

## Supplementary Material

### Smiles rearrangement for the synthesis of diarylamines

Xiao Tian,<sup>a</sup> Ren-Min Wu,<sup>a</sup> Gang Liu,<sup>a</sup> Zhu-Bo Li,<sup>a</sup> He-Lin Wei,<sup>a</sup> Hao Yang,<sup>b</sup>  
Dong-Soo Shin,<sup>c</sup> Li-Ying Wang,<sup>a</sup> Hua Zuo<sup>a,\*</sup>

<sup>a</sup>College of Pharmaceutical Sciences, Southwest University,  
Chongqing, 400715, China

<sup>b</sup>College of Horticulture and Landscape Architecture, Southwest University,  
Chongqing, 400715, China

<sup>c</sup>Department of Chemistry, Changwon National University, Changwon, 641-773,  
South Korea

E-mail: [zuohua@swu.edu.cn](mailto:zuohua@swu.edu.cn)

#### Table of Contents

1. General remarks	S1
2. General procedure of Ligand-free Smiles Rearrangement for the Synthesis of Diarylamines <b>3</b>	S2
3. Synthesis and analytical data of <b>3a-u</b>	S2
4. References	S9
5. Copies of NMR and MS spectra for compounds	S10

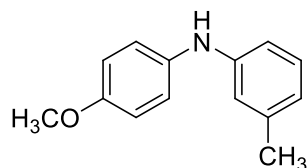
#### 1. General remarks

<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were recorded in CDCl<sub>3</sub> (300 MHz for <sup>1</sup>H NMR and 75 MHz for <sup>13</sup>C NMR, respectively) with tetramethylsilane as the internal reference on Bruker Advance 300 FT spectrometer. Chemical shifts were reported in parts per million. Mass spectra (MS) were measured by ESI. CDCl<sub>3</sub> were used as delivered from Sigma-Aldrich. Silica gel (70-230 mesh) was used for flash column chromatography. All the reactions were monitored by TLC using 0.25 mm silica gel plates (Merck 60F254) with UV indicator. The microwave-assisted reaction time is the hold time at the final temperature. Unless otherwise noted, other reagents were obtained from commercial suppliers and used without further purification.

## 2. General Procedure for the Smiles Rearrangement for the Synthesis of Diarylamines (3)

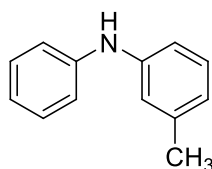
To a magnetically stirred solution of the appropriate arylamine **2** (1.0 mmol) and Cs<sub>2</sub>CO<sub>3</sub> (3.2 mmol) in dry DMF cooled by ice bath were added chloroacetyl chloride (1.2 mmol) and substituted phenol **1** (1.0 mmol). The reaction mixture was then stirred for 30 min at room temperature and placed into microwave oven (600W, 150 °C) and irradiated for 30-80 min. The solvent was removed under vacuum and water (20 mL) was added into the residue. The mixture was then extracted by ethyl acetate (4 x 30 mL). The combined organic layers were dried over anhydrous MgSO<sub>4</sub> and evaporated under vacuum to give the crude product. Pure product was obtained by column chromatography on silica gel.

## 3. Synthesis and analytical data of (3a-u)



### Scheme S1. *N*-(4-Methoxyphenyl)-3-methylbenzenamine **3a**.<sup>1</sup>

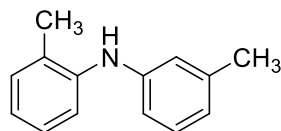
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a gray solid. Mp 72-75 °C (lit.<sup>1</sup> 75-76 °C). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 2.28 (s, 3H; CH<sub>3</sub>), 3.80 (s, 3H; OCH<sub>3</sub>), 5.45 (s, br, 1H; NH), 6.64-7.24 (m, 8H; ArH) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ 21.5 (CH<sub>3</sub>), 55.6 (OCH<sub>3</sub>), 112.8 (CH), 114.2 (CH), 114.6 (CH), 116.3 (CH), 120.5 (CH), 122.2 (CH), 129.1 (CH), 135.9 (C), 139.1 (C), 145.1 (C), 155.2 (C) ppm.



### Scheme S2. 3-Methyl-*N*-phenylbenzenamine **3b**.<sup>2</sup>

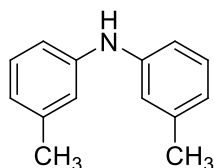
Following the general procedure, the crude product was purified over a silica gel

column using petroleum ether to give a yellow liquid.  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  2.29 (s, 3H;  $\text{CH}_3$ ), 5.58 (s, 1H; NH), 6.85-7.28 (m, 9H;  $\text{ArH}$ ) ppm.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  20.7 ( $\text{CH}_3$ ), 116.8 (CH), 117.8 (CH), 118.9 (CH), 120.2 (CH), 120.9 (CH), 129.3 (CH), 129.8 (CH), 130.9 (CH), 140.2 (C), 143.9 (C) ppm.



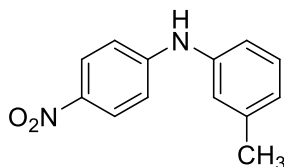
**Scheme S3.** 3-Methyl-*N*-*o*-tolylbenzenamine **3c**.<sup>3</sup>

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a yellow liquid.  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  2.22 (s, 3H;  $\text{CH}_3$ ), 2.28 (s, 3H;  $\text{CH}_3$ ), 5.29 (s, br, 1H; NH), 6.69-7.23 (m, 9H;  $\text{ArH}$ ) ppm.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  17.8 ( $\text{CH}_3$ ), 21.45 ( $\text{CH}_3$ ), 114.5 (CH), 118.1 (CH), 118.8 (CH), 121.3 (CH), 121.8 (CH), 126.7 (CH), 128.1 (C), 129.1 (CH), 130.8 (CH), 139.1 (C), 141.2 (C), 143.8 (C) ppm.



**Scheme S4.** *dim*-Tolylamine **3d**.<sup>4</sup>

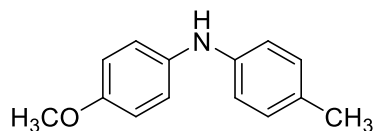
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a colorless liquid.  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  2.25 (s, 6H;  $\text{CH}_3$ ), 5.46 (s, br, 1H; NH), 6.69 (d,  $J = 7.2$  Hz, 2H;  $\text{ArH}$ ), 6.79-6.83 (m, 4H;  $\text{ArH}$ ), 7.07-7.12 (m, 2H;  $\text{ArH}$ ). ppm.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  21.4 ( $\text{CH}_3$ ), 114.8 (CH), 118.5 (CH), 121.6 (CH), 129.0 (CH), 139.0 (C), 143.1 (C) ppm.



**Scheme S5.** 3-Methyl-*N*-(4-nitrophenyl)benzenamine **3e**.

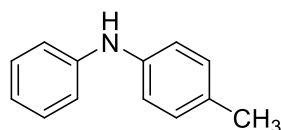
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 130-133 °C.  $^1\text{H}$  NMR (300

MHz, CDCl<sub>3</sub>):  $\delta$  2.37 (s, 3H; CH<sub>3</sub>), 6.29 (s, br, 1H; NH), 6.92 (d,  $J$  = 8.7 Hz, 2H; ArH), 6.97-7.02 (m, 3H; ArH), 7.25-7.27 (m, 1H, ArH), 8.11 (d,  $J$  = 8.5 Hz, 2H; ArH) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  21.4 (CH<sub>3</sub>), 113.6 (CH), 119.0 (CH), 122.6 (CH), 125.5 (CH), 126.2 (CH), 129.5 (C), 139.4 (C), 139.6 (C), 139.7 (C), 150.3 (C) ppm. MS (ESI, m/z)(%): 229 (8) [M+1], 212 (57), 182 (74), 167 (100).



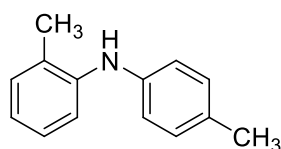
**Scheme S6.** *N*-(4-Methoxyphenyl)-4-methylbenzenamine **3f**.<sup>5</sup>

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a gray solid. Mp 80-82 °C (lit.<sup>5</sup> 82 °C). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  2.27 (s, 3H; CH<sub>3</sub>), 3.78 (s, 3H; OCH<sub>3</sub>), 5.38 (s, br, 1H; NH), 6.83-6.85 (m, 4H; ArH), 7.00-7.04 (m, 4H; ArH) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  20.5 (CH<sub>3</sub>), 55.6 (OCH<sub>3</sub>), 114.6 (CH), 116.5 (CH), 121.1 (CH), 129.3 (C), 129.8 (CH), 136.6 (C), 142.4 (C), 154.7 (C) ppm.



**Scheme S7.** 4-Methyl-*N*-phenylbenzenamine **3g**.<sup>6</sup>

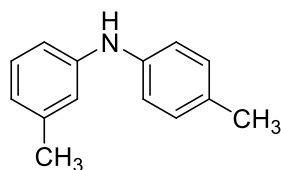
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a white solid. Mp 85-87 °C (lit.<sup>6</sup> 87 °C). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  2.24 (s, 3H; CH<sub>3</sub>), 5.49 (s, br, 1H; NH), 6.54-7.22 (m, 9H; ArH) ppm.



**Scheme S8.** 4-Methyl-*N*-*o*-tolylbenzenamine **3h**.<sup>7</sup>

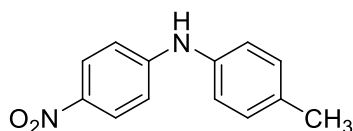
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a yellow viscous oil. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  2.25 (s, 3H; CH<sub>3</sub>), 2.30 (s, 3H; CH<sub>3</sub>), 5.29 (s, br, 1H; NH), 6.85-6.95 (m, 3H; ArH), 7.06-7.24 (m, 5H; ArH) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  17.8 (CH<sub>3</sub>),

20.6 (CH<sub>3</sub>), 117.2 (CH), 118.6 (CH), 121.0 (CH), 126.7 (CH), 126.9 (C), 129.8 (CH), 130.4 (C), 130.8 (CH), 141.0 (C), 142.0 (C) ppm.



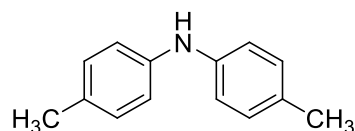
**Scheme S8.** 4-Methyl-*N*-*m*-tolylbenzenamine **3i**.<sup>8</sup>

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a yellow viscous oil. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 2.27 (d, 6H; CH<sub>3</sub>), 5.49 (s, br, 1H; NH), 6.68 (d, *J* = 7.2 Hz, 1H; Ar*H*), 6.80–7.21 (m, 7H; Ar*H*) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ 20.6 (CH<sub>3</sub>), 21.5 (CH<sub>3</sub>), 113.9 (CH), 117.5 (CH), 118.8 (CH), 121.1 (CH), 129.1 (CH), 129.8 (CH), 130.7 (C), 139.1 (C), 140.3 (C), 143.8 (C) ppm.



**Scheme S9.** 4-Methyl-*N*-(4-nitrophenyl)benzenamine **3j**.<sup>9</sup>

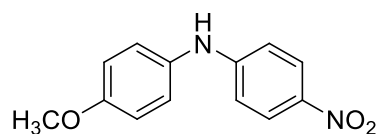
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 132–135 °C (lit.<sup>9</sup> 137 °C). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 2.36 (s, 6H; CH<sub>3</sub>), 6.29 (s, br, 1H; NH), 6.86 (d, *J* = 9.0 Hz, 2H; Ar*H*), 7.11 (d, *J* = 8.1 Hz, 2H; Ar*H*), 7.19 (d, *J* = 8.0 Hz, 2H; Ar*H*), 8.08 (d, *J* = 9.0 Hz, 2H; Ar*H*) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ 20.9 (CH<sub>3</sub>), 113.1 (CH), 122.6 (CH), 126.2 (CH), 130.2 (CH), 134.8 (C), 136.6 (C), 139.2 (C), 150.8 (C) ppm.



**Scheme S10.** dip-Tolylamine **3k**.<sup>10</sup>

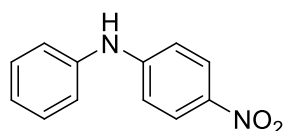
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a light yellow solid. Mp 74–77 °C (lit.<sup>10</sup> 73–75 °C). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 2.28 (s, 6H; CH<sub>3</sub>), 5.49 (s, br, 1H; NH), 6.93 (d, *J* = 8.0 Hz, 4H; Ar*H*), 7.05 (d, *J* = 8.0 Hz, 4H; Ar*H*) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):

$\delta$  20.6 (CH<sub>3</sub>), 117.9 (CH), 129.8 (CH), 130.1 (C), 141.1 (C) ppm.



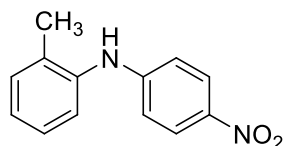
**Scheme S11.** *N*-(4-Methoxyphenyl)-4-nitrobenzenamine **3l**.<sup>11</sup>

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 149-152 °C (lit.<sup>11</sup> 152-153 °C). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  3.84 (s, 3H; OCH<sub>3</sub>), 6.16 (s, 1H; NH), 6.76 (d, *J* = 8.8 Hz, 2H; Ar*H*), 6.94 (d, *J* = 8.4 Hz, 2H; Ar*H*), 7.16 (d, *J* = 8.4 Hz, 2H; Ar*H*), 8.08 (d, *J* = 8.8 Hz, 2H; Ar*H*) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  55.5 (OCH<sub>3</sub>), 112.6 (CH), 114.9 (CH), 125.5 (CH), 126.3 (CH), 131.9 (C), 139.0 (C), 151.7 (C), 157.4 (C) ppm.



**Scheme S12.** 4-Nitro-*N*-phenylbenzenamine **3m**.<sup>12</sup>

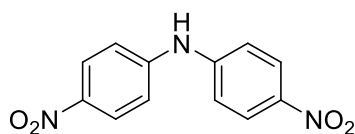
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 131-133 °C (lit.<sup>12</sup> 131 °C). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  6.40 (s, 1H; NH), 6.94 (d, *J* = 9.0 Hz, 2H; Ar*H*), 7.14-7.42 (m, 5H; Ar*H*), 8.11 (d, *J* = 9.0 Hz, 2H; Ar*H*) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  113.6 (CH), 121.9 (CH), 124.6 (C), 126.2 (CH), 139.4 (C), 139.6 (C), 150.2 (C) ppm.



**Scheme S13.** 4-Nitro-*N*-*o*-tolylbenzenamine **3n**.

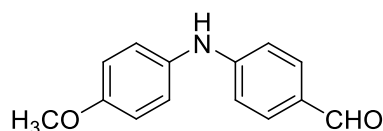
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 130-133 °C. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  2.25 (s, 3H; CH<sub>3</sub>), 6.10 (s, 1H; NH), 6.72 (d, *J* = 8.9 Hz, 2H; Ar*H*), 7.18-7.31 (m, 4H; Ar*H*), 8.08 (d, *J* = 8.9 Hz, 2H; Ar*H*) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  17.8 (CH<sub>3</sub>), 113.0 (CH), 124.7 (CH), 126.1 (CH), 126.2 (CH), 127.1 (CH),

131.4 (CH), 133.2 (C), 137.5 (C), 139.1 (C), 151.3 (C) ppm. MS (ESI,  $m/z$ )(%): 229 (9) [M+1], 212 (100), 182 (77), 168 (94).



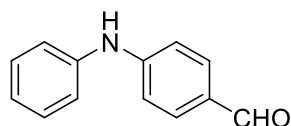
**Scheme S14.** 3-methyl-*N*-(3-nitrophenyl)benzenamine **3o**.<sup>13</sup>

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a yellow solid. Mp 145-147 °C (lit.<sup>13</sup> 146 °C); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 4.36 (s, br, 1H; NH), 6.63 (d,  $J = 8.9$  Hz, 2H; ArH), 7.21-7.26 (m, 3H; ArH), 8.1 (d,  $J = 8.8$  Hz, 1H; ArH), 8.2 (d,  $J = 8.9$  Hz, 2H; ArH) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ 113.2 (CH), 117.2 (CH), 125.9 (CH), 126.2 (C) ppm.



**Scheme S15.** 4-(4-methoxyphenylamino)benzaldehyde **3p**.<sup>14</sup>

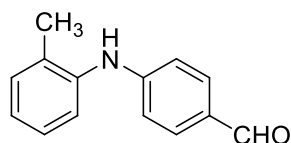
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 108-111 °C (lit.<sup>14</sup> 113 °C). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 3.83 (s, 3H; OCH<sub>3</sub>), 6.08 (s, 1H; NH), 6.85 (d,  $J = 8.4$  Hz, 2H; ArH), 6.92 (d,  $J = 8.7$  Hz, 2H; ArH), 7.16 (d,  $J = 8.7$  Hz, 2H; ArH), 7.70 (d,  $J = 8.4$  Hz, 2H; ArH), 9.75 (s, 1H; CHO) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ 55.5 (OCH<sub>3</sub>), 113.4 (CH), 114.8 (CH), 125.1 (CH), 127.8 (C), 132.2 (CH), 132.6 (C), 151.4 (C), 157.0 (C), 190.2 (CHO) ppm.



**Scheme S16.** 4-(phenylamino)benzaldehyde **3q**.<sup>15</sup>

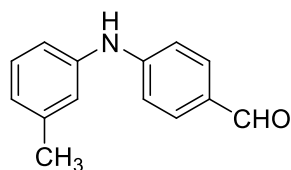
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 94-97 °C (lit.<sup>15</sup> 95-97 °C). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 6.38 (s, 1H; NH), 7.02 (d,  $J = 8.2$  Hz, 2H; ArH), 7.09-7.39 (m, 5H; ArH), 7.74 (d,  $J = 8.2$  Hz, 2H; ArH), 9.78 (s, 1H; CHO) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ 114.4 (CH), 121.3 (CH), 123.8 (CH), 128.4 (C), 129.5

(CH), 132.1 (CH), 140.0 (C), 149.8 (C), 190.4 (CHO) ppm.



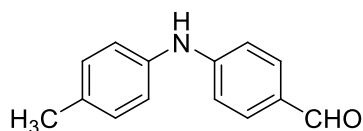
**Scheme S17.** 4-(*o*-toluidino)benzaldehyde **3r**.

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 85-87 °C. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 2.25 (s, 3H; CH<sub>3</sub>), 6.00 (s, 1H; NH), 6.82 (d, *J* = 8.4 Hz, 2H; ArH), 7.13-7.27 (m, 4H; ArH), 7.71 (d, *J* = 8.4 Hz, 2H; ArH), 9.76 (s, 1H; CHO) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ 17.9 (CH<sub>3</sub>), 113.8 (CH), 124.1 (CH), 125.4 (CH), 127.0 (CH), 127.9 (C), 131.3 (CH), 132.1 (CH), 132.6 (C), 138.0 (C), 151.0 (C), 190.3 (CHO) ppm. MS (ESI, *m/z*)(%): 212 (28) [M+1], 184 (12), 183 (9), 182 (14), 169 (52), 168 (24), 103 (48), 88 (100), 75 (11), 60 (10).



**Scheme S18.** 4-(*m*-toluidino)benzaldehyde **3s**.

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 117-119 °C. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 2.34 (s, 3H; CH<sub>3</sub>), 6.37 (s, 1H; NH), 6.92-7.24 (m, 6H; ArH), 7.71-7.74 (d, *J* = 8.3 Hz, 2H; ArH), 9.77 (s, 1H; CHO) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ 21.4 (CH<sub>3</sub>), 114.4 (CH), 118.3 (CH), 121.9 (CH), 124.7 (CH), 128.2 (C), 129.3 (CH), 132.1 (CH), 139.5 (C), 139.9 (C), 150.0 (C), 190.4 (CHO) ppm. MS (ESI, *m/z*)(%): 212 (33) [M+1], 183 (21), 169 (69), 103 (81), 88 (100), 75 (34), 73 (6), 60 (21).

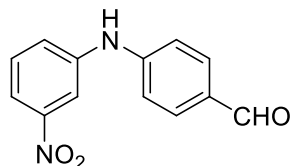


**Scheme S19.** 4-(*p*-toluidino)benzaldehyde **3t**.

Following the general procedure, the crude product was purified over a silica gel



column using petroleum ether to give a brown solid. Mp 85-88 °C. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 2.35 (s, 3H; CH<sub>3</sub>), 6.20 (s, 1H; NH), 6.95 (d, *J* = 8.4 Hz, 2H; ArH), 7.10 (d, *J* = 8.1 Hz, 2H; ArH), 7.18 (d, *J* = 8.1 Hz, 2H; ArH), 7.72 (d, *J* = 8.4 Hz, 2H; ArH), 9.77 (s, 1H; CHO) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ 20.8 (CH<sub>3</sub>), 113.9 (CH), 122.1 (CH), 128.1 (C), 130.1 (CH), 132.1 (CH), 134.0 (C), 137.2 (C), 150.5 (C), 190.3 (CHO) ppm.



#### Scheme S20. 4-(3-nitrophenylamino)benzaldehyde **3u**.

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a yellow solid. Mp 152-155 °C. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 6.35 (s, 1H; NH), 7.13 (d, *J* = 8.1 Hz, 2H; ArH), 7.49-7.52 (m, 2H; ArH), 7.83 (d, *J* = 8.1 Hz, 2H; ArH), 7.87-8.04 (m, 2H; ArH), 9.87 (s, 1H; CHO) ppm. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ 114.1 (CH), 116.1 (CH), 117.6 (CH), 122.3 (C), 125.2 (C), 130.4 (C), 132.1 (CH), 142.1 (C), 147.6 (C), 148.5 (C), 190.3 (CHO) ppm. MS (ESI, *m/z*)(%): 243 (16) [M+1], 197 (42), 168 (80), 167 (100).

## 4. References

1. Guram, Anil S.; Buchwald, Stephen L. *J. Am. Chem. Soc.* **1994**, *116*, 7901.
2. Reddy, C. V.; Kingston, J. V.; Verkade, J. G. *J. Org. Chem.* **2008**, *73*, 3047.
3. Altman, R. A.; Anderson, K. W.; Buchwald, S. L. *J. Org. Chem.* **2008**, *73*, 5167.
4. Saavedra, C.; Hernández, R.; Boto, A.; Alvarez, E. *J. Org. Chem.* **2009**, *74*, 4720.
5. Desmarets, C.; Schneider, R.; Fort, Y. *J. Org. Chem.* **2002**, *67*, 3029.
6. Gao, C. Y.; Yang, L. M. *J. Org. Chem.* **2008**, *73*, 1624.
7. Shen, Q. L.; Hartwig, J. F. *Org. Lett.* **2008**, *10*, 4109.
8. Kabalka, G. W.; Zhou, L. L. *Org. Lett.* **2006**, *3*, 320.
9. Hughes, G. M. K.; Saunders, B. C. *J. Chem. Soc.* **1956**, *20*, 3814.
10. Artamkina, G. A.; Sergeev, A. G.; Shtern, M. M.; Beletskaya, I. P. *J. Org. Chem.* **2006**, *42*, 1683.
11. McNulty, James; Cheekoor, Sreedhar; Bender, Timothy P.; Coggan, Jennifer A. *European J. Org. Chem.* **2007**, *9*, 1423.
12. Wadia, M. S.; Patil, D. V. *Synth. Commun.* **2003**, *33*, 2725.
13. Sheremeteva, T. V.; Gusinskaya, V. A. *Seriya Khimicheskay.* **1966**, *4*, 695.
14. Fukuzaki, E.; Nishide, H. *J. Am. Chem. Soc.* **2006**, *128*, 996.

15. Brown, Ursula, M.; Carter, P. H. *J. Chem. Soc.* **1958**, *9*, 1843.

**5. Copies of NMR and MS spectra for compounds**



Current Data Parameters  
 NAME WRM-1H  
 EXPNO 12  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091022  
 Time 18.00  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 24  
 DS 0  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 64  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 DI 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

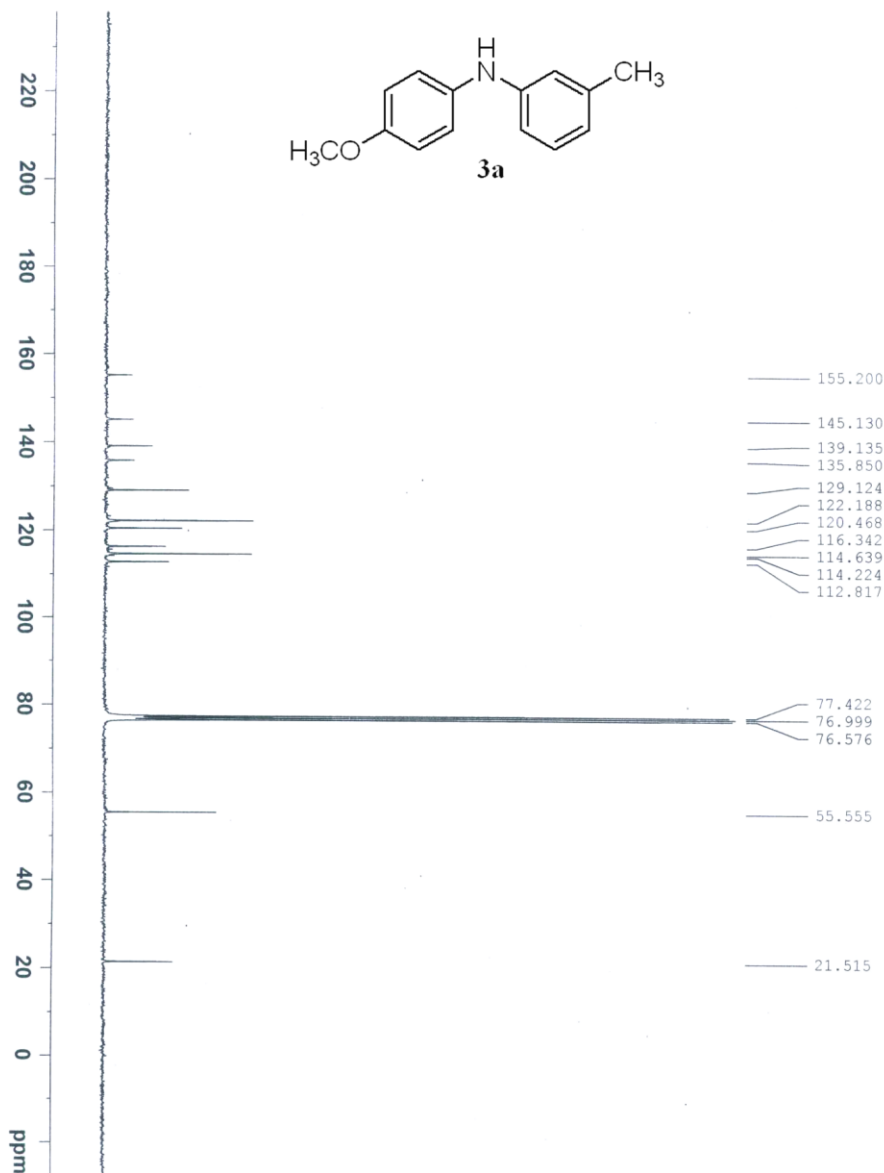
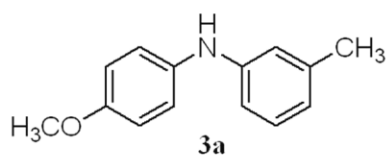
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.1700088 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 20.00 cm  
 CY 0.00 cm  
 FL1 14.939 PPM  
 FL 4484.33 Hz  
 FZP -5.033 ppm  
 F2 -1510.88 Hz  
 FPMCM 0.99863 ppm/cm  
 HZCM 299.76022 Hz/cm



TX-1-3



155.200  
145.130  
139.135  
135.850  
129.124  
122.188  
120.468  
116.342  
114.639  
114.224  
112.817  
  
77.422  
76.999  
76.576  
  
55.555  
  
21.515



Current Data Parameters  
NAME WRM-13C  
EXPNO 6  
PROCNO 1

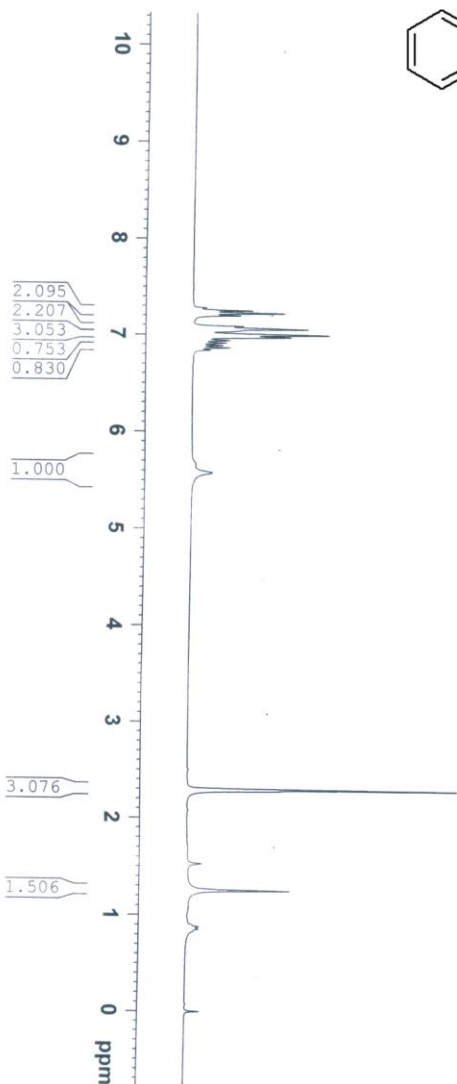
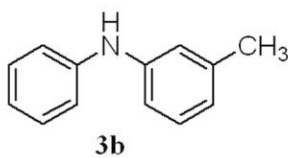
F2 - Acquisition Parameters

Date\_ 20091026  
Time 12.02  
INSTRUM av300  
PROBHD 5 mm QNP 1H/13  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 3938  
DS 0  
SWH 30120.482 Hz  
FDRS 0.459602 Hz  
AQ 1.0879476 sec  
RG 4096  
DW 16.600 usec  
DE 6.00 usec  
TE 67.32 K  
D1 2.5000000 sec  
d11 0.0300000 sec  
MCREST 0.0100000 sec  
MCMKR 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.50 usec  
PL1 4.00 dB  
SFO1 75.4866643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 19.04 dB  
SFO2 300.1710453 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4778096 MHz  
WDW EM  
SSB 0  
LB 3.50 Hz  
GB 0  
PC 1.40



7.2833  
 7.2562  
 7.2300  
 7.2041  
 7.0925  
 7.0663  
 7.0058  
 6.9835  
 6.9466  
 6.9200  
 6.8949  
 6.8704  
 6.8462  
 5.6670  
 5.5809

2.2972  
 2.2839  
  
 1.5298  
 1.2539  
 0.8789  
 0.8555  
 0.8347  
  
 -0.0005

LG-1-26



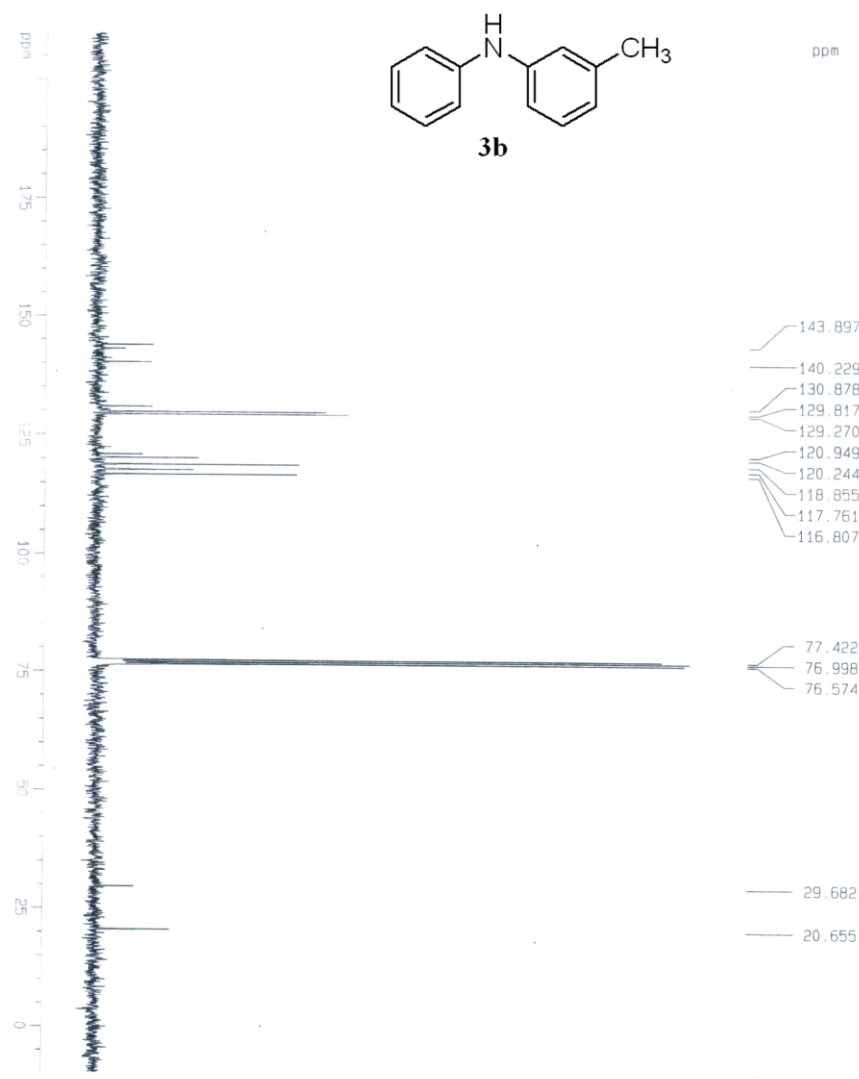
Current Data Parameters  
 NAME LG-1H  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20091106  
 Time 11.31  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 0  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 3.2  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.1700150 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00



LG-1-26

Current Data Parameters  
 Name: LG-13C  
 ExpNO: 1  
 PROCNO: 1

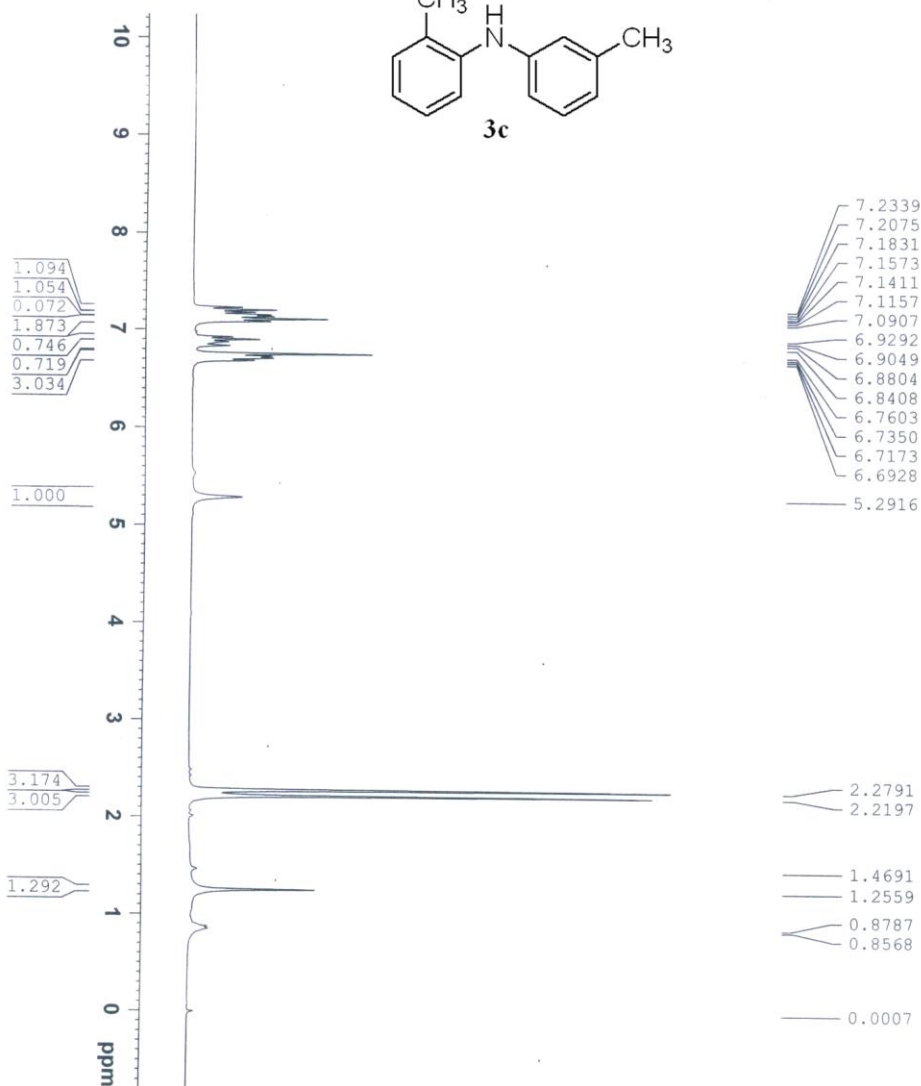
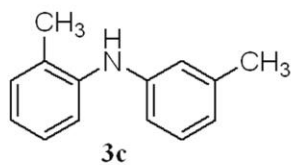
F2 - Acquisition Parameters  
 Date\_: 20091109  
 Time: 10.43  
 INSTRUM: AV300  
 PROBP2: 5 mm QNP 1H/13  
 PULPROG: zgpg  
 TO: 65536  
 SOLVENT: CDCl3  
 NS: 161  
 DS: 0  
 SM: 30120.482 Hz  
 FIDRES: 0.459502 Hz  
 AQ: 1.0879476 sec  
 RG: 6502  
 DM: 16.600 usec  
 DE: 57.02 usec  
 TE: 300.2 K  
 D1: 3.00000000 sec  
 d11: 0.03000000 sec  
 MCREST: 0.00000000 sec  
 KMASK: 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1: 13C  
 P1: 12.50 usec  
 PL1: 4.00 dB  
 SFO1: 75.4686643 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CHOPRG2: waltz16  
 NUC2: 1H  
 PCPD2: 80.00 usec  
 PL2: 2.00 dB  
 PL12: 19.04 dB  
 SFO2: 300.1370493 MHz

F2 - Processing parameters  
 SI: 32768  
 SF: 75.4778123 MHz  
 NDM: EM  
 SSB: 0  
 LB: 3.50 Hz  
 GB: 0  
 PC: 1.40

1D NMR D101 Parameters  
 CX: 20.00 cm  
 CP: 0.00 cm  
 F1P: 209.724 DDM  
 F2P: 15830.26 Hz  
 F3P: 31.721 DDM  
 F4P: -33.093 Hz  
 DSIWCA: 10.37223 DDM/cm  
 HZCW: 628.19763 Hz/cm



IG-1-21



Current Data Parameters  
 NAME LG-1H  
 EXPNO 6  
 PROCNO 1

F2 - Acquisition Parameters

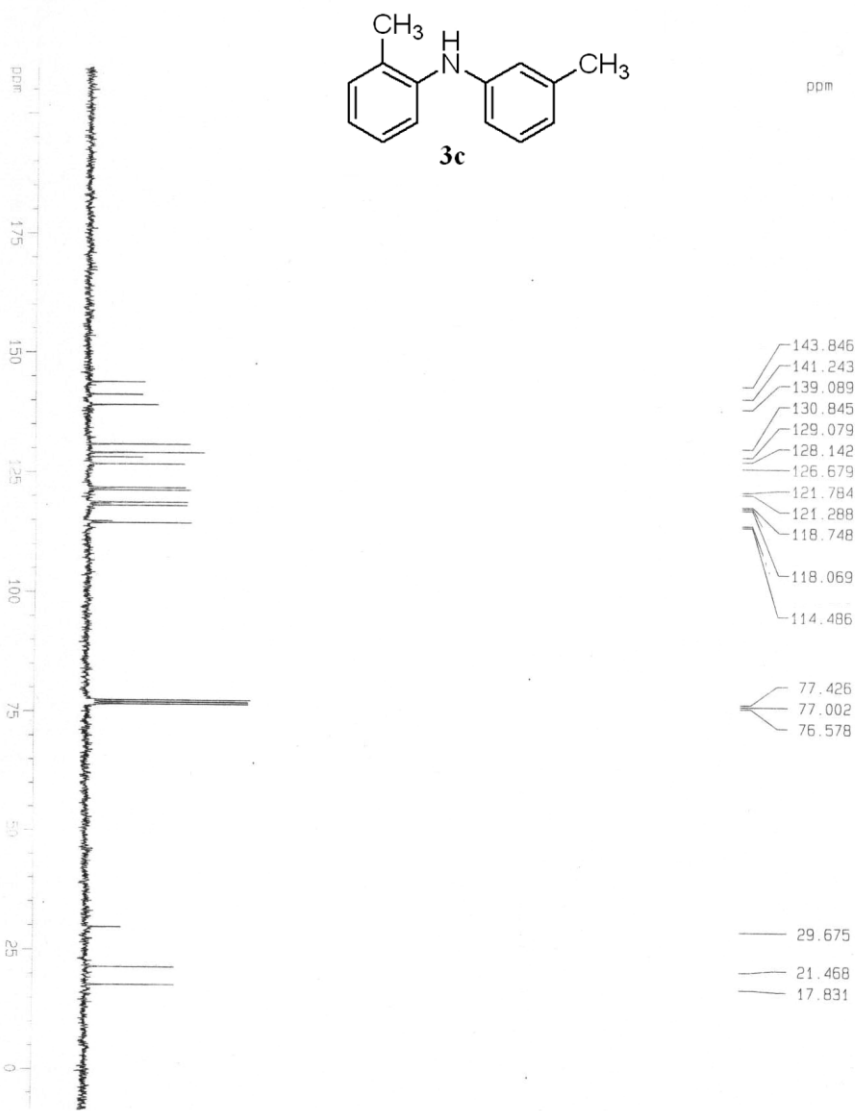
Date\_ 20091106  
 Time\_ 11.27  
 INSTRUM av300  
 PROBRD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 0  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 3.2  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 DI 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====

NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters

SI 16384  
 SF 300.1700381 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00



LG-1-21-

Current Data Parameters  
 NAME LG-13C  
 EXPNO 7  
 PROCNO 1

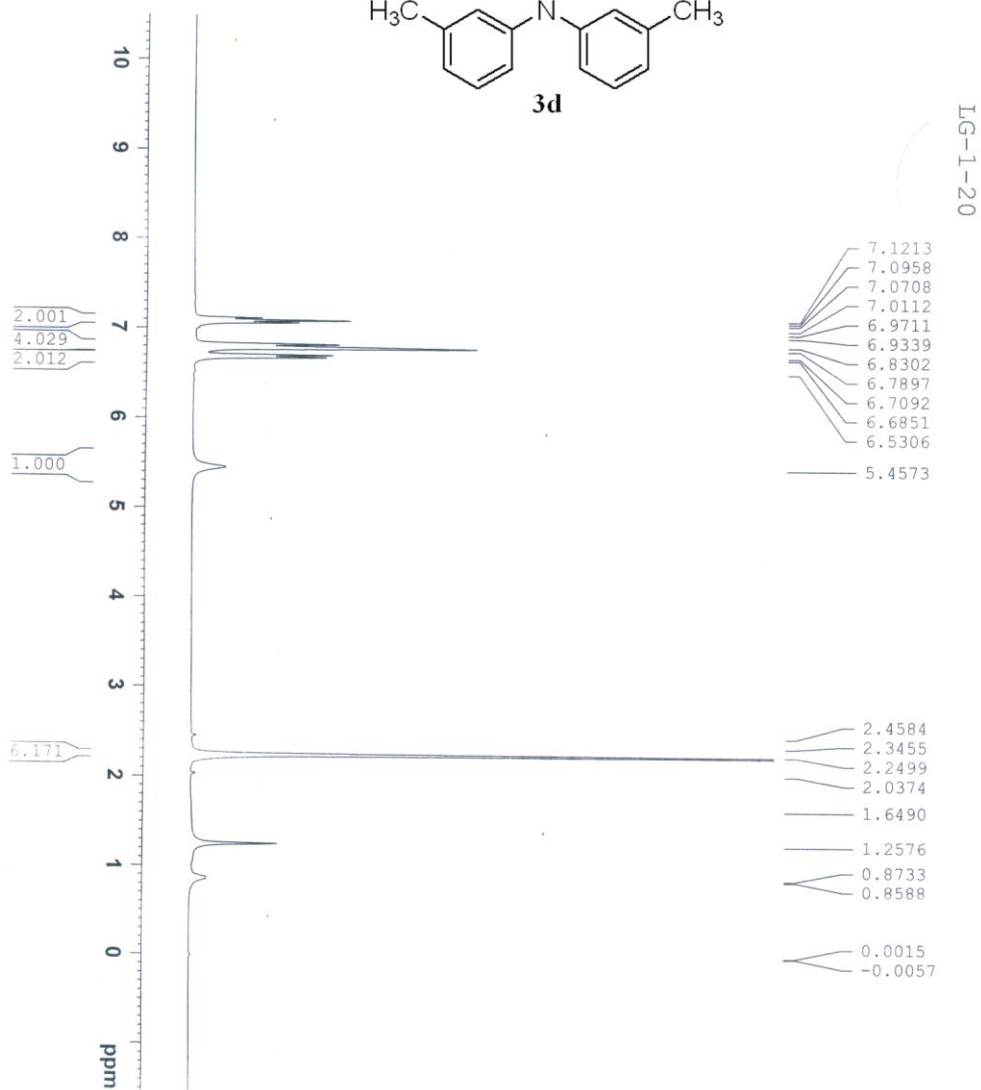
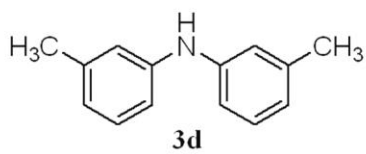
F2 - Acquisition Parameters  
 Date\_ 20091109  
 Time 10:57  
 INSTRUM svt300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TO 62395  
 SOLVENT CDCl3  
 NS 51  
 DS 0  
 SWH 30120.482 Hz  
 FIDRES 0.459602 Hz  
 AQ 1.0879476 sec  
 RG 6502  
 DM 16.600 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 3.00000000 sec  
 d11 0.03000000 sec  
 MCHREST 0.00000000 sec  
 MCMRK 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 12.50 usec  
 PL1 0.00 dB  
 SFO1 75.4689613 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NUC2 1H  
 P1 80.00 usec  
 PL2 2.00 dB  
 PL12 19.04 dB  
 SFO2 300.171053 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.478197 MHz  
 MDX EM  
 SSB 0  
 LB 3.50 Hz  
 GB 0  
 PC 1.40

1D NMR Plot parameters  
 EX 0.00 cm  
 CY 0.00 cm  
 FIP 209.635 ppm  
 FI 15822.88 Hz  
 F2P -8.592 ppm  
 F2 -848.55 Hz  
 FWHM 10.9143 ppm/cm  
 HZCM 823.57086 Hz/cm



- 7.1213
- 7.0958
- 7.0708
- 7.0112
- 6.9711
- 6.9339
- 6.8302
- 6.7897
- 6.7092
- 6.6851
- 6.5306
- 5.4573
  
- 2.4584
- 2.3455
- 2.2499
- 2.0374
- 1.6490
- 1.2576
- 0.8733
- 0.8588
  
- 0.0015
- 0.0057

```

Current Data Parameters
NAME      LG-1H
EXPNO    2
PROCNO   1

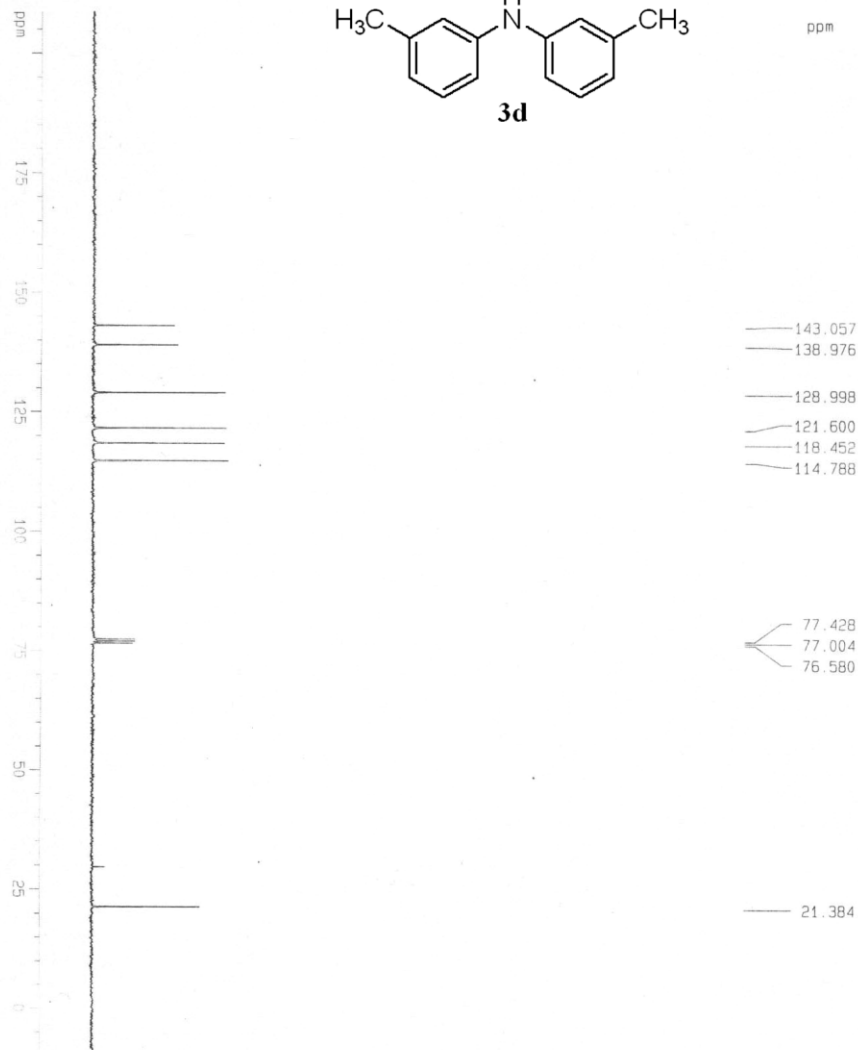
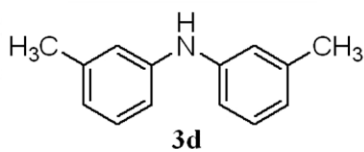
F2 - Acquisition Parameters
Date_    20091106
Time     11.00
INSTRUM  av300
PROBHD   5 mm QNP 1H/13
PULPROG  zg
TD        32768
SOLVENT  CDCl3
NS        8
DS        0
SMH       5995.204 Hz
FIDRES    0.182959 Hz
AQ        2.7329011 sec
RG         3.2
DE        83.400 usec
TE        6.00 usec
D1        673.2 K
MCREST    3.00000000 sec
MCWRRK    0.01500000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        11.25 usec
PL1       2.00 dB
SFO1      300.1714955 MHz

F2 - Processing parameters
SI         16384
SF         300.1700791 MHz
RDM        8192
SBB        0
LB         1.00 Hz
GB         0
PC         1.00
    
```







- 143.057
- 138.976
- 128.998
- 121.600
- 118.452
- 114.788
- 77.428
- 77.004
- 76.580
- 21.384

LG-1-20

Current Data Parameters  
 NAME LG-13C  
 EXPNO 4  
 PROCNO 1

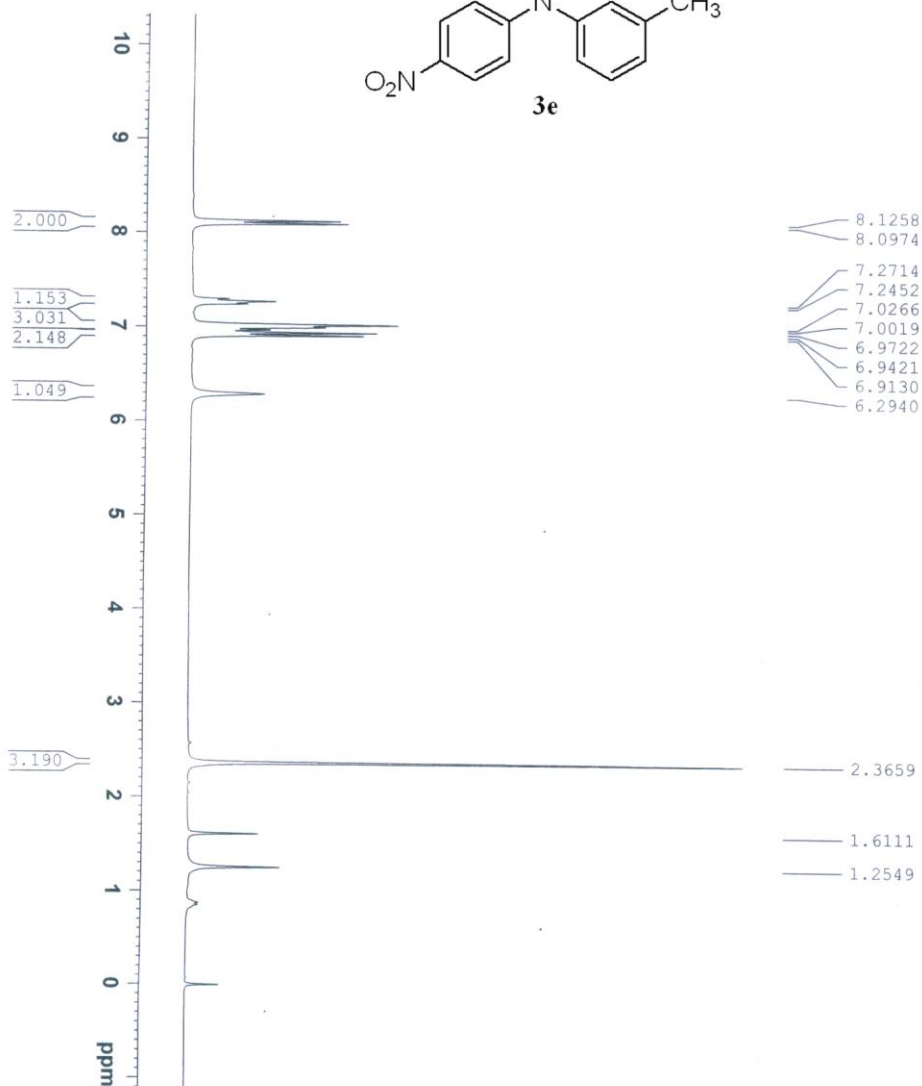
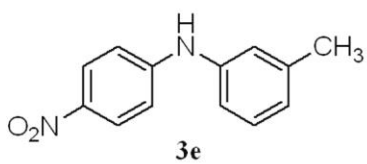
F2 - Acquisition Parameters  
 Date\_ 20091109  
 Time 10:25  
 INSTRUM AV300  
 PROBRD 5 mm QNP 1H/13  
 PULPROG zgpg  
 TO 65536  
 SOLVENT CDCl3  
 NS 28  
 DS 0  
 SWH 30120.482 Hz  
 FIDRES 0.43692 Hz  
 AQ 1.067550 sec  
 RG 16.500 usec  
 DE 6.00 usec  
 TE 673.2 K  
 O1 3.0000000 sec  
 O1 0.0300000 sec  
 MCHPREST 0.0000000 sec  
 MCHPRK 0.0150000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 12.50 usec  
 PL1 4.00 dB  
 SFO1 75.468843 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NUC2 1H  
 P2 90.00 usec  
 PL2 2.00 dB  
 PL12 19.04 dB  
 SFO2 300.1710453 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.477852 MHz  
 MDW EM  
 SSB 0  
 LB 3.50 Hz  
 GB 0  
 PC 1.40

10 NMR D101 parameters  
 CX 20.00 cm  
 CY 20.00 cm  
 ELP 200.000 ppm  
 F1 15760.000 Hz  
 F2 -8.811 MHz  
 F2 -665.00 Hz  
 PPMDCM 10.88077 ppm/cm  
 HZDCM 821.25732 Hz/cm



WHL-1-8



```

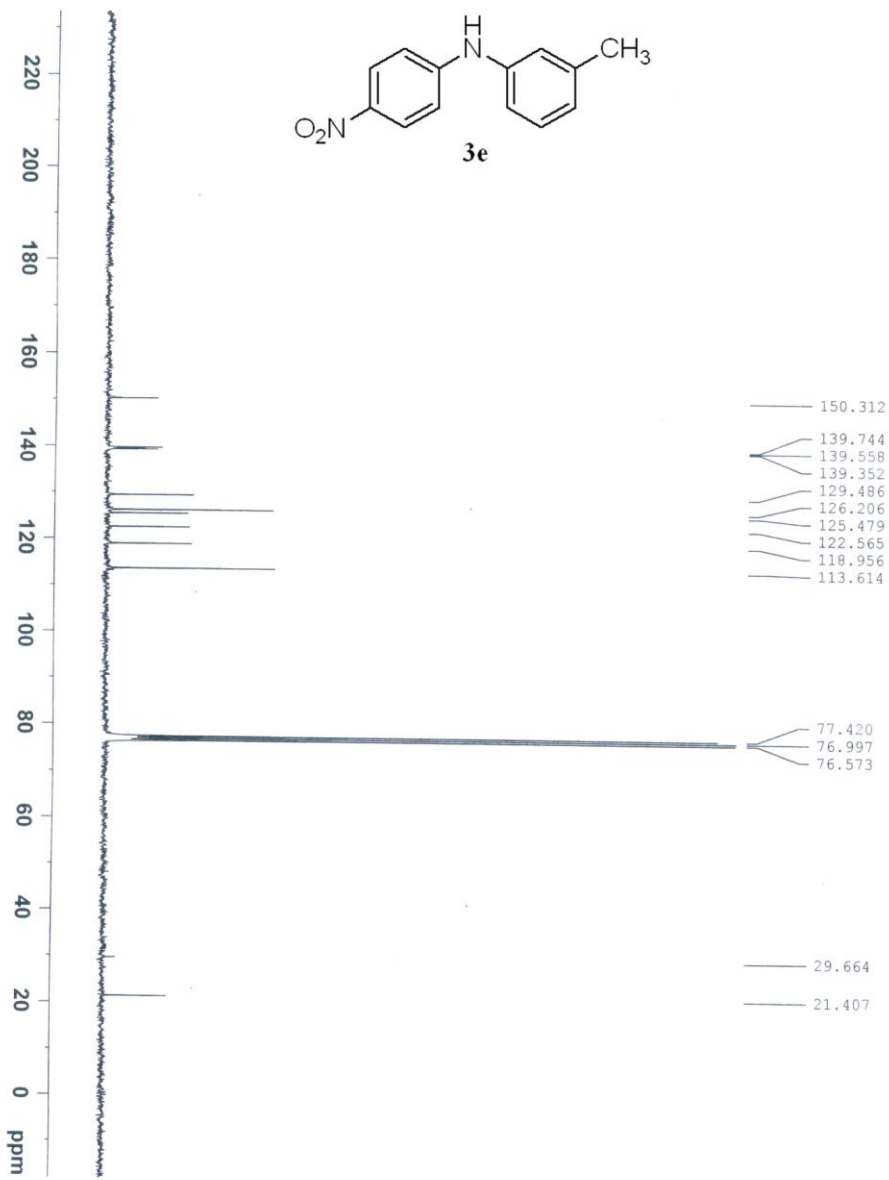
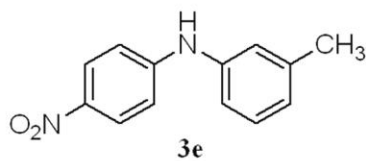
Current Data Parameters
NAME          WHL-1H
EXPNO        2
PROCNO       1

F2 - Acquisition Parameters
Date_        20091106
Time         10.53
INSTRUM     av300
PROBHD      5 mm QNP 1H/13
PULPROG     zgpg30
TD           32768
SOLVENT     CDCl3
NS           16
DS           0
SWH          5995.204 Hz
FIDRES       0.182959 Hz
AQ           2.7329011 sec
RG           64
RG           64
DW           83.400 usec
DE           6.00 usec
TE           673.2 K
D1           3.00000000 sec
MCREST      0.00000000 sec
MCMRK       0.01500000 sec

===== CHANNEL f1 =====
NUC1         1H
P1           11.25 usec
PL1          2.00 dB
SFO1         300.1714955 MHz

F2 - Processing parameters
SI           300.1700048 MHz
WDW          EM
SSB          0
IB           0
GB           0
PC           1.00
    
```

WHL-1-8



150.312  
139.744  
139.558  
139.352  
129.486  
126.206  
125.479  
122.565  
118.956  
113.614

77.420  
76.997  
76.573

29.664  
21.407



Current Data Parameters  
NAME LG-3JC  
EXPNO 9  
PROCNO 1

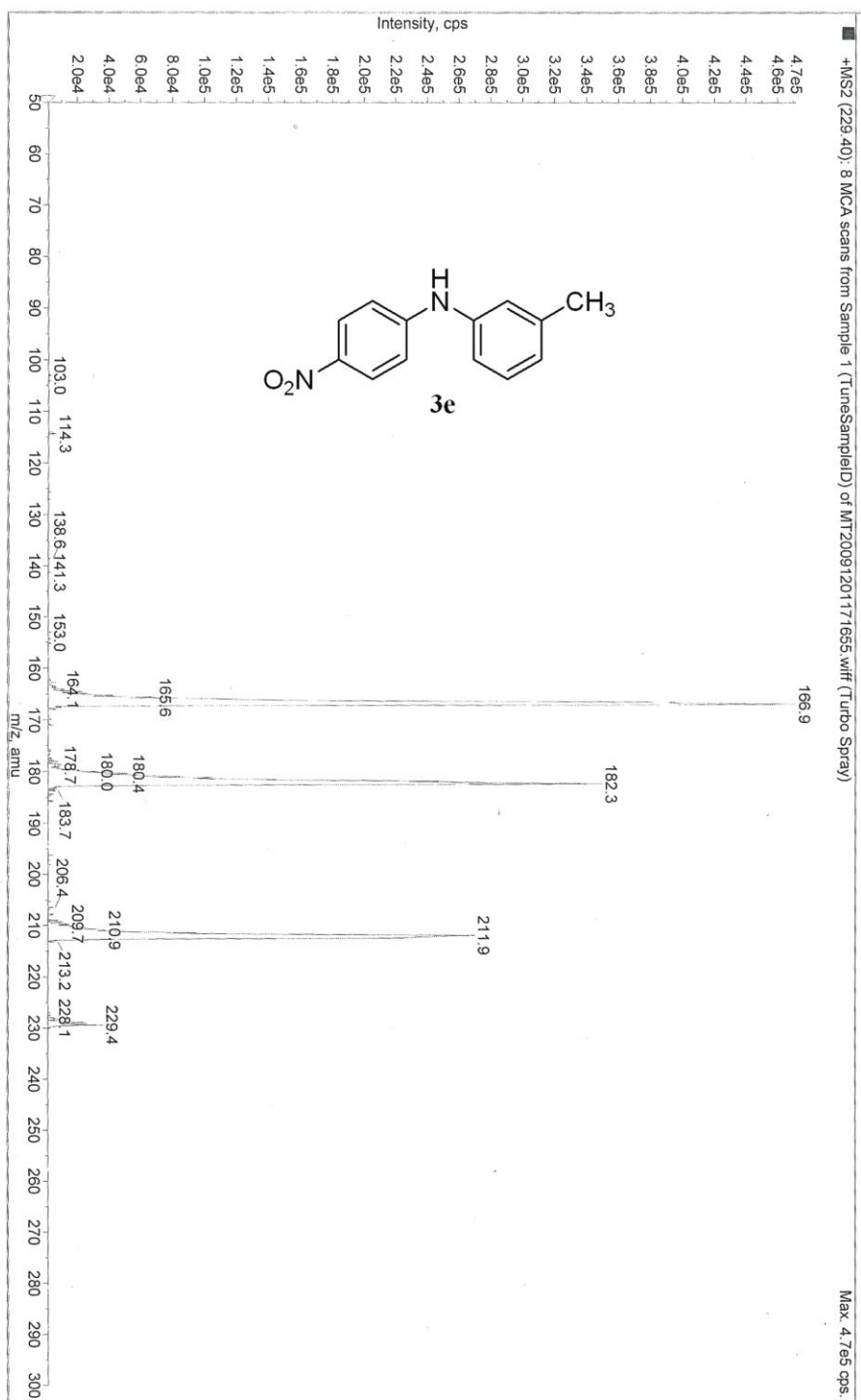
F2 - Acquisition Parameters  
Date\_ 20091109  
Time 17:20  
INSTRUM av300  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1001  
DS 0  
SWH 30720.482 Hz  
FIDRES 0.459602 Hz  
AQ 1.0879476 sec  
RG 6502  
DW 16.600 usec  
DE 6.00 usec  
TE 673.2 K  
D1 3.00000000 sec  
d11 0.03000000 sec  
MCREST 0.00000000 sec  
MCWRRK 0.01500000 sec

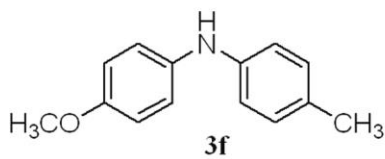
===== CHANNEL f1 =====  
NUC1 13C  
P1 12.50 usec  
PL1 4.00 dB  
SFO1 75.4868643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 19.04 dB  
SFO2 300.1710453 MHz

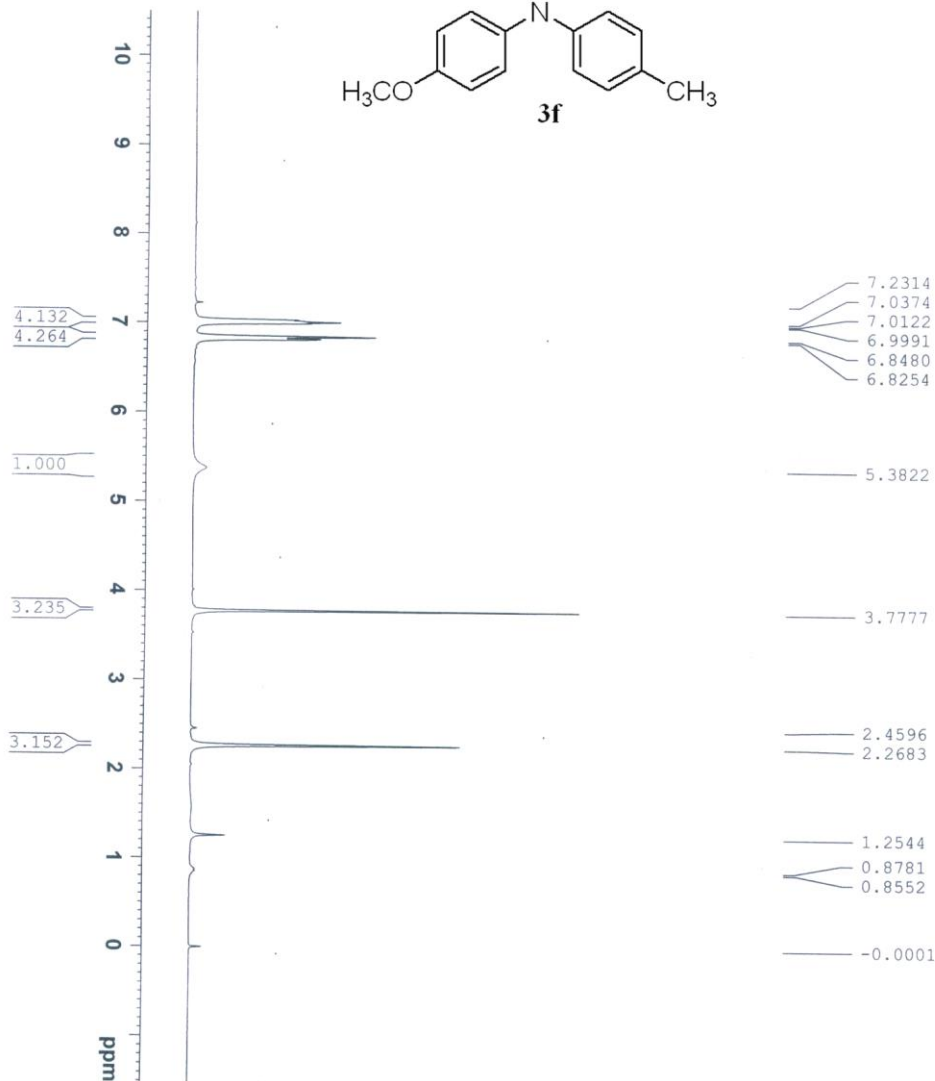
F2 - Processing parameters  
SI 32768  
SF 75.478105 MHz  
WDW EM  
SSB 0  
LB 3.50 Hz  
GB 1.40  
PC 1.40

WHL-18 MS





TX-2-3



Current Data Parameters  
 NAME TX-1H  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20091106  
 Time\_ 11:34  
 INSTRUM 4V300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG 32768  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 0  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 3.2  
 DM 83.400 usec  
 DE 6.400 usec  
 TE 673.2 K  
 D1 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRK 0.01500000 sec

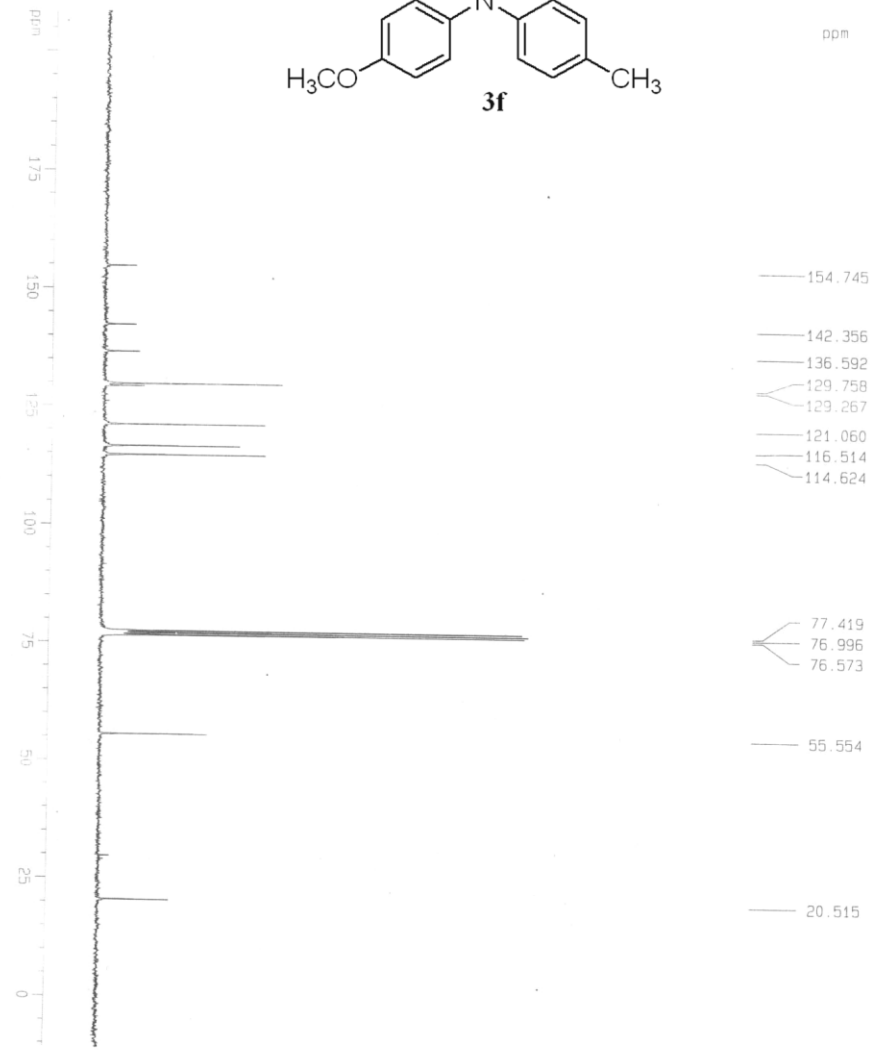
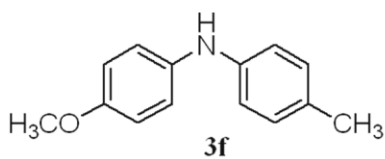
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters

SI 16384  
 SF 300.1700132 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters

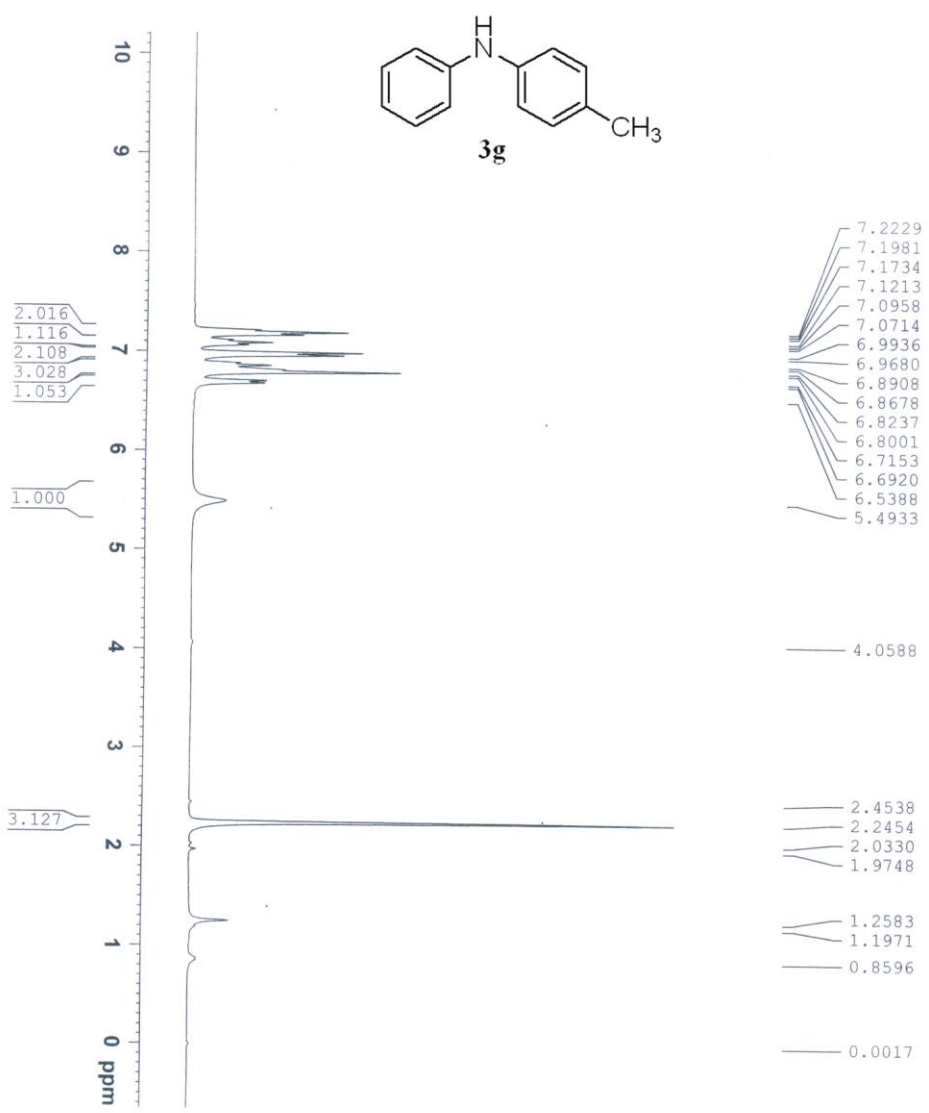
CX 20.00 cm  
 CY 0.00 cm  
 F1P 14.925 ppm  
 F1 4479.94 Hz  
 F2P -5.048 ppm  
 F2 -1515.27 Hz  
 PPMCM 0.99863 ppm/cm  
 HZCM 299.76022 Hz/cm



TX-2-3

```

Current Data Parameters
NAME          LO-12
EXPNO        11
PROCNO       1
-----
F2 - Acquisition Parameters
Date_        20091109
Time         19 24
INSTRUM     av300
PROBHD      5 mm QNP 1H/13
PULPROG     zgpg30
TD           65536
SOLVENT     CDCl3
NS           1443
DS           0
SWH          30120.482 Hz
FIDRES      0.495602 Hz
AQ          1.0979476 sec
RG           6502
AQ           18.800 usec
DE           67.00 usec
TE           300.2 K
D1           3.00000000 sec
d11          0.03000000 sec
MORREST     0.00000000 sec
KORPRK      0.01500000 sec
-----
***** CHANNEL f1 *****
NUC1         13C
P1           12.50 usec
PL1          4.00 dB
SFO1         75.4858643 MHz
-----
***** CHANNEL f2 *****
CHPROG2     waltz16
NUC2         1H
P2           80.00 usec
PL2          2.00 dB
PL12         19.04 dB
SFO2         300.1370493 MHz
-----
F2 - Processing parameters
SI           32768
SF           75.4778123 MHz
WDW          EM
SSB          0
LB           3.50 Hz
GB           0
PC           1.40
-----
10 NMR plot parameters
CX           20.00 cm
CY           0.00 cm
F1P          208.508 DPM
F2P          15737.72 Hz
F2R          -10.947 DPM
F2          10.9524 Hz
NUC1PROB    828.19793 Hz/7%
NUC2PROB    828.19793 Hz/7%
    
```



IG-1-25



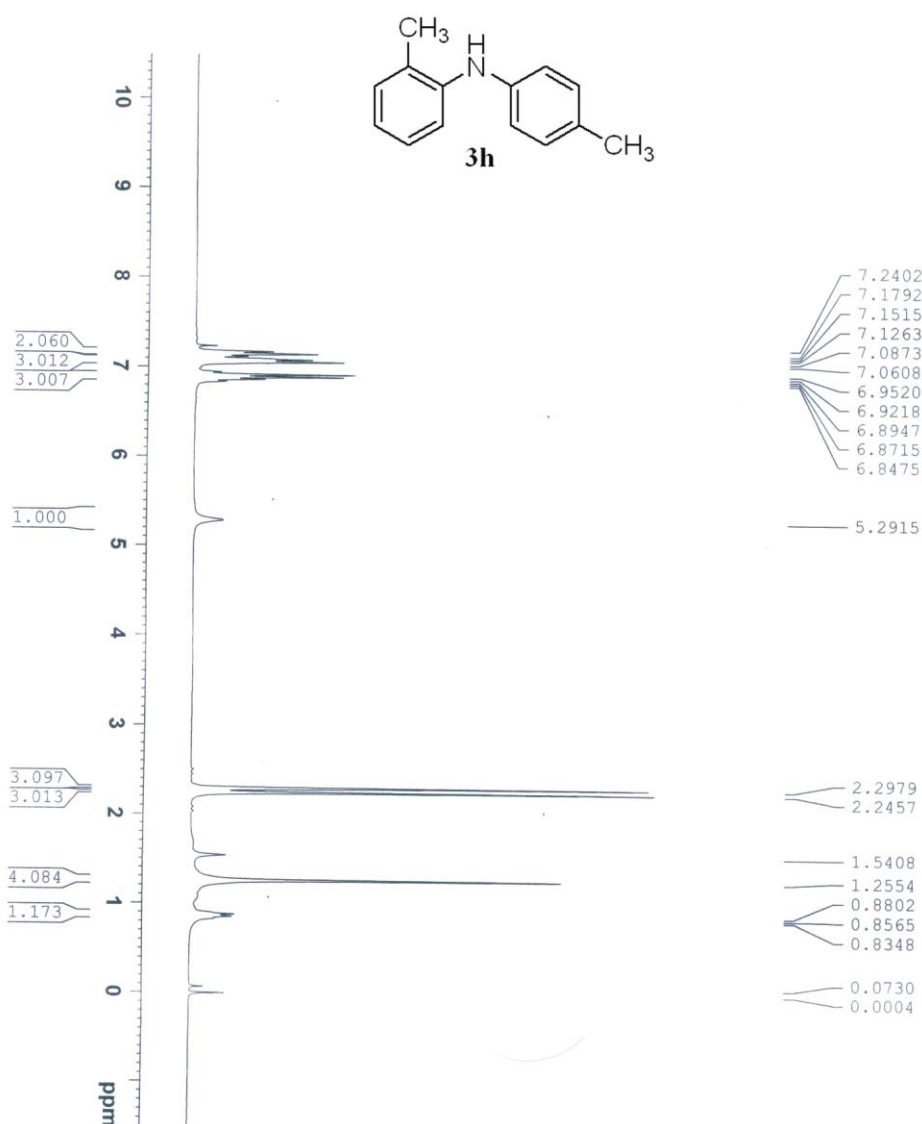
Current Data Parameters  
 NAME IG-1H  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091106  
 Time 11.12  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 0

SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 3.2  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.1700787 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00



LG-1-X



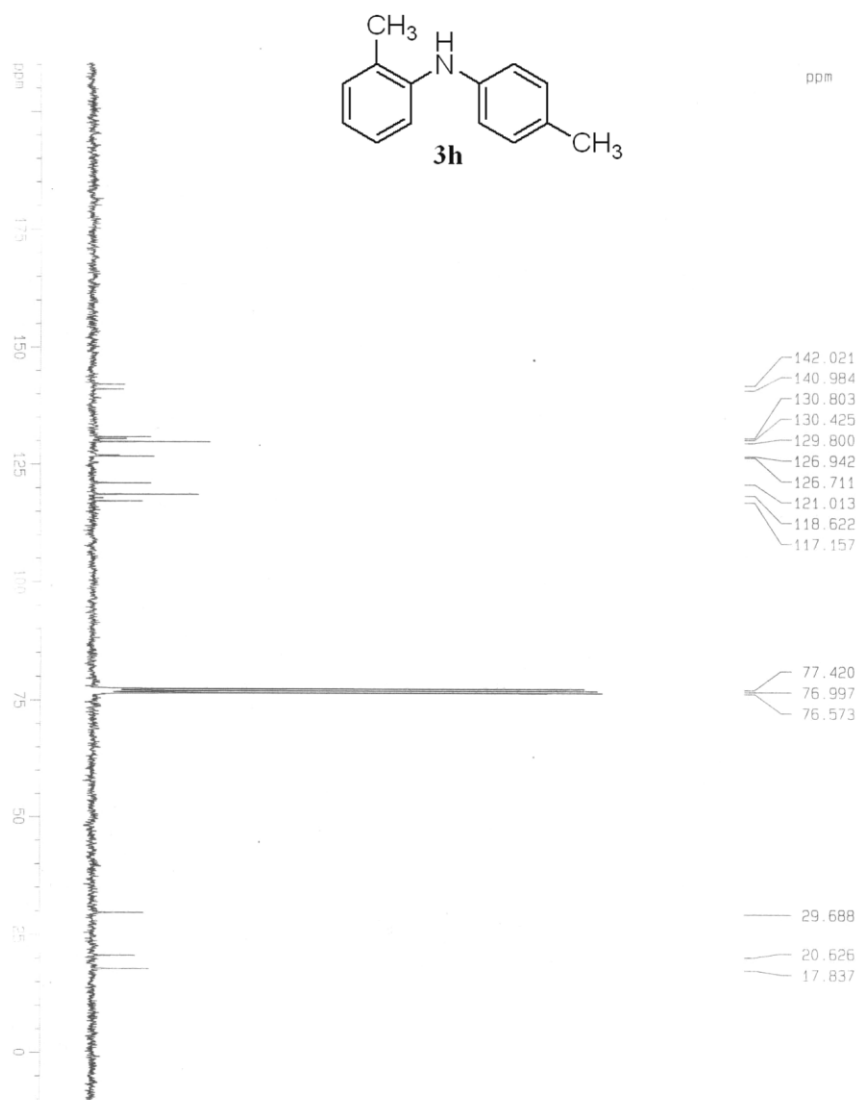
Current Data Parameters  
 NAME LG-1h  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091106  
 Time 11.20  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 0  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 3.2  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCMRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.1700103 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00





LG-1-x

Current Data Parameters  
 NAME LG-13C  
 EXPNO 3  
 PROCNO 1

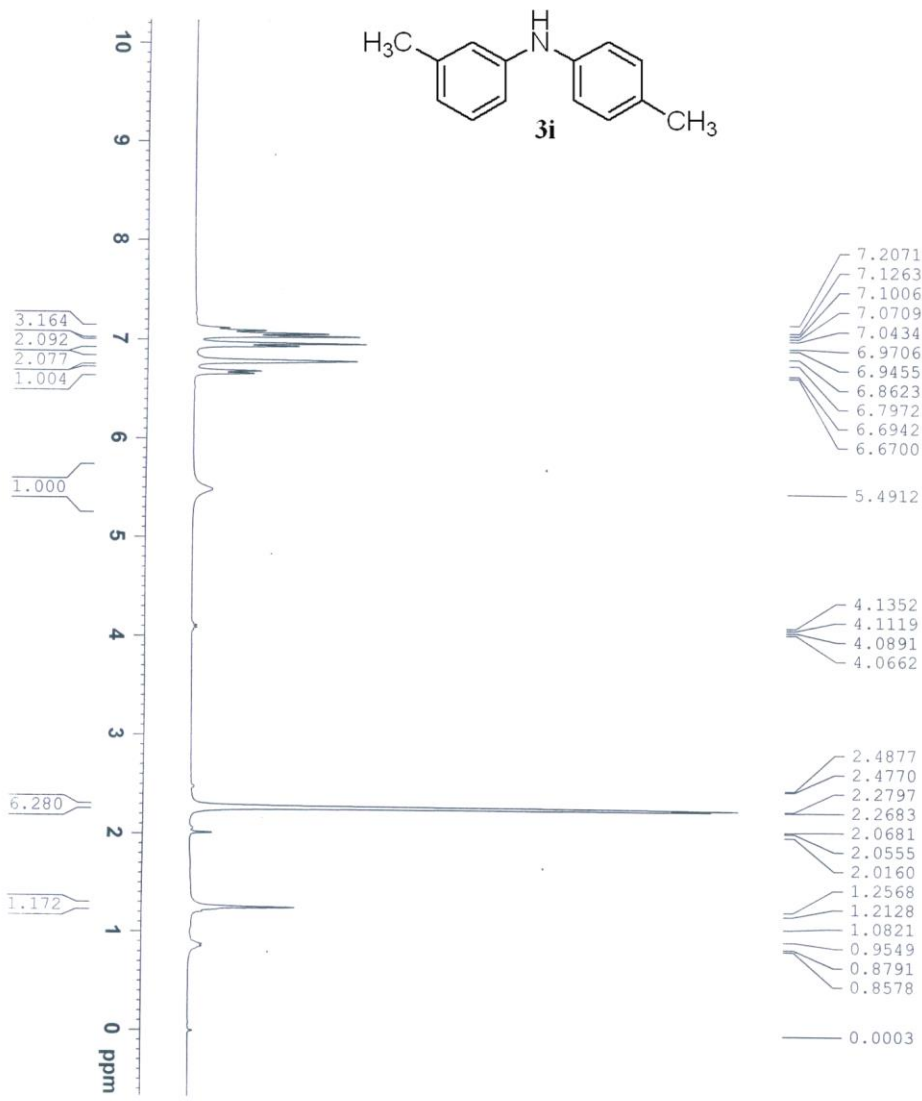
F2 - Acquisition Parameters  
 Date\_ 20091109  
 Time 10.04  
 INSTRUM 4v300  
 PULPROG 5 mm DNP 14v13  
 TD 65536  
 FIDRES 0.2313  
 SOLVENT CDCl3  
 NS 637  
 DS 0  
 SMH 30120.482 Hz  
 FIDRES 0.459602 Hz  
 AQ 1.0873476 sec  
 RG 6502  
 DM 15.600 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 3.00000000 sec  
 d11 0.03000000 sec  
 WDETECT 0.00000000 sec  
 KWARK 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 12.50 usec  
 PL1 0 dB  
 SFO1 75.468643 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 PPRPG2 waltz16  
 NUCE2 1H  
 PPRPG2 80.00 usec  
 PL2 2.00 dB  
 PL12 19.04 dB  
 SFO2 300.1710453 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4778105 MHz  
 MDX EM  
 SSB 0  
 LB 3.50 Hz  
 GB 0  
 PC 1.40

1D NMR Plot parameters:  
 CX 20.00 cm  
 CY 0.00 cm  
 FIP 210.371 DDM  
 FI 15879.35 Hz  
 FAP -10.309 DDM  
 FZ -776.13 Hz  
 PPMCN 11.03403 DDM/CD  
 HZCN 832.82446 Hz/CD

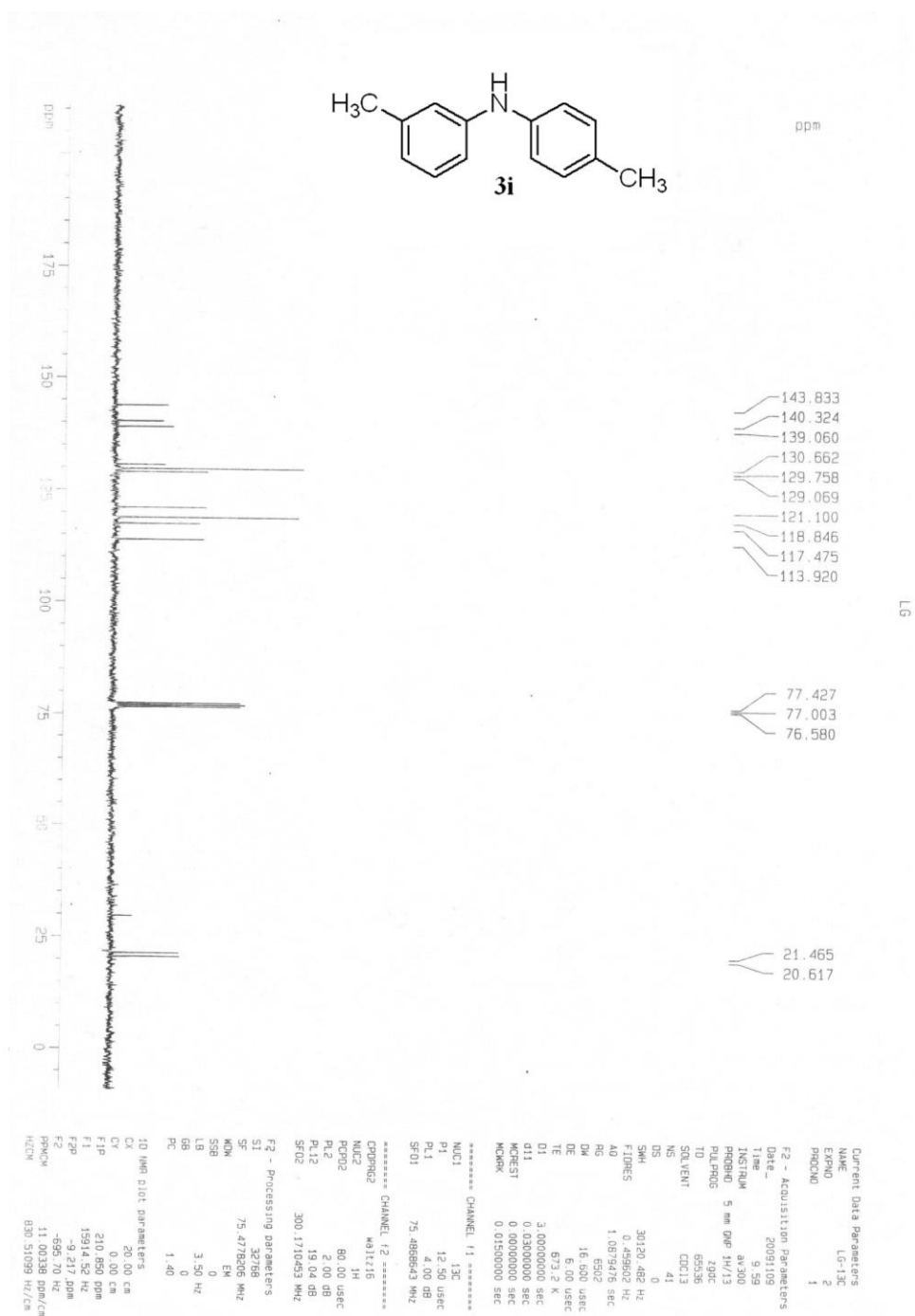


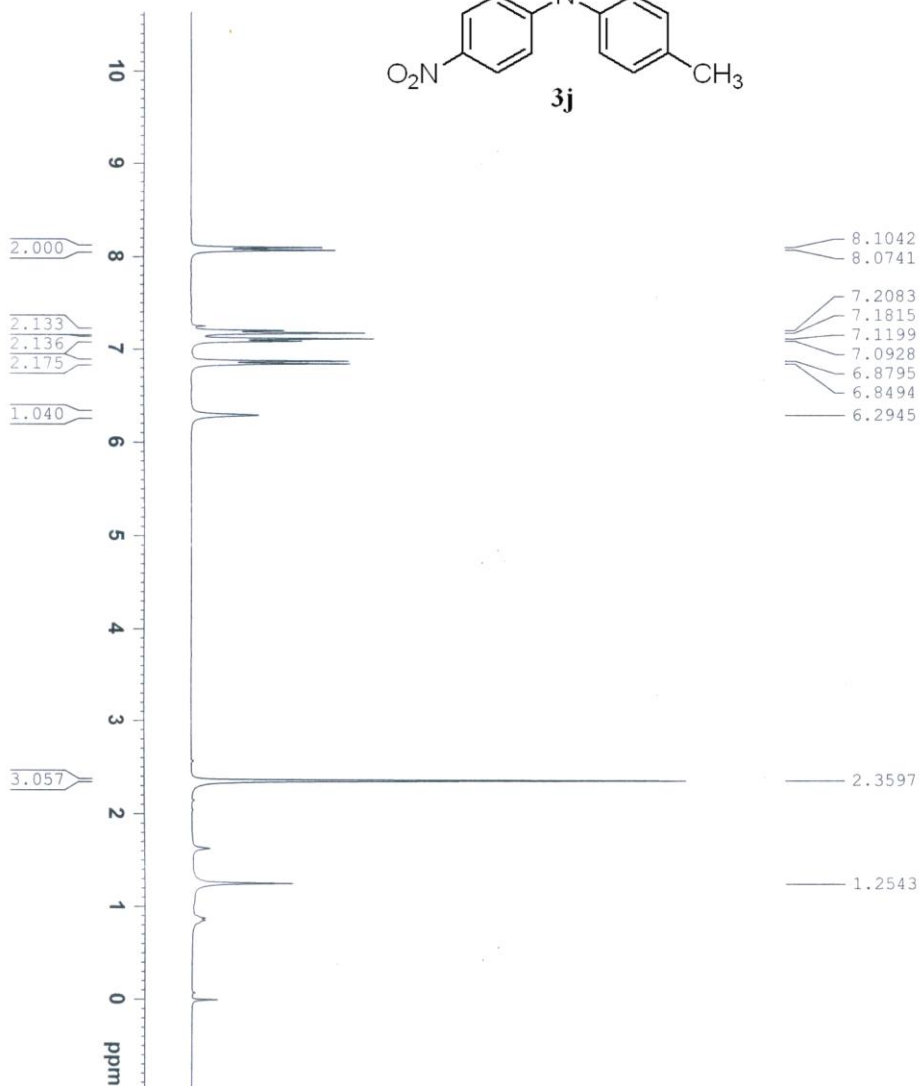
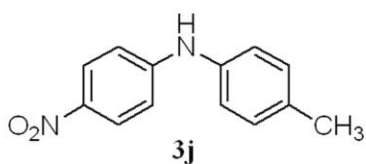
LG



```

Current Data Parameters
NAME          LG-1H
EXPNO         1
PROCNO        1
=====
F2 - Acquisition Parameters
Date_         20091106
Time          10.56
INSTRUM      av300
PROBHD       5 mm QNP 1H/13
PULPROG      zgpg30
TD           32768
SOLVENT      CDCl3
NS           8
DS           0
SWH          5995.204 Hz
FIDRES       0.182959 Hz
AQ           2.7329011 sec
RG           3.2
DW           83.400 usec
DE           6.00 usec
TE           673.2 K
D1           3.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec
=====
CHANNEL F1
NUC1          1H
P1           11.25 usec
PL1          2.00 dB
SFO1         300.1714955 MHz
=====
F2 - Processing parameters
SI           16384
SF           300.1700396 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.00
    
```





WRM-1-7



Current Data Parameters  
 NAME WRM-1H  
 EXPNO 10  
 PROCNO 1

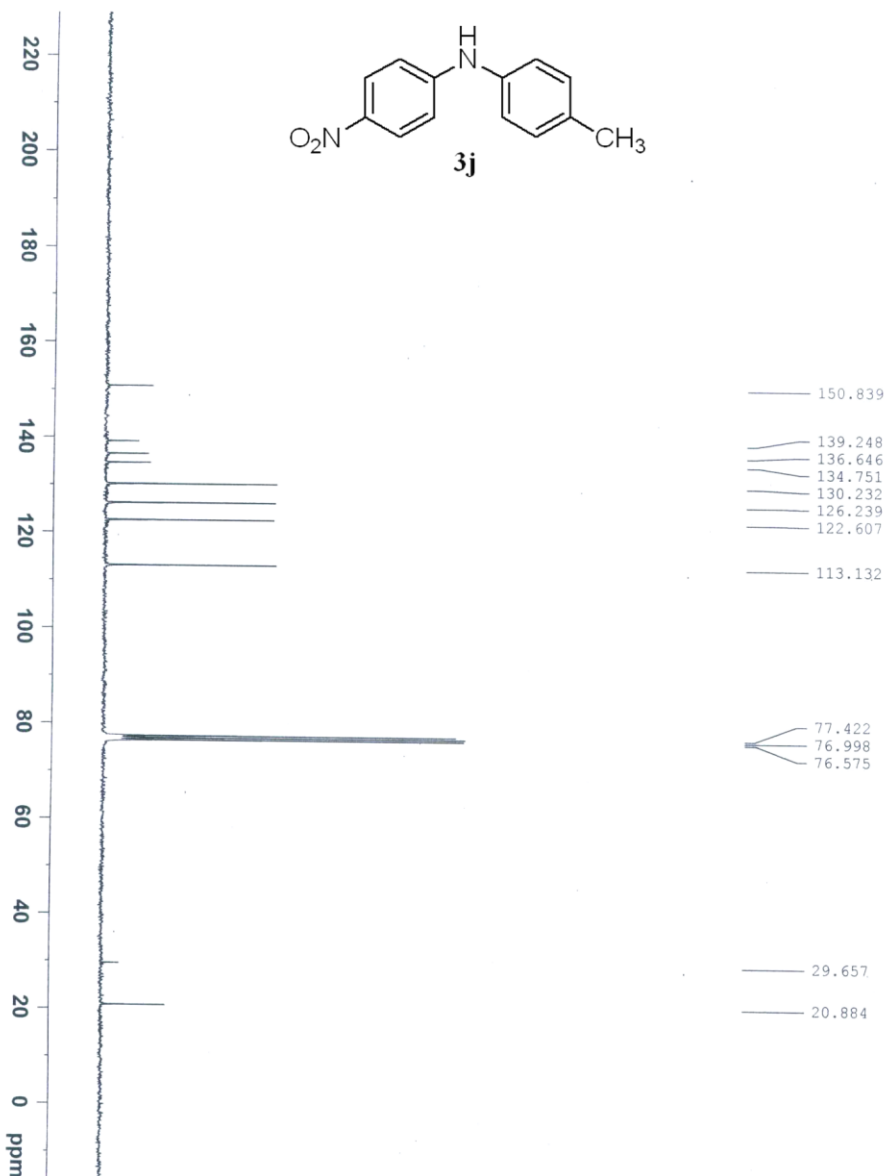
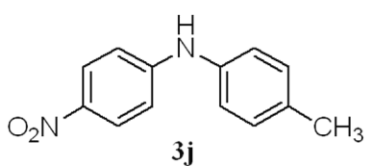
F2 - Acquisition Parameters

Date\_ 20091022  
 Time\_ 17.47  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 2048  
 DS 4  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 64  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 3.00000000 sec  
 WCREST 0.00000000 sec  
 MCWRRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.1700055 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

WRM-1-7



Current Data Parameters  
 NAME WRM-13C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20091026  
 Time 20:53  
 INSTRUM 80 300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 873  
 DS 0  
 SWH 30120.482 Hz  
 FIDRES 0.459602 Hz  
 AQ 1.0879476 sec  
 RG 4096  
 DW 16.600 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 2.50000000 sec  
 d11 0.03000000 sec  
 MCREST 0.00000000 sec  
 MCWRRK 0.01500000 sec

===== CHANNEL f1 =====

NUC1 13C  
 P1 12.50 usec  
 PL1 4.00 dB  
 SFO1 75.4868543 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 2.00 dB  
 PL12 19.04 dB  
 SFO2 300.1170453 MHz

F2 - Processing parameters

SF 327.68 MHz  
 WDWDW 75.4778114 MHz  
 SSB 0  
 LB 3.50 Hz  
 GB 1.40  
 PC 1.40



LG-1-30



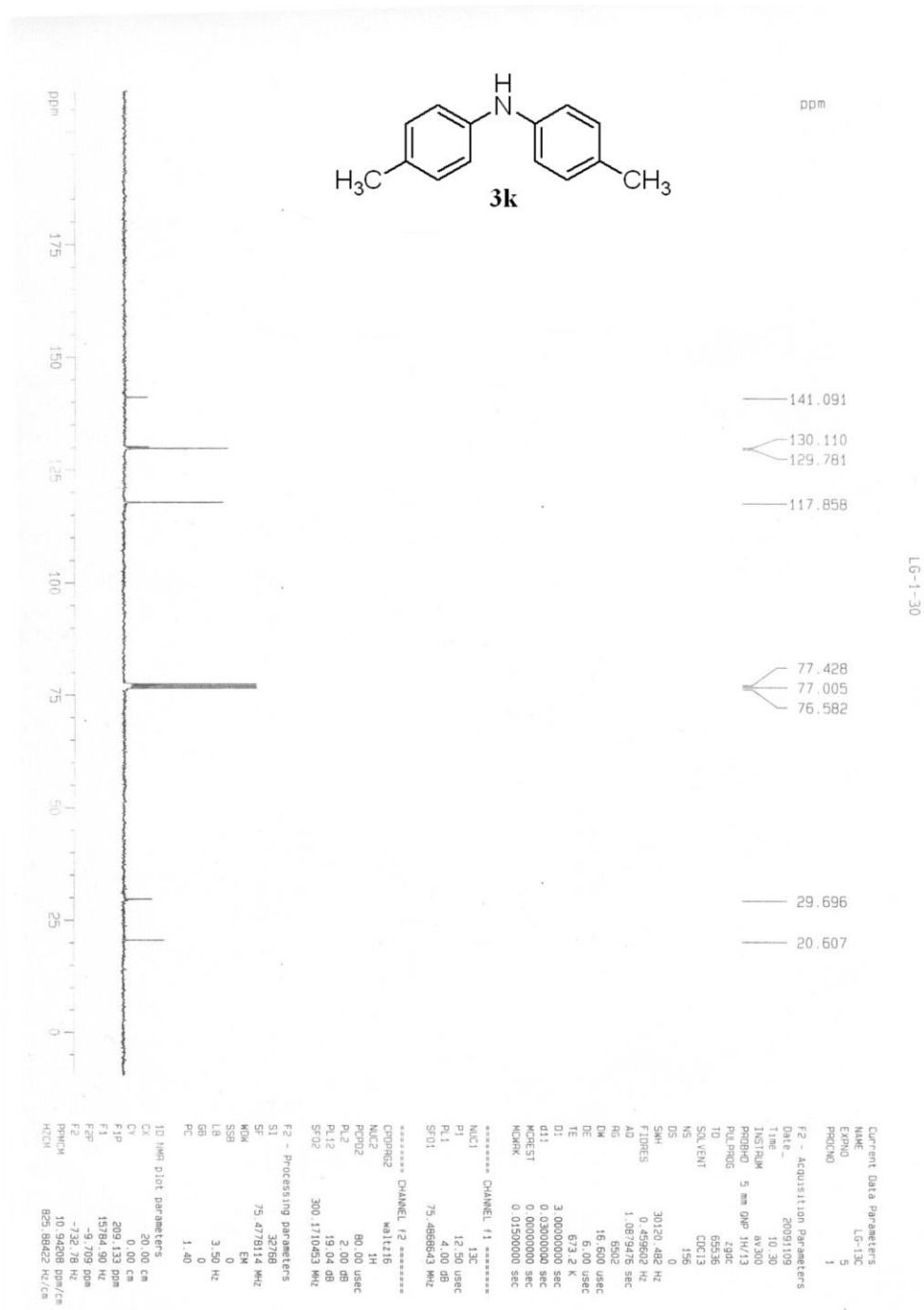
```

Current Data Parameters
NAME      LG-1H
EXPNO    5
PROCNO   1

F2 - Acquisition Parameters
Date_    20091106
Time     11.24
INSTRUM  av300
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        32768
SOLVENT  CDCl3
NS        8
DS        0
SMH       5995.204 Hz
FIDRES    0.182959 Hz
AQ         2.7329011 sec
RG         3.2
DE         83.400 usec
TE         6.00 usec
D1         673.2 K
MCREST    3.00000000 sec
MCMARK    0.01500000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        11.25 usec
PL1       2.00 dB
SFO1      300.1714955 MHz

F2 - Processing parameters
SI         16384
SF         300.1700150 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00
    
```





WRM-1-2



Current Data Parameters  
 NAME WRM-1H  
 EXNO 9  
 PROCNO 1

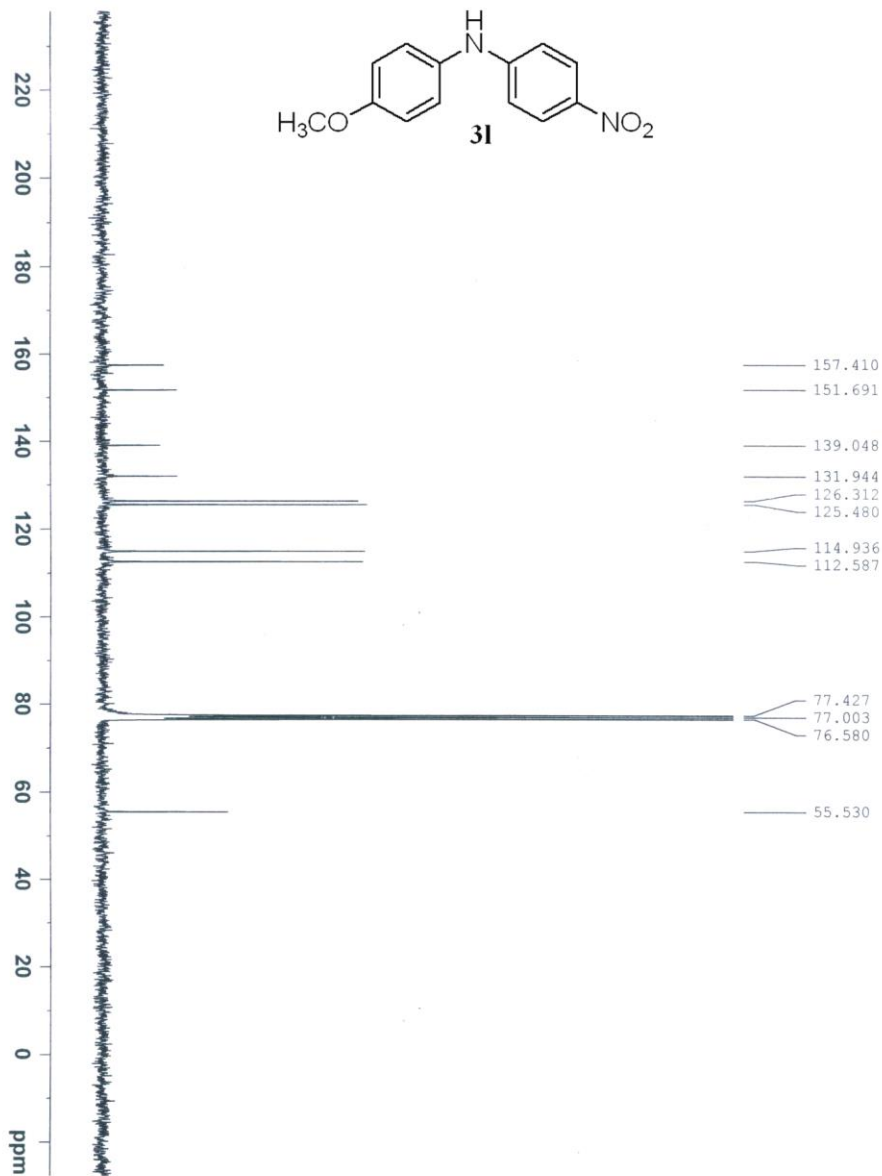
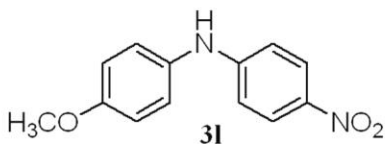
F2 - Acquisition Parameters  
 Date\_ 20091022  
 Time\_ 17.42  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 24  
 DS 0  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 64  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.1700037 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00



WRM-1-2



- 157.410
- 151.691
- 139.048
- 131.944
- 126.312
- 125.480
- 114.936
- 112.587
- 77.427
- 77.003
- 76.580
- 55.530



Current Data Parameters  
 NAME WRM-1-3C  
 EXPNO 4  
 PROCNO 1

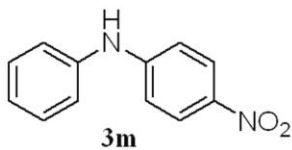
F2 - Acquisition Parameters

Date\_ 20091025  
 Time 15:44  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgdc  
 TD 65536  
 SOLVENT CDCl3  
 NS 1006  
 DS 0  
 SWH 30120.482 Hz  
 FIDRES 0.459602 Hz  
 AQ 1.0579476 sec  
 RG 11385.2  
 DW 16.600 usec  
 DE 2.00 usec  
 TE 300.2 K  
 D1 2.5000000 sec  
 d11 0.03000000 sec  
 MCWV 0.01500000 sec  
 MCWVR 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 12.50 usec  
 PL1 4.00 dB  
 SFO1 75.4886643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waliz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 2.00 dB  
 PL12 19.04 dB  
 SFO2 300.1710453 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4778096 MHz  
 WDW EM  
 SSB 0  
 LB 3.50 Hz  
 GB 0  
 PC 140



WRM-1-19



Current Data Parameters  
 NAME WRM-1H  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091022  
 Time 17.03

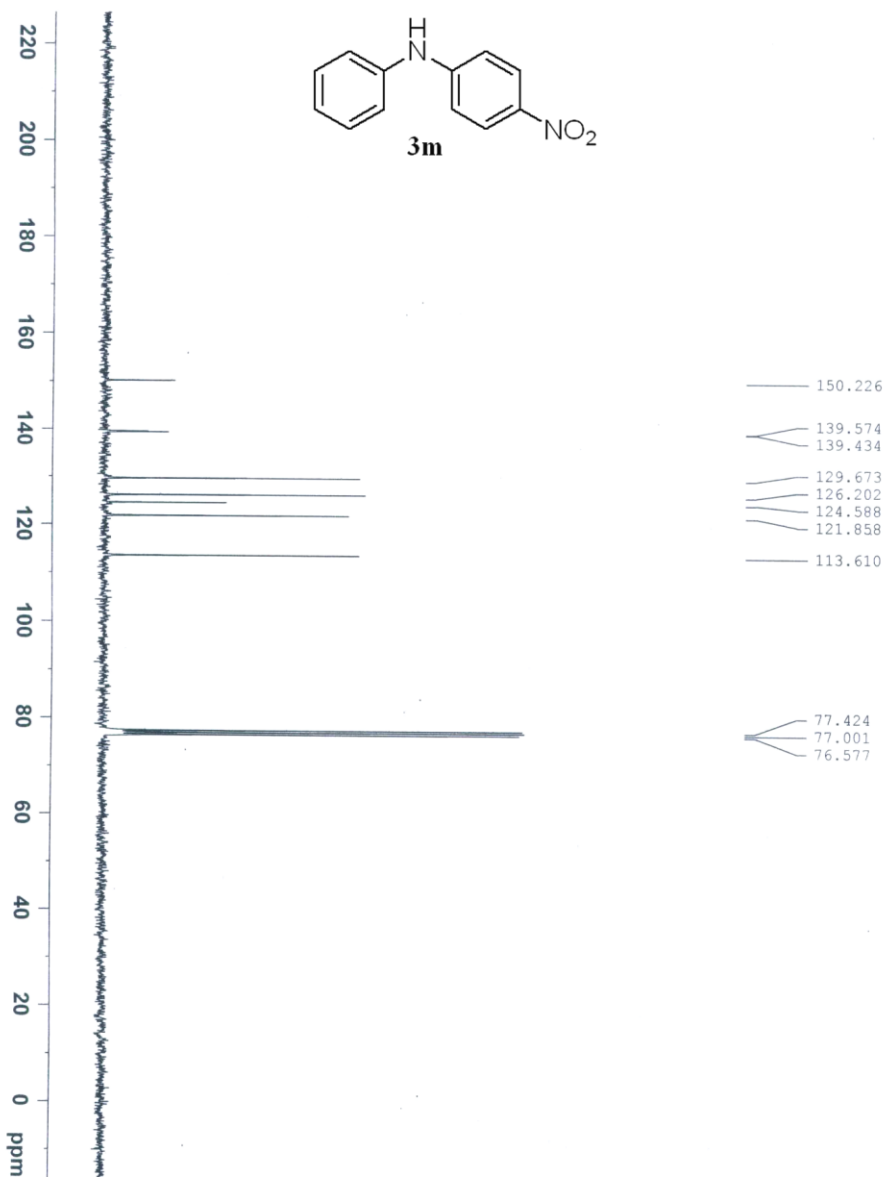
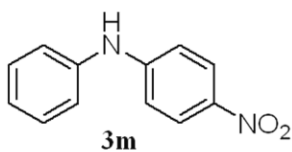
INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 ID zgpg30  
 SOLVENT CDCl3  
 NS 24  
 DS 0

SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 64  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 DI 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.170052 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

WRM-1-19



150.226
139.574
139.434
129.673
126.202
124.588
121.858
113.610
77.424
77.001
76.577



Current Data Parameters  
 NAME WRM-13C  
 EXPNO 8  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20091026  
 Time 19.07  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 234  
 DS 0  
 SWH 30120.482 Hz  
 FIDRES 0.459602 Hz  
 AQ 1.0879476 sec  
 RG 4096  
 DW 16.600 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 2.50000000 sec  
 d11 0.03000000 sec  
 MCREST 0.00000000 sec  
 MCWRRK 0.01500000 sec

===== CHANNEL f1 =====

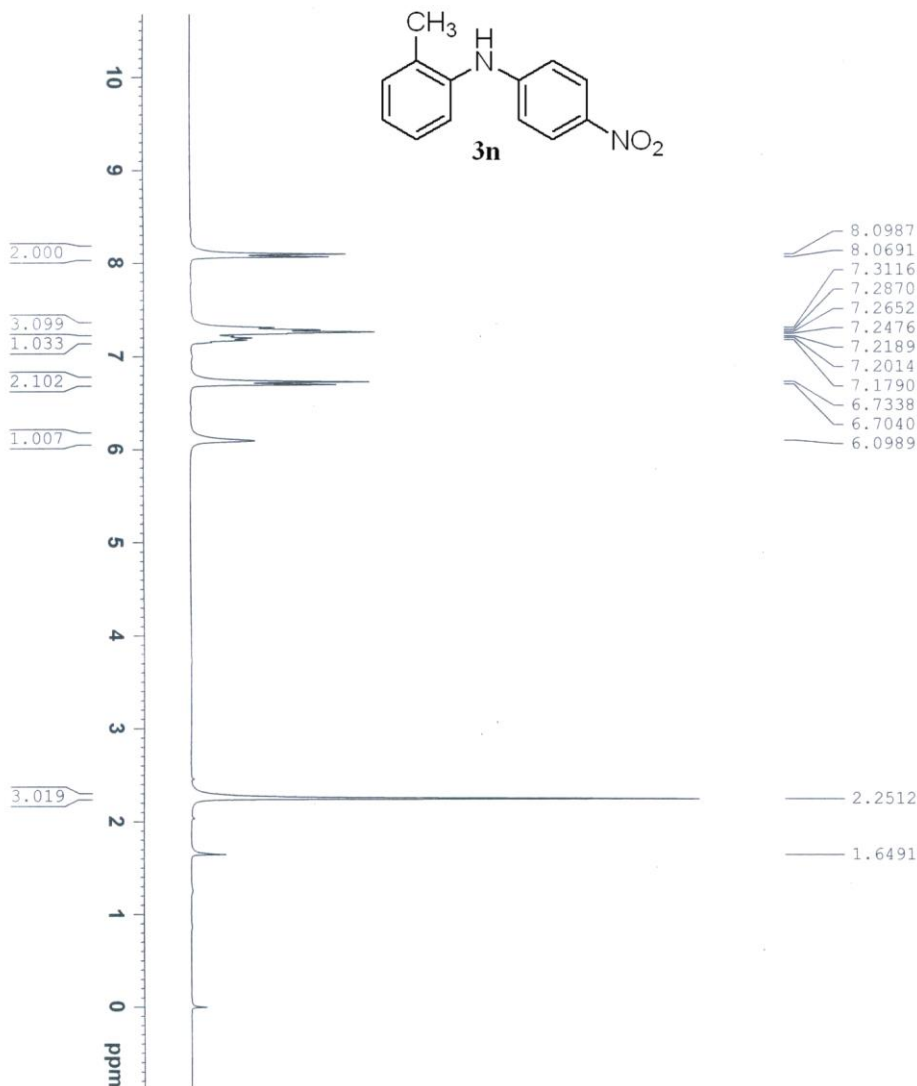
NUC1 <sup>13</sup>C  
 P1 12.50 usec  
 PL1 4.00 dB  
 SFO1 75.4858643 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 80.00 usec  
 PL2 2.00 dB  
 PL12 19.04 dB  
 SFO2 300.1710453 MHz

F2 - Processing parameters

SE 32.768  
 WINDW EM  
 SSB 0  
 GB 3.50 Hz  
 LB 0  
 PC 1.40



WRM-1-20



Current Data Parameters  
 NAME WRM-1H  
 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091022  
 Time\_ 17.22

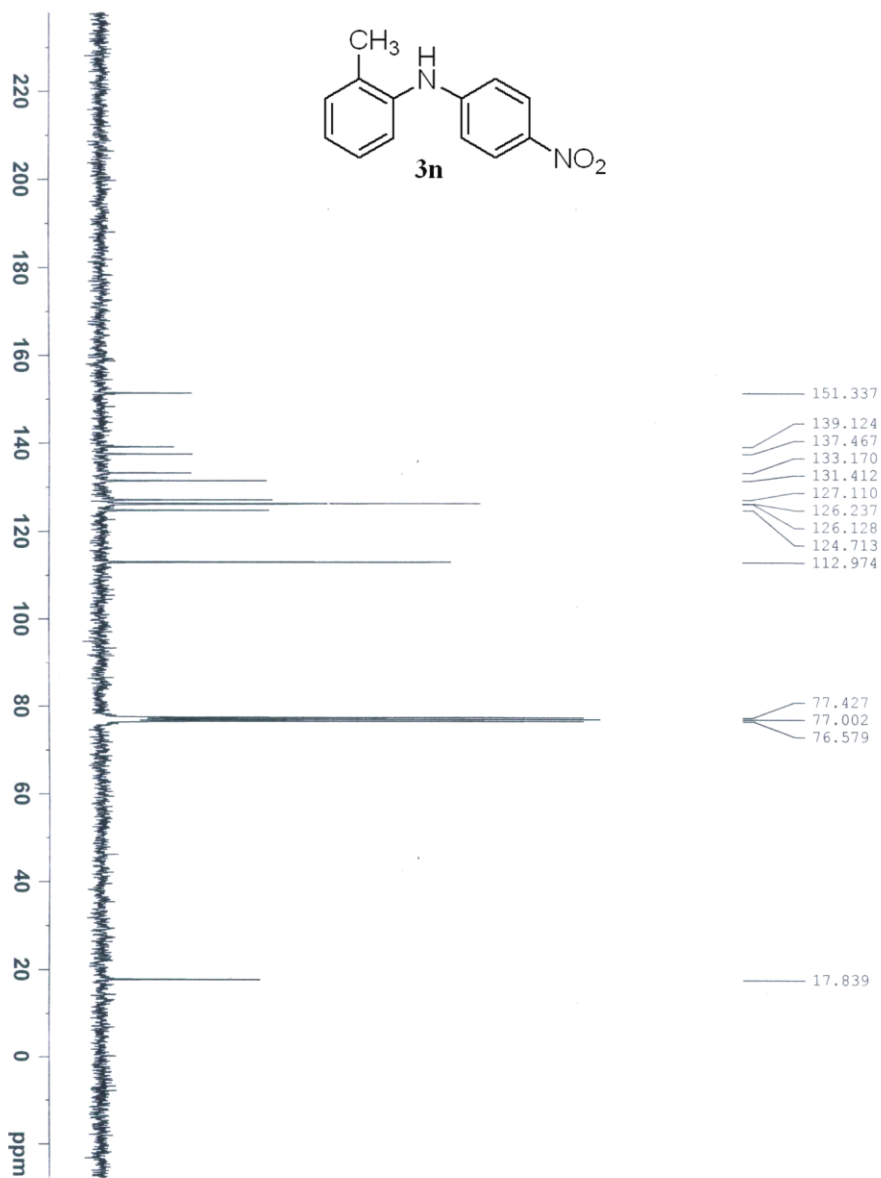
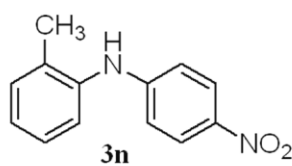
INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 24

DS 0  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 64  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 DI 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.170052 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

WRM-1-20



151.337  
139.124  
137.467  
133.170  
131.412  
127.110  
126.237  
126.128  
124.713  
112.974

77.427  
77.002  
76.579

17.839



Current Data Parameters  
NAME WRM-13C  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters

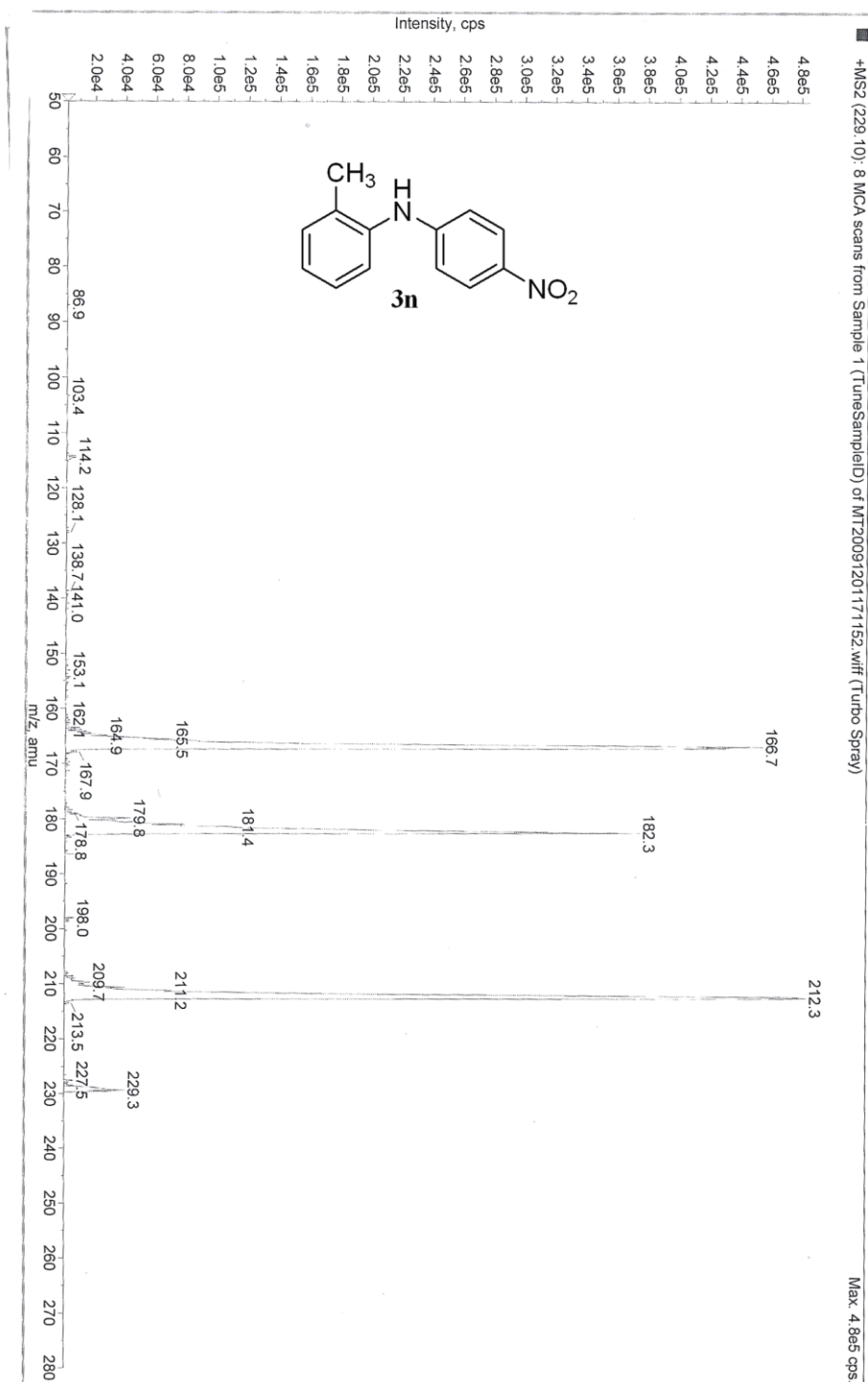
Date\_ 20091025  
Time 9:14  
INSTRUM av300  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg  
TD 65536  
SOLVENT CDCl3  
NS 208  
DS 0  
SWH 30120.482 Hz  
FIDRES 0.459602 Hz  
AQ 1.0879476 sec  
RG 11585.2  
DW 16.600 usec  
DE 6.00 usec  
TE 67.32 K  
D1 2.5000000 sec  
d11 0.0300000 sec  
MCREST 0.0100000 sec  
MCWPRK 0.01500000 sec

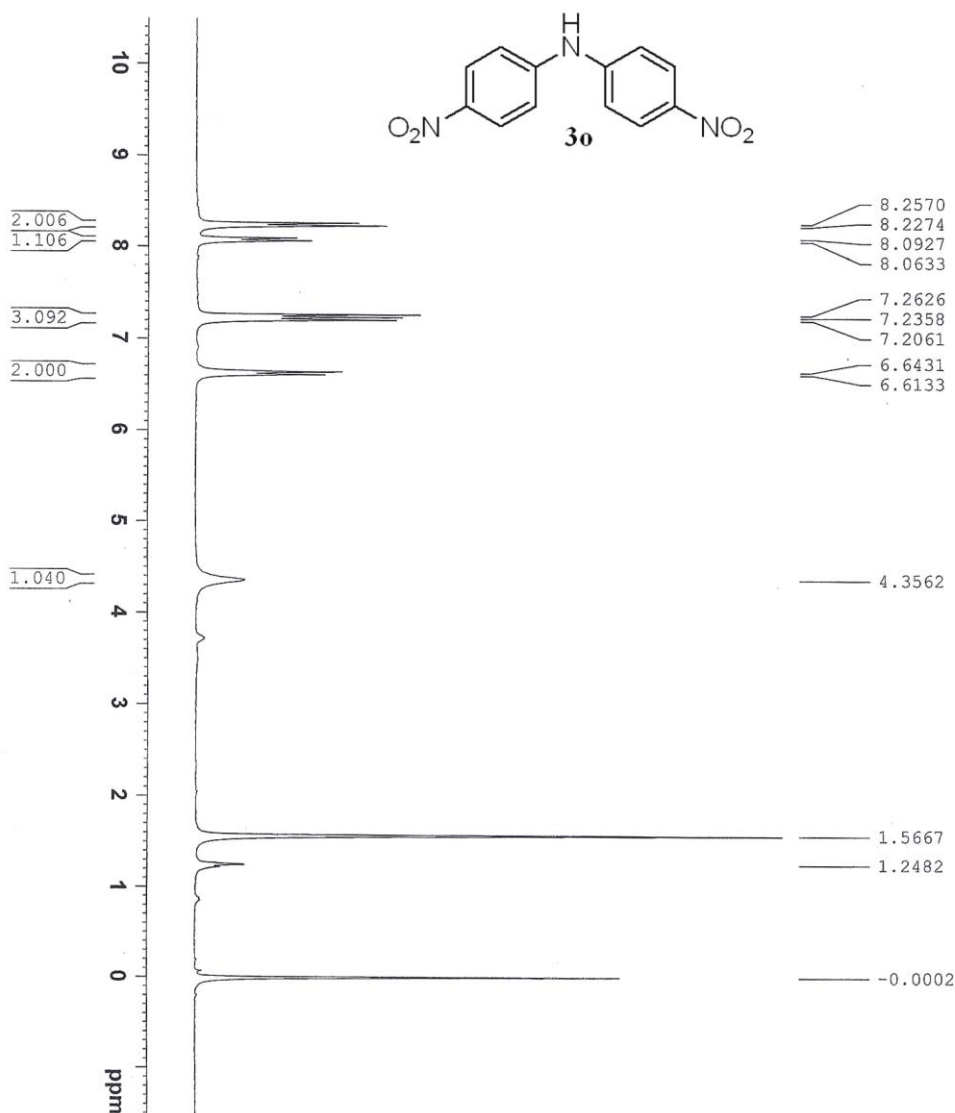
==== CHANNEL f1 =====  
NUC1 13C  
P1 12.50 usec  
PL1 4.00 dB  
SFO1 75.486643 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 19.04 dB  
SFO2 300.1710453 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4778133 MHz  
WDW EM  
SSB 0  
LB 3.50 Hz  
GB 0  
PC 1.40

WJRM-1-20 M22





WRM-1-14



Current Data Parameters  
 NAME WRM-1H  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091022  
 Time\_ 16:44

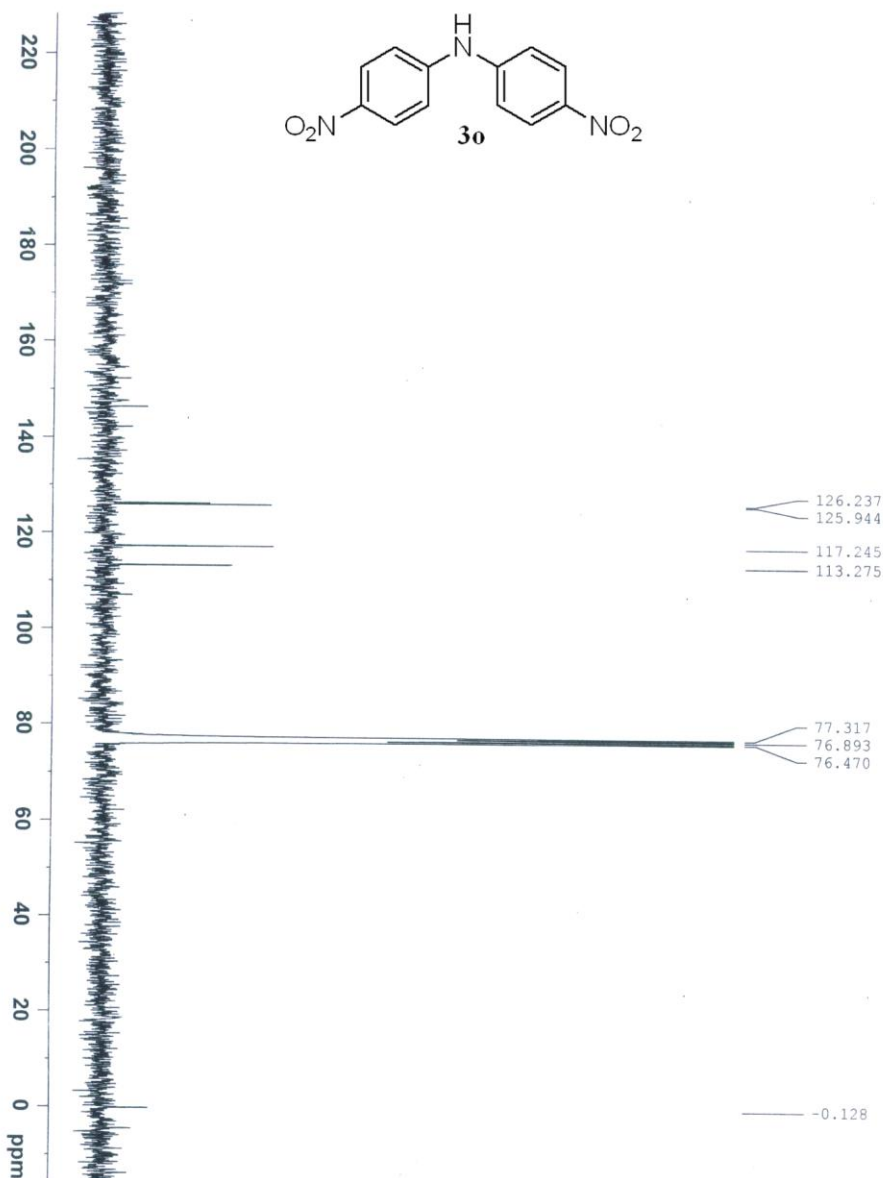
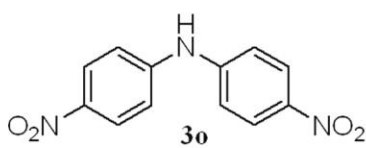
INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 24  
 DS 0

SWH 5895.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 64  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.1700041 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

WRM-1-14



Current Data Parameters  
 NAME WRM-13C  
 EXPNO 11  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 2008-10-27  
 Time 2:08  
 INSTRUM av300  
 PROBD 5 mm QNP 1H/13  
 PULPROG zgpg  
 TD 65536  
 SOLVENT CDCl3  
 NS 4096  
 DS 0  
 SWH 30120.482 Hz  
 FIDRES 0.093902 Hz  
 AQ 1.08749 sec  
 RG 4096  
 DW 16.600 usec  
 DE 6.00 usec  
 TE 63.32 K  
 D1 2.500000 usec  
 d11 0.03000000 sec  
 MCREST 0.00000000 sec  
 MCMRK 0.01500000 sec

===== CHANNEL f1 =====

NUC1 13C  
 P1 12.50 usec  
 PL1 4.00 dB  
 SFO1 75.4866643 MHz

===== CHANNEL f2 =====

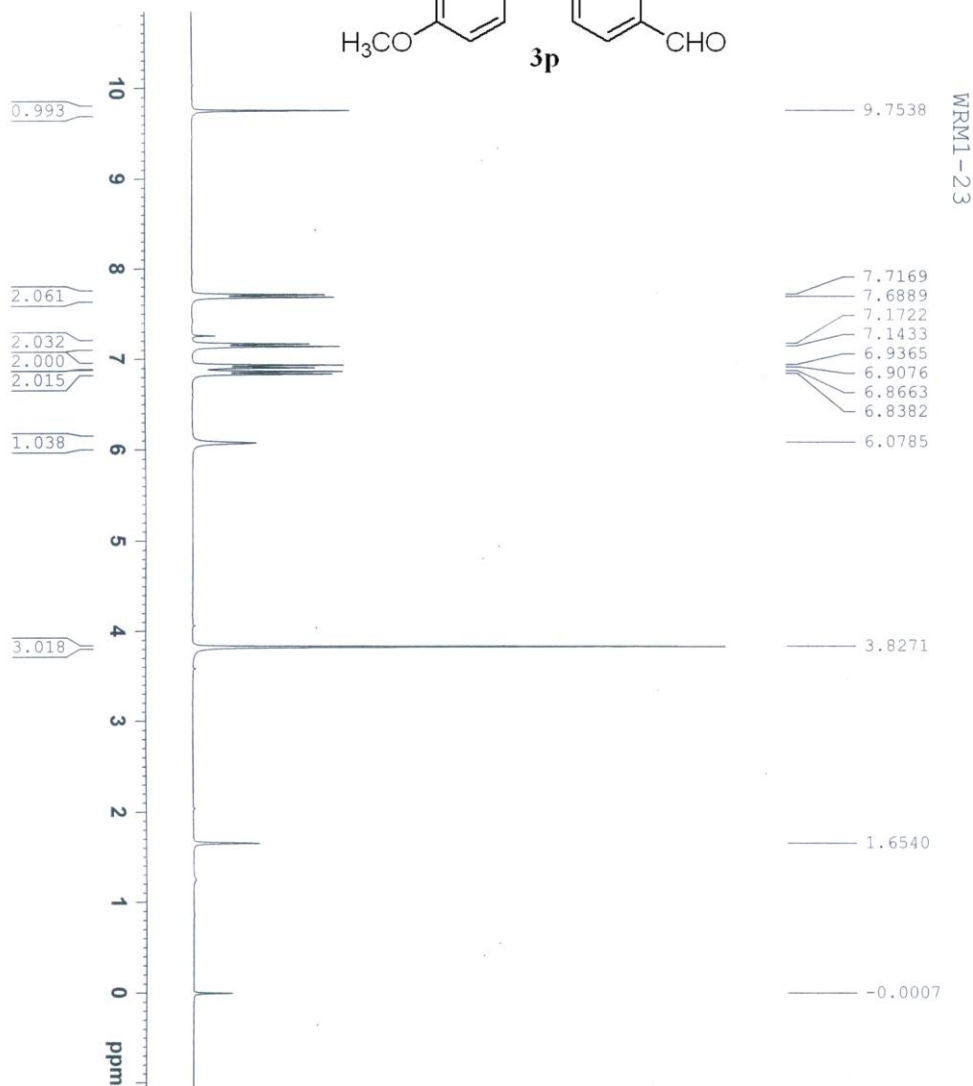
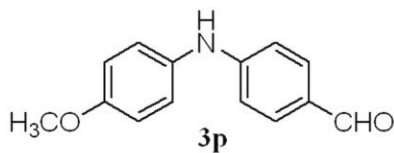
CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 2.00 dB  
 P2 19.04 dB  
 SFO2 300.1710453 MHz

F2 - Processing parameters

SI 32768  
 SF 75.4778151 MHz  
 VSWR 0  
 SSB EM  
 LB 350 Hz  
 GB 0  
 PC 1.40

1D NMR pdt parameters  
 CX 20.00 cm  
 CY 0.00 cm  
 F1P 319.473 ppm  
 F2P 2413.15 Hz  
 F2 600734 Hz  
 PPMCM 19.95920 ppm/cm  
 HZCM 1506.02417 Hz/cm





WRM1-23



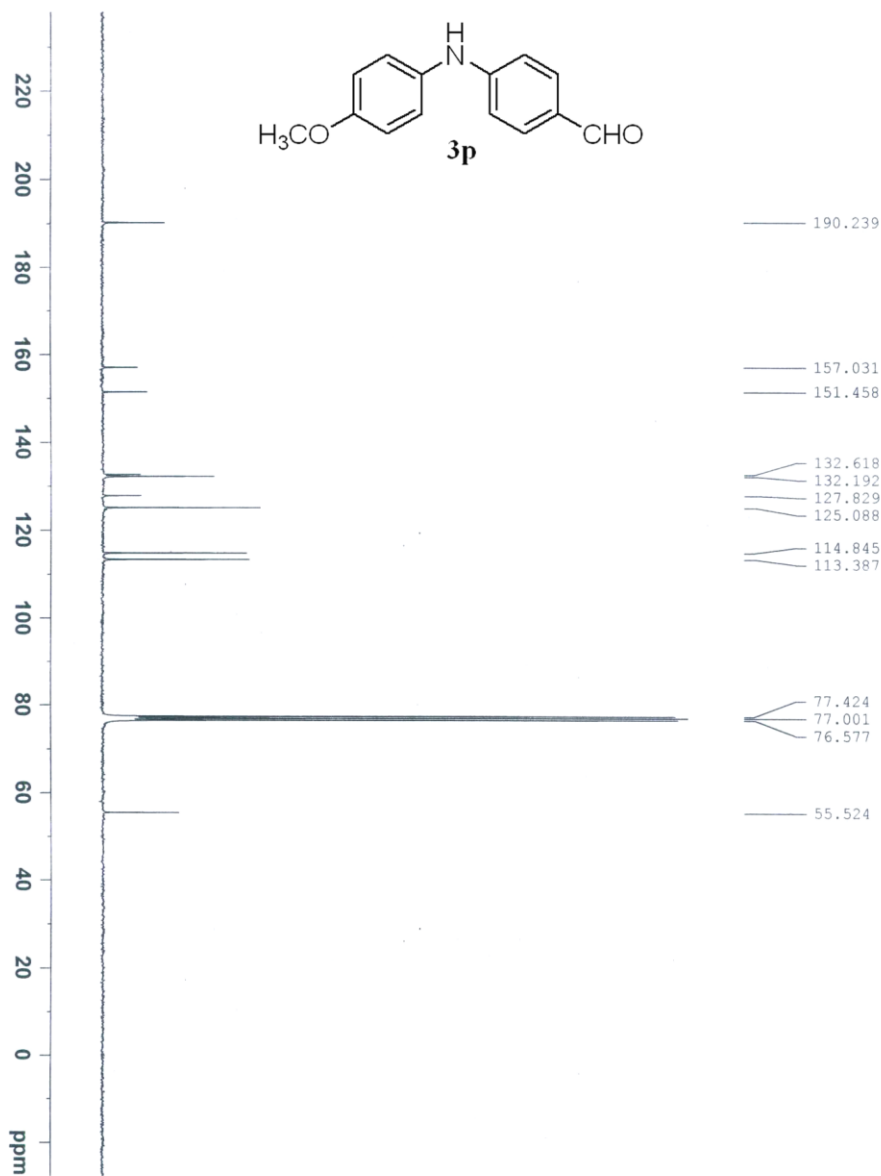
Current Data Parameters  
 NAME WRM-1H  
 EXNO 3  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20091022  
 Time\_ 17.10  
 INSTRUM av300  
 PROBD 5 mm QNP 1H/13  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 24  
 DS 0  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 64  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 DI 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.1700041 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00



WRM-1-23



Current Data Parameters  
 NAME WRM-13C  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091025  
 Time 9:25

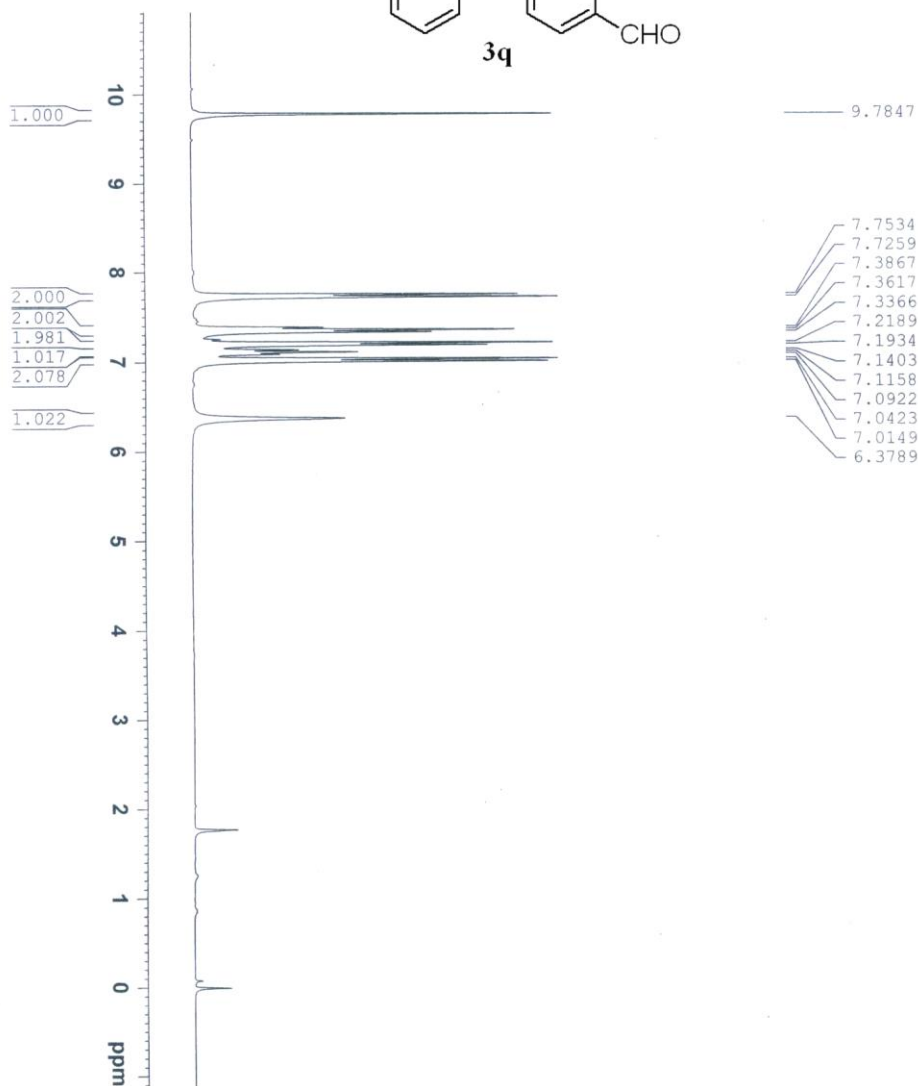
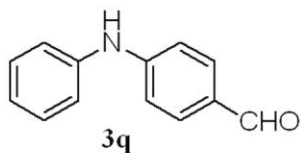
INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgdc  
 TD 65536  
 SOLVENT CDCl3  
 NS 5268  
 DS 0

SWH 30120.482 Hz  
 FIDRES 0.459602 Hz  
 AQ 1.0879476 sec  
 RG 11586.2  
 DW 6.600 usec  
 DE 6.90 usec  
 TE 600.130000 sec  
 D1 2.50000000 sec  
 d11 0.03000000 sec  
 MCREST 0.00000000 sec  
 MCWVRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 12.50 usec  
 PL1 4.00 dB  
 SFO1 75.4866643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 2.00 dB  
 PL12 19.04 dB  
 SFO2 300.1710453 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4778087 MHz  
 WDW EM  
 SSB 0  
 LB 3.50 Hz  
 GB 0  
 PC 1.40



MRM-1-22

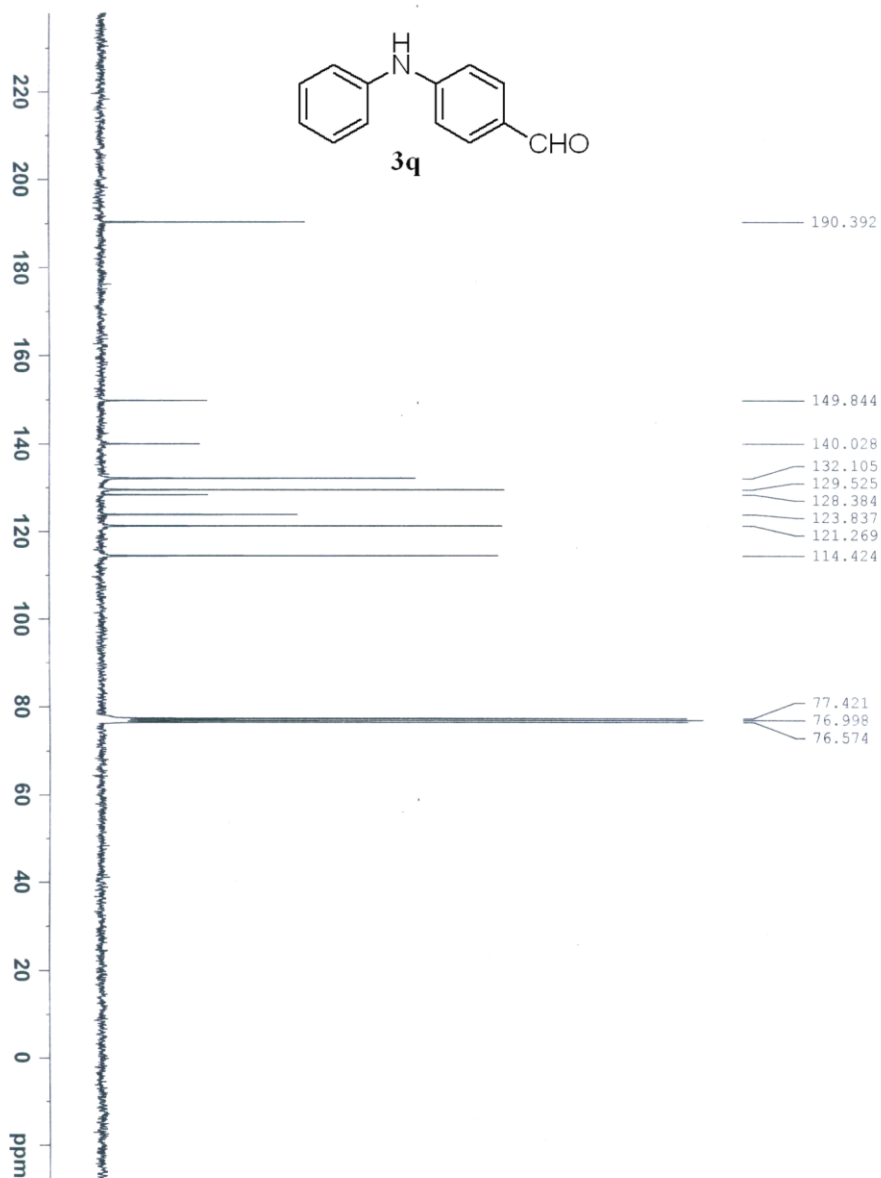


Current Data Parameters  
 NAME MRM-1H  
 EXPNO 6  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091022  
 Time\_ 17.28  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 24  
 DS 0  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 64  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 DI 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.1700059 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME WRM-13C  
 EXPNO 1  
 PROCNO 1

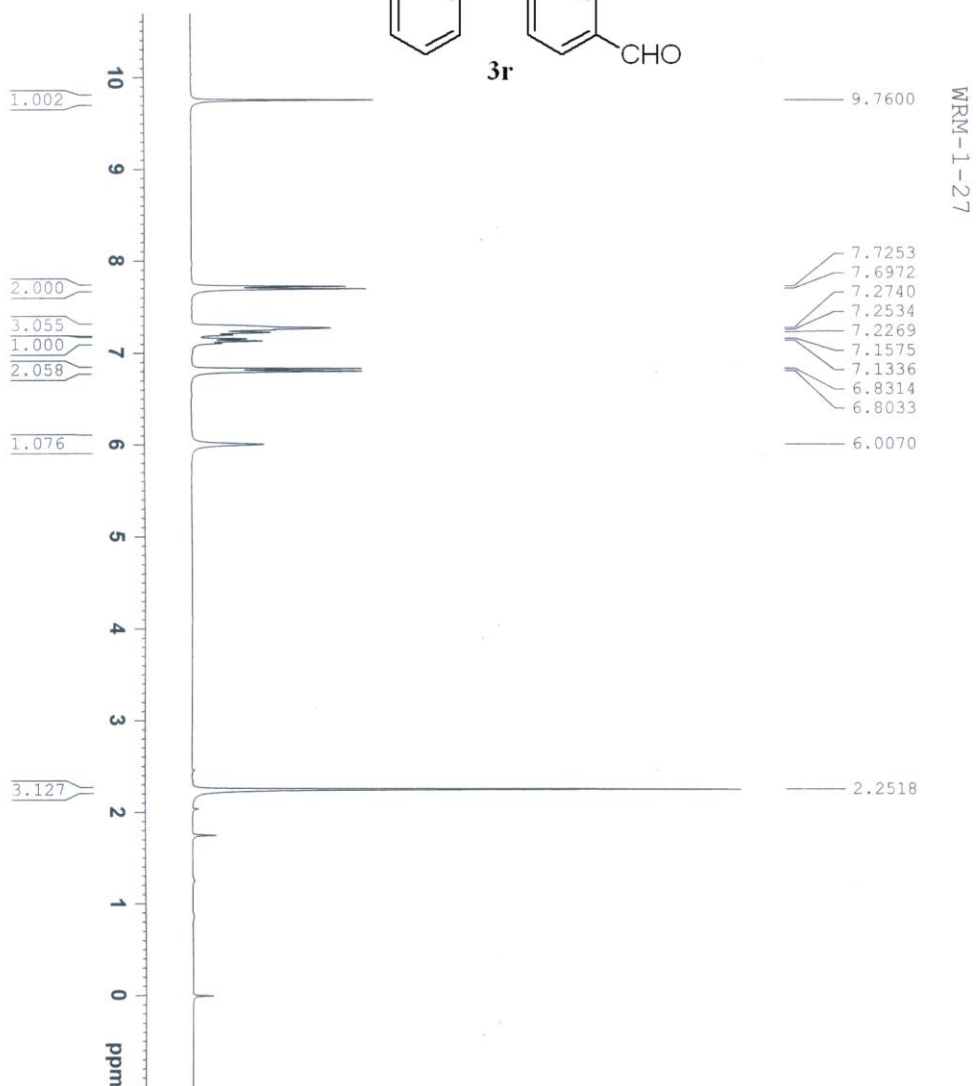
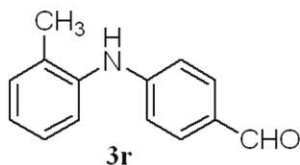
F2 - Acquisition Parameters

Date\_ 20091025  
 Time 8.37  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgdc  
 TD 65536  
 SOLVENT CDCl3  
 NS 506  
 DS 0  
 SWH 30120.482 Hz  
 FIDRES 0.459602 Hz  
 AQ 1.0879476 sec  
 RG 11585.2  
 DW 16.600 usec  
 DE 6.90 usec  
 TE 673.2 K  
 TD 2.5903200 sec  
 d11 0.0300000 sec  
 MCREST 0.0000000 sec  
 MCWPRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 12.50 usec  
 PL1 4.00 dB  
 SFO1 75.4866443 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 2.00 dB  
 PL12 19.04 dB  
 SFO2 300.1710453 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4778133 MHz  
 WDW EM  
 SSB 0  
 LB 3.50 Hz  
 GB 0  
 PC 1.40



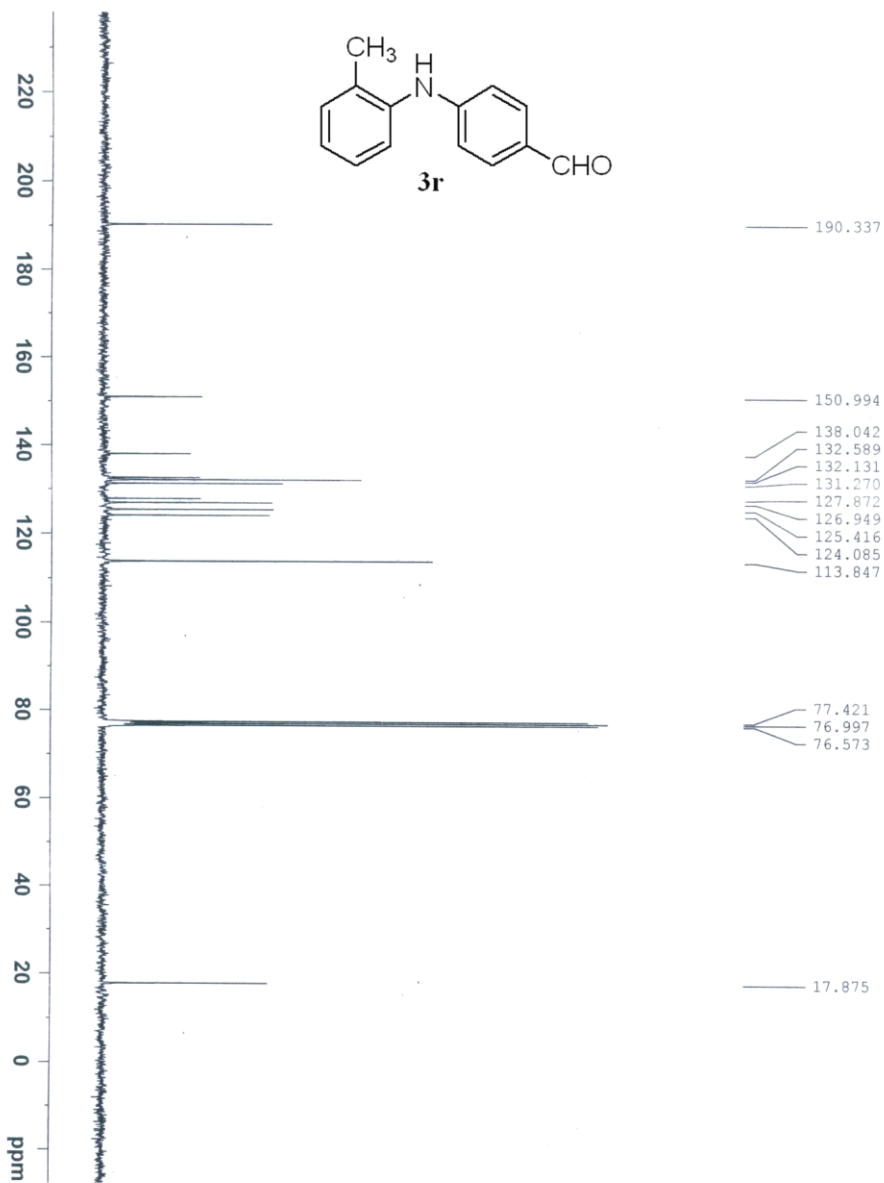
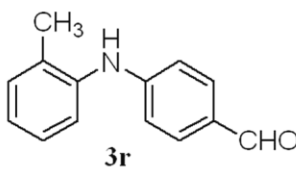
Current Data Parameters  
 NAME WRM-1H  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091022  
 Time 17.16  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 24  
 DS 0  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 64  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 DI 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.1700056 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

WRM-1-27



Current Data Parameters  
 NAME WRM-13C  
 EXPNO 7  
 PROCNO 1



F2 - Acquisition Parameters

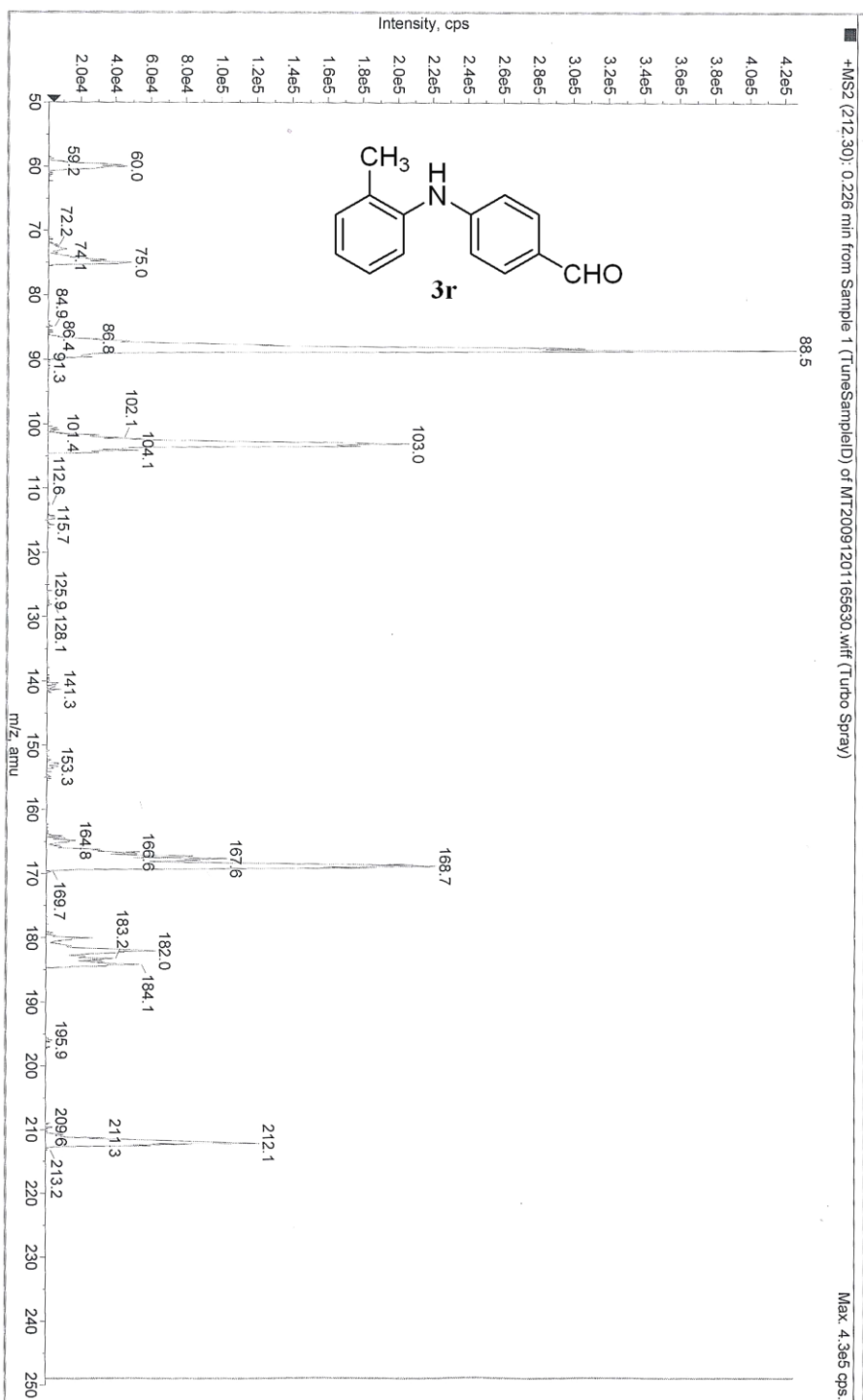
Date 20091026  
 Time 16:30  
 INSTRUM av300  
 PROBHD 5 mm QNP-1H/13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 396  
 DS 0  
 SWH 30120.482 Hz  
 FIDRES 0.459602 Hz  
 AQ 1.0879476 sec  
 RG 4096  
 DW 16.600 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 2.50000000 sec  
 d11 0.03000000 sec  
 MCREST 0.00000000 sec  
 MCWRRK 0.01500000 sec

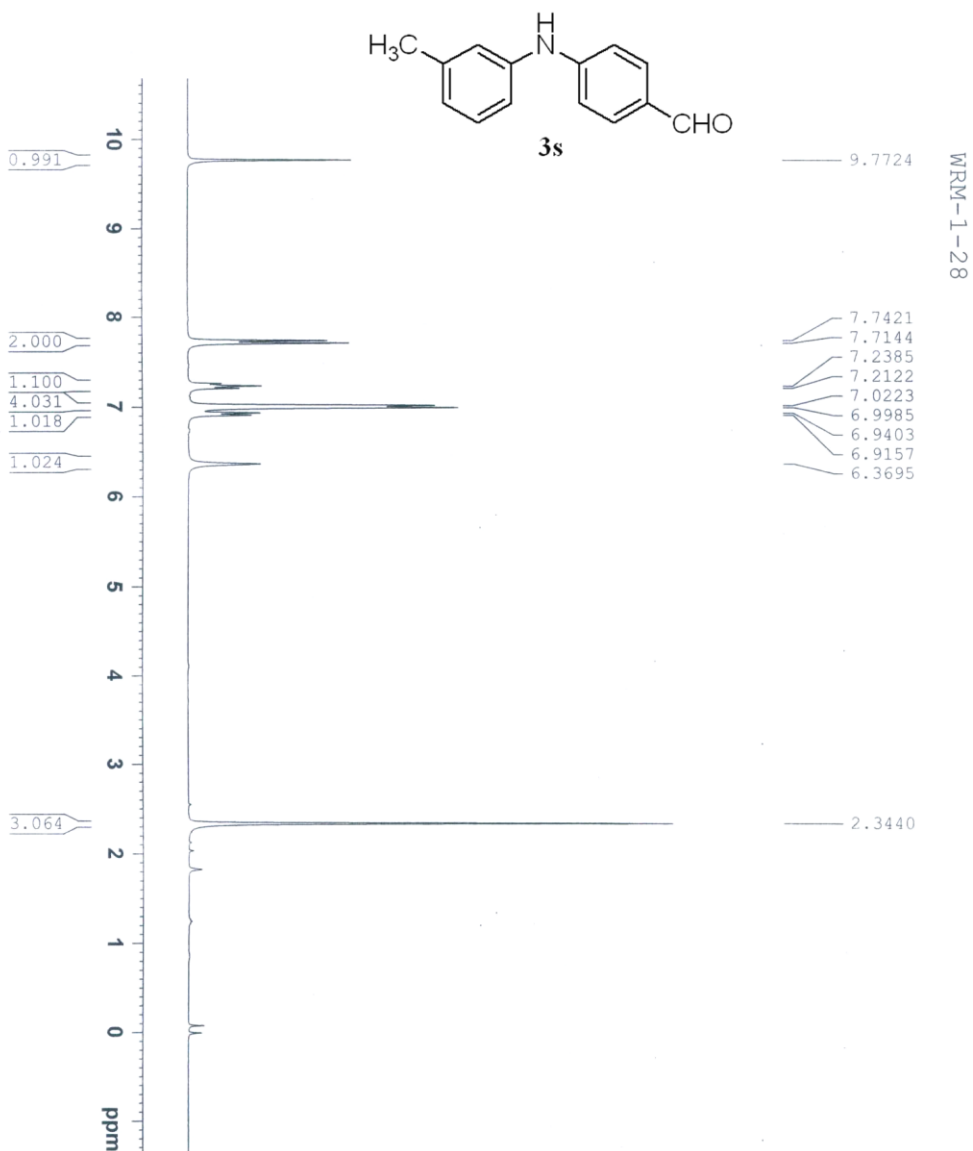
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 12.50 usec  
 PL1 4.00 dB  
 SFO1 75.4866943 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 NO2 80.00 usec  
 NO2D2 2.00 dB  
 PL2 19.04 dB  
 SFO2 300.1710453 MHz

F2 - Processing parameters  
 SF 75.4778133 MHz  
 WDW EM  
 SSB 0  
 LB 3.50 Hz  
 GB 0  
 PC 1.40

NMR-121 MS





Current Data Parameters  
 NAME WRM-1H  
 EXPNO 8  
 PROCNO 1

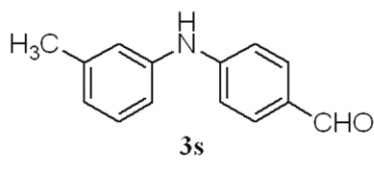
F2 - Acquisition Parameters  
 Date\_ 20091022  
 Time\_ 17.36  
 INSTRUM 4V300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 65536  
 ID 1  
 SOLVENT CDCl3  
 NS 24  
 DS 0  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 64  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 DL 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCMRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUCL1 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

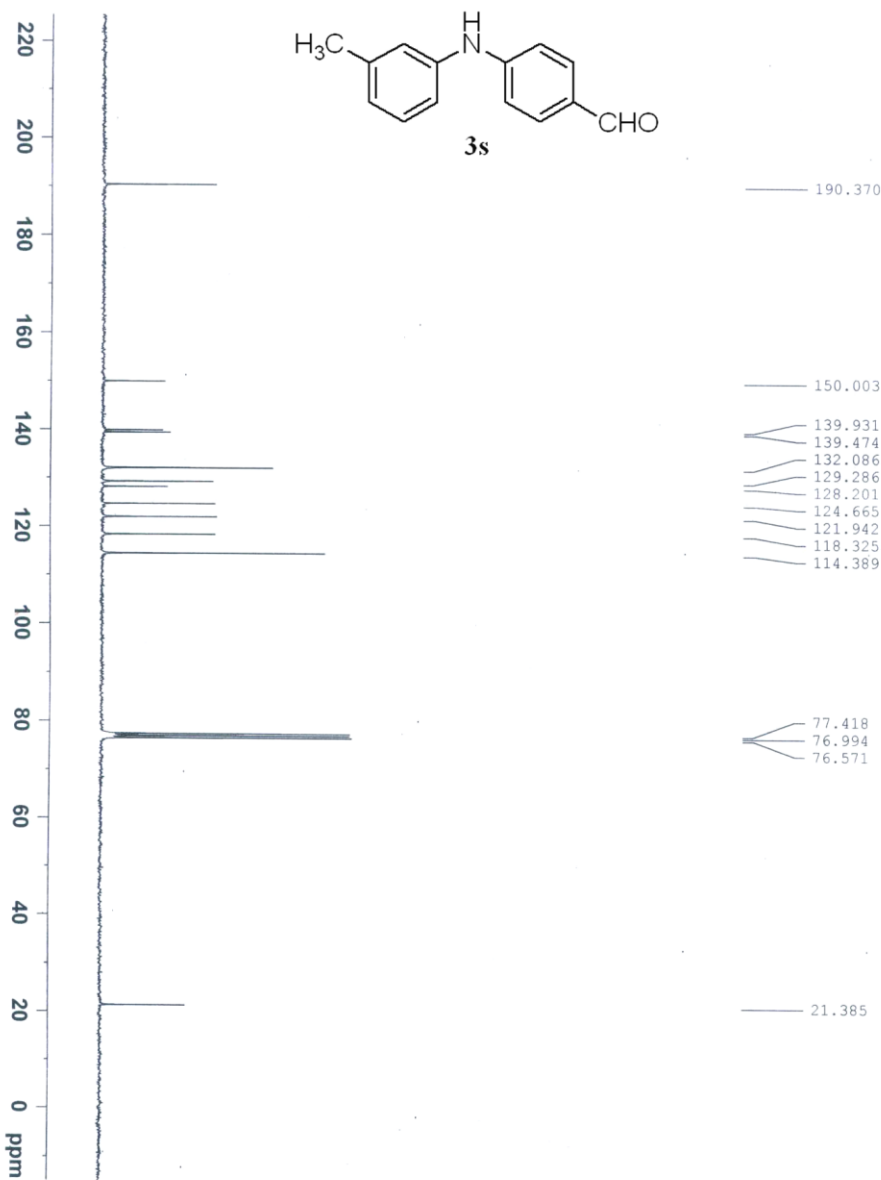
F2 - Processing parameters  
 SI 16384  
 SF 300.170081 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 20.00 cm  
 CY 0.00 cm  
 FIP 14.942 ppm  
 FI 4485.06 Hz  
 FPP -5.031 ppm  
 F2 -1510.14 Hz  
 PPM1M 0.99853 ppm/cm  
 PPM2M 299.76022 Hz/cm





WRM-1-28



- 190.370
- 150.003
- 139.931
- 139.474
- 132.086
- 129.286
- 128.201
- 124.665
- 121.942
- 118.325
- 114.389
- 77.418
- 76.994
- 76.571
- 21.385



Current Data Parameters  
 NAME WRM-13C  
 EXPNO 9  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091028  
 Time 19:56  
 INSTRUM acq100  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 629  
 DS 0

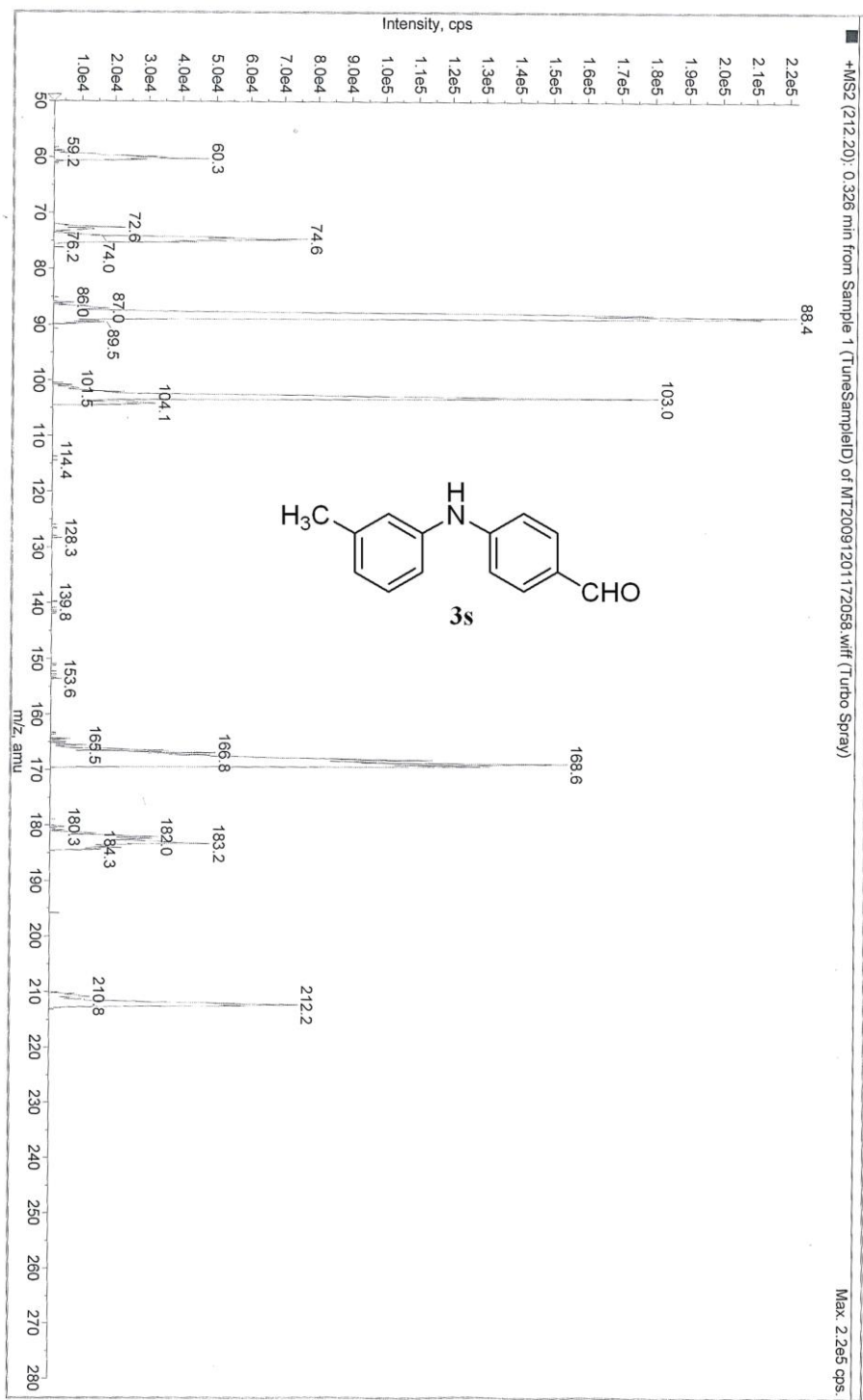
SWH 30120.482 Hz  
 FIDRES 0.459602 Hz  
 AQ 1.0879476 sec  
 RG 4096  
 DW 16.600 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 2.50000000 sec  
 d11 0.03000000 sec  
 MCREST 0.00000000 sec  
 MCWRRK 0.01500000 sec

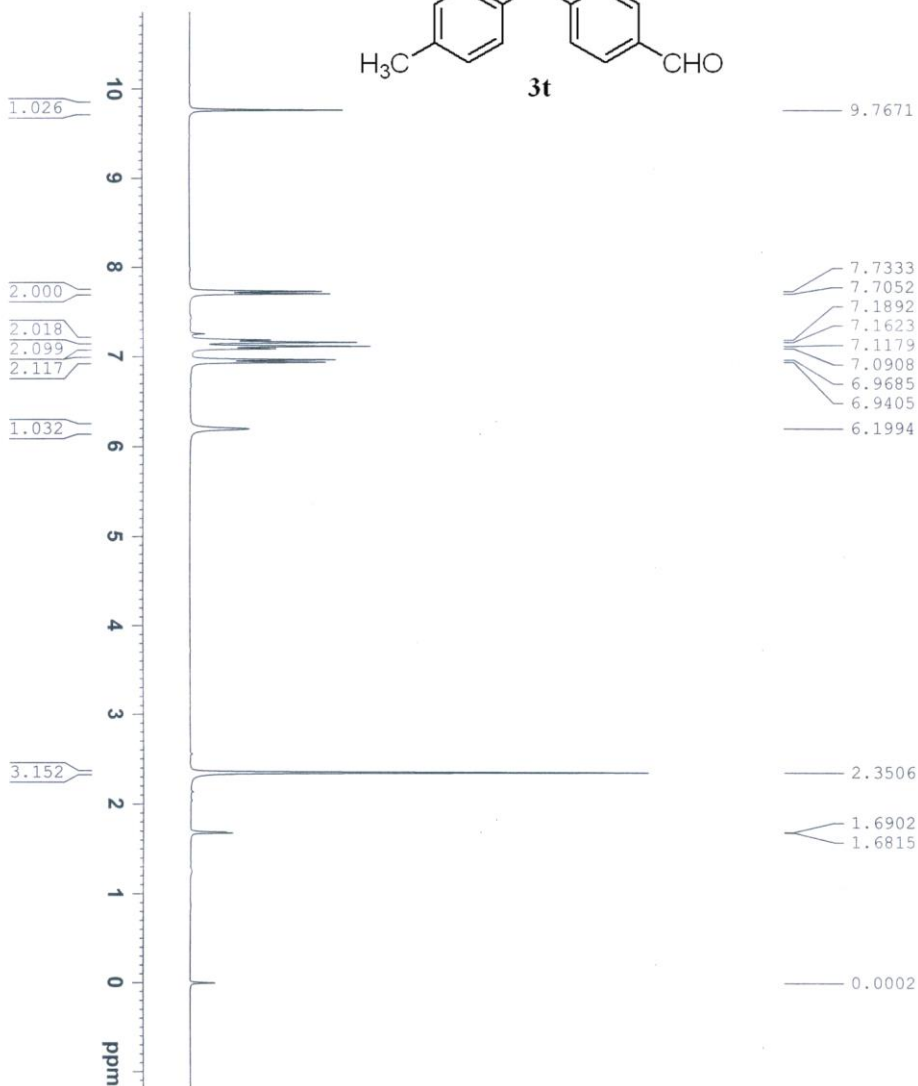
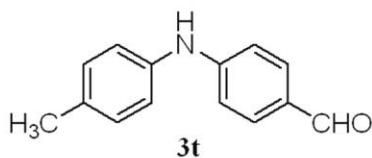
==== CHANNEL f1 =====  
 NUC1 13C  
 P1 12.50 usec  
 PL1 4.00 dB  
 SFO1 75.4868643 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 2.00 dB  
 PL12 19.04 dB  
 SFO2 300.1710453 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4778151 MHz  
 WDW EM  
 SSB 0  
 GB 3.50 Hz  
 CB 0  
 PC 1.40

W846-1-28 K52.



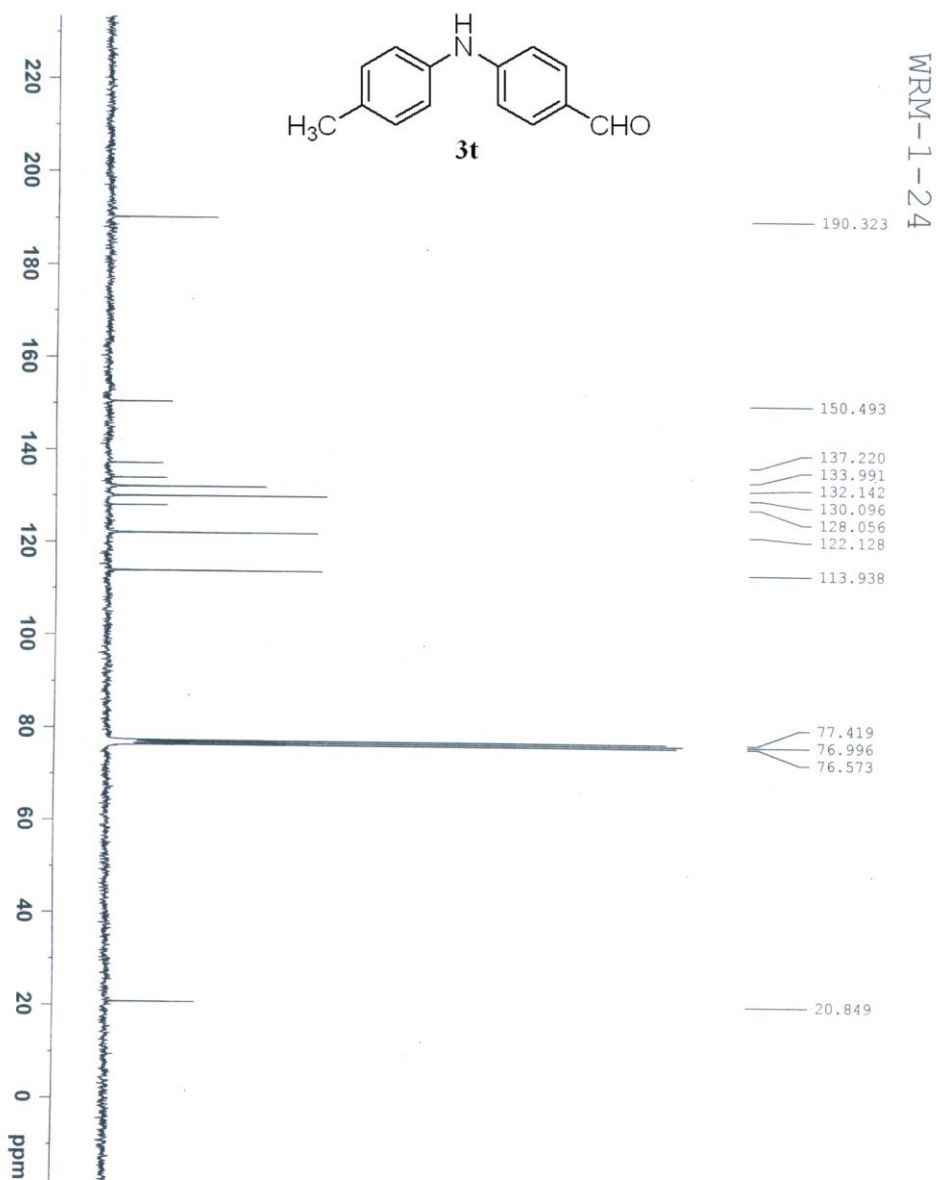


Current Data Parameters  
 NAME RRM-1H  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091022  
 Time 17.33  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 24  
 DS 0  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 64  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 673.2 K  
 D1 3.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUCL 1H  
 P1 11.25 usec  
 PL1 2.00 dB  
 SFO1 300.1714955 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.170052 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME WRM-13C  
 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20091025  
 Time 16.03  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 TDPROG zgpg30  
 SOLVENT CDCl3  
 NS 475  
 DS 0

SI 307.20482 Hz

FIDRES 0.22442 Hz

AQ 1.087476 sec

RG 11585.2

DW 18.600 usec

DE 6.00 usec

TE 300.2 K

D1 2.500000 sec

d11 0.03000000 sec

MCREST 0.00000000 sec

MCWIRK 0.01500000 sec

===== CHANNEL f1 =====

NUC1 13C

PC 12.50 usec

PL1 4.00 dB

SFO1 75.486843 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 80.00 usec

PL2 2.00 dB

SFO2 300.1710453 MHz

F2 - Processing parameters

SI 327.68

WDW 75.477814 MHz

SSB 0 EM

LB 3.50 Hz

GB 0

PC 1.40

1D NMR-pi4 parameters

CX 20.00 cm

CY 0.00 cm

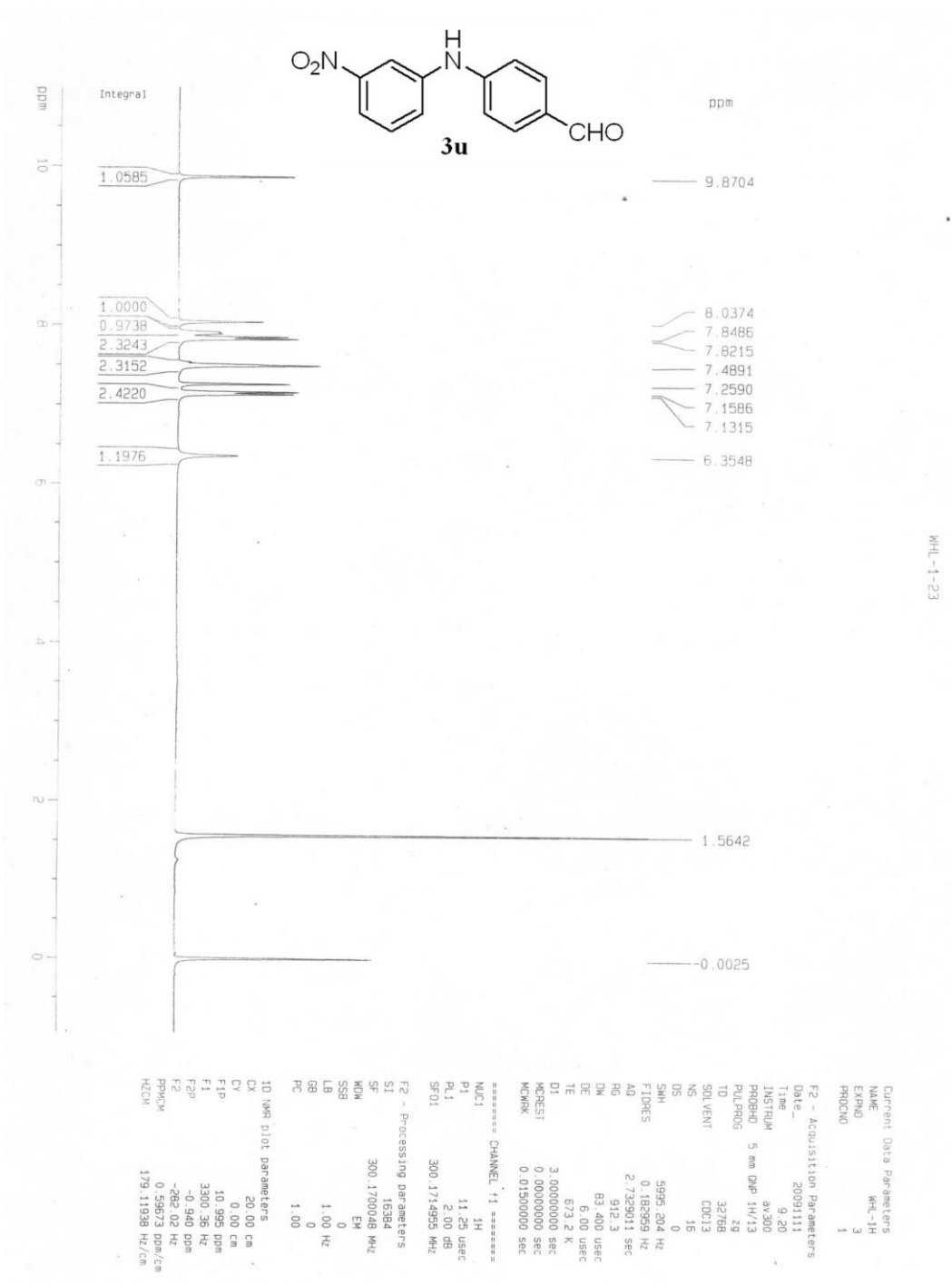
F1P 208.520 ppm

F2P 159.850 Hz

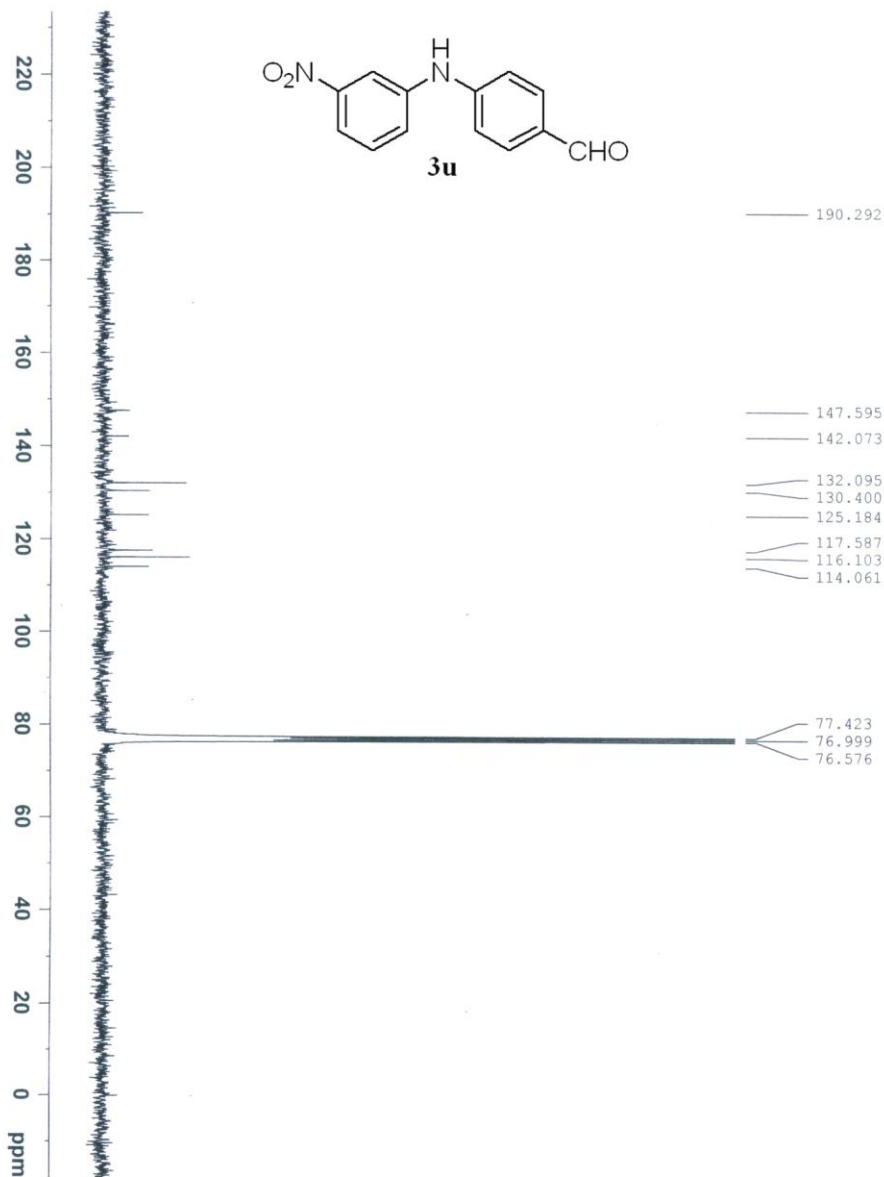
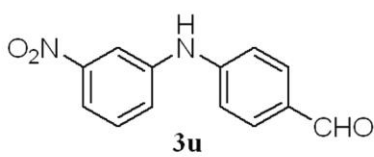
F2 159.850 ppm

PPMCM 10.91143 ppm/cm

HZCM 823.57086 Hz/cm



WHL-1-23



Current Data Parameters  
 NAME WRM-13C  
 EXPNO 15  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20091111  
 Time 17.15  
 INSTRUM av300  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg  
 TD 65536  
 SOLVENT CDCl3  
 NS 6144  
 DS 0  
 SWH 30120.482 Hz  
 FIDRES 0.459602 Hz  
 AQ 1.0879476 sec  
 RG 6902  
 DW 16.600 usec  
 DE 6.90 usec  
 TE 673.2 K  
 D1 2.5000000 sec  
 d11 0.0300000 sec  
 MCOREST 0.0100000 sec  
 MCVNKR 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 12.50 usec  
 PL1 4.00 dB  
 SFO1 75.486643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 2.00 dB  
 PL12 19.04 dB  
 SFO2 300.1710453 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.47789059 MHz  
 WDW EM  
 SSB 0  
 LB 3.50 Hz  
 GB 0  
 PC 1.40

WHL-1-23 MS<sub>n</sub>

