

## Supporting Information for

### Synthesis of Substituted Indole from 2-Aminobenzaldehyde through [1,2]-Aryl Shift

*Patrick Levesque and Pierre-André Fournier\**

Merck Frosst Center for Therapeutic Research,  
16711 Trans Canada Hwy, Kirkland, Qc, Canada, H9H 3L1

PierreAndreFournier@gmail.com

#### Contents:

Experimental .....	2
Copies of $^1\text{H}$ and $^{13}\text{C}$ Spectra.....	21

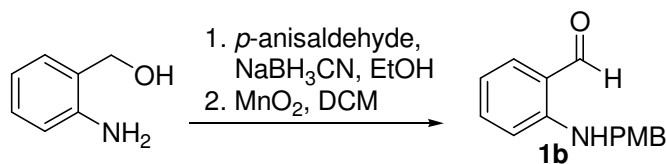
## Experimental

**General Experimental:** Unless otherwise noted, all reactions were carried out with magnetic stirring in flame-dried, round-bottom flasks under nitrogen. Plastic syringes were purged with nitrogen prior to use. Benzyl bromide was passed through basic alumina and benzaldehyde was freshly distilled prior to use. All other solvents and reagents were used as supplied (analytical or HPLC grade) without prior purification. Compounds **1a<sup>i</sup>**, **1c<sup>ii</sup>**, **1n<sup>iii</sup>** and **1o<sup>iv</sup>** were prepared according to literature procedures.

TLC was performed with glass-backed silica gel plates and visualized either by UV detection (254 nm) or potassium permanganate (KMnO<sub>4</sub>) stain. Flash column chromatography was performed on an automated column chromatography platform. NMR spectra were recorded on 500 or 400 MHz NMR instruments in CDCl<sub>3</sub>. High resolution mass spectra (HRMS) were recorded using electrospray ionization on a Time of Flight (TOF) mass spectrometer.

## Experimental

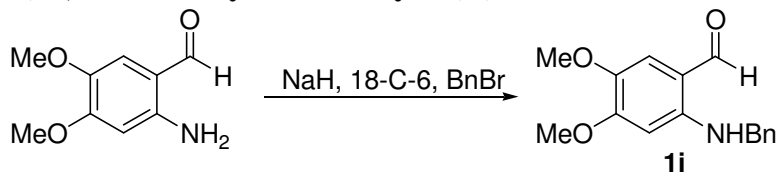
### 2-[(4-Methoxyphenyl)methylamino]benzaldehyde (**1b**)



To a solution of 2-aminobenzyl alcohol (41 mmol) in DCE (0.2 M) was added *p*-anisaldehyde (1.1 eq) followed by sodium cyanoborohydride (5 eq). The solution was stirred at room temperature overnight. NaHCO<sub>3</sub> (aq) was added and the aqueous phase was washed with DCM 3 times. The combined organic layers were dried over MgSO<sub>4</sub>, filtered and concentrated *in vacuo*. The crude residue was purified by flash chromatography to yield 2-[(4-methoxyphenyl)methylamino]benzyl alcohol in 68% yield. The alcohol (4.1 mmol) was dissolved in DCM (0.28 M) and MnO<sub>2</sub> (6 equiv.) was added. The solution was stirred at room temperature for 48 hours and filtered over a silica pad. The pad was rinsed with DCM before the organic solvent was removed. The residue was purified by flash chromatography to yield title compound **1b** as a yellow solid in 76% yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 9.80 (s, 1 H); 8.63 (s, 1 H); 7.44 (d, J = 7.72 Hz, 1 H); 7.31-7.26 (m, 1 H); 7.21 (d, J = 8.19 Hz, 2 H); 6.83 (d, J = 8.28 Hz, 2

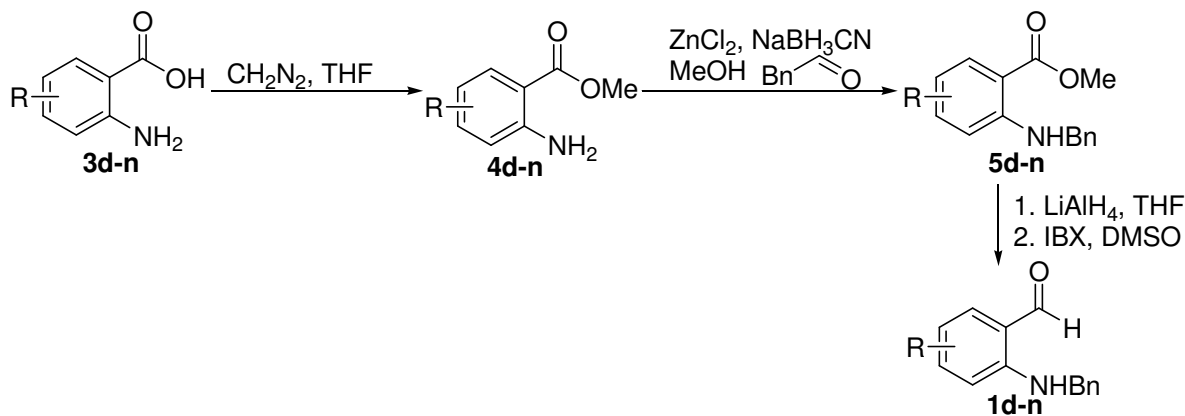
H); 6.65 (t, J = 7.45 Hz, 1 H); 6.61 (d, J = 8.56 Hz, 1 H); 4.36 (d, J = 4.82 Hz, 2 H); 3.75 (s, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 194.1, 158.9, 150.6, 136.7, 135.8, 130.2, 128.3, 118.6, 115.2, 114.2, 111.3, 55.3, 46.1. HRMS (ESI) m/z calculated for C<sub>15</sub>H<sub>16</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 242.11756, found 242.11776.

### 2-(benzylamino)-4,5-dimethoxy-benzaldehyde (**1i**)



To a solution of 2-amino-4,5-dimethoxy-benzaldehyde<sup>v</sup> (1.2 mmol) in THF (1M) was added NaH (1.2 equiv.) and 18-crown-6 (0.1 equiv.). The solution was stirred for 20 minutes before benzyl bromide (1 equiv.) in solution in THF (1M) was added. The solution was stirred at room temperature for 24 hours before a saturated solution of aqueous NH<sub>4</sub>Cl was added. The aqueous layer was extracted (3x) with EtOAc. The combined organic layers were dried over MgSO<sub>4</sub>, filtered and concentrated *in vacuo*. The crude residue was purified by flash chromatography to yield the title compound **1i** in 16% yield as an orange oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 9.70 (s, 1 H); 8.97 (s, 1 H); 7.40-7.27 (m, 5 H); 6.94 (s, 1 H); 6.10 (s, 1 H); 4.50 (s, 2 H); 3.86 (s, 3 H); 3.79 (s, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 191.1, 156.7, 148.4, 140.1, 138.4, 128.8, 127.4, 127.1, 117.2, 111.1, 94.3, 56.6, 55.8, 47.0. HRMS (ESI) m/z calculated for C<sub>16</sub>H<sub>17</sub>NO<sub>3</sub>Na [M+Na]<sup>+</sup>, 294.11061, found 294.10996.

### Synthesis of aldehydes **1d** to **1f** and **1j** to **1n**



### General Procedure 1 for the methylation of 2-aminobenzoic acids

To a solution of 2-amino-benzoic acid (1.0 equiv.) in EtOAc or THF (0.1 M) was added a 1M solution of diazomethane in Et<sub>2</sub>O (5.0 equiv.) and the solution was stirred for 1 hour. Acetic acid (4.0 equiv.) was added to stop the reaction. The reaction mixture was poured into a saturated aqueous solution of NaHCO<sub>3</sub> and it was extracted (3x) with EtOAc. The combined organic layers were dried over MgSO<sub>4</sub>, filtered and concentrated *in vacuo* to furnish methyl 2-aminobenzoate (71-100% yields). No further purification of these products was necessary.

#### **General Procedure 2 for the reductive amination of methyl 2-aminobenzoates**

To a solution of methyl 2-aminobenzoate (1.0 equiv.), benzaldehyde (2.0 equiv.), and zinc chloride (1.7 equiv.) in MeOH (0.50 M) was added sodium cyanoborohydride (1.7 equiv.) at room temperature. The mixture was stirred at room temperature for 2-12 hours (if any starting material was still visible by TLC after this time, the mixture was refluxed for 1-2 hour). A saturated solution of aqueous NH<sub>4</sub>Cl was added to the mixture and the later was extracted (3x) with EtOAc. The combined organic layers were dried over MgSO<sub>4</sub>, filtered and concentrated *in vacuo*. The crude residue was purified by flash chromatography to yield the corresponding methyl 2-(benzylamino)benzoate (15-99% yields).

#### **General Procedure 3 for the LiAlH<sub>4</sub> reduction of methyl 2-(benzylamino)benzoates**

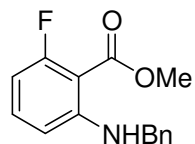
To a solution of methyl 2-(benzylamino)benzoate (1.0 equiv.) in THF (0.100 M) is added LAH (3.5 equiv.) in portions at 0 °C. The mixture is stirred for 30-60 minutes while warming up to room temperature. The reaction is stopped by adding a saturated aqueous solution of ammonium chloride. The mixture is extracted 3x with EtOAc and the combined organic layers are dried over MgSO<sub>4</sub>, filtered, and concentrated *in vacuo*. The crude residue is then used crude in the IBX oxidation reaction (if sufficiently clean) or purified by flash chromatography before being oxidized. This furnishes [2-(benzylamino)phenyl]methanol (?-? % yields).

#### **General Procedure 4 for the oxidation of [2-(benzylamino)phenyl]methanol with IBX**

IBX (1.2 equiv.) is stirred in DMSO (0.400 M) until dissolution and the solution is added to a solution of [2-(benzylamino)phenyl]methanol in DMSO (0.400 M) and stirred for 30 minutes. Water is added to stop the reaction and the white precipitate is filtered of and

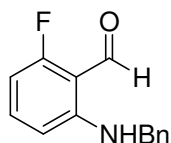
rinned with DCM. The filtrate is extracted 3x with DCM and the combined organic layers are washed 1x with brine, 1x with 10% Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> (aq), and 1x with water before it is dried over MgSO<sub>4</sub>, filtered once again and concentrate *in vacuo*. The crude residue is purified by flash chromatography to yield 2-(benzylamino)benzaldehyde (?-?% yields).

#### Methyl 2-(benzylamino)-6-fluorobenzoate (**5d**)



The corresponding methyl ester **4d** was obtained in 97% yield from corresponding 2-aminobenzoic acid **3d** (6.45 mmol) as a yellow solid using general procedure 1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.12r (dd, J = 14.46, 7.23 Hz, 1 H); 6.45-6.29 (m, 2 H); 5.73 (s, 2 H); 3.89 (s, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 167.4 (d), 164.7 (s), 162.1 (s), 151.7 (d), 133.8 (d), 112.1 (d), 103.8 (d), 51.9 (s). HRMS (ESI) m/z calculated for C<sub>8</sub>H<sub>9</sub>FNO<sub>2</sub> [M+H]<sup>+</sup>, 170.0612, found 170.0618. Reductive amination was performed on the crude ester (6.22 mmol) using general procedure 2 to give the title compound **5d** in 88% yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.04 (s, 1 H); 7.35-7.12 (m, 5 H); 6.41-6.26 (m, 2 H); 4.40 (d, J = 5.51 Hz, 2 H); 3.89 (s, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 168.2 (d), 165.2 (s), 162.6 (s), 152.0 (d), 138.5 (s), 134.5 (d), 128.8 (s), 127.4 (s), 127.2 (s), 107.4 (d), 103.0 (d), 52.0 (s), 47.6 (s). HRMS (ESI) m/z calculated for C<sub>15</sub>H<sub>15</sub>FNO<sub>2</sub> [M+H]<sup>+</sup>, 260.10813, found 260.10861.

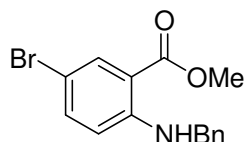
#### 2-(Benzylamino)-6-fluorobenzaldehyde (**1d**)



Methyl 2-(benzylamino)-6-fluorobenzoate **5d** (5.3 mmol) in DCM (0.100 M) is added DIBAL-H (3.5 equiv.; 1.5M in toluene) at -78 °C. The mixture is stirred for 30 minutes and the reaction is stopped by adding a saturated aqueous solution of ammonium chloride. The mixture is extracted 3x with DCM and the combined organic layers are dried over MgSO<sub>4</sub>, filtered, and concentrated *in vacuo*. The residue is filtered on a silica gel pad, eluting with 1:1 EtOAc:hexanes to give the crude benzylic alcohol in 74% yield. This crude alcohol (4 mmol) was oxidized using general conditions 4 to give the title

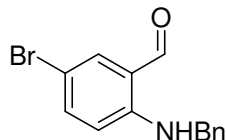
compound **1d** as a yellow solid in 54 % yield from the corresponding [2-(benzylamino)phenyl]methanol. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 10.30 (s, 1 H); 9.14 (s, 1 H); 7.37-7.19 (m, 6 H); 6.38 (d, J = 8.70 Hz, 1 H); 6.27 (dd, J = 11.13, 8.02 Hz, 1 H); 4.45 (d, J = 5.78 Hz, 2 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 189.3, 189.2, 168.3, 165.7, 152.0, 152.0, 137.9, 137.3, 137.2, 128.8, 127.5, 127.0, 107.8, 107.5, 107.5, 101.1, 100.9, 46.9. HRMS (ESI) m/z calculated for C<sub>14</sub>H<sub>13</sub>FNO [M+H]<sup>+</sup>, 230.09757, found 230.09801.

#### Methyl 2-(benzylamino)-5-bromobenzoate (**5e**)



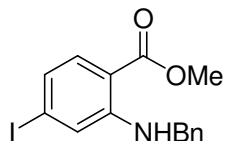
Reductive amination was performed on the commercially available methyl 2-amino-5-bromobenzoate (**4e**) (8.7 mmol) using general procedure 2 to give the title compound **5e** as a yellow solid in 99% yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.04 (d, J = 2.49 Hz, 1 H); 7.42-7.25 (m, 6 H); 6.64 (d, J = 8.95 Hz, 1 H); 4.44 (s, 2 H); 3.87 (s, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 168.1, 149.8, 138.3, 137.2, 133.9, 128.9, 128.8, 127.4, 127.1, 127.1, 113.7, 111.7, 106.3, 51.8, 47.0. HRMS (ESI) m/z calculated for C<sub>15</sub>H<sub>15</sub>BrNO<sub>2</sub> [M+H]<sup>+</sup>, 320.0281, found 320.0302.

#### 2-(Benzylamino)-5-bromobenzaldehyde (**1e**)



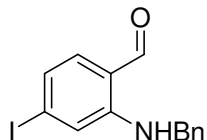
Methyl 2-(benzylamino)-5-bromobenzoate (**5e**) was reduced to the corresponding benzylic alcohol in quantitative yield using general procedure 3. The crude alcohol was directly oxidized using general procedure 4 to give the title compound **1e** as a yellow solid in 89% yield over 2 steps from **5e**. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 9.79 (s, 1 H); 8.73 (s, 1 H); 7.59 (d, J = 2.53 Hz, 1 H); 6.55 (d, J = 8.98 Hz, 1 H); 4.47 (s, 2 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 193.0, 149.4, 138.5, 138.4, 137.8, 128.9, 127.6, 127.0, 120.0, 113.7, 106.5, 46.8. HRMS (ESI) m/z calculated for C<sub>14</sub>H<sub>12</sub>BrNO [M+H]<sup>+</sup>, 290.01750, found 290.01754.

#### Methyl 2-(benzylamino)-4-iodobenzoate (**5f**)



The corresponding methyl ester **4f** was obtained in quantitative yield from corresponding 2-aminobenzoic acid **3f** (3.8 mmol) as a yellow solid using general procedure 1.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.13-7.03 (m, 1 H); 6.75 (d,  $J = 7.86$  Hz, 1 H); 6.58 (d,  $J = 8.28$  Hz, 1 H); 4.85 (s, 2 H); 3.93 (s, 2 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  167.7, 149.0, 134.1, 132.2, 119.7, 115.0, 52.2. HRMS (ESI)  $m/z$  calculated for  $\text{C}_8\text{H}_9\text{INO}_2$   $[\text{M}+\text{H}]^+$ , 277.96725, found 277.96785. Reductive amination was performed on the crude ester (1.8 mmol) using the general procedure 2 to give the title compound **5f** as a yellow solid in 73% yield.  $\text{ZnI}_2$  was employed instead of  $\text{ZnCl}_2$  to prevent halide replacement (when using  $\text{ZnCl}_2$  under the standard conditions, the 4-chlorobenzoate was isolated).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.11 (s, 1 H); 7.57 (d,  $J = 8.43$  Hz, 1 H); 7.41-7.22 (m, 5 H); 7.05 (s, 1 H); 6.94 (d,  $J = 8.47$  Hz, 1 H); 4.39 (s, 2 H); 3.84 (s, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  168.9, 151.4, 138.2, 132.7, 128.9, 127.6, 127.4, 124.3, 120.7, 109.8, 103.1, 51.8, 47.2. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{15}\text{H}_{15}\text{INO}_2$   $[\text{M}+\text{H}]^+$ , 368.01420, found 368.01609.

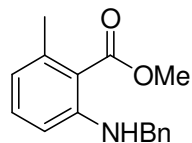
### 2-(Benzylamino)-4-iodobenzaldehyde (**1f**)



To a solution of methyl 2-(benzylamino)-4-iodobenzoate **5f** (1.3 mmol) in DCM (0.100 M) is added DIBAL-H (3.5 equiv.; 1.5M in toluene) at  $-78$  °C. The mixture is stirred for 30 minutes and the reaction is stopped by adding a saturated aqueous solution of ammonium chloride. The mixture is extracted 3x with DCM and the combined organic layers are dried over  $\text{MgSO}_4$ , filtered, and concentrated *in vacuo*. The residue is filtered on a silica gel pad, eluting with 1:1 EtOAc:hexanes to give the crude benzylic alcohol (yellow solid) in 85% yield. This crude alcohol (1.1 mmol) was oxidized using general conditions 4 to give the title compound **1f** as a yellow solid in 76 % yield from the corresponding [2-(benzylamino)phenyl]methanol.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  9.77 (s, 1 H); 8.69 (s, 1 H); 7.40-7.26 (m, 5 H); 7.17-7.02 (m, 3 H); 4.42 (d,  $J = 5.67$  Hz, 2

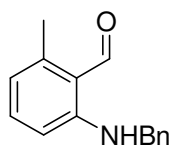
H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  193.7, 150.7, 137.6, 129.0, 127.7, 127.3, 124.8, 120.6, 118.0, 105.3, 46.8. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{14}\text{H}_{12}\text{INO}$   $[\text{M}+\text{H}]^+$ , 338.0036, found 338.0031.

### Methyl 2-(benzylamino)-6-methylbenzoate (**5j**)



The corresponding methyl ester **4j** was obtained in quantitative yield from corresponding 2-aminobenzoic acid **3j** (6.6 mmol) as a white solid using general procedure 1.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.12-7.03 (m, 1 H); 6.53 (d,  $J = 7.83$  Hz, 2 H); 5.10 (s, 2 H); 3.89 (s, 3 H); 2.43 (s, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  169.6, 149.1, 140.1, 132.0, 120.3, 114.5, 113.8, 51.3, 22.9. HRMS (ESI)  $m/z$  calculated for  $\text{C}_9\text{H}_{12}\text{NO}_2$   $[\text{M}+\text{H}]^+$ , 166.0863, found 166.0899. Reductive amination was performed on the crude ester (6.5 mmol) using the general procedure 2 to give the title compound **5j** as a yellow solid in 76% yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.12 (dd,  $J = 16.35, 8.06$  Hz, 1 H); 6.49 (d,  $J = 7.95$  Hz, 1 H); 4.39 (s, 1 H); 3.88 (s, 1 H); 2.44 (s, 2 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  170.3, 149.9, 140.5, 139.2, 132.5, 132.4, 128.7, 128.6, 127.2, 127.1, 119.4, 113.3, 109.6, 109.5, 51.4, 51.4, 47.6, 47.5, 23.5, 23.4. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{16}\text{H}_{18}\text{NO}_2$   $[\text{M}+\text{H}]^+$ , 256.1332, found 256.1362.

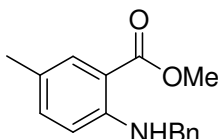
### 2-(Benzylamino)-6-methylbenzaldehyde (**1j**)



Methyl 2-(benzylamino)-6-methylbenzoate (**5j**) (5.0 mmol) was reduced to the corresponding benzylic alcohol (yellow solid) in 82% yield using general procedure 3.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.04-6.96 (m, 1 H); 6.54-6.44 (m, 2 H); 4.64 (s, 2 H); 4.29 (s, 2 H); 2.26 (s, 3 H); 1.91 (d,  $J = 11.07$  Hz, 1 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  147.8, 139.6, 136.4, 129.0, 128.6, 127.4, 127.1, 122.7, 119.6, 109.5, 58.9, 48.0, 19.8. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{15}\text{H}_{18}\text{NO}$   $[\text{M}+\text{H}]^+$ , 228.1383, found 228.1439. The crude alcohol (3.9 mmol) was directly oxidized using general procedure 4 to give the title compound **1j** as a yellow solid in 70% yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  10.38 (s, 1

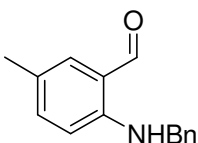
H); 9.43 (s, 1 H); 7.35-7.23 (m, 5 H); 7.19 (t, J = 7.93 Hz, 1 H); 6.52 (d, J = 8.63 Hz, 1 H); 6.41 (d, J = 7.21 Hz, 1 H); 4.47 (s, 2 H); 2.58 (s, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 192.5, 151.7, 143.6, 138.5, 136.1, 128.8, 127.3, 127.0, 118.0, 116.2, 110.4, 46.7, 19.3. HRMS (ESI) m/z calculated for C<sub>15</sub>H<sub>16</sub>NO [M+H]<sup>+</sup>, 226.12264, found 226.12280.

### Methyl 2-(benzylamino)-5-methylbenzoate (**5k**)



The corresponding methyl ester **4k** was obtained in quantitative yield from corresponding 2-aminobenzoic acid **3k** (6.6 mmol) as a white solid using general procedure 1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.57 (s, 1 H); 7.01 (d, J = 8.30 Hz, 1 H); 6.51 (d, J = 8.30 Hz, 1 H); 5.46 (s, 2 H); 3.78 (s, 3 H); 2.14 (s, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 168.7, 148.4, 135.4, 131.0, 125.6, 117.0, 110.8, 51.6, 20.4. HRMS (ESI) m/z calculated for C<sub>9</sub>H<sub>12</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 166.0863, found 166.0879. Reductive amination was performed on the crude ester (6.5 mmol) using the general procedure 2 to give the title compound **5k** as a yellow solid in 71% yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.04 (s, 1 H); 7.78 (s, 1 H); 7.43-7.33 (m, 4 H); 7.17 (d, J = 8.61 Hz, 1 H); 6.61 (d, J = 8.56 Hz, 1 H); 4.49 (s, 2 H); 3.91 (s, 3 H); 2.27 (s, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 168.9, 149.0, 139.0, 135.5, 131.3, 128.5, 126.9, 123.5, 111.7, 109.9, 51.2, 46.9, 20.0. HRMS (ESI) m/z calculated for C<sub>16</sub>H<sub>18</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 256.13321, found 256.13346.

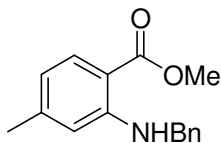
### 2-(Benzylamino)-5-methylbenzaldehyde (**1k**)



Methyl 2-(benzylamino)-5-methylbenzoate (**5k**) (4.4 mmol) was reduced to the corresponding benzylic alcohol (yellow solid) in quantitative yield using general procedure 3. The crude alcohol (4.4 mmol) was directly oxidized using general procedure 4 to give the title compound **1k** as a yellow solid in 71% yield over 2 steps from **5k**. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 9.80 (s, 1 H); 8.59 (s, 1 H); 7.34-7.19 (m, 5 H); 7.12 (d, J = 8.59 Hz, 1 H); 6.53 (d, J = 8.58 Hz, 1 H); 4.42 (d, J = 5.86 Hz, 2 H);

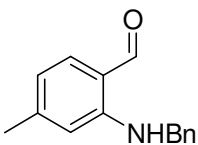
2.22 (s, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  194.1, 148.8, 138.6, 137.1, 136.3, 128.8, 127.3, 127.0, 124.3, 118.6, 111.5, 77.5, 46.7, 20.1. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{15}\text{H}_{16}\text{NO}$   $[\text{M}+\text{H}]^+$ , 226.12264, found 226.12322.

#### Methyl 2-(benzylamino)-4-methylbenzoate (**5I**)



The corresponding methyl ester **4I** was obtained in quantitative yield from corresponding 2-aminobenzoic acid **3I** (6.6 mmol) as a white solid using general procedure 1.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.74 (d,  $J = 8.10$  Hz, 1 H); 6.50-6.43 (m, 2 H); 5.76 (s, 2 H); 3.85 (s, 3 H); 2.26 (s, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  168.6, 150.6, 144.9, 131.2, 117.8, 116.8, 108.4, 51.4, 21.6. HRMS (ESI)  $m/z$  calculated for  $\text{C}_9\text{H}_{12}\text{NO}_2$   $[\text{M}+\text{H}]^+$ , 166.0863, found 166.0896. Reductive amination was performed on the crude ester (6.5 mmol) using the general procedure 2 to give the title compound **5I** as a yellow solid in 98% yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.27 (s, 1 H); 7.81 (d,  $J = 8.12$  Hz, 1 H); 7.38-7.23 (m, 5 H); 6.51 (s, 1 H); 6.46 (d,  $J = 8.16$  Hz, 1 H); 4.44 (s, 2 H); 3.84 (s, 3 H); 2.26 (s, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  169.2, 150.7, 145.6, 138.7, 131.7, 128.8, 127.4, 127.4, 117.0, 112.4, 108.3, 51.6, 47.5, 22.3. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{16}\text{H}_{18}\text{NO}_2$   $[\text{M}+\text{H}]^+$ , 256.1332, found 256.1393.

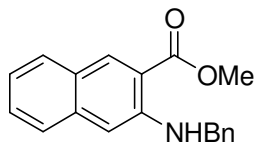
#### 2-(Benzylamino)-4-methylbenzaldehyde (**II**)



Methyl 2-(benzylamino)-4-methylbenzoate (**5I**) (4.4 mmol) was reduced to the corresponding benzylic alcohol (yellow solid) in quantitative yield using general procedure 3. The crude alcohol (4.4 mmol) was directly oxidized using general procedure 4 to give the title compound **II** as a yellow solid in 82% yield over 2 steps from **5I**.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  9.79 (s, 1 H); 8.75 (s, 1 H); 7.39-7.23 (m, 6 H); 6.53 (d,  $J = 7.87$  Hz, 1 H); 6.46 (s, 1 H); 4.46 (s, 2 H); 2.27 (s, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  193.4, 150.7, 147.3, 138.4, 136.8, 128.8, 127.4, 127.2, 117.1, 117.0,

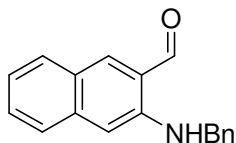
111.5, 46.7, 22.6. HRMS (ESI)  $m/z$  calculated for  $C_{15}H_{16}NO$   $[M+H]^+$ , 226.1226, found 226.1251.

### Methyl 3-(benzylamino) naphthalene-2-carboxylate (**5m**)



The corresponding methyl ester **4m** was obtained in 71% yield from corresponding 2-aminobenzoic acid **3m** (5.3 mmol) as a white solid using general procedure 1.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  8.52 (s, 1 H); 7.74 (d,  $J = 8.28$  Hz, 1 H); 7.55 (d,  $J = 8.41$  Hz, 1 H); 7.43 (t,  $J = 7.55$  Hz, 1 H); 7.21 (t,  $J = 7.50$  Hz, 1 H); 7.00 (s, 1 H); 5.60 (s, 2 H); 3.98 (s, 3 H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ ):  $\delta$  168.3, 146.1, 137.4, 133.5, 129.3, 128.8, 126.1, 125.2, 122.5, 114.7, 110.0, 52.0. HRMS (ESI)  $m/z$  calculated for  $C_{12}H_{12}NO_2$   $[M+H]^+$ , 202.0863, found 202.0884. Reductive amination was performed on the crude ester (3.8 mmol) using the general procedure 2 to give the title compound **5m** as a yellow solid in 97% yield.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  8.53 (s, 1 H); 7.93 (s, 1 H); 7.69 (d,  $J = 8.18$  Hz, 1 H); 7.51 (d,  $J = 8.37$  Hz, 1 H); 7.44-7.21 (m, 6 H); 7.19-7.11 (m, 1 H); 6.84 (s, 1 H); 4.50 (s, 2 H); 3.93 (s, 3 H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ ):  $\delta$  168.8, 146.6, 138.9, 137.8, 133.9, 129.3, 128.9, 128.7, 127.3, 127.2, 125.7, 125.1, 122.2, 114.2, 105.1, 52.0, 47.6. HRMS (ESI)  $m/z$  calculated for  $C_{19}H_{18}NO_2$   $[M+H]^+$ , 292.1332, found 292.1361.

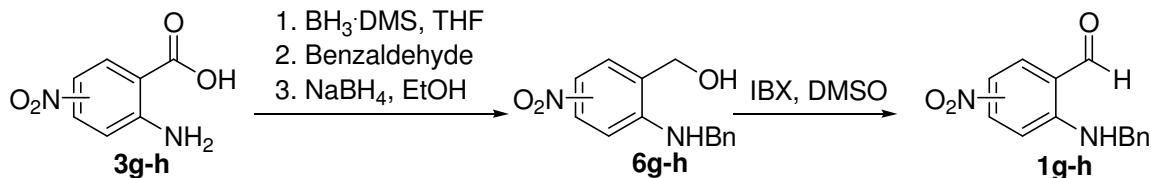
### 3-(benzylamino) naphthalene-2-carbaldehyde (**1m**)



Methyl 3-(benzylamino)-naphthalene-2-carboxylate (**5m**) (3.7 mmol) was reduced to the corresponding benzylic alcohol (yellow solid) in quantitative yield using general procedure 3. The crude alcohol (3.7 mmol) was directly oxidized using general procedure 4 to give the title compound **1m** as an orange solid in 78% yield over 2 steps from **5m**.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  10.06 (s, 1 H); 8.10 (s, 1 H); 8.04 (s, 1 H); 7.72 (d,  $J = 8.25$  Hz, 1 H); 7.50 (d,  $J = 8.44$  Hz, 1 H); 7.16 (t,  $J = 7.50$  Hz, 1 H); 6.77 (s, 1 H); 4.51 (d,  $J = 5.60$  Hz, 2 H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ ):  $\delta$  195.0, 146.2, 140.8,

138.6, 138.4, 130.0, 129.4, 128.8, 127.4, 127.3, 126.0, 125.5, 122.5, 122.2, 104.9, 47.2.  
HRMS (ESI)  $m/z$  calculated for  $C_{18}H_{16}NO$   $[M+H]^+$ , 262.12264, found 262.12296.

### Synthesis of aldehydes **1g** and **1h**



### General Procedure 5 for the borane reduction of anthranilic acid

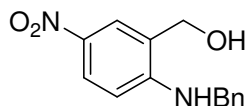
To a solution of anthranilic acid **3** (1.0 equiv.) in THF (0.280 M) is added borane-methyl sulfide complex (6.0 equiv.) and the solution was stirred at room temperature for 24 hours. The reaction was stopped at room temperature by addition of methanol until the solution had stopped bubbling. The solvent was evaporated *in vacuo* and the residue was filtered on a silica gel pad eluting with 50% EtOAc in Hexanes yielding (2-aminophenyl)methanol (99% yield).

### General Procedure 6 for aminal formation with benzaldehyde and reduction with $NaBH_4$ of (2-aminophenyl)methanol

To a solution of (2-aminophenyl)methanol (1.0 equiv.) in 2-propanol (0.266 M) is added benzaldehyde (1.1 equiv.) followed by chloroacetic acid (0.1 equiv.). The mixture is stirred for 1-5 days at room temperature (if after 1 day there is no progress, the reaction is refluxed for 48 hours) until all starting material is gone by NMR. The solvent is evaporated *in vacuo* and this corresponding crude aminal is used without further purification.

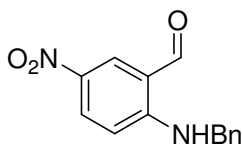
To a solution of the crude aminal in ethanol (0.200 M) is added sodium borohydride (1.0 equiv.) and the mixture is refluxed for 1-2 hours. Once all the starting material has reacted, the reaction is stopped by adding a saturated aqueous solution of ammonium chloride and the ethanol is evaporated *in vacuo* before the solution is extracted 3x with EtOAc, dried over  $MgSO_4$ , filtered, and concentrated *in vacuo*. The crude residue is purified by flash chromatography to furnish [2-(benzylamino)phenyl]methanol ( $\geq 95\%$  yields)

**[2-(benzylamino)-5-nitrophenyl]methanol (6g):**



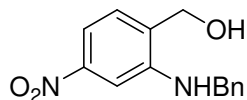
The corresponding benzylic alcohol was obtained in 80% yield from corresponding 2-aminobenzoic acid **3g** (5.5 mmol) using general procedure 5. The crude alcohol (3.95 mmol) was used to form an aminor using general procedure 6 yielding the title compound **6g** as an orange solid in 95% yield over 2 steps from the benzylic alcohol. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.07 (dd, J = 9.06, 2.64 Hz, 1 H); 8.00 (d, J = 2.63 Hz, 1 H); 7.40-7.27 (m, 5 H); 6.60 (d, J = 9.07 Hz, 1 H); 4.76 (s, 2 H); 4.49 (s, 2 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 153.0, 137.6, 137.0, 129.0, 127.8, 127.2, 126.5, 125.2, 123.3, 109.5, 64.2, 47.4. HRMS (ESI) m/z calculated for C<sub>14</sub>H<sub>15</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>, 259.10772, found 259.10843.

**2-(Benzylamino)-5-nitrobenzaldehyde (1g)**



[2-(benzylamino)-5-nitrophenyl]methanol (**6g**) (3.7 mmol) was oxidized using general procedure 4 to give the title compound **1g** as an orange solid in 76% yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 9.90 (s, 1 H); 9.43 (s, 1 H); 8.49 (s, 1 H); 8.19 (d, J = 9.24 Hz, 1 H); 7.41-7.28 (m, 5 H); 6.71 (d, J = 9.34 Hz, 1 H); 4.58 (d, J = 5.76 Hz, 2 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 193.2, 154.0, 136.9, 136.4, 133.6, 130.9, 129.2, 128.1, 127.1, 117.2, 111.7, 47.1. HRMS (ESI) m/z calculated for C<sub>14</sub>H<sub>13</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>, 257.0921, found 257.0919.

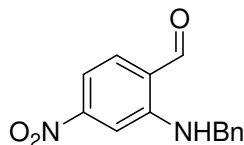
**[2-(benzylamino)-4-nitrophenyl]methanol (6h):**



The corresponding benzylic alcohol was obtained in 99% yield from corresponding 2-aminobenzoic acid **3h** (5.5 mmol) using general procedure 5. The crude alcohol (5.4 mmol) was used to form an aminor using general procedure 6 yielding the title compound **6h** as an orange solid in 72% yield over 2 steps from the benzylic alcohol. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.46 (d, J = 8.22 Hz, 1 H); 7.42 (s, 1 H); 7.40-7.32 (m, 4 H); 7.32-7.26 (m, 1 H); 7.16 (d, J = 8.10 Hz, 1 H); 5.53 (s, 1 H); 4.73 (s, 2 H); 4.42 (d, J = 5.04

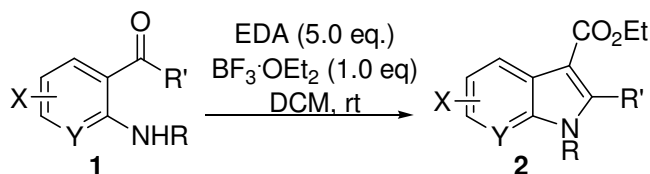
Hz, 2 H); 1.85 (s, 1 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  149.2, 148.0, 138.0, 130.3, 129.0, 128.9, 127.6, 127.5, 111.5, 105.0, 64.0, 47.7. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{14}\text{H}_{15}\text{N}_2\text{O}_3$   $[\text{M}+\text{H}]^+$ , 259.1077, found 259.1075.

### 2-(Benzylamino)-4-nitrobenzaldehyde (**1h**)



[2-(benzylamino)-4-nitrophenyl]methanol (**6h**) (3.6 mmol) was oxidized using general procedure 4 to give the title compound **1h** as a red solid in 94% yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  10.01 (s, 1 H); 8.96 (s, 1 H); 7.70 (d,  $J = 8.39$  Hz, 1 H); 7.54 (s, 1 H); 7.49 (dd,  $J = 8.37, 2.18$  Hz, 1 H); 7.46-7.30 (m, 5 H); 4.56 (d,  $J = 5.68$  Hz, 2 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  193.6, 152.3, 150.6, 137.9, 137.0, 129.0, 127.9, 127.3, 121.4, 109.3, 106.6, 46.9. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{14}\text{H}_{13}\text{N}_2\text{O}_3$   $[\text{M}+\text{H}]^+$ , 257.0921, found 257.0919.

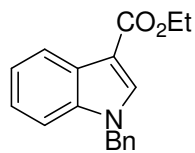
### Synthesis of indoles **2a-2o**



### General Procedure 7 for the synthesis of indoles **2a-2o**

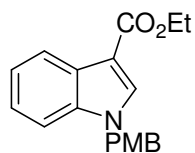
To a solution of aldehyde **1** (1.0 equiv.) and EDA (5.0 eq) in DCM (0.2 M) at  $0^\circ\text{C}$  was added  $\text{BF}_3\cdot\text{Et}_2\text{O}$  (1.0 eq) dropwise. The ice bath was removed upon completion of the addition and the solution was stirred at room temperature. The reaction is monitored by TLC of LC-MS and when complete consumption of aldehyde **1** is observed, the reaction mixture was poured into a saturated aqueous solution of  $\text{NaHCO}_3$  and it was extracted (3x) with DCM. The combined organic layers were dried over  $\text{MgSO}_4$ , filtered and concentrated *in vacuo* to yield an orange oil. The crude residue was purified by flash chromatography to yield indole **2**.

### Ethyl 1-benzylindole-3-carboxylate (**2a**)



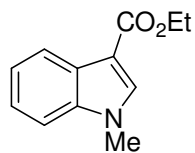
Obtained from the corresponding aldehyde **1a** (0.47 mmol) using general procedure 7 to give the title compound **2a** as a light yellow solid in 74% yield. Characterization matches that of literature.<sup>vi</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.26 (d, J = 7.64 Hz, 1 H); 7.90 (s, 1 H); 7.37-7.24 (m, 6 H); 7.19 (d, J = 6.76 Hz, 2 H); 5.37 (s, 2 H); 4.53-4.36 (m, 2 H); 1.47 (t, J = 7.10 Hz, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 164.7, 136.4, 135.6, 134.2, 128.6, 127.7, 126.6, 126.4, 122.5, 121.6, 121.4, 109.9, 107.5, 59.3, 50.3, 14.2. HRMS (ESI) m/z calculated for C<sub>18</sub>H<sub>18</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 280.1338, found 280.1344.

### Ethyl 1-(4-methoxybenzyl) indole-3-carboxylate (**2b**)



Obtained from the corresponding aldehyde **1b** (0.41 mmol) using general procedure 7 to give the title compound **2b** as a light yellow solid in 77% yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.14 (d, J = 7.54 Hz, 1 H); 7.77 (s, 1 H); 7.27 (d, J = 7.73 Hz, 1 H); 7.25-7.14 (m, 2 H); 7.05 (d, J = 8.24 Hz, 2 H); 6.79 (d, J = 8.28 Hz, 2 H); 5.19 (s, 2 H); 4.32 (dd, J = 14.22, 7.11 Hz, 2 H); 3.72 (s, 3 H); 1.36 (t, J = 7.11 Hz, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 165.7, 159.5, 136.7, 134.4, 128.6, 127.9, 126.9, 122.8, 122.0, 121.8, 114.4, 110.3, 107.7, 59.7, 55.3, 50.2, 14.6. HRMS (ESI) m/z calculated for C<sub>19</sub>H<sub>20</sub>NO<sub>3</sub> [M+H]<sup>+</sup>, 310.14377, found 310.14303.

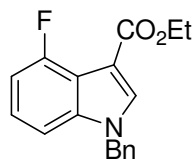
### Ethyl 1-methylindole-3-carboxylate (**2c**)



Obtained from the corresponding aldehyde **1c** (0.74 mmol) using general procedure 7 to give the title compound **2c** as a light yellow solid in 74% yield. Characterization matches that of literature.<sup>vii</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.27-8.22 (m, 1 H); 7.77 (s, 1 H); 7.33 (d, J = 3.58 Hz, 3 H); 4.43 (q, J = 7.09 Hz, 2 H); 3.76 (s, 3 H); 1.47 (t, J = 7.09 Hz,

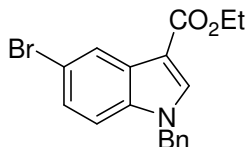
3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.6, 137.7, 135.7, 127.2, 123.2, 122.3, 122.1, 110.3, 107.6, 60.1, 33.8, 15.2. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{12}\text{H}_{14}\text{NO}_2$   $[\text{M}+\text{H}]^+$ , 204.1025, found 204.1022.

**Ethyl 1-benzyl-4-fluoroindole-3-carboxylate (2d)**



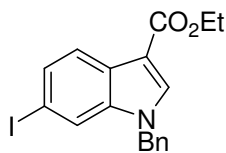
Obtained from the corresponding aldehyde **1d** (0.44 mmol) using general procedure 7 to give the title compound **2d** as a light yellow solid in 85% yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.88 (s, 1 H); 7.39-7.30 (m, 3 H); 7.22-7.07 (m, 4 H); 6.97 (dd,  $J = 10.20$ , 7.96 Hz, 1 H); 5.33 (s, 2 H); 4.40 (q,  $J = 7.10$  Hz, 2 H); 1.43 (t,  $J = 7.18$  Hz, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  163.9 (s), 157.5 (s), 155.4 (s), 139.6 (d), 135.5 (d), 129.1 (s), 128.3 (s), 127.0 (s), 123.7 (d), 114.9 (d), 108.0 (d), 107.3 (d), 106.5 (d), 60.1 (s), 51.0 (s), 14.5 (s). HRMS (ESI)  $m/z$  calculated for  $\text{C}_{18}\text{H}_{17}\text{FNO}_2$   $[\text{M}+\text{H}]^+$ , 298.12378, found 298.12455.

**Ethyl 1-benzyl-5-bromoindole-3-carboxylate (2e)**



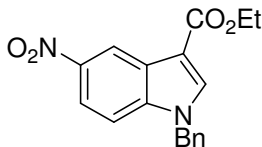
Obtained from the corresponding aldehyde **1e** (0.46 mmol) using general procedure 7 to give the title compound **2e** as a light yellow solid in 85% yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.33 (s, 1 H); 7.82 (s, 1 H); 7.46-7.14 (m, 5 H); 7.17-7.07 (m, 3 H); 5.28 (s, 2 H); 4.38 (q,  $J = 7.14$  Hz, 2 H); 1.41 (t,  $J = 7.14$  Hz, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.7, 135.6, 135.5, 135.4, 129.2, 128.5, 128.4, 127.1, 126.0, 124.6, 115.8, 111.9, 107.7, 60.1, 51.0, 14.7. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{18}\text{H}_{17}\text{BrNO}_2$   $[\text{M}+\text{H}]^+$ , 358.04372, found 358.04346.

### Ethyl 1-benzyl-6-iodoindole-3-carboxylate (**2f**)



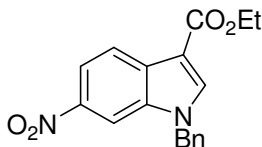
Obtained from the corresponding aldehyde **1f** (0.30 mmol) using general procedure 7 to give the title compound **2f** as a light yellow solid in 86% yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.98 (d,  $J = 8.42$  Hz, 1 H); 7.78 (s, 1 H); 7.70 (s, 1 H); 7.58 (d,  $J = 8.43$  Hz, 1 H); 7.36 (t,  $J = 6.80$  Hz, 3 H); 7.16 (d,  $J = 6.70$  Hz, 2 H); 5.31 (s, 2 H); 4.41 (dd,  $J = 14.22, 7.11$  Hz, 2 H); 1.44 (t,  $J = 7.10$  Hz, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.7, 138.0, 135.5, 134.7, 130.9, 129.1, 128.4, 127.0, 126.2, 123.5, 119.3, 108.2, 87.1, 60.0, 50.7, 14.6. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{18}\text{H}_{17}\text{INO}_2$   $[\text{M}+\text{H}]^+$ , 406.02985, found 406.02856.

### Ethyl 1-benzyl-5-nitroindole-3-carboxylate (**2g**)



Obtained from the corresponding aldehyde **1g** (0.30 mmol) using general procedure 7 to give the title compound **2g** as a light yellow solid in 84% yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  9.13 (d,  $J = 2.26$  Hz, 1 H); 8.16 (dd,  $J = 9.08, 2.29$  Hz, 1 H); 8.01 (s, 1 H); 7.41-7.35 (m, 4 H); 7.20-7.16 (m, 2 H); 5.41 (s, 2 H); 4.46 (q,  $J = 7.13$  Hz, 2 H); 1.47 (t,  $J = 7.13$  Hz, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.1, 143.7, 139.5, 137.3, 135.0, 129.4, 128.8, 127.2, 126.3, 119.1, 118.7, 110.7, 110.4, 60.5, 51.4, 14.7. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_4$   $[\text{M}+\text{H}]^+$ , 325.11828, found 325.11741.

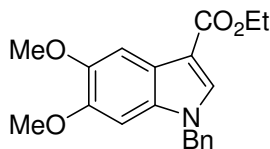
### Ethyl 1-benzyl-6-nitroindole-3-carboxylate (**2h**)



Obtained from the corresponding aldehyde **1h** (0.39 mmol) using general procedure 7 to give the title compound **2h** as a light yellow solid in 86% yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.33-8.23 (m, 2 H); 8.13 (dd,  $J = 8.92, 1.97$  Hz, 1 H); 8.08 (s, 1 H); 7.37 (d,  $J = 7.23$  Hz, 3 H); 7.21 (d,  $J = 6.81$  Hz, 2 H); 5.43 (s, 2 H); 4.42 (q,  $J = 7.12$  Hz, 2 H);

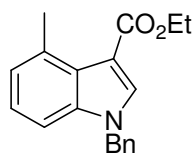
1.48-1.40 (m, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.1, 144.0, 138.8, 135.5, 134.8, 131.5, 129.3, 128.7, 127.2, 122.1, 117.2, 108.9, 107.2, 60.3, 51.2, 14.5. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_4$   $[\text{M}+\text{H}]^+$ , 325.1183, found 325.1184.

**Ethyl 1-benzyl-5,6-dimethoxyindole-3-carboxylate (2i)**



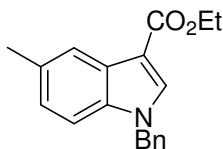
Obtained from the corresponding aldehyde **1i** (0.18 mmol) using general procedure 7 to give the title compound **2i** as a light yellow solid in 52% yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.73 (s, 1 H); 7.72 (s, 1 H); 7.39-7.28 (m, 3 H); 7.17 (d,  $J = 7.01$  Hz, 2 H); 6.74 (s, 1 H); 5.32 (s, 2 H); 4.40 (q,  $J = 7.12$  Hz, 2 H); 4.00 (s, 3 H); 3.87 (s, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.3, 147.5, 146.7, 136.0, 132.5, 131.0, 129.0, 128.1, 126.9, 120.1, 107.4, 103.0, 93.5, 59.6, 56.2, 50.9, 14.6. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{20}\text{H}_{22}\text{NO}_4$   $[\text{M}+\text{H}]^+$ , 340.1543, found 340.1544.

**Ethyl 1-benzyl-4-methylindole-3-carboxylate (2j)**



Obtained from the corresponding aldehyde **1j** (0.44 mmol) using general procedure 7 to give the title compound **2j** as a light yellow solid in 57% yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.92 (s, 1 H); 7.39-7.28 (m, 3 H); 7.18-7.14 (m, 4 H); 7.07 (t,  $J = 4.11$  Hz, 1 H); 5.35 (s, 2 H); 4.37 (q,  $J = 7.11$  Hz, 2 H); 2.92 (s, 3 H); 1.42 (t,  $J = 7.11$  Hz, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.8, 137.6, 136.2, 135.8, 132.9, 129.1, 128.1, 127.0, 125.6, 124.1, 123.2, 108.9, 108.1, 59.9, 50.8, 22.7, 14.6. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{19}\text{H}_{20}\text{NO}_2$   $[\text{M}+\text{H}]^+$ , 294.14886, found 294.14873.

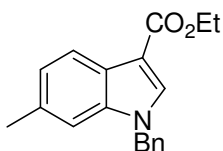
**Ethyl 1-benzyl-5-methylindole-3-carboxylate (2k)**



Obtained from the corresponding aldehyde **1k** (0.44mmol) using general procedure 7 to give the title compound **2k** as a light yellow solid in 71% yield.  $^1\text{H}$  NMR (400 MHz,

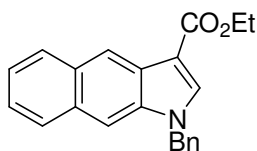
CDCl<sub>3</sub>):  $\delta$  7.78 (s, 1 H); 7.59 (s, 1 H); 7.13-7.00 (m, 3 H); 6.98-6.87 (m, 3 H); 6.83 (d,  $J = 8.42$  Hz, 1 H); 5.08 (s, 2 H); 4.16 (q,  $J = 7.11$  Hz, 2 H); 2.26 (s, 3 H); 1.19 (t,  $J = 7.11$  Hz, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  165.25, 136.15, 135.17, 134.55, 131.56, 128.98, 128.10, 127.17, 127.01, 124.50, 121.50, 110.02, 107.28, 59.69, 50.76, 21.63, 14.67. HRMS (ESI)  $m/z$  calculated for C<sub>19</sub>H<sub>20</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 294.14886, found 294.14857.

**Ethyl 1-benzyl-6-methylindole-3-carboxylate (2l)**



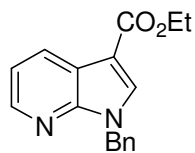
Obtained from the corresponding aldehyde **1l** (0.44 mmol) using general procedure 7 to give the title compound **2l** as a light yellow solid in 72% yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.12 (d,  $J = 8.10$  Hz, 1 H); 7.82 (s, 1 H); 7.40-7.31 (m, 3 H); 7.22-7.12 (m, 4 H); 5.33 (s, 2 H); 4.42 (q,  $J = 7.12$  Hz, 2 H); 2.49 (s, 3 H); 1.50-1.42 (t, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  165.2, 137.2, 136.2, 134.1, 132.9, 129.0, 128.1, 127.0, 124.7, 123.8, 121.5, 110.2, 107.8, 59.7, 50.5, 21.9, 14.7. HRMS (ESI)  $m/z$  calculated for C<sub>19</sub>H<sub>20</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 294.14886, found 294.14865.

**Ethyl 1-benzyl-benzo[*f*]indole-3-carboxylate (2m)**



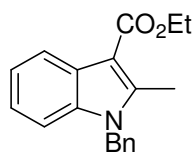
Obtained from the corresponding aldehyde **1m** (0.38 mmol) using general procedure 7 to give the title compound **2m** as a white solid in 80% yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.77 (s, 1 H); 8.09 (s, 2 H); 7.93-7.87 (m, 1 H); 7.73 (s, 1 H); 7.46-7.41 (m, 2 H); 7.39-7.31 (m, 3 H); 7.25-7.19 (m, 2 H); 5.43 (s, 2 H); 4.49 (q,  $J = 7.11$  Hz, 2 H); 1.51 (t,  $J = 7.11$  Hz, 3 H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  165.0, 138.9, 137.2, 135.9, 130.3, 129.9, 129.1, 128.6, 128.2, 127.6, 127.4, 127.1, 124.6, 123.7, 119.9, 106.9, 106.3, 59.9, 50.8, 14.7. HRMS (ESI)  $m/z$  calculated for C<sub>22</sub>H<sub>20</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 330.14866, found 330.14858.

### Ethyl 1-benzyl-7-azaindole-3-carboxylate (**2n**)



Obtained from the corresponding aldehyde **1n** (0.26 mmol) using general procedure 7 to give the title compound **2n** as a white solid in 52% yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.43 (d,  $J = 8.00$  Hz, 1 H); 8.39 (d,  $J = 4.73$  Hz, 1 H); 8.04-7.75 (m, 1 H); 7.26-7.11 (m, 6 H); 5.43 (s, 2 H); 4.34 (q,  $J = 7.14$  Hz, 2 H); 1.35 (t,  $J = 7.16$  Hz, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.3, 147.9, 144.1, 136.6, 133.9, 129.9, 128.8, 128.0, 127.8, 119.0, 118.1, 106.4, 59.9, 48.2, 14.6. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_2$   $[\text{M}+\text{H}]^+$ , 281.12845, found 281.12906.

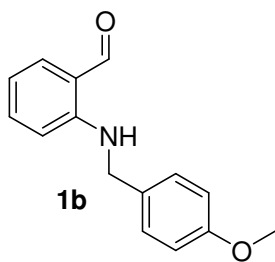
### Ethyl 1-benzyl-2-methylindole-3-carboxylate (**2o**)



Obtained from the corresponding aldehyde **1o** (0.26 mmol) using general procedure 7 to give the title compound **2o** as a white solid in 46% yield. Characterization matches that of literature.<sup>viii</sup>  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.21 (d,  $J = 7.96$  Hz, 1 H); 7.33-7.19 (m, 6 H); 7.05-6.99 (m, 2 H); 5.40 (s, 2 H); 4.46 (q,  $J = 7.12$  Hz, 2 H); 2.78 (s, 3 H); 1.51 (t,  $J = 7.11$  Hz, 3 H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  166.2, 145.2, 136.4, 129.0, 127.7, 126.8, 126.0, 122.3, 121.8, 121.6, 121.6, 109.5, 104.7, 59.5, 46.5, 14.7, 11.9. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{19}\text{H}_{20}\text{NO}_2$   $[\text{M}+\text{H}]^+$ , 294.14886, found 294.14897.

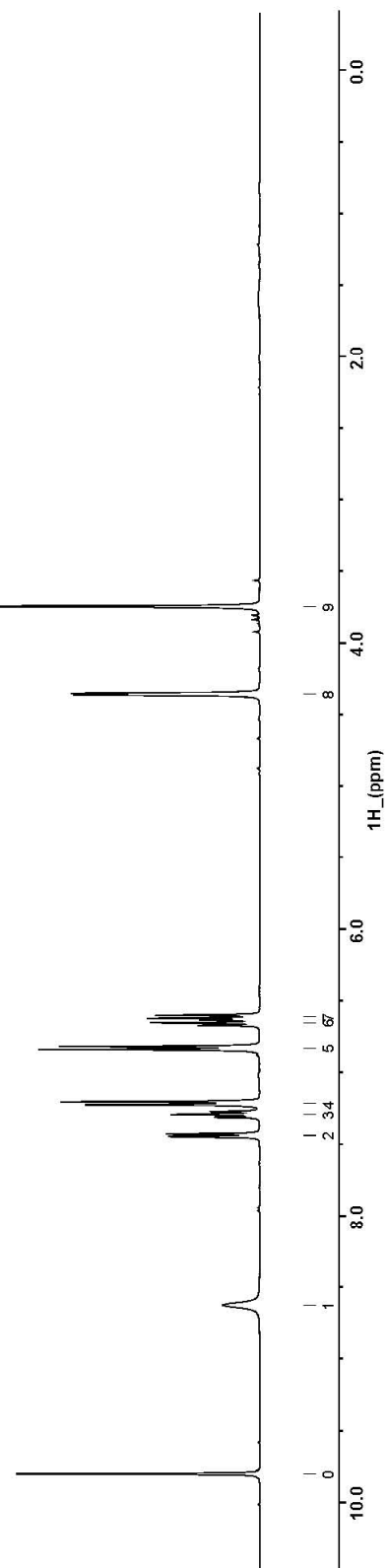
- 
- (i) Yotphan, S.; Bergman, R. G.; Ellman, J. A. *Org. Lett.* **2009**, 7, 1511.
  - (ii) Lee, Y. R.; Hung, T. V. *Tetrahedron* **2008**, 64, 7338.
  - (iii) Fadda, A. A.; Abdelrazek, F. M.; El-Habbal, M. M. *Indian J. Chem., Sect B* **1986**, 25B, 194.
  - (iv) Bella, A. F.; Slawin, A. M. Z.; Walton, J. C. *J. Org. Chem.* **2004**, 69, 5926.
  - (v) Yang, D.; Guo, W.; Cai, Y.; Jiang, L.; Jiang, K.; Wu, X. *Heteroatom Chemistry* **2008**, 19, 229.
  - (vi) Farghaly, A.-R. A. H. *J. Chin. Chem. Soc.*, **2004**, 51, 147.
  - (vii) Majchrzak, M. J.; Simchen, G. *Synthesis* **1986**, 956.
  - (viii) Patent application, Beard, R. L.; Donello, J. E.; Yuan, H.; Colon, D. F.; Duong, T.; Liu, X.; Hu, Y. U.S. Patent 60,774,102, **2006**.

# Copies of $^1\text{H}$ and $^{13}\text{C}$ Spectra

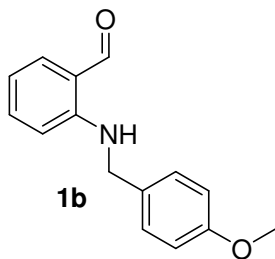


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 Proton Characterization of 2-amino-PMB-benzaldehyde

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4	7.21	d	1.99	8.19
5	6.83	d	1.95	8.28
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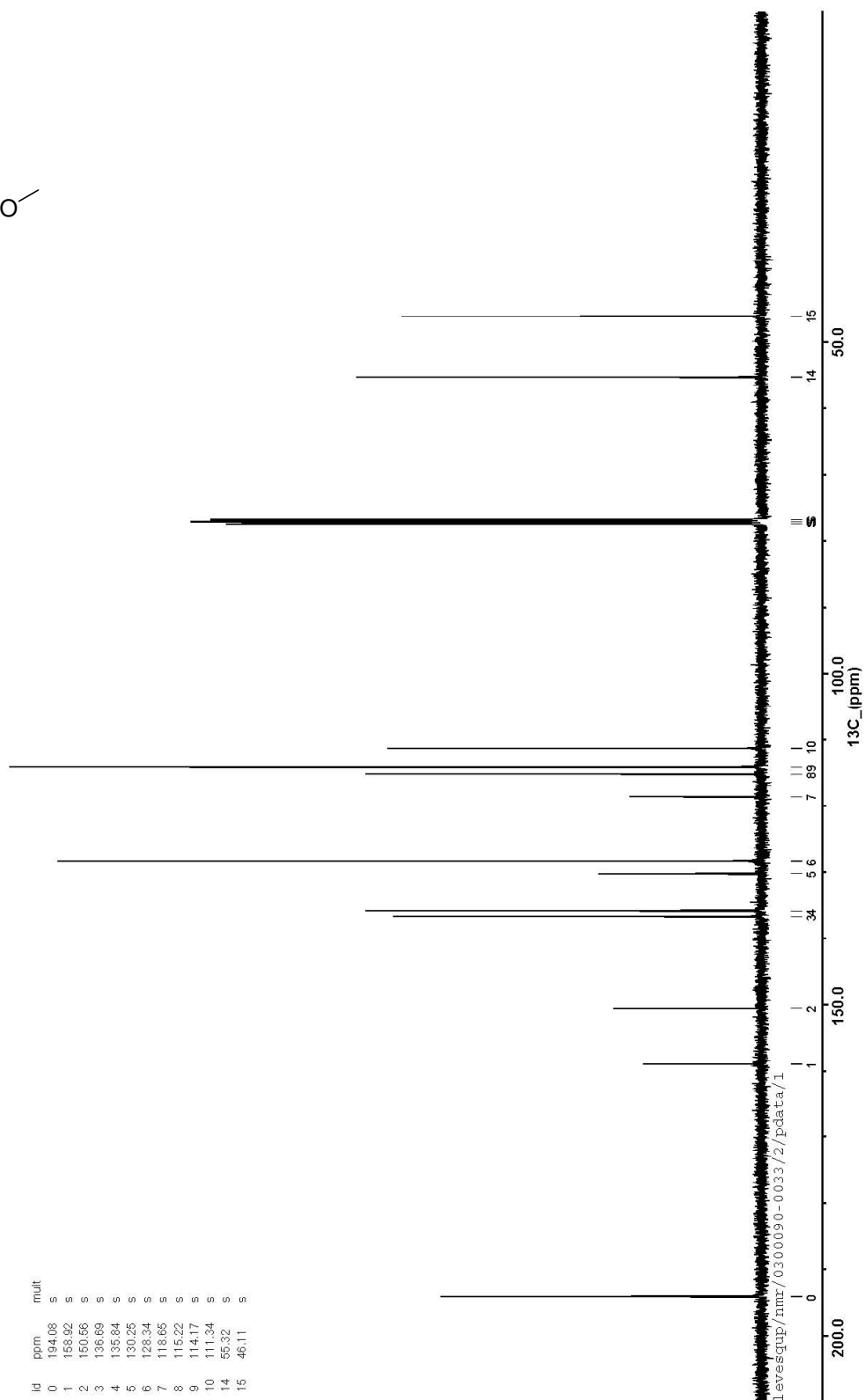


$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of 2-[(4-methoxyphenyl)methylamino]benzaldehyde (**1b**)

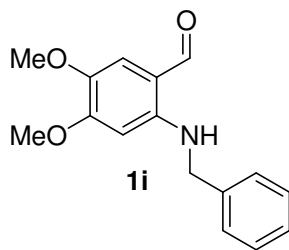


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 Carbon Characterization of 2-amino-PMB-benzaldehyde

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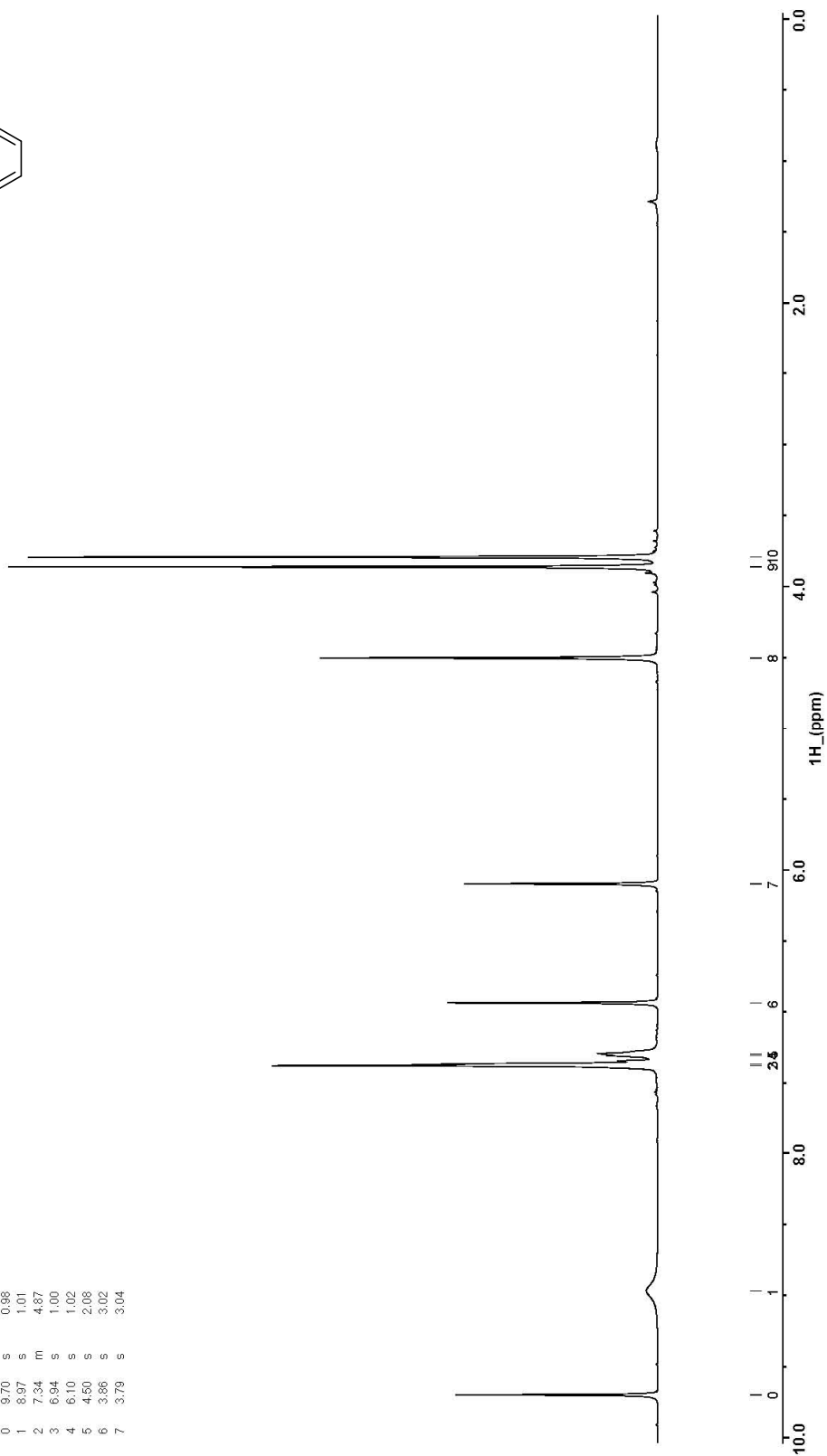
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of 2-[(4-methoxyphenyl)methylamino]benzaldehyde (**1b**)



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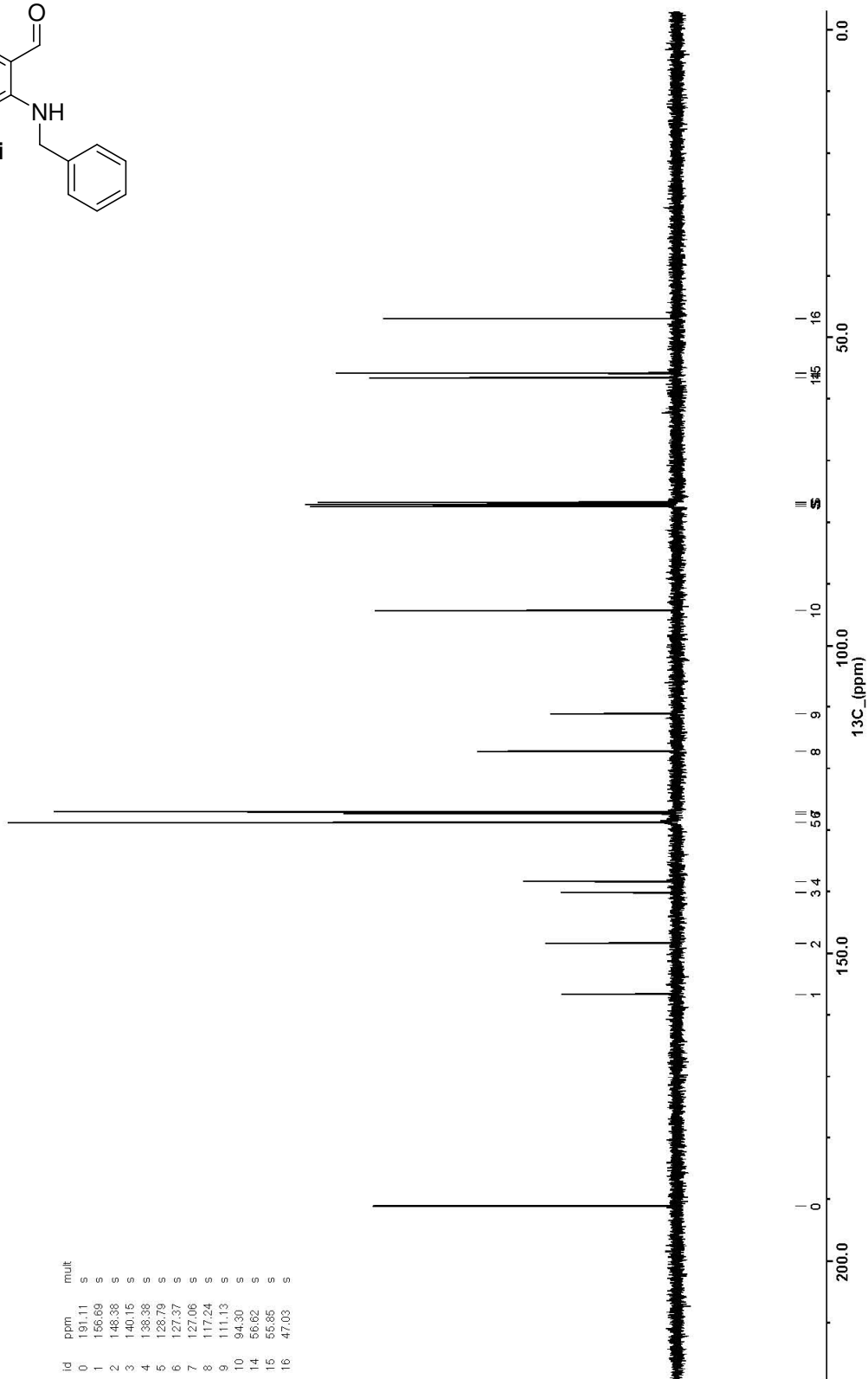
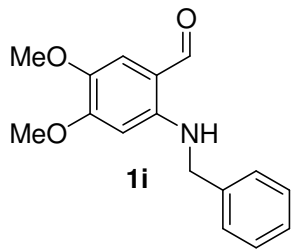


<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of 2-(benzylamino)-4,5-dimethoxy-benzaldehyde (**1i**)

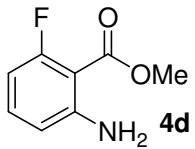
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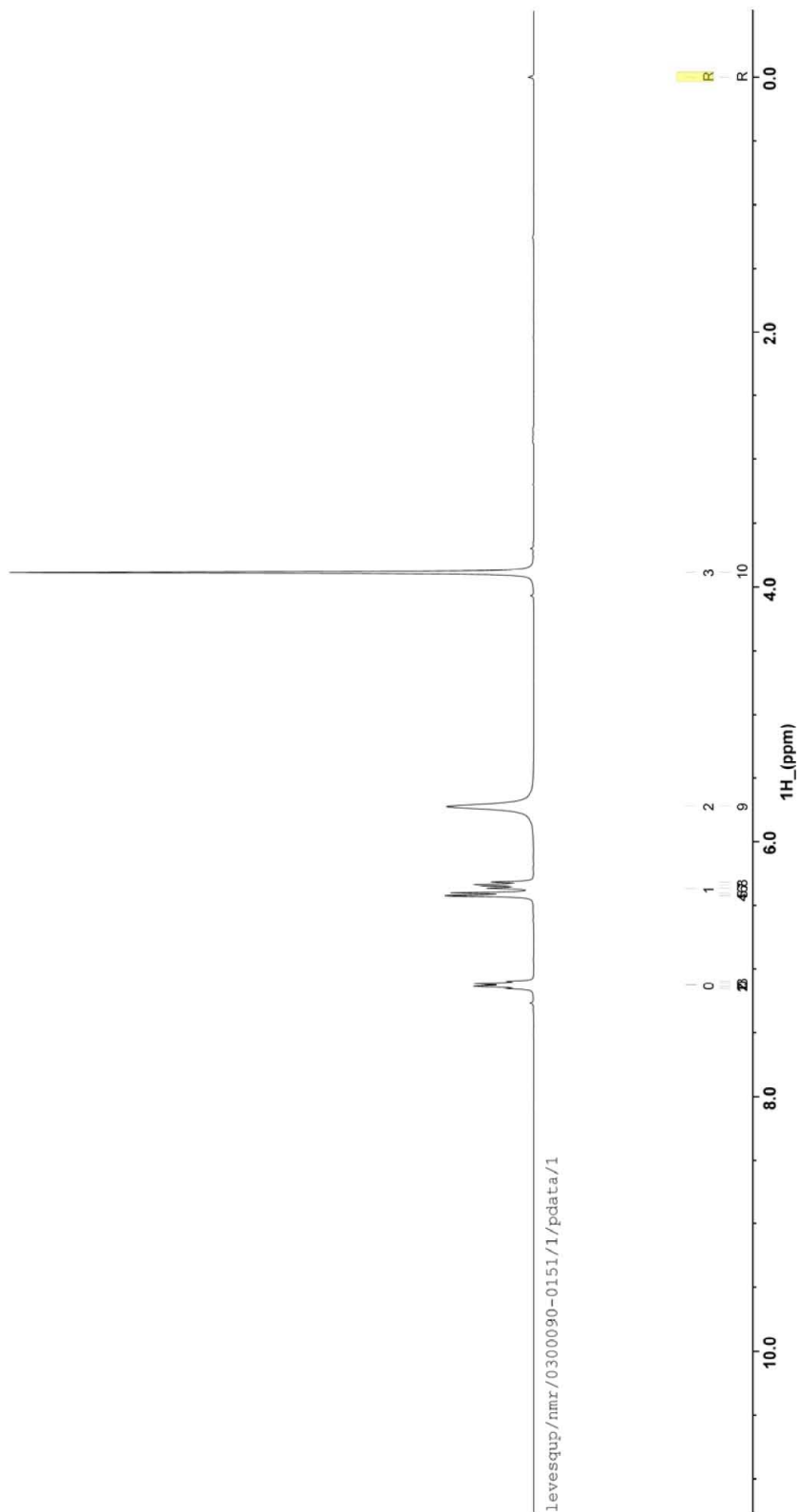
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of 2-(benzylamino)-4,5-dimethoxy-benzaldehyde (**1i**)



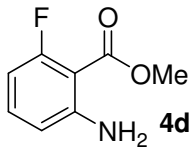
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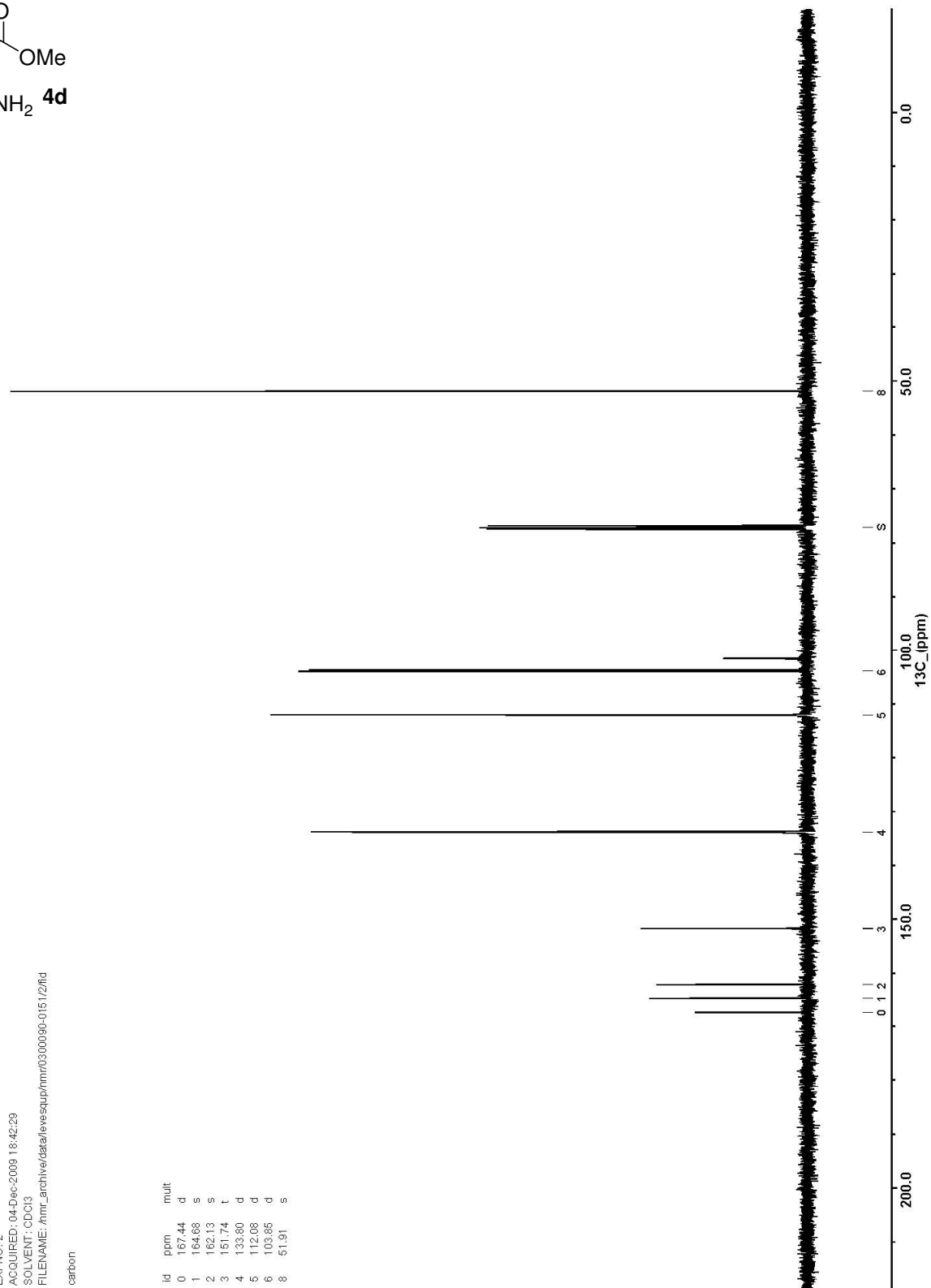
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of methyl 2-amino-6-fluorobenzoate (**4d**)



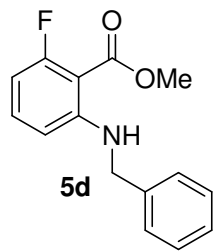
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carbon

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8	51.91	s



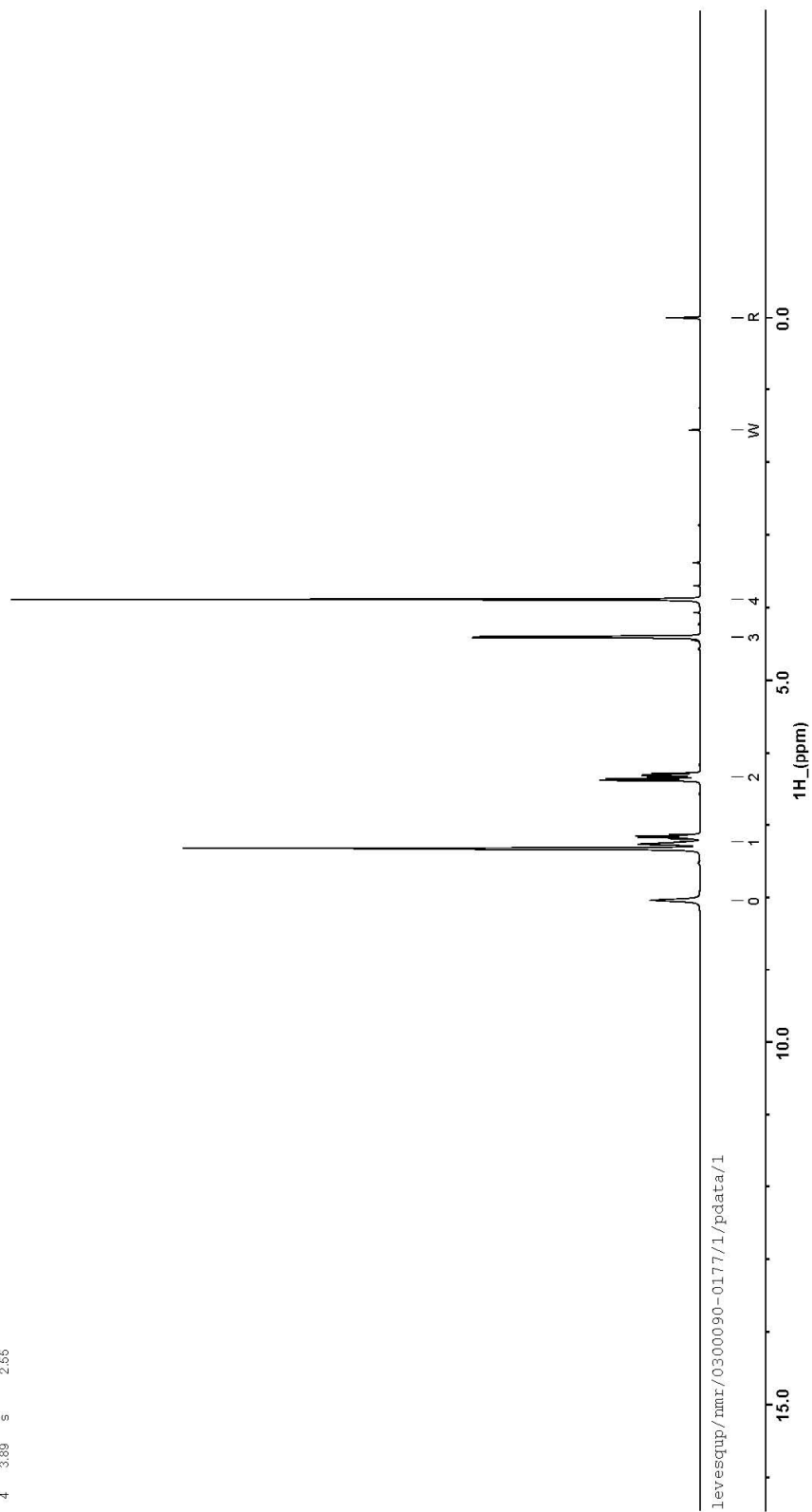
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of methyl 2-amino-6-fluorobenzoate (**4d**)



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4	3.89	s	2.85	

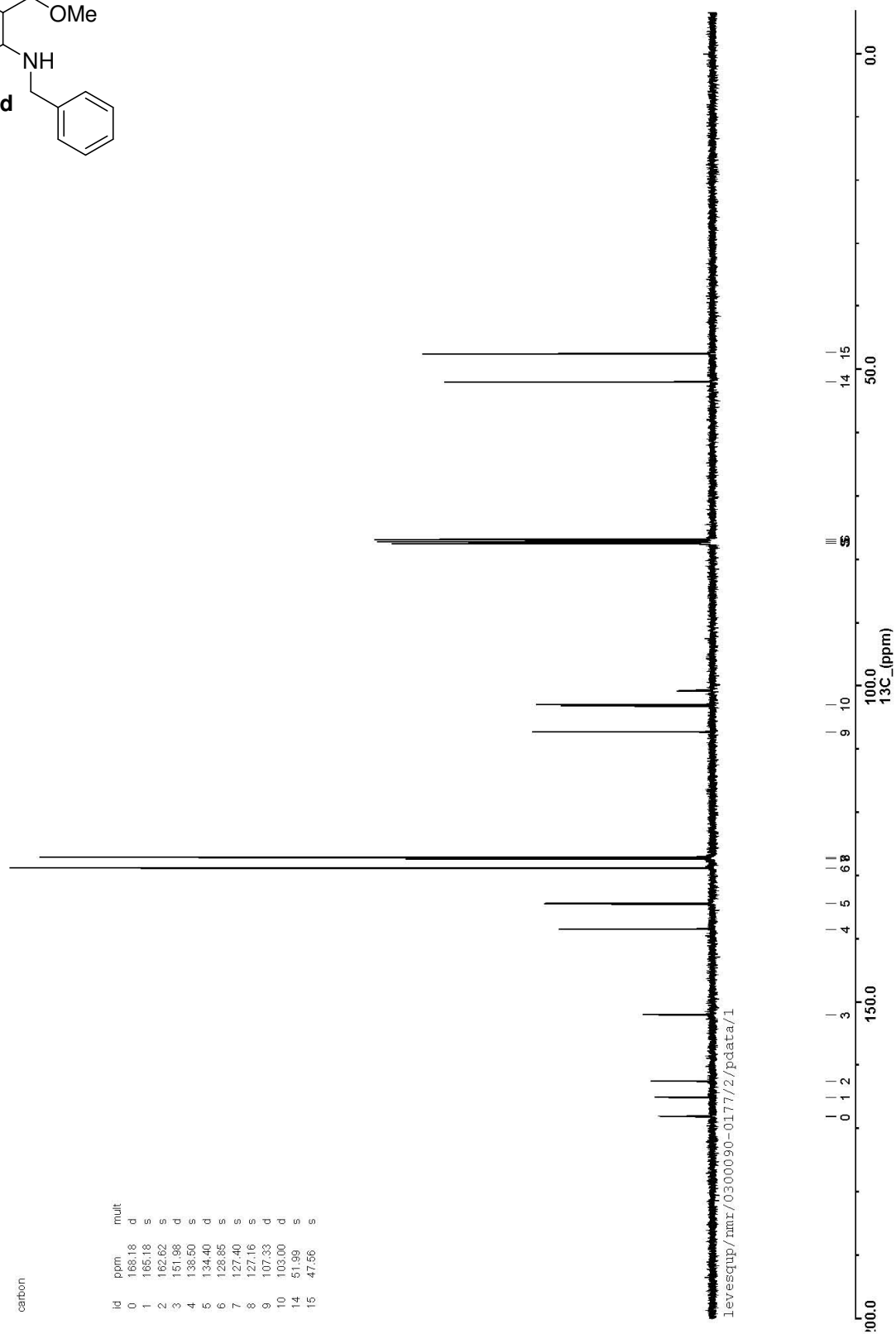
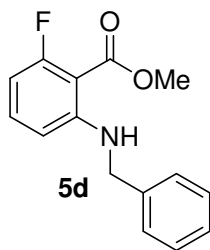


$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of methyl 2-(benzylamino)-6-fluorobenzoate (**5d**)

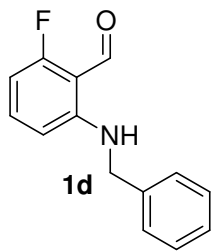
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carbon

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7	127.40	s
8	127.16	s
9	107.33	d
10	103.00	d
14	51.99	s
15	47.56	s



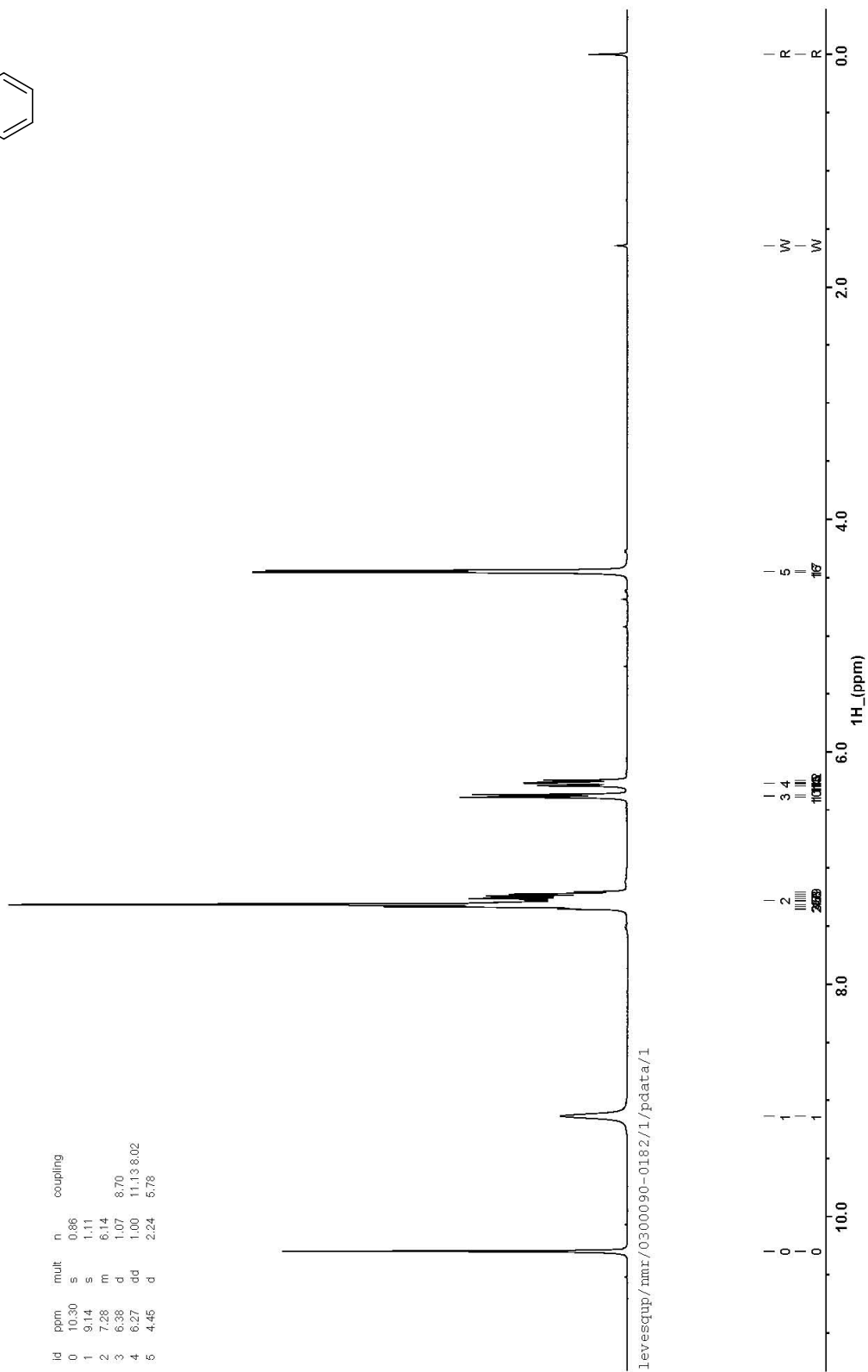
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of methyl 2-(benzylamino)-6-fluorobenzoate (**5d**)



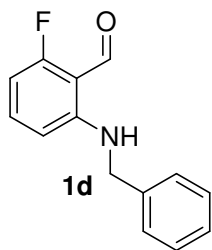
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 BOOK: 0300090-0182  
 EXPNO: 1  
 ACQUIRED: 21-Dec-2009 07:45:25  
 SOLVENT: CDCl3  
 FILENAME: rml\_archive\data\levesq\nmr\0300090-0182/1fid

proton

ld	ppm	mult	n	coupling
0	10.30	s	0.86	
1	9.14	s	1.11	
2	7.28	m	6.14	
3	6.38	d	1.07	8.70
4	6.27	dd	1.00	11.13-8.02
5	4.45	d	2.24	5.78



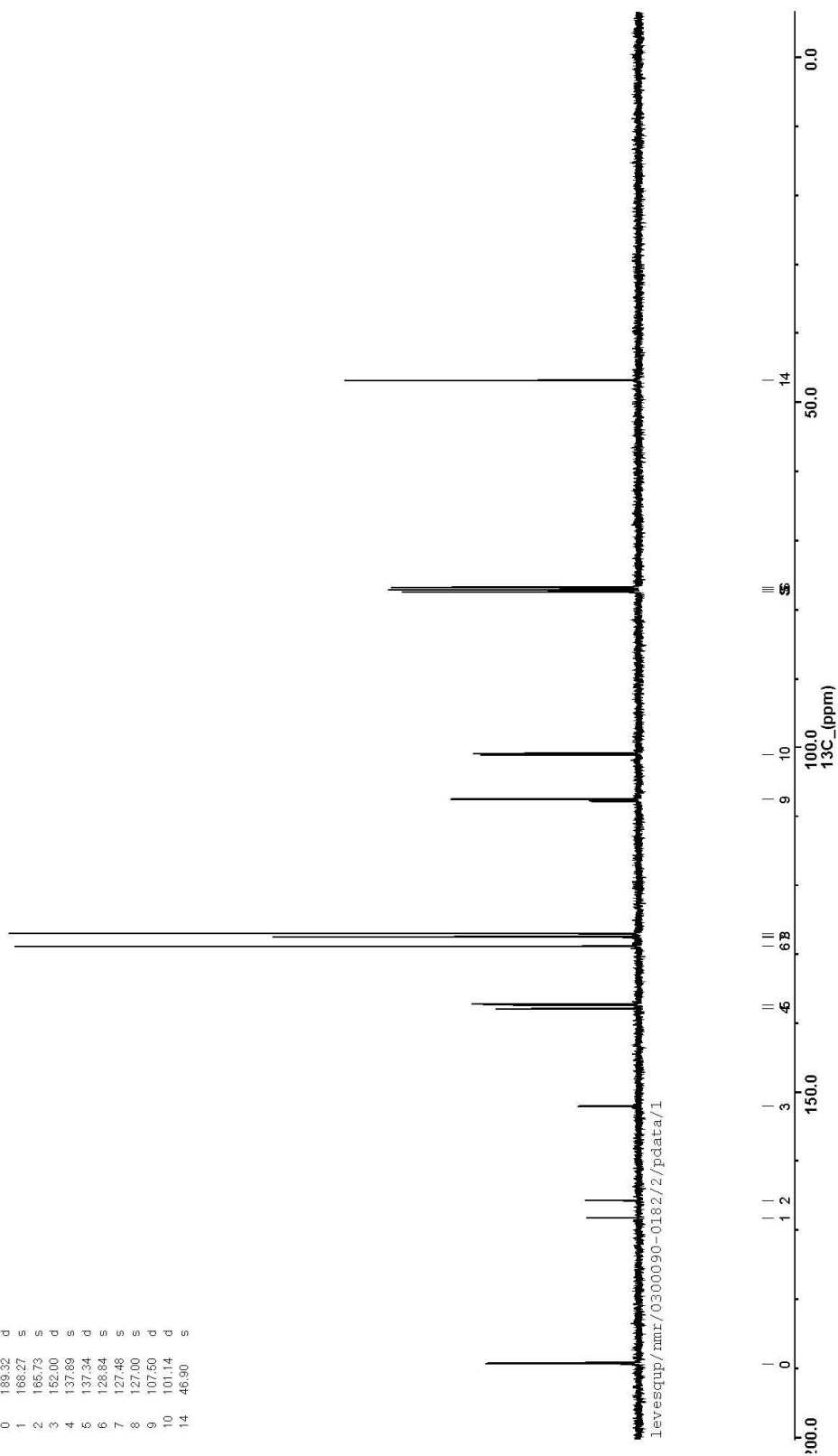
<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of 2-(benzylamino)-6-fluorobenzaldehyde (**1d**)



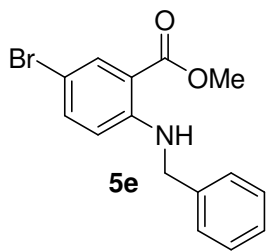
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 SOLVENT: CDCl3  
 FILENAME: rmt\_archive\data\levesq\nmr\0300090-0182\fid

carbon

id	ppm	mult
0	189.32	d
1	168.27	s
2	165.73	s
3	152.00	d
4	137.89	s
5	137.34	d
6	128.84	s
7	127.48	s
8	127.00	s
9	107.50	d
10	101.14	d
14	46.90	s



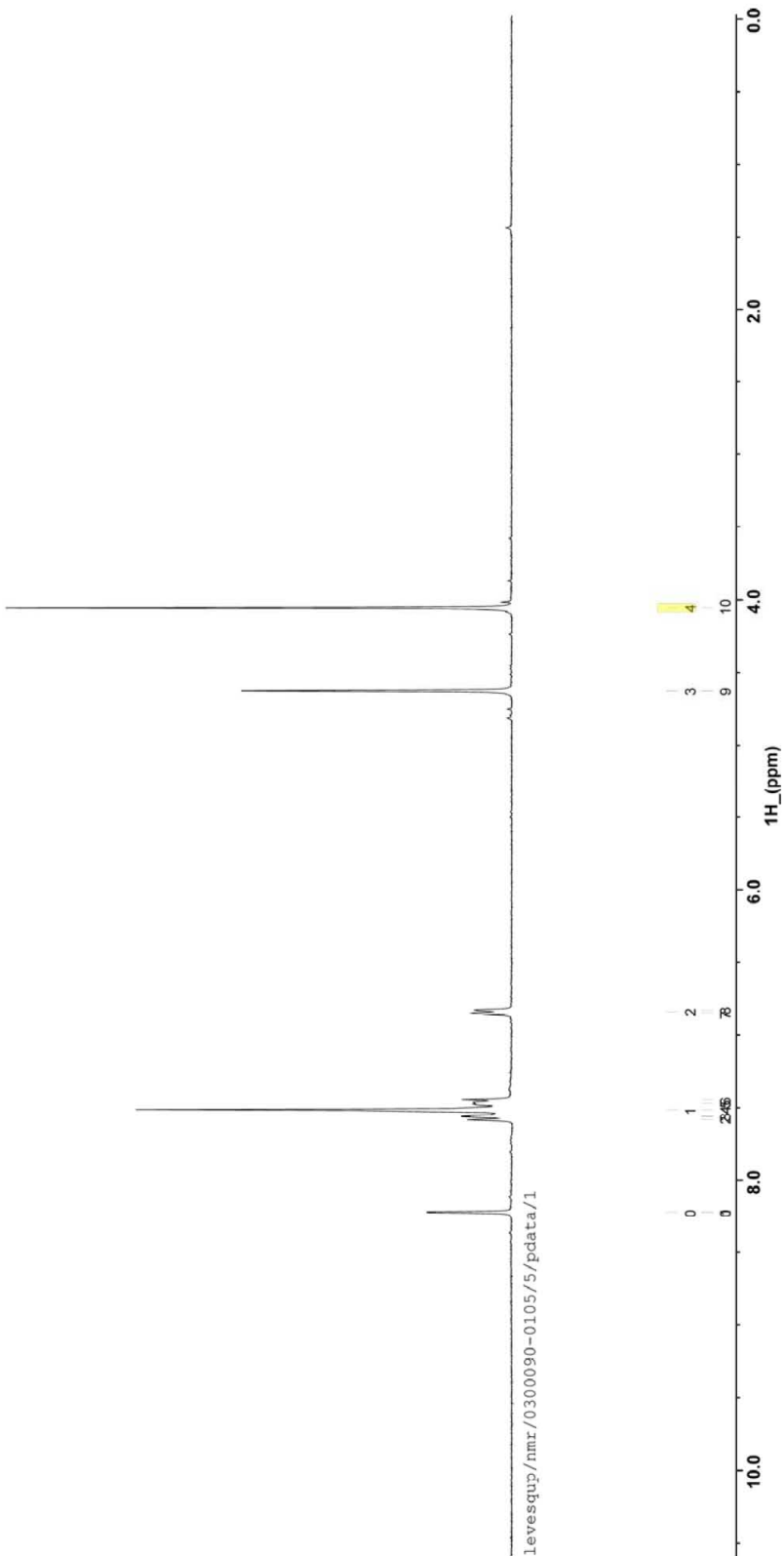
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of 2-(benzylamino)-6-fluorobenzaldehyde (**1d**)



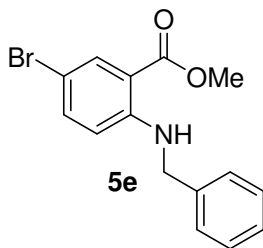
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 ACQUIRED: 12-Nov-2009 13:18:40  
 SOLVENT: CDCl3  
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proton

id	ppm	mult	n	coupling
0	8.22	d	1.00	2.38
1	7.51	m	6.44	
2	6.84	d	1.21	9.00
3	4.52	s	2.17	
4	4.05	s	3.14	



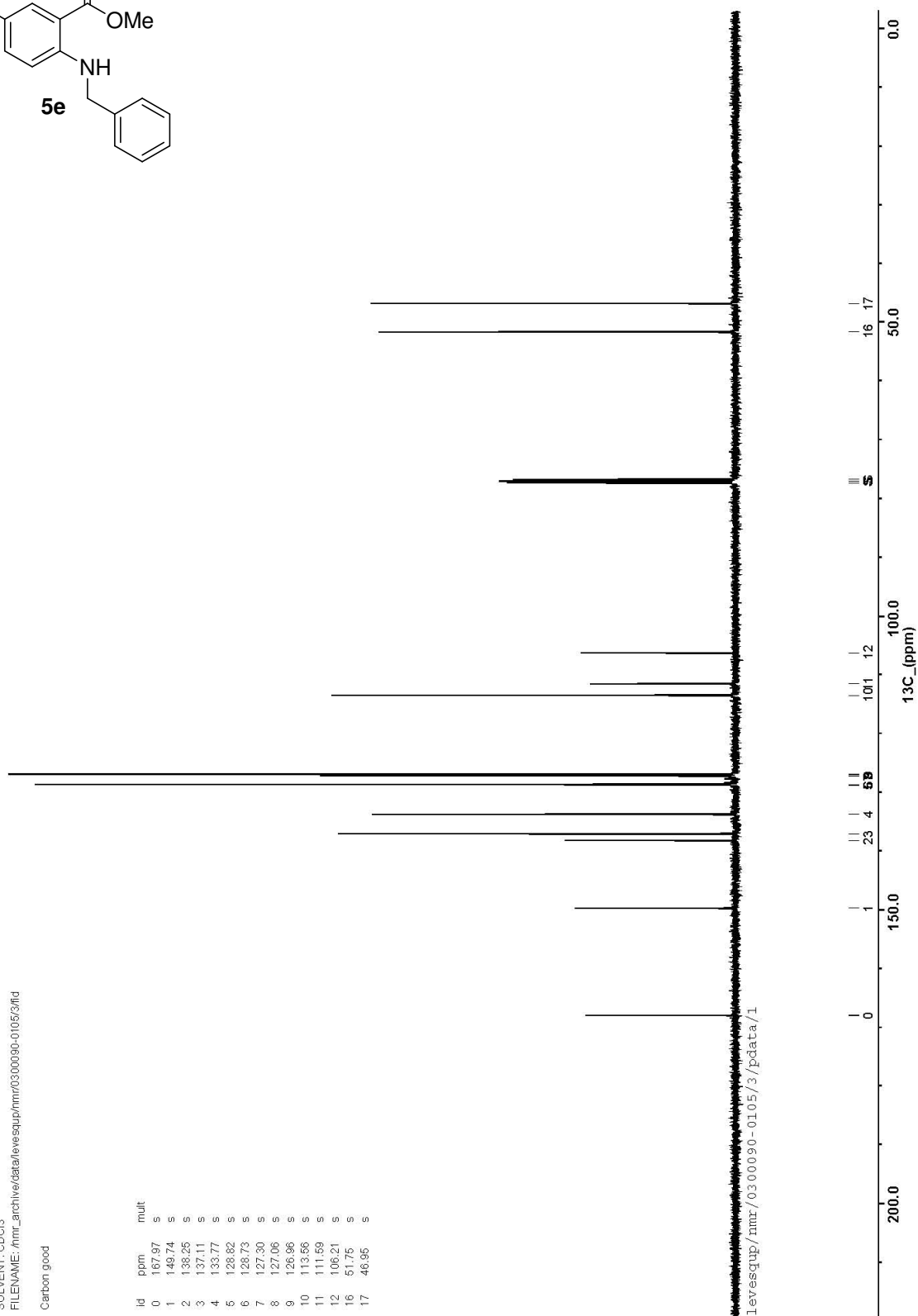
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of methyl 2-(benzylamino)-5-bromobenzoate (**5e**)



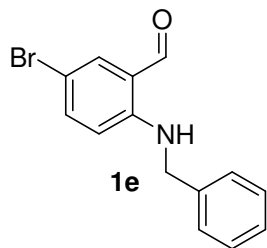
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Carbon good

id	ppm	mult
0	167.97	s
1	149.74	s
2	138.25	s
3	137.11	s
4	133.77	s
5	128.82	s
6	128.73	s
7	127.30	s
8	127.06	s
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10	113.66	s
11	111.59	s
12	106.21	s
16	51.75	s
17	46.95	s



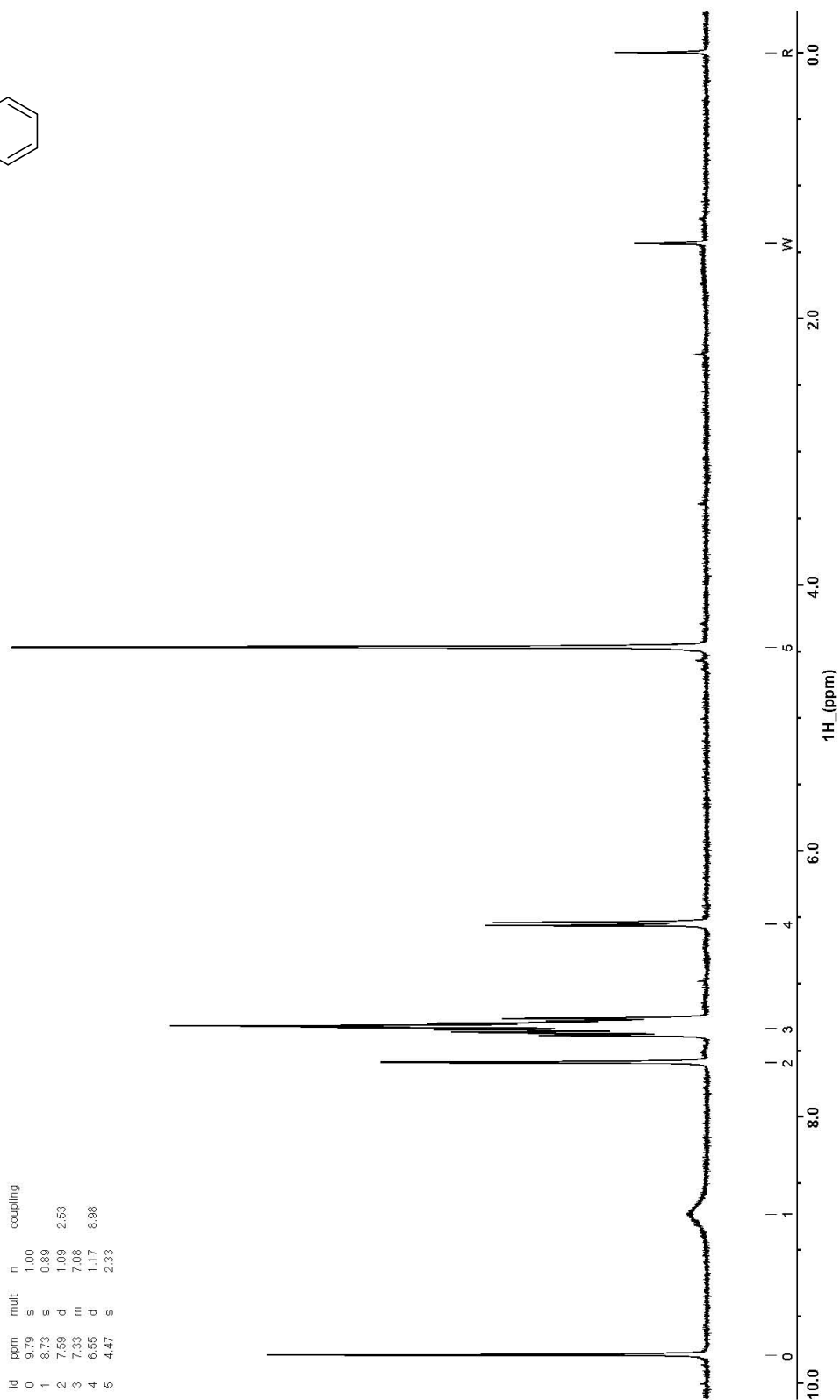
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of methyl 2-(benzylamino)-5-bromobenzoate (**5e**)



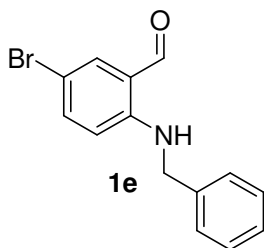
USER: lvevsq  
 BOOK: 0300090-0115  
 EXPNO: 4  
 ACQUIRED: 13-Nov-2009 14:27:09  
 SOLVENT: CDCl3  
 FILENAME: rml\_archive\data/lvevsq/rmr0300090-0115/4fid

proton tms

ld	ppm	mult	n	coupling
0	9.79	s	1.00	
1	8.73	s	0.89	
2	7.59	d	1.09	2.53
3	7.33	m	7.08	
4	6.55	d	1.17	8.98
5	4.47	s	2.33	



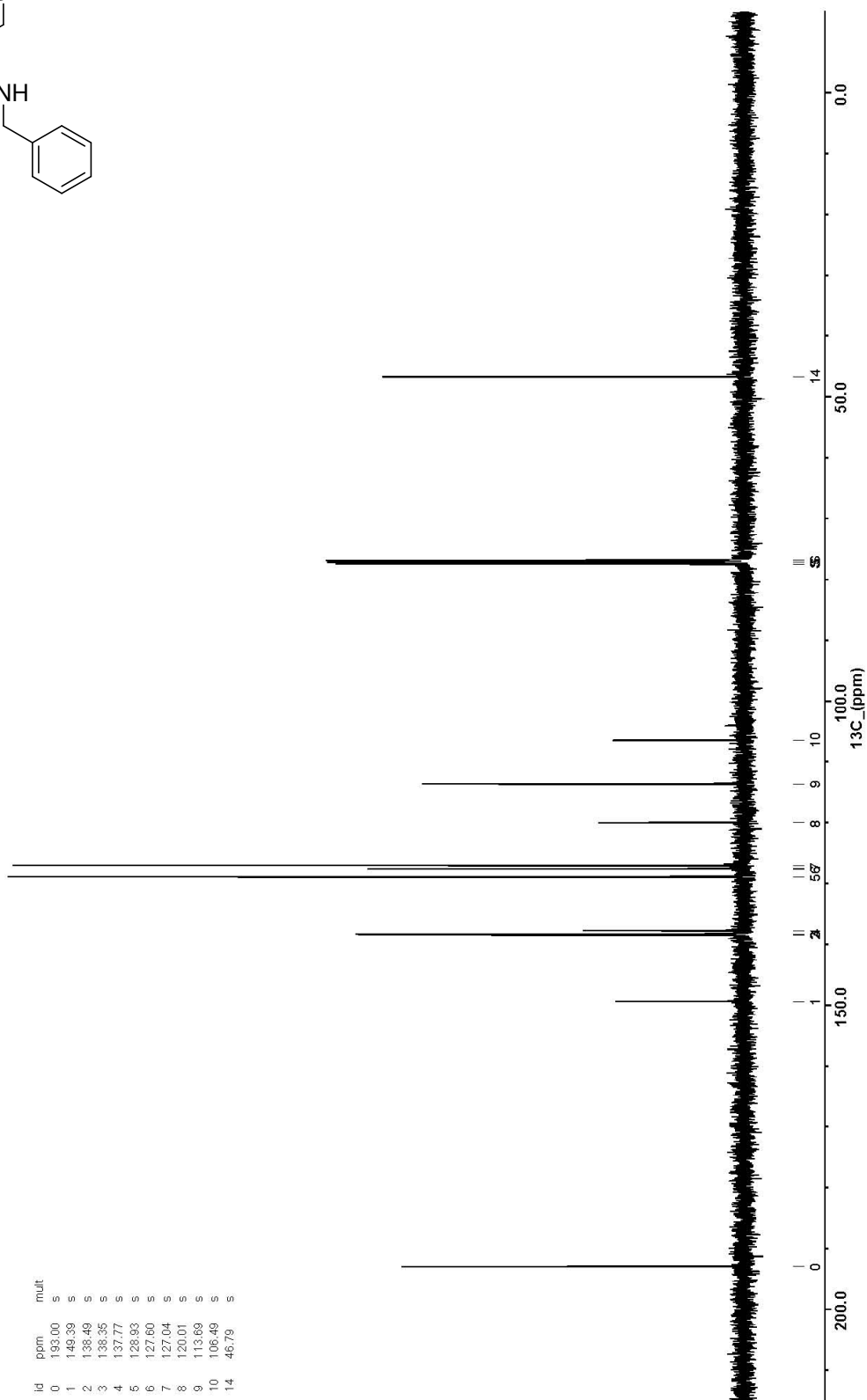
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of 2-(benzylamino)-5-bromobenzaldehyde (**1e**)



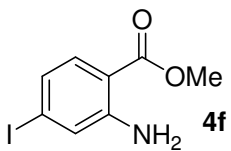
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 EXPNO: 2  
 ACQUIRED: 13-Nov-2009 14:10:08  
 SOLVENT: CDCl3  
 FILENAME: rml\_archive\data\levesq\mrmr0300090-01152.fid

carbon

id	ppm	mult
0	193.00	s
1	149.39	s
2	138.49	s
3	138.35	s
4	137.77	s
5	128.83	s
6	127.60	s
7	127.04	s
8	120.01	s
9	113.69	s
10	106.49	s
14	46.79	s



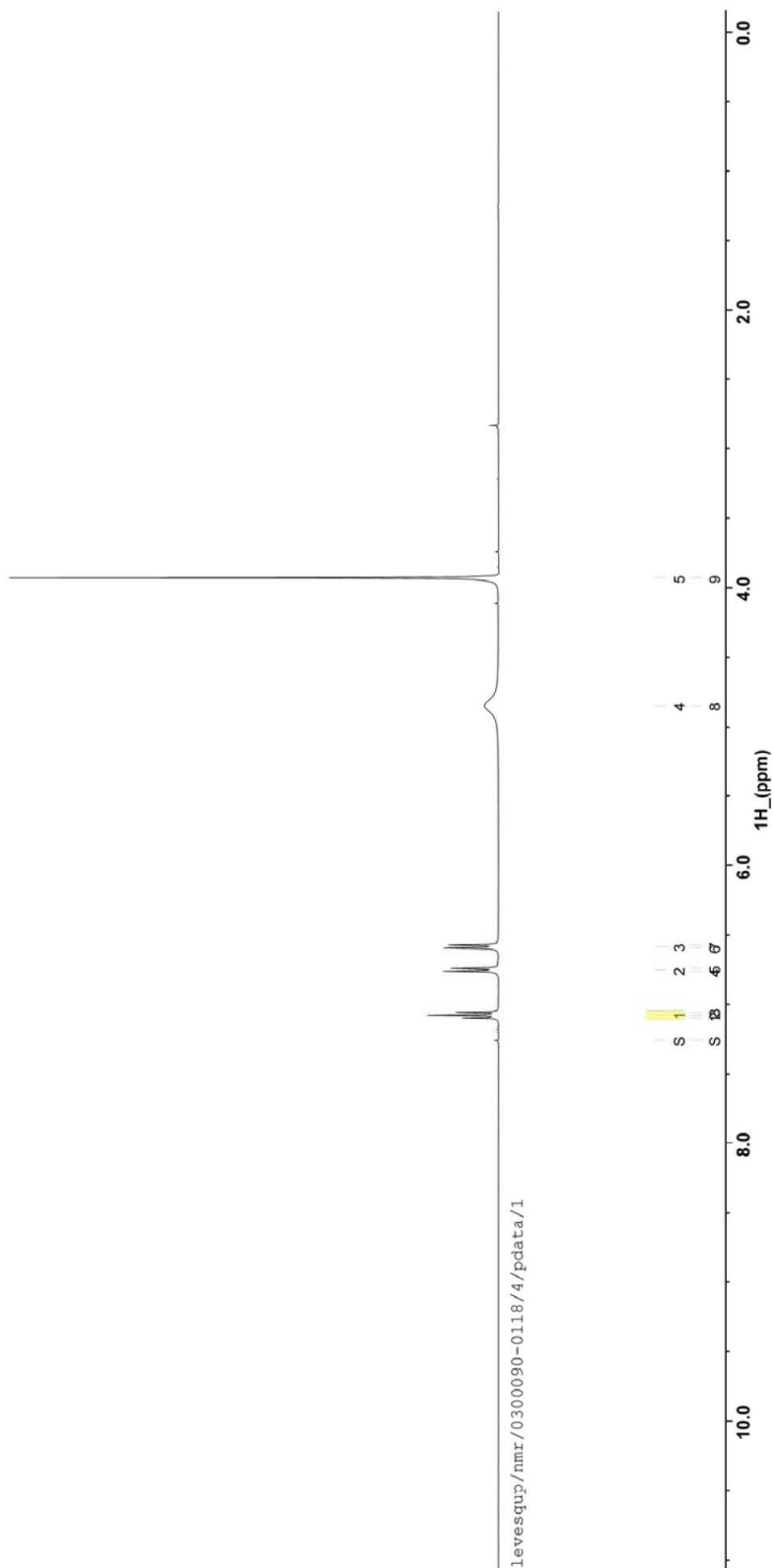
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of 2-(benzylamino)-5-bromobenzaldehyde (**1e**)



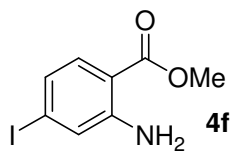
USER: levesq  
 BOOK: 0300090-0118  
 EXPNO: 4  
 ACQUIRED: 17-Nov-2009 14:18:20  
 SOLVENT: CDCl3  
 FILENAME: nmr\_archive\data/levesq/nmr/0300090-0118/1d

proton

id	ppm	mult	n	coupling
1	7.98	m	0.87	
2	6.75	d	1.00	7.86
3	6.58	d	1.07	8.28
4	4.95	s	2.39	
5	3.93	s	2.49	



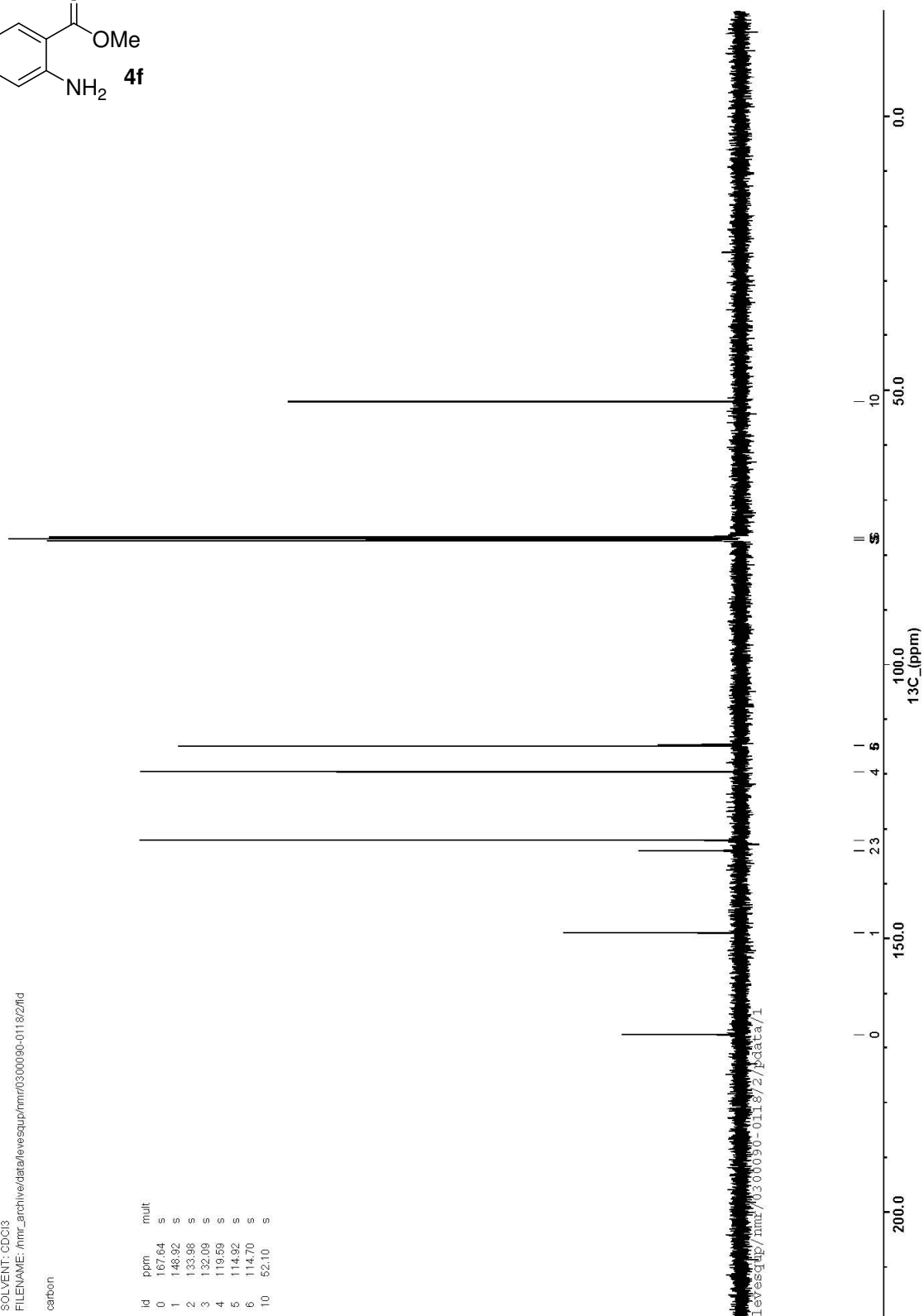
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of methyl 2-amino-4-iodobenzoate (**4f**)



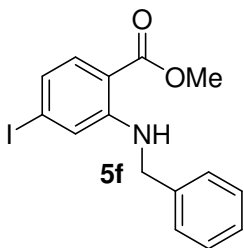
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 BOOK: 0300090-0118  
 EXPNO: 2  
 ACQUIRED: 17.Nov.2009 12:41:01  
 SOLVENT: CDCl3  
 FILENAME: nmr\_archive\data\levesqtp\nmr\0300090-0118/2fid

carbon

id	ppm	mult
0	167.64	s
1	148.92	s
2	133.86	s
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4	119.69	s
5	114.92	s
6	114.70	s
10	52.10	s



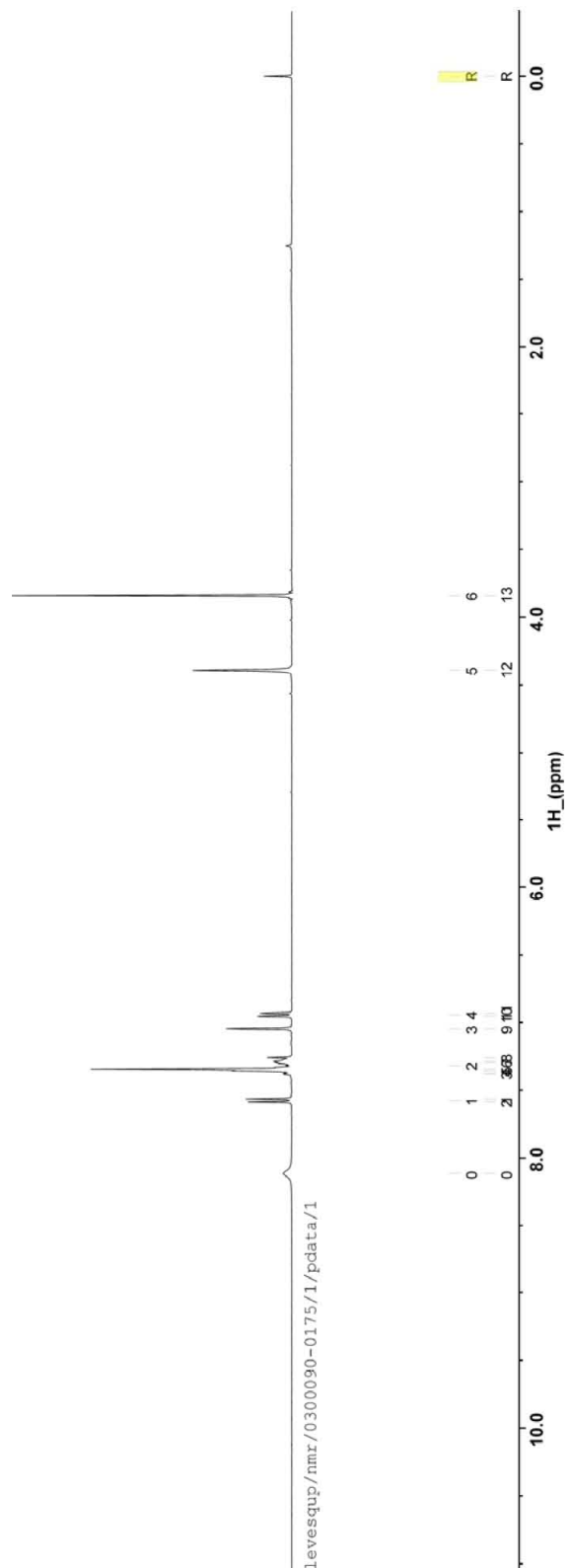
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of methyl 2-amino-4-iodobenzoate (**4f**)



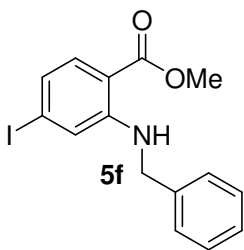
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 BOOK: 0300090-0175  
 EXPNO: 1  
 ACQUIRED: 16-Dec-2009 18:33:38  
 SOLVENT: CDCl3  
 FILENAME: nmr\_archive\data\levesq\nmr\0300090-0175\1.fid

proton

id	ppm	mult	n	coupling
0	8.11	s	0.91	
1	7.57	d	1.00	8.43
2	7.32	m	4.78	
3	7.05	s	1.06	
4	6.94	d	1.01	8.47
5	4.39	s	2.03	
6	3.84	s	3.12	



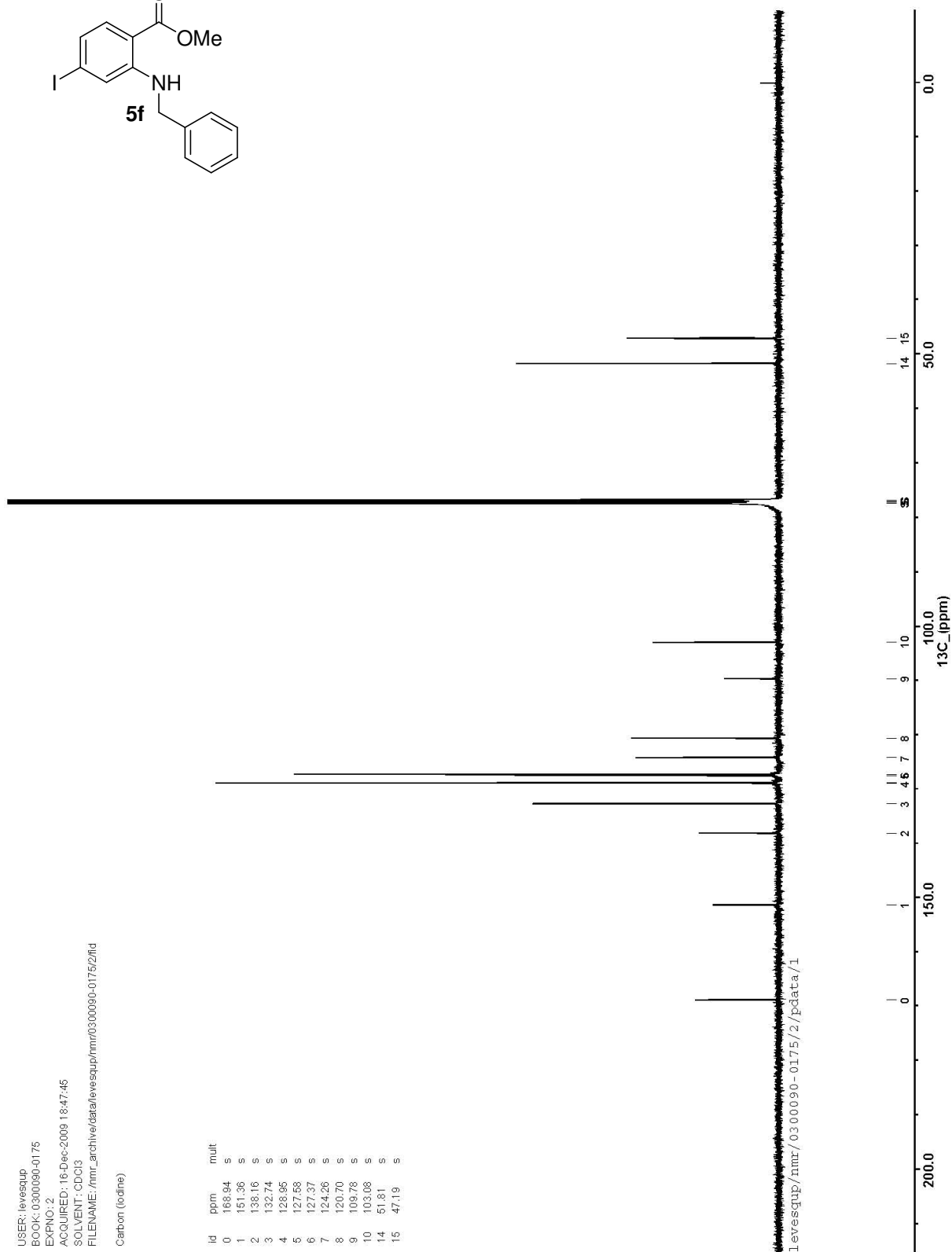
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of methyl 2-(benzylamino)-4-iodobenzoate (**5f**)



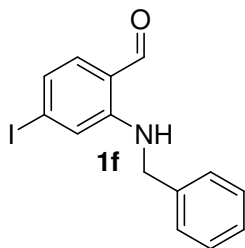
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 BOOK: 0300090-0175  
 EXPNO: 2  
 ACQUIRED: 16-Dec-2009 18:47:46  
 SOLVENT: CDCl3  
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Carbon (offset)

id	ppm	mult
0	168.84	s
1	151.36	s
2	138.16	s
3	132.74	s
4	128.95	s
5	127.68	s
6	127.37	s
7	124.26	s
8	120.70	s
9	109.78	s
10	103.08	s
14	51.81	s
15	47.19	s



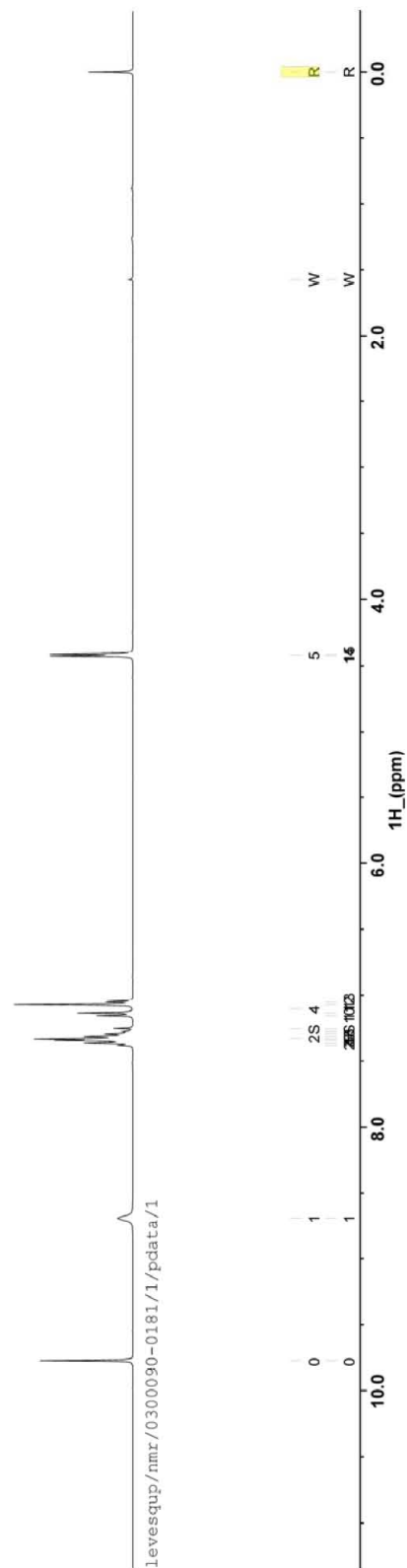
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of methyl 2-(benzylamino)-4-iodobenzoate (**5f**)



USER: levesq  
 BOOK: 0300090-0181  
 EXPNO: 1  
 ACQUIRED: 18-Dec-2009 15:56:17  
 SOLVENT: CDCl3  
 FILENAME: nmr\_archive\data\levesq\nmr\0300090-0181\fid

proton

id	ppm	mult	n	coupling
0	9.77	s	1.00	
1	8.59	s	1.18	
2	7.33	m	5.24	
4	7.10	m	3.33	
5	4.42	d	2.39	5.67

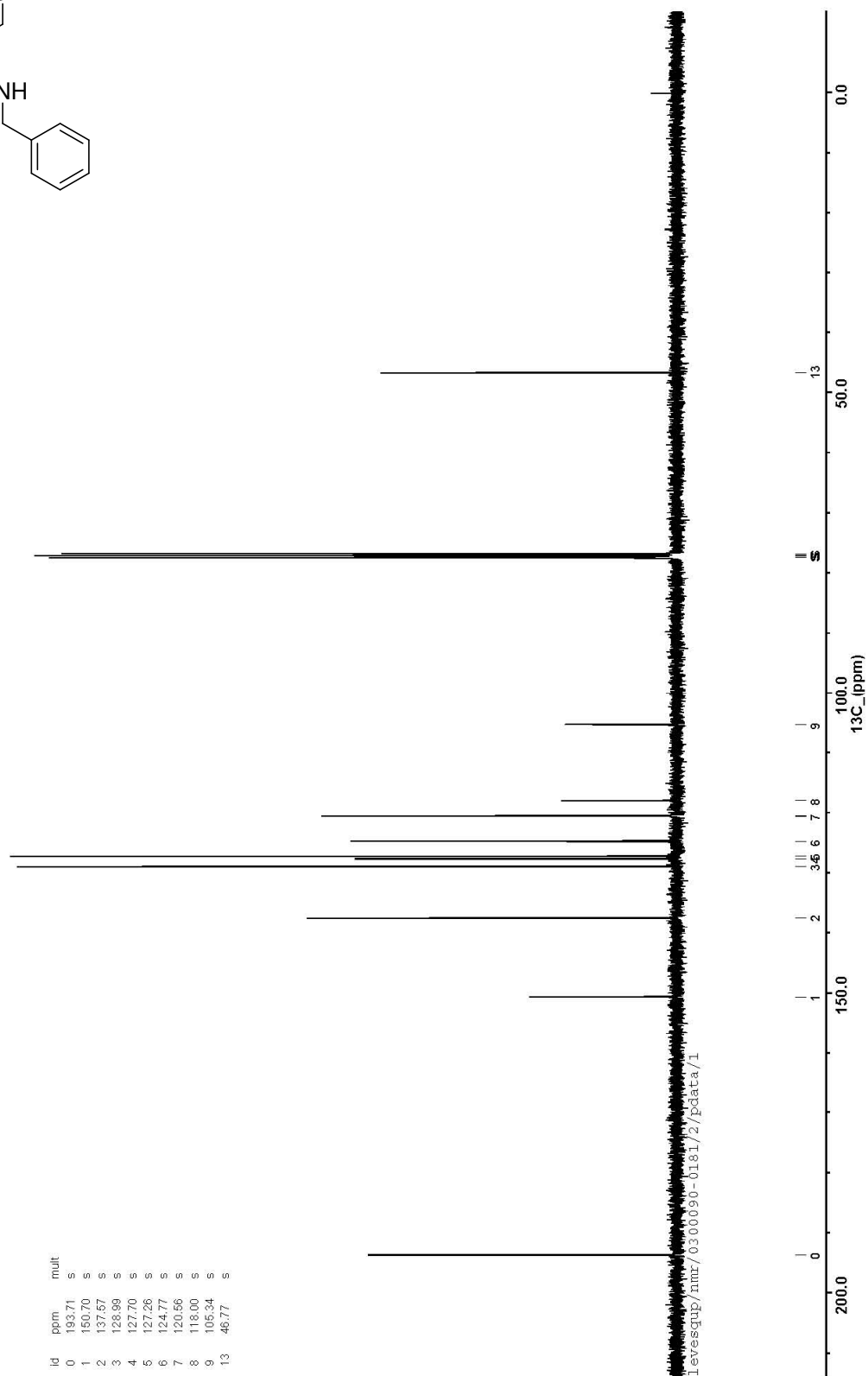
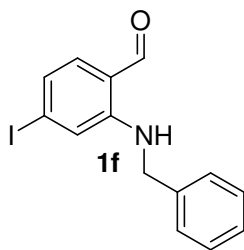


$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of 2-(benzylamino)-4-iodobenzaldehyde (**1f**)

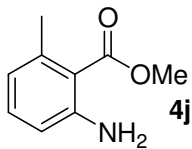
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BOOK: 0300090-0181  
EXPNO: 2  
ACQUIRED: 18-Dec-2009 16:04:05  
SOLVENT: CDCl3  
FILENAME: rmmr\_archive\data\levesq\mrmr\0300090-0181\2\fid

carbon

id	ppm	mult
0	193.71	s
1	150.70	s
2	137.57	s
3	128.99	s
4	127.70	s
5	127.26	s
6	124.77	s
7	120.66	s
8	118.00	s
9	105.34	s
13	46.77	s



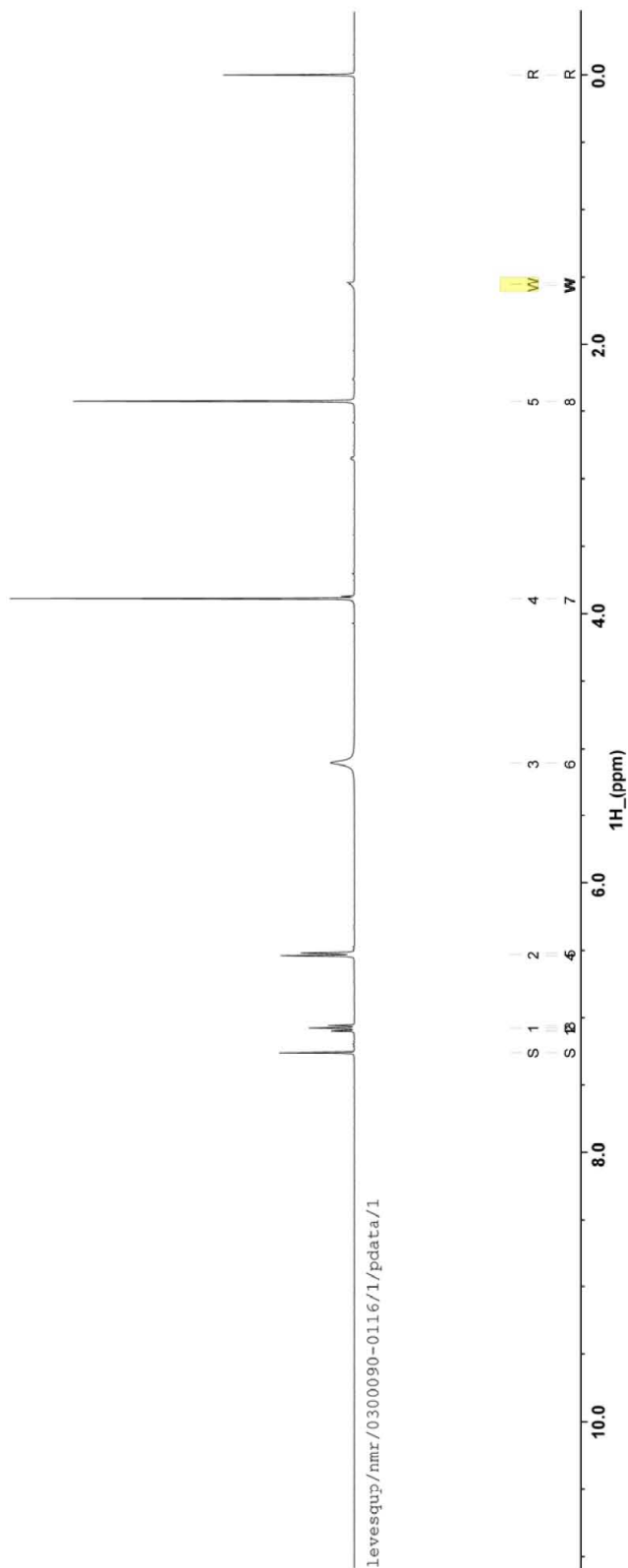
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of 2-(benzylamino)-4-iodobenzaldehyde (**1f**)



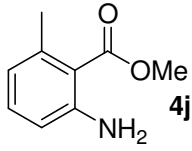
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 EXPNO: 1  
 ACQUIRED: 18-Nov-2009 13:54:23  
 SOLVENT: CDCl3  
 FILENAME: /mmr\_archive/data/levesq/mmr/0300090-0116/1fid

proton

id	ppm	mult	n	coupling
1	7.08	m	1.00	
2	6.53	d	2.05	7.83
3	5.10	s	1.89	
4	3.89	s	3.18	
5	2.43	s	3.33	



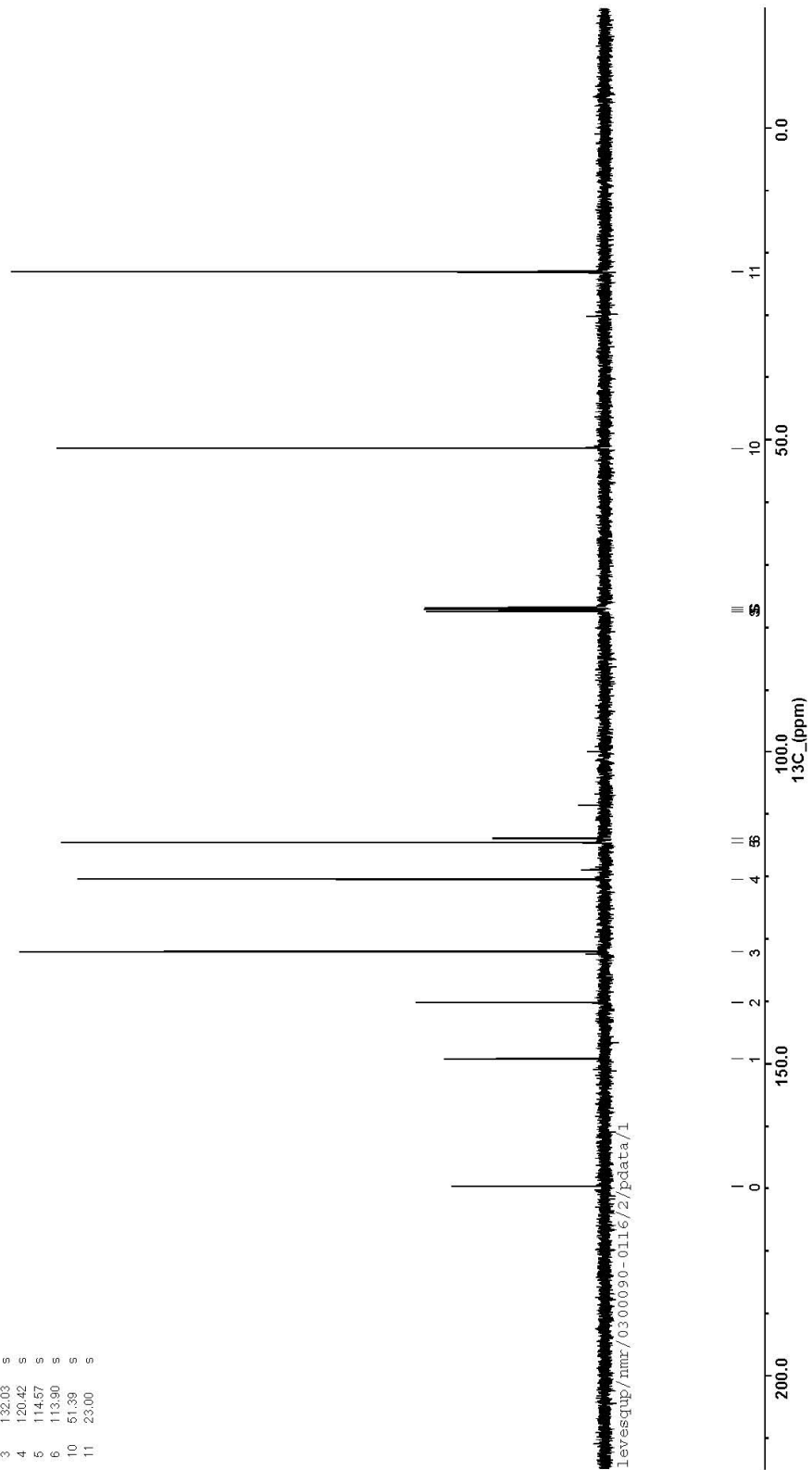
<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of methyl 2-amino-6-methylbenzoate (**4j**)



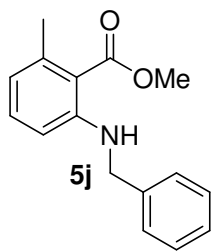
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 BOOK: 0300090-0116  
 EXPNO: 2  
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 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levescup/nmr/0300090-0116/2/flc

carbon

id	ppm	mult
0	169.72	s
1	149.18	s
2	140.17	s
3	132.03	s
4	120.42	s
5	114.57	s
6	113.90	s
10	51.39	s
11	23.00	s



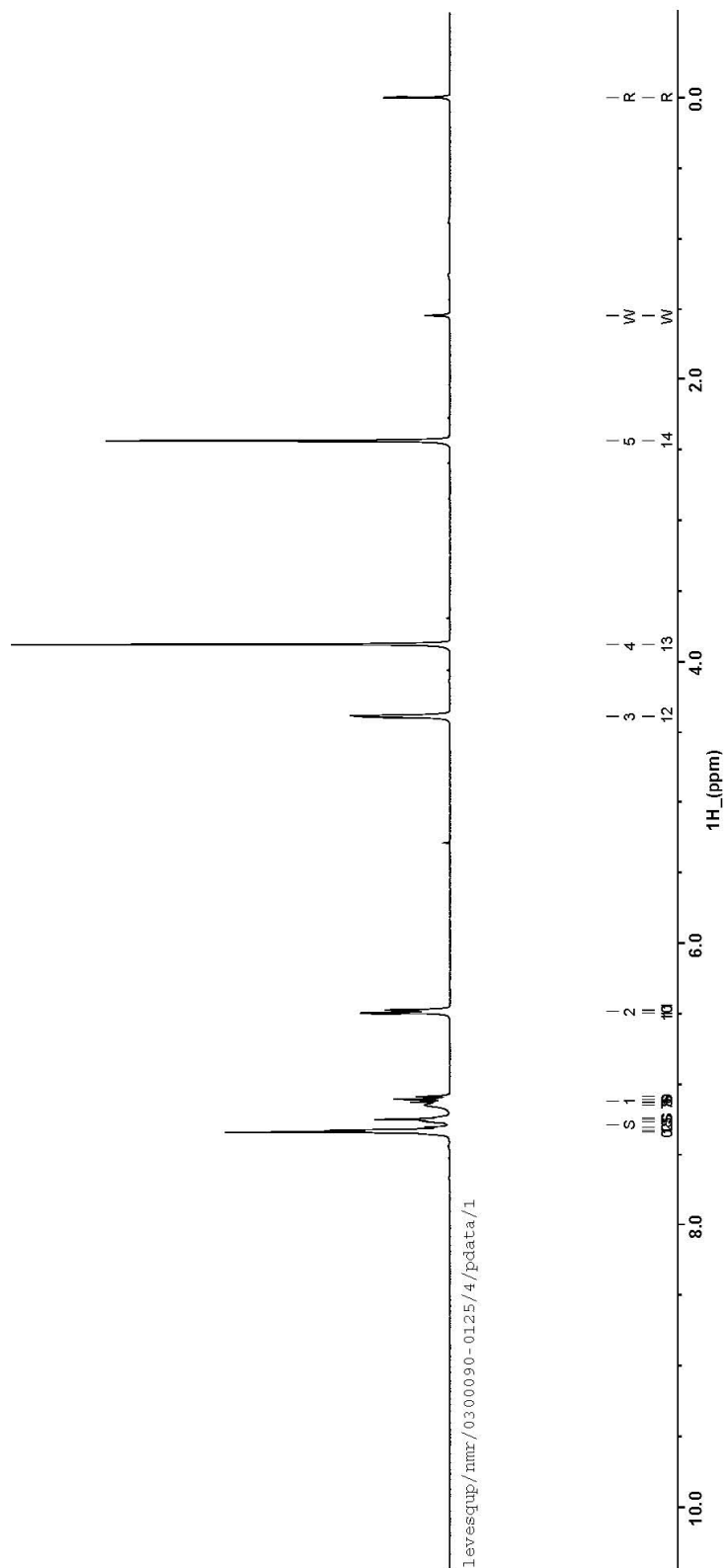
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of methyl 2-amino-6-methylbenzoate (**4j**)



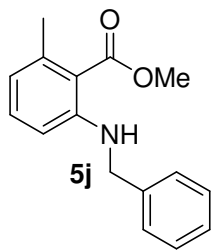
USER: levesq  
 BOOK: 0300090-0125  
 EXPNO: 4  
 ACQUIRED: 24-Nov-2009 16:39:31  
 SOLVENT: CDCl3  
 FILENAME: /hmr\_archive/data/levesq/hmr/0300090-0125/4/fid

proton

id	ppm	mult	n	coupling
1	7.12	dd	1.00	16.35/8.06
2	6.49	d	1.24	7.95
3	4.39	s	1.45	
4	3.88	s	1.42	
5	2.44	s	1.65	



$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of methyl 2-(benzylamino)-6-methylbenzoate (**5j**)

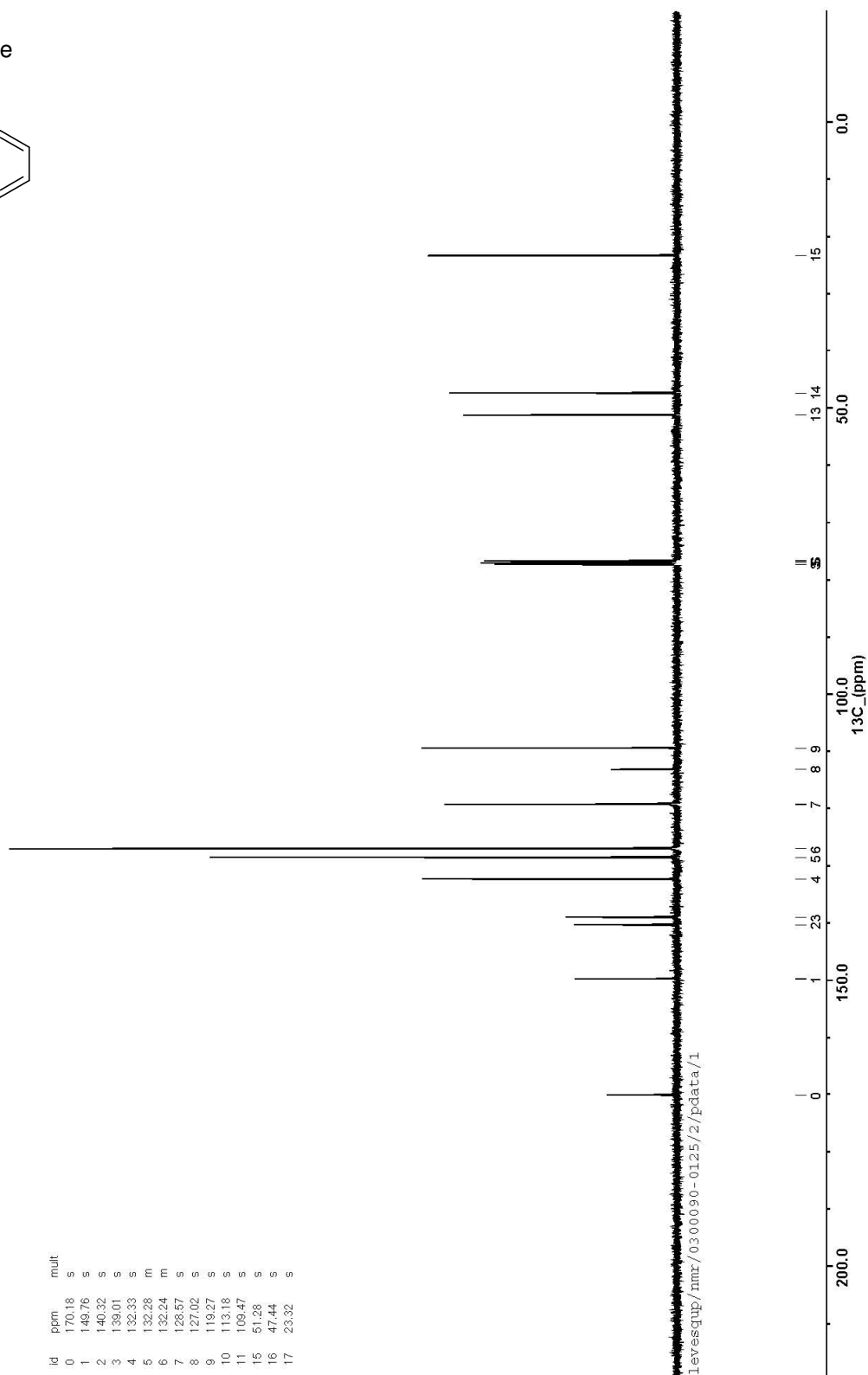


USER: levescup  
 BOOK: 0300090-0125  
 EXPNO: 2  
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 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levescup/nmr/0300090-0125/2/flc

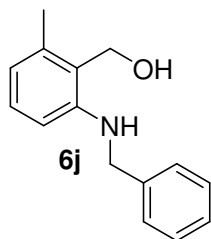
carbon

id	ppm	mult
0	170.18	s
1	149.76	s
2	140.32	s
3	139.01	s
4	132.33	s
5	132.28	m
6	132.24	m
7	128.67	s
8	127.02	s
9	119.27	s
10	113.16	s
11	109.47	s
15	51.28	s
16	47.44	s
17	23.32	s

levescup/nmr/0300090-0125/2/pdata/1



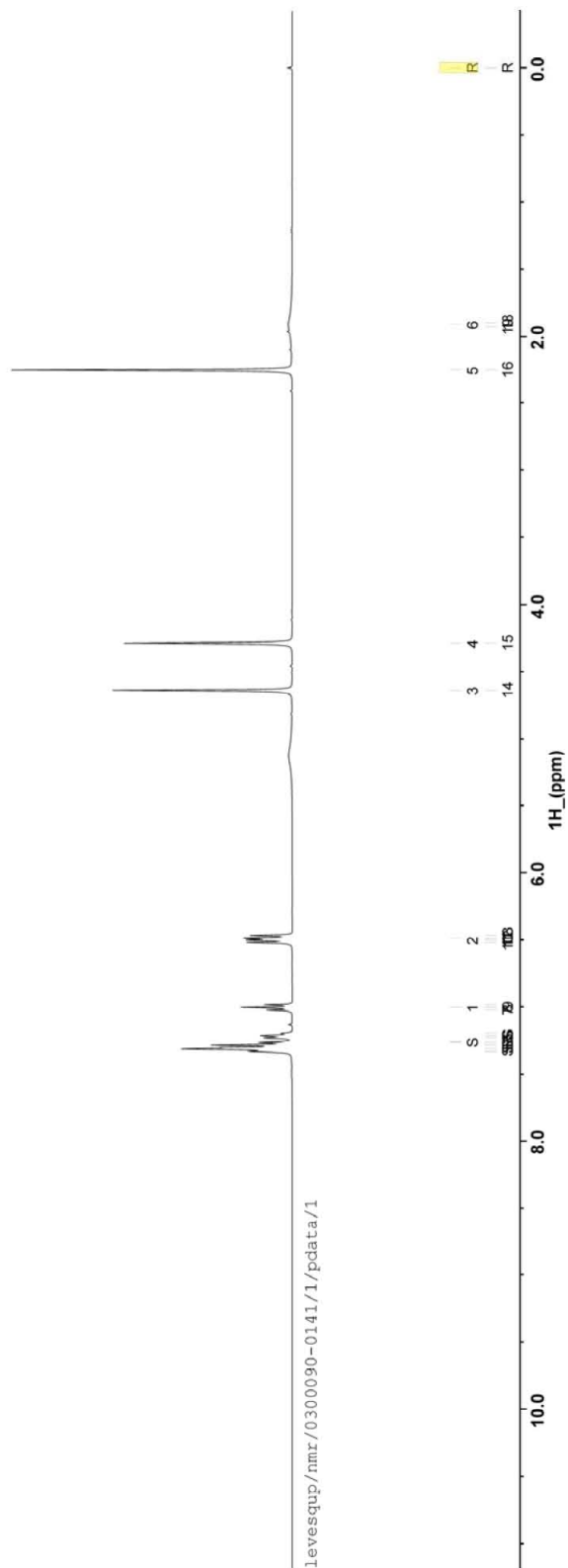
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of methyl 2-(benzylamino)-6-methylbenzoate (**5j**)



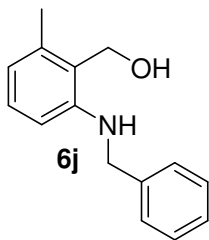
USER: levesqup  
 BOOK: 0300090-0141  
 EXPNO: 1  
 ACQUIRED: 07-Dec-2009 13:32:00  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levesqup/nmr/0300090-0141/1.fid

proton

id	ppm	mult	n	coupling
1	7.00	m	1.00	
2	6.49	m	2.00	
3	4.84	s	2.00	
4	4.29	s	2.05	
5	2.26	s	3.00	
6	1.91	d	1.07	11.07



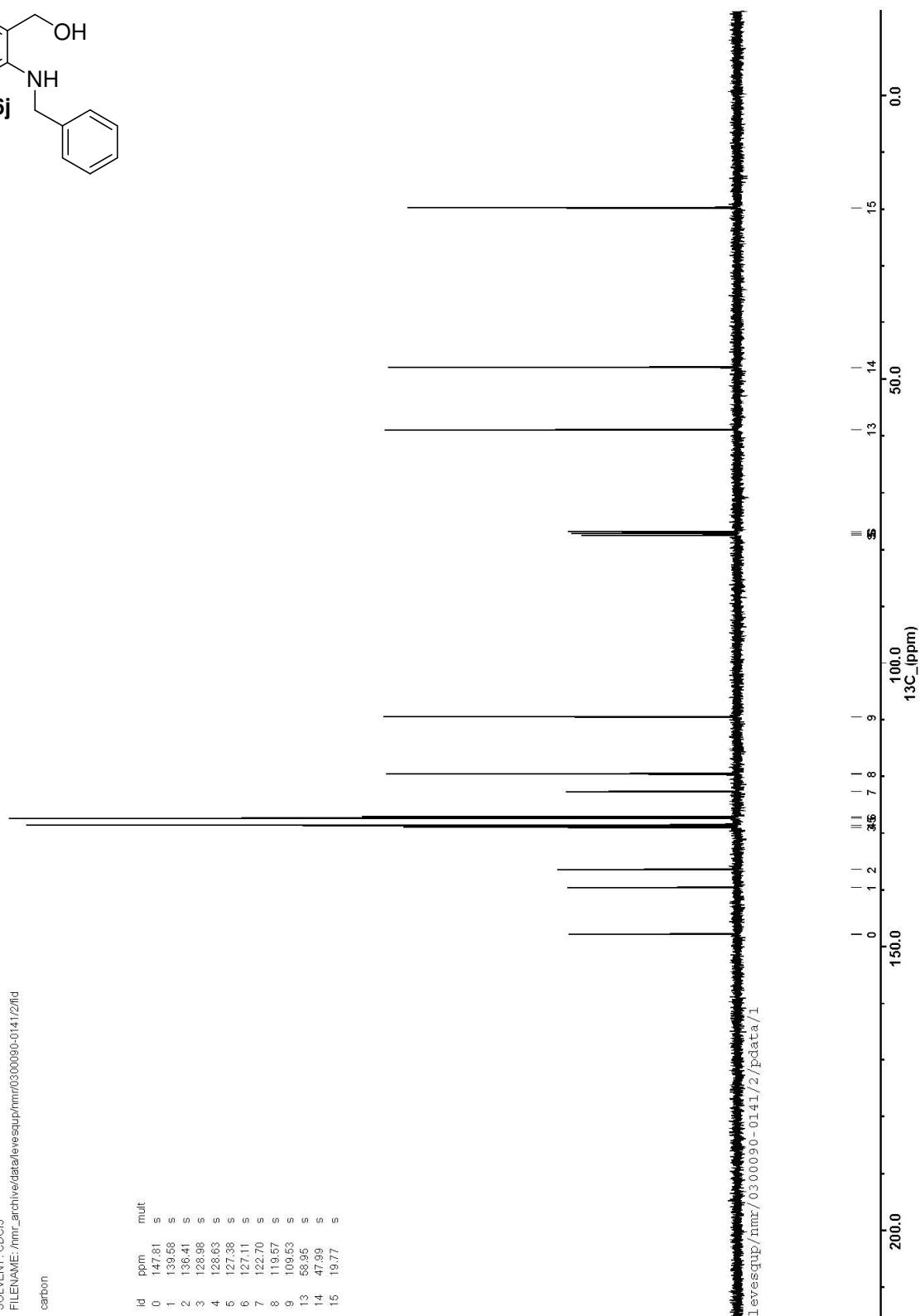
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of [2-(benzylamino)-6-methylphenyl]methanol (**6j**)



USER: levescup  
 BOOK: 0300090-0141  
 EXPNO: 2  
 ACQUIRED: 07-Dec-2009 13:37:31  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levescup/nmr/0300090-0141/2/fid

carbon

id	ppm	mult
0	147.81	s
1	139.68	s
2	136.41	s
3	128.98	s
4	128.63	s
5	127.38	s
6	127.11	s
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8	119.57	s
9	109.53	s
13	58.95	s
14	47.99	s
15	19.77	s

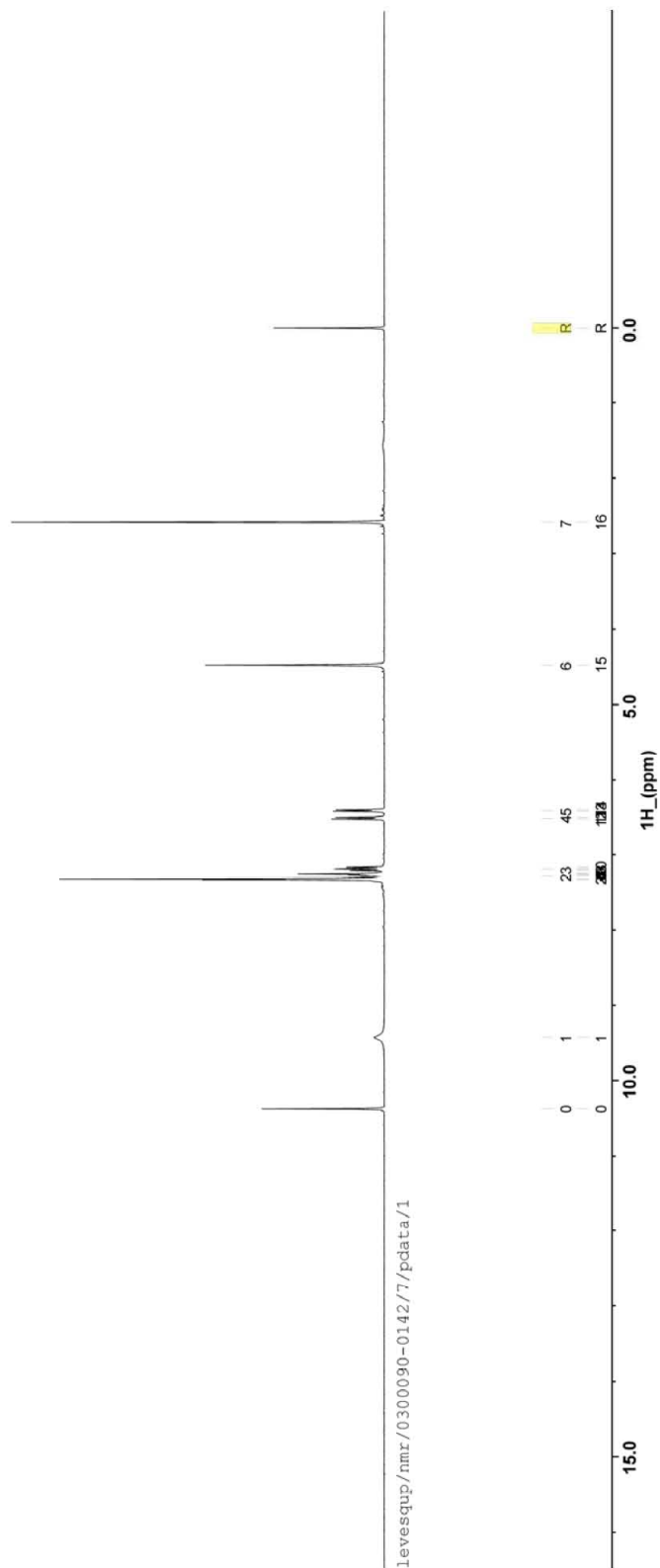
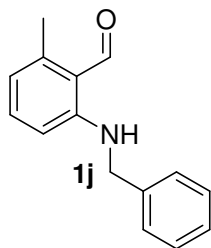


$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of [2-(benzylamino)-6-methylphenyl]methanol (**6j**)

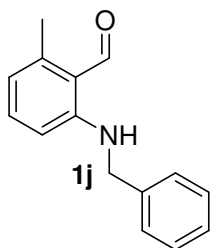
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BOOK: 0300090-0142  
EXPNO: 7  
ACQUIRED: 09-Dec-2009 13:39:19  
SOLVENT: CDCl3  
FILENAME: /nmr\_archive/data/levesqup/nmr/0300090-0142/7/fid

proton

id	ppm	mult	n	coupling
0	10.38	s	0.88	
1	9.43	s	0.96	
2	7.29	m	4.86	
3	7.19	t	1.02	7.93
4	6.52	d	1.02	8.63
5	6.41	d	1.00	7.21
6	4.47	s	1.97	
7	2.90	s	2.90	



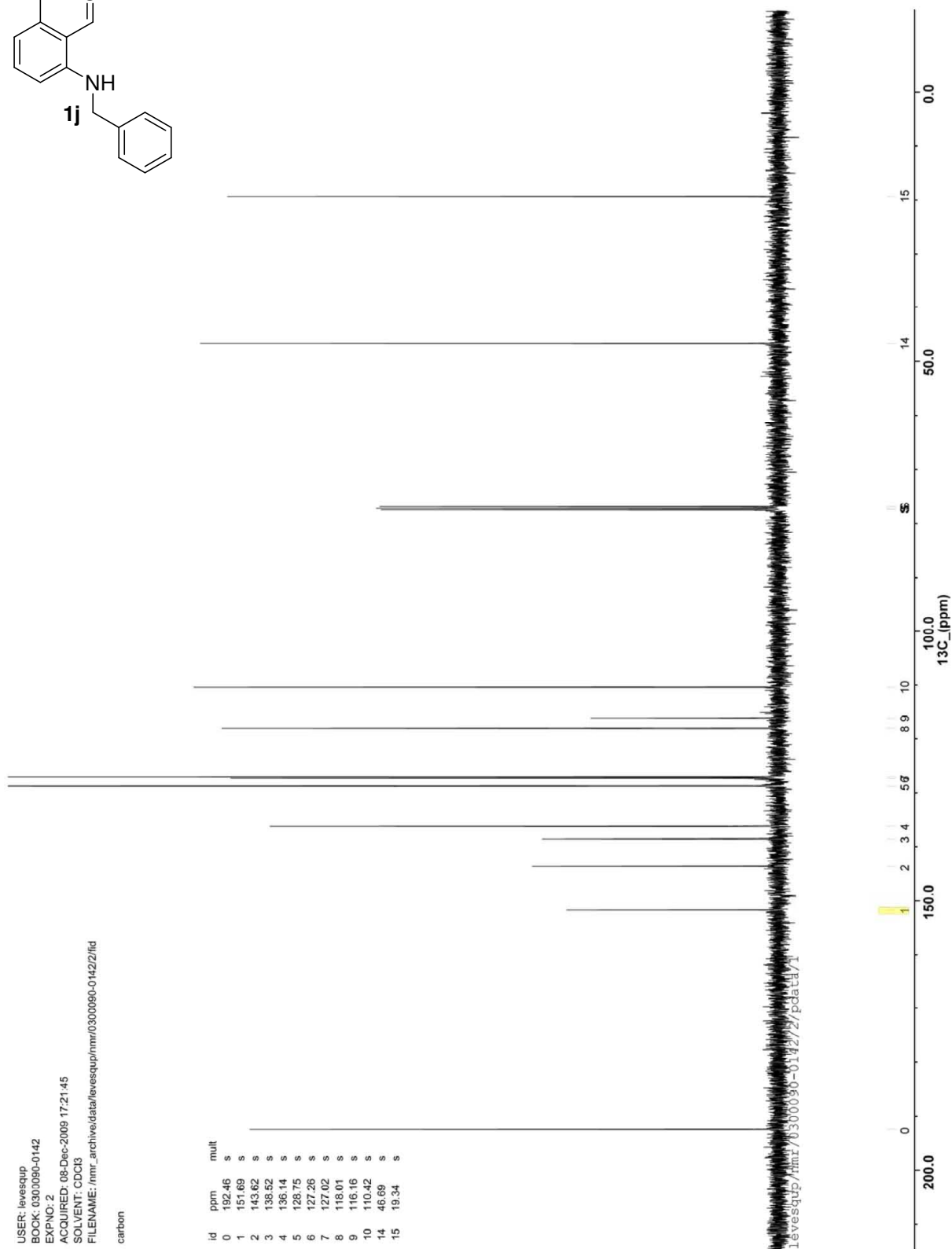
<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of 2-(benzylamino)-6-methylbenzaldehyde (**1j**)



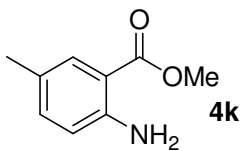
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 BOOK: 0300090-0142  
 EXPNO: 2  
 ACQUIRED: 08-Dec-2009 17:21:45  
 SOLVENT: CDCl3  
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carbon

id	ppm	mult
0	192.46	s
1	151.69	s
2	143.62	s
3	136.52	s
4	136.14	s
5	128.75	s
6	127.26	s
7	127.02	s
8	118.01	s
9	116.16	s
10	110.42	s
14	46.69	s
15	19.34	s



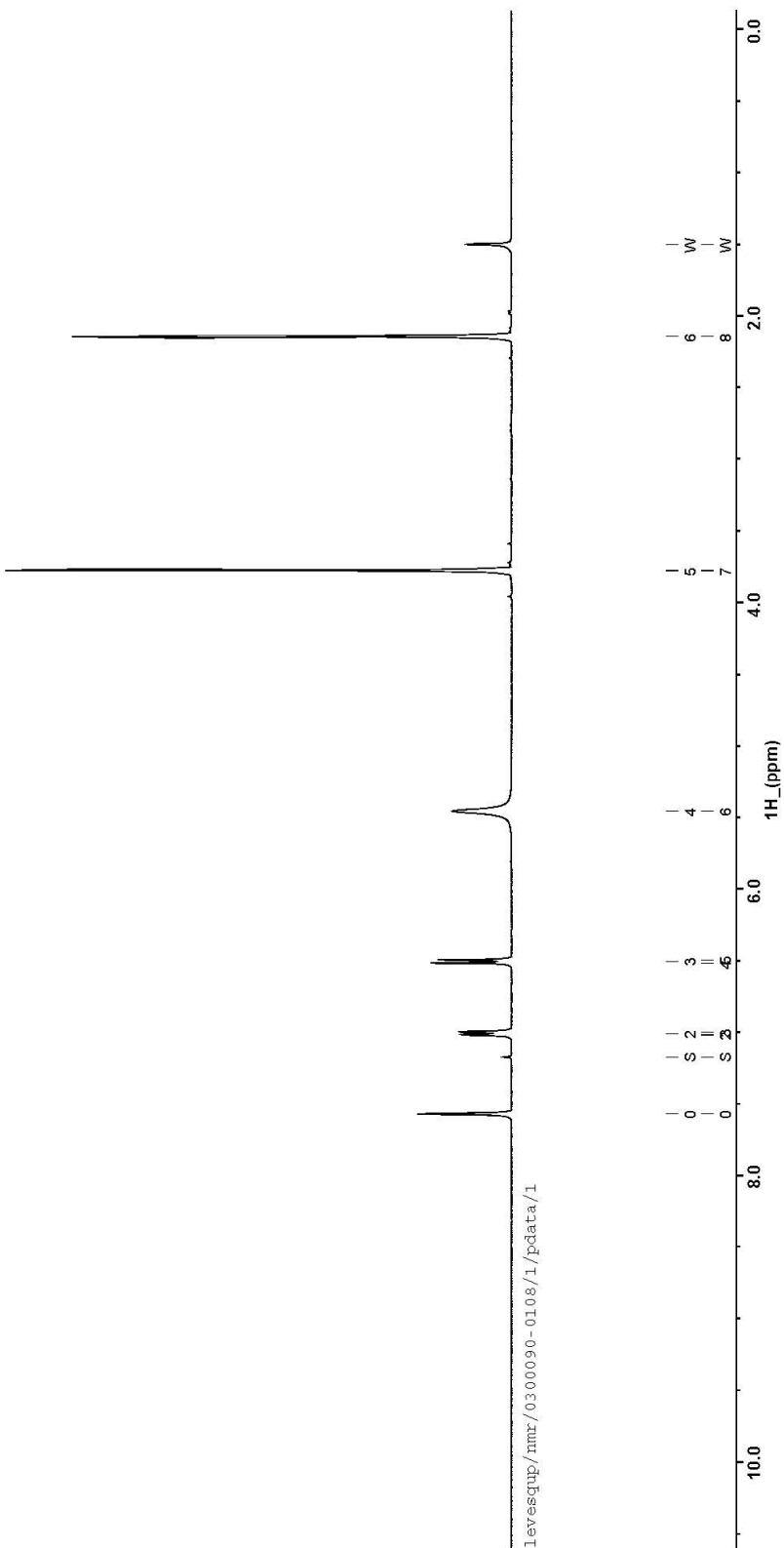
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of 2-(benzylamino)-6-methylbenzaldehyde (**1j**)



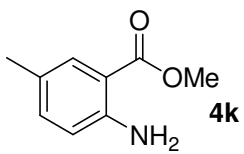
USER: levescup  
 BOOK: 0300090-0108  
 EXPNO: 1  
 ACQUIRED: 11-Nov-2009 11:42:08  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levescup/nmr/0300090-0108/1/fid

Proton

id	ppm	mult	n	coupling
0	7.57	s	1.02	
2	7.01	d	1.04	8.30
3	6.51	d	1.00	8.30
4	5.46	s	1.99	
5	3.78	s	2.87	
6	2.14	s	2.96	



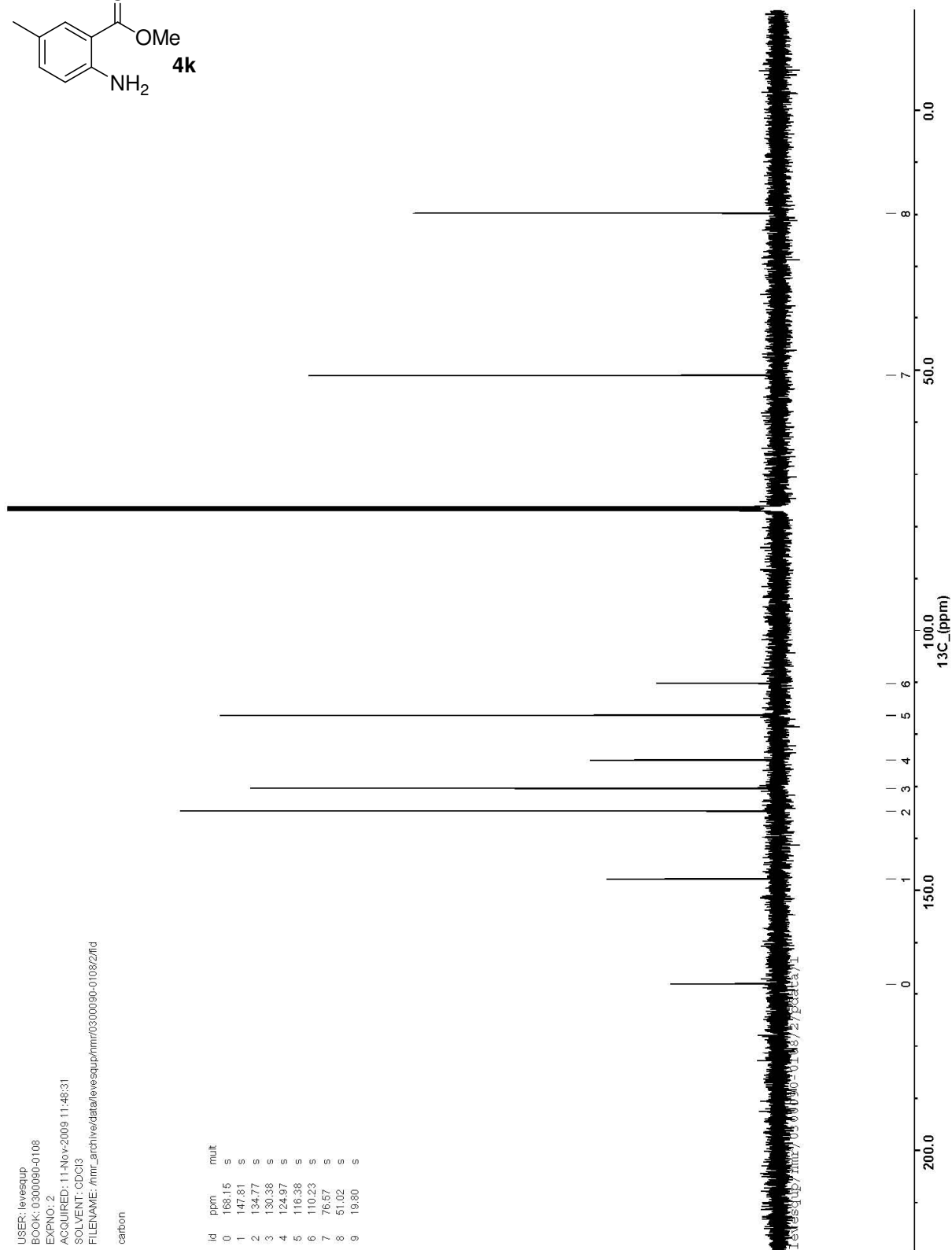
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of methyl 2-amino-5-methylbenzoate (**4k**)



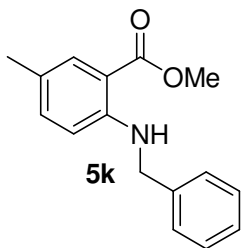
USER: levescup  
 BOOK: 0300090-0108  
 EXPNO: 2  
 ACQUIRED: 11-Nov-2009 11:48:31  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levescup/nmr/0300090-0108/2/flc

carbon

id	ppm	mult
0	168.15	s
1	147.81	s
2	134.77	s
3	130.38	s
4	124.97	s
5	116.38	s
6	110.23	s
7	76.57	s
8	51.02	s
9	19.80	s



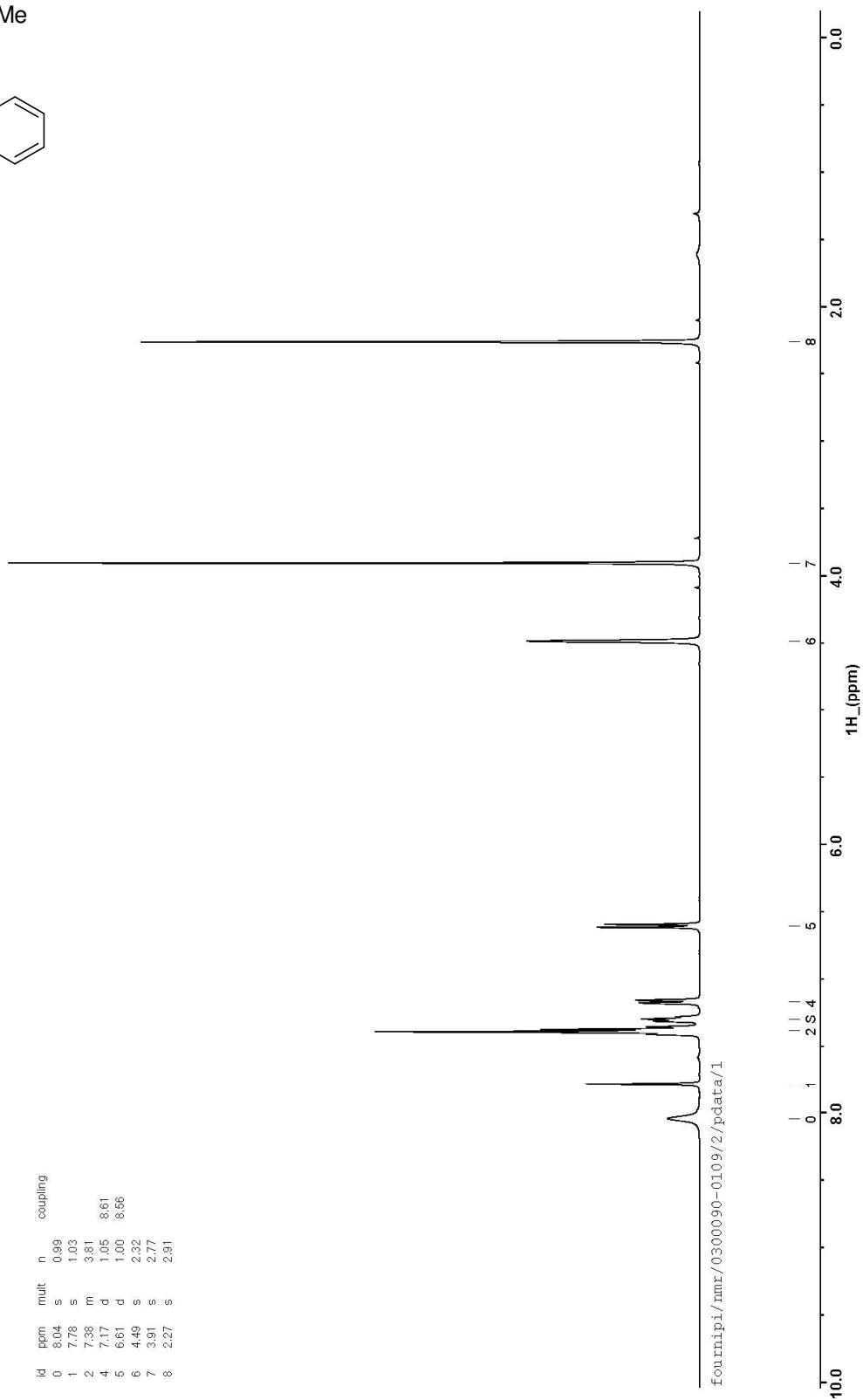
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of methyl 2-amino-5-methylbenzoate (**4k**)



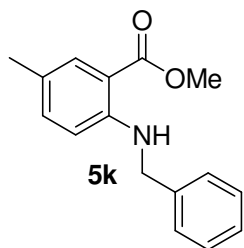
USER: fourmpi  
 BOOK: 0300090-0109  
 EXPNO: 2  
 ACQUIRED: 19-Jan-2010 18:30:11  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/fourmpi/nmr/0300090-0109/2/fid

proton

id	ppm	mult	n	coupling
0	8.04	s	0.99	
1	7.78	s	1.03	
2	7.58	m	3.81	
4	7.17	d	1.05	8.61
5	6.61	d	1.00	8.56
6	4.49	s	2.32	
7	3.91	s	2.77	
8	2.27	s	2.91	



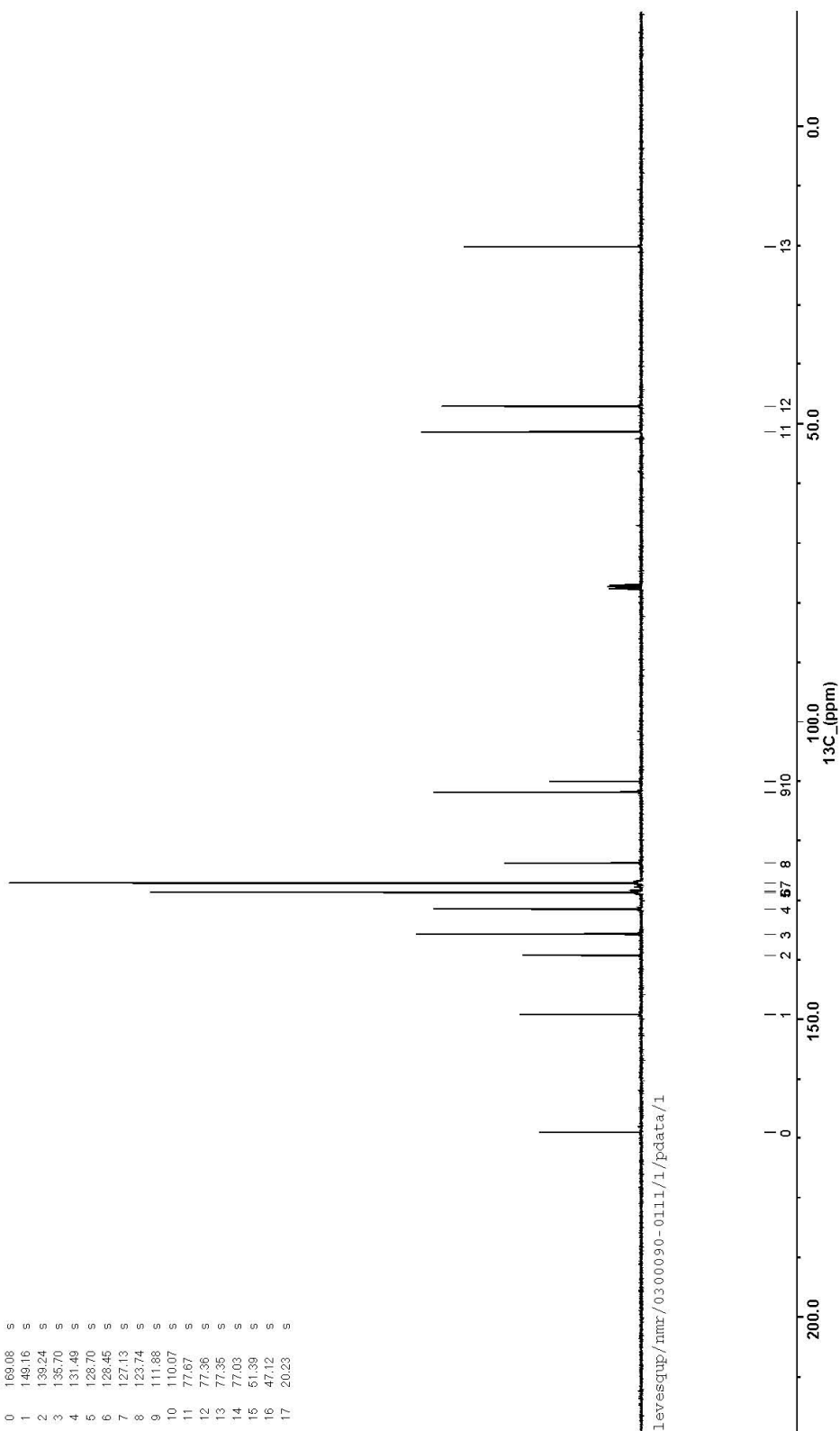
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of methyl 2-(benzylamino)-5-methylbenzoate (**5k**)



USER: levescup  
 BOOK: 0300090-0111  
 EXPNO: 1  
 ACQUIRED: 16-Nov-2009 16:20:45  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levescup/nmr/0300090-0111/1.fid

carbon

id	ppm	mult
0	169.08	s
1	149.16	s
2	139.24	s
3	136.70	s
4	131.49	s
5	128.70	s
6	128.45	s
7	127.13	s
8	123.74	s
9	111.88	s
10	110.07	s
11	77.67	s
12	77.36	s
13	77.35	s
14	77.03	s
15	51.39	s
16	47.12	s
17	20.23	s

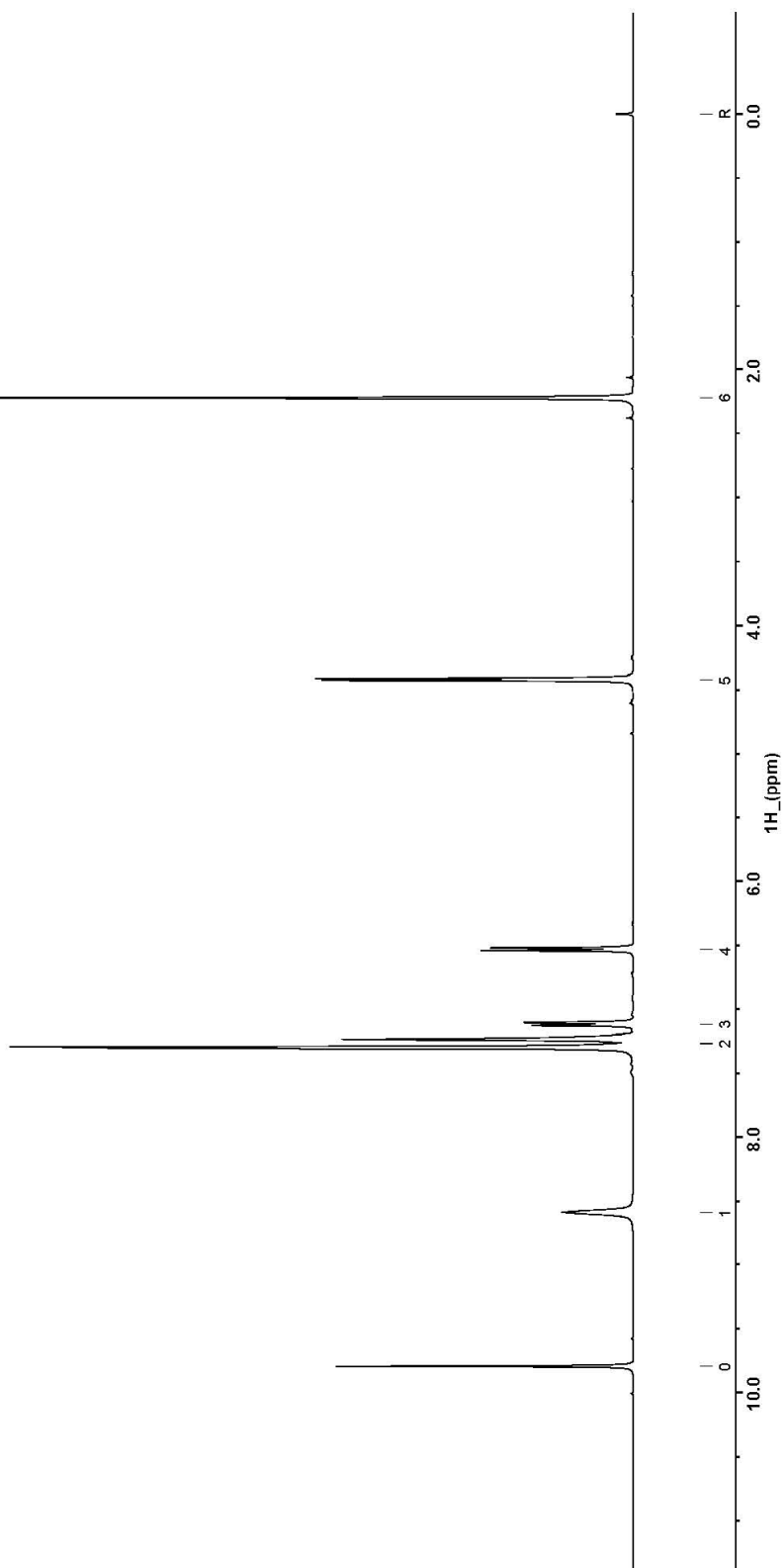
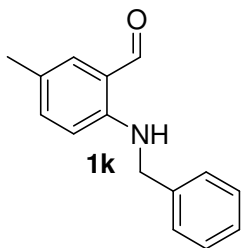


<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of methyl 2-(benzylamino)-5-methylbenzoate (**5k**)

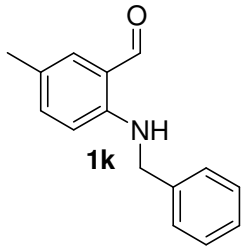
USER: levescup  
BOOK: 0300090-0174  
EXPNO: 1  
ACQUIRED: 16-Dec-2009 10:38:41  
SOLVENT: CDCl3  
FILENAME: /nmr\_archive/data/levescup/nmr/0300090-0174/1rfd

proton

id	ppm	mult	n	coupling
0	9.80	s	0.87	
1	8.59	s	1.01	
2	7.27	m	5.05	
3	7.12	d	1.00	8.59
4	6.53	d	0.97	8.58
5	4.42	d	2.02	5.86
6	2.22	s	2.82	



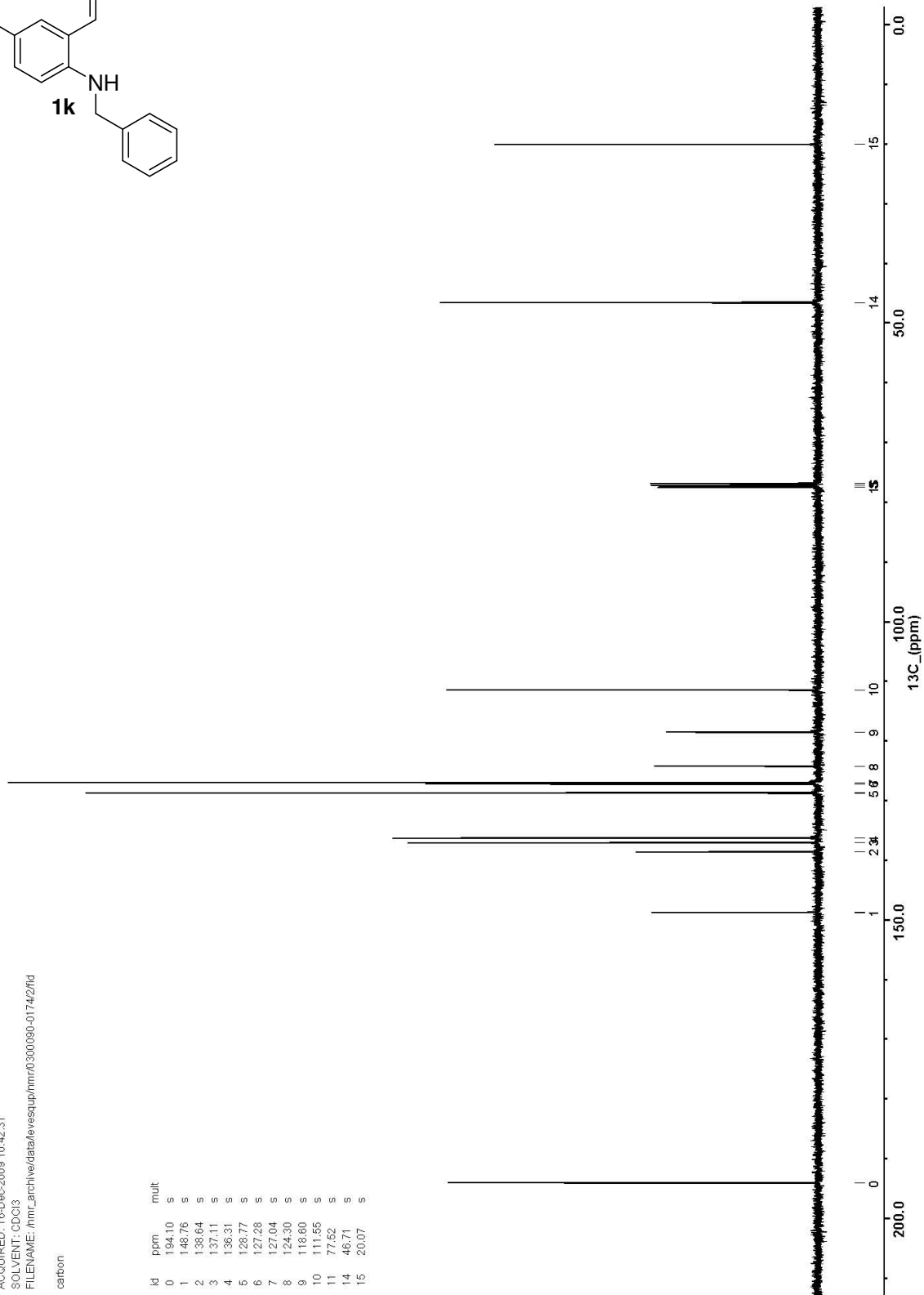
<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of 2-(benzylamino)-5-methylbenzaldehyde (**1k**)



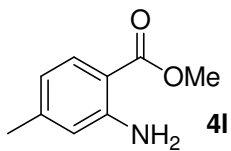
USER: levescup  
 BOOK: 0300090-0174  
 EXPNO: 2  
 ACQUIRED: 16-Dec-2009 10:42:31  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levescup/nmr/0300090-0174/2fid

carbon

id	ppm	mult
0	194.10	s
1	148.76	s
2	138.64	s
3	137.11	s
4	136.31	s
5	128.77	s
6	127.28	s
7	127.04	s
8	124.30	s
9	118.60	s
10	111.55	s
11	77.52	s
14	46.71	s
15	20.07	s



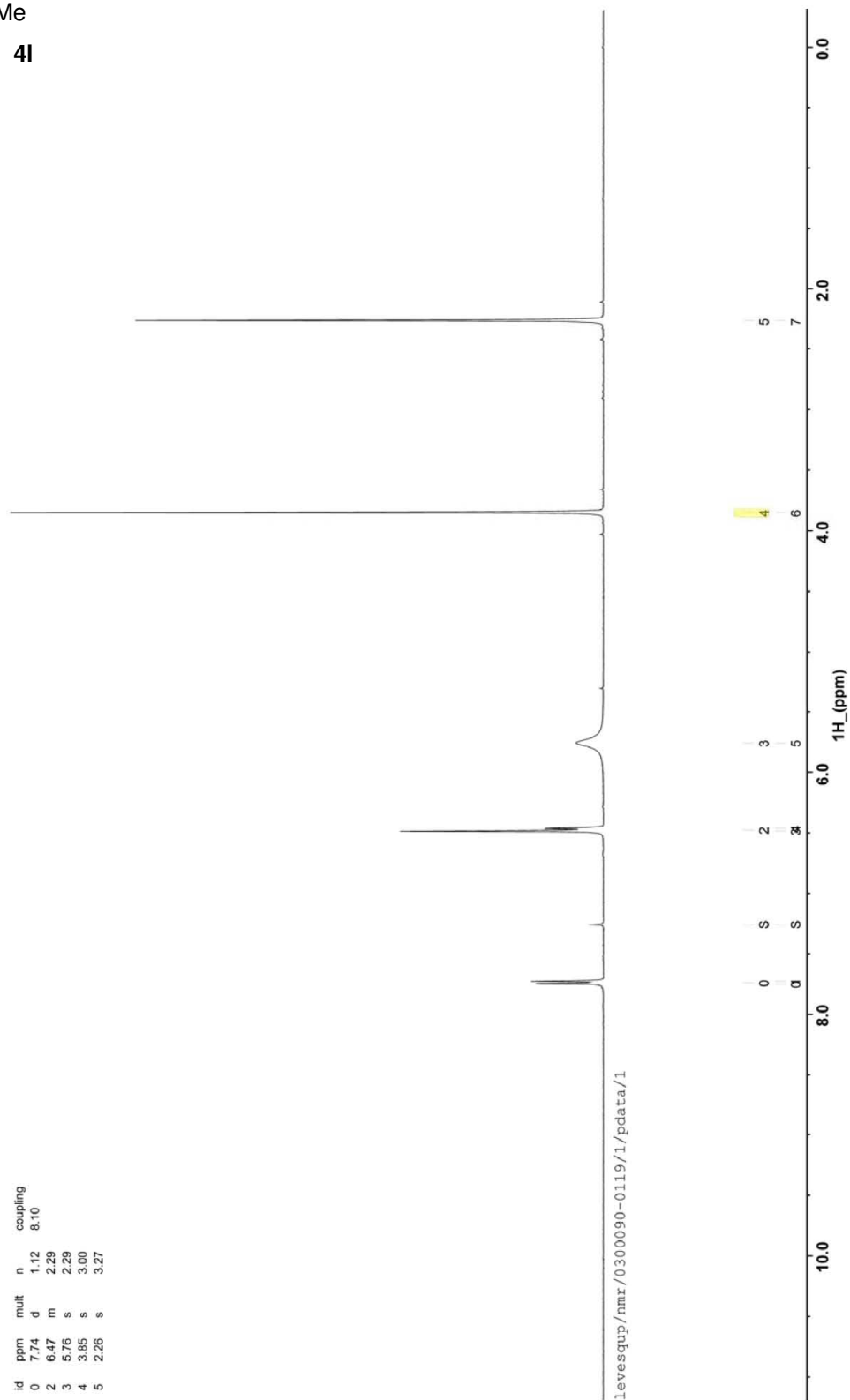
<sup>13</sup>C NMR Spectrum (101 MHz, CDCl<sub>3</sub>) of 2-(benzylamino)-5-methylbenzaldehyde (**1k**)



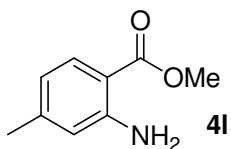
USER: levesqup  
 BOOK: 0300090-0119  
 EXPNO: 1  
 ACQUIRED: 17-Nov-2009 16:02:33  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levesqup/nmr/0300090-0119/1/fid

proton

id	ppm	mult	n	coupling
0	7.74	d	1.12	8.10
2	6.47	m	2.28	
3	5.76	s	2.28	
4	3.95	s	3.00	
5	2.26	s	3.27	



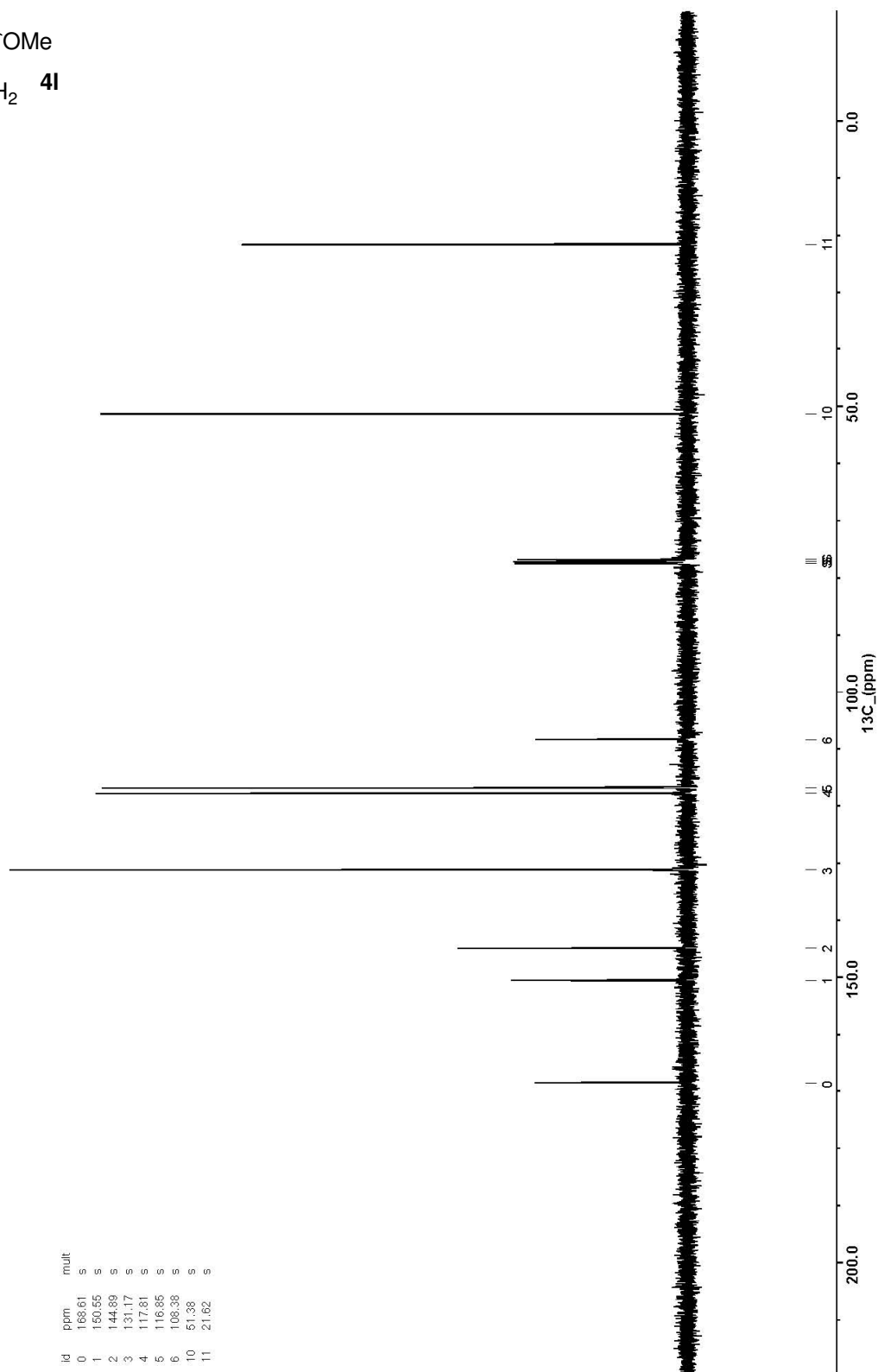
<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of methyl 2-amino-4-methylbenzoate (**4I**)



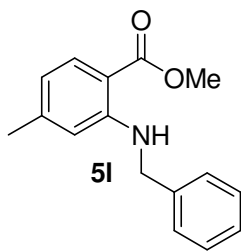
USER: levescup  
 BOOK: 0300090-0119  
 EXPNO: 2  
 ACQUIRED: 17-Nov-2009 16:08:10  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levescup/nmr/0300090-0119/2/fid

carbon

id	ppm	mult
0	168.61	s
1	150.55	s
2	144.89	s
3	131.17	s
4	117.81	s
5	116.85	s
6	108.38	s
10	51.38	s
11	21.62	s



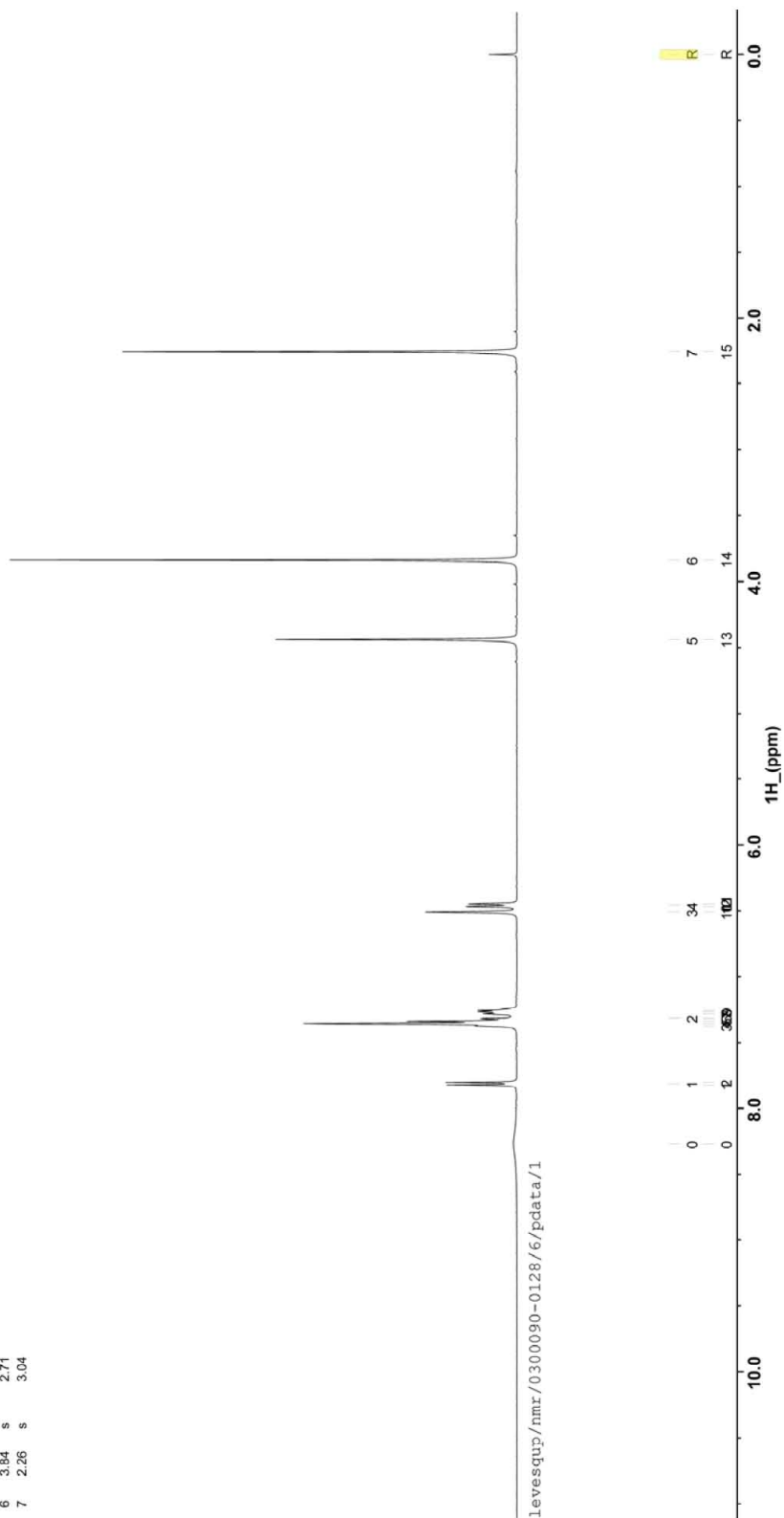
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of methyl 2-amino-4-methylbenzoate (**41**)



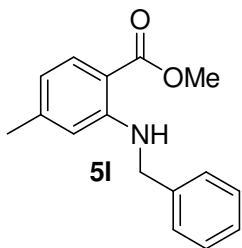
USER: levesqup  
 BOOK: 0300090-0128  
 EXPNO: 6  
 ACQUIRED: 24-Nov-2009 14:02:20  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levesqup/nmr/0300090-0128/6/fid

proton

id	ppm	mult	n	coupling
0	8.27	s	0.99	
1	7.81	d	1.00	8.12
2	7.31	m	5.34	
3	6.51	s	1.13	
4	6.46	d	1.11	8.16
5	4.44	s	2.13	
6	3.84	s	2.71	
7	2.26	s	3.04	



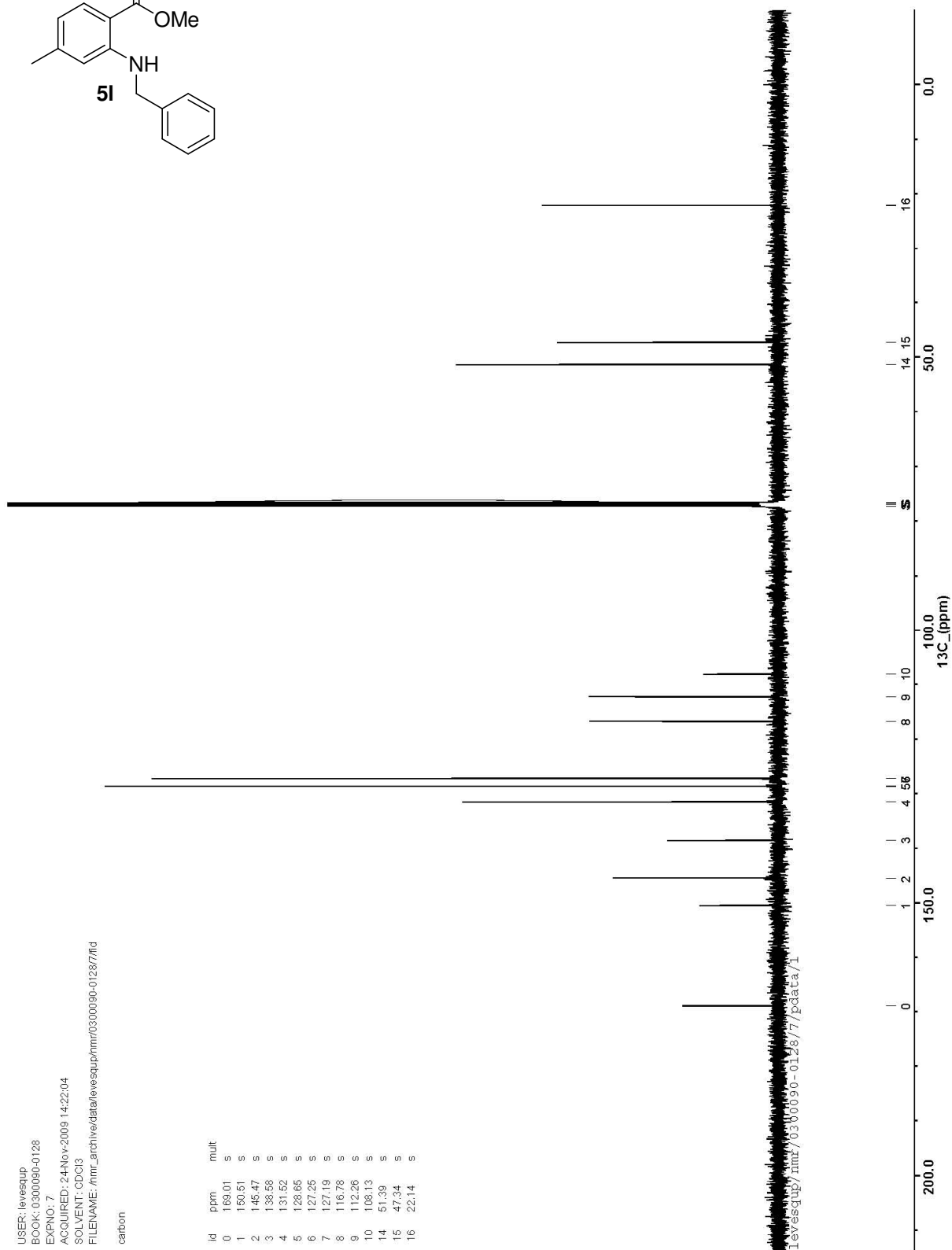
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of methyl 2-(benzylamino)-4-methylbenzoate (**51**)



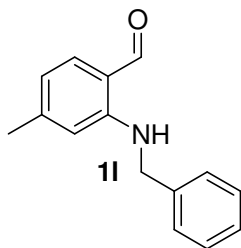
USER: levescup  
 BOOK: 0300090-0128  
 EXPNO: 7  
 ACQUIRED: 24-Nov-2009 14:22:04  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levescup/nmr/0300090-0128/7.ftc

carbon

id	ppm	mult
0	169.01	s
1	150.51	s
2	145.47	s
3	138.58	s
4	131.82	s
5	128.65	s
6	127.25	s
7	127.19	s
8	116.78	s
9	112.26	s
10	106.13	s
14	51.39	s
15	47.34	s
16	22.14	s



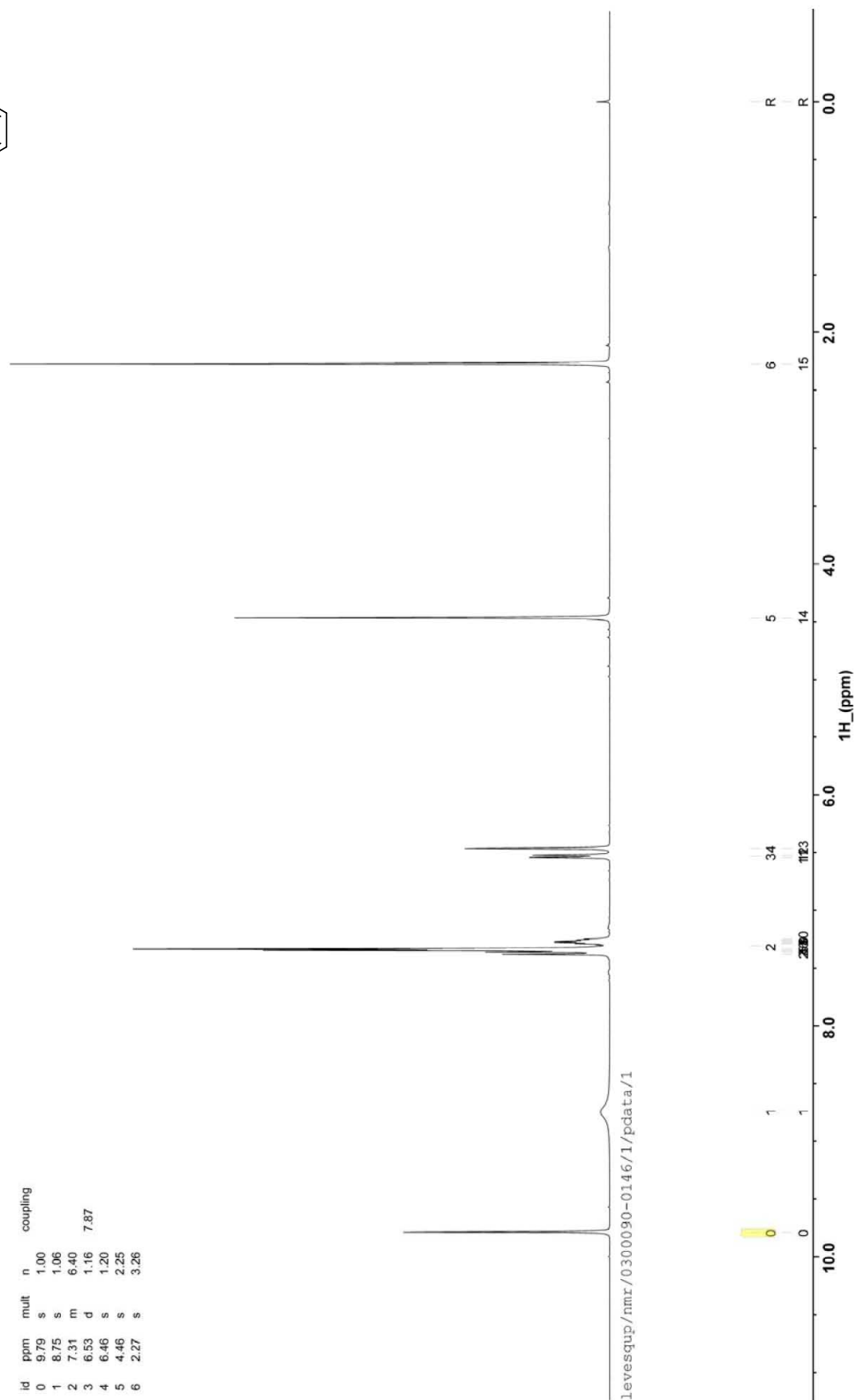
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of methyl 2-(benzylamino)-4-methylbenzoate (**51**)



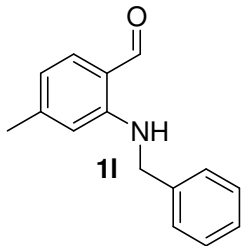
USER: levesqup  
 BOOK: 0300090-0146  
 EXPNO: 1  
 ACQUIRED: 14-Dec-2009 14:35:40  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levesqup/nmr/0300090-0146/1.fid

proton

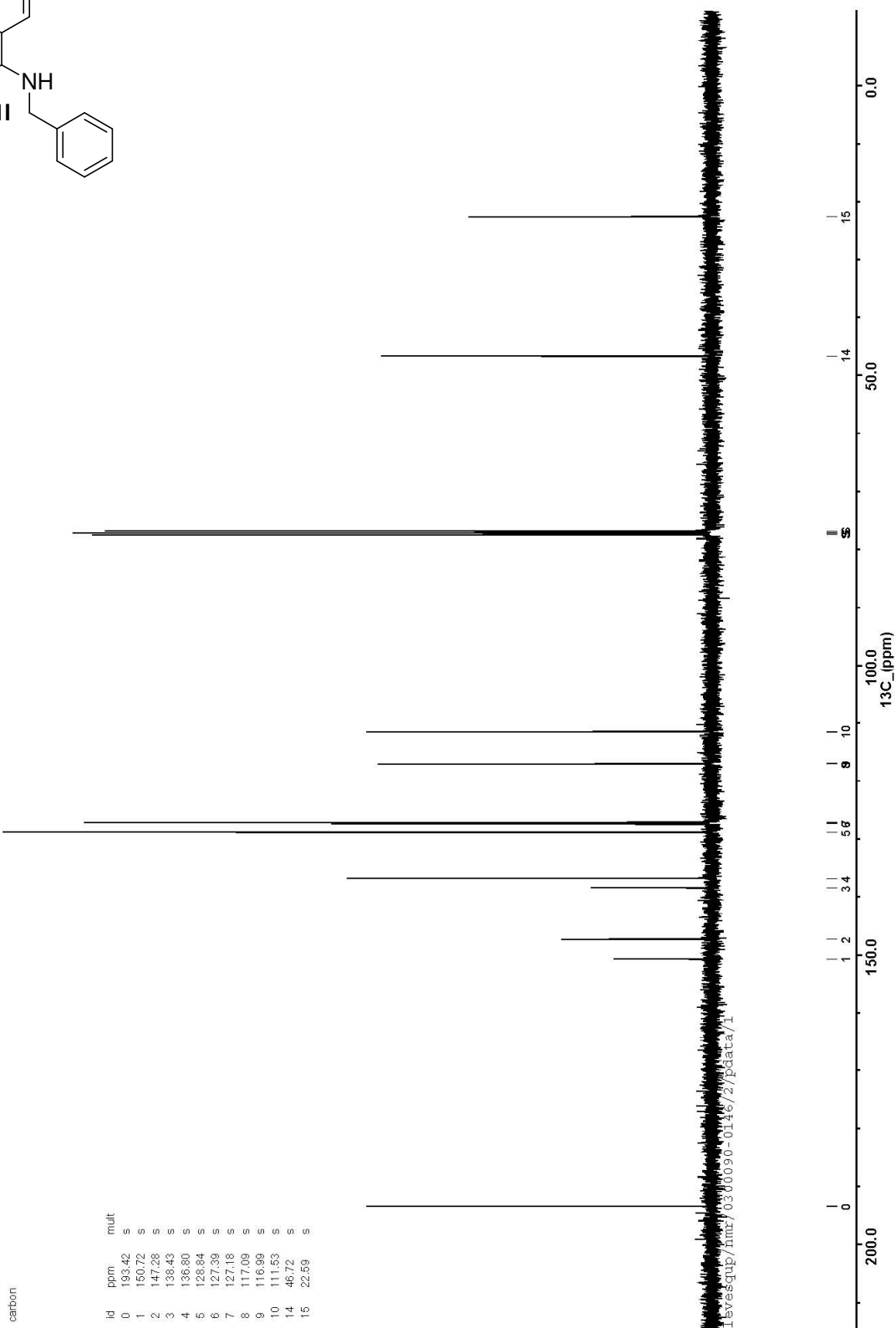
id	ppm	mult	n	coupling
0	9.79	s	1.00	
1	8.75	s	1.06	
2	7.31	m	6.40	
3	6.53	d	1.16	7.87
4	6.46	s	1.20	
5	4.46	s	2.25	
6	2.27	s	3.26	



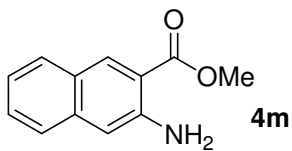
<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of 2-(benzylamino)-4-methylbenzaldehyde (**II**)



USER: levescup  
 BOOK: 0300090-0146  
 EXPNO: 2  
 ACQUIRED: 14-Dec-2009 14:40:47  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levescup/nmr/0300090-0146/2/flc



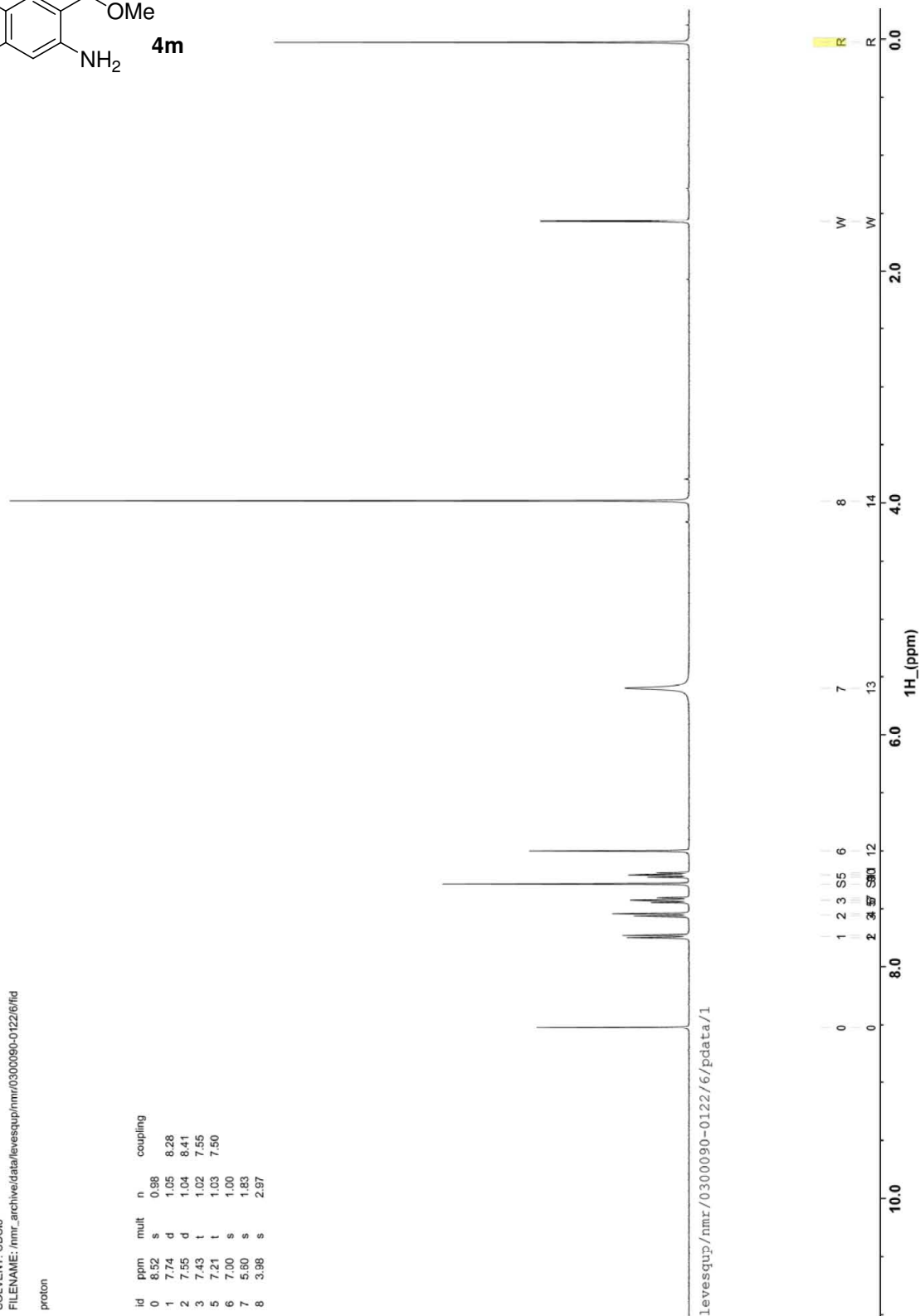
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of 2-(benzylamino)-4-methylbenzaldehyde (**11**)



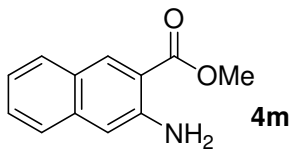
USER: levesqup  
 BOOK: 0300090-0122  
 EXPNO: 6  
 ACQUIRED: 23-Nov-2009 12:17:15  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levesqup/nmr/0300090-0122/6/fid

proton

id	ppm	mult	n	coupling
0	8.52	s	0.98	
1	7.74	d	1.05	8.28
2	7.55	d	1.04	8.41
3	7.43	t	1.02	7.55
5	7.21	t	1.03	7.50
6	7.00	s	1.00	
7	5.80	s	1.83	
8	3.98	s	2.97	



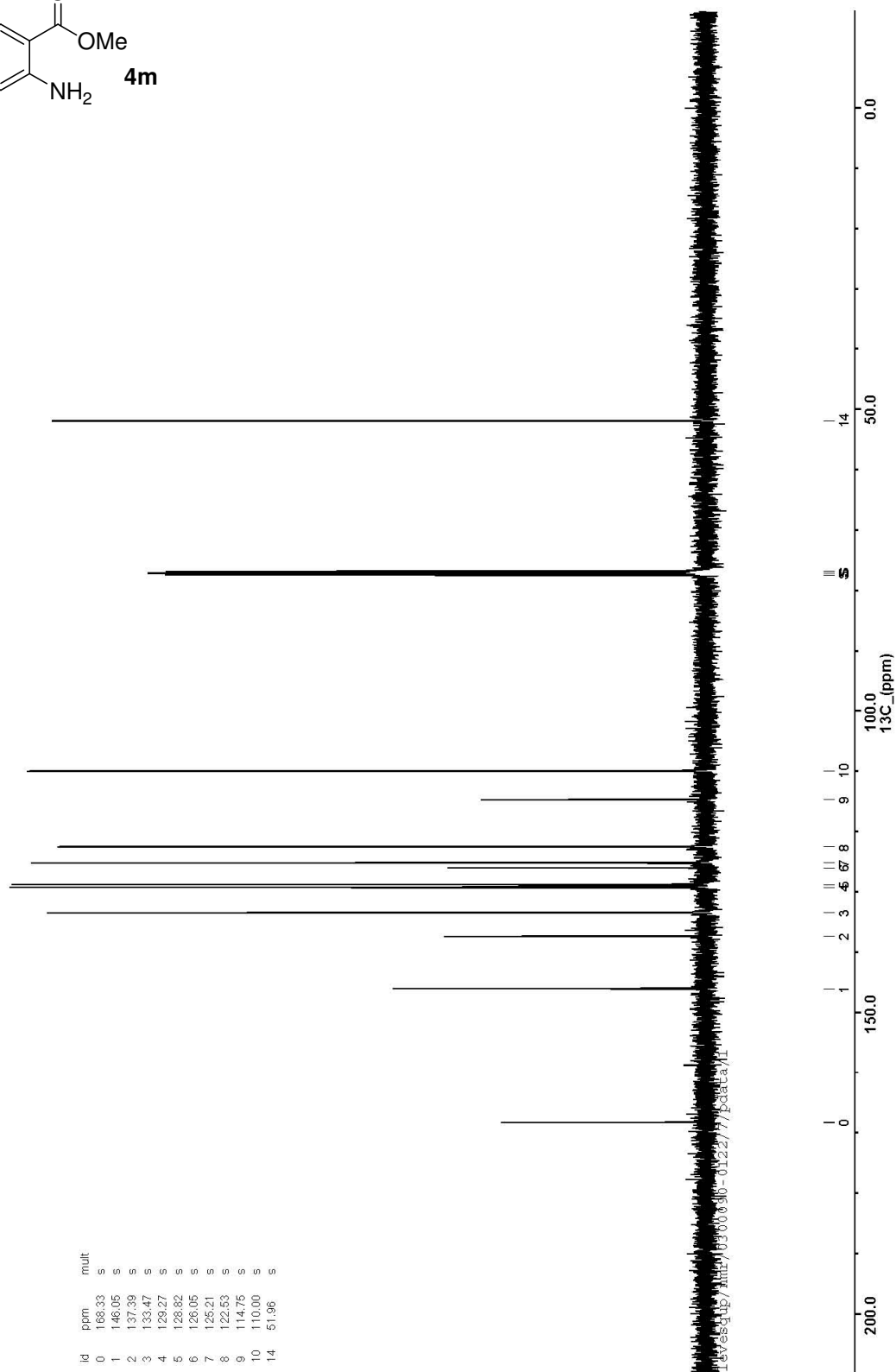
<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of methyl 3-aminonaphthalene-2-carboxylate (**4m**)



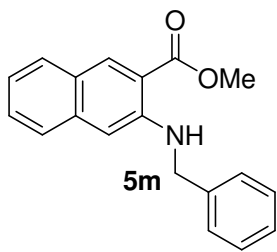
USER: levescup  
 BOOK: 0300090-0122  
 EXPNO: 7  
 ACQUIRED: 23/Nov-2009 12:42:04  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levescup/nmr/0300090-01227.ft3

carbon

id	ppm	mult
0	168.33	s
1	146.05	s
2	137.39	s
3	133.47	s
4	129.27	s
5	128.82	s
6	126.05	s
7	125.21	s
8	122.53	s
9	114.75	s
10	110.00	s
14	51.96	s



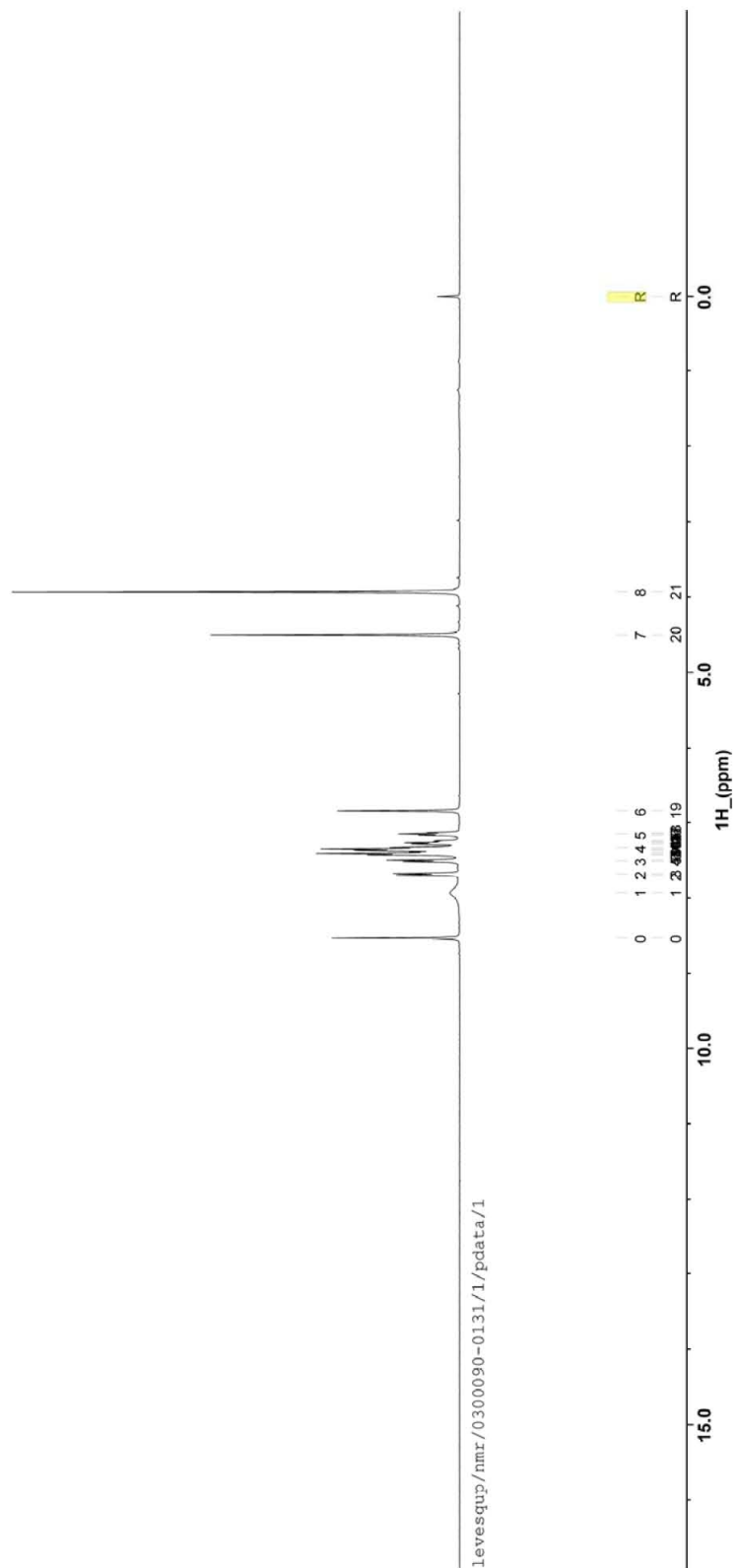
<sup>13</sup>C NMR Spectrum (101 MHz, CDCl<sub>3</sub>) of methyl 3-aminonaphthalene-2-carboxylate (**4m**)



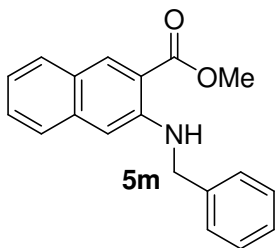
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 BOOK: 0300090-0131  
 EXPNO: 1  
 ACQUIRED: 25-Nov-2009 11:30:21  
 SOLVENT: CDCl3  
 FILENAME: nmr\_archive\data\levesqup\nmr\0300090-0131\1.fid

proton

id	ppm	mult	n	coupling
0	8.53	s	0.88	
1	7.93	s	1.00	
2	7.89	d	1.05	8.18
3	7.51	d	1.05	8.37
4	7.33	m	5.93	
5	7.15	m	1.02	
6	6.84	s	0.84	
7	4.50	s	1.90	
8	3.93	s	2.63	



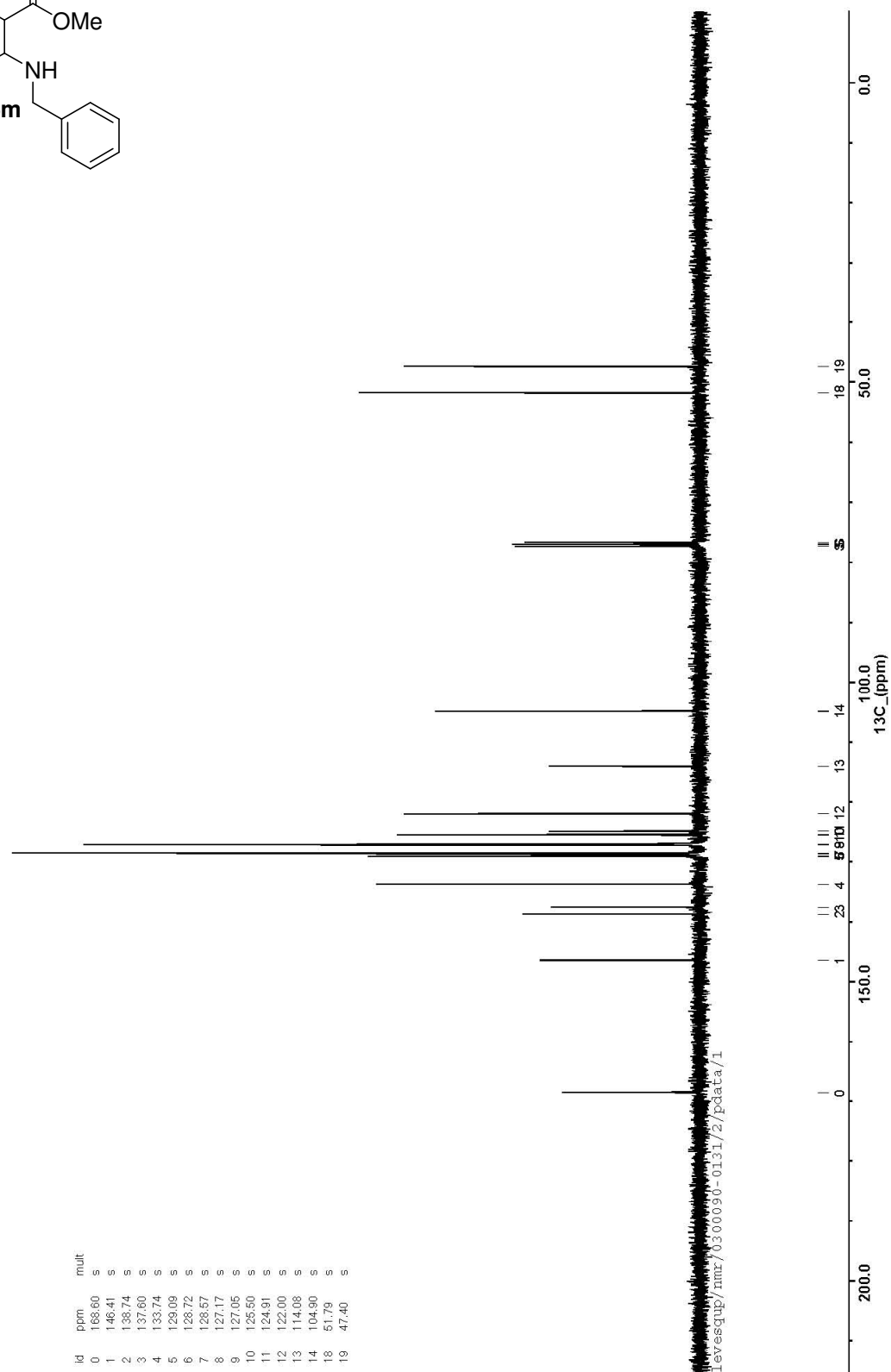
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of methyl 3-(benzylamino)naphthalene-2-carboxylate (**5m**)



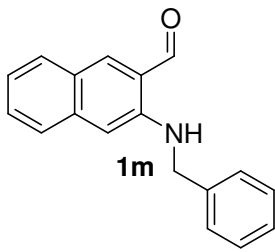
USER: levesqup  
 BOOK: 0300090-0131  
 EXPNO: 2  
 ACQUIRED: 26Nov-2009 11:36:15  
 SOLVENT: CDCl3  
 FILENAME: nmr\_archive\data\levesqup\nmr\0300090-0131\2fid

carbon

id	ppm	mult
0	168.60	s
1	146.41	s
2	138.74	s
3	137.00	s
4	133.74	s
5	129.09	s
6	128.72	s
7	128.57	s
8	127.17	s
9	127.05	s
10	125.50	s
11	124.91	s
12	122.00	s
13	114.08	s
14	104.90	s
18	51.79	s
19	47.40	s



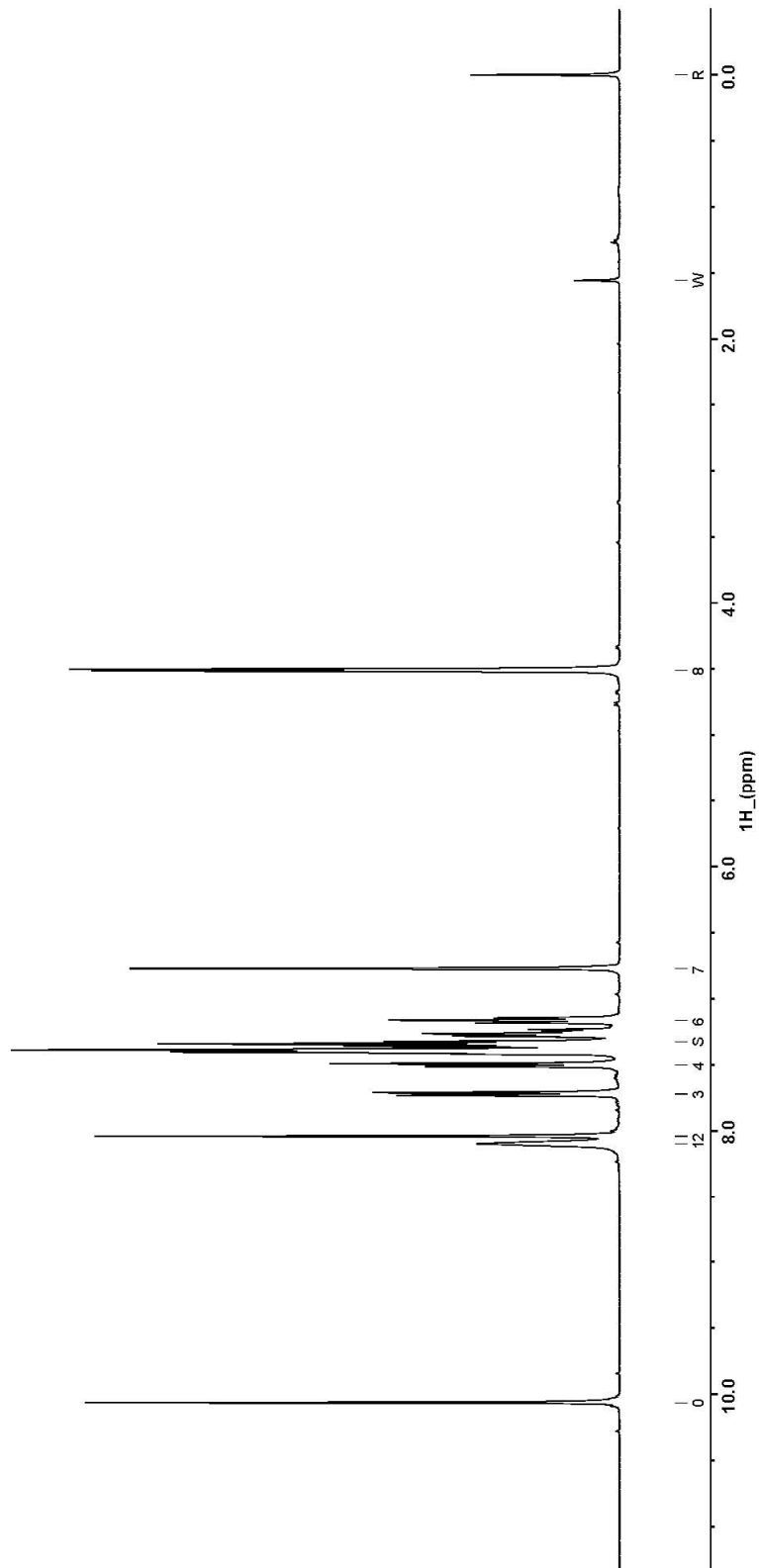
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of methyl 3-(benzylamino)  
 naphthalene-2-carboxylate (**5m**)



USER: levesq  
 BOOK: 0300090-0148  
 EXPNO: 1  
 ACQUIRED: 16-Dec-2009 10:51:34  
 SOLVENT: CDCl3  
 FILENAME: rml\_archive\data\levesq\fmr0300090-0148/1fid

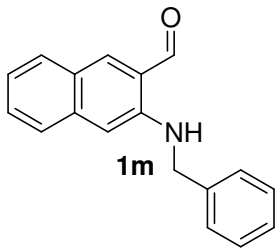
proton

id	ppm	mult	n	coupling
0	10.06	s	0.94	
1	8.10	s	1.10	
2	8.04	s	1.00	
3	7.72	d	1.01	8.25
4	7.50	d	1.04	8.44
6	7.16	t	1.01	7.50
7	6.77	s	1.00	
8	4.51	d	2.13	5.60



<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of 3-(benzylamino) naphthalene-2-carbaldehyde

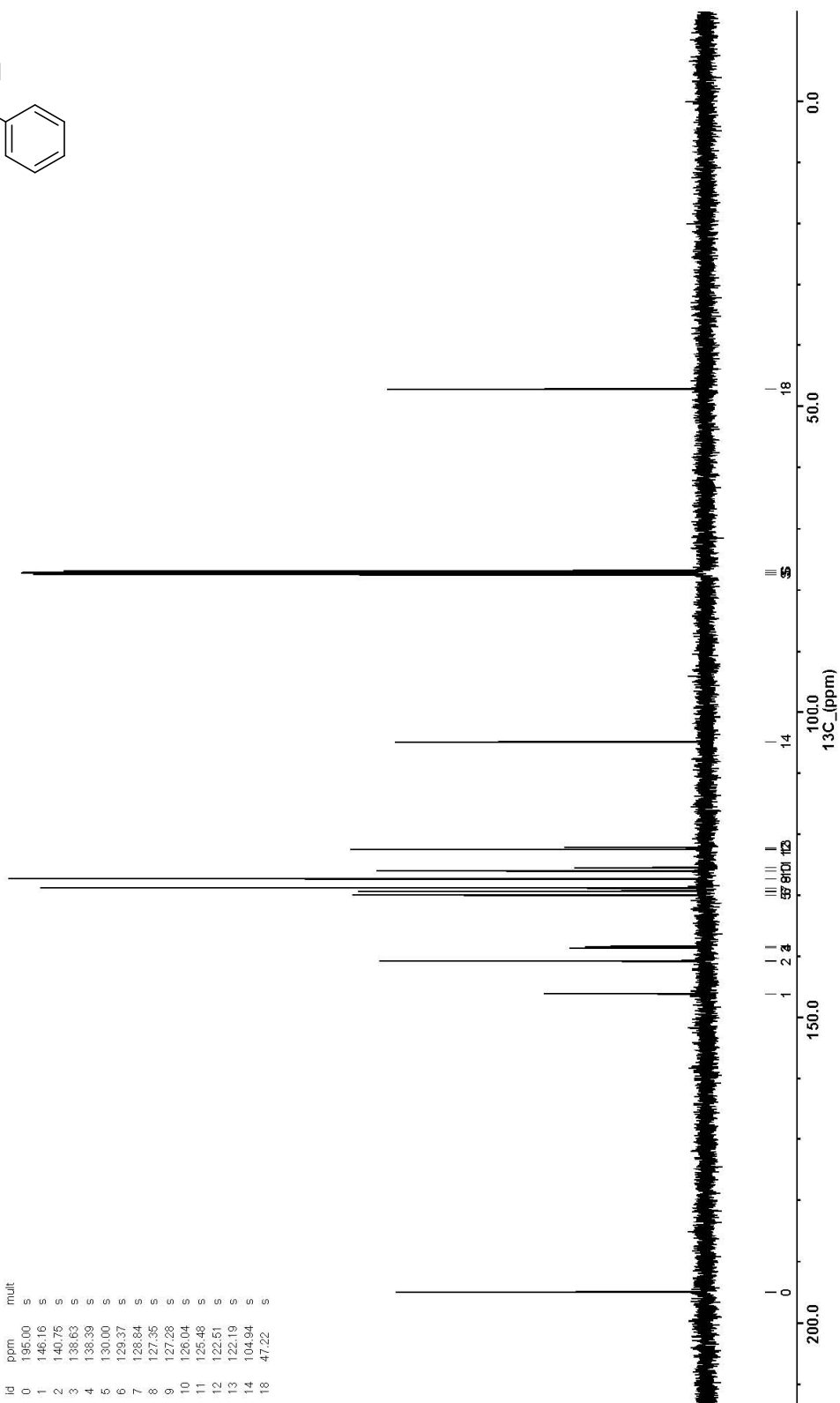
(**1m**)



USER: levesq  
 BOOK: 0300090-0148  
 EXPNO: 2  
 ACQUIRED: 16-Dec-2009 10:57:29  
 SOLVENT: CDCl3  
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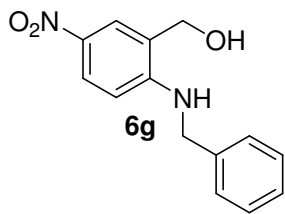
carbon

id	ppm	mult
0	195.00	s
1	146.16	s
2	140.75	s
3	138.63	s
4	138.39	s
5	130.00	s
6	129.37	s
7	128.84	s
8	127.35	s
9	127.28	s
10	126.04	s
11	125.48	s
12	122.51	s
13	122.19	s
14	104.94	s
18	47.22	s



$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of 3-(benzylamino) naphthalene-2-carbaldehyde

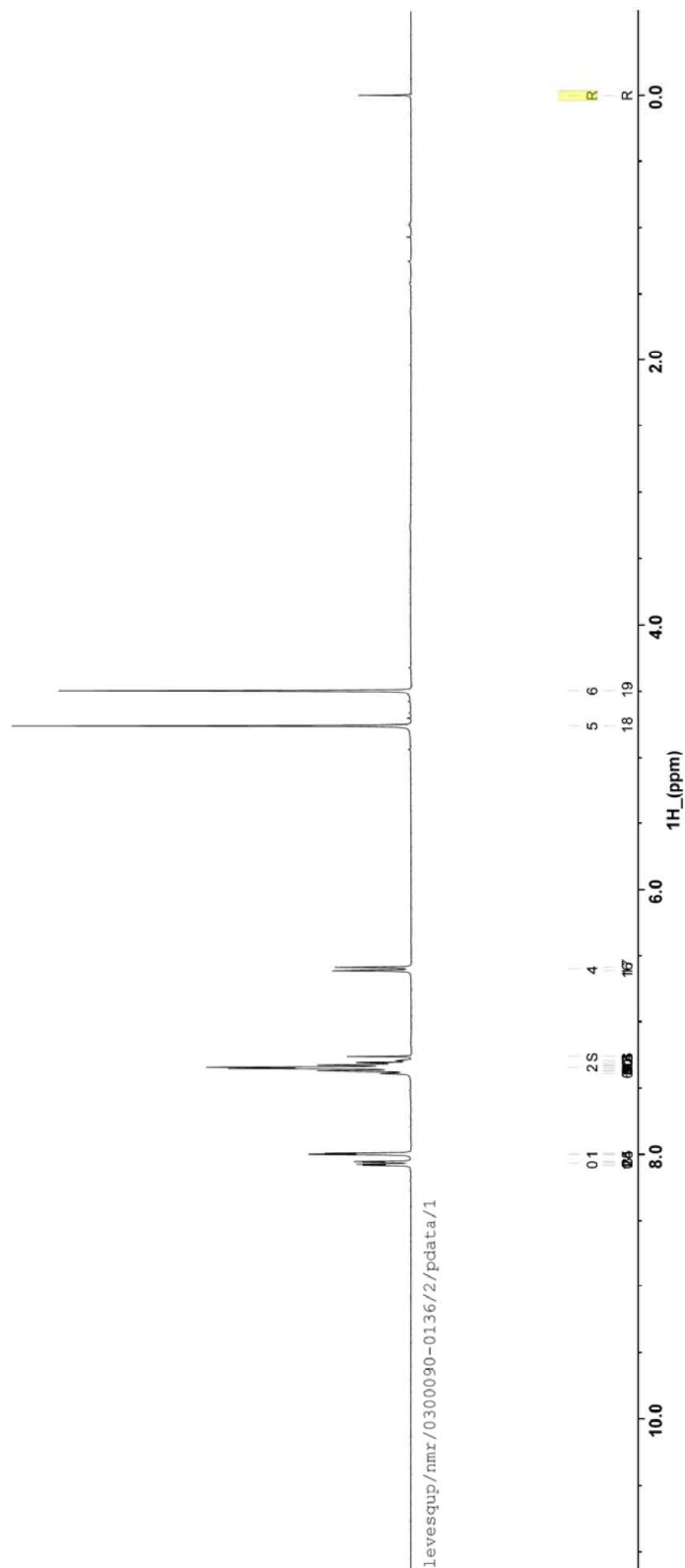
(**1m**)



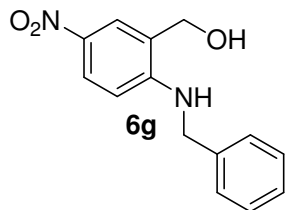
USER: levesq  
 BOOK: 0300090-0136  
 EXPNO: 2  
 ACQUIRED 04-Dec-2009 13:03:51  
 SOLVENT: CDCl3  
 FILENAME: nmr\_archive\data\levesq\nmr\0300090-0136/2/fid

Proton

id	ppm	mult	n	coupling
0	8.07	dd	1.00	9.06, 2.64
1	8.00	d	1.02	2.63
2	7.34	m	4.94	
4	6.80	d	1.07	9.07
5	4.76	s	2.09	
6	4.49	s	2.17	



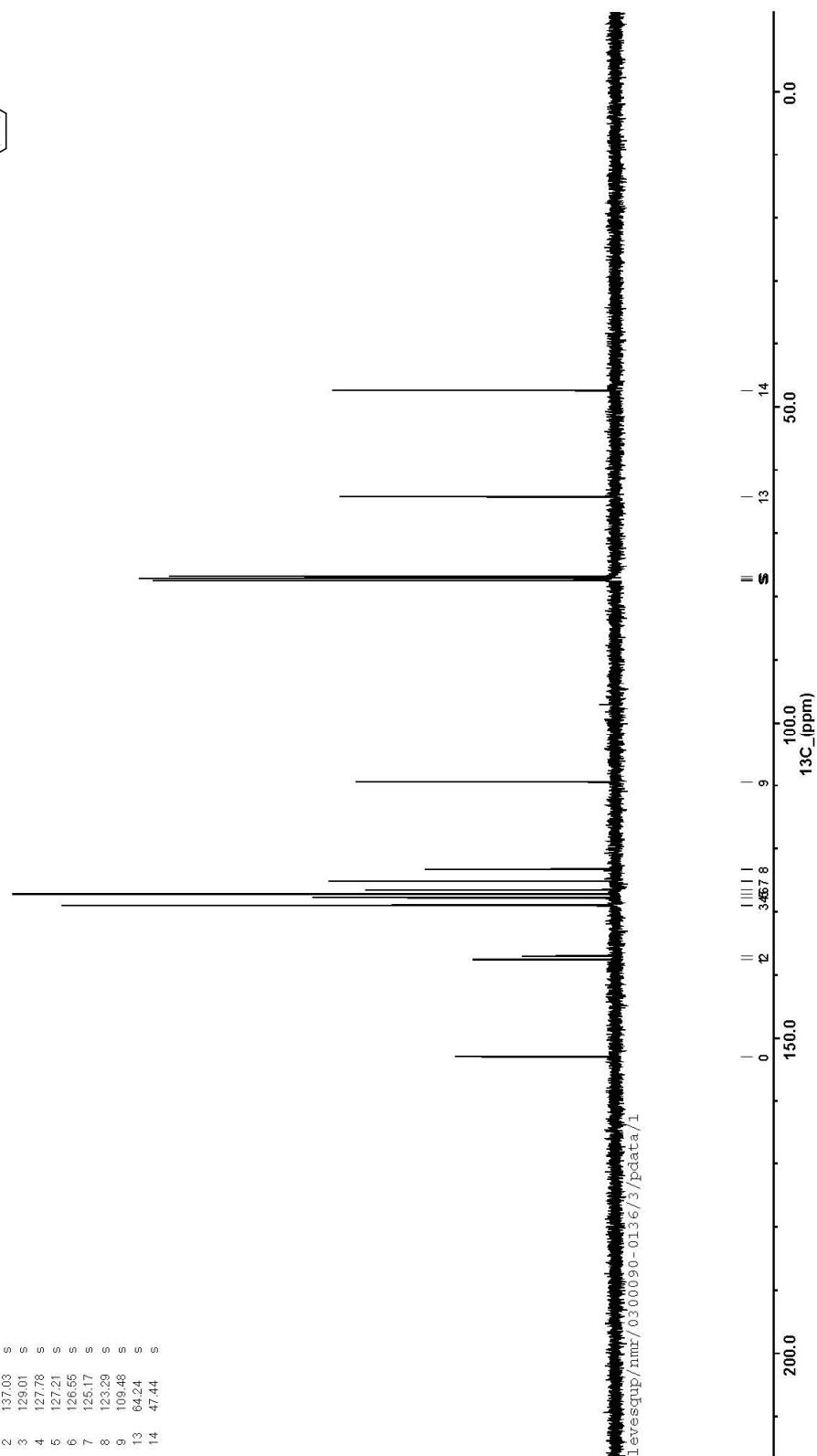
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of [2-(benzylamino)-5-nitrophenyl]methanol (**6g**)



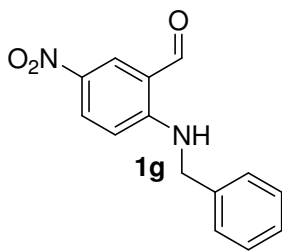
USER: levesq  
 BOOK: 0300090-0136  
 EXPNO: 3  
 ACQUIRED: 04-Dec-2009 13:12:40  
 SOLVENT: CDCl3  
 FILENAME: rmmr\_archive\data\levesq\mnr\0300090-0136/3.fid

carbon

id	ppm	mult
0	152.96	s
1	137.68	s
2	137.03	s
3	129.01	s
4	127.78	s
5	127.21	s
6	126.65	s
7	125.17	s
8	123.29	s
9	109.48	s
13	64.24	s
14	47.44	s



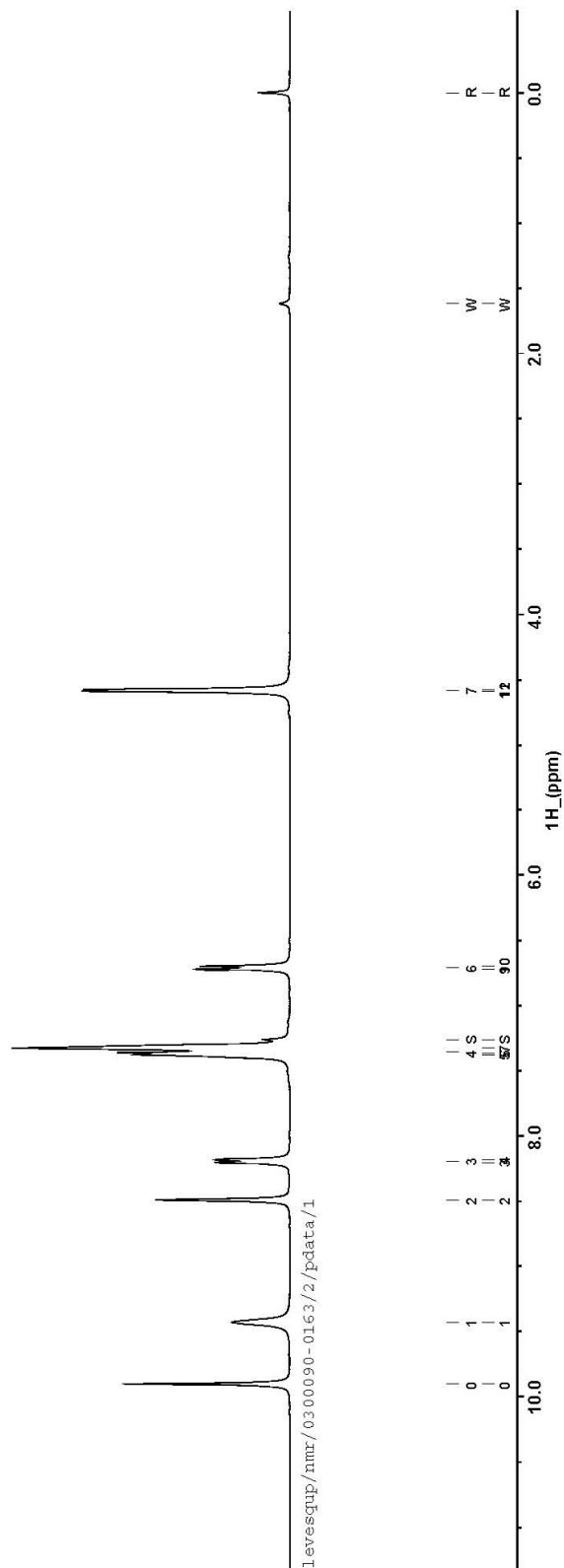
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of [2-(benzylamino)-5-nitrophenyl]methanol (**6g**)



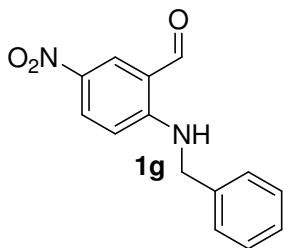
USER: lveesq  
 BOOK: 0300090-0163  
 EXPNO: 2  
 ACQUIRED: 10-Dec-2009 15:14:20  
 SOLVENT: CDCl3  
 FILENAME: rnmr\_archive\data/lveesq/nmr/0300090-0163/2fid

proton

ld	ppm	mult	n	coupling
0	9.90	s	0.87	
1	9.43	s	1.02	
2	8.48	s	0.95	
3	8.19	d	0.96	9.24
4	7.35	m	5.00	
6	6.71	d	0.99	9.34
7	4.58	d	2.04	5.76



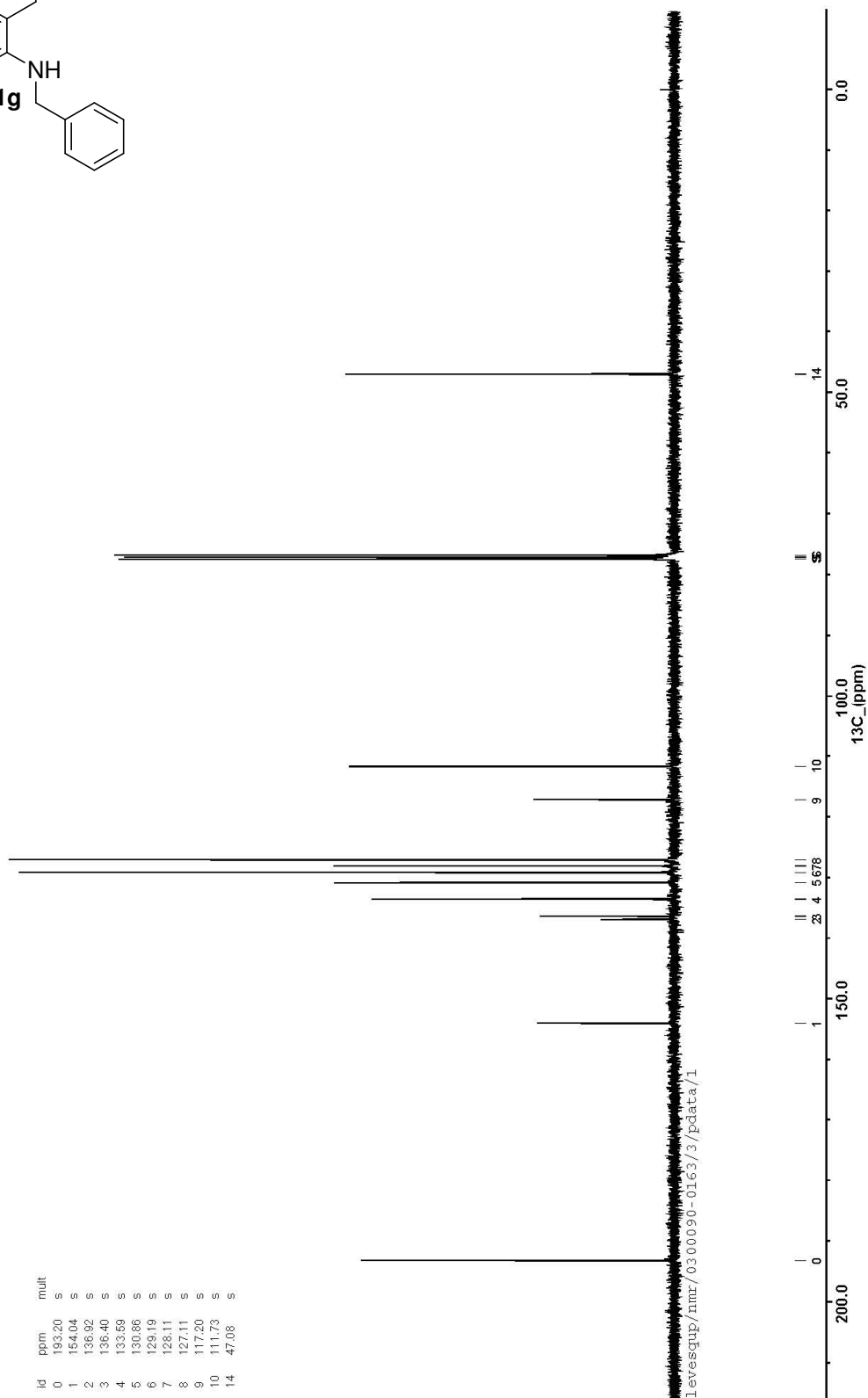
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of 2-(benzylamino)-5-nitrobenzaldehyde (**1g**)



USER: lveesq  
 BOOK: 0300090-0163  
 EXPNO: 3  
 ACQUIRED: 10-Dec-2009 15:19:34  
 SOLVENT: CDCl3  
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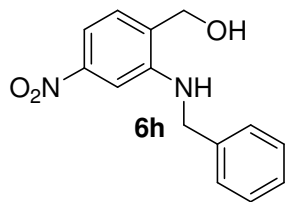
carbon

id	ppm	mult
0	193.20	s
1	154.04	s
2	136.92	s
3	136.40	s
4	133.59	s
5	130.86	s
6	129.19	s
7	128.11	s
8	127.11	s
9	117.20	s
10	111.79	s
14	47.06	s



$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of 2-(benzylamino)-5-nitrobenzaldehyde (**1g**)

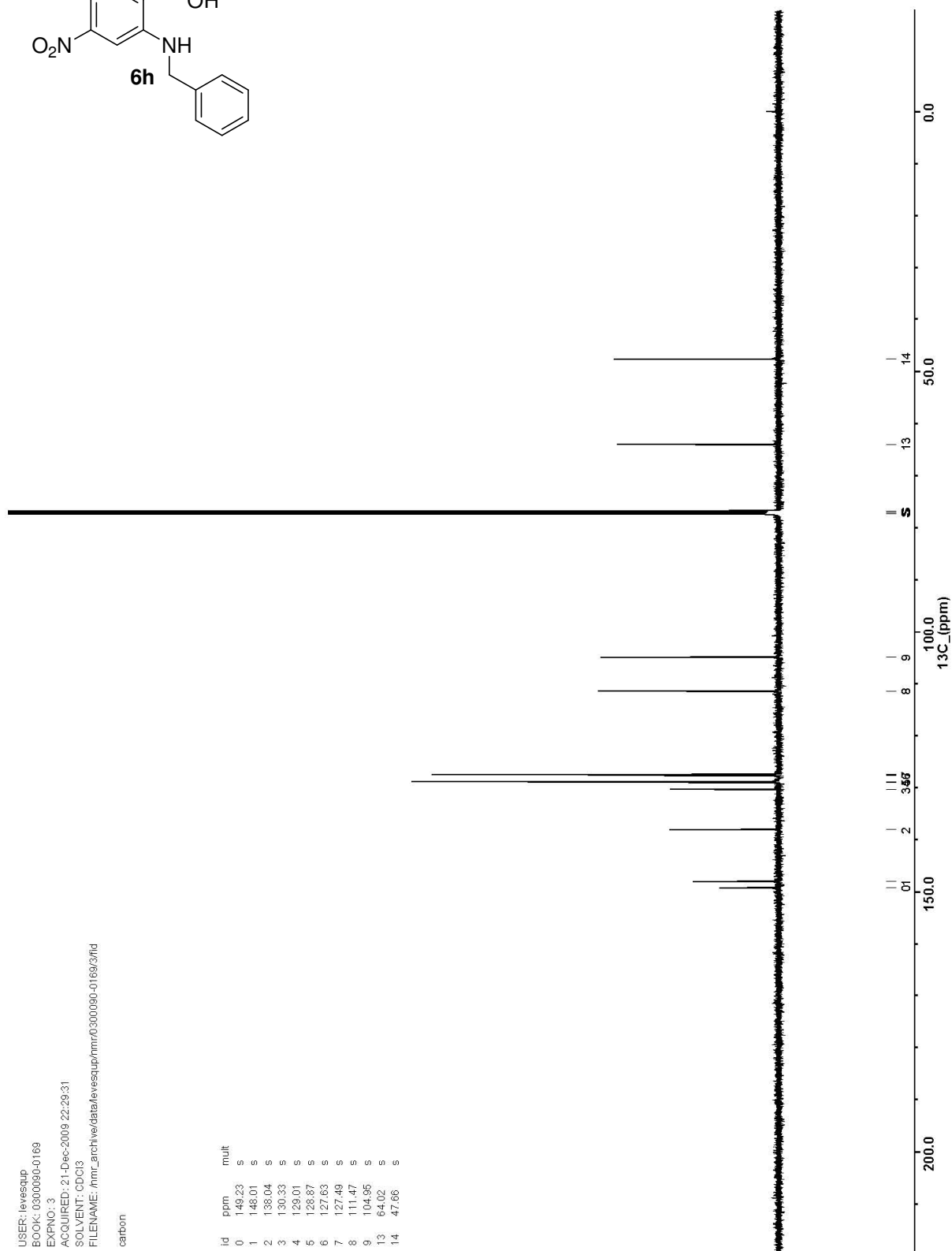




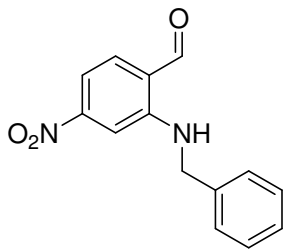
USER: levescup  
 BOOK: 0300090-0169  
 EXPNO: 3  
 ACQUIRED: 21-Dec-2009 22:29:31  
 SOLVENT: CDCl3  
 FILENAME: /nmr\_archive/data/levescup/nmr/0300090-0169/3fid

carbon

id	ppm	mult
0	149.23	s
1	148.01	s
2	136.04	s
3	130.33	s
4	129.01	s
5	128.87	s
6	127.63	s
7	127.49	s
8	111.47	s
9	104.95	s
13	64.02	s
14	47.66	s



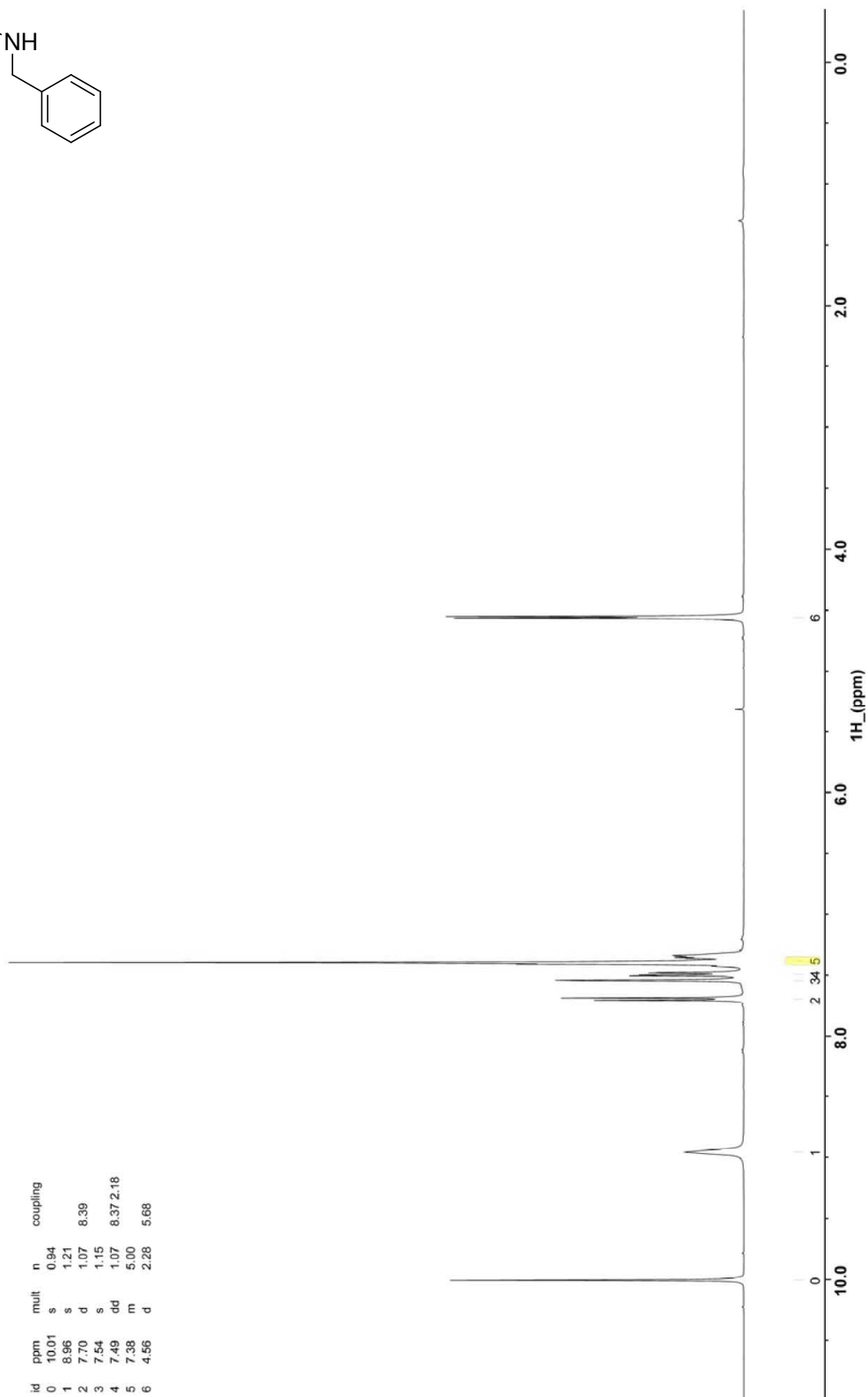
<sup>13</sup>C NMR Spectrum (101 MHz, CDCl<sub>3</sub>) of [2-(benzylamino)-4-nitrophenyl]methanol (**6h**)



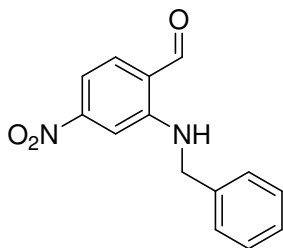
USER: fourmpi  
 BOOK: 0283254-0084  
 EXPNO: 1  
 ACQUIRED: 03-Mar-2010 10:04:26  
 SOLVENT: CDCl3  
 FILENAME: nmr\_archive\data/fourmpi/nmr/0283254-0084/1.fid

clean proton

id	ppm	mult	n	coupling
0	10.01	s	0.94	
1	8.96	s	1.21	
2	7.70	d	1.07	8.39
3	7.54	s	1.15	
4	7.49	dd	1.07	8.37 2.18
5	7.38	m	5.00	
6	4.56	d	2.28	5.68



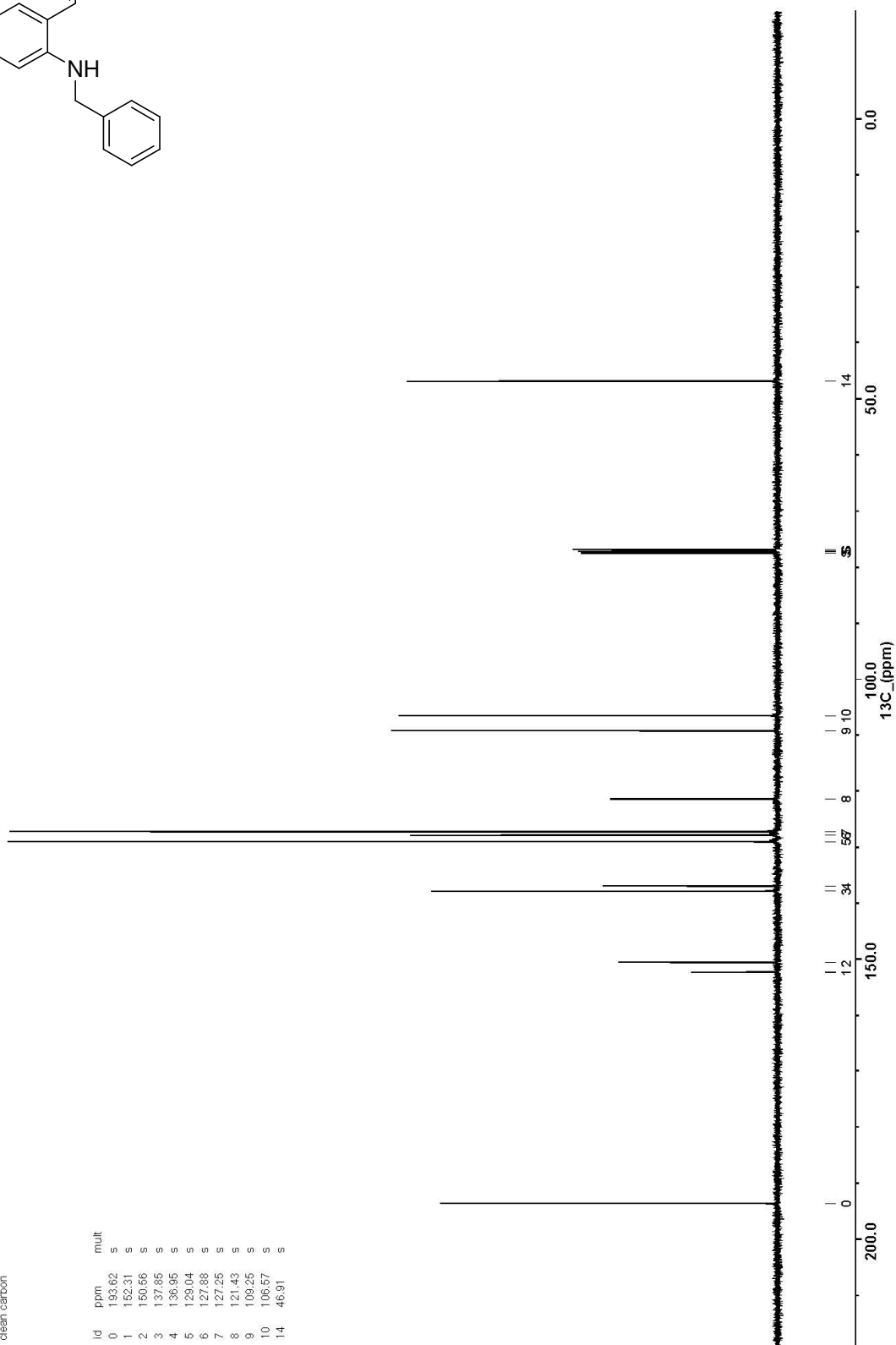
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of 2-(benzylamino)-4-nitrobenzaldehyde (**1h**)



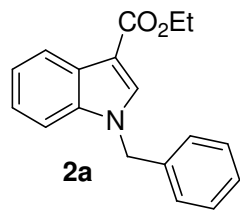
USER: fourmpi  
 BOOK: 0283264-0084  
 EXPNO: 2  
 ACQUIRED: 03-Mar-2010 10:12:34  
 SOLVENT: CDCl3  
 FILENAME: rmt\_archive\data\fourmpi\rmt\0283264-0084\2fid

clean carbon

id	ppm	mult
0	193.62	s
1	152.31	s
2	150.56	s
3	137.85	s
4	136.95	s
5	129.04	s
6	127.88	s
7	127.25	s
8	121.43	s
9	109.25	s
10	106.57	s
14	46.91	s

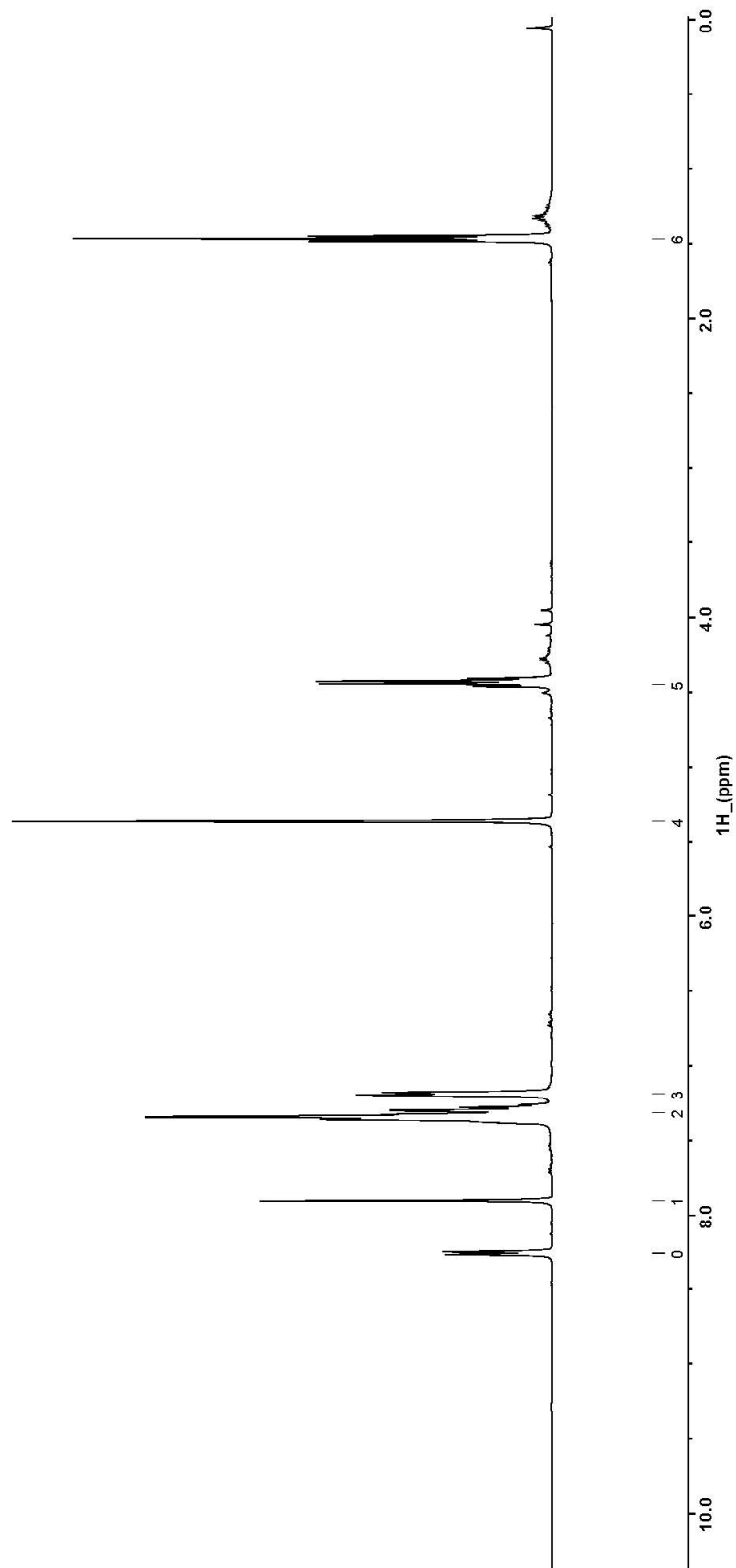


$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of 2-(benzylamino)-4-nitrobenzaldehyde (**1h**)

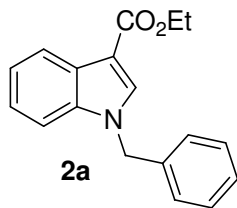


Parameters  
 DATE Dec 03 2009  
 TEMP 300  
 SOLVENT CDCl3  
 SEQUENCE zg30  
 F1 Parameters  
 SF 400.18000  
 SW 8278.15  
 SIZE 32768

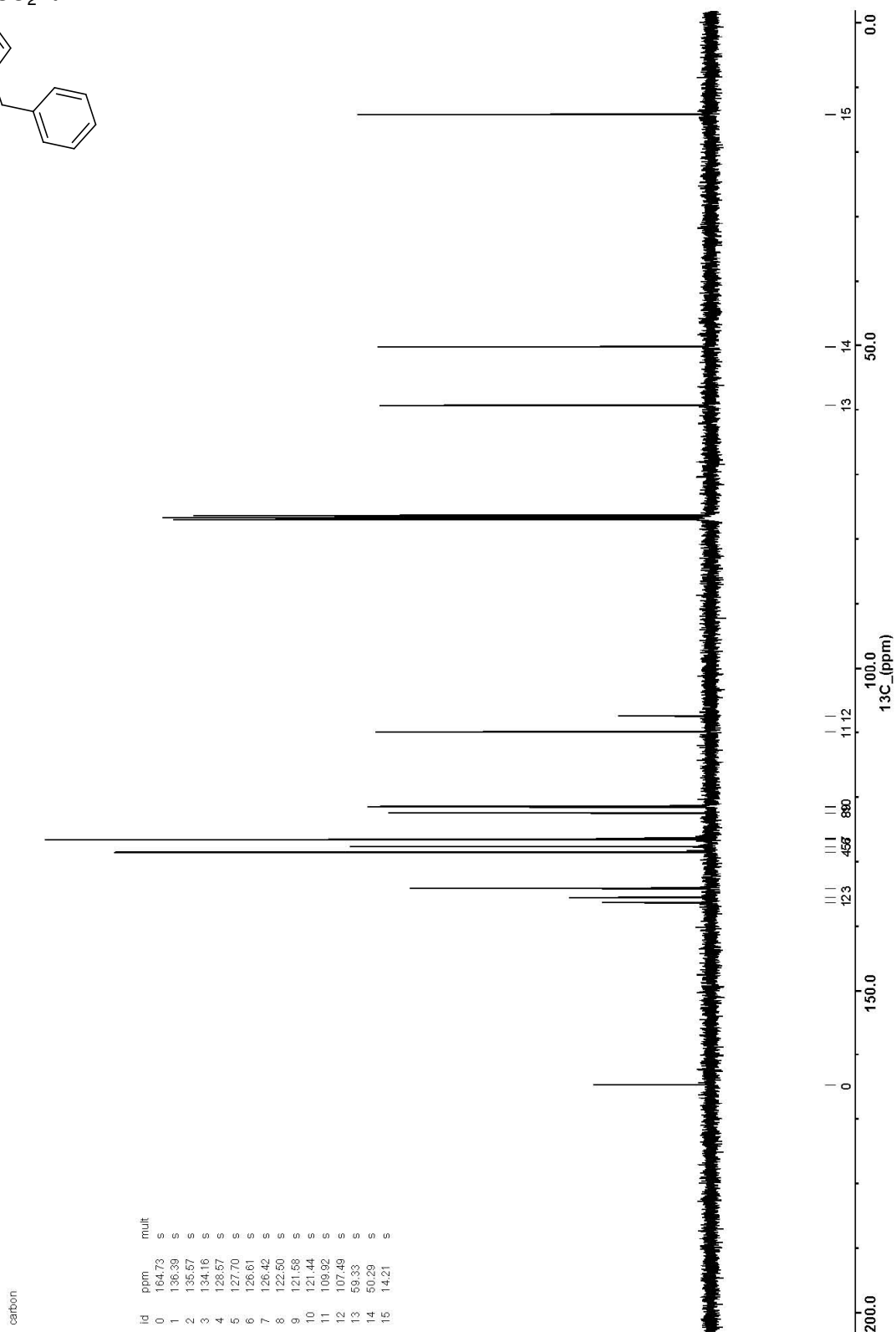
id	ppm	mult	n	coupling
0	8.26	d	1.00	7.64
1	7.90	s	0.85	
2	7.31	m	5.98	
3	7.19	d	2.09	6.76
4	5.37	s	2.01	
5	4.45	m	2.00	
6	1.47	t	2.97	7.10



<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of ethyl 1-benzylindole-3-carboxylate (**2a**)

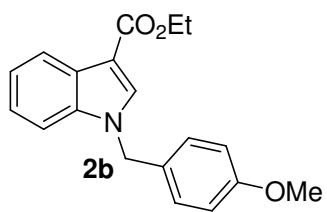


USER: levesqup  
 BOOK: 0300090-0157  
 EXPNO: 2  
 ACQUIRED: 03-Dec-2009 15:32:23  
 SOLVENT: CDCl3  
 FILENAME: rmt\_archive\data\levesqup\rmt0300090-01572.fid



$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of ethyl 1-benzylindole-3-carboxylate (**2a**)

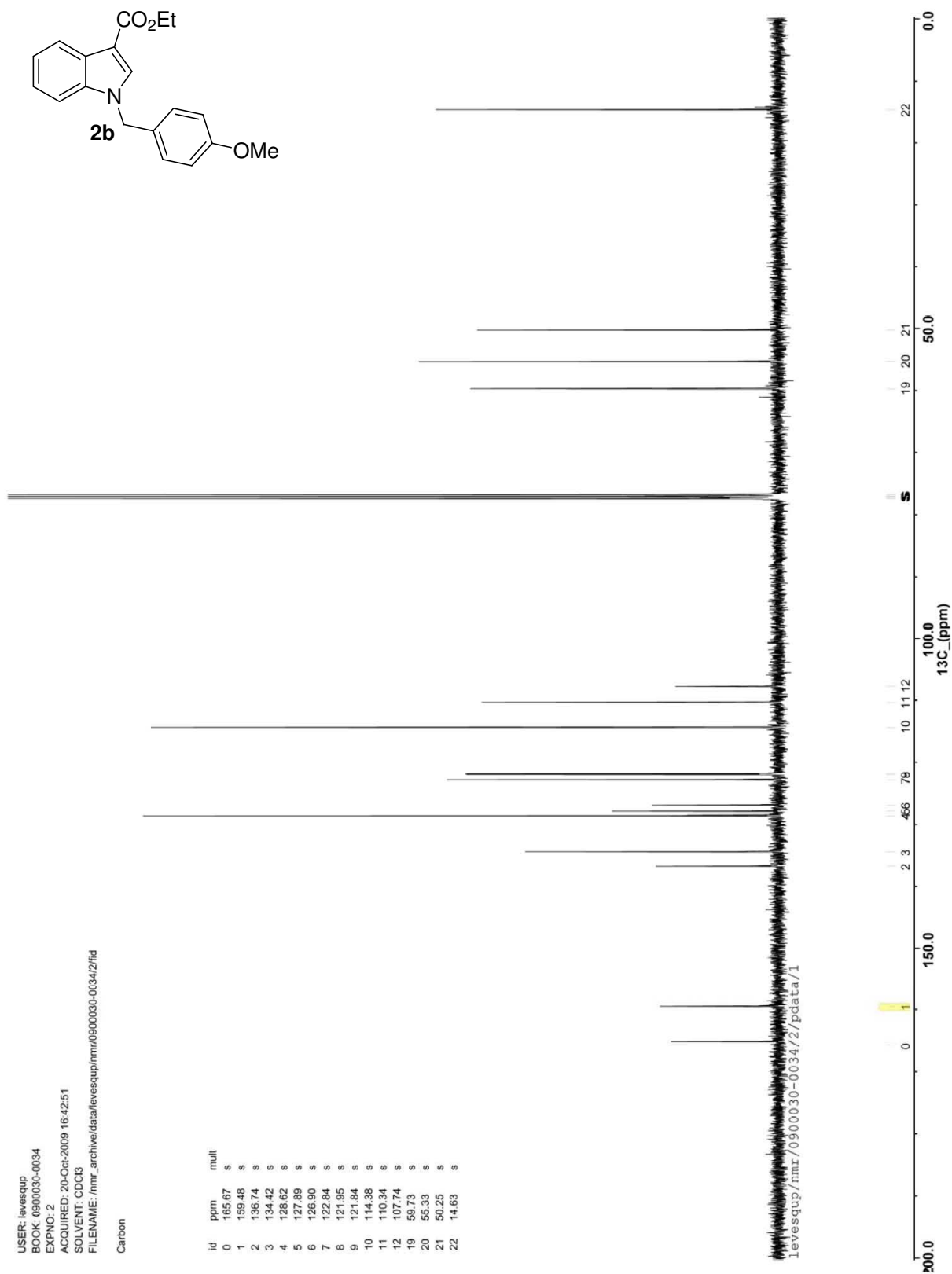




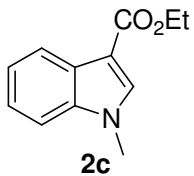
USER: levesqup  
 BOOK: 0900030-0034  
 EXPNO: 2  
 ACQUIRED: 20-Oct-2009 16:42:51  
 SOLVENT: CDCl3  
 FILENAME: nmr\_archive\data\levesqup\nmr\0900030-0034\2\fid

Carbon

id	ppm	mult
0	165.67	s
1	159.48	s
2	136.74	s
3	134.42	s
4	128.62	s
5	127.89	s
6	126.90	s
7	122.84	s
8	121.95	s
9	121.84	s
10	114.38	s
11	110.34	s
12	107.74	s
19	59.73	s
20	55.33	s
21	50.25	s
22	14.63	s



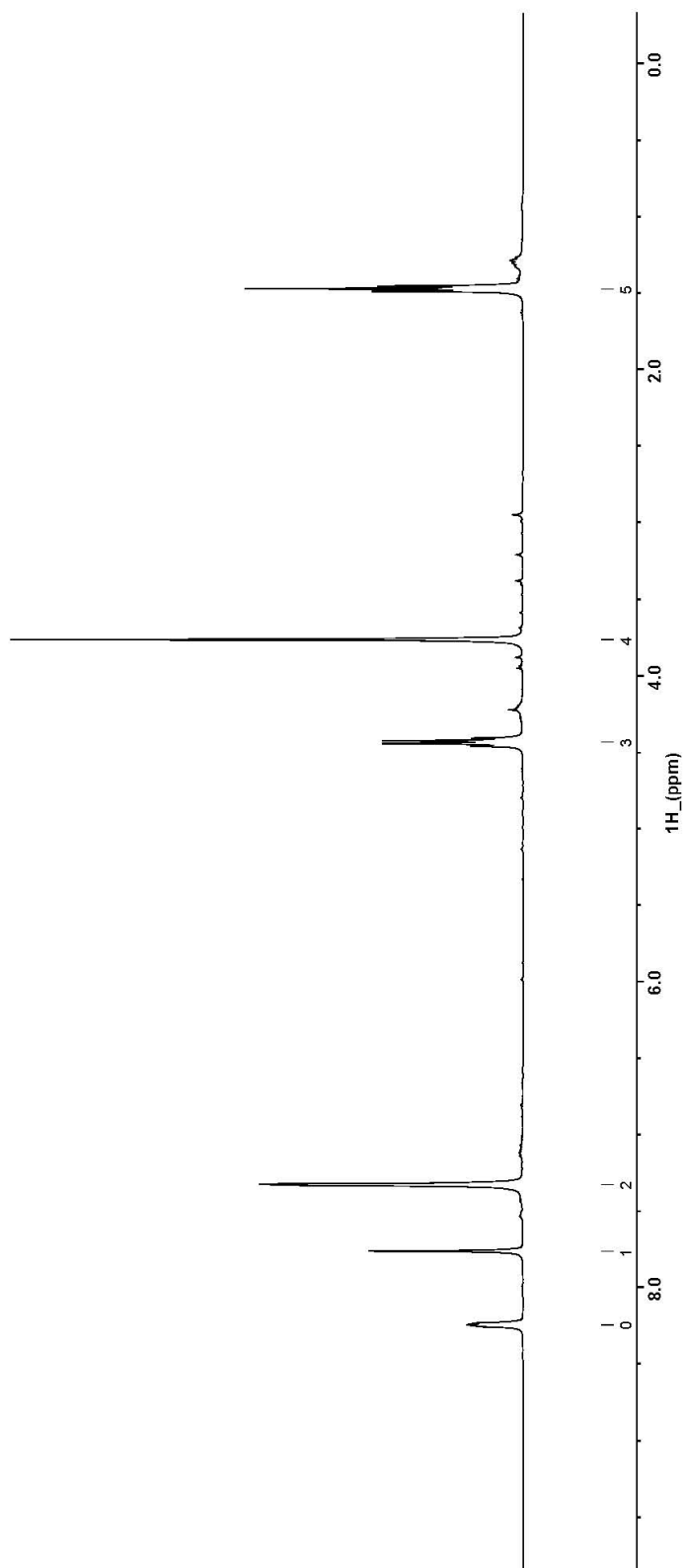
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of ethyl 1-benzylindole-3-carboxylate (**2b**)



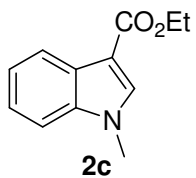
USER: fourmpi  
 BOOK: 0300026-0081  
 EXPNO: 1  
 ACQUIRED: 27-Jul-2010 17:02:31  
 SOLVENT: CDCl3  
 FILENAME: rml\_archive\data\fourmpi\rmf0300026-0081.fid

Proton

id	ppm	mult	n	coupling
0	8.25	m	1.00	
1	7.77	s	0.82	
2	7.33	d	3.02	3.68
3	4.43	q	2.07	7.09
4	3.76	s	2.77	
5	1.47	t	3.10	7.09



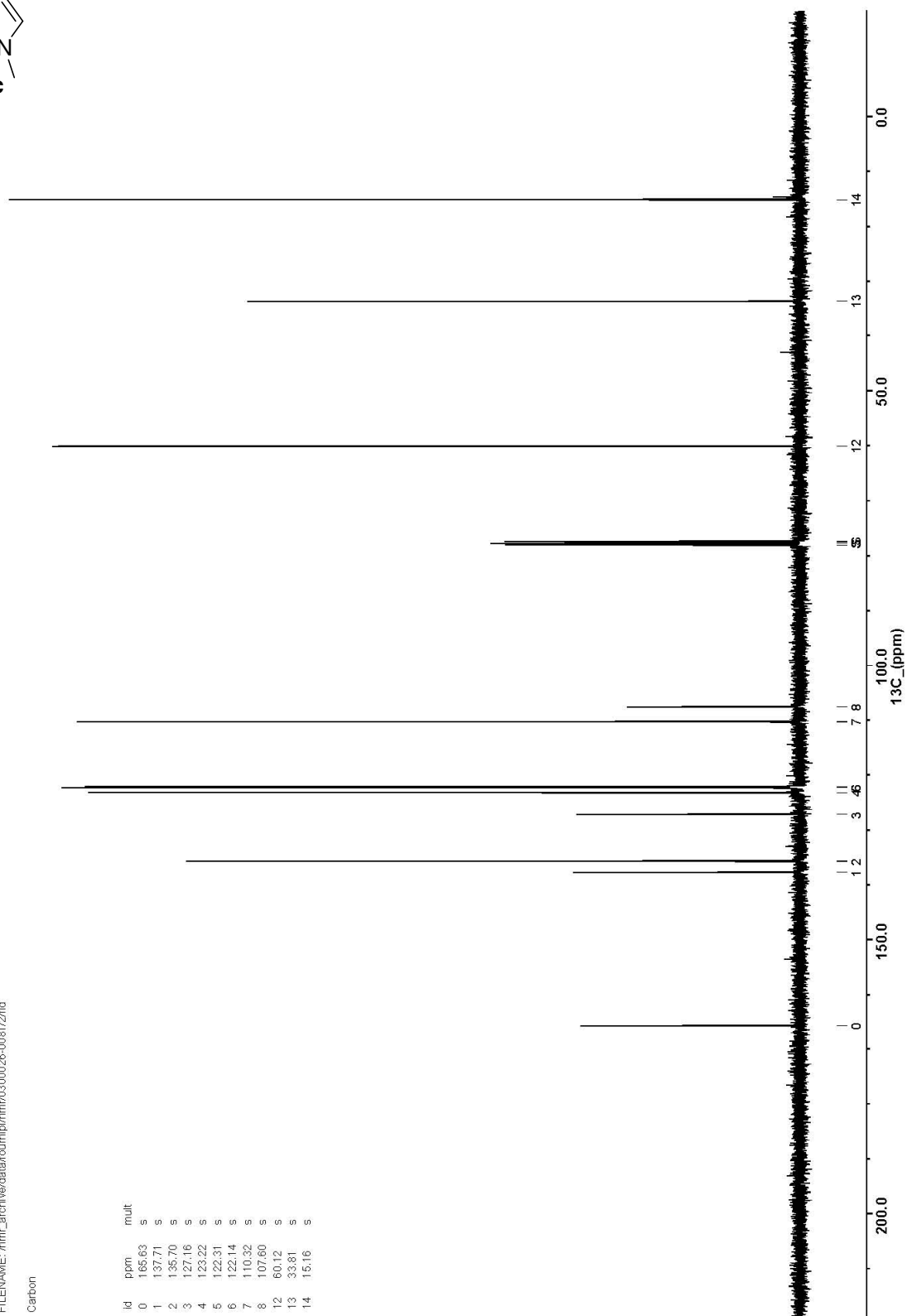
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of ethyl 1-methylindole-3-carboxylate (**2c**)



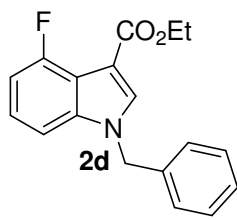
USER: fourmpi  
 BOOK: 0300026-0081  
 EXPNO: 2  
 ACQUIRED: 27-Jul-2010 17:08:28  
 SOLVENT: CDCl3  
 FILENAME: rml\_archive\datafourmpi\rml\0300026-0081\2.fid

Carbon

Id	ppm	mult
0	165.63	s
1	137.71	s
2	135.70	s
3	127.16	s
4	123.22	s
5	122.31	s
6	122.14	s
7	110.32	s
8	107.60	s
12	60.12	s
13	33.81	s
14	15.16	s



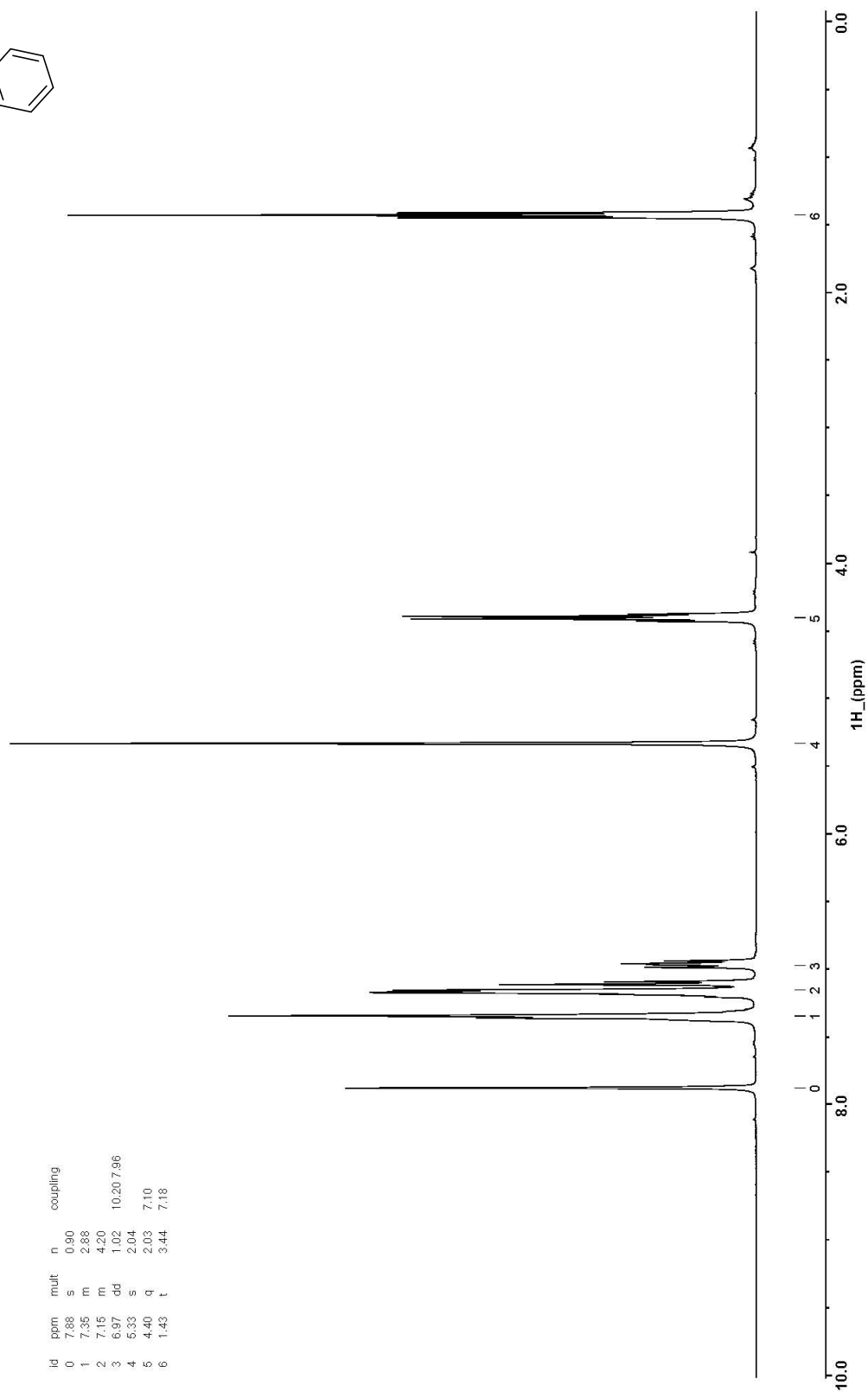
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of ethyl 1-methylindole-3-carboxylate (**2c**)



USER: fourmpi  
 BOOK: 0283264-0076  
 EXPNO: 6  
 ACQUIRED: 15-Jan-2010 10:24:10  
 SOLVENT: CDCl3  
 FILENAME: rmt\_archive\data\fourmpi\rmt\0283264-0076\6.fid

proton

id	ppm	mult	n	coupling
0	7.88	s	0.80	
1	7.35	m	2.88	
2	7.15	m	4.20	
3	6.97	dd	1.02	10.20 7.96
4	5.33	s	2.04	
5	4.40	q	2.03	7.10
6	1.43	t	3.44	7.18

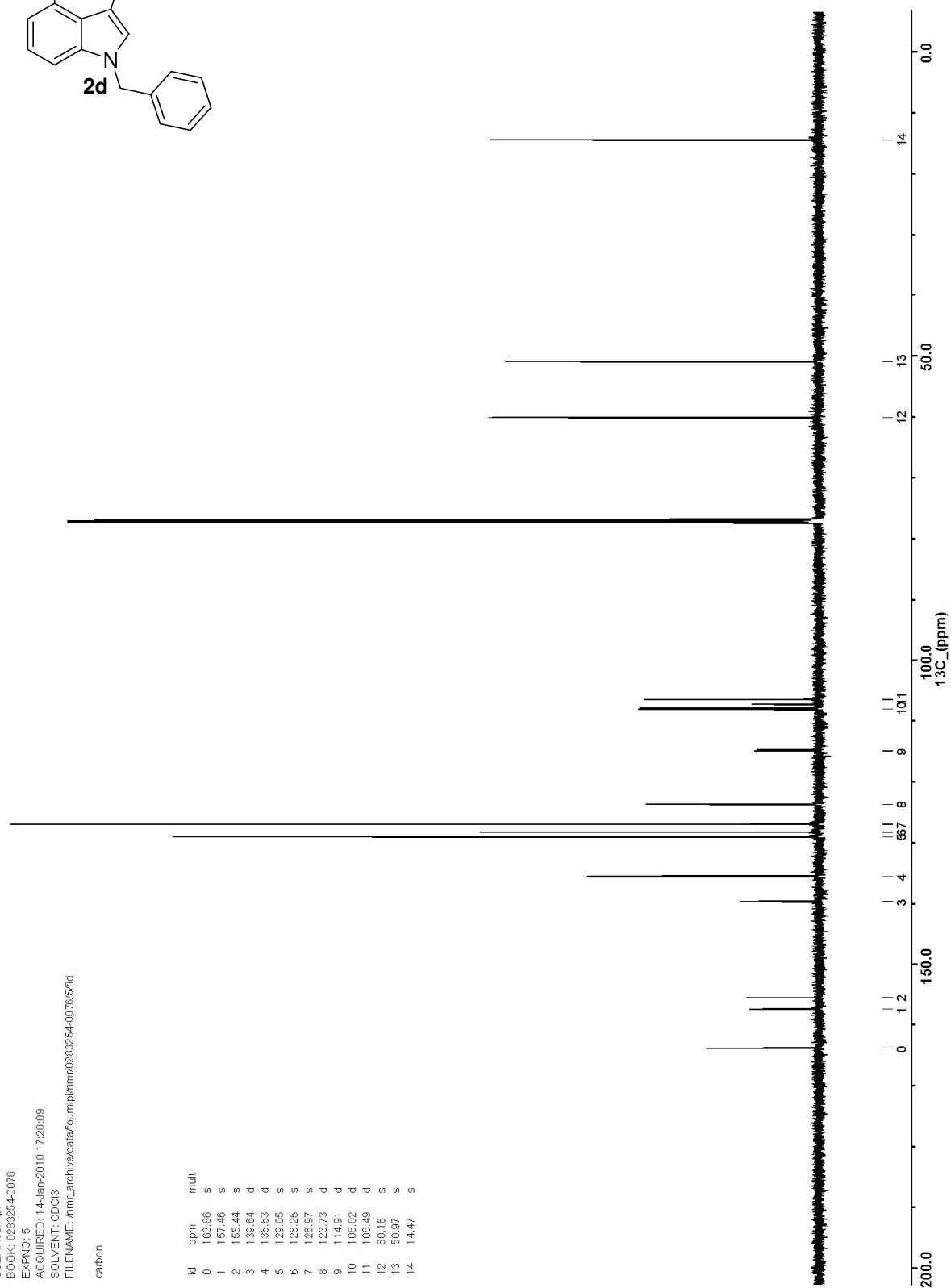


<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-4-fluoroindole-3-carboxylate (**2d**)

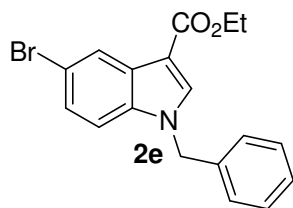
USER: fourmpi  
BOOK: 0283254-0076  
EXPNO: 5  
ACQUIRED: 14-Jan-2010 17:20:09  
SOLVENT: CDCl3  
FILENAME: rml\_archive\datafourmpi\rml\0283254-0076\5.fid

carbon

id	ppm	mult
0	163.86	s
1	157.46	s
2	155.44	s
3	139.64	d
4	135.53	d
5	129.05	s
6	128.25	s
7	126.97	s
8	123.73	d
9	114.91	d
10	108.02	d
11	106.49	d
12	60.15	s
13	50.97	s
14	14.47	s

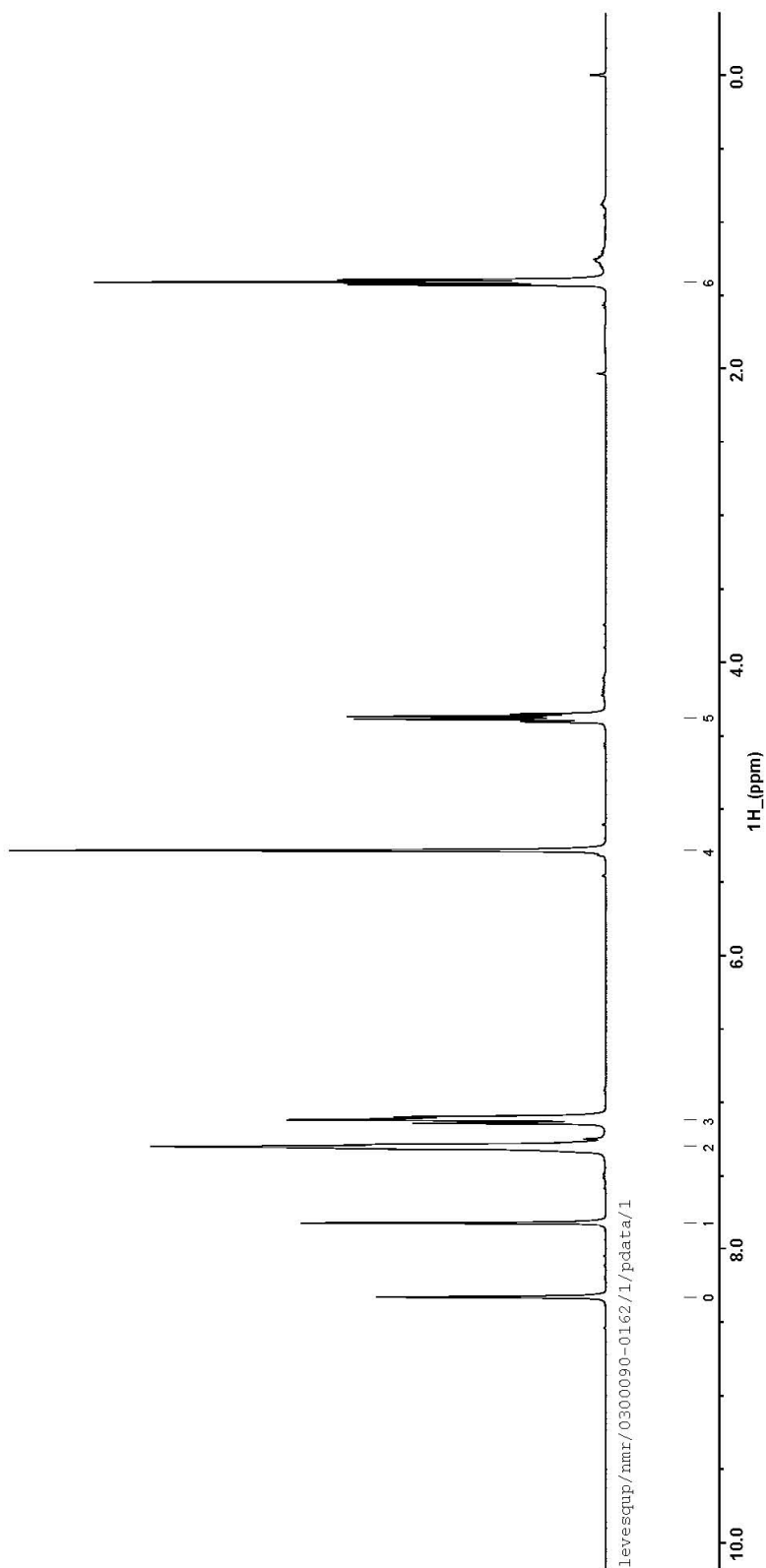


<sup>13</sup>C NMR Spectrum (101 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-4-fluoroindole-3-carboxylate (**2d**)



Parameters  
 DATE Dec 03 2009  
 TEMP 300  
 SOLVENT CDCl3  
 SEQUENCE zg30  
 F1 Parameters  
 SF 400.18000  
 SW 8278.15  
 SIZE 32768

id	ppm	mult	n	coupling
0	8.33	s	1.00	
1	7.82	s	1.00	
2	7.30	m	4.54	
3	7.12	m	3.27	
4	5.28	s	2.22	
5	4.38	q	2.16	7.14
6	1.41	t	3.27	7.14

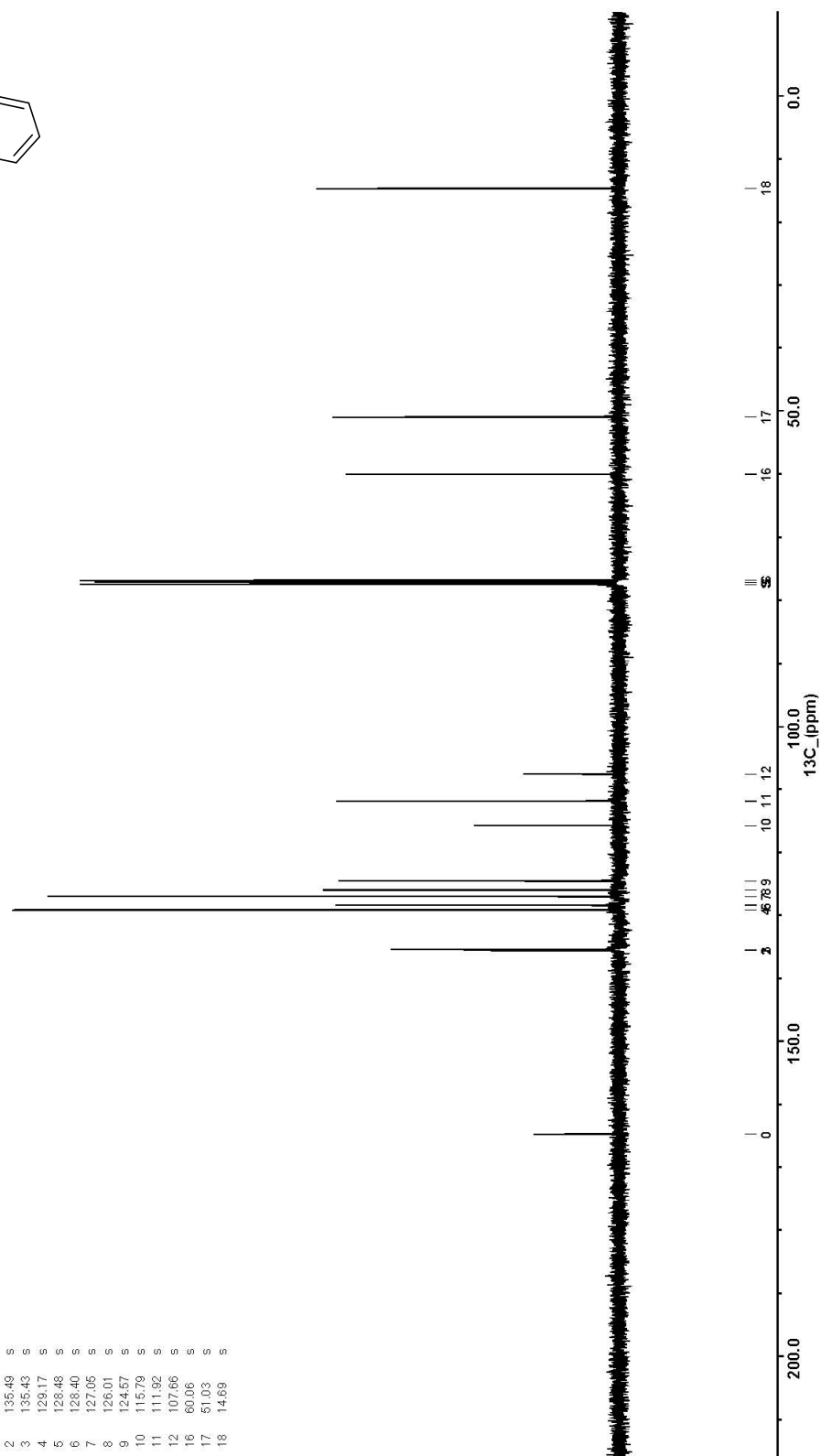
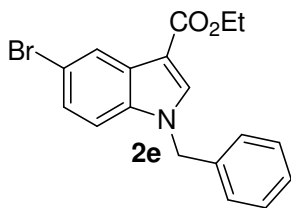


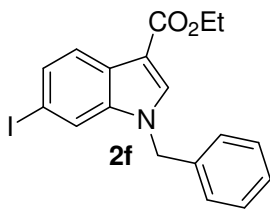
<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-5-bromoindole-3-carboxylate (**2e**)

USER: leveq  
BOOK: 0300090-0162  
EXPNO: 2  
ACQUIRED: 03-Dec-2009 14:42:12  
SOLVENT: CDCl3  
FILENAME: rmmi\_archive\data\leveq\mnr\0300090-0162\fid

carbon

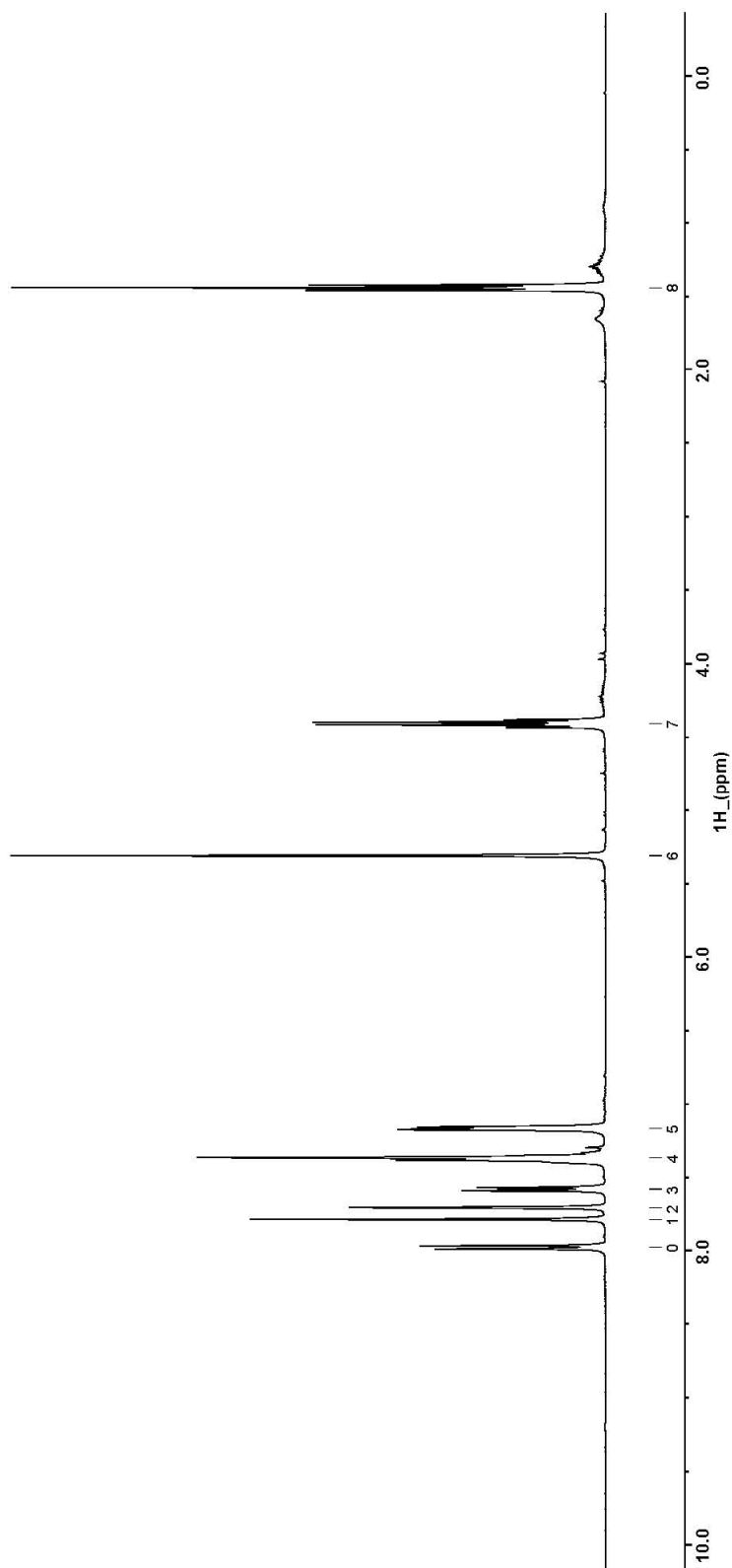
id	ppm	mult
0	164.70	s
1	135.61	s
2	135.49	s
3	135.43	s
4	129.17	s
5	128.48	s
6	128.40	s
7	127.05	s
8	126.01	s
9	124.57	s
10	115.79	s
11	111.92	s
12	107.66	s
16	60.06	s
17	51.03	s
18	14.69	s





USER: fourmpi  
 BOOK: 0283264-0071  
 EXPNO: 1  
 ACQUIRED: 06-Jan-2010 15:35:25  
 SOLVENT: CDCl3  
 FILENAME: rmt\_archive\data\fourmpi\rmt\0283264-0071.fid  
 proton f35

id	ppm	mult	n	coupling
0	7.98	d	0.88	8.42
1	7.78	s	0.85	
2	7.70	s	1.00	
3	7.68	d	1.05	8.43
4	7.37	m	2.91	
5	7.16	m	2.11	
6	5.31	s	2.01	
7	4.41	q	2.03	7.11
8	1.44	t	3.01	7.10

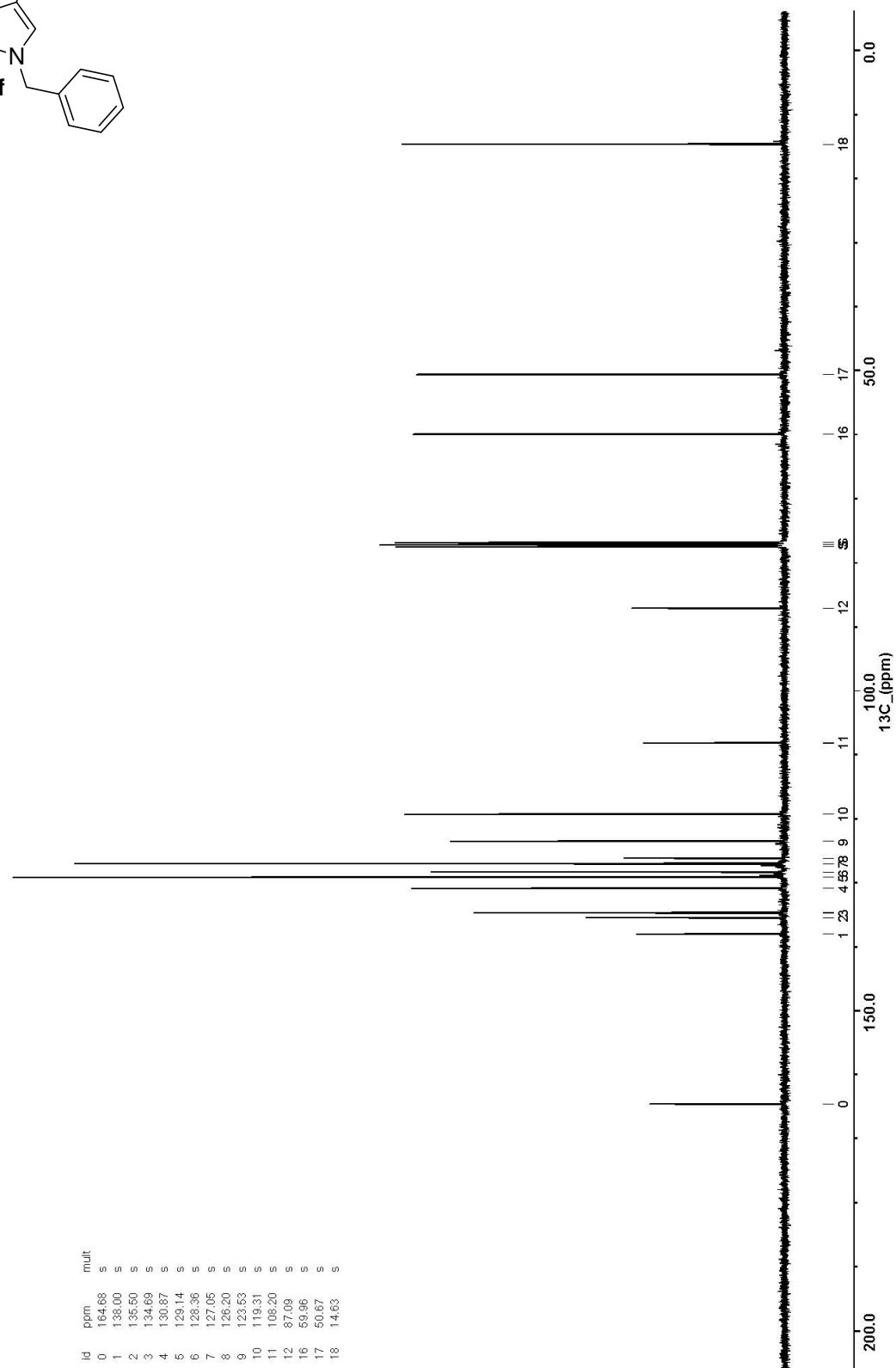
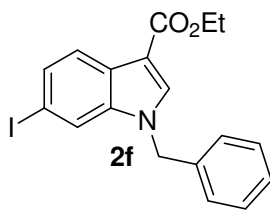


<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-6-iodoindole-3-carboxylate (**2f**)

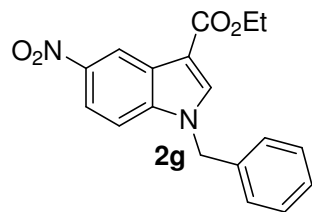
USER: fourmpi  
BOOK: 0283264-0071  
EXPNO: 2  
ACQUIRED: 06-Jan-2010 17:39:21  
SOLVENT: CDCl3  
FILENAME: rmt\_archive\data\fourmpi\rmt\0283264-0071\2fid

carbon

id	ppm	mult
0	164.68	s
1	138.00	s
2	135.50	s
3	134.69	s
4	130.87	s
5	129.14	s
6	128.36	s
7	127.05	s
8	126.20	s
9	123.53	s
10	119.31	s
11	108.20	s
12	87.09	s
16	59.96	s
17	50.67	s
18	14.63	s



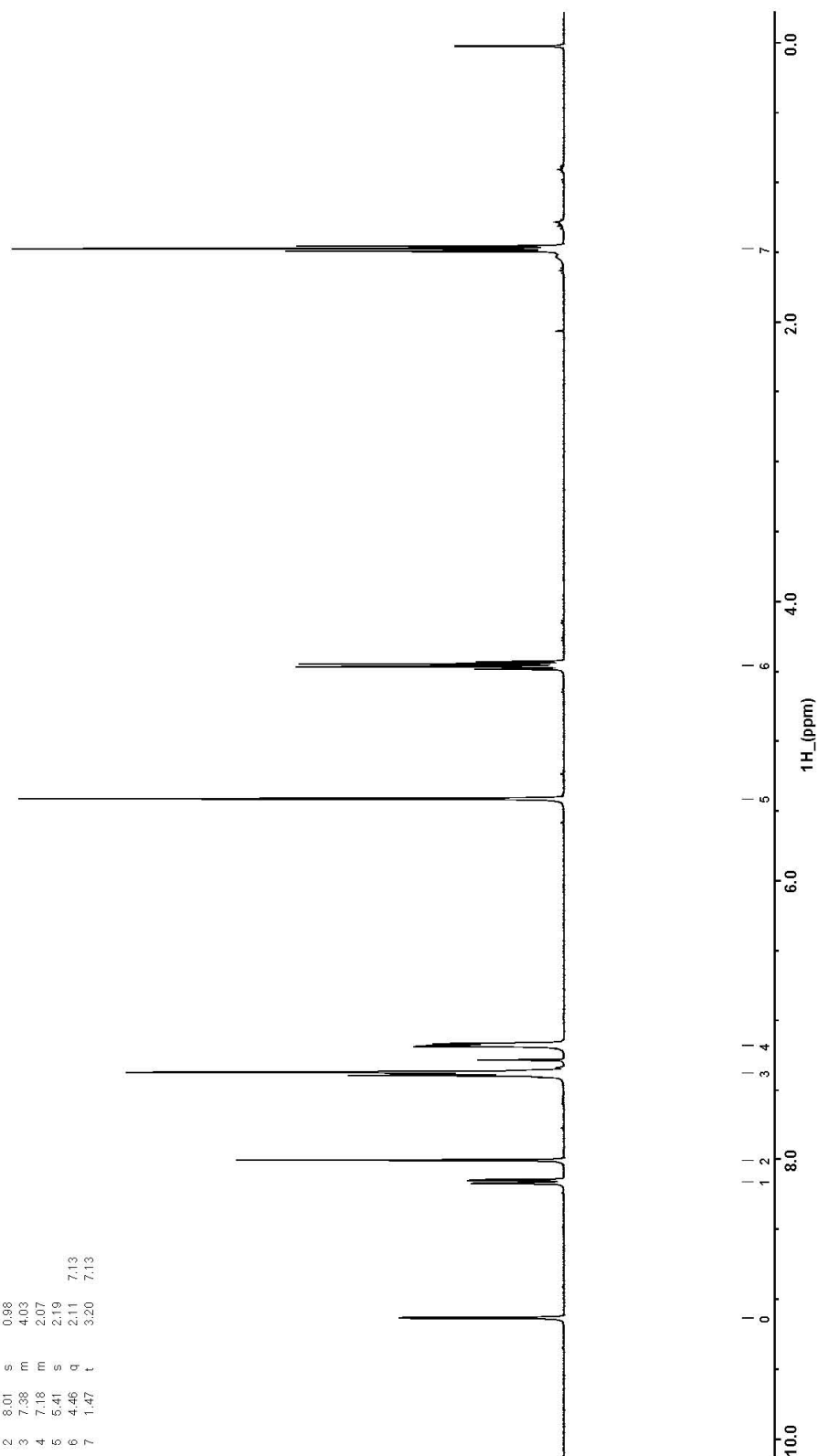
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of ethyl 1-benzyl-6-iodoindole-3-carboxylate (**2f**)



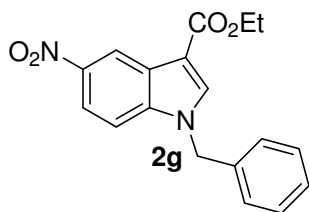
USER: leveq  
 BOOK: 0300090-0171  
 EXPNO: 5  
 ACQUIRED: 14-Dec-2009 07:20:40  
 SOLVENT: CDCl3  
 FILENAME: rmmr\_archive\data\leveq\hmr\0300090-0171\5fid

proton

id	ppm	mult	n	coupling
0	9.13	d	0.94	2.26
1	8.16	dd	1.00	9.08 2.29
2	8.01	s	0.88	
3	7.38	m	4.03	
4	7.18	m	2.07	
5	5.41	s	2.19	7.13
6	4.46	q	2.11	7.13
7	1.47	t	3.20	7.13



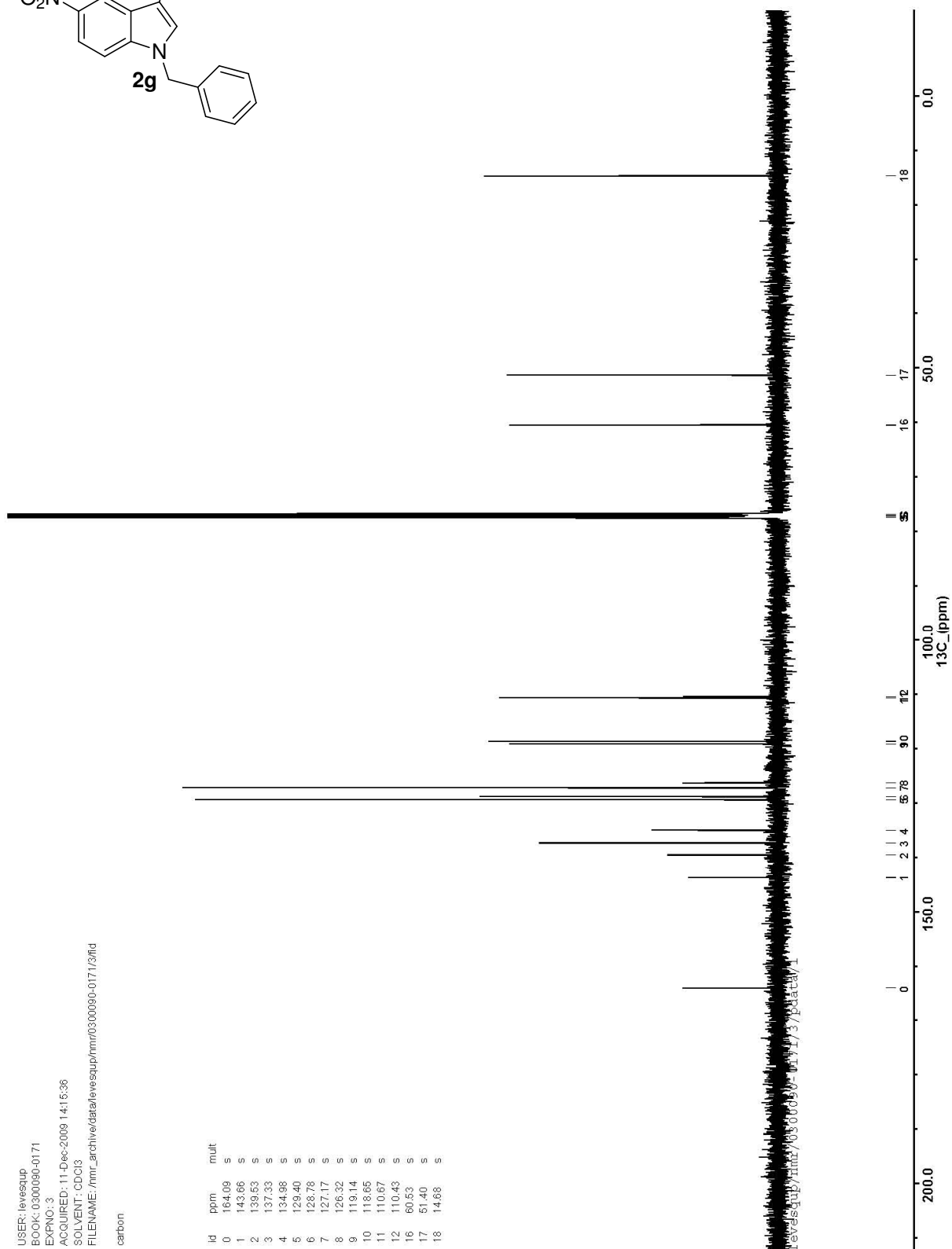
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of ethyl 1-benzyl-5-nitroindole-3-carboxylate (**2g**)



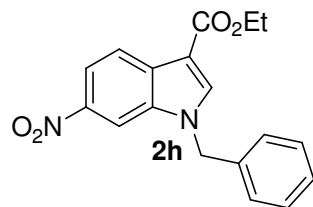
USER: levesqup  
 BOOK: 0300090-0171  
 EXPNO: 3  
 ACQUIRED: 11-Dec-2009 14:15:36  
 SOLVENT: CDCl3  
 FILENAME: rmmr\_archive\data\levesqup\mnr\0300090-0171\3.fid

carbon

id	ppm	mult
0	164.09	s
1	143.66	s
2	139.63	s
3	137.33	s
4	134.98	s
5	129.40	s
6	128.78	s
7	127.17	s
8	126.32	s
9	119.14	s
10	118.65	s
11	110.67	s
12	110.43	s
16	60.53	s
17	51.40	s
18	14.68	s



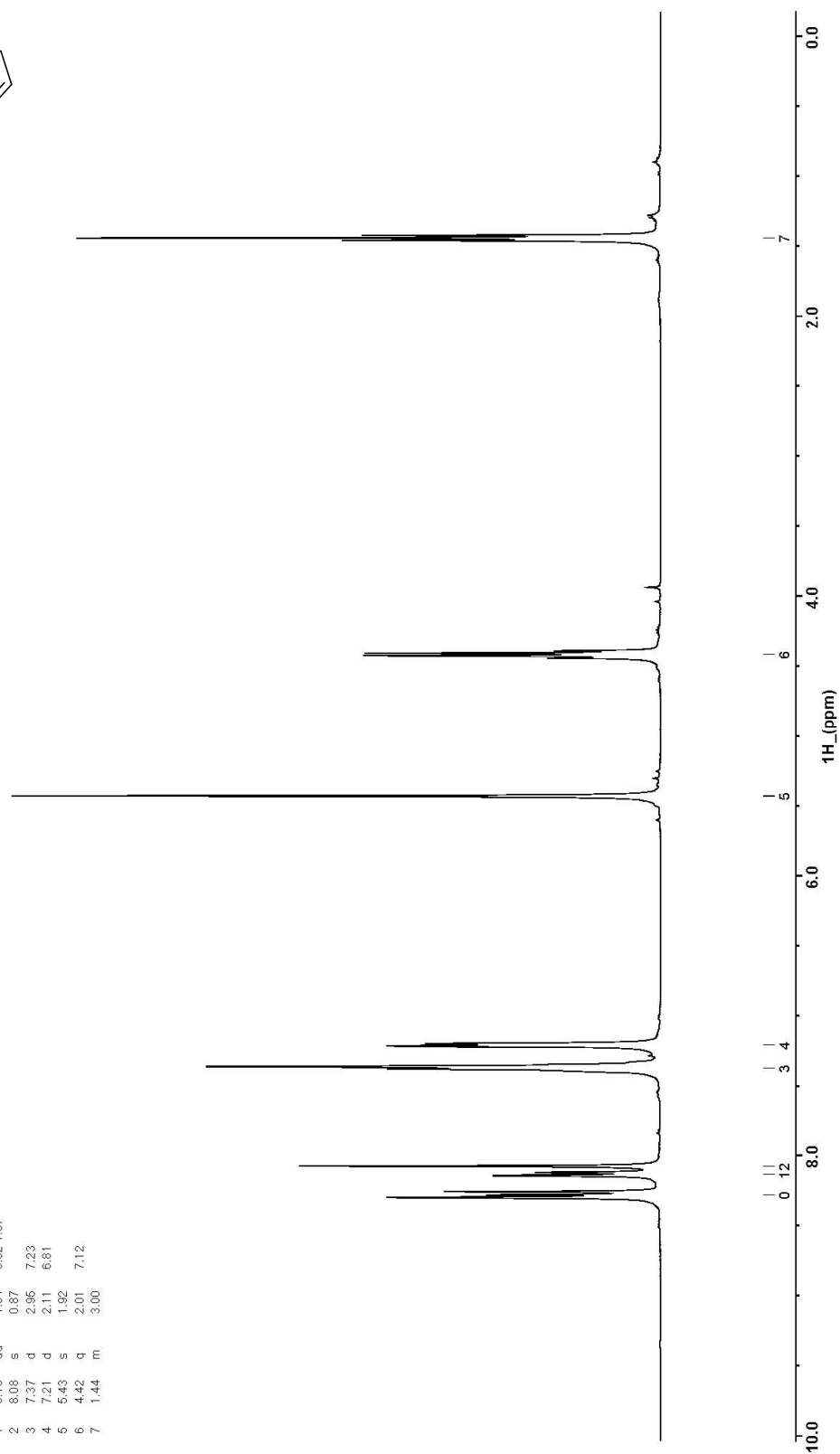
<sup>13</sup>C NMR Spectrum (101 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-5-nitroindole-3-carboxylate (**2g**)



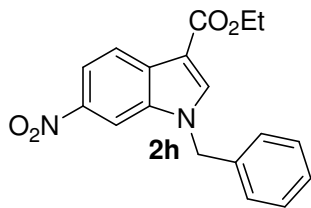
USER: fourmpi  
 BOOK: 0283264-0086  
 EXPNO: 5  
 ACQUIRED: 19-Mar-2010 17:32:48  
 SOLVENT: CDCl3  
 FILENAME: rml\_archive\data\fourmpi\rml\0283264-0086\5fid

proton

id	ppm	mult	n	coupling
0	8.28	m	1.99	
1	8.13	dd	1.04	8.92 1.97
2	8.08	s	0.87	
3	7.37	d	2.95	7.23
4	7.21	d	2.11	6.81
5	5.43	s	1.92	
6	4.42	q	2.01	7.12
7	1.44	m	3.00	



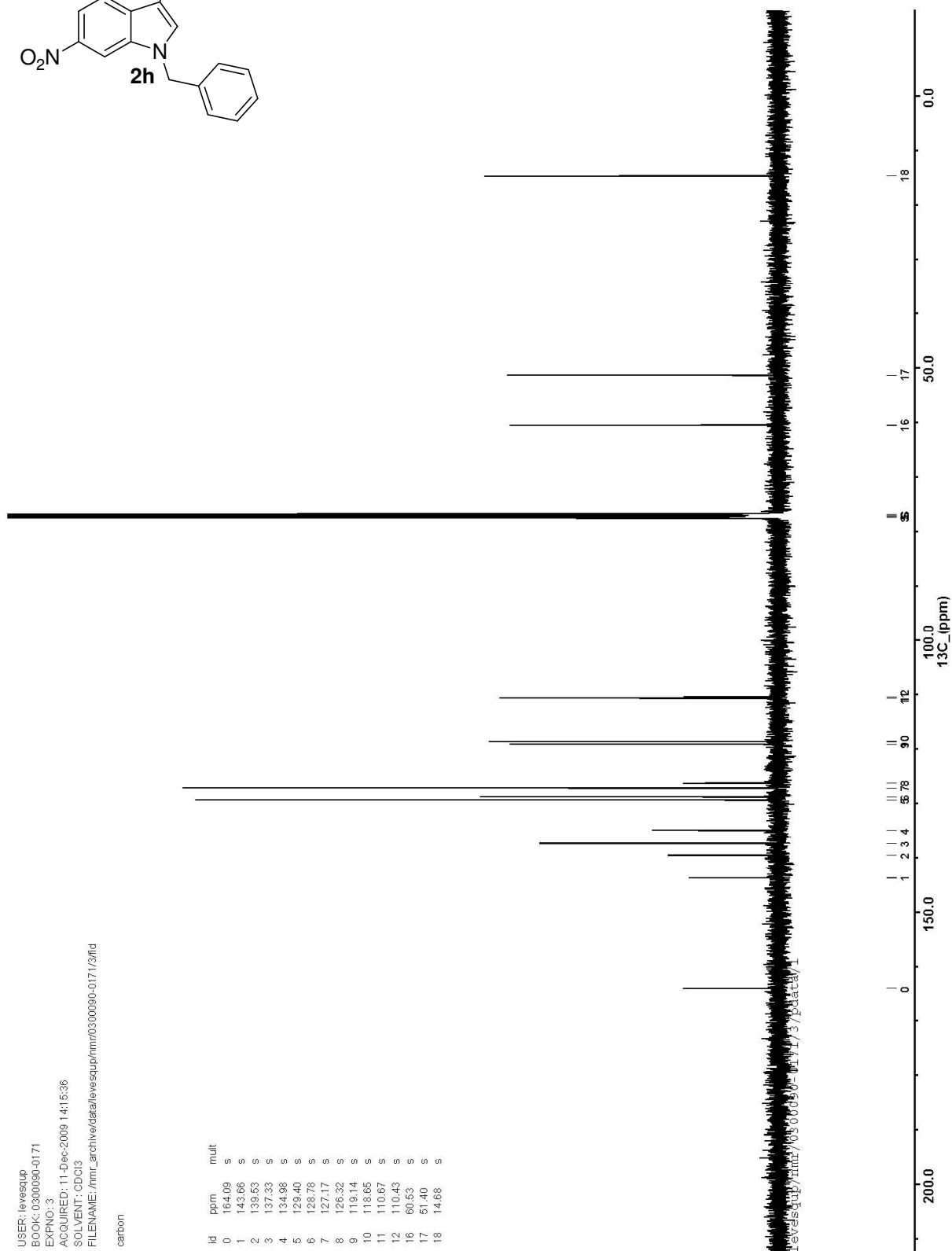
$^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of ethyl 1-benzyl-6-nitroindole-3-carboxylate (**2h**)



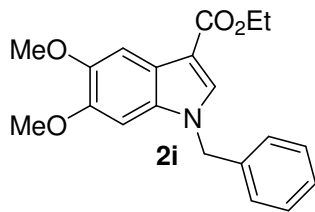
USER: levesq  
 BOOK: 0300090-0171  
 EXPNO: 3  
 ACQUIRED: 11-Dec-2009 14:15:36  
 SOLVENT: CDCl3  
 FILENAME: rmmr\_archive\data\levesq\mnr\0300090-0171\3.fid

carbon

id	ppm	mult
0	164.09	s
1	143.66	s
2	139.63	s
3	137.33	s
4	134.98	s
5	129.40	s
6	128.78	s
7	127.17	s
8	126.32	s
9	119.14	s
10	118.65	s
11	110.67	s
12	110.43	s
16	60.53	s
17	51.40	s
18	14.68	s



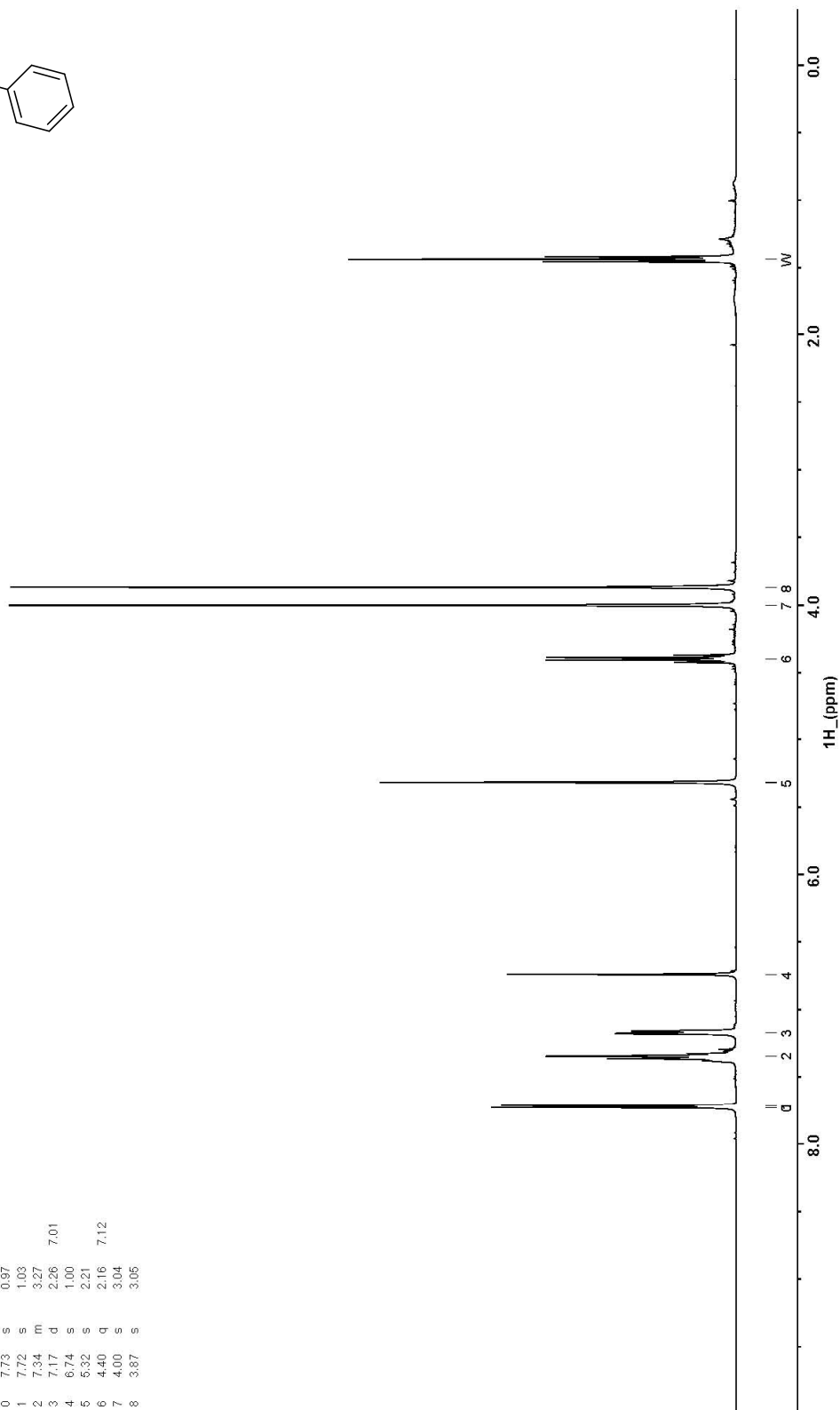
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of ethyl 1-benzyl-6-nitroindole-3-carboxylate (**2h**)



USER: fourmpi  
 BOOK: 0283254-0095  
 EXPNO: 5  
 ACQUIRED: 08-Apr-2010 11:06:58  
 SOLVENT: CDCl3  
 FILENAME: rml\_archive\data/fourmpi/rmf/0283254-0095/5fid

proton

id	ppm	mult	n	coupling
0	7.73	s	0.97	
1	7.72	s	1.03	
2	7.34	m	3.27	
3	7.17	d	2.26	7.01
4	6.74	s	1.00	
5	5.32	s	2.21	
6	4.40	q	2.16	7.12
7	4.00	s	3.04	
8	3.87	s	3.05	

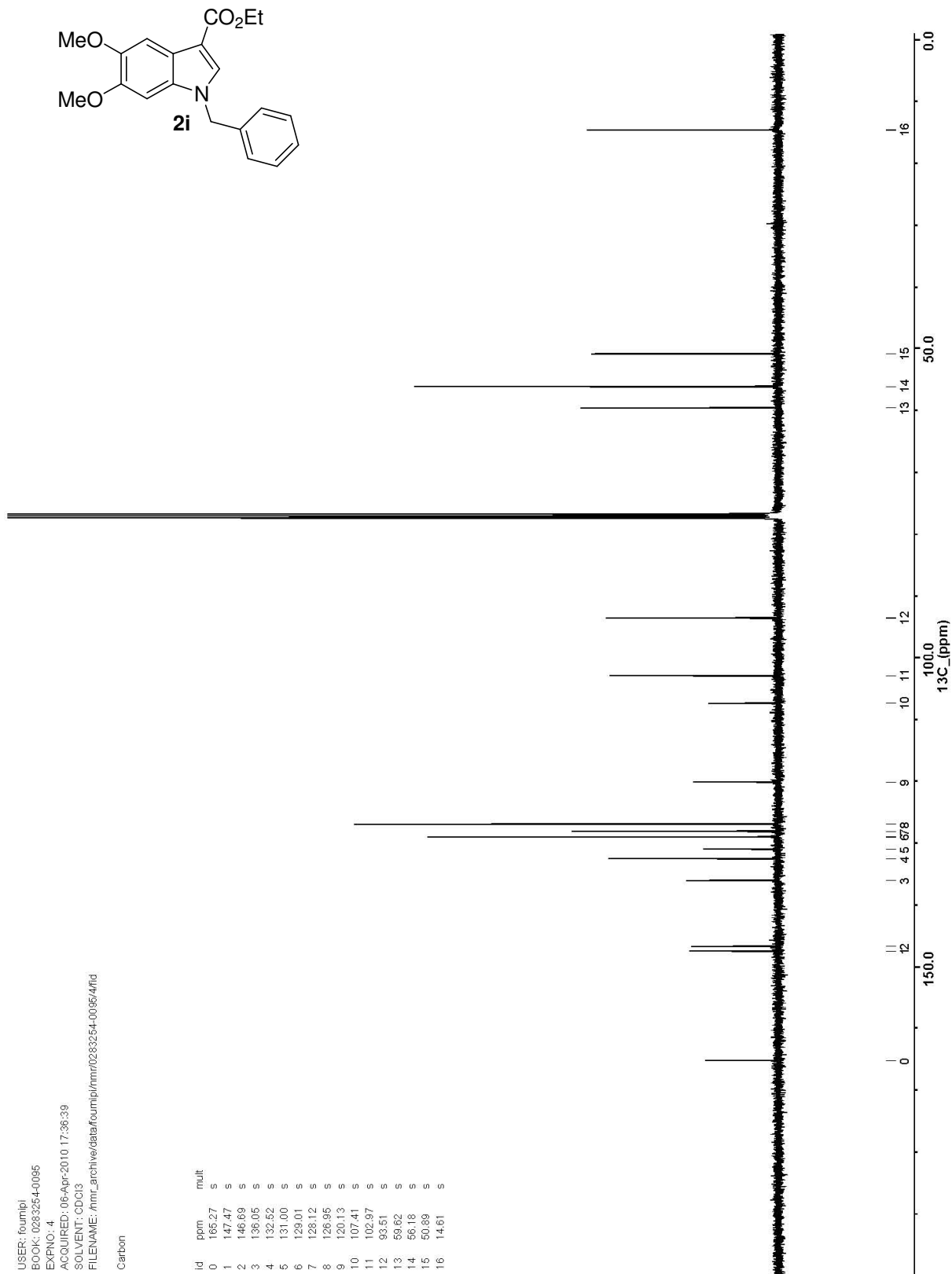


<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-5,6-dimethoxyindole-3-carboxylate (**2i**)

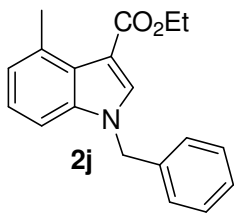
USER: fourmpi  
BOOK: 0283264-0095  
EXPNO: 4  
ACQUIRED: 06-Apr-2010 17:36:39  
SOLVENT: CDCl3  
FILENAME: rmi\_archive\data\fourmpi\rmf0283264-0095\4.fid

Carbon

id	ppm	mult
0	165.27	s
1	147.47	s
2	146.69	s
3	136.05	s
4	132.52	s
5	131.00	s
6	129.01	s
7	128.12	s
8	126.95	s
9	120.13	s
10	107.41	s
11	102.97	s
12	93.51	s
13	59.62	s
14	56.18	s
15	50.89	s
16	14.61	s



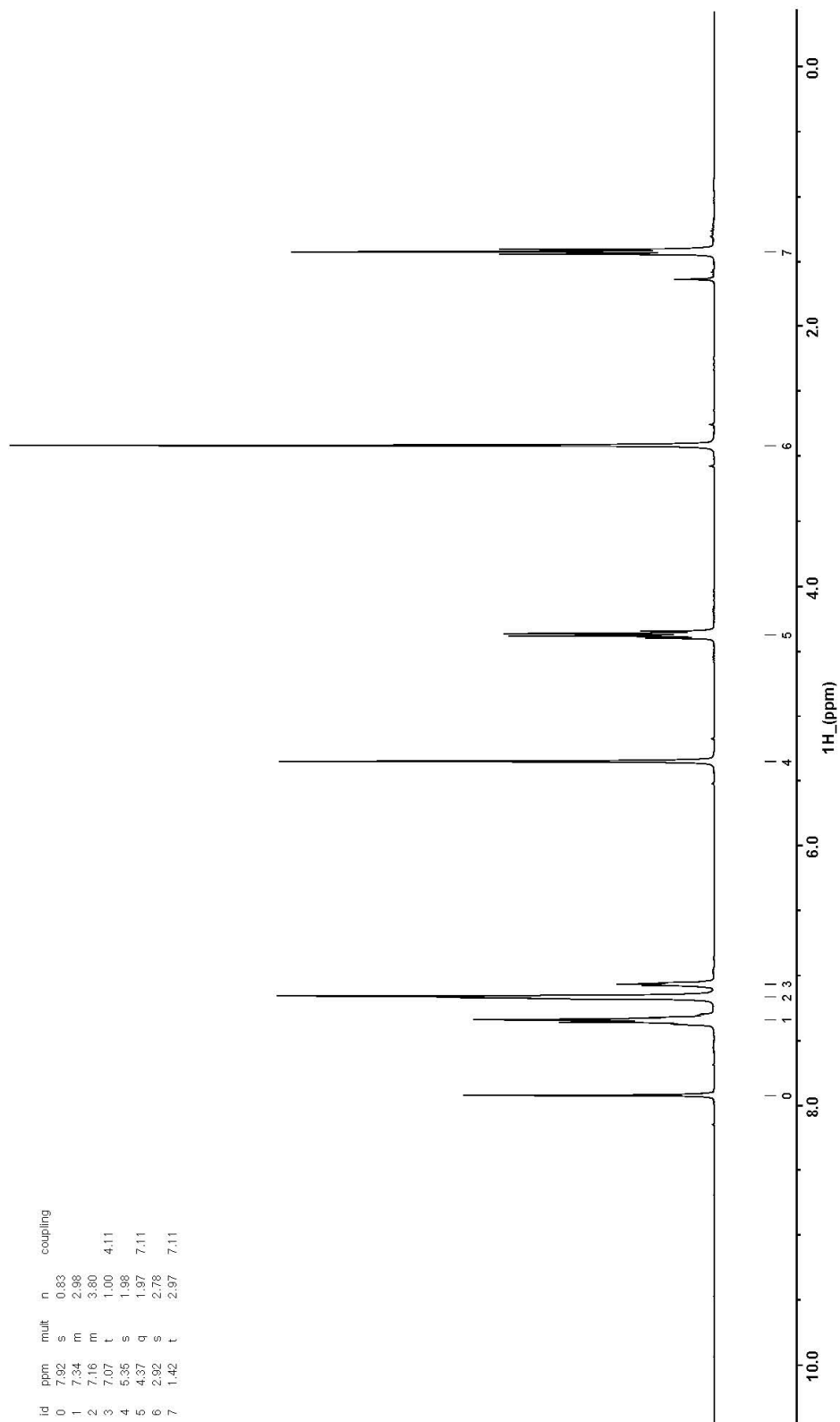
<sup>13</sup>C NMR Spectrum (101 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-5,6-dimethoxyindole-3-carboxylate (**2i**)



USER: fourmpi  
 BOOK: 0300090-0170  
 EXPNO: 2  
 ACQUIRED: 18-Jan-2010 11:25:39  
 SOLVENT: CDCl3  
 FILENAME: fmr\_archive\datafourmpi/fmr/0300090-01702/fid

24

id	ppm	mult	n	coupling
0	7.92	s	0.83	
1	7.34	m	2.98	
2	7.16	m	3.80	
3	7.07	t	1.00	4.11
4	5.35	s	1.98	
5	4.37	q	1.97	7.11
6	2.92	s	2.78	
7	1.42	t	2.97	7.11

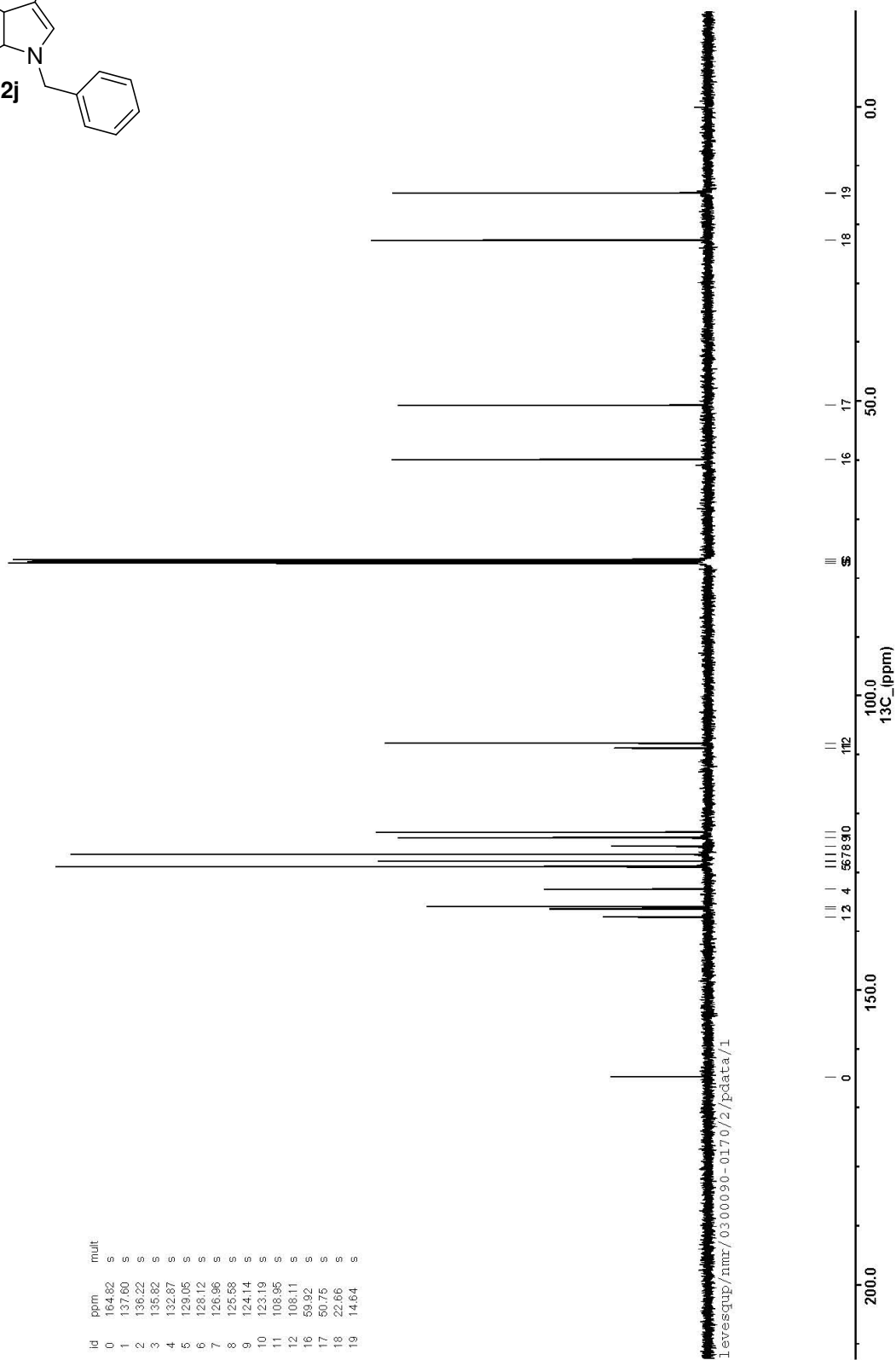
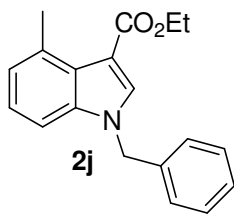


<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-4-methylindole-3-carboxylate (**2j**)

USER: levequp  
BOOK: 0300090-0170  
EXPNO: 2  
ACQUIRED: 11-Dec-2009 08:29:54  
SOLVENT: CDCl3  
FILENAME: rmmr\_archive\data\levequp\hmr\0300090-0170\2.fid

carbon

id	ppm	mult
0	164.82	s
1	137.60	s
2	136.22	s
3	135.82	s
4	132.87	s
5	129.05	s
6	128.12	s
7	126.96	s
8	125.58	s
9	124.14	s
10	123.19	s
11	108.95	s
12	108.11	s
16	59.92	s
17	50.75	s
18	22.66	s
19	14.64	s

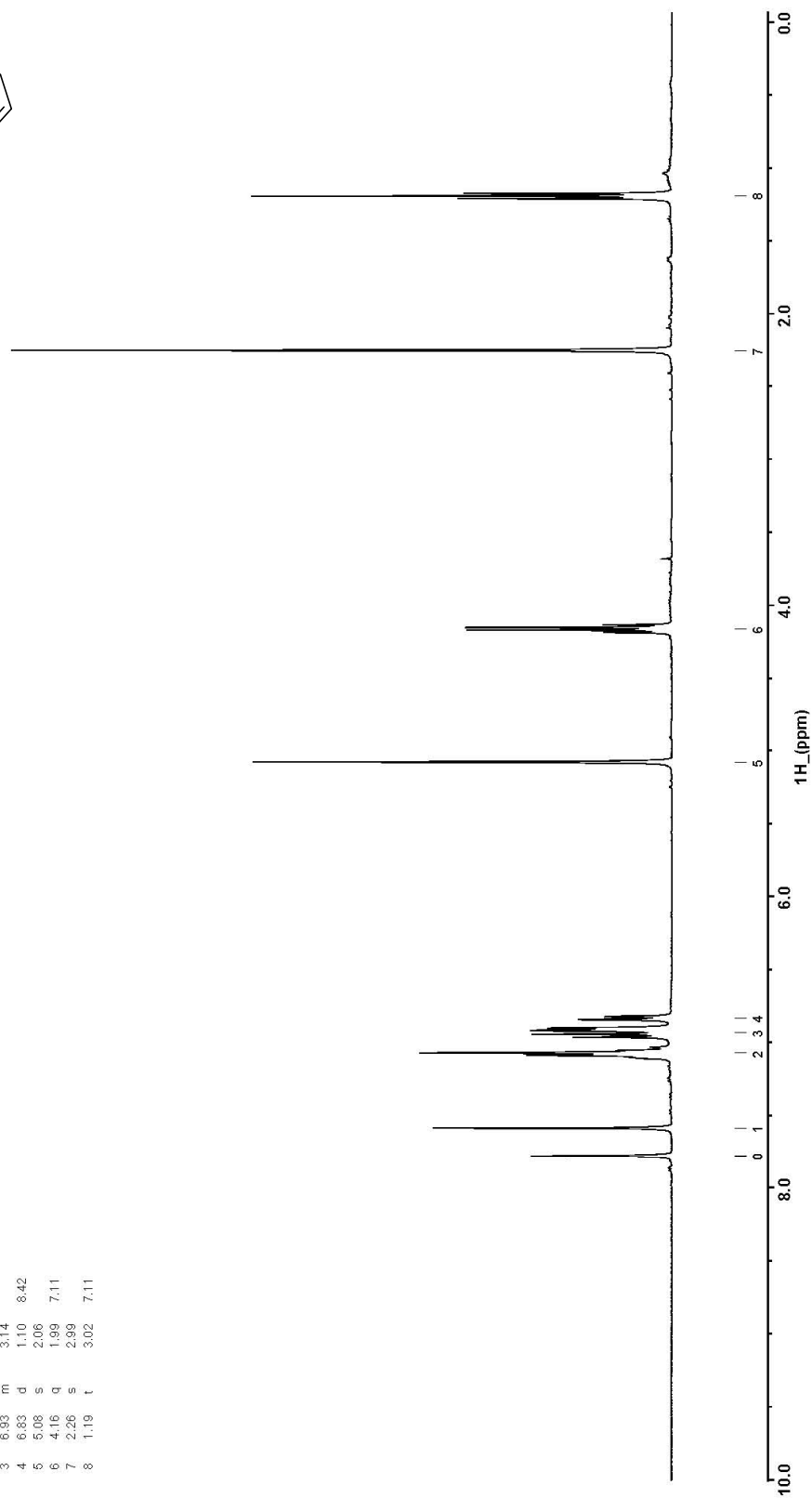
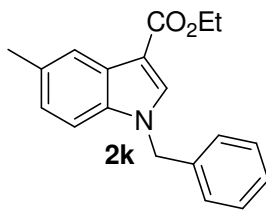


$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of ethyl 1-benzyl-4-methylindole-3-carboxylate (**2j**)

USER: lveqsup  
BOOK: 0300090-0184  
EXPNO: 1  
ACQUIRED: 05-Jan-2010 11:08:49  
SOLVENT: CDCl3  
FILENAME: rmmr\_archive\data\lveqsup\mnr\0300090-0184\fid

clean proton

id	ppm	mult	n	coupling
0	7.78	s	1.00	
1	7.59	s	0.86	
2	7.07	m	3.09	
3	6.93	m	3.14	
4	6.83	d	1.10	8.42
5	5.08	s	2.06	
6	4.16	q	1.99	7.11
7	2.26	s	2.99	
8	1.19	t	3.02	7.11

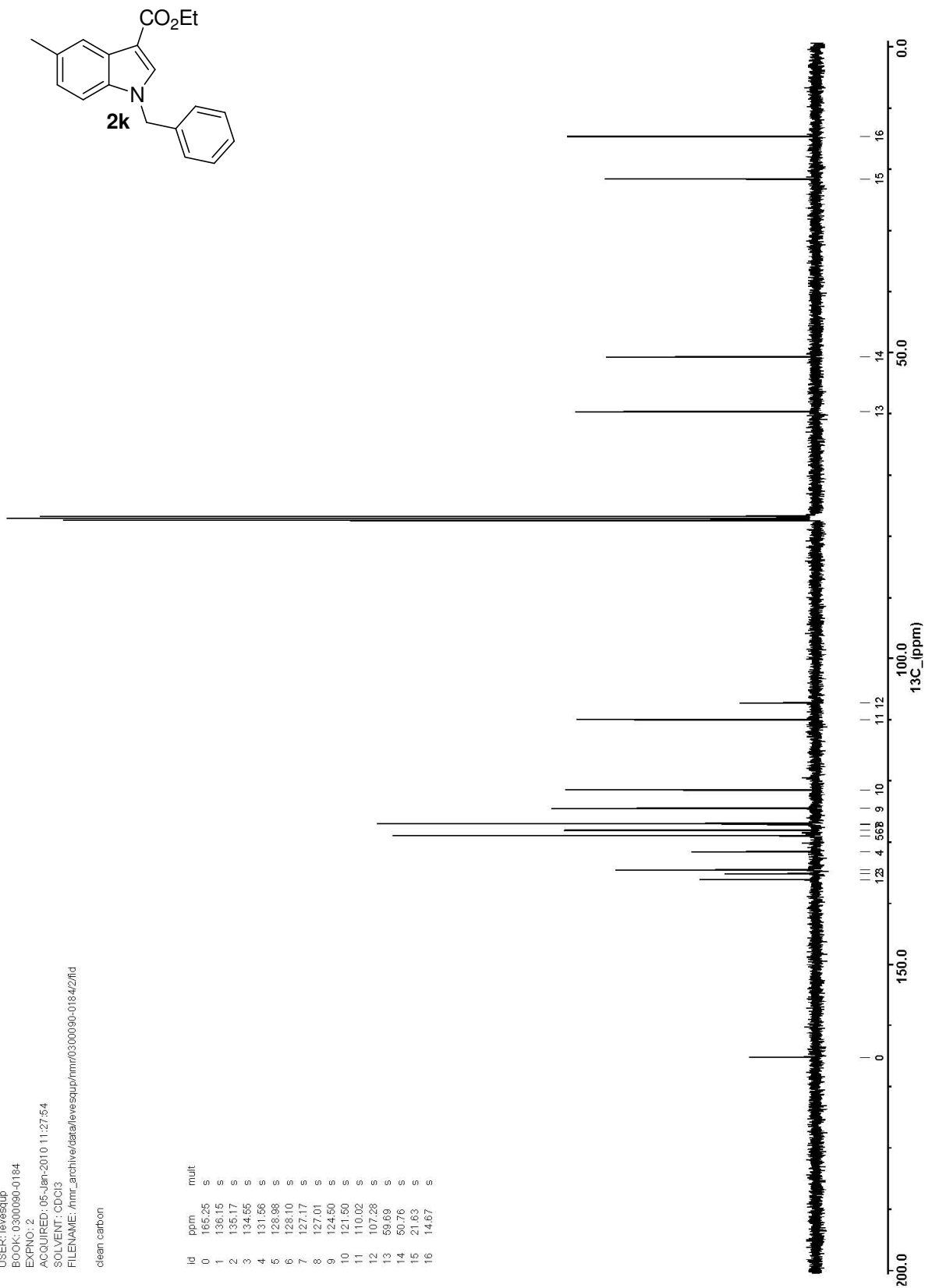


<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-5-methylindole-3-carboxylate (**2k**)

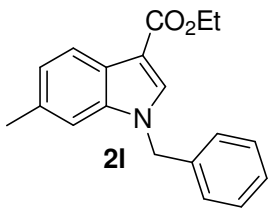
USER: leveq  
BOOK: 0300090-0184  
EXPNO: 2  
ACQUIRED: 05-Jan-2010 11:27:54  
SOLVENT: CDCl3  
FILENAME: rmmr\_archive\data\leveq\mrmr\0300090-0184\2fid

clean carbon

id	ppm	mult
0	165.25	s
1	136.15	s
2	135.17	s
3	134.66	s
4	131.66	s
5	128.88	s
6	128.10	s
7	127.17	s
8	127.01	s
9	124.50	s
10	121.50	s
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12	107.28	s
13	69.69	s
14	50.76	s
15	21.63	s
16	14.67	s



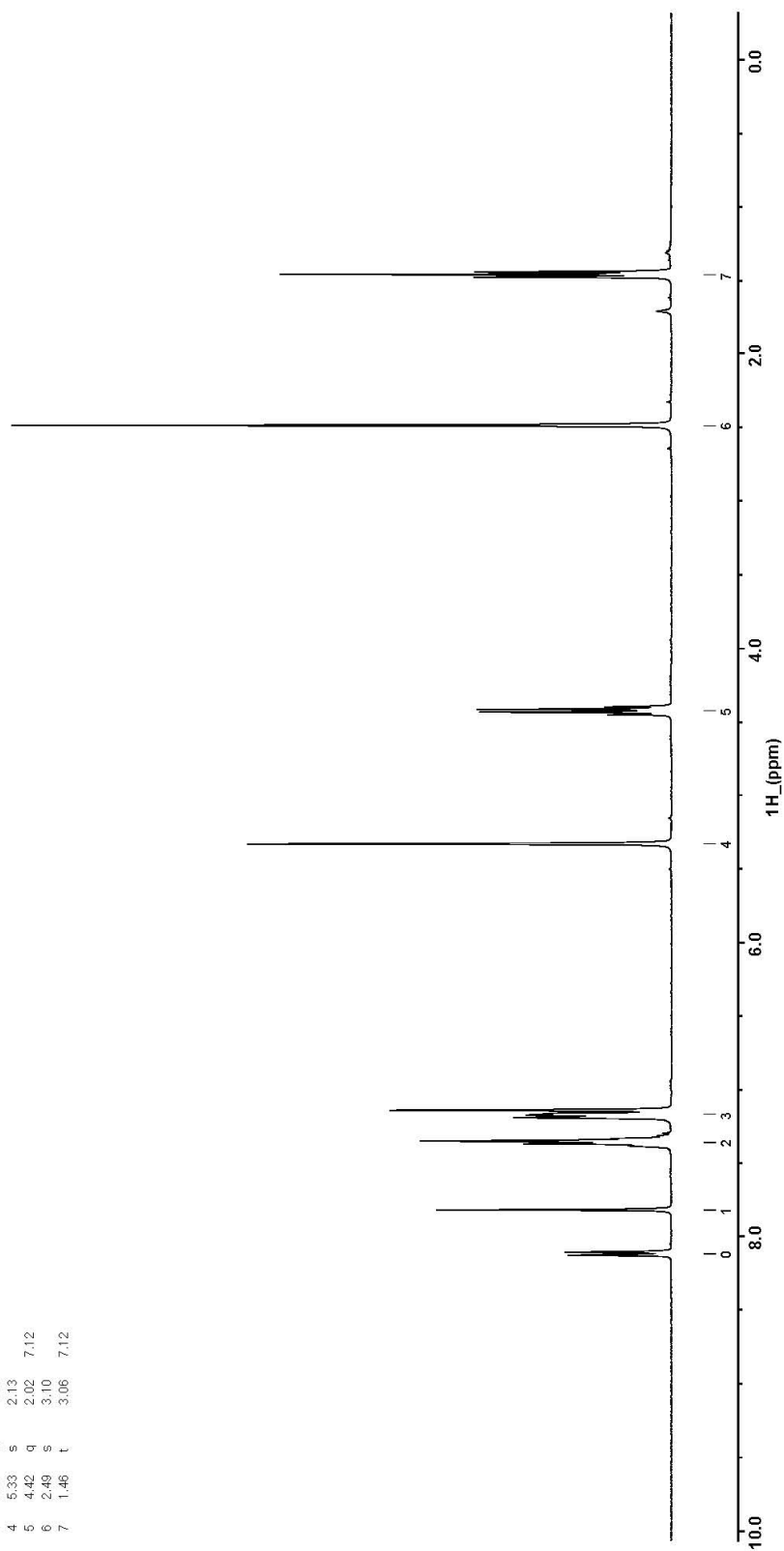
<sup>13</sup>C NMR Spectrum (101 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-5-methylindole-3-carboxylate (**2k**)



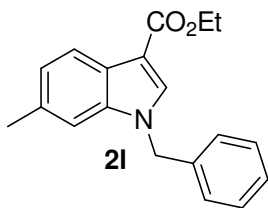
USER: fourmpi  
 BOOK: 0300090-0172  
 EXPNO: 2  
 ACQUIRED: 19-Jan-2010 18:35:51  
 SOLVENT: CDCl3  
 FILENAME: /mnt\_archive/data/fourmpi/mr/0300090-0172/2f/d

proton

id	ppm	mult	n	coupling
0	8.12	d	1.01	8.10
1	7.62	s	0.92	
2	7.36	m	2.93	
3	7.17	m	4.00	
4	6.33	s	2.13	
5	4.42	q	2.02	7.12
6	2.49	s	3.10	
7	1.46	t	3.06	7.12



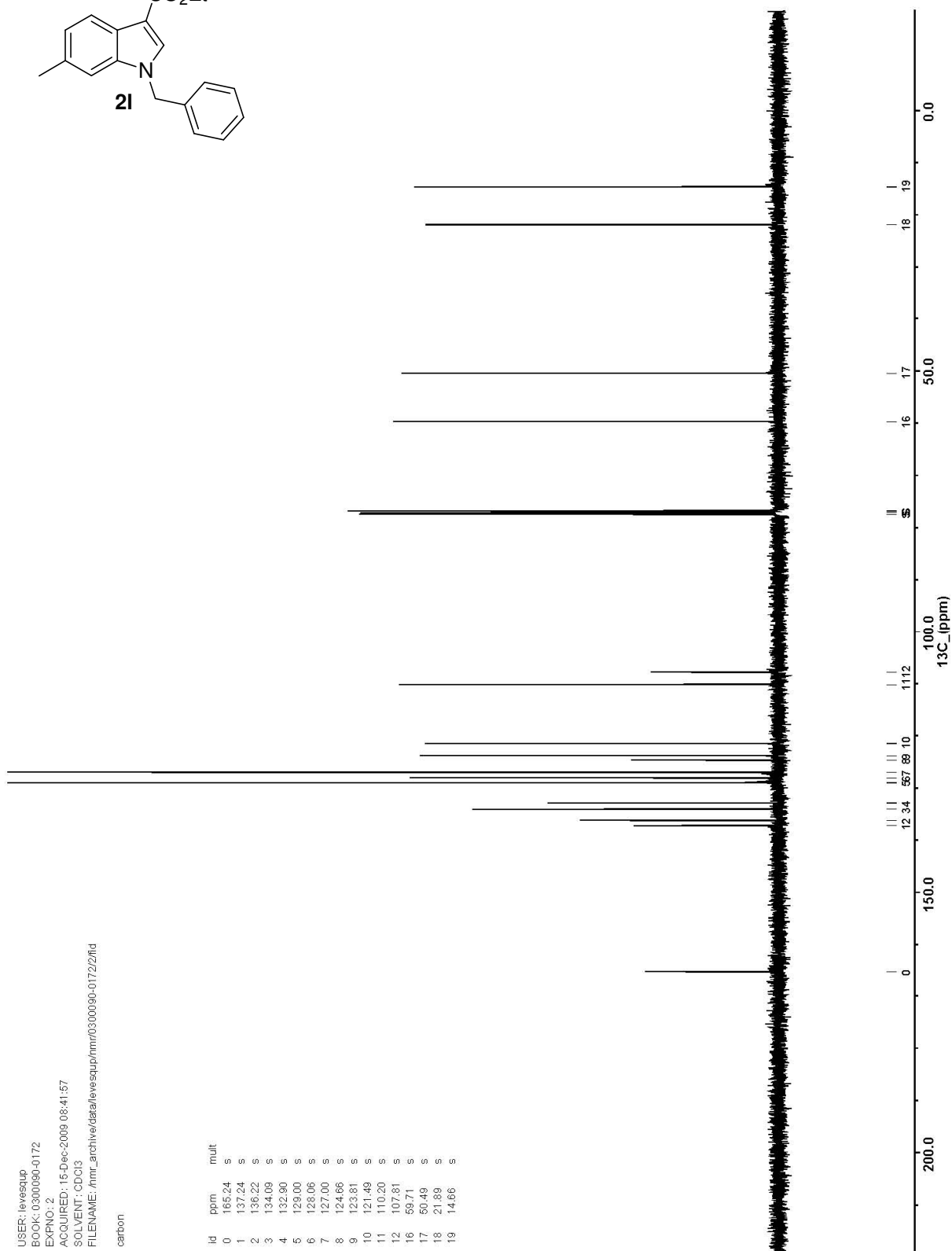
<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-6-methylindole-3-carboxylate (**21**)



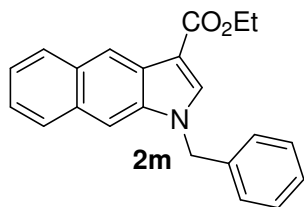
USER: levesq  
 BOOK: 0300090-0172  
 EXPNO: 2  
 ACQUIRED: 15-Dec-2009 08:41:57  
 SOLVENT: CDCl3  
 FILENAME: rmt\_archive\data\levesq\hmr\0300090-0172\fid

carbon

id	ppm	mult
0	165.24	s
1	137.24	s
2	136.22	s
3	134.09	s
4	132.90	s
5	129.00	s
6	128.06	s
7	127.00	s
8	124.66	s
9	123.81	s
10	121.49	s
11	110.20	s
12	107.81	s
16	69.71	s
17	60.49	s
18	21.89	s
19	14.66	s



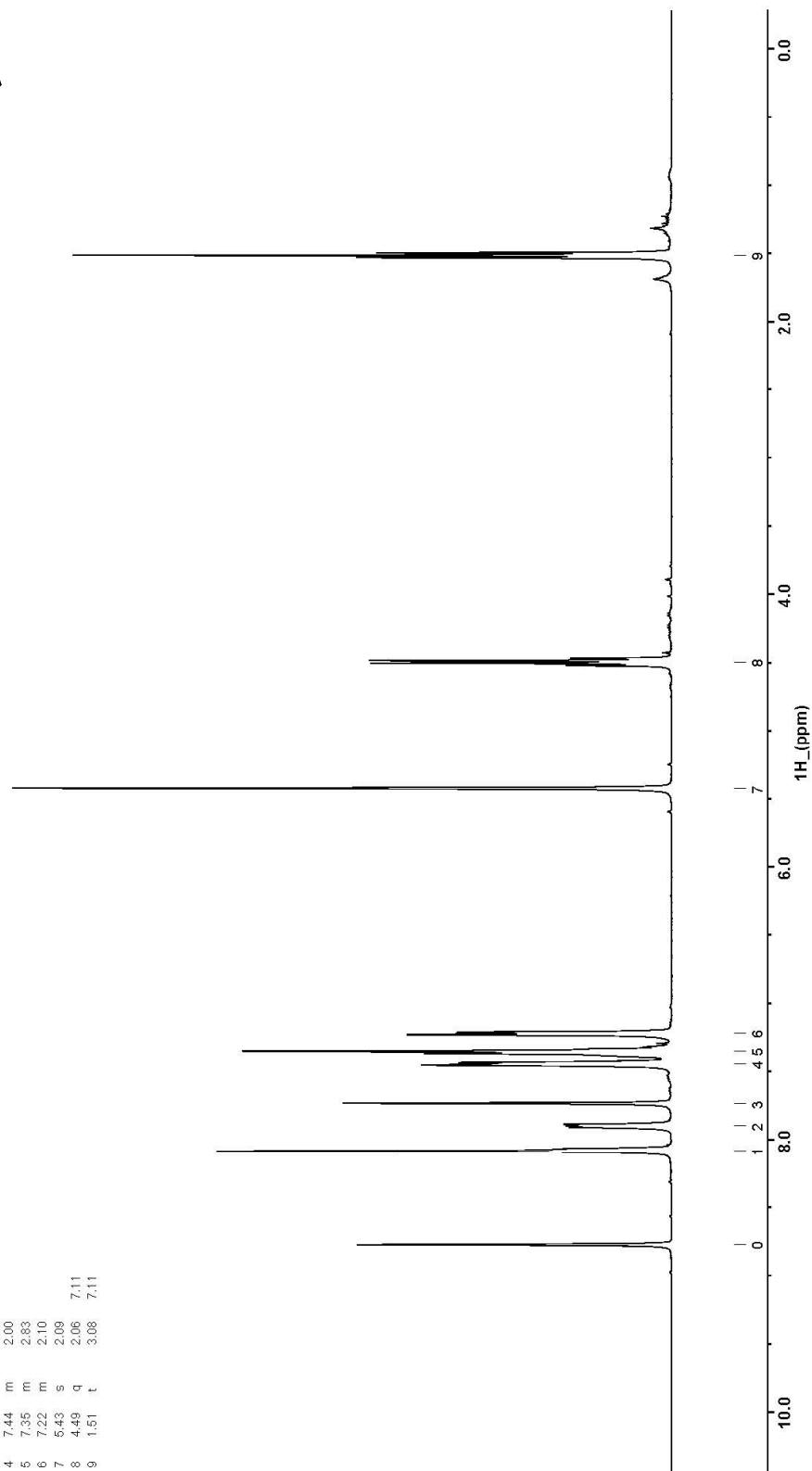
<sup>13</sup>C NMR Spectrum (101 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-6-methylindole-3-carboxylate (**21**)



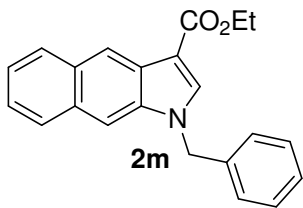
USER: fourmpi  
 BOOK: 0300090-0183  
 EXPNO: 1  
 ACQUIRED: 02-Feb-2010 17:53:00  
 SOLVENT: CDCl3  
 FILENAME: rml\_archive\datafourmpi\rmf0300090-0183/1.fid

proton

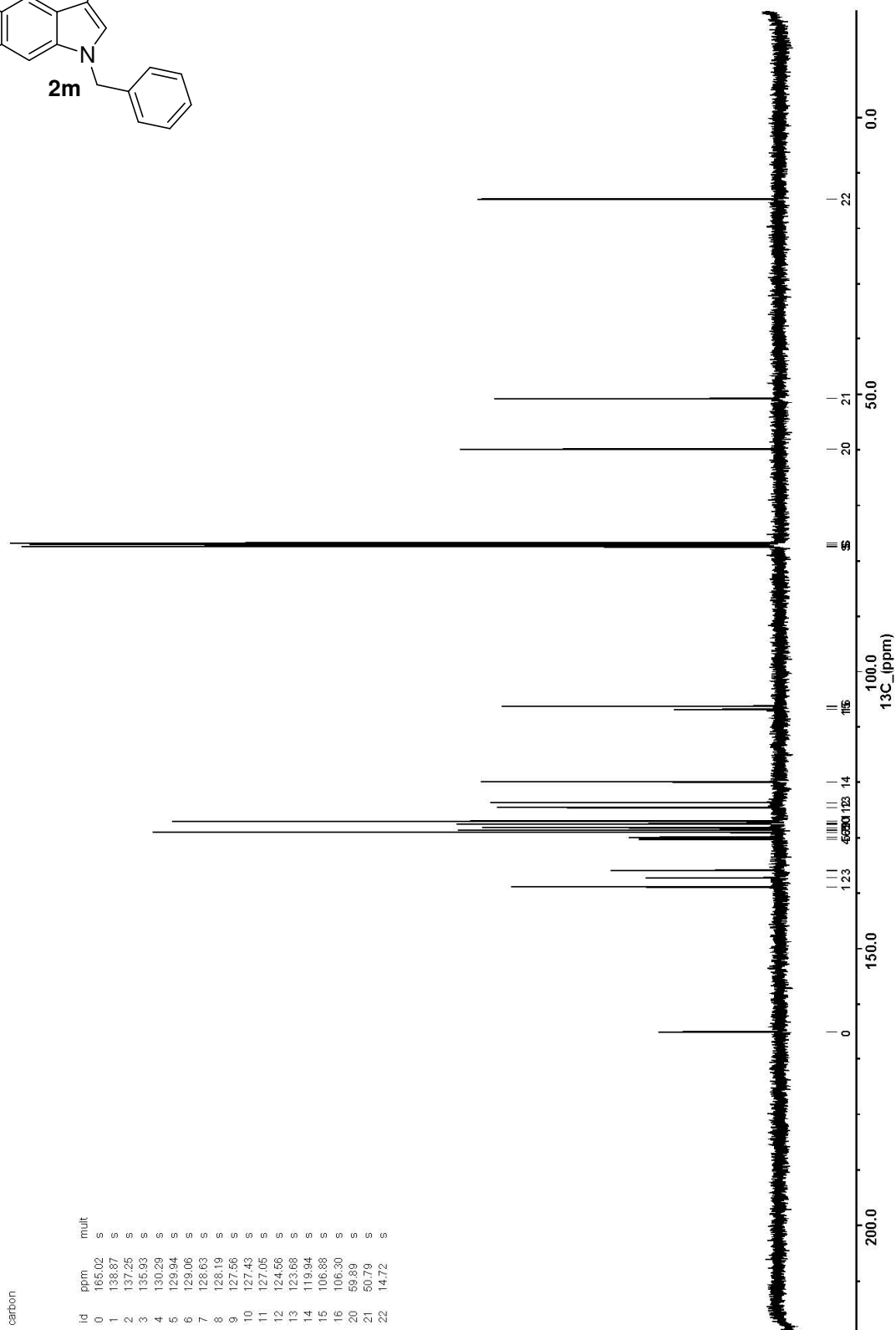
id	ppm	mult	n	coupling
0	8.77	s	0.98	
1	8.09	s	1.61	
2	7.90	m	1.08	
3	7.73	s	1.03	
4	7.44	m	2.00	
5	7.35	m	2.83	
6	7.22	m	2.10	
7	6.43	s	2.09	
8	4.49	q	2.06	7.11
9	1.51	t	3.08	7.11



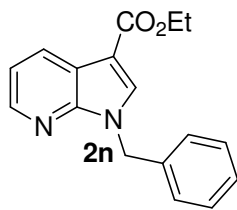
<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-benzo[f]indole-3-carboxylate (**2m**)



USER: fourmpi  
 BOOK: 0300090-0183  
 EXPNO: 2  
 ACQUIRED: 02-Feb-2010 18:01:55  
 SOLVENT: CDCl3  
 FILENAME: rmm\_archive\data\fourmpi\rmm\0300090-0183\2f.fid



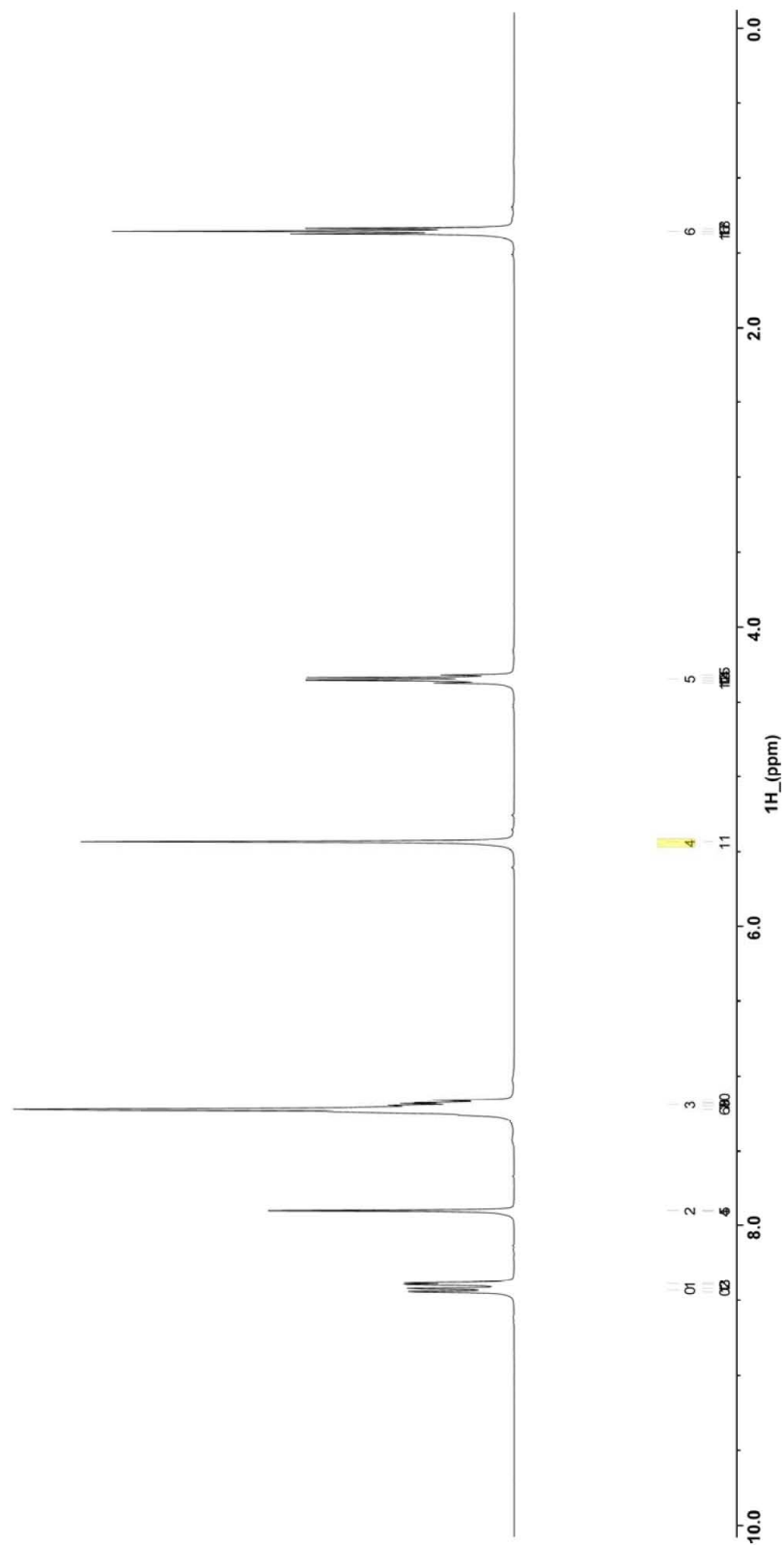
$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of ethyl 1-benzyl-benzof[7]indole-3-carboxylate (**2m**)



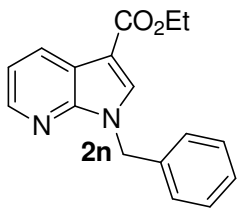
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 BOOK: 0283254-0098  
 EXPNO: 1  
 ACQUIRED: 19-Apr-2010 16:13:22  
 SOLVENT: CDCl3  
 FILENAME: nmr\_archive\data/fourmpi/nmr/0283254-0098/fid

proton

id	ppm	mult	n	coupling
0	8.43	d	1.14	8.00
1	8.39	d	1.09	4.73
2	7.90	m	0.87	
3	7.19	m	5.89	
4	5.43	s	2.00	
5	4.34	q	2.15	7.14
6	1.35	t	3.16	7.16

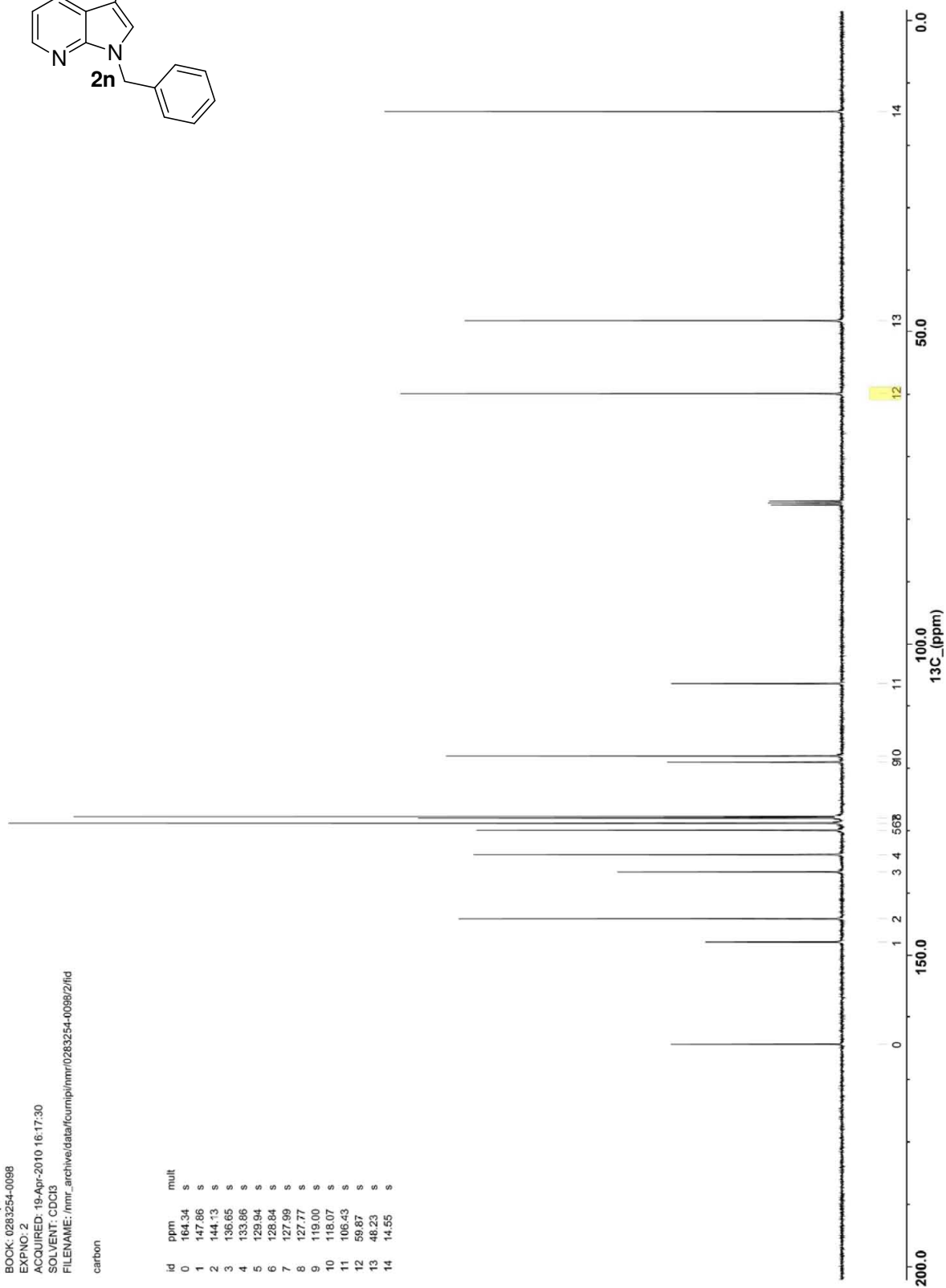


<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-7-azaindole-3-carboxylate (**2n**)

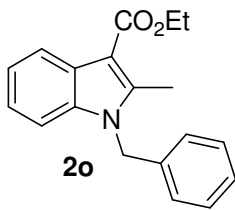


USER: fourmpi  
 BOOK: 0283254-0098  
 EXPNO: 2  
 ACQUIRED: 19-Apr-2010 16:17:30  
 SOLVENT: CDCl3  
 FILENAME: nmr\_archive\data\fourmpi\mr\0283254-0098\2.fid

id	ppm	mult
0	164.34	s
1	147.86	s
2	144.13	s
3	136.65	s
4	133.86	s
5	129.94	s
6	128.64	s
7	127.99	s
8	127.77	s
9	119.00	s
10	118.07	s
11	106.43	s
12	59.87	s
13	48.23	s
14	14.55	s



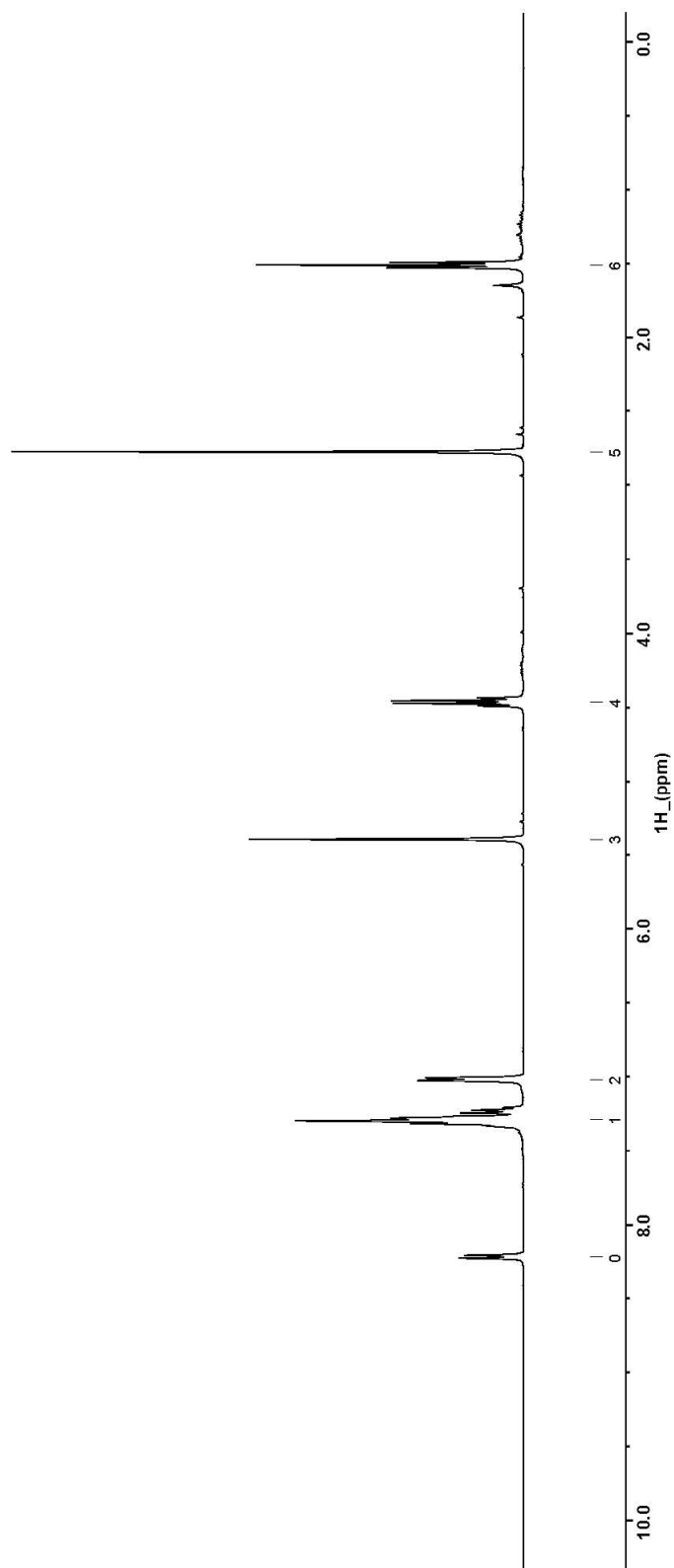
<sup>13</sup>C NMR Spectrum (101 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-7-azaindole-3-carboxylate (**2n**)



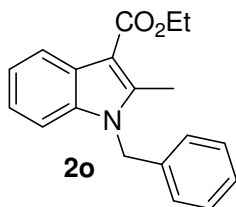
USER: foumipi  
 BOOK: 0283254-0108  
 EXPNO: 2  
 ACQUIRED: 29-Jul-2010 09:02:52  
 SOLVENT: CDCl3  
 FILENAME: /mnt\_archive/data/foumipi/mmr/0283254-0108/2/fid

proton

id	ppm	mult	n	coupling
0	8.22	d	1.00	7.98
1	7.29	d	5.48	8.68
2	7.02	m	2.07	
3	6.40	s	2.06	
4	4.46	q	2.03	7.12
5	2.78	s	2.86	
6	1.51	m	3.03	



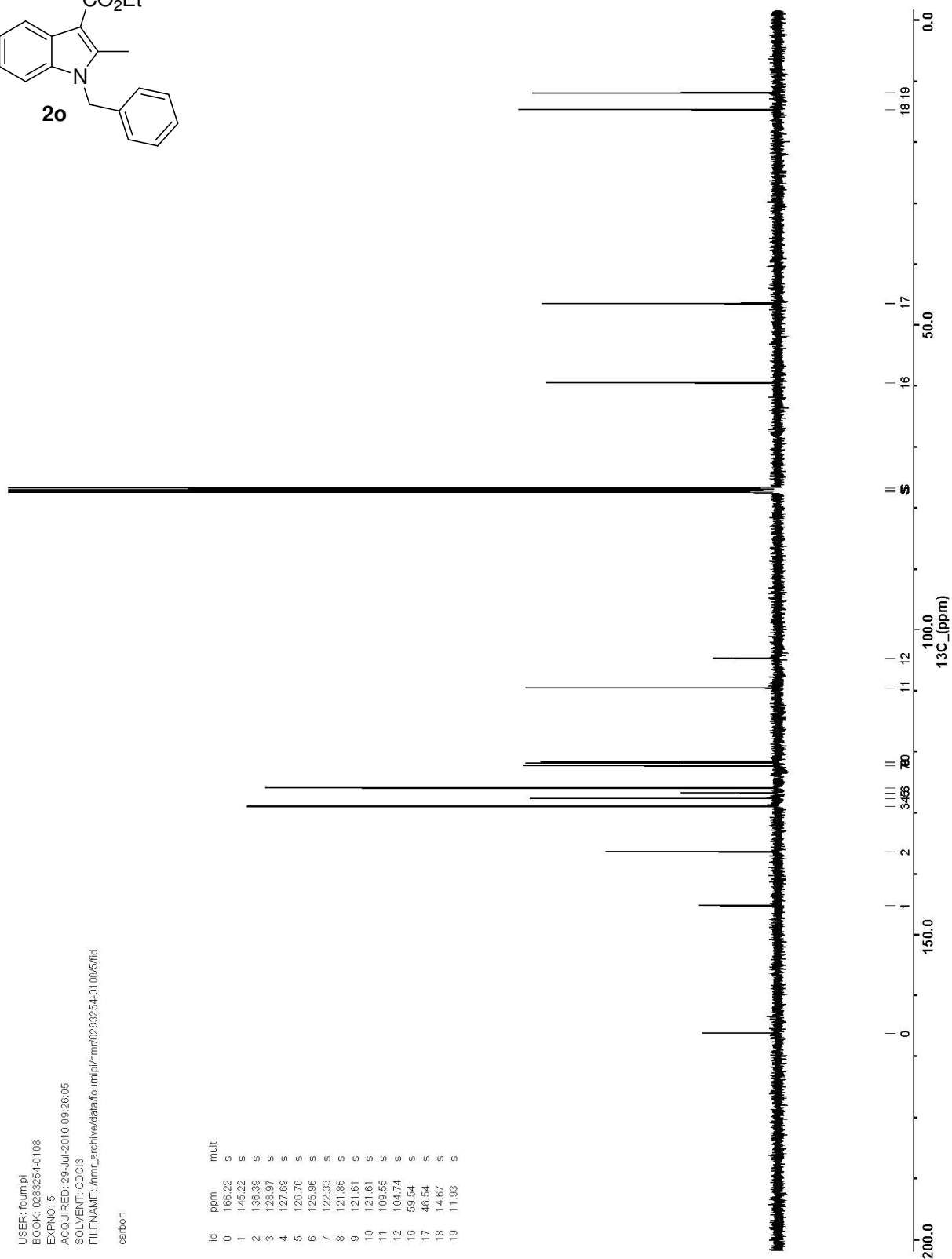
<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of ethyl 1-benzyl-2-methylindole-3-carboxylate (**2o**)



USER: founmpi  
 BOOK: 0283264-0108  
 EXPNO: 5  
 ACQUIRED: 29-Jul-2010 09:26:05  
 SOLVENT: CDCl3  
 FILENAME: /nmt\_archive/data/founmpi/nmr/0283264-0108/5fid

carbon

id	ppm	mult
0	166.22	s
1	145.22	s
2	136.30	s
3	128.97	s
4	127.69	s
5	126.76	s
6	125.96	s
7	122.33	s
8	121.85	s
9	121.61	s
10	121.61	s
11	109.55	s
12	104.74	s
16	59.54	s
17	46.54	s
18	14.67	s
19	11.93	s



$^{13}\text{C}$  NMR Spectrum (101 MHz,  $\text{CDCl}_3$ ) of ethyl 1-benzyl-2-methylindole-3-carboxylate (**2o**)