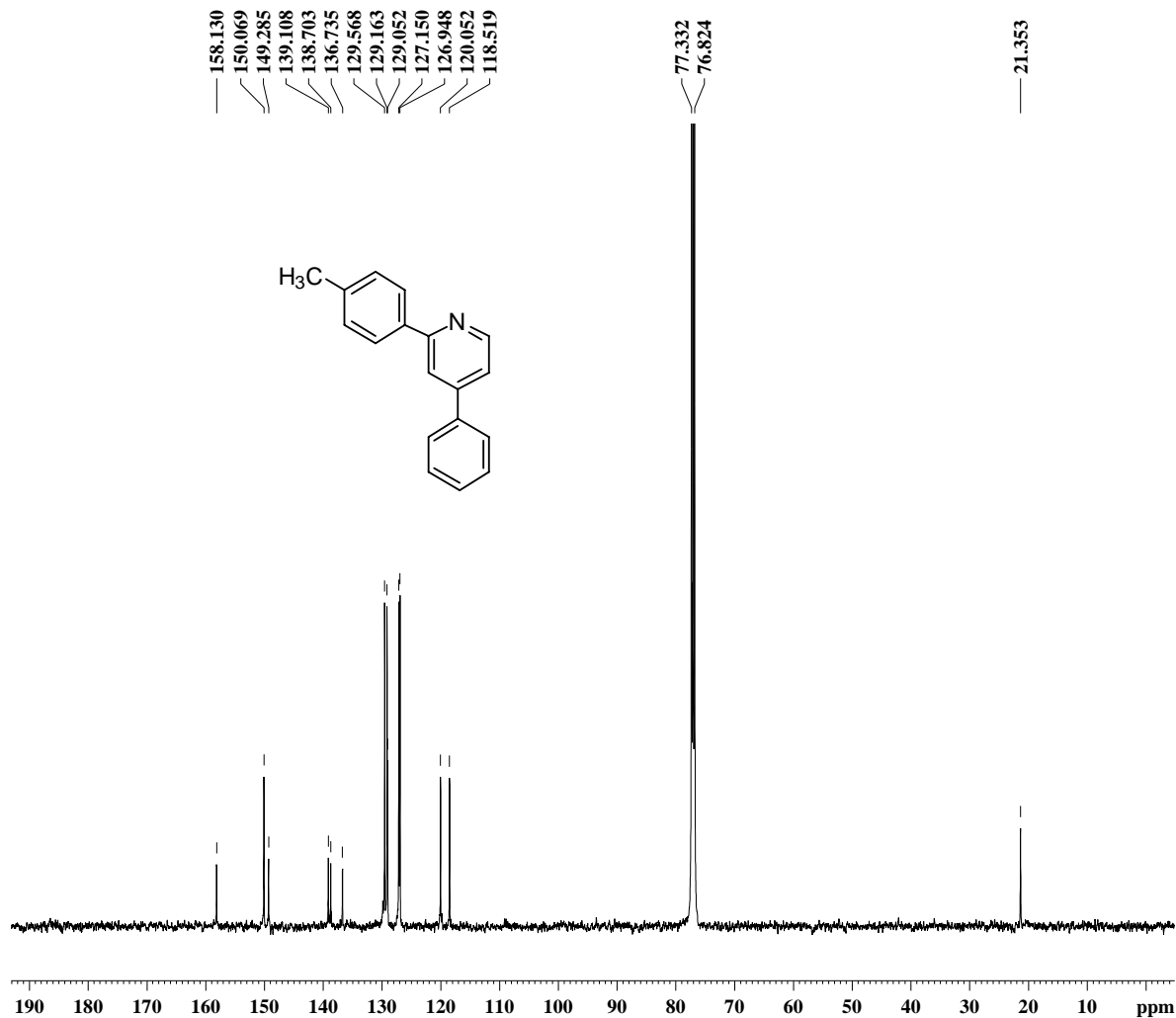
WSW1014-2 1H 2011 11 28



NAME WSW1014-2  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20111128  
 Time 19.32  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 362  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 296.9 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300139 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW1014-2 13C 1D 2011 12 01



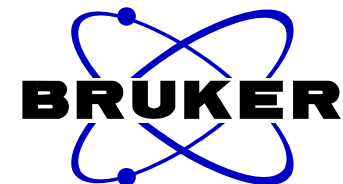
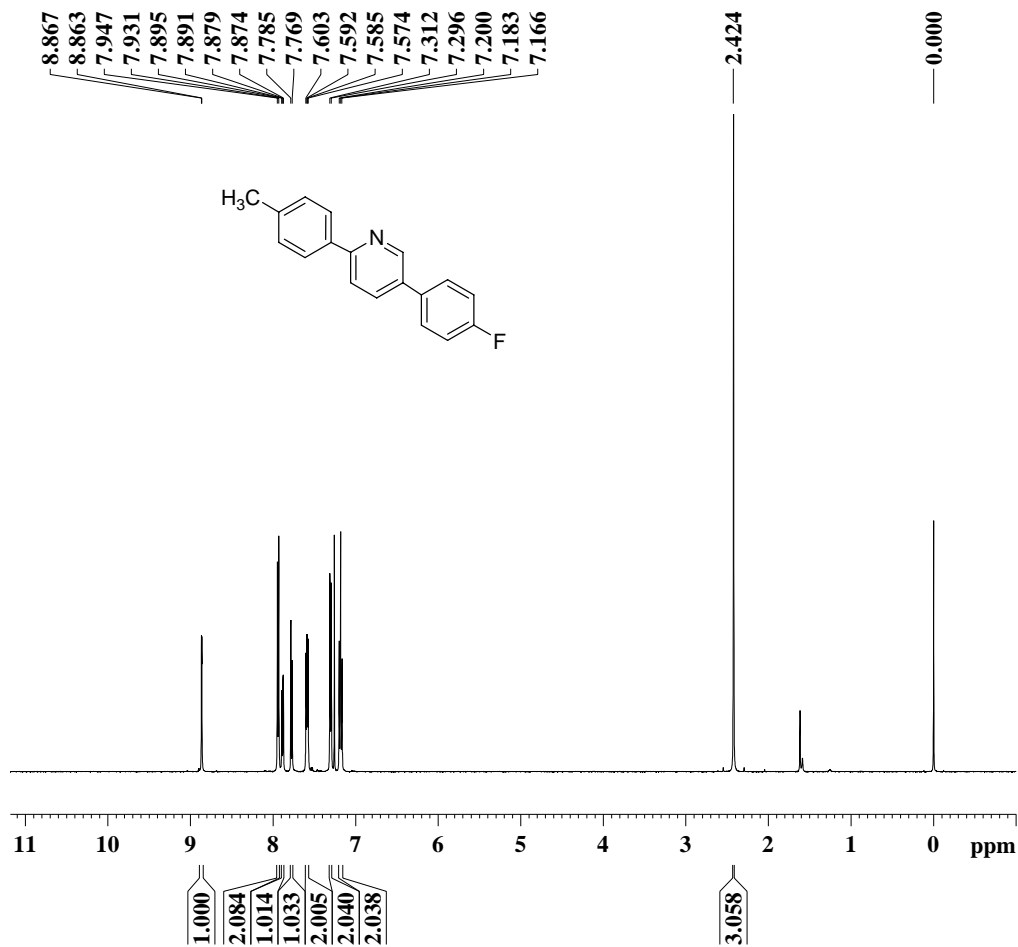
NAME WSW1014-2  
EXPNO 2  
PROCNO 1  
Date\_ 20111201  
Time 14.56  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1081  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 295.7 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326387 MHz  
WDW EM  
SSB 0  
LB 6.00 Hz  
GB 0  
PC 2.00

Compound 3j

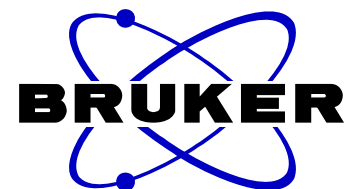
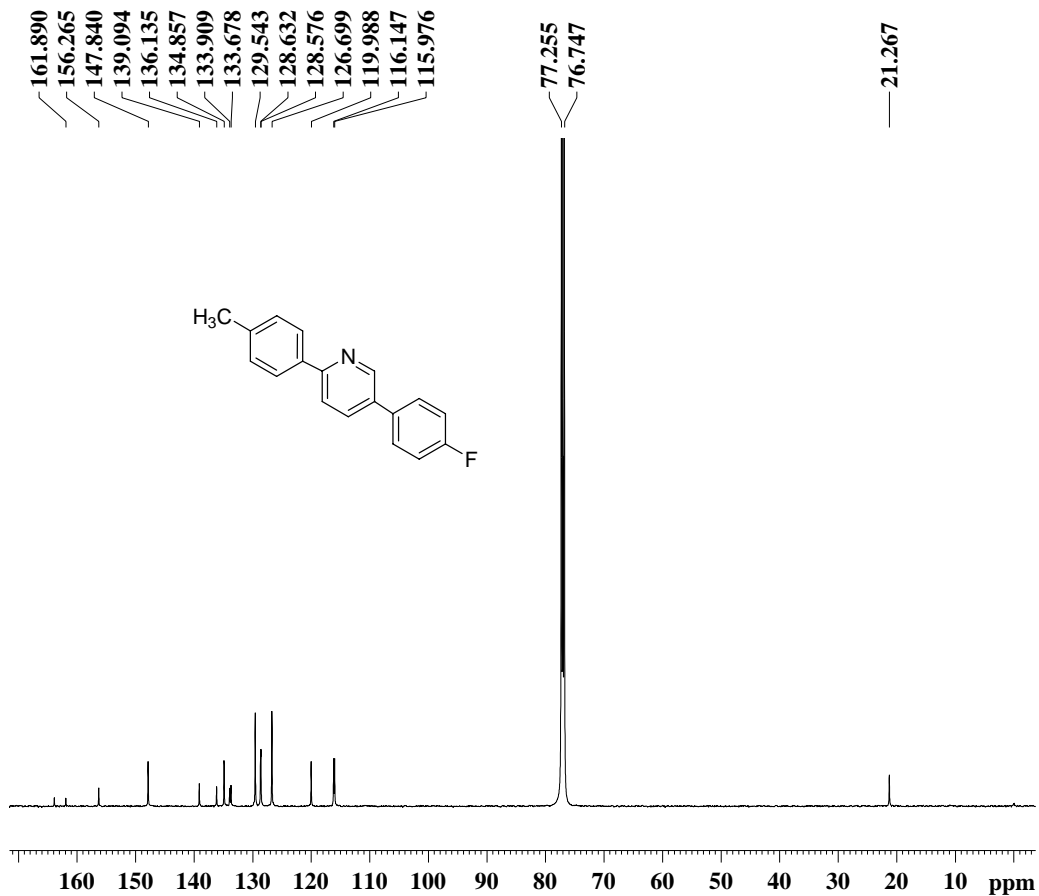
WSW1129-1 1H 2011 12 14



NAME WSW1129-1  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20111214  
 Time 18.25  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 456  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 294.0 K  
 D1 2.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300111 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW1129-1 13C 1D 2011 12 18



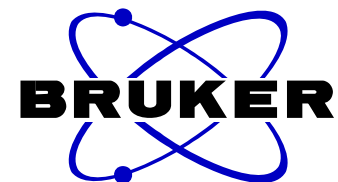
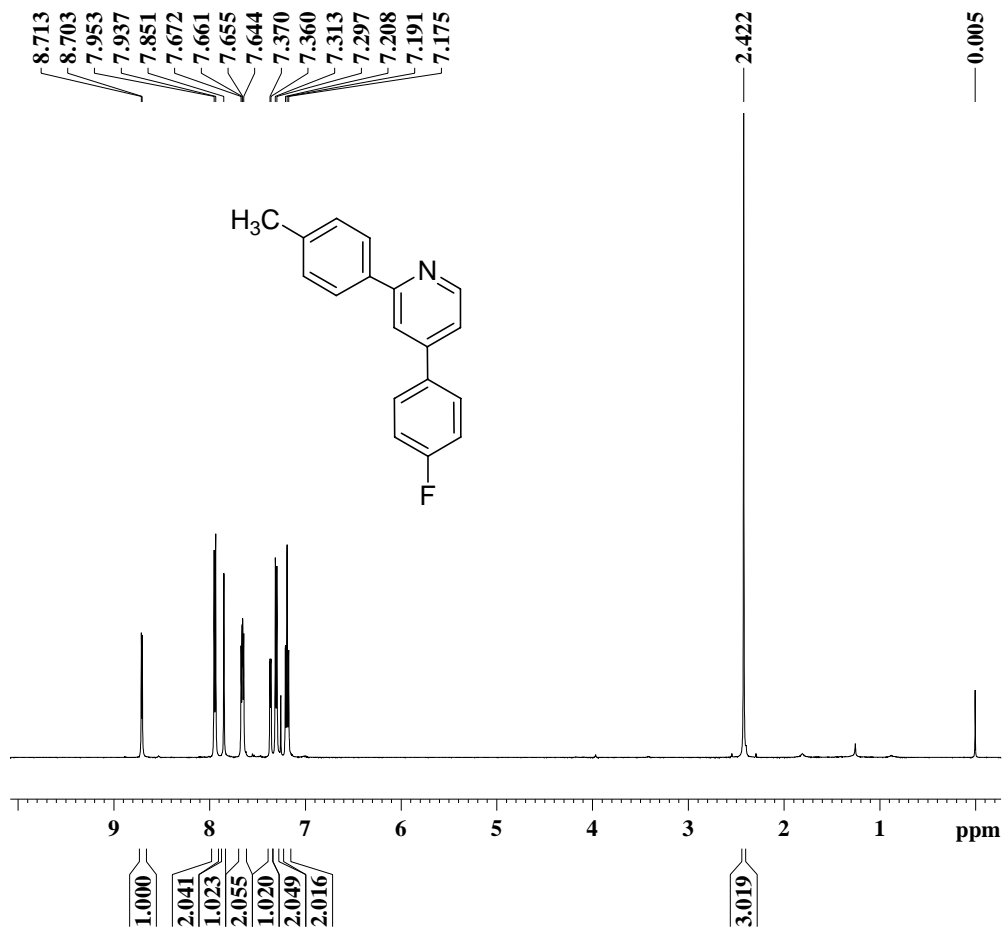
NAME WSW1129-1  
EXPNO 2  
PROCNO 1  
Date\_ 20111218  
Time 21.55  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 10755  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 297.2 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326428 MHz  
WDW EM

Compound 4j

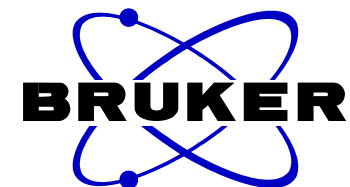
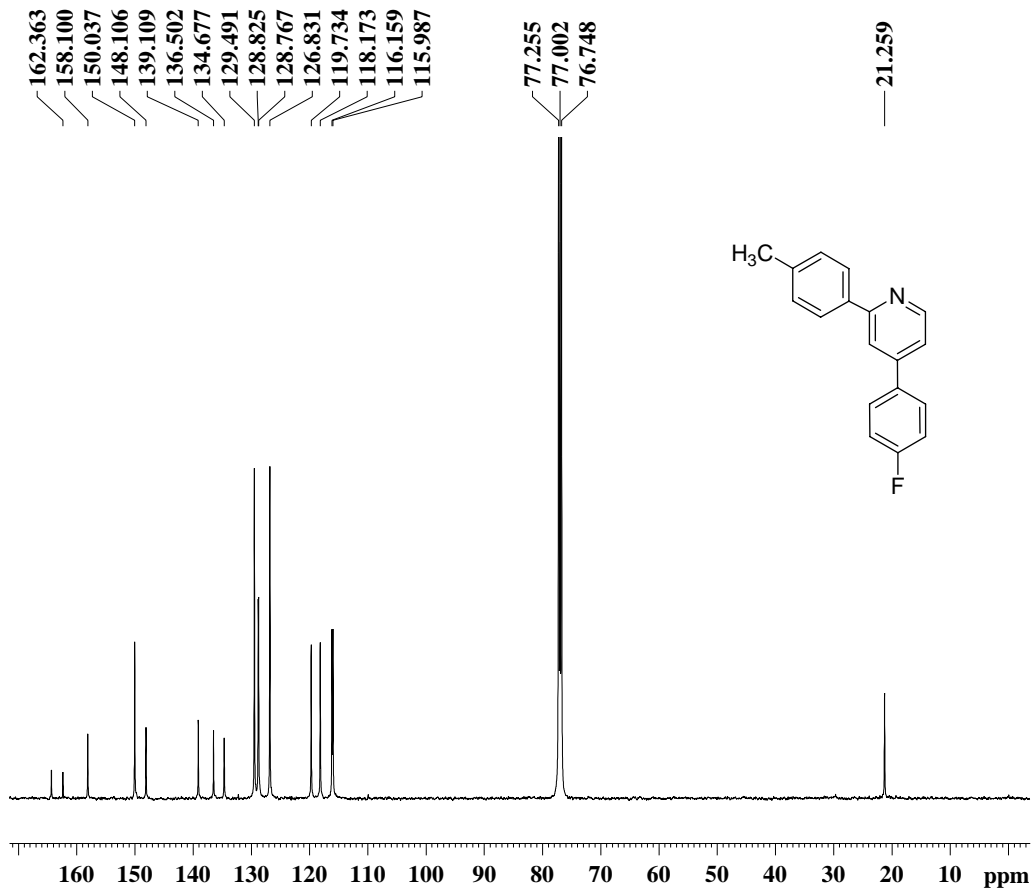
WSW1129-2 1H 2011 12 14



NAME WSW1129-2  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20111214  
 Time 18.29  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 228  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 294.0 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300111 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

wsw1129-2 13C 1D 2011 12 19



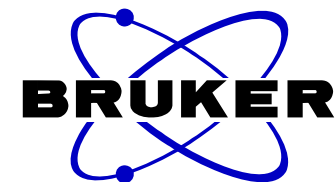
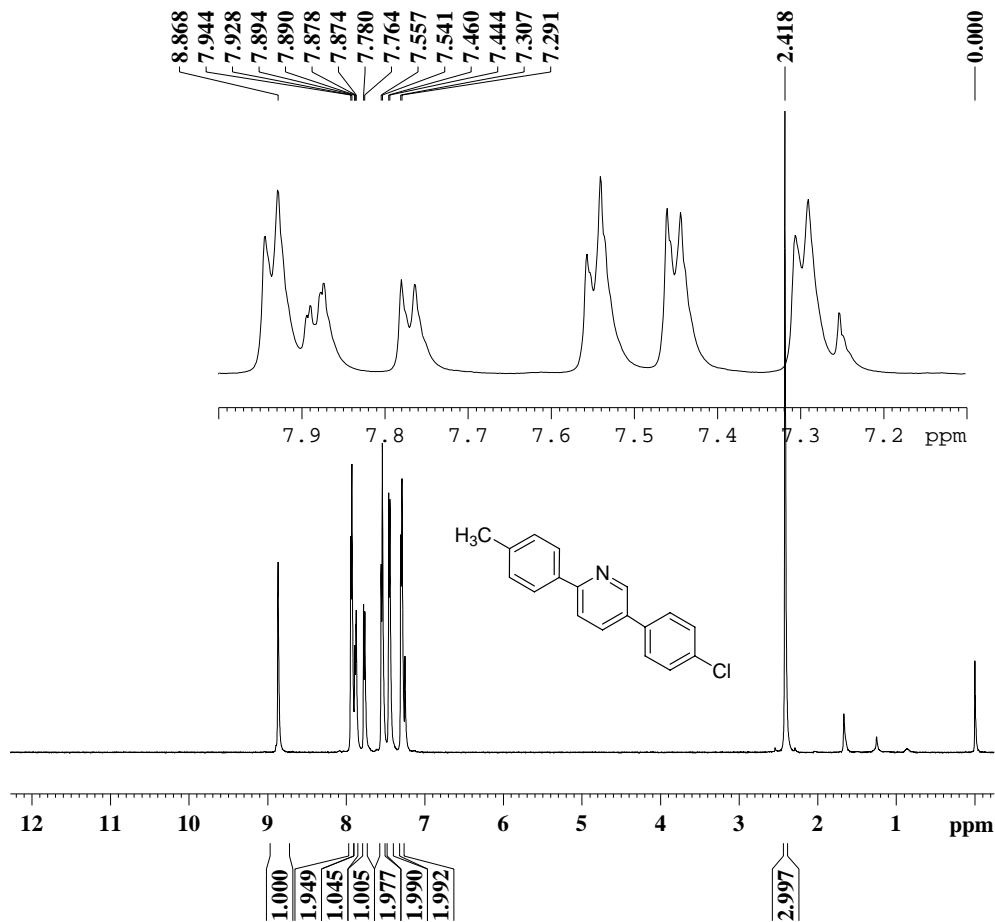
NAME WSW1129-2  
EXPNO 21  
PROCNO 1  
Date\_ 20111219  
Time 14.28  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1955  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 1290  
DW 15.300 usec  
DE 6.00 usec  
TE 294.8 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326512 MHz  
WDW EM

Compound **3k**

WSW1104-1 1H 2011 11 10

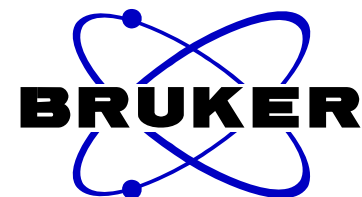
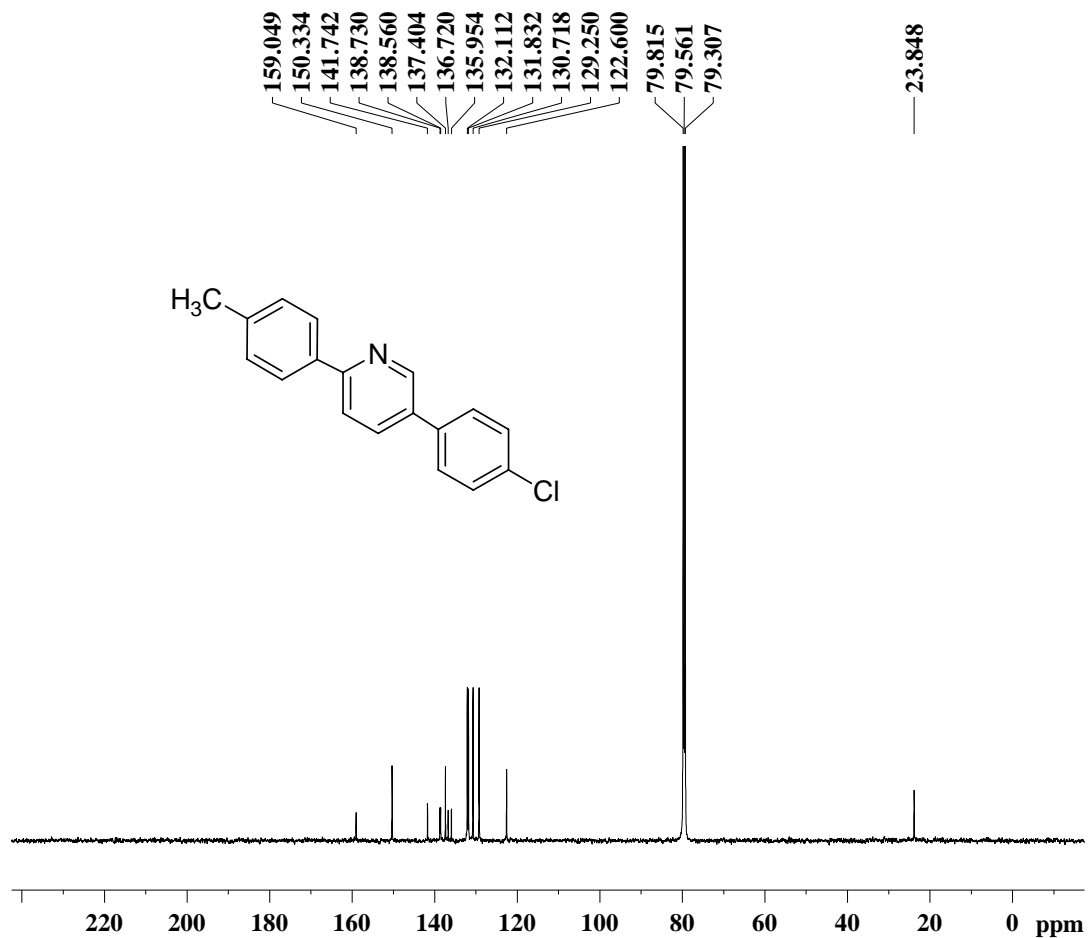


NAME WSW1104-1  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20111110  
 Time 19.45  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.638500 sec  
 RG 287  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 295.9 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300138 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00



WSW1104-1 13C 1D 2011 11 15



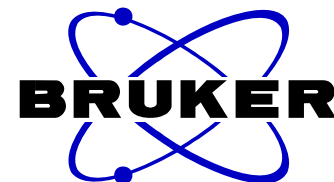
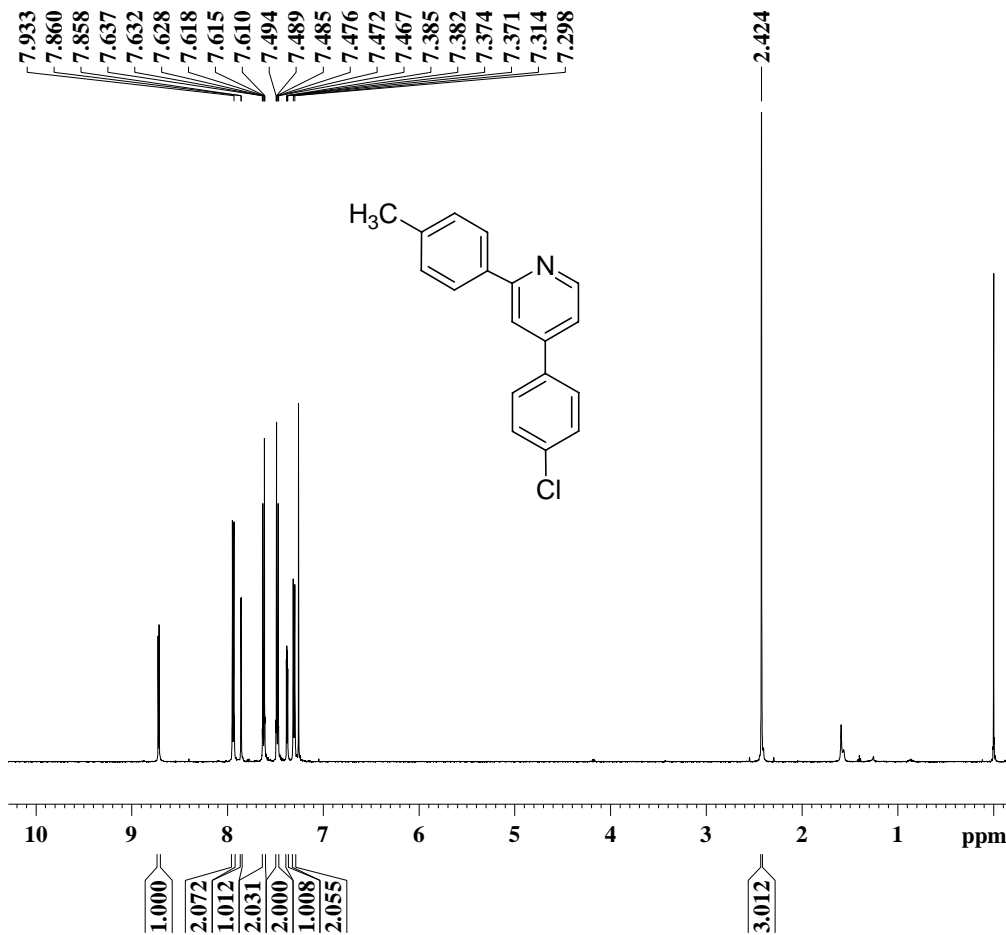
NAME WSW1104-1  
EXPNO 2  
PROCNO 1  
Date\_ 20111115  
Time 10.40  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1045  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 297.0 K  
D1 2.0000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

=====  
CHANNEL f1  
=====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

=====  
CHANNEL f2  
=====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7323258 MHz  
WDW EM

Compound **4k**

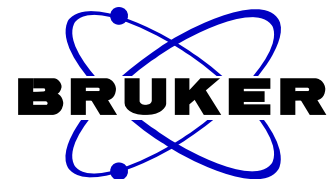
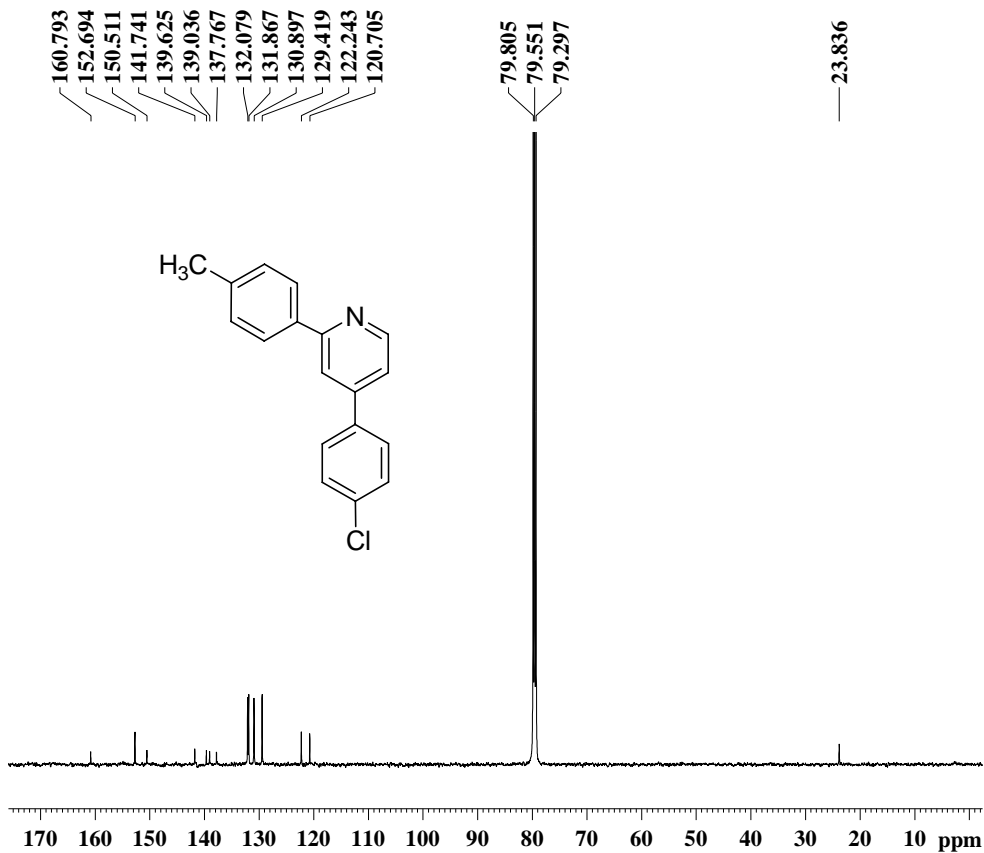
WSW1104-3 1H 2011 11 10



NAME WSW1104-3  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20111110  
 Time 19.50  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 575  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 295.8 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300111 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW1104-3 13C ID 2011 11 15



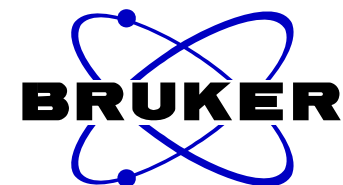
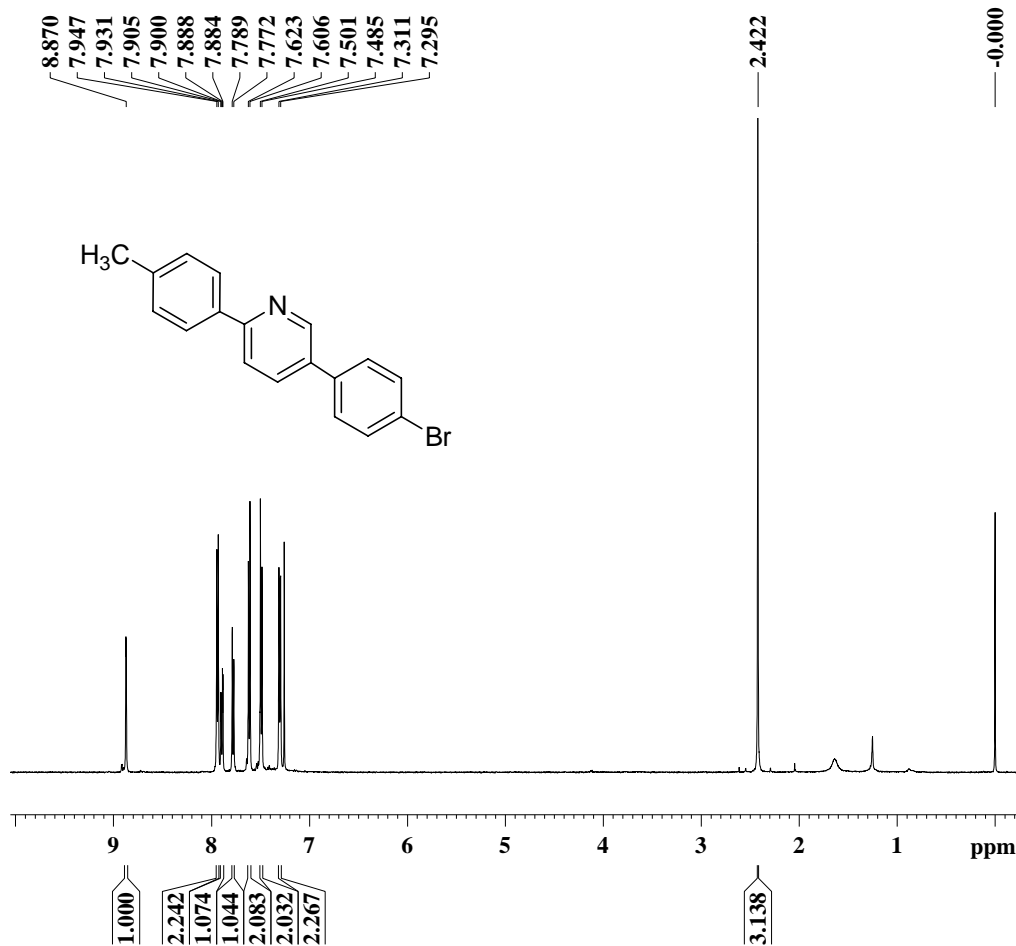
NAME WSW1104-3  
EXPNO 2  
PROCNO 1  
Date\_ 20111115  
Time 12.21  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1447  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 297.1 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7323258 MHz  
WDW EM

Compound 3I

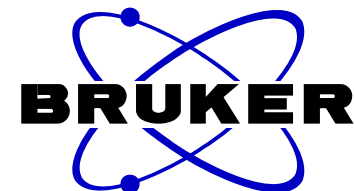
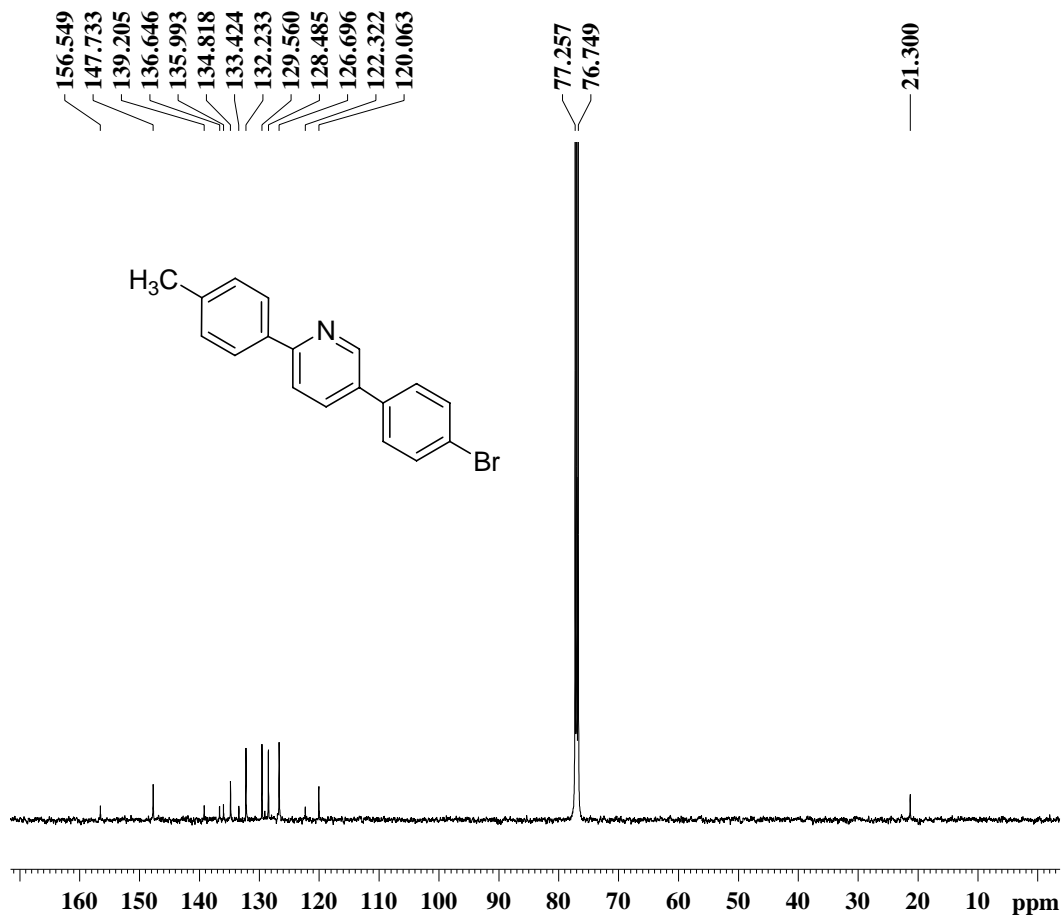
WSW1201-1 1H 2011 12 14



NAME WSW1201-1  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20111214  
 Time 18.33  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 456  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 294.0 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300111 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW1201-1 13C 1D 2011 12 18



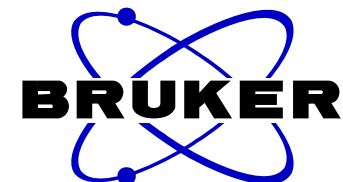
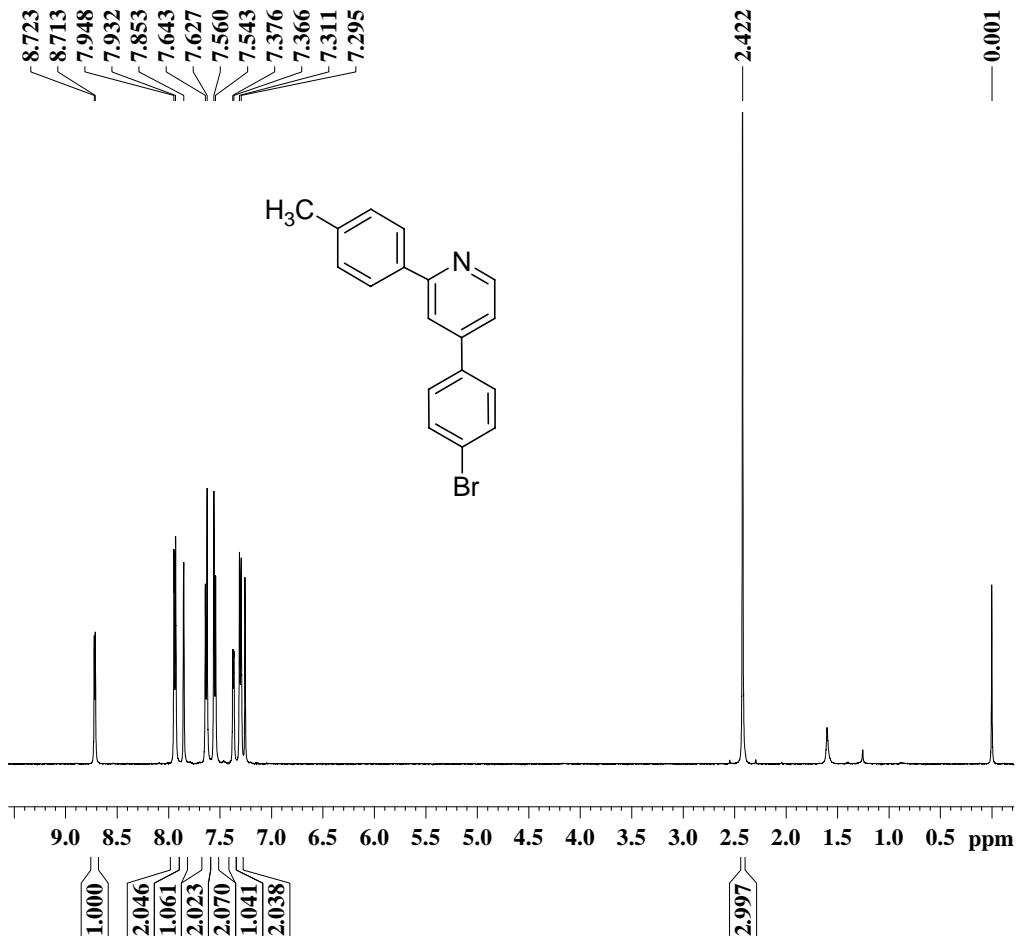
NAME WSW1201-1  
EXPNO 2  
PROCNO 1  
Date\_ 20111218  
Time 21.25  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 433  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 296.3 K  
D1 2.0000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

=====  
CHANNEL f1  
=====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

=====  
CHANNEL f2  
=====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326468 MHz  
WDW EM

Compound 4I

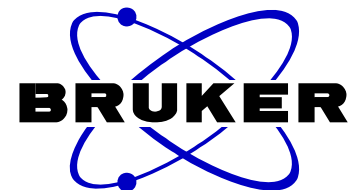
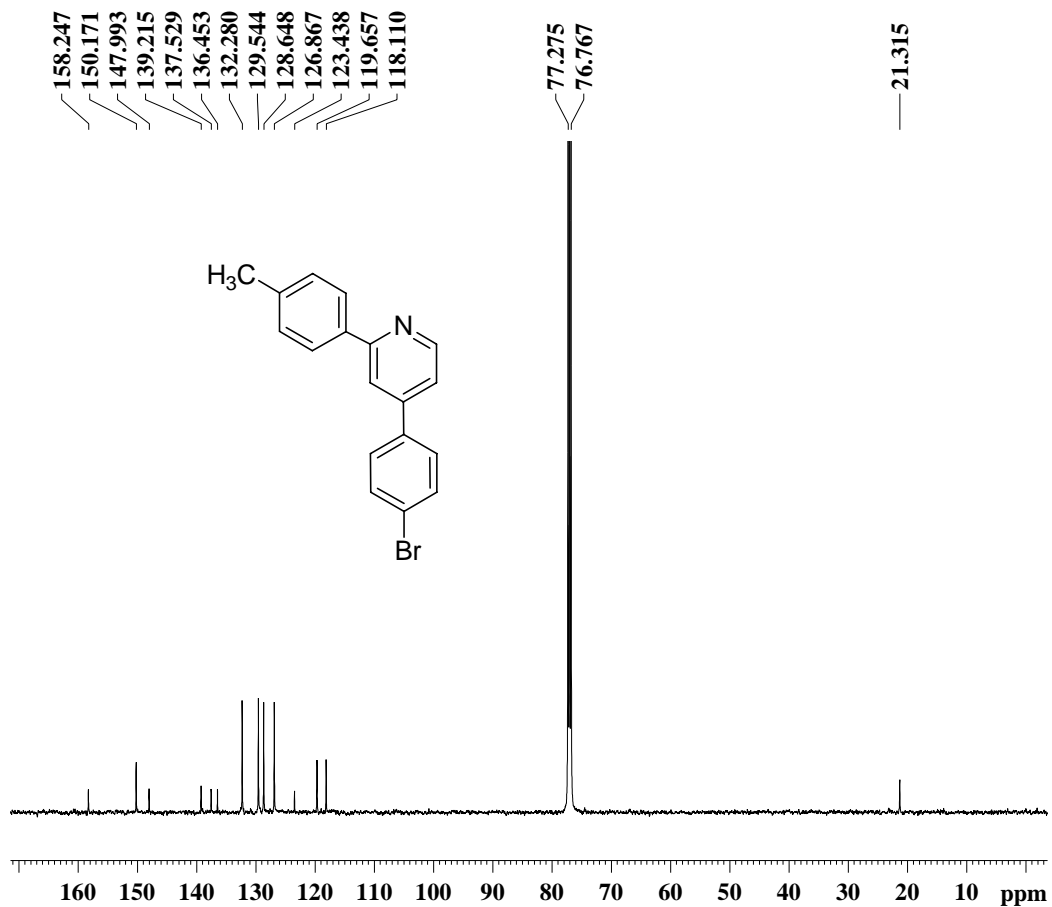
WSW1201-2 1H 2011 12 21



NAME WSW1201-2  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20111221  
 Time 19.45  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 456  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300111 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW1201-2 13C ID 2011 12 27



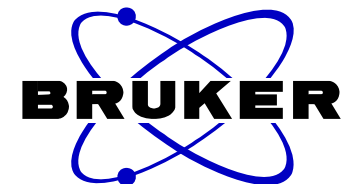
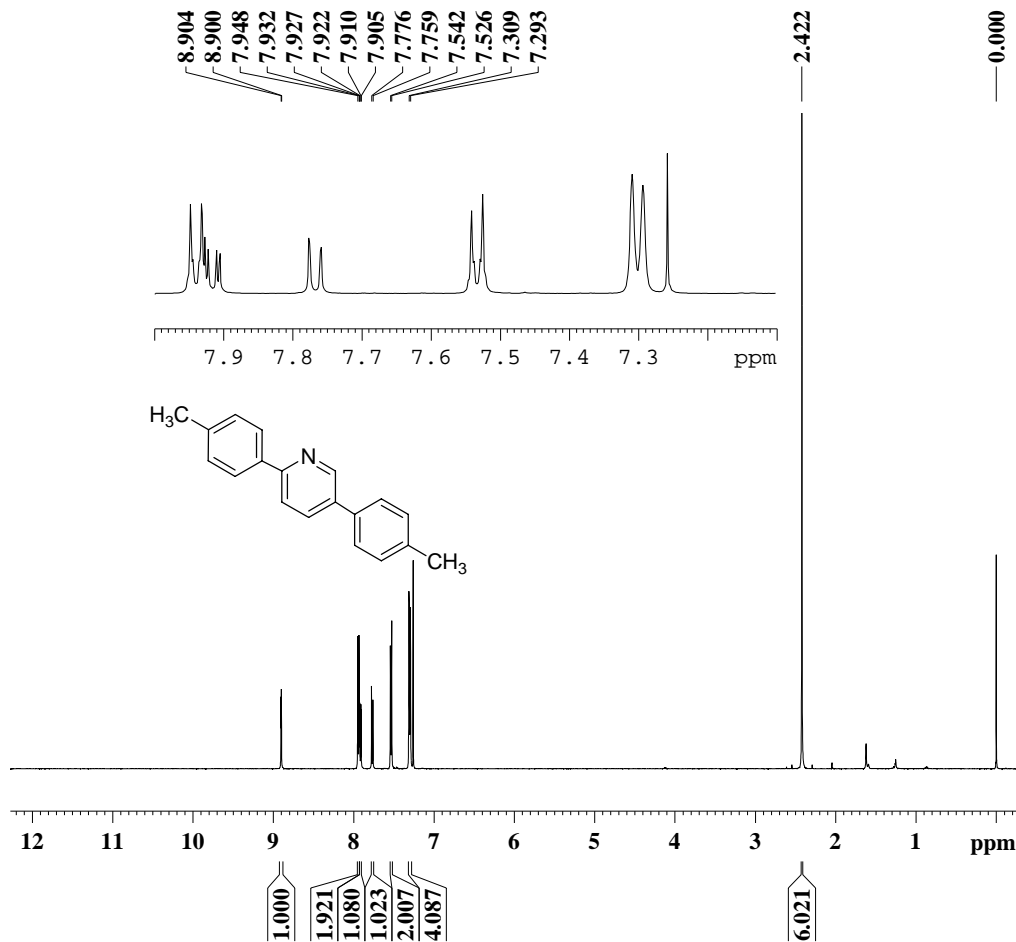
NAME WSW1201-2  
EXPNO 2  
PROCNO 1  
Date\_ 20111227  
Time 8.25  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 784  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 292.2 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326468 MHz  
WDW EM

Compound **3m**

WSW1122-1 1H 2011 12 14

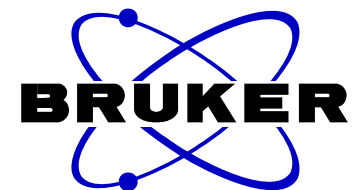
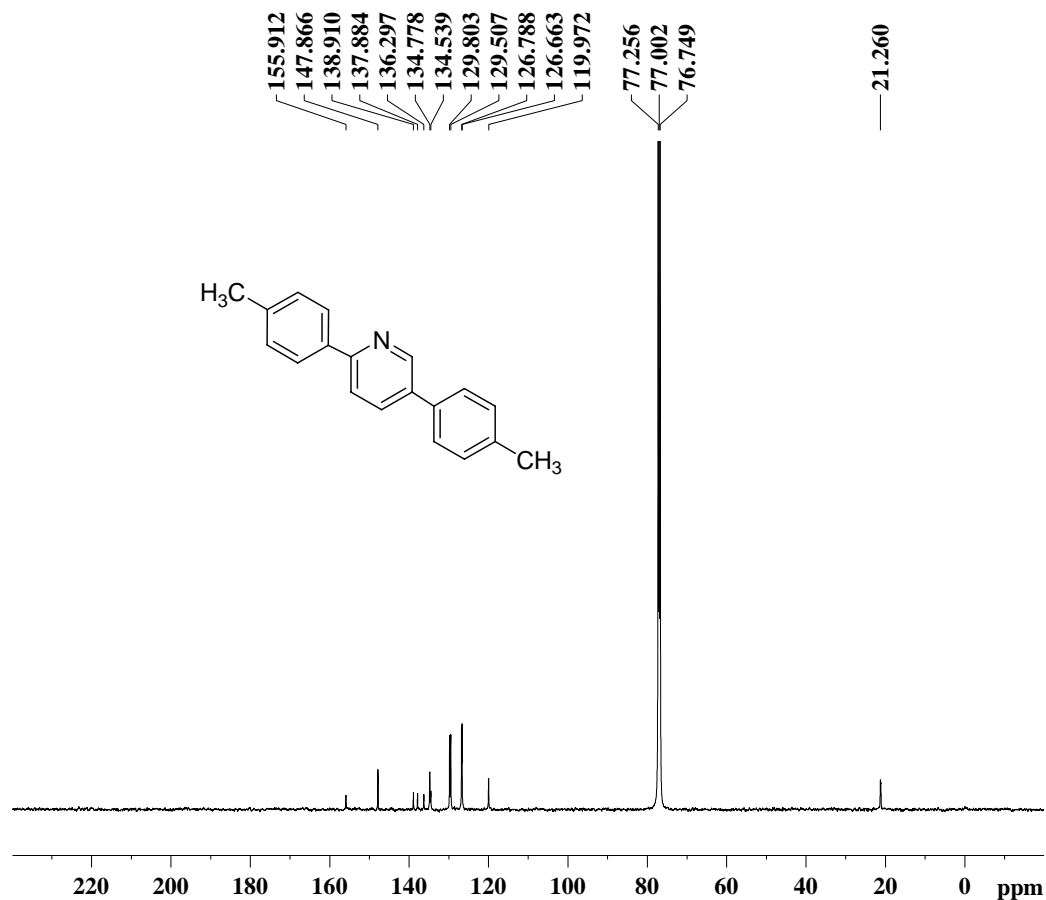


NAME WSW1122-1  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20111214  
 Time 18.00  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 575  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 294.1 K  
 D1 2.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300111 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00



wsw1122-1 13C 1D 2011 12 17



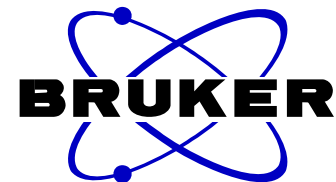
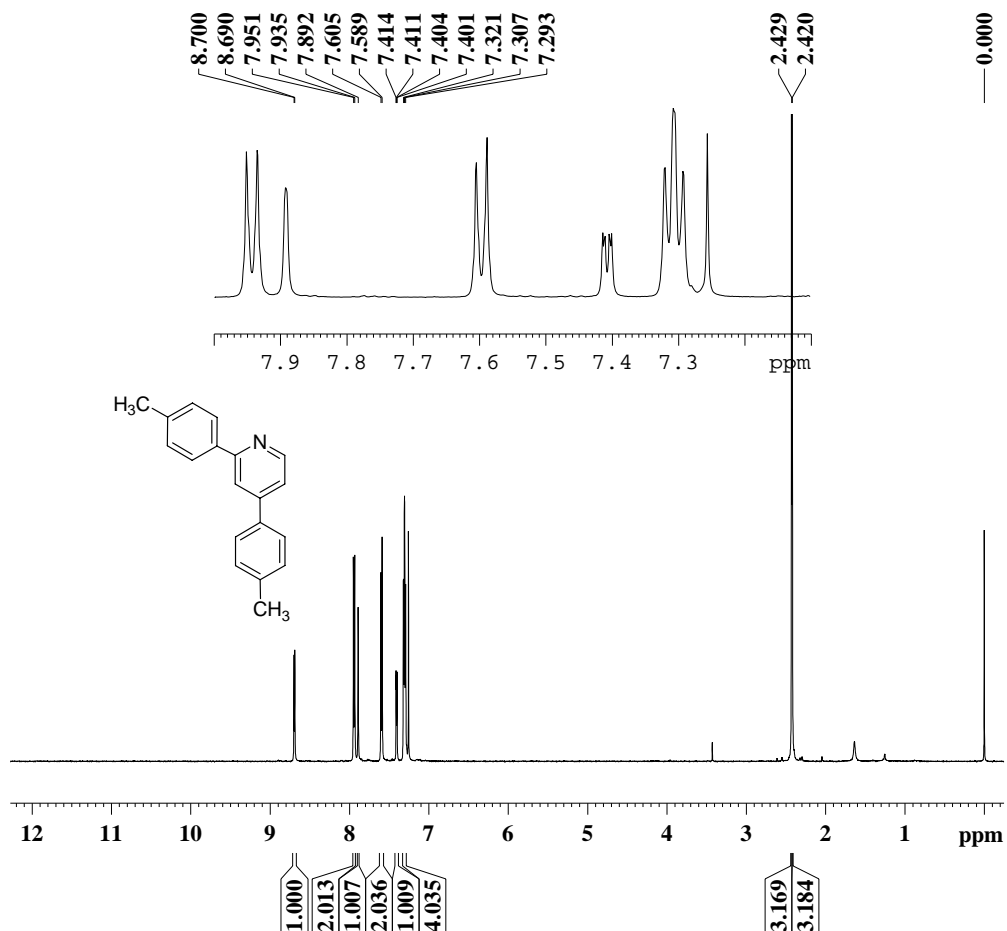
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EXPNO 21  
PROCNO 1  
Date\_ 20111217  
Time 9.38  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2171  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 1290  
DW 15.300 usec  
DE 6.00 usec  
TE 297.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326450 MHz  
WDW EM

Compound **4m**

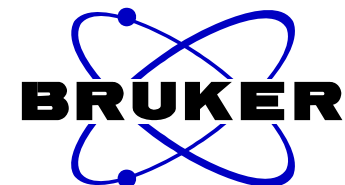
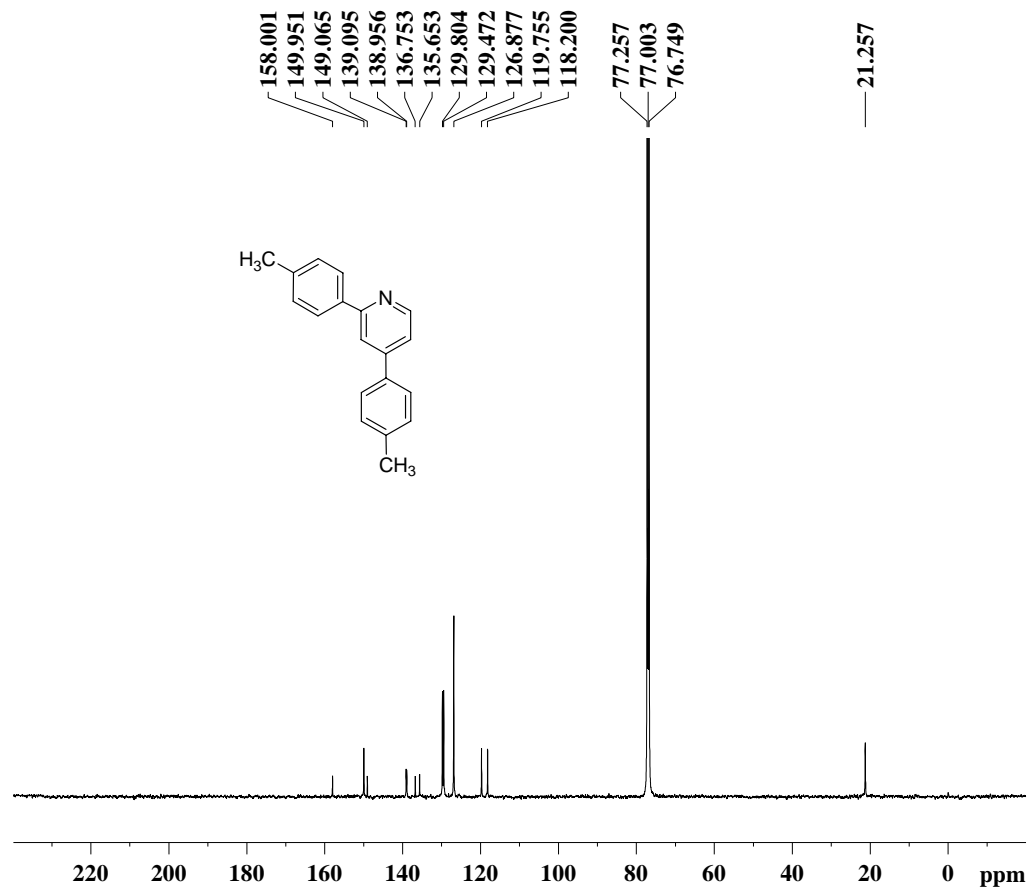
WSW1122-2 1H 2011 12 14



NAME WSW1122-2  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20111214  
 Time 18.22  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 456  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 294.0 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300119 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

wsw1122-2 13C 1D 2011 12 19



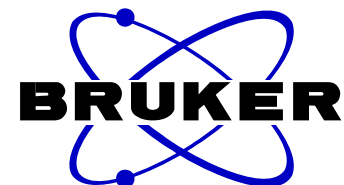
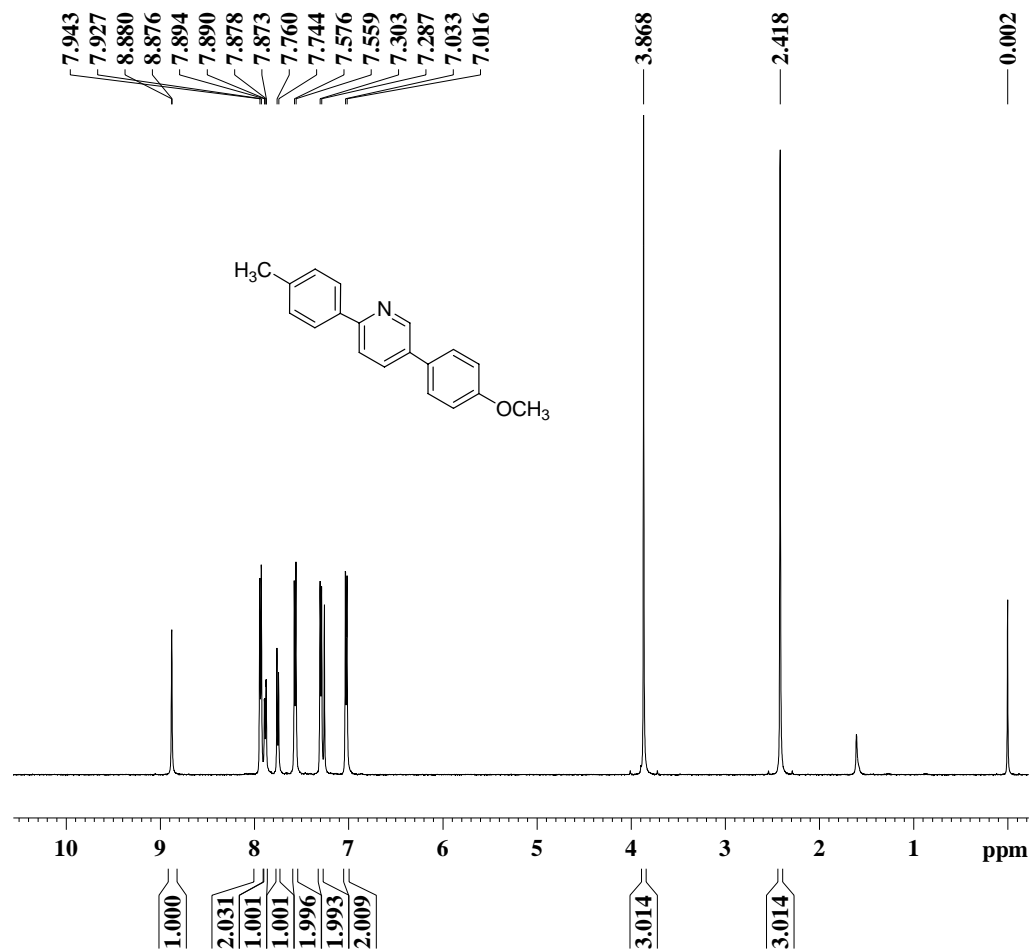
NAME WSW1122-2  
EXPNO 21  
PROCNO 1  
Date\_ 20111219  
Time 11.21  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1900  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 1290  
DW 15.300 usec  
DE 6.00 usec  
TE 294.9 K  
D1 2.00000000 sec  
dL1 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326484 MHz  
WDW EM

Compound **3n**

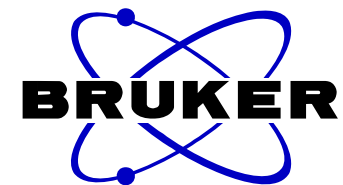
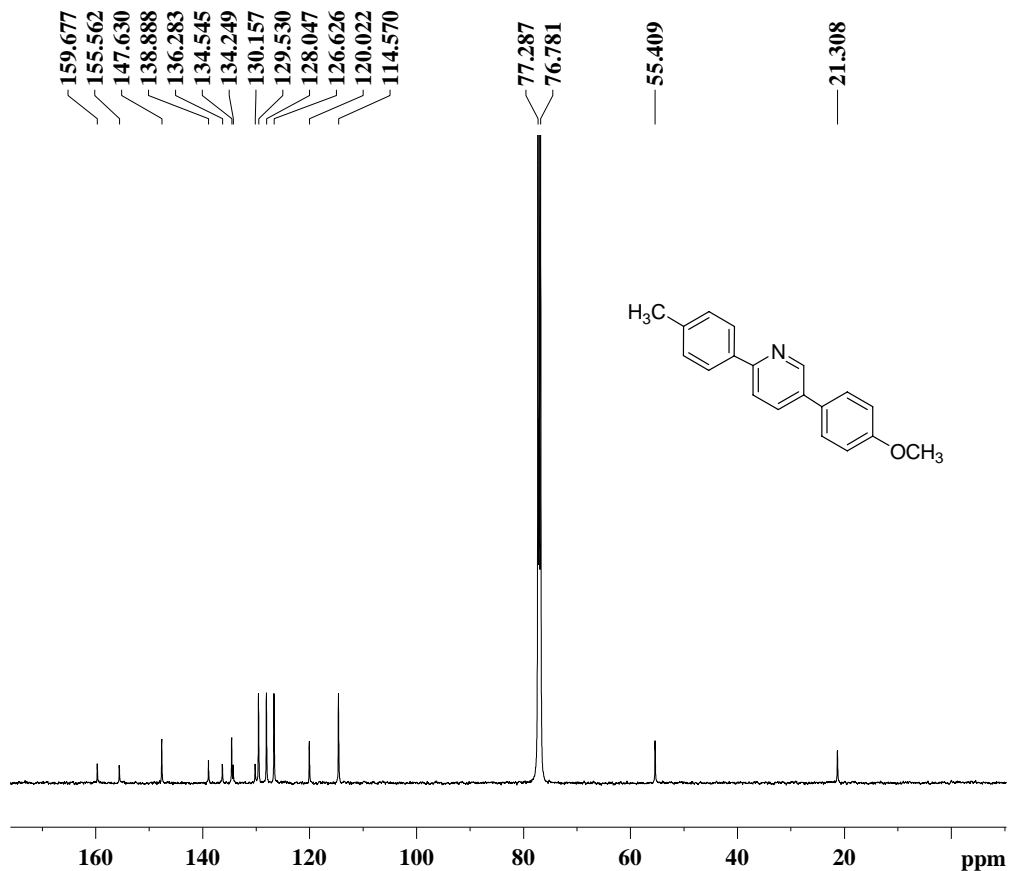
WSW1209-2 1H 2011 12 21



NAME WSW1209-2  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20111221  
 Time 19.52  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 456  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300111 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW1209-2 13C 1D 2011 12 26



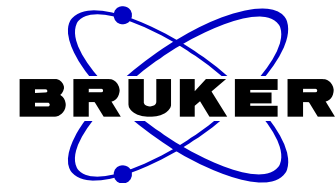
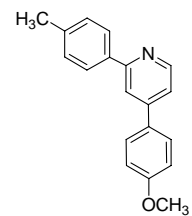
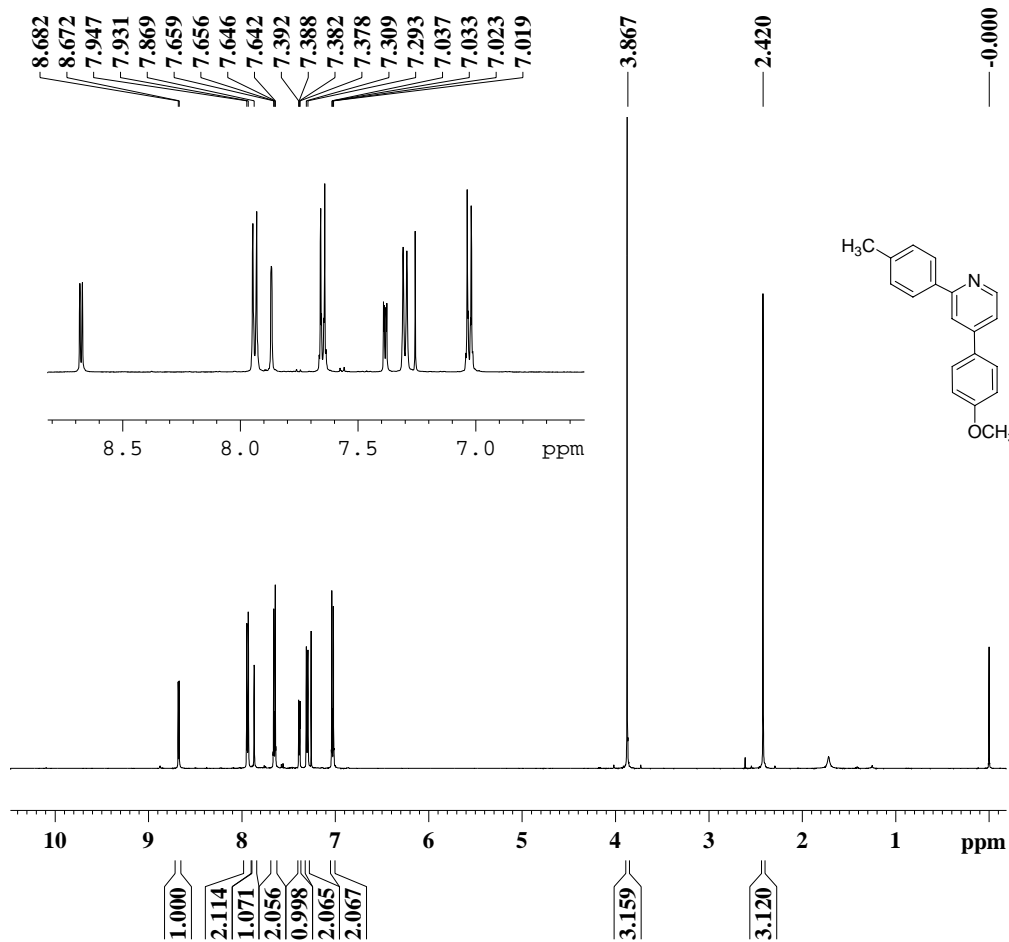
NAME WSW1209-2  
EXPNO 2  
PROCNO 1  
Date\_ 20111226  
Time 13.10  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 3344  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 18400  
DW 15.300 usec  
DE 6.00 usec  
TE 294.4 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326428 MHz  
WDW EM

Compound **4n**

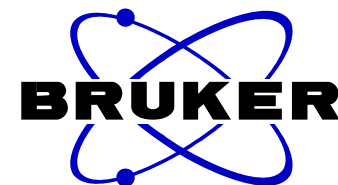
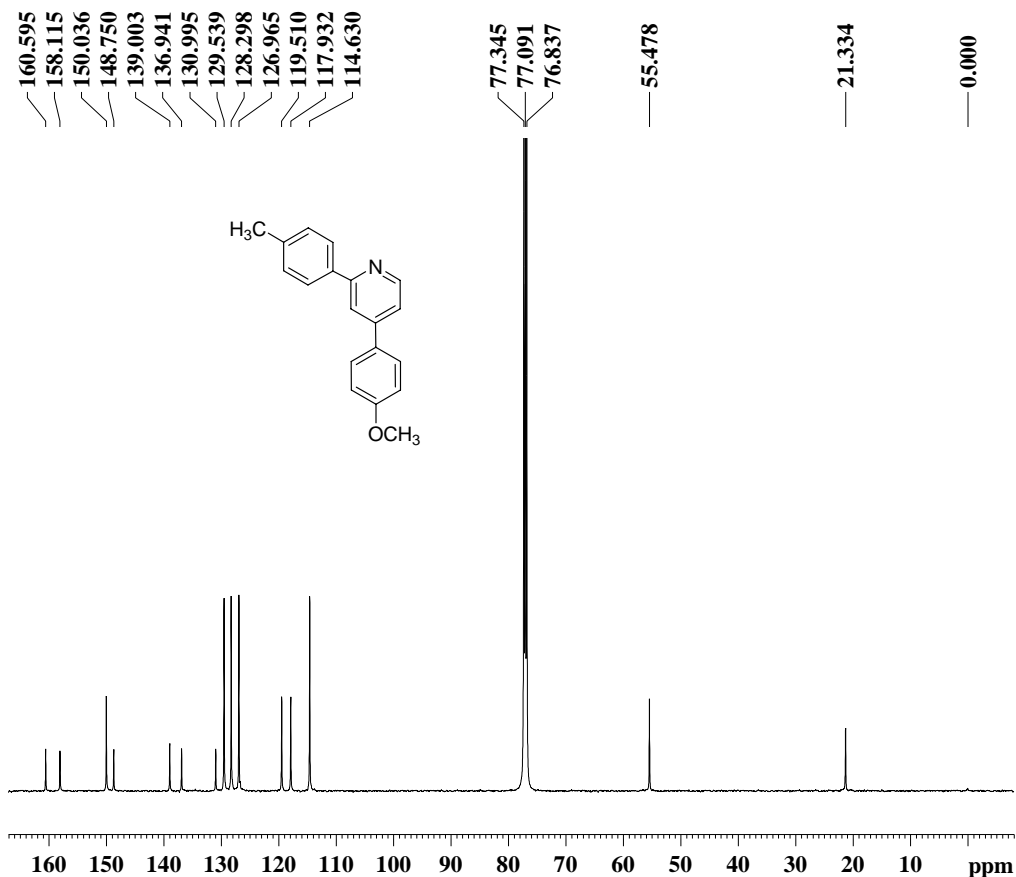
WSW1209-3 1H 2012 01 04



NAME WSW1209-3  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20120104  
 Time 10.39  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 322  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 291.6 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300115 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW1209-3 13C 1D 2012 03 21



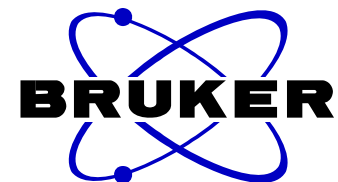
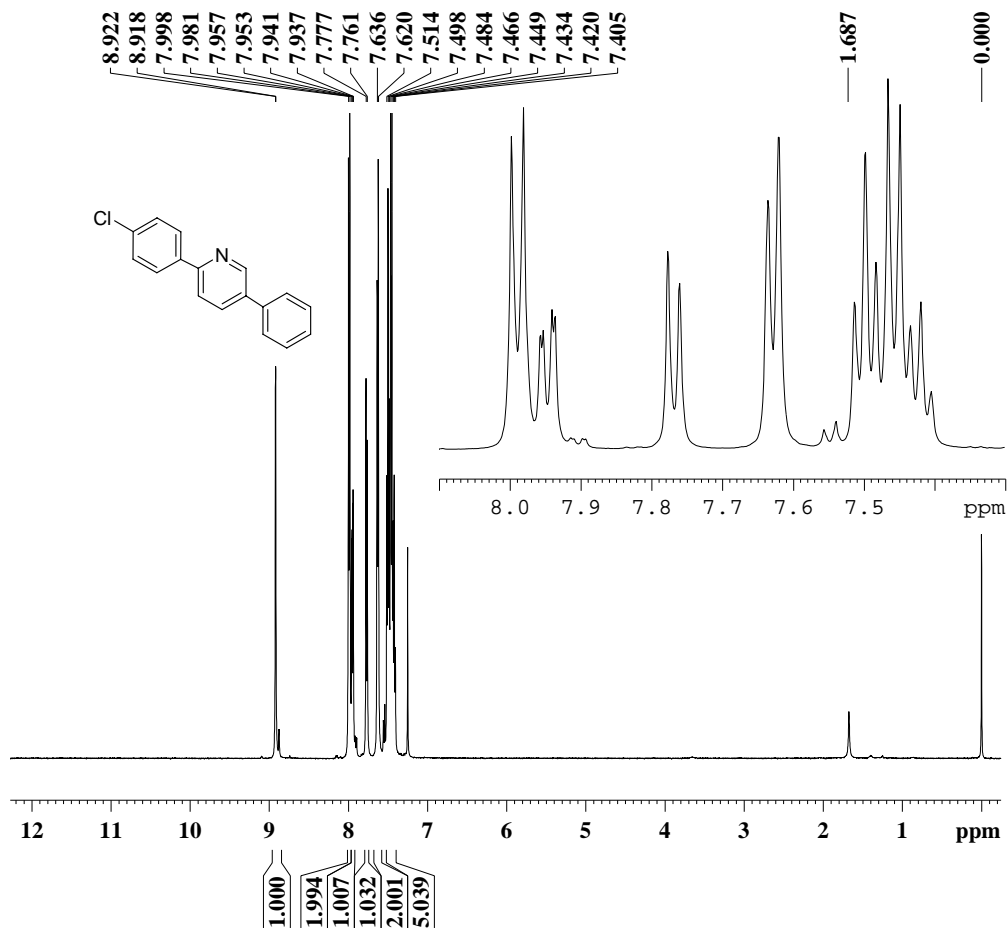
NAME WSW1209-3  
EXPNO 2  
PROCNO 1  
Date\_ 20120322  
Time 7.27  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 11376  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 9200  
DW 15.300 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326332 MHz  
WDW EM

Compound **3o**

WSW0409-1 1H 2012 04 16

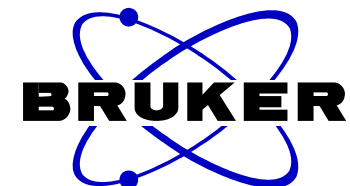
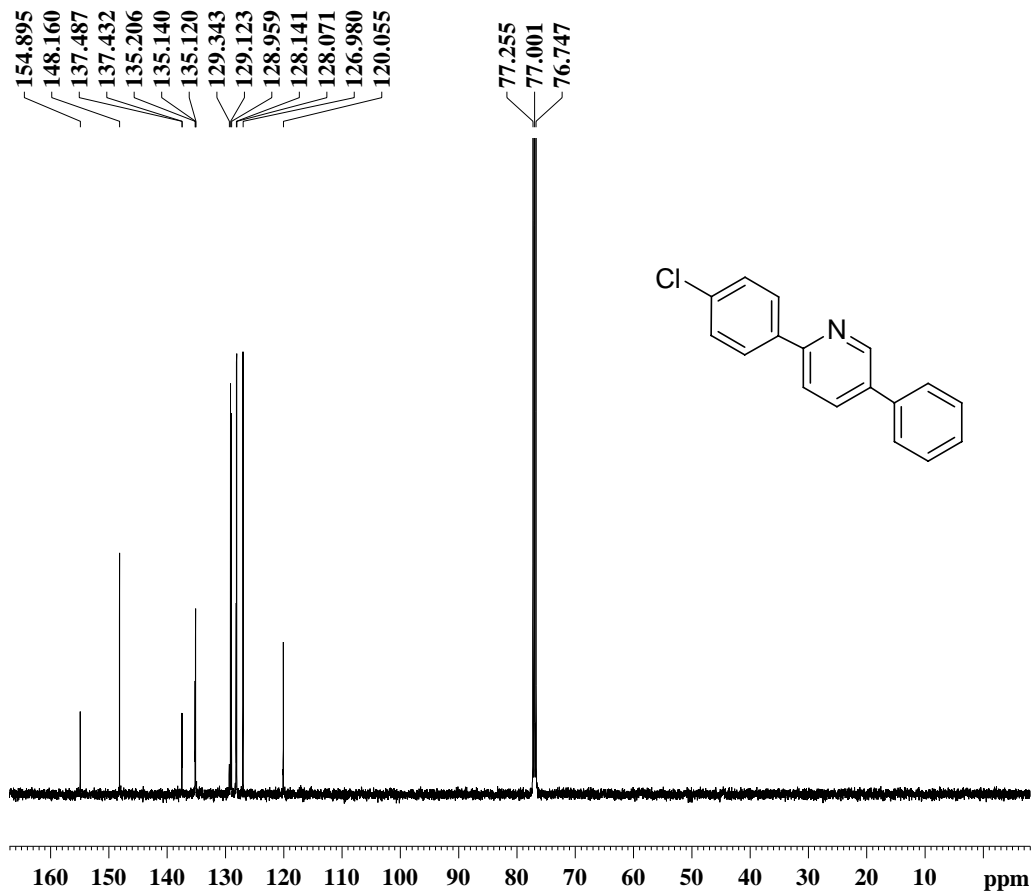


NAME WSW0409-1  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20120417  
 Time 8.23  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 287  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 293.7 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300134 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00



wsn0409-1 13C 1D 2012 04 23



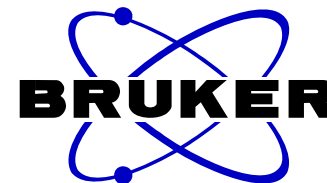
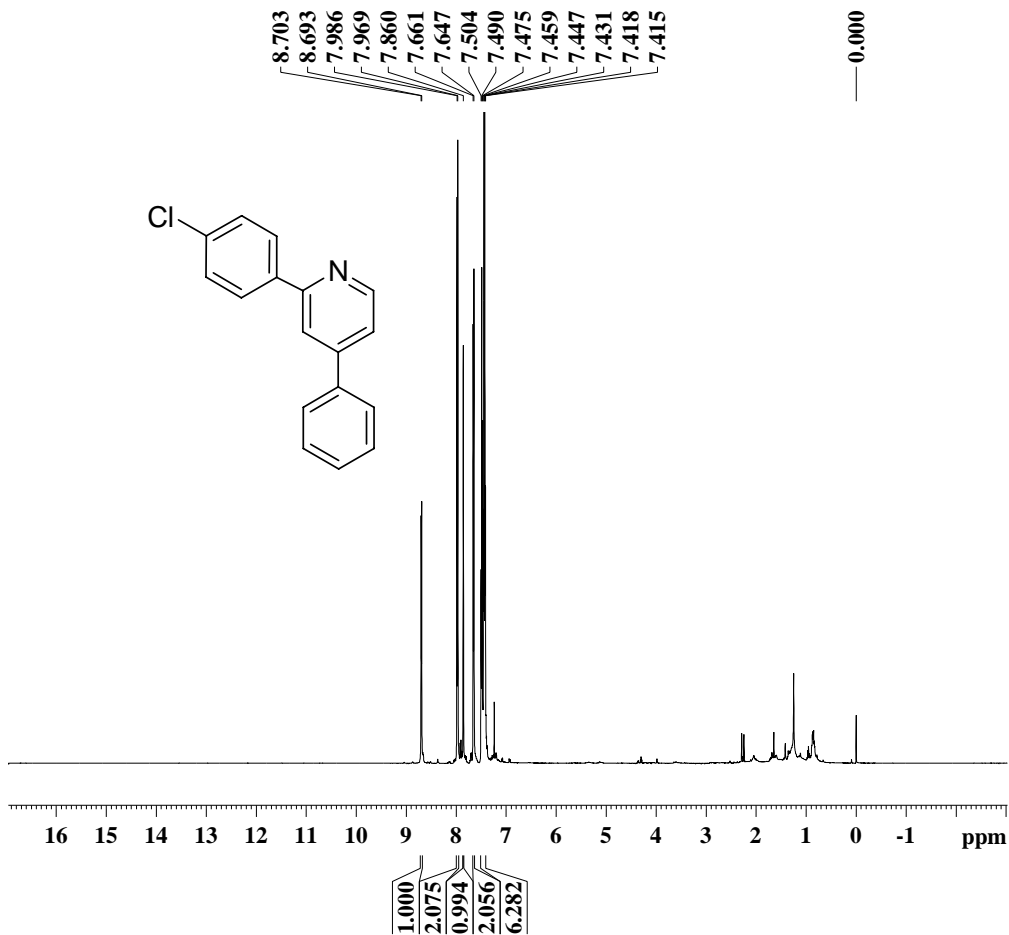
NAME WSW0409-1  
EXPNO 2  
PROCNO 11  
Date\_ 20120423  
Time 12.50  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 500  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 8200  
DW 15.300 usec  
DE 6.00 usec  
TE 298.9 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326452 MHz  
WDW EM

Compound 4o

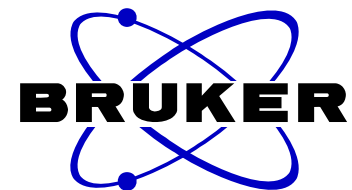
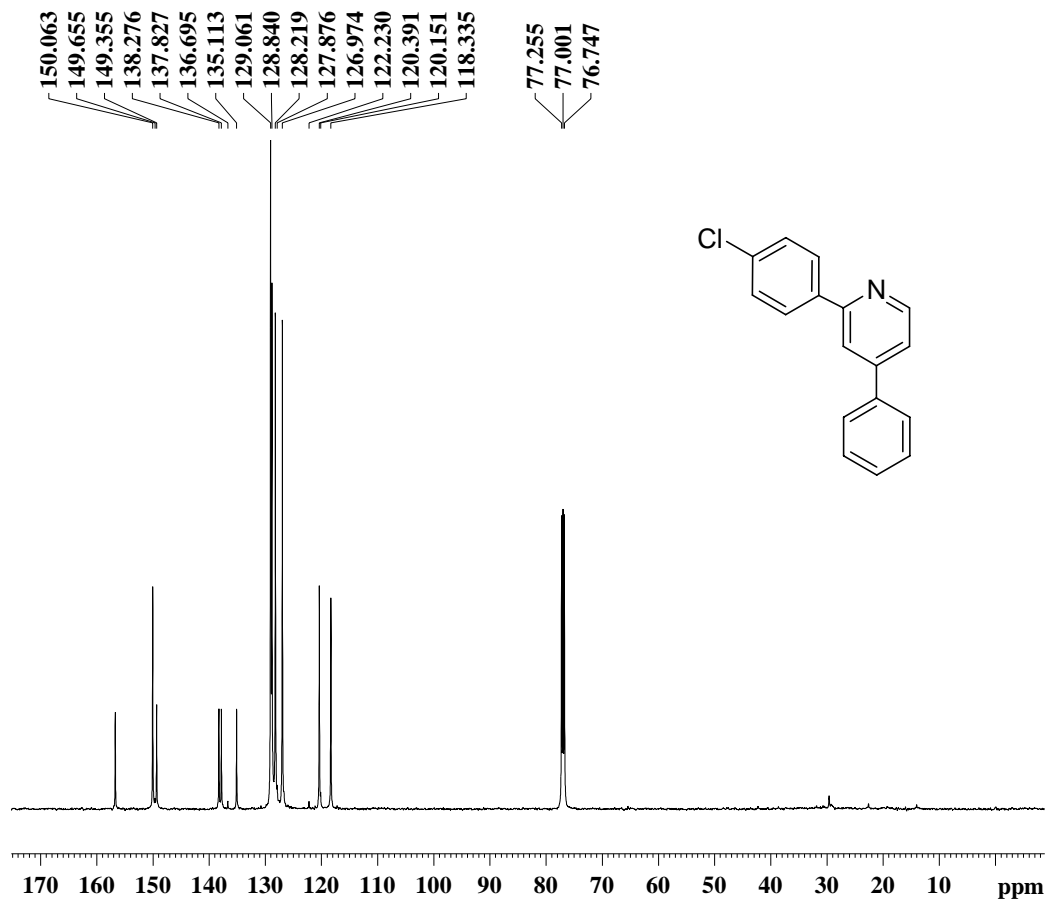
WSW0409-2 1H 2012 04 16



NAME WSW0409-2  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20120417  
 Time 9.00  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.6385000 sec  
 RG 80.6  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 293.7 K  
 D1 2.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz  
 SI 16384  
 SF 500.0300208 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

wsw0409-2 13C 1D 2012 04 23



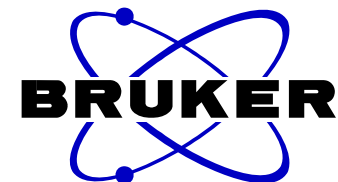
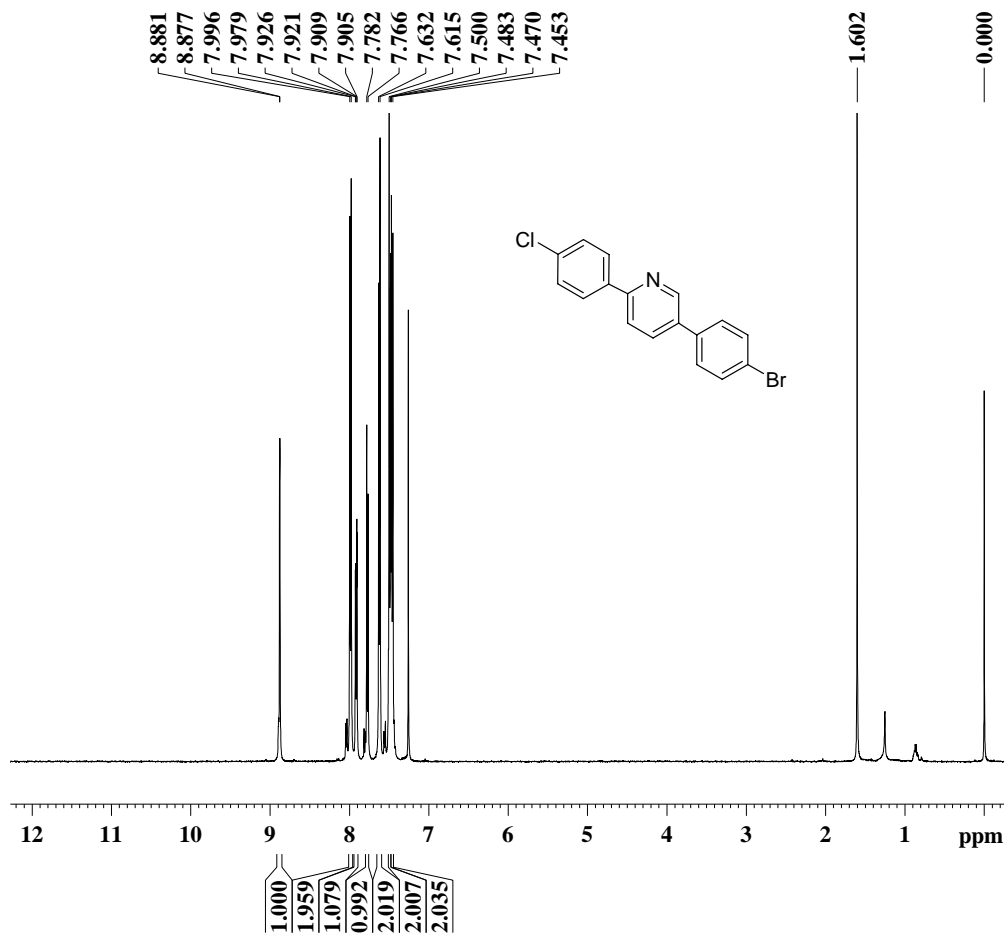
NAME WSW0409-2  
EXPNO 2  
PROCNO 11  
Date\_ 20120423  
Time 14.23  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1600  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 8200  
DW 15.300 usec  
DE 6.00 usec  
TE 299.6 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.8999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326555 MHz  
WDW EM

Compound **3p**

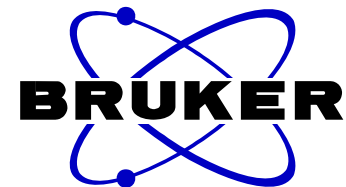
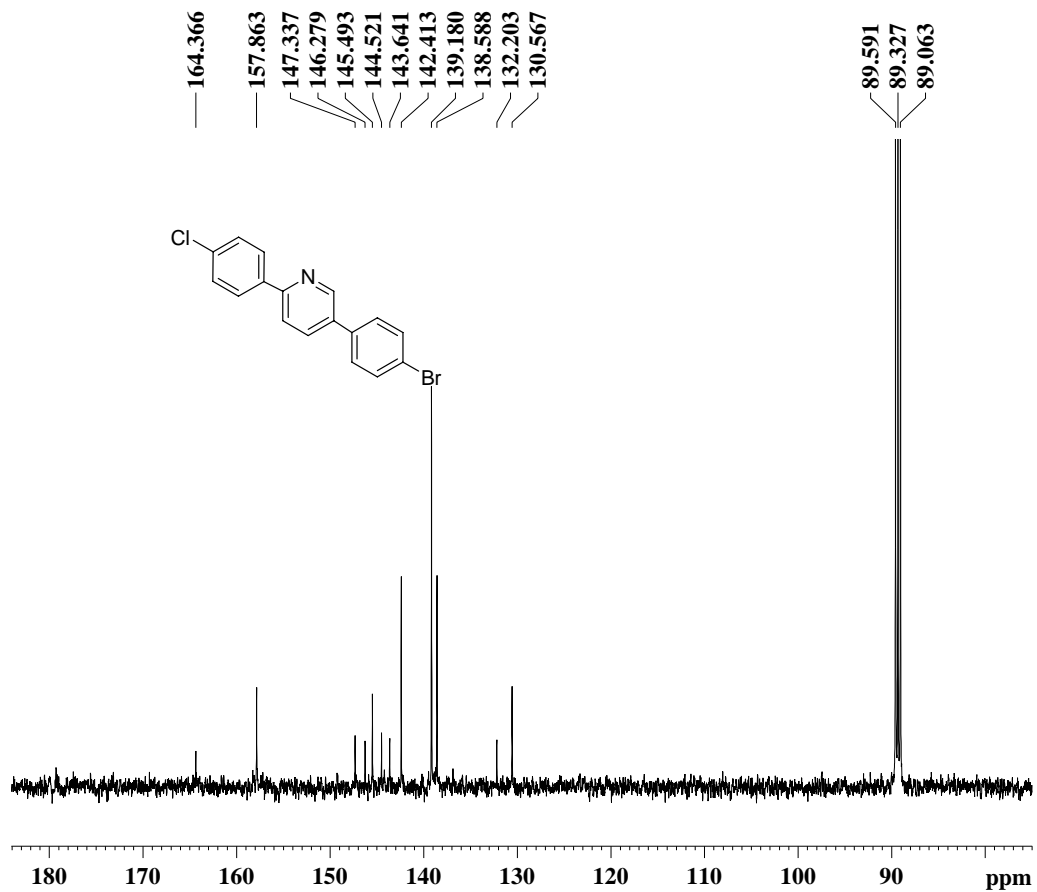
WSW0630-1 1H 1D 2012 09 10



NAME WSW0630-1  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20120910  
 Time 7.35  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 16384  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8193000 sec  
 RG 512  
 DW 50.000 usec  
 DE 8.00 usec  
 TE 296.8 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.00 usec  
 PL1 2.00 dB  
 SFO1 500.0338500 MHz  
 SI 16384  
 SF 500.0300102 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW0630-1 13C 1D 2012 09 13



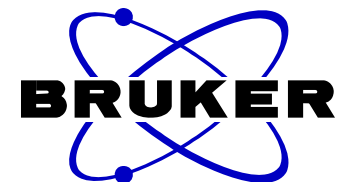
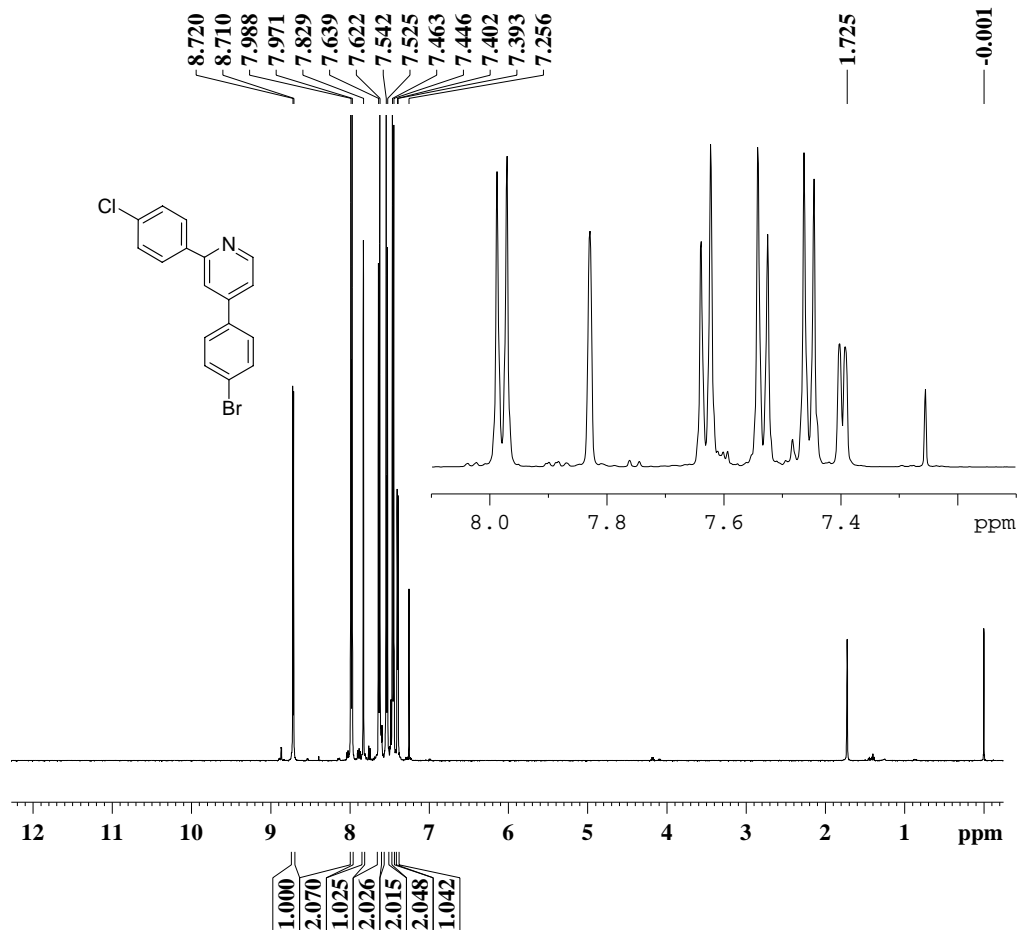
NAME WSW0630-1  
EXPNO 2  
PROCNO 1  
Date\_ 20120913  
Time 16.04  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 2622  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 912  
DW 15.300 usec  
DE 6.00 usec  
TE 301.8 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 20

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.20 usec  
PL1 3.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 17.70 dB  
PL13 17.70 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7313930 MHz  
WDW EM

Compound **4p**

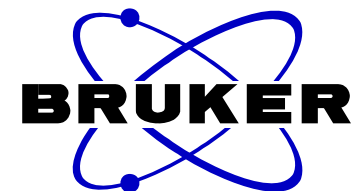
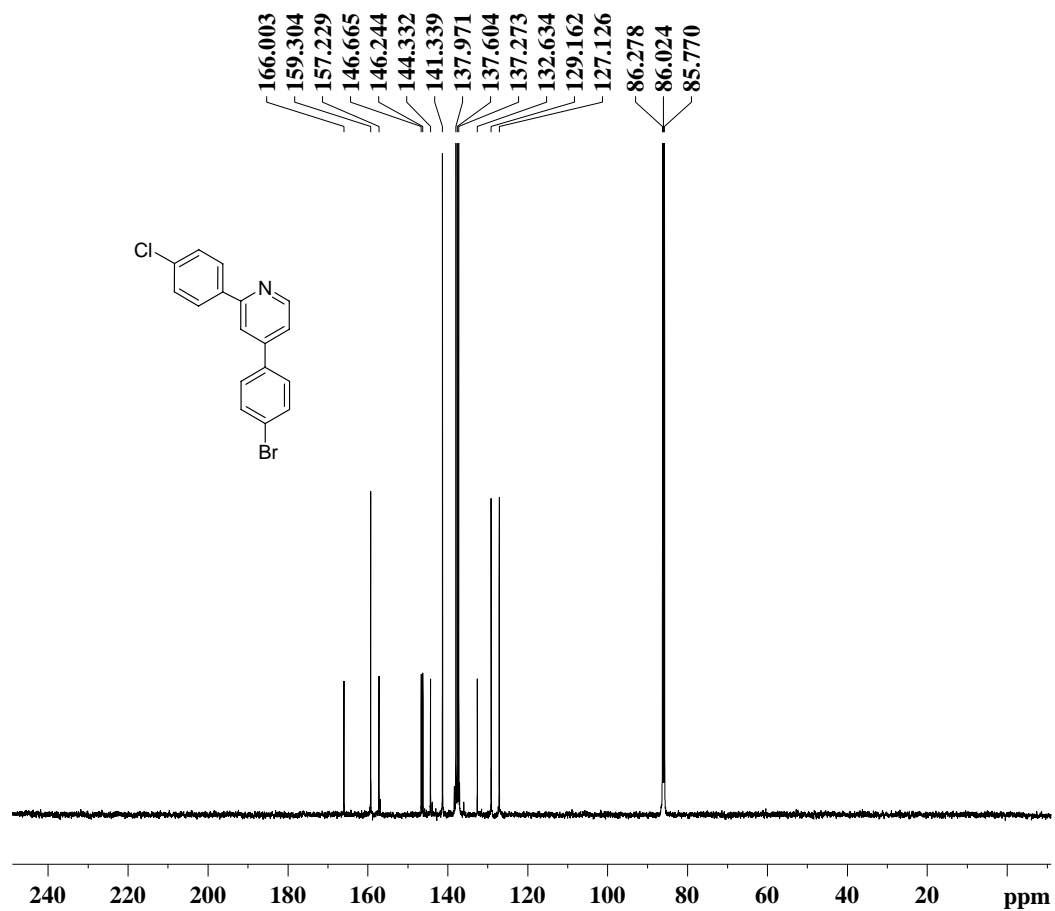
WSW0630-2 1H 1D 2012 09 10



NAME WSW0630-2  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20120910  
 Time 7.40  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 16384  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8193000 sec  
 RG 256  
 DW 50.000 usec  
 DE 8.00 usec  
 TE 296.9 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.00 usec  
 PL1 2.00 dB  
 SFO1 500.0338500 MHz  
 SI 16384  
 SF 500.0300118 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW0630-2 13C 1D 2012 09 13



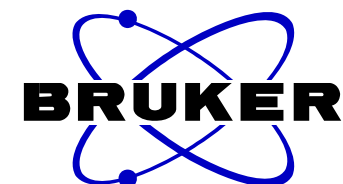
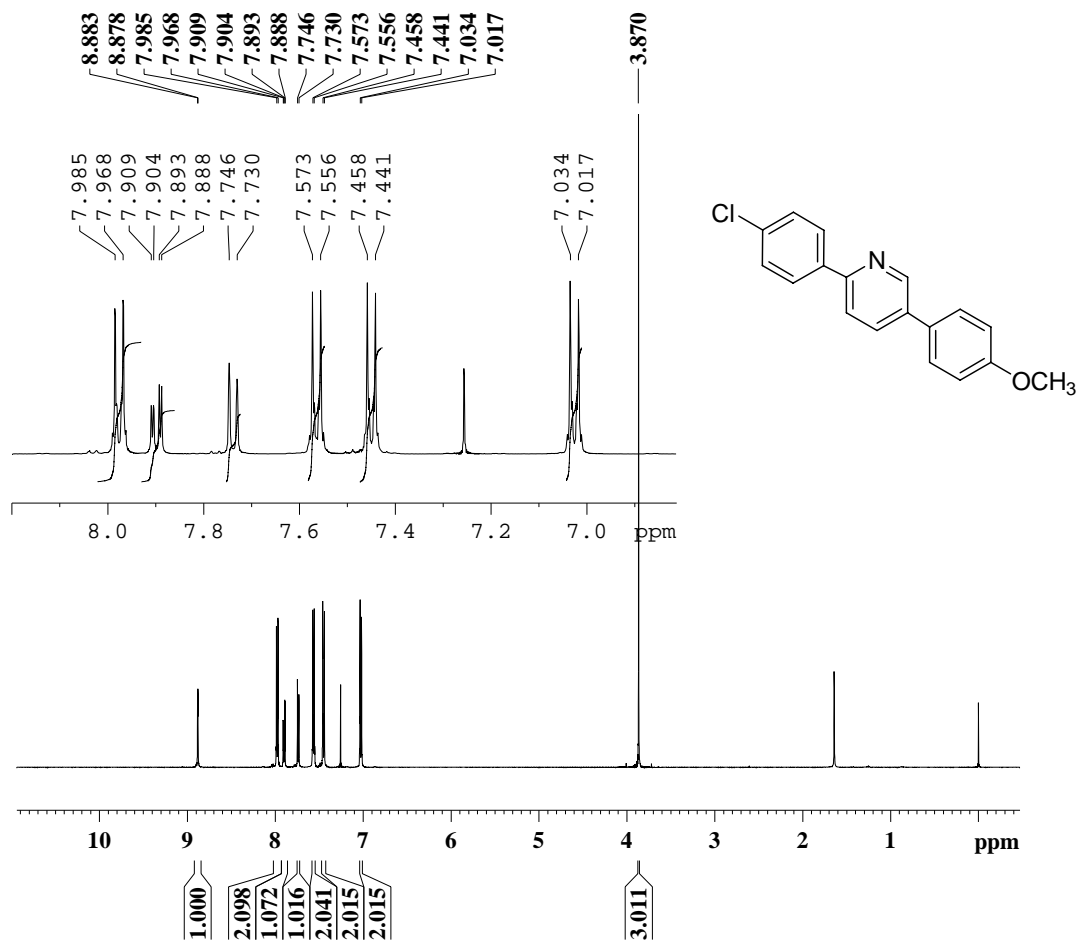
NAME WSW0630-2  
EXPNO 2  
PROCNO 1  
Date\_ 20120913  
Time 10.07  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 798  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 912  
DW 15.300 usec  
DE 6.00 usec  
TE 300.5 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 10

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.20 usec  
PL1 3.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 17.70 dB  
PL13 17.70 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7315152 MHz  
WDW EM

Compound **3q**

WSW0704-1 1H 1D 2012 09 17

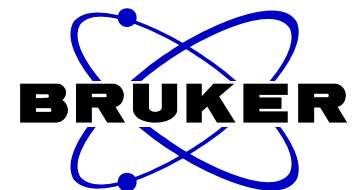
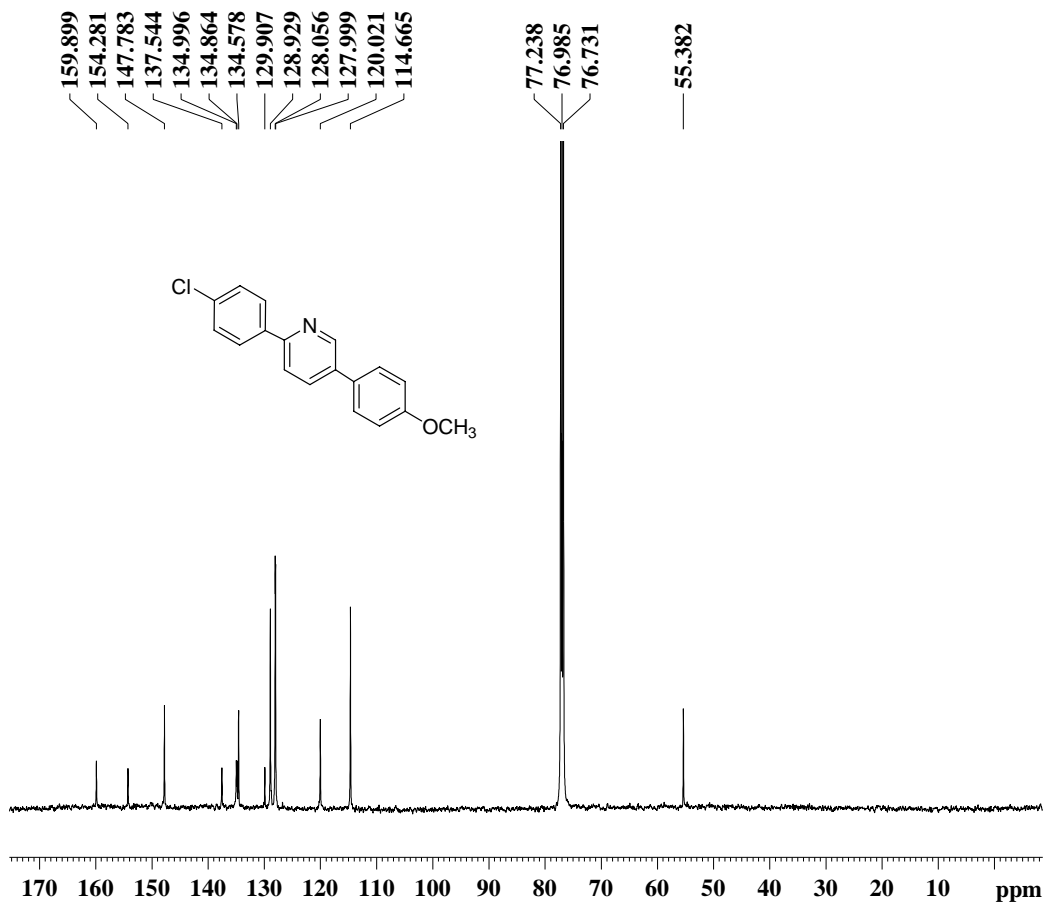


NAME WSW0704-1  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20120919  
 Time 19.17  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 16384  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8193000 sec  
 RG 256  
 DW 50.000 usec  
 DE 8.00 usec  
 TE 297.5 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.00 usec  
 PL1 2.00 dB  
 SFO1 500.0338500 MHz  
 SI 16384  
 SF 500.0300118 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00



WSW0704-1 13C 1D 2012 09 24



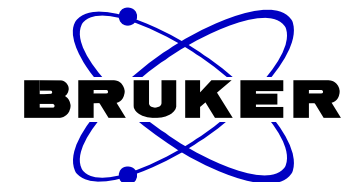
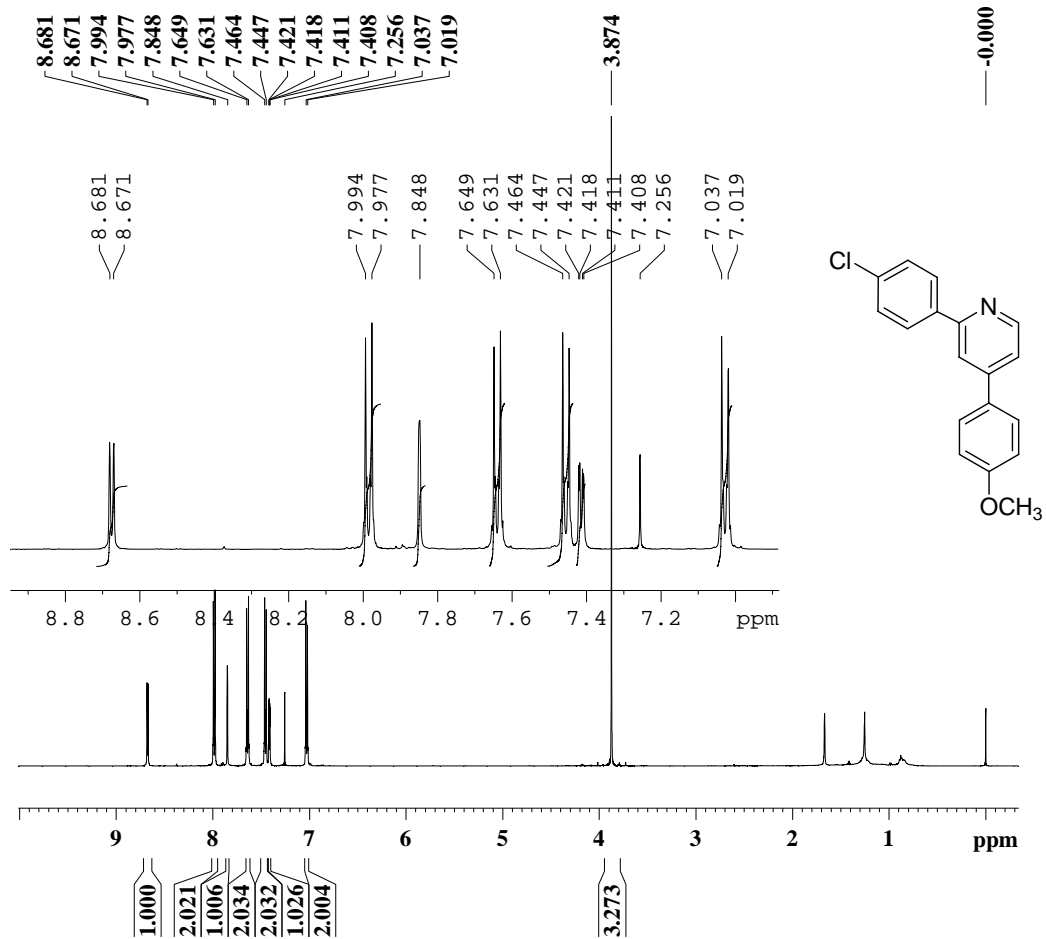
NAME WSW0704-1  
EXPNO 2  
PROCNO 1  
Date\_ 20120924  
Time 8.50  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1439  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 912  
DW 15.300 usec  
DE 6.00 usec  
TE 304.2 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 20

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.20 usec  
PL1 3.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 17.70 dB  
PL13 17.70 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326435 MHz  
WDW EM

Compound **4q**

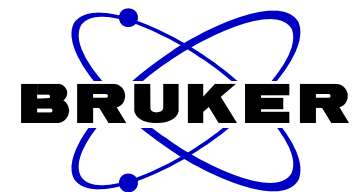
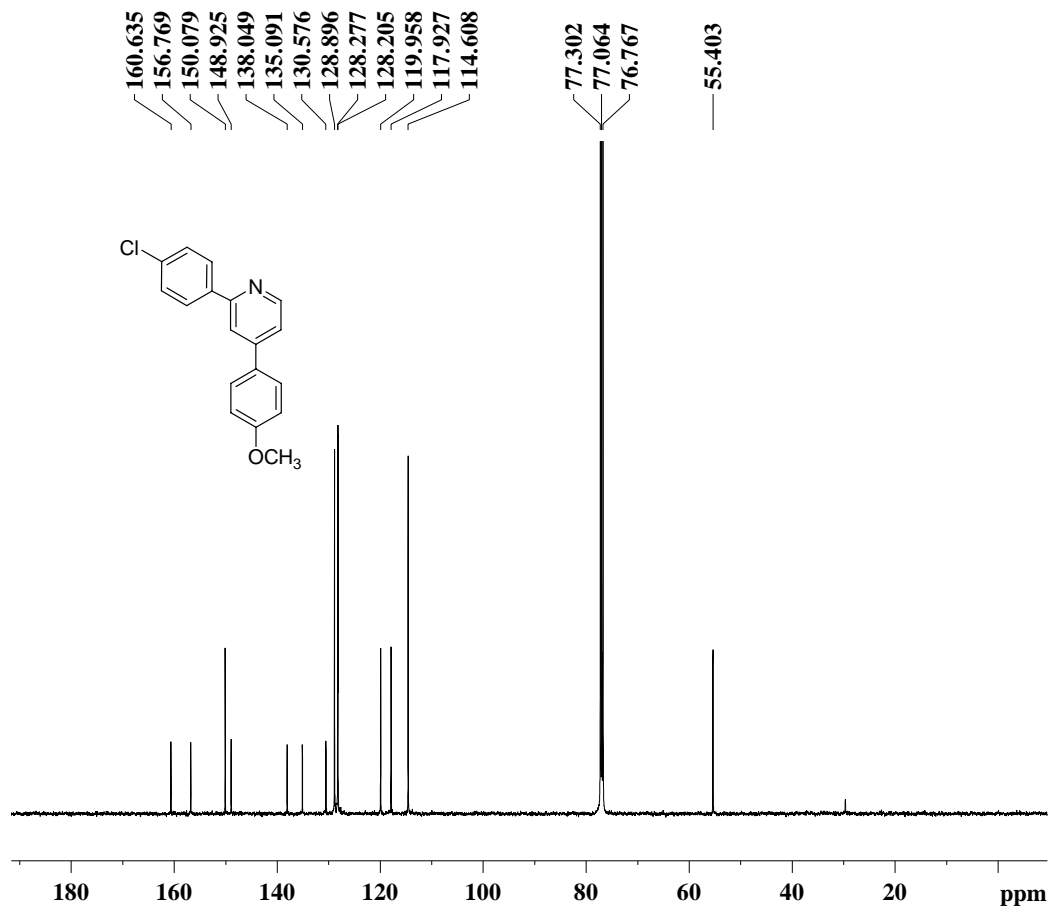
WSW0704-2 1H 1D 2012 09 17



NAME WSW0704-2  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20120919  
 Time 19.20  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 16384  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8193000 sec  
 RG 256  
 DW 50.000 usec  
 DE 8.00 usec  
 TE 297.4 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.00 usec  
 PL1 2.00 dB  
 SFO1 500.0338500 MHz  
 SI 16384  
 SF 500.0300118 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW0704-2 13C 1D 2012 09 24



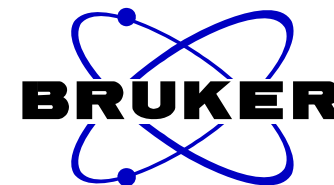
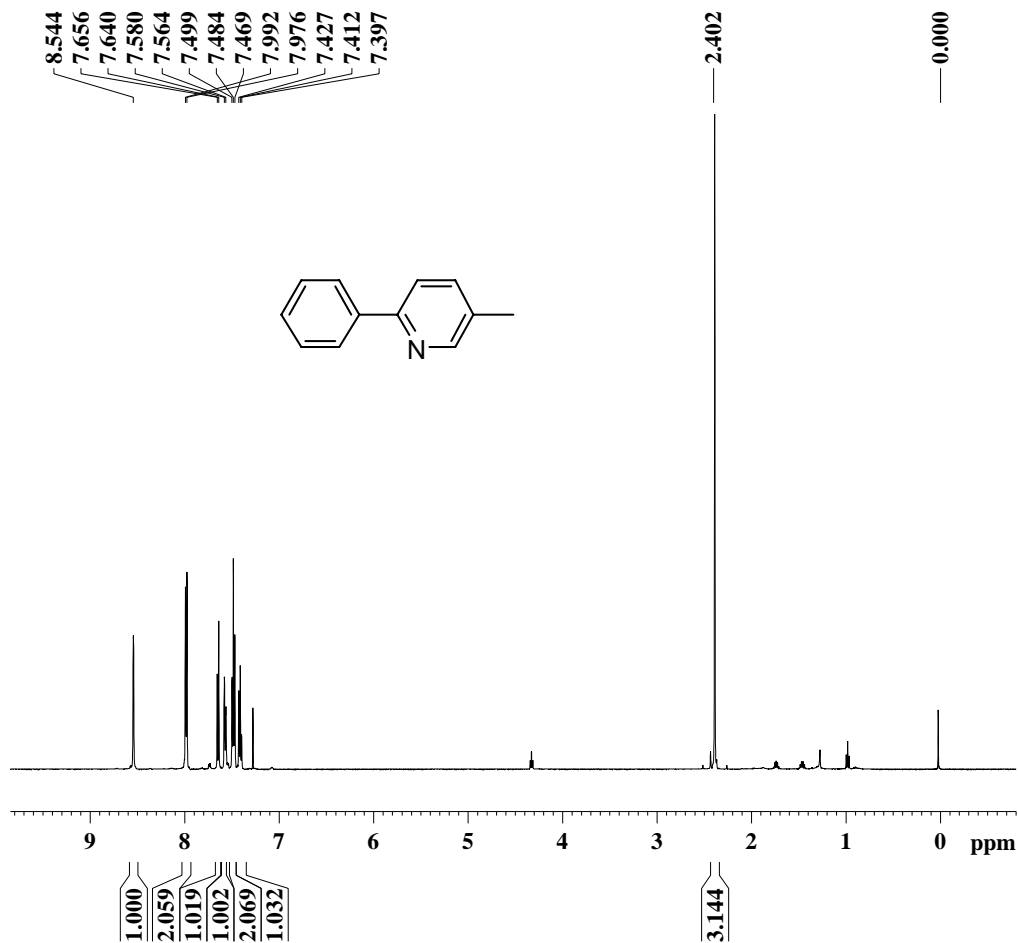
NAME WSW0704-2  
EXPNO 2  
PROCNO 1  
Date\_ 20120924  
Time 10.40  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2105  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 912  
DW 15.300 usec  
DE 6.00 usec  
TE 303.3 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 20

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.20 usec  
PL1 3.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 17.70 dB  
PL13 17.70 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326456 MHz  
WDW EM

Compound **3r**

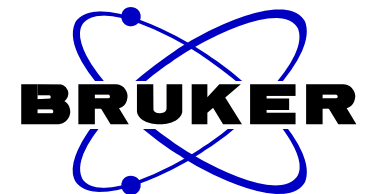
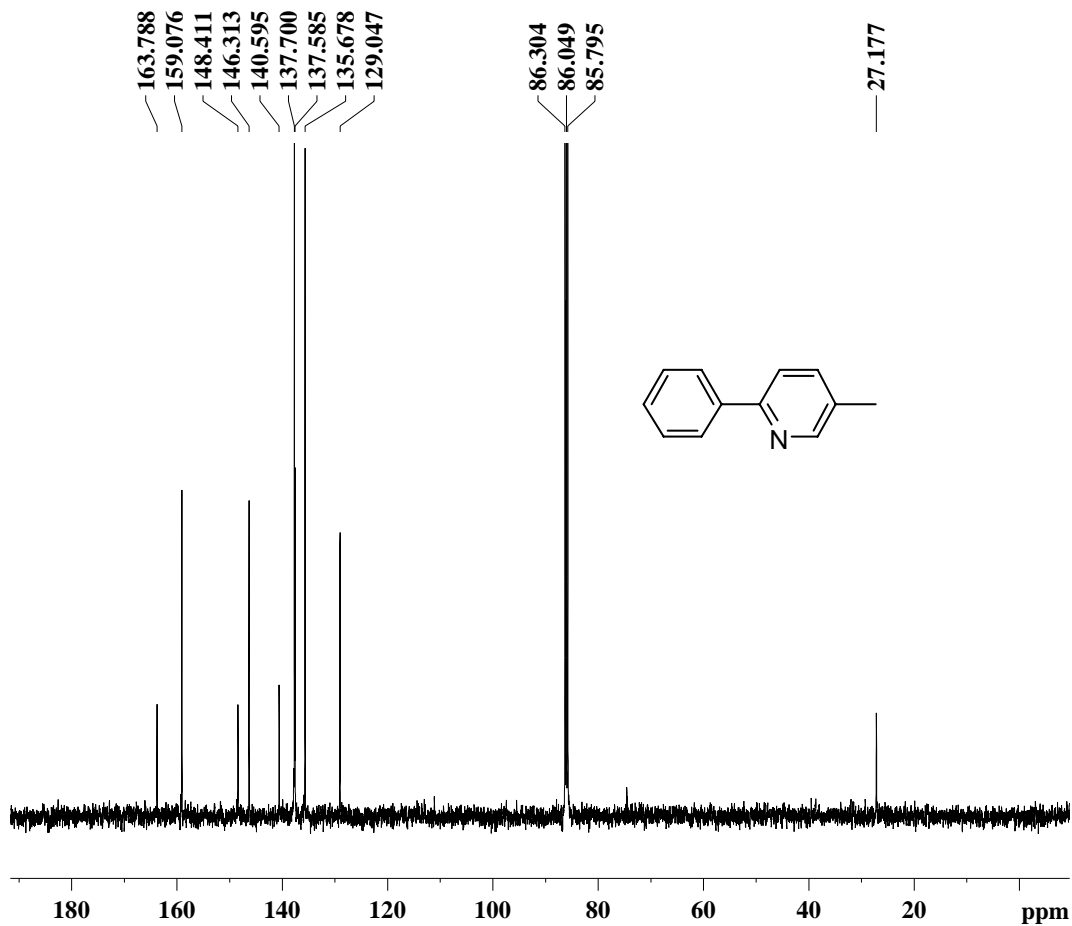
WSW1107-1 1H 1D 2013 01 03



NAME WSW1107-1  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20121225  
 Time 20.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 16384  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8193000 sec  
 RG 50.8  
 DW 50.000 usec  
 DE 8.00 usec  
 TE 291.1 K  
 D1 1.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.00 usec  
 PL1 2.00 dB  
 SFO1 500.0338500 MHz  
 SI 16384  
 SF 500.0299998 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 10.00

WSW1107-1 13C 1D 2013 01 07



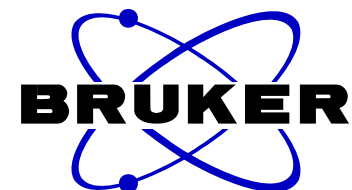
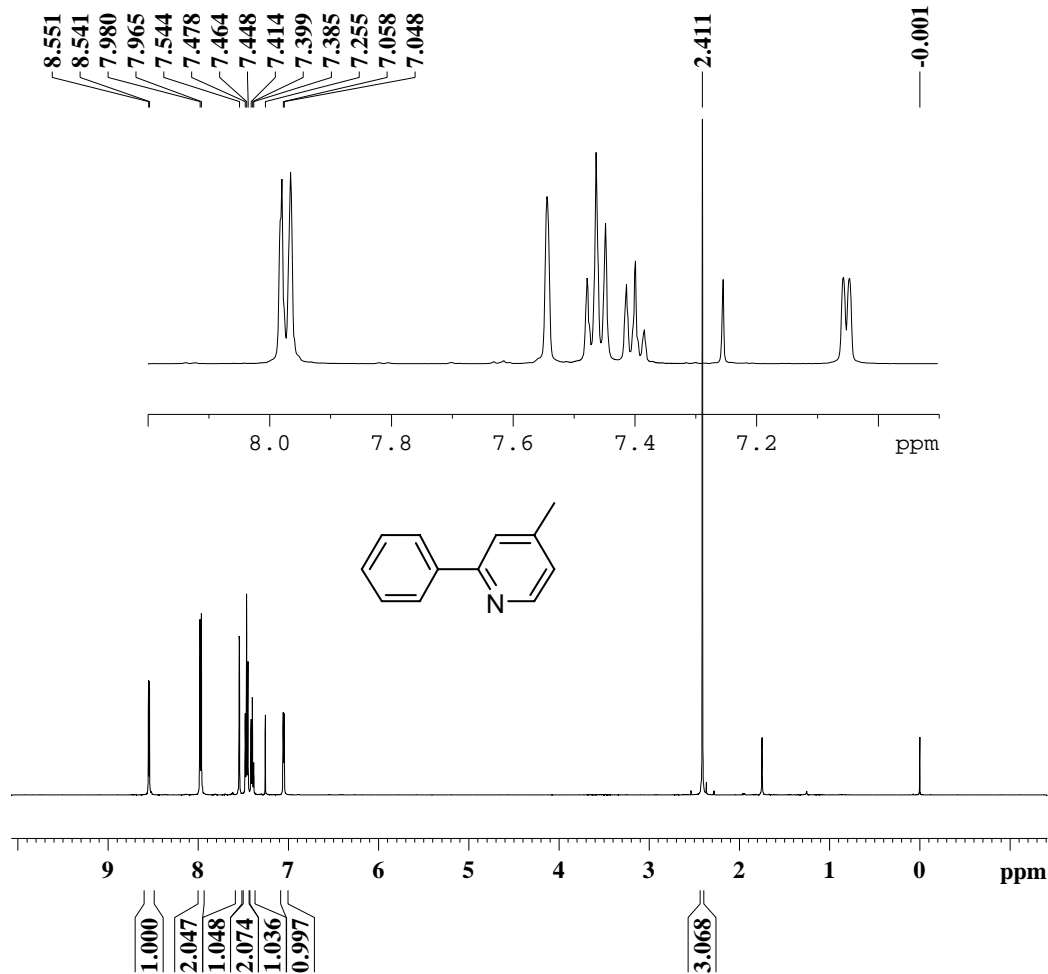
NAME WSW1107-1  
EXPNO 2  
PROCNO 1  
Date\_ 20130107  
Time 19.51  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 57  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 1440  
DW 15.300 usec  
DE 6.00 usec  
TE 292.8 K  
D1 2.0000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 10

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.20 usec  
PL1 3.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 17.70 dB  
PL13 17.70 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7315152 MHz  
WDW EM

Compound **4r**

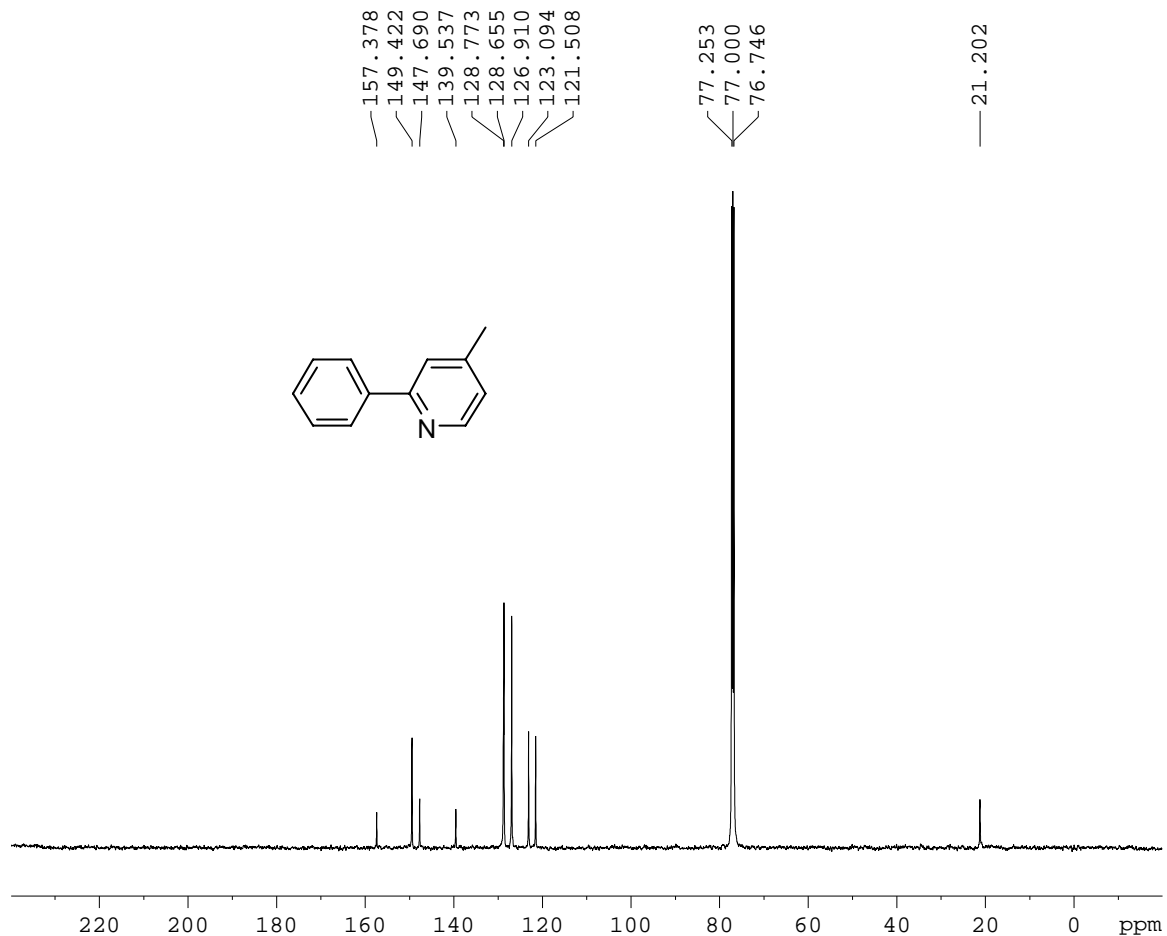
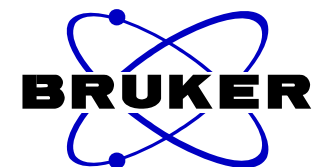
wsw1107-2-c 1H 1D 2013 09 24



NAME wsw1107-2-c  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20130924  
 Time 11.09  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 16384  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8193000 sec  
 RG 287  
 DW 50.000 usec  
 DE 8.00 usec  
 TE 297.5 K  
 D1 1.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.00 usec  
 PL1 2.00 dB  
 SFO1 500.0338500 MHz  
 SI 16384  
 SF 500.0300120 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

wsw1107-2-c 13C 2013 09 22



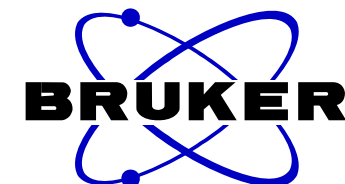
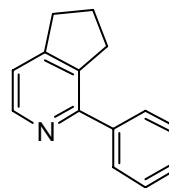
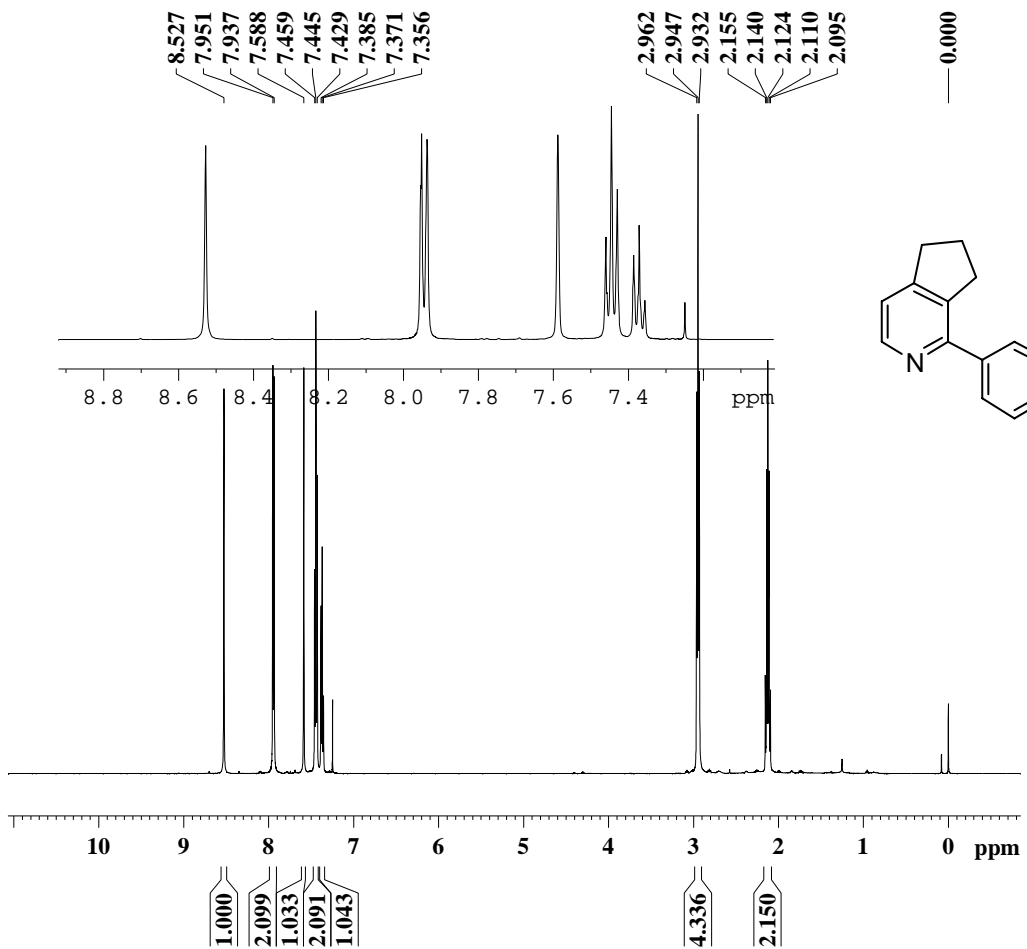
NAME wsw1107-2-c  
EXPNO 2  
PROCNO 1  
Date\_ 20130924  
Time 12.00  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1649  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 1820  
DW 15.300 usec  
DE 6.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 40

=====  
CHANNEL f1  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SFO1 125.7464750 MHz

=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326470 MHz  
WDW EM  
SSB 0  
LB 10.00 Hz  
GB 0  
PC 1.00

Compound **6a**

WSW140310 1H 1D 2014 01 19



NAME WSW140310  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20140319  
 Time 17.30  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 16384  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8193000 sec  
 RG 203  
 DW 50.000 usec  
 DE 8.00 usec  
 TE 673.2 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.00 usec  
 PL1 2.00 dB  
 SFO1 500.0338500 MHz  
 SI 16384  
 SF 500.0300165 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 6.00



WSW140310

13C 1D

2014 03 20

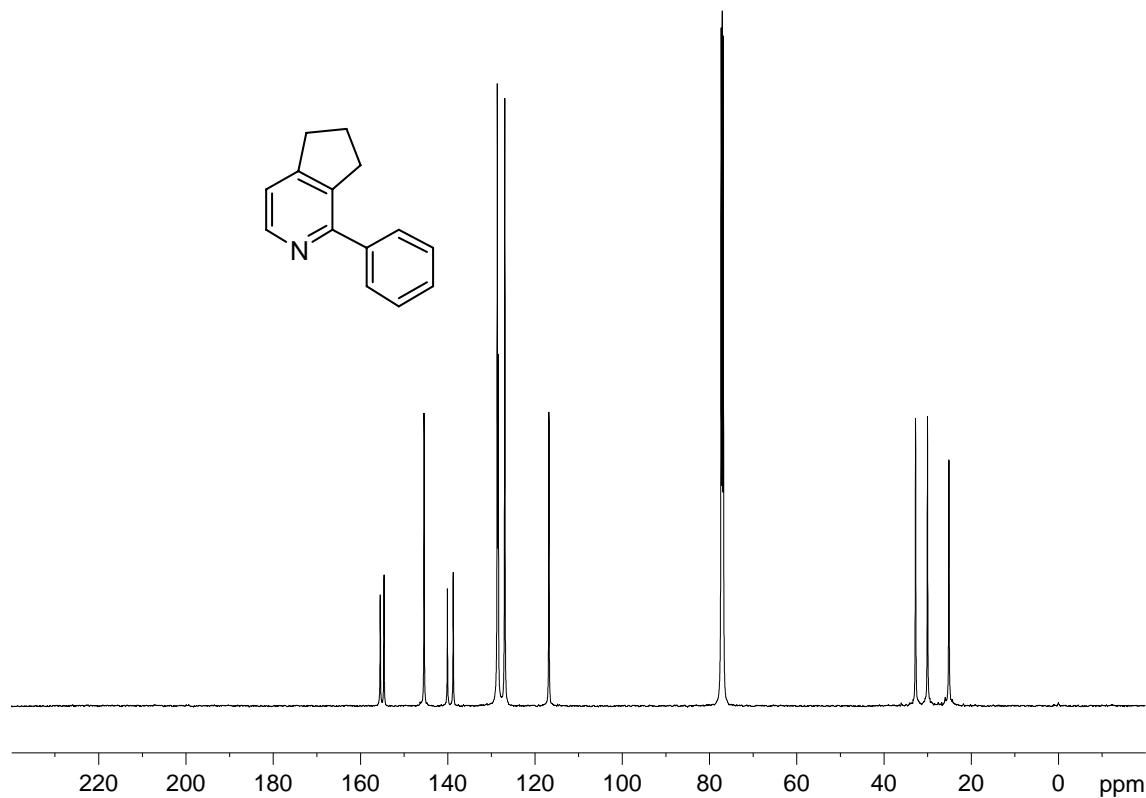
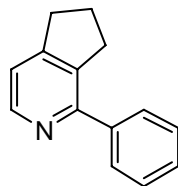


155.420  
154.606  
145.368  
140.025  
138.684  
128.582  
128.360  
126.865  
116.758

77.274  
77.023  
76.772

29.980  
25.061

0.006



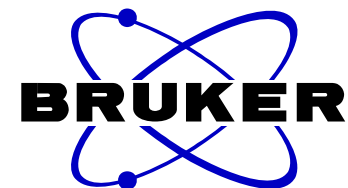
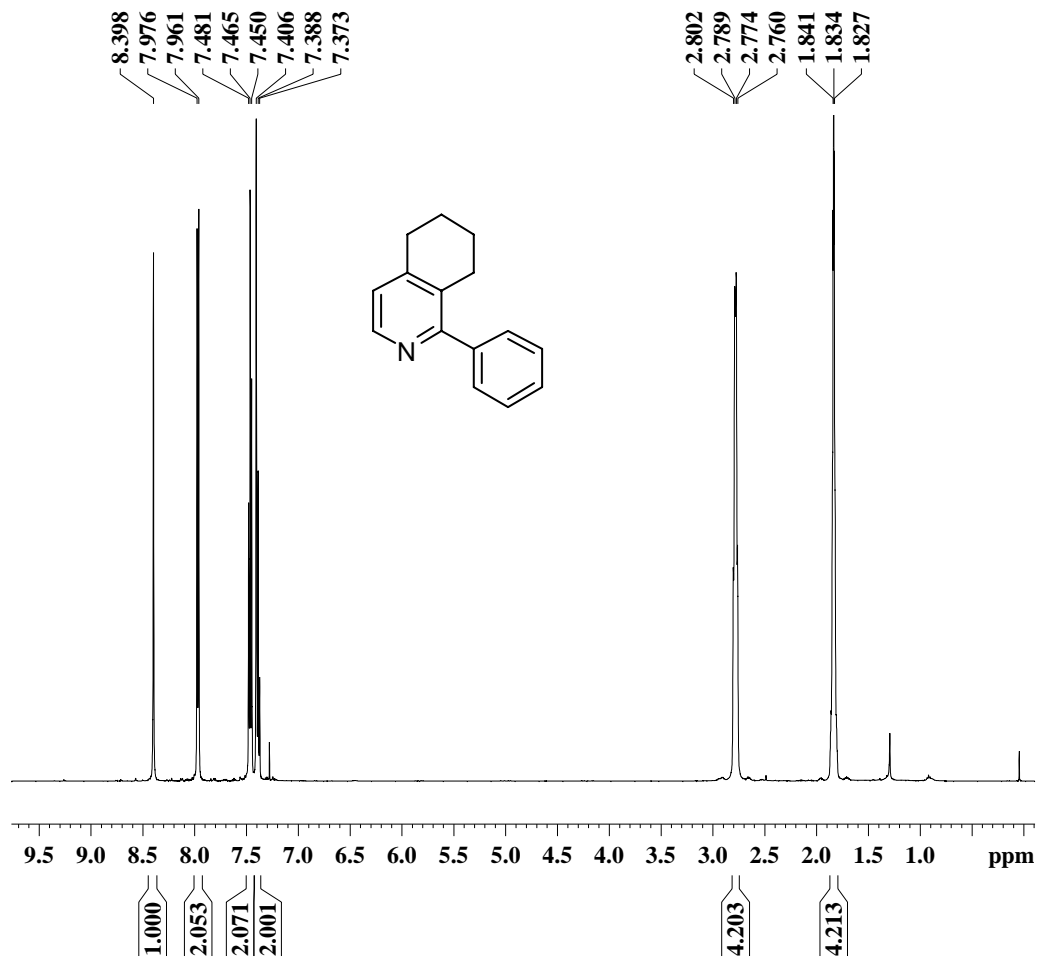
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EXPNO 2  
PROCNO 1  
Date\_ 20140320  
Time 21.33  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 12216  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 1820  
DW 15.300 usec  
DE 6.00 usec  
TE 673.2 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 20

==== CHANNEL f1 =====  
NUC1 13C  
P1 12.20 usec  
PL1 3.00 dB  
SFO1 125.7464750 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 17.70 dB  
PL13 17.70 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326485 MHz  
WDW EM  
SSB 0  
LB 12.00 Hz  
GB 0  
PC 1.00

Compound **6b**

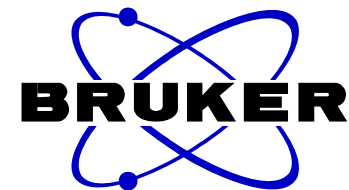
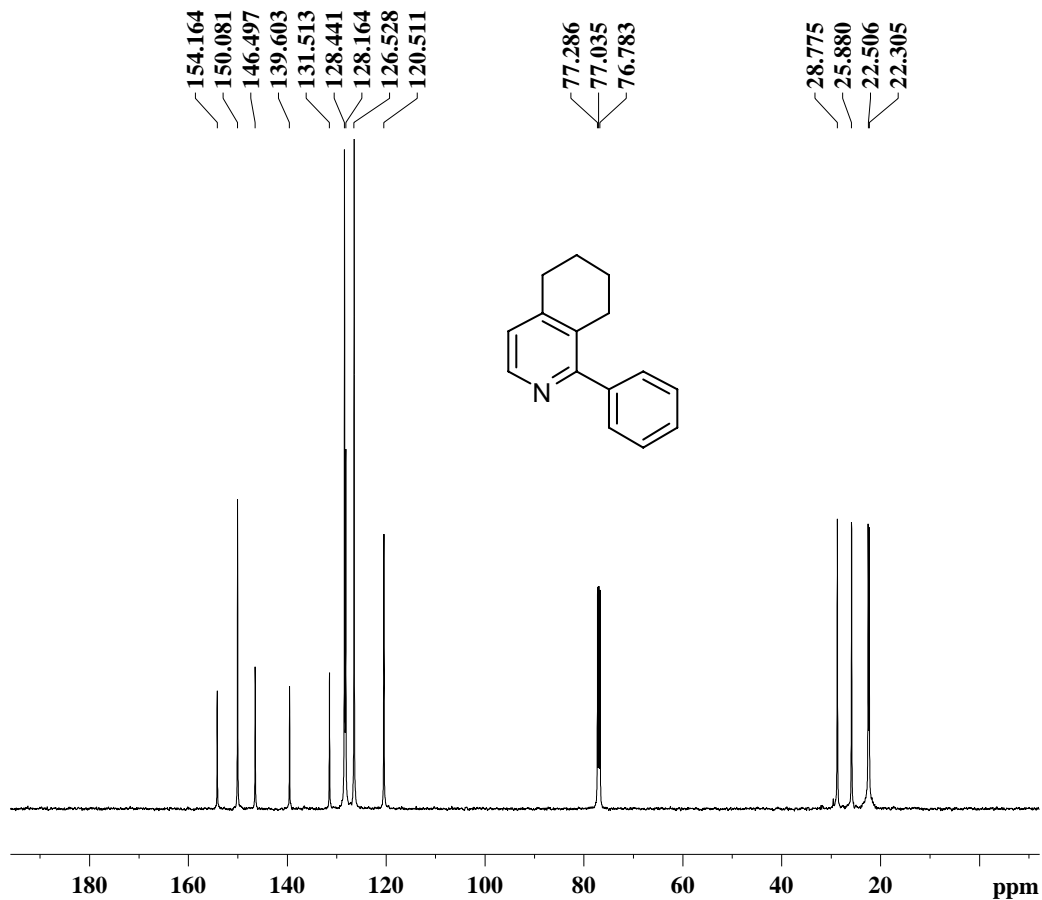
WSW1031 1H 1D 2012 12 03



NAME WSW1031  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20121203  
 Time 19.08  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 16384  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8193000 sec  
 RG 50.8  
 DW 50.000 usec  
 DE 8.00 usec  
 TE 293.2 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.00 usec  
 PL1 2.00 dB  
 SFO1 500.0338500 MHz  
 SI 16384  
 SF 500.0299998 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

WSW1031 13C ID 2012 12 06



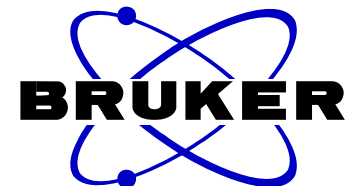
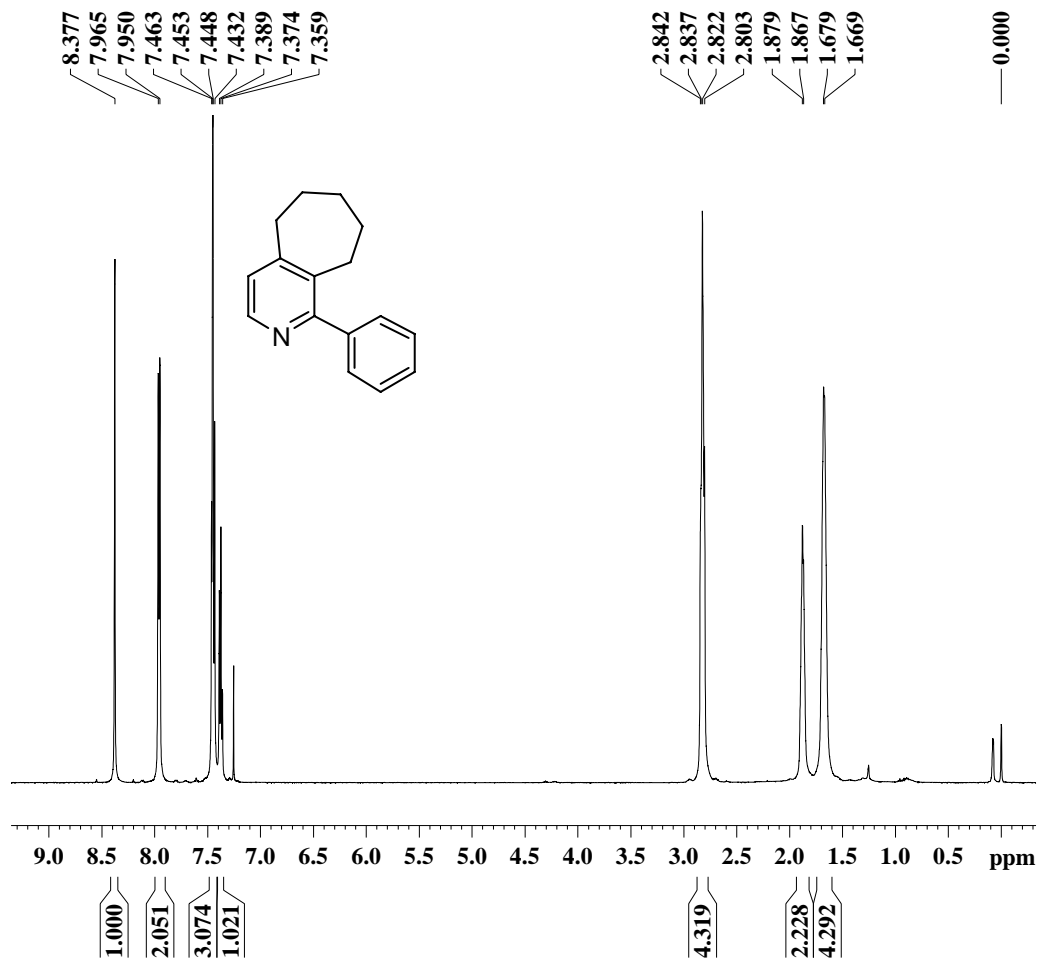
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EXPNO 2  
PROCNO 1  
Date\_ 20121206  
Time 10.57  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 464  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 8200  
DW 15.300 usec  
DE 6.00 usec  
TE 294.9 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 50

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.20 usec  
PL1 3.00 dB  
SFO1 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 17.70 dB  
PL13 17.70 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326667 MHz  
WDW EM

Compound **6c**

WSW140311 1H 1D 2014 01 19



NAME WSW140311  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20140319  
 Time 17.36  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 16384  
 SOLVENT CDCl3  
 NS 16  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8193000 sec  
 RG 203  
 DW 50.000 usec  
 DE 8.00 usec  
 TE 673.2 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.00 usec  
 PL1 2.00 dB  
 SFO1 500.0338500 MHz  
 SI 16384  
 SF 500.0300139 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

WSW140311

13C 1D

2014 03 22

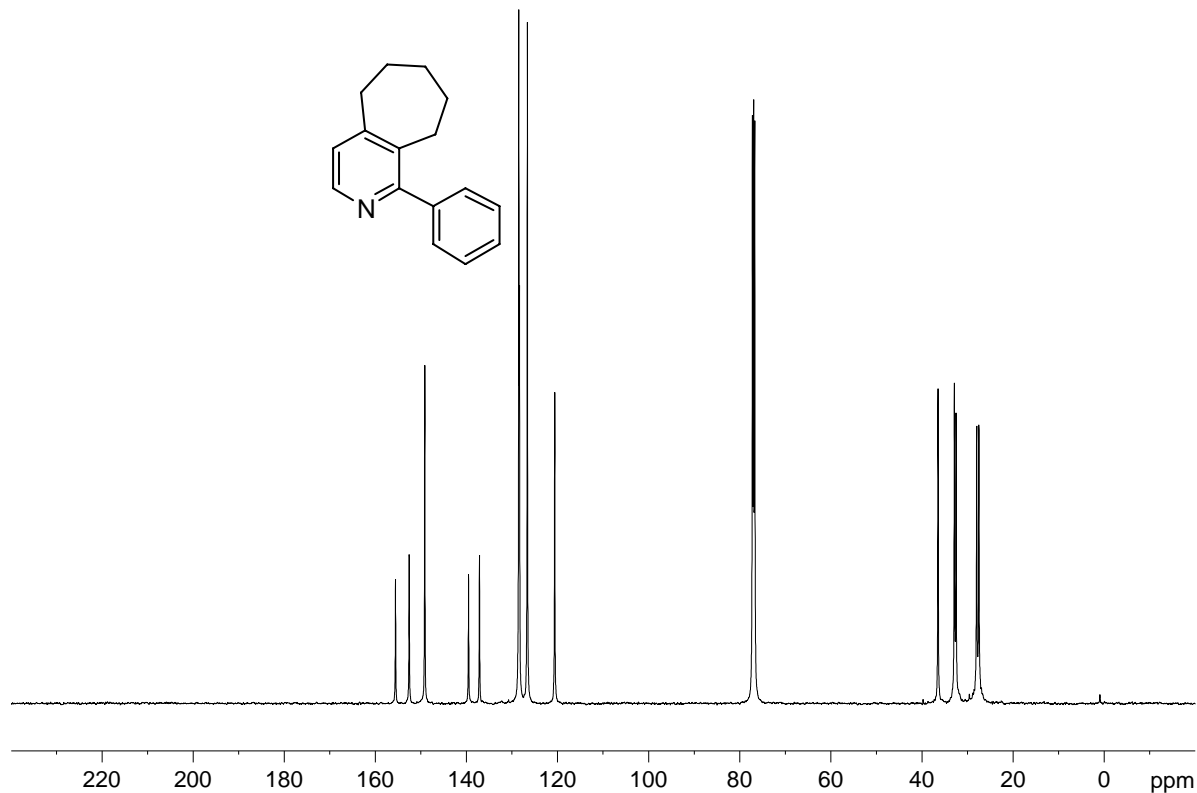
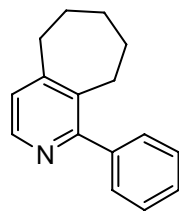


155.647  
152.643  
149.231  
139.618  
137.212  
128.593  
128.425  
126.690  
120.694

77.291  
77.039  
76.781

36.544  
32.954  
32.592  
28.062  
27.577

0.000



NAME WSW140311  
EXPNO 2  
PROCNO 1  
Date\_ 20140322  
Time 10.59  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 5649  
DS 2  
SWH 32679.738 F  
FIDRES 0.498653 F  
AQ 1.0027661 s  
RG 1820  
DW 15.300 u  
DE 6.00 u  
TE 673.2 K  
D1 2.0000000 s  
d11 0.0300000 s  
DELTA 1.89999998 s  
TD0 20

==== CHANNEL f1 =====  
NUC1 13C  
P1 12.20 u  
PL1 3.00 c  
SF01 125.7464750 M

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 u  
PL2 2.00 c  
PL12 17.70 c  
PL13 17.70 c  
SF02 500.0355000 M  
SI 32768  
SF 125.7326485 M  
WDW EM  
SSB 0