

Room-Temperature Highly Efficient Suzuki-Miyaura Reactions in Water in the  
Presence of Stilbazo

*Yi-Yuan Peng,<sup>a,b\*</sup> Jinbiao Liu,<sup>a</sup> Xiaoli Lei,<sup>a</sup> and Zenlan Yin<sup>a</sup>*

<sup>a</sup>Key Laboratory of Green Chemistry, Jiangxi Province and College of Chemistry,  
Jiangxi Normal University, Nanchang, Jiangxi 330022, China

<sup>b</sup>College of Life Science, Jiangxi Normal University, Nanchang, Jiangxi 330022,  
China

[Yiyuanpeng@yahoo.com](mailto:Yiyuanpeng@yahoo.com)

**Supporting Information**

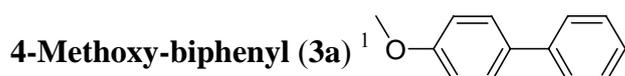
**List of Contents**

<b>1. Typical experimental procedure for the palladium-catalyzed Suzuki-Miyaura cross-coupling reaction in H<sub>2</sub>O</b>	<b>S1</b>
<b>2. Analytical data</b>	<b>S2-S6</b>
<b>3. References</b>	<b>S6</b>
<b>4. NMR spectra</b>	<b>S7-S26</b>
<b>1. Typical experimental procedure for the palladium-catalyzed Suzuki-Miyaura cross-coupling reaction in H<sub>2</sub>O.</b>	

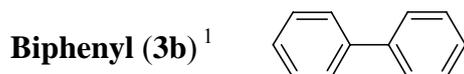
Stilbazo (5 mol %) was added to a mixture of ArX (0.2 mmol) and arylboronic acid (0.22 mmol), K<sub>2</sub>CO<sub>3</sub> (0.4 mmol) and H<sub>2</sub>O (1 mL) in a 5-mL round-bottom flask filled with N<sub>2</sub>. The reaction mixture was stirred at room temperature for an appropriate time until complete conversion of aryl halide took place (monitored by TLC). After

completion, the mixture was extracted with  $\text{CH}_2\text{Cl}_2$  (3×3 mL) and the combined organic extracts were dried over anhydrous sodium sulfate and evaporated under vacuum, leaving the crude product, which was purified by column chromatography to afford the corresponding products.

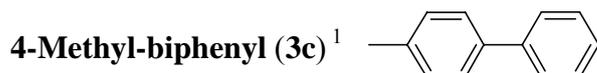
## 2. Analytical data for 3a-3k and 4a-4j



White solid; mp 88–90 °C; <sup>1</sup>H NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.56–7.52 (m, 4H), 7.41 (t,  $J = 7.2$  Hz, 2H), 7.30 (t,  $J = 7.2$ , 1H), 6.99 (d,  $J = 8.4$  Hz, 2H), 3.85 (s, 3H); <sup>13</sup>C NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.1, 140.8, 133.8, 128.7, 128.2, 126.8, 126.7, 114.2, 55.4.



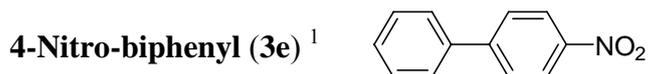
White solid; mp 68–70 °C; <sup>1</sup>H NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 8.0$  Hz, 4H), 7.46 (t,  $J = 7.6$  Hz, 4H), 7.37 (t,  $J = 7.6$  Hz, 2H); <sup>13</sup>C NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  141.2, 128.7, 127.2, 127.1.



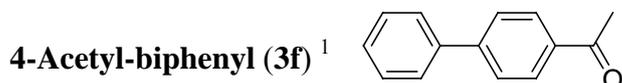
White solid; mp 44–46 °C; <sup>1</sup>H NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.58 (t,  $J = 7.6$  Hz, 2H), 7.49 (d,  $J = 8.0$  Hz, 2H), 7.43–7.39 (m, 2H), 7.33 (t,  $J = 7.6$  Hz, 1H), 7.25 (t,  $J = 8.0$  Hz, 2H), 2.38 (s, 3H).



Colorless liquid; <sup>1</sup>H NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  2.27 (s, 3H), 7.24–7.26 (m, 4H), 7.31–7.36 (m, 3H), 7.39–7.46 (m, 2H).



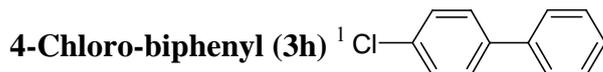
Yellow solid; mp 112–114°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.31 (d, *J* = 8.8 Hz, 2H), 7.75 (d, *J* = 8.8 Hz, 2H), 7.64 (t, *J* = 8.8 Hz, 2H), 7.52-7.43 (m, 3H).



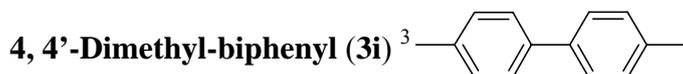
White solid; mp 116–118°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.04 (d, *J* = 8.0 Hz, 2H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.49-7.38 (m, 3H), 2.64 (s, 3H).



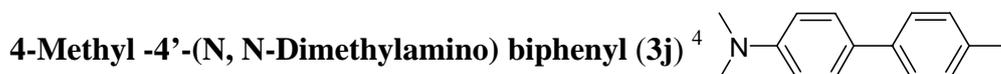
White solid; mp 121-123°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.56-7.49 (m, 4H), 7.41 (t, *J* = 7.6Hz, 2H), 7.27 (m, 1H), 6.82 (d, *J* = 8.8Hz, 2H), 2.99 (s, 6H).



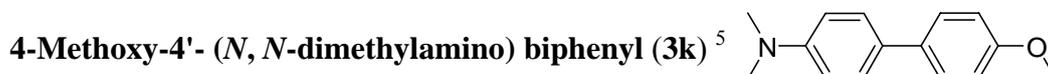
White solid; mp 77-79°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.56-7.48 (m, 4H), 7.46-7.34 (m, 5H).



White solid; mp 118-120°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.48 (d, *J* = 8.0 Hz, 4H), 7.24 (d, *J* = 8.0 Hz, 4H), 2.38 (s, 6H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 138.2, 136.7, 129.4, 129.1, 126.8, 21.1.

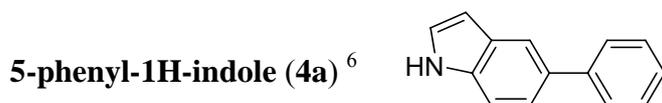


Gray solid; mp 132-133°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.49 (d, *J* = 8.8 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 8.0Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 2H), 2.98 (s, 6H), 2.36 (s, 3H).

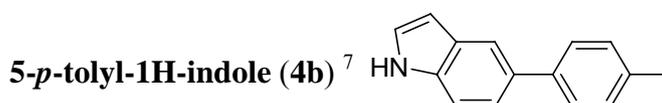


Gray solid; mp 156-157 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.49 (d, *J* = 8.8 Hz,

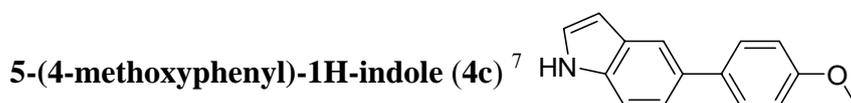
2H), 7.46 (d,  $J = 9.2$  Hz, 2H), 6.95 (d,  $J = 8.4$  Hz, 2H), 6.81 (d,  $J = 8.4$  Hz, 2H), 3.09 (s, 3H), 2.98 (s, 6H).



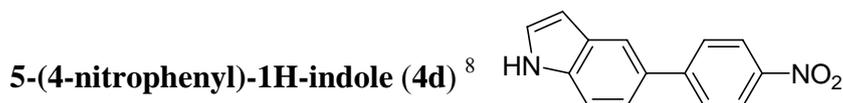
White solid; mp 68-70°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.15 (s, 1H), 7.86 (s, 1H), 7.66 (d,  $J = 8.0$  Hz, 2H), 7.45-7.41 (m, 4H), 7.31 (t,  $J = 6.8$  Hz, 1H), 7.24-7.23 (m, 1H), 6.61 (t,  $J = 4.8$  Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  142.5, 135.3, 133.4, 128.7, 128.4, 127.3, 124.9, 122.0, 120.8, 119.3, 111.3, 103.1.



White solid; mp: 78-79°C <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 8.24 (br s, 1H), 7.83 (s, 1H), 7.66 (d,  $J = 8.0$  Hz, 2H), 7.49 (s, 2H), 7.25-6.99 (m, 3H), 6.60 (s, 1H), 2.39 (s, 3H).

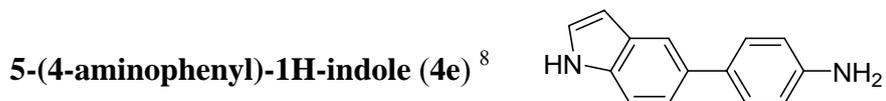


White solid; mp 109-110°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.14 (br s, 1H), 7.80 (s, 1H), 7.58-7.56 (m, 2H), 7.46-7.38 (m, 2H), 7.22 (t,  $J = 2.4$  Hz, 1H), 6.99-6.96 (m, 2H), 6.59 (t,  $J = 2.4$  Hz, 1H), 3.85 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  158.5, 135.2, 135.0, 133.1, 128.4, 128.2, 124.6, 121.8, 118.8, 118.7, 111.2, 103.0, 55.9.

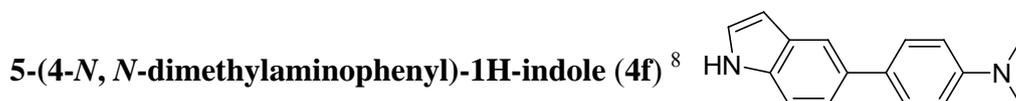


Yellow solid; mp 132-133°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.30-8.28 (m, 3H), 7.92 (d,  $J = 0.8$  Hz, 1H), 7.80-7.78 (m, 2H), 7.52-7.46 (m, 2H), 7.30-7.23 (m, 1H),

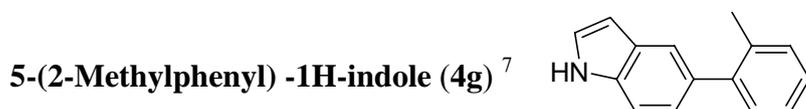
6.65 (t,  $J = 2.0$  Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  149.1, 146.3, 136.1, 130.8, 128.5, 127.6, 125.6, 124.1, 120.0, 111.8, 103.4.



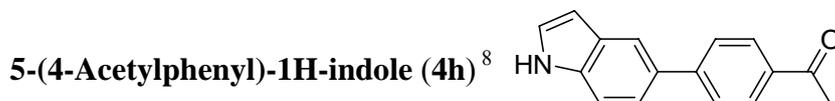
Gray solid; mp: 126-127°C;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  10.98 (br s, 1H), 7.64 (s, 1H), 7.39-25 (m, 5H), 6.64 (d,  $J = 8.4$  Hz, 2H), 6.42 (t,  $J = 2.0$  Hz, 1H), 5.04 (br s 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  147.0, 134.6, 132.0, 129.6, 128.1, 127.2, 126.9, 125.6, 125.4, 119.8, 116.6, 114.6, 111.5, 101.2.



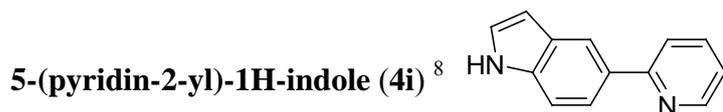
White solid; mp 138-140°C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.14 (br s, 1H), 7.80 (s, 1H), 7.57 (d,  $J = 8.8$  Hz, 2H), 7.42 (s, 2H), 7.22 (t,  $J = 2.4$  Hz, 1H), 6.89 (d,  $J = 6.8$  Hz, 2H), 6.58 (s, 1H), 2.99 (s, 6H).



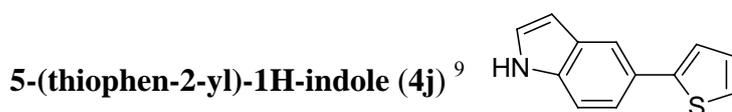
White solid; mp: 65-66°C  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.12 (s, 1H), 7.64 (m, 1H), 7.41-7.37 (m, 1H), 7.31-7.10 (m, 6H), 6.55 (s, 1H), 2.30 (s, 1H).



White solid; mp 135-137°C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.30 (br s, 1H), 8.04 (d,  $J = 8.0$  Hz, 2H), 7.91 (d,  $J = 8.0$  Hz, 1H), 7.76 (d,  $J = 8.4$  Hz, 2H), 7.51-7.46 (m, 2H), 7.25 (t,  $J = 8.4$  Hz, 1H), 6.63 (t,  $J = 2.4$  Hz, 1H), 2.64 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  169.0, 147.3, 135.8, 135.0, 131.9, 128.9, 128.4, 127.2, 125.3, 121.8, 119.7, 111.4, 103.1, 26.6.



White solid; mp: 122-124°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.69 (d, *J* = 4.8 Hz, 1H), 8.34 (br s, 1H), 8.27 (s, 1H), 7.89 (d, *J* = 8.8 Hz, 1H), 7.79-7.71 (m, 2H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.25 (t, *J* = 3.2 Hz, 1H), 7.23-7.16 (m, 1H), 6.63 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 158.7, 149.44, 136.67, 136.4, 131.5, 128.3, 124.9, 121.4, 121.1, 120.4, 119.6, 111.2, 103.4.



White solid; mp 118-120°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.14 (br s, 1H), 7.88 (d, *J* = 8.8 Hz, 1H), 7.48-7.36 (m, 4H), 7.27-7.21 (m, 2H), 6.57(s, 1H).

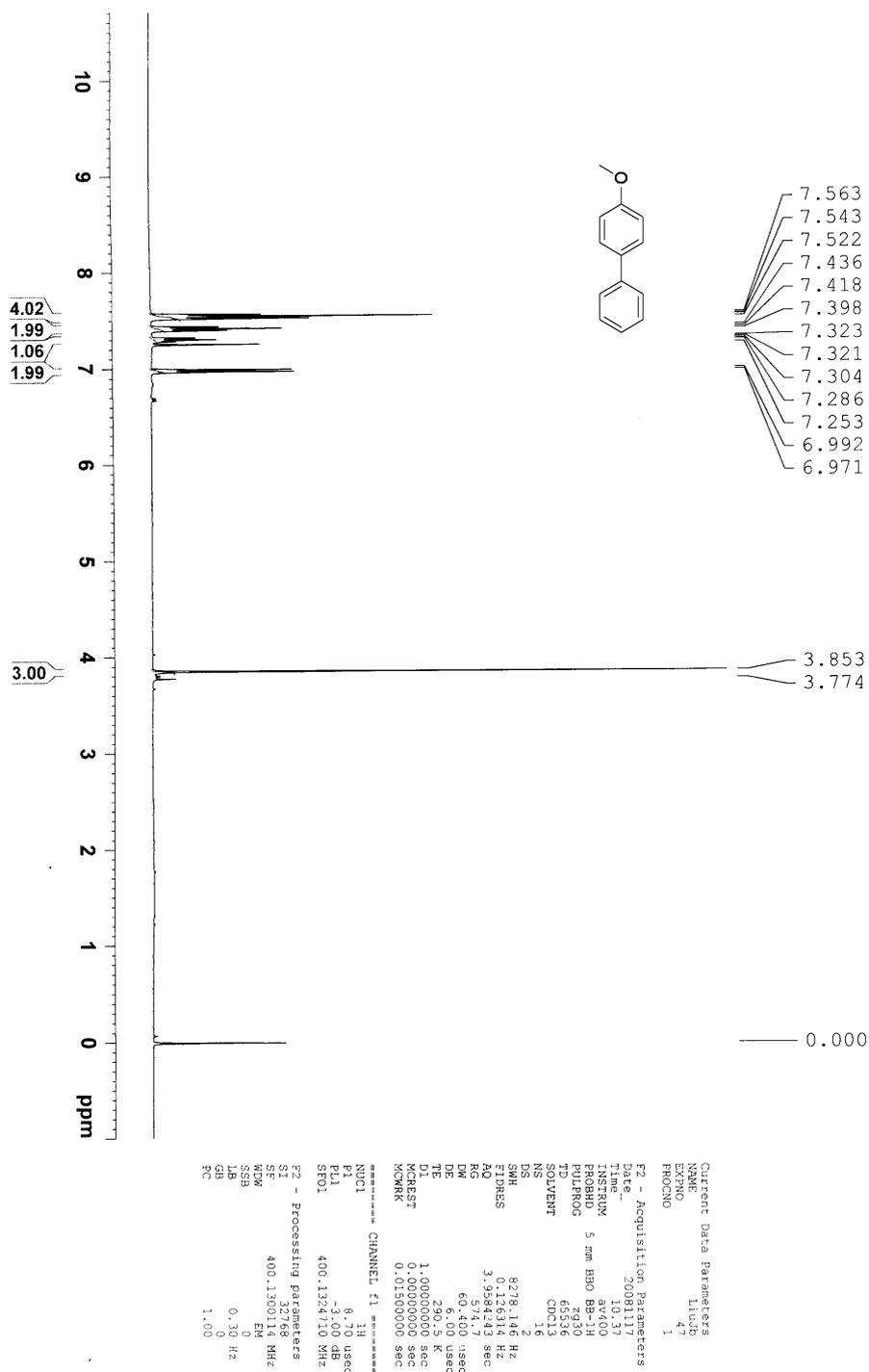
### 3. References

1. (a) H. J. Li, W. J. Liu and Y. X. Xie, *J. Org. Chem.* 2005, **70**, 5409. (b) J. H. Li and W. J. Liu, *Org. Lett.* 2004, **6**, 2809.
2. A. G. Molander and B. Biolatto, *J. Org. Chem.* 2003, **68**, 4302.
3. C. Amatore, C. Cammoun and A. Jutand, *Eur. J. Org. Chem.* 2008, **73**, 4567.
4. K. Inada and N. Miyaura, *Tetrahedron*, 2000, **56**, 8657.
5. E. Tatsuki, F. Keigo, E. Mayuko, K. Masayuki and K. Masanori, *Adv. Syn. & Cata.*; 2004, **346**, 1685.
6. S. W. Michael and D. Philip, *J. Org. Chem.* 2004, **69**, 1137.
7. M. Guobin, P. Ye, L. B. Yu and B. M. Carmen *J. Org. Chem.* 2005, **70**, 2332
8. *PCT Int. Appl.* 2006, 292.

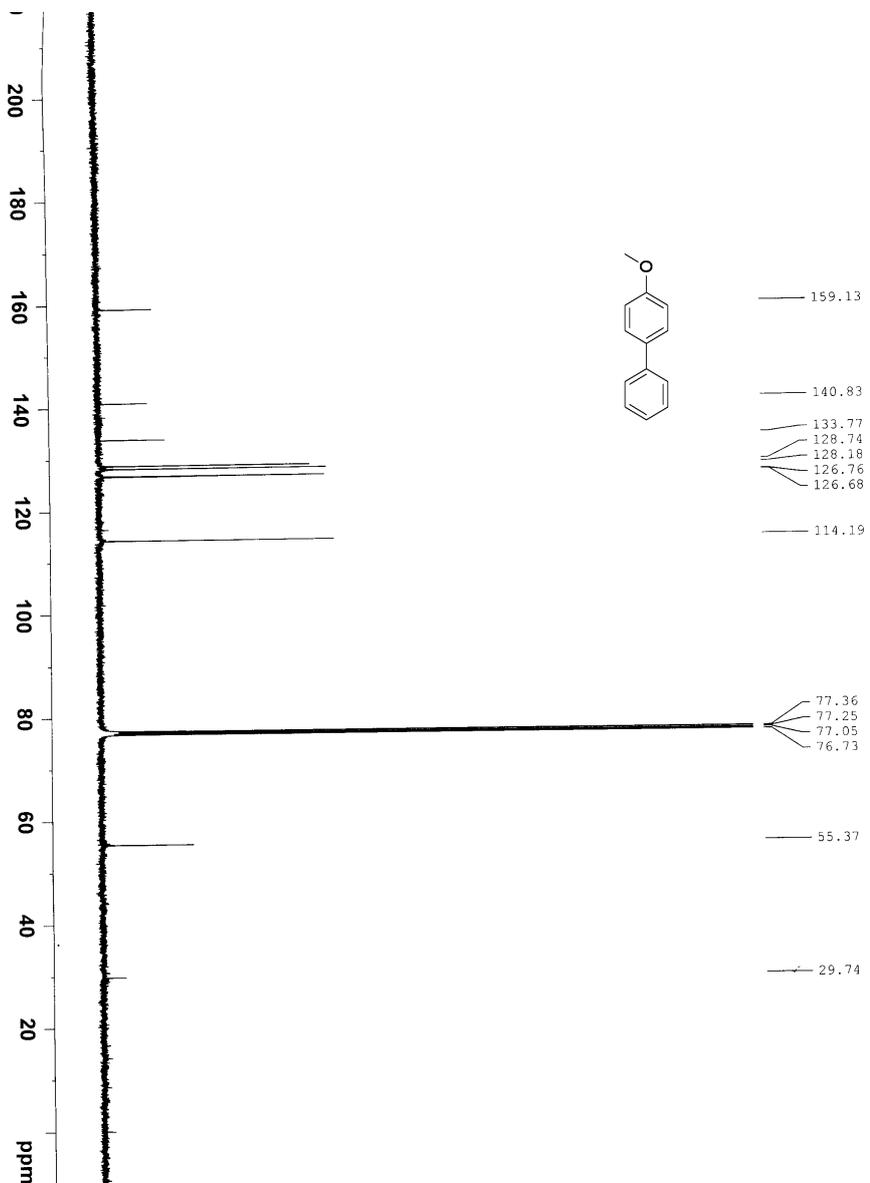
9. A. S. Sarac, S. O. Sarioglan, T. Dziomba and E. Sezer, *European Polymer Journal* 2007, **43**, 3392.

## 4. NMR spectra

### 4-Methoxy-biphenyl (3a)



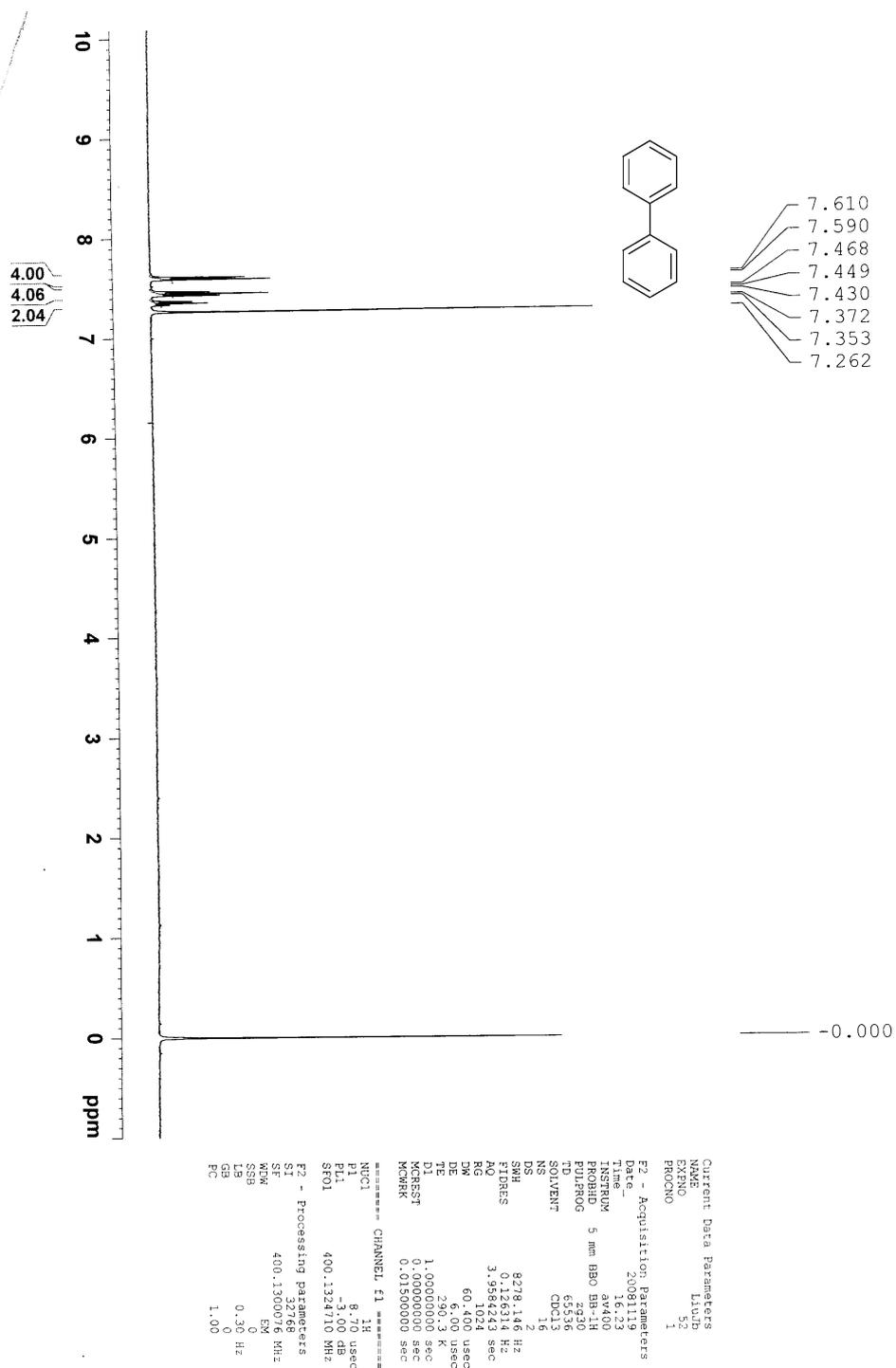
### 4-Methoxy-biphenyl (3a)



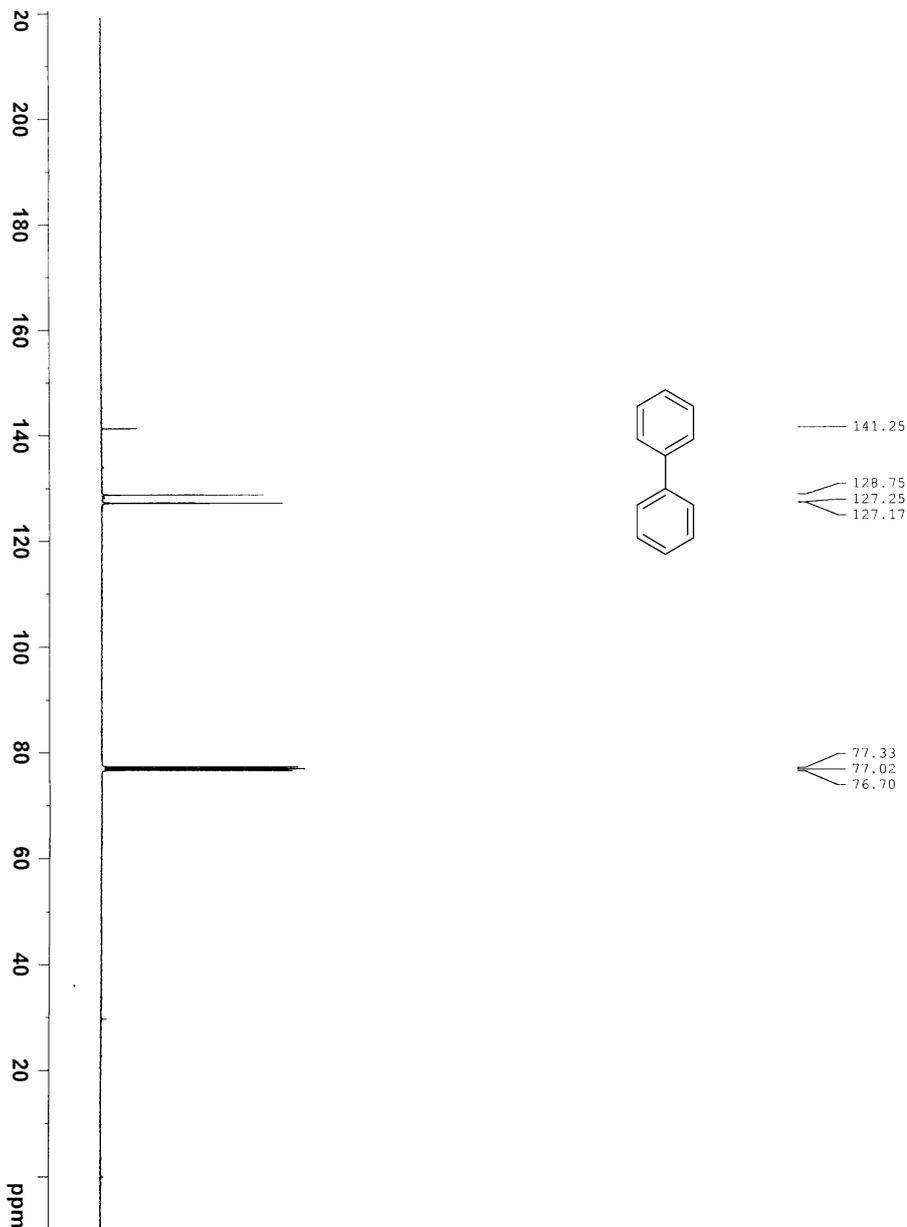
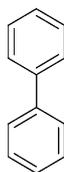
```

Current Data Parameters
NAME          L1003
EXPNO        31
PROCNO       31
=====
F2 - Acquisition Parameters
Date_         20081119
Time          14.53
INSTRUM      av400
PROBHD       5 mm BBO BB-1H
PULPROG      zgpg30
TD            65536
SOLVENT      CDCl3
NS           1438
DS            4
SWH           23980.814 Hz
FIDRES        0.365918 Hz
AQ            1.3664756 sec
RG            9195.2
DW            20.890 usec
DE            294.9 usec
TE            300.2 K
d1            2.00000000 sec
d11           0.03000000 sec
d12           0.00000000 sec
MCPRK        0.01500000 sec
=====
CHANNEL F1
NUC1          13C
P1            130 usec
PL1           -2.00 dB
SFO1         100.6282838 MHz
=====
CHANNEL F2
=====
CPDPRG2      waltz16
NUC2          1H
NUC2         80.00 usec
PCPD2        1.00 dB
PL2          12.97 dB
PL12         20.00 dB
SFO2         400.1316005 MHz
=====
F2 - Processing parameters
SI            32768
SF           100.6127690 MHz
WDW           EM
SSB           0
GB            0
PC            1.40
  
```

### Biphenyl (3b)



### Biphenyl (3b)



```

Current Data Parameters
NAME          Luub
EXPNO        34
PROCNO       1

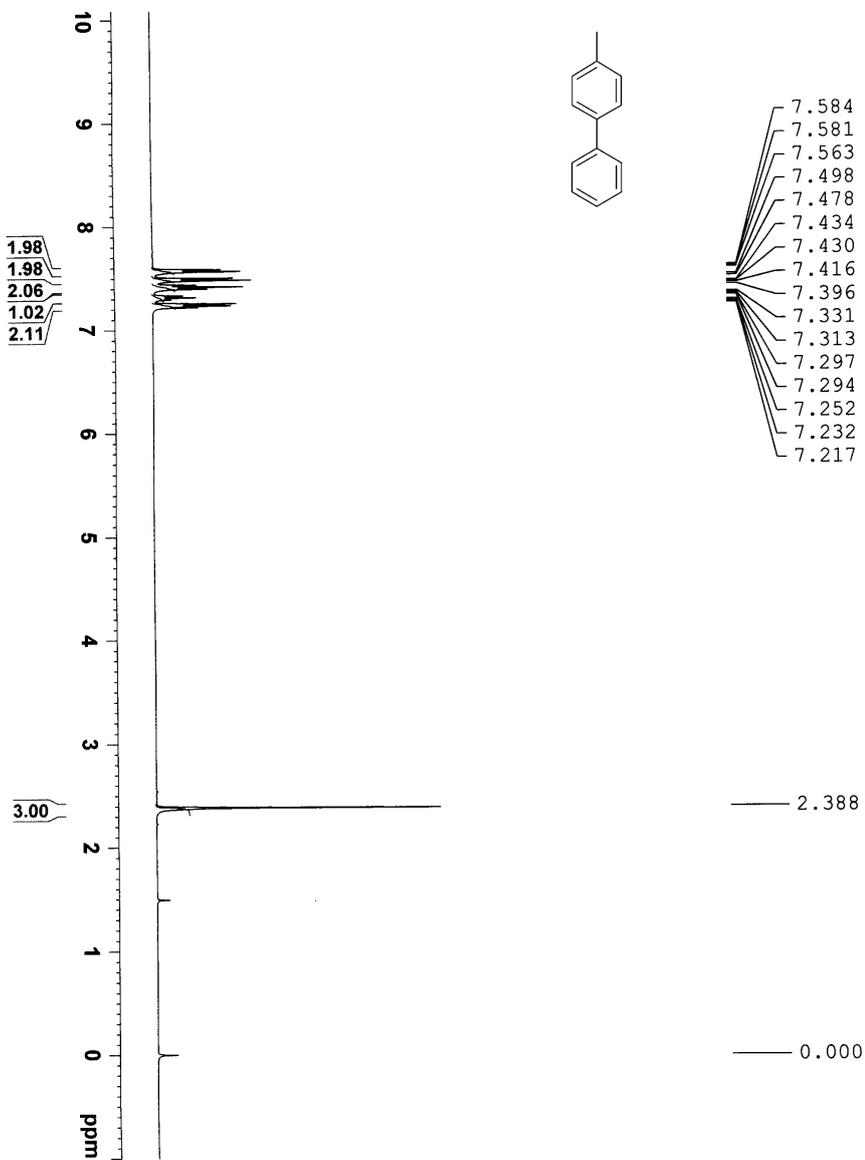
F2 - Acquisition Parameters
Date_        20080928
Time         12.33
INSTRUM      aw400
PROBHD       5 mm BBO BB-1H
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           1024
DS           4
SWH          23980.814 Hz
FIDRES       0.365918 Hz
AQ           1.3664756 sec
RG           11585.2
DE           20.890 usec
TE           297.8 K
D1           2.00000000 sec
d11          0.03000000 sec
ICREST       0.00000000 sec
MORPH        0.01500000 sec

===== CHANNEL f1 =====
NUC1          13C
P1            8.50 usec
PL1          -2.00 dB
SFO1         100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
RGPD2        80.00 usec
P12          3.00 dB
P13          16.27 dB
P14          20.00 dB
SFO2         400.1318005 MHz

F2 - Processing parameters
SI           32768
SF           100.6127707 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.00
    
```

### 4-Methyl-biphenyl (3c)



- 7.584
- 7.581
- 7.563
- 7.498
- 7.478
- 7.434
- 7.430
- 7.416
- 7.396
- 7.331
- 7.313
- 7.297
- 7.294
- 7.252
- 7.232
- 7.217

- 2.388
- 0.000

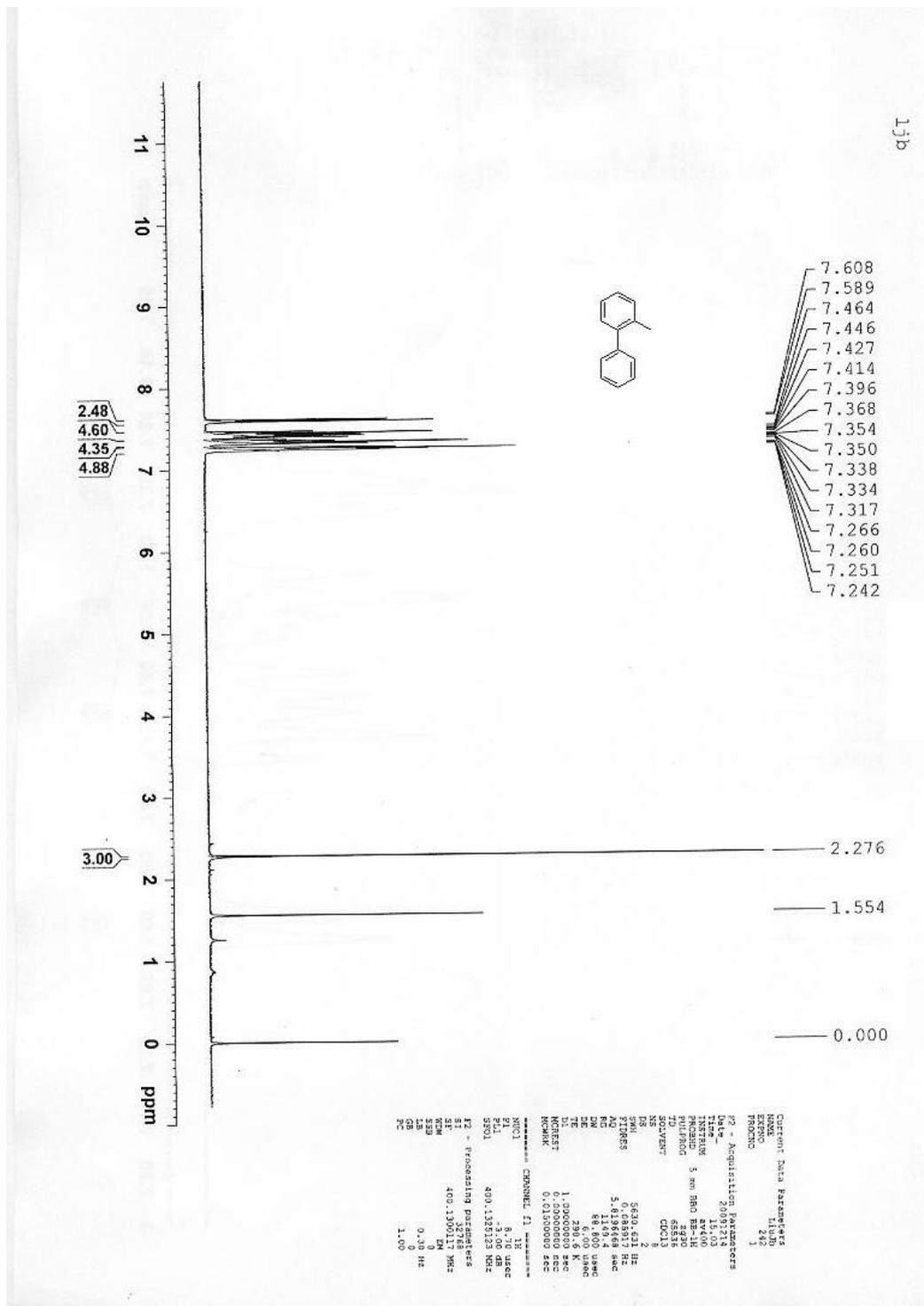
Current Data Parameters  
 NAME Liub  
 EXPNO 62  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090318  
 Time 16:55  
 INSTRUM av400  
 PROBRD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 65536  
 SFO1 400.1324710  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8278.144 Hz  
 FWH 0.126314 Hz  
 AQ 3.9584243 sec  
 RG 574.7  
 DM 60.400 usec  
 DE 25.00 usec  
 TE 300.2 K  
 D1 1.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRRK 0.01500000 sec

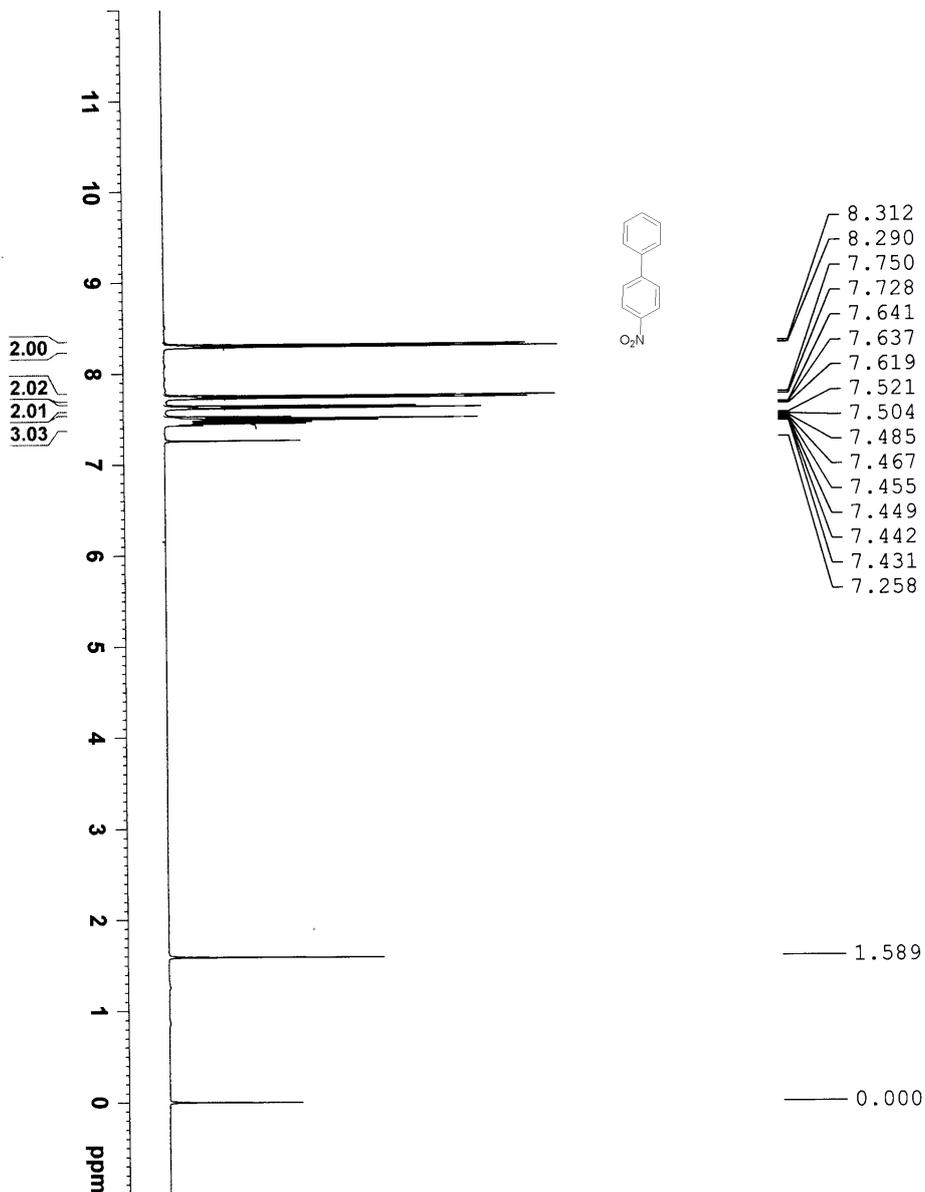
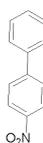
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 8.70 usec  
 PL1 -3.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300257 MHz  
 WDW EM  
 SSB 0 Hz  
 GB 0 Hz  
 PC 1.00

### 2-Methyl-biphenyl (3d)



### 4-Nitro-biphenyl (3e)



- 8.312
- 8.290
- 7.750
- 7.728
- 7.641
- 7.637
- 7.619
- 7.521
- 7.504
- 7.485
- 7.467
- 7.455
- 7.449
- 7.442
- 7.431
- 7.258

- 1.589
- 0.000

Current Data Parameters  
 NAME p1  
 EXNO 1  
 PROCNO 1

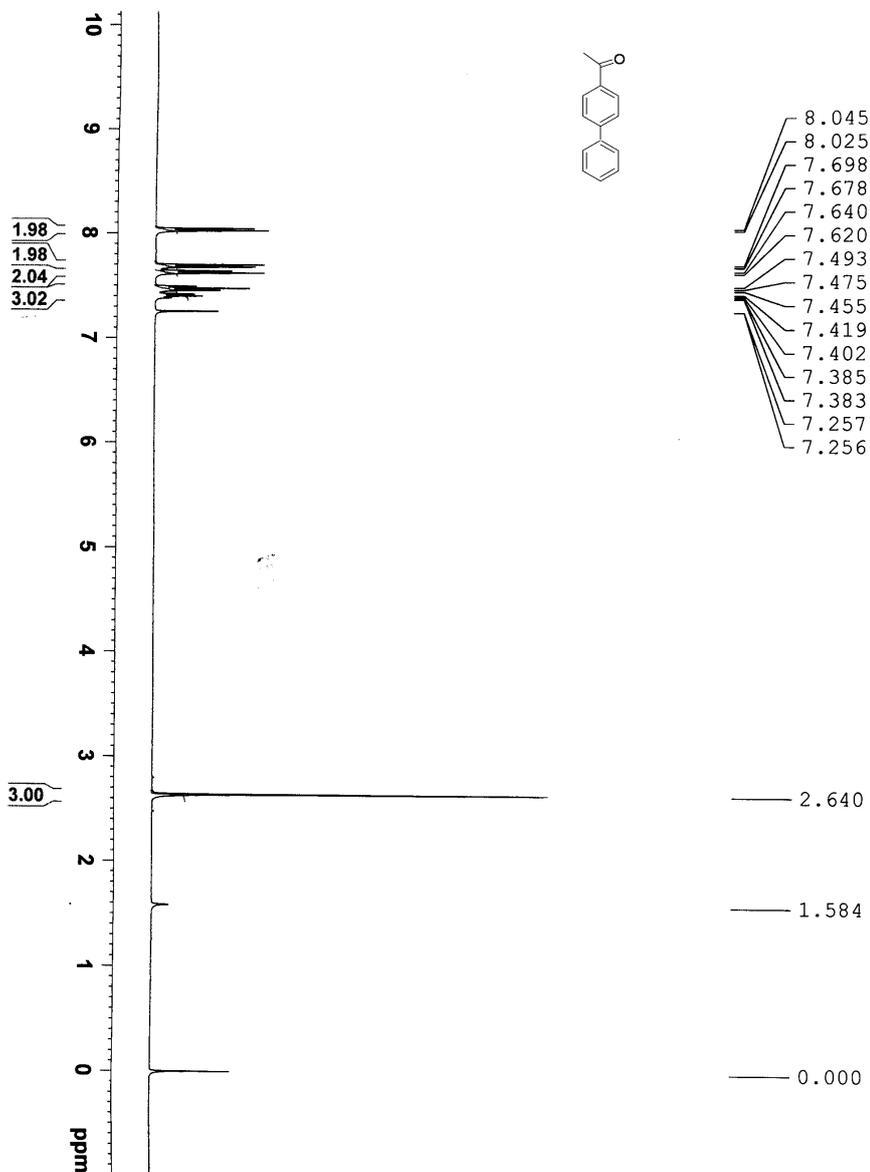
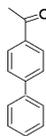
F2 - Acquisition Parameters  
 Date\_ 20090313  
 Time\_ 15.28  
 INSTRUM av400  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 FIDRES 0.126314 Hz  
 AQ 3.9584243 sec  
 RG 60.000 usec  
 DM 1.000 usec  
 DE 6.00 usec  
 TE 291.3 K  
 D1 1.00000000 sec  
 MCKEAT 0.00000000 sec  
 MCMRRK 0.01500000 sec

===== CHANNEL F1 =====  
 NUC1 1H  
 P1 8.70 usec  
 PL1 -3.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300829 MHz  
 KF 1  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

S14

### 4-Acetyl-biphenyl (3f)



8.045  
 8.025  
 7.698  
 7.678  
 7.640  
 7.620  
 7.493  
 7.475  
 7.455  
 7.419  
 7.402  
 7.385  
 7.383  
 7.257  
 7.256

2.640  
 1.584  
 0.000

1.98  
 1.98  
 2.04  
 3.02

3.00

ppm

```

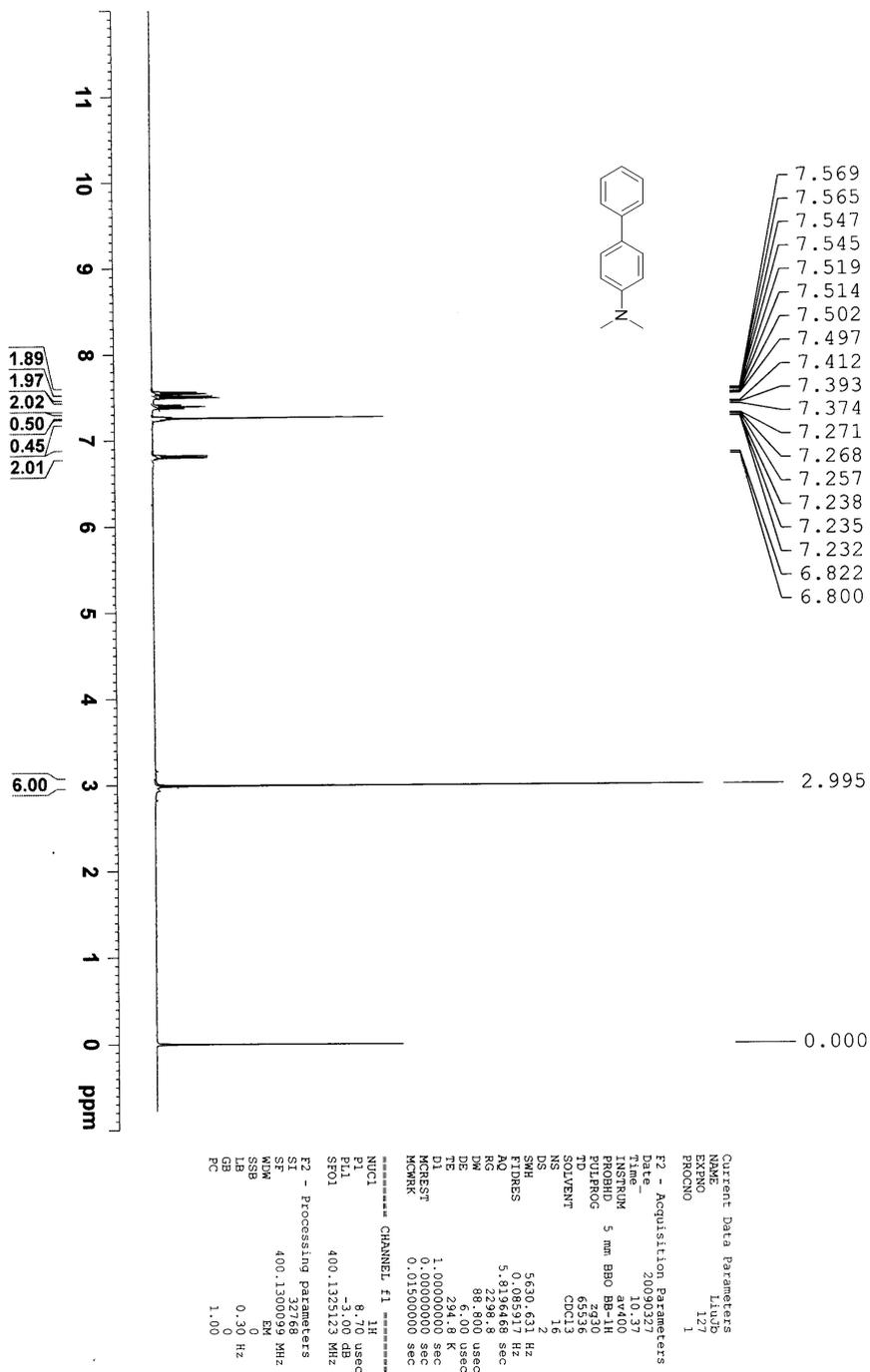
Current Data Parameters
NAME          Liubb
EXPNO         63
PROCNO        1

F2 - Acquisition Parameters
Date_         20080320
Time          15:05
INSTRUM       av400
PROBHD        5 mm BBO BB-1H
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            2
DS            2
SWH           8278.146 Hz
FIDRES       0.126314 Hz
AQ           3.392643 sec
RG           624.45
DM           60.100 usec
DE           6.00 usec
TE           296.15 K
T1           1.0000000 sec
T2           0.0000000 sec
MCRBSM       0.01500000 sec
MCWPRK       0.01500000 sec

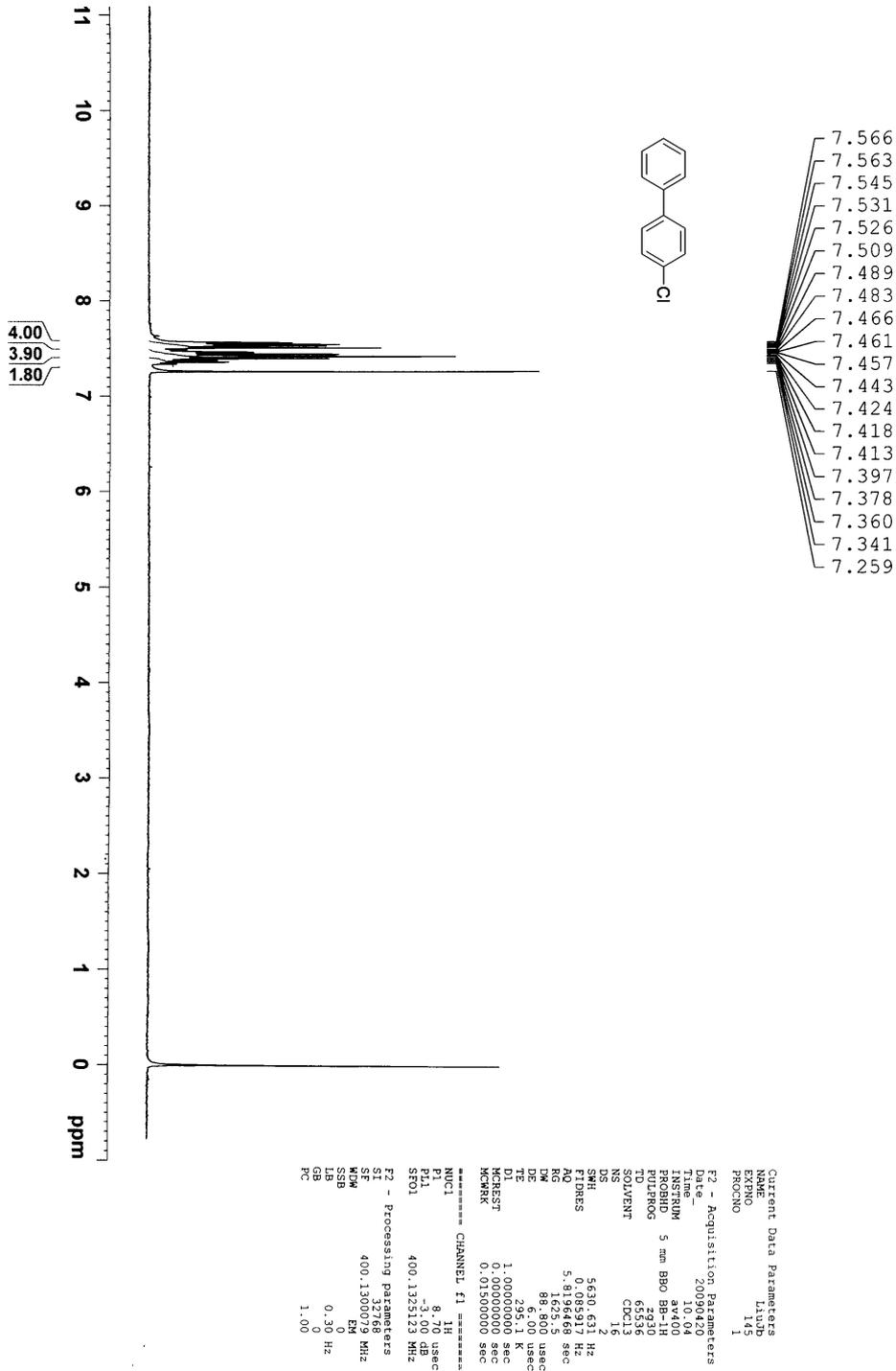
===== CHANNEL f1 =====
NUC1          1H
P1            9.10 usec
PL1          -3.70 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI           32768
SF           400.1300000 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
    
```

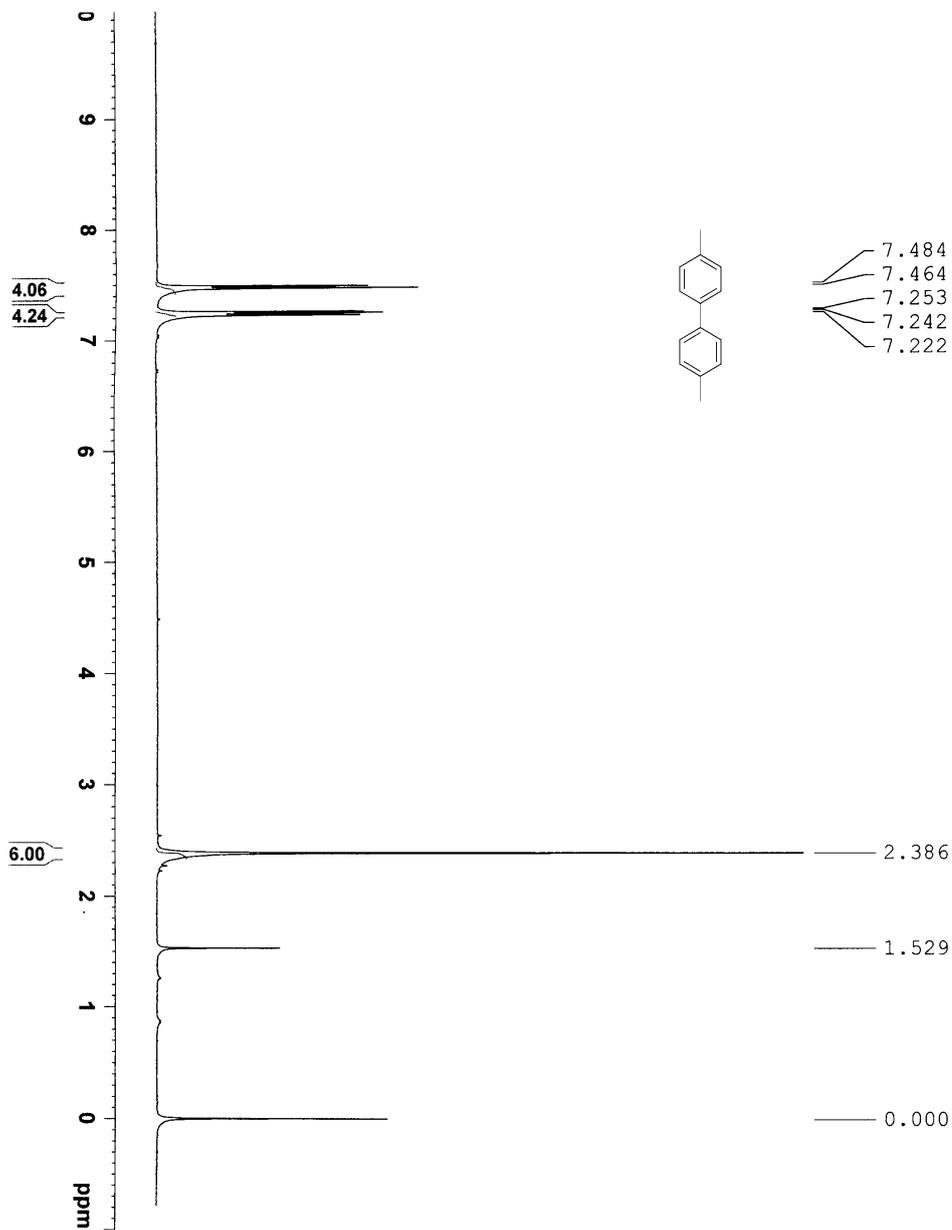
4- (N, N-dimethylamino) biphenyl (3g)



### 4-Chloro-biphenyl (3h)



4, 4'-Dimethyl-biphenyl (3i)



```

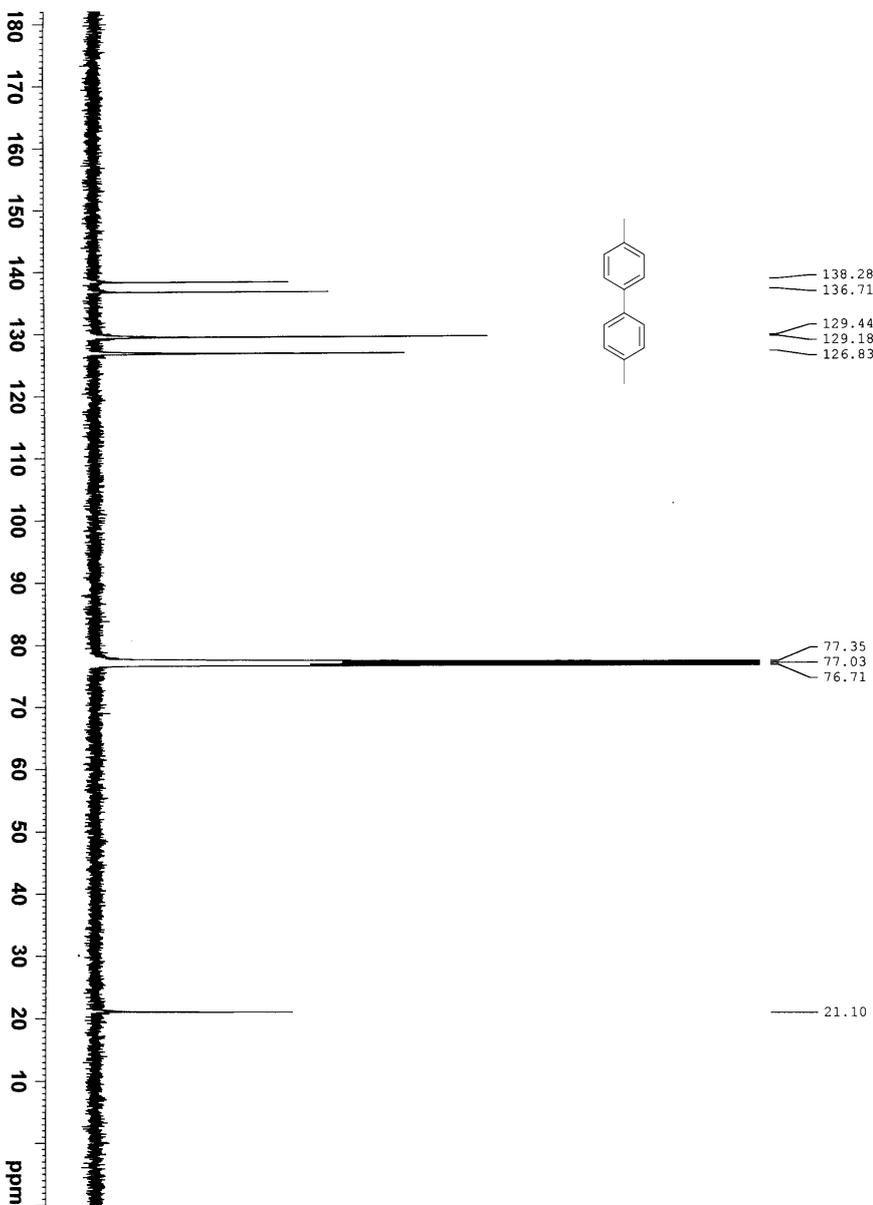
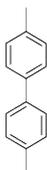
Current Data Parameters
NAME      Liutp
EXPNO    138
PROCNO   1

F2 - Acquisition Parameters
Date_    20090413
Time     15.37
INSTRUM  av400
PROBHD   5 mm BBO BB-4H
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       5630.63 Hz
AQ        0.086917 Hz
RG        1448.2
DM        89.800 usec
DE        5.00 usec
TE        298.0 K
D1        1.00000000 sec
MCHRGST  0.00000000 sec
MCKMR    0.01500000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        8.70 usec
PL1       0.00 dB
SFO1      400.1326129 MHz

F2 - Processing parameters
SI        32768
SF        400.1300110 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

### 4, 4'-Dimethyl-biphenyl (3i)



138.28  
 136.71  
 129.44  
 129.18  
 126.83

77.35  
 77.03  
 76.71

21.10

```

Current Data Parameters
NAME      Liuid
EXPNO    144
PROCNO   1

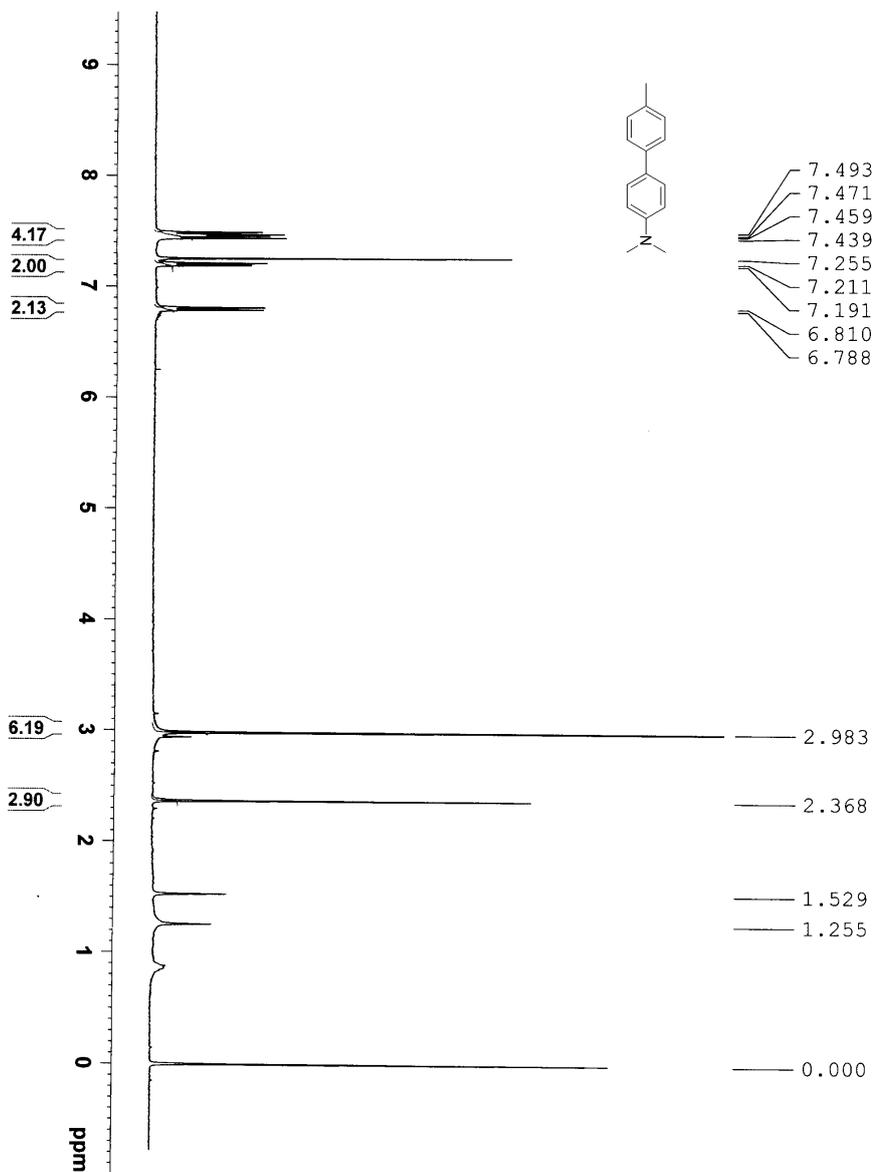
F2 - Acquisition Parameters
Date_    20090415
Time     23.17
INSTRUM  5 mm BBO BB-1H
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        6144
DS        4
SWH       23980.814 Hz
FIDRES    0.365918 Hz
AQ        1.3664756 sec
RG        9195.2
DM        20.850 usec
DE        5.00 usec
PE        25.00 usec
D1        2.0000000 sec
d11       0.03000000 sec
MCREST    0.0000000 sec
MCWRK     0.01500000 sec

===== CHANNEL f1 =====
NUC1      13C
P1        8.50 usec
PL1       2.00 dB
SFO1     100.628299 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -3.00 dB
PL12      16.27 dB
PL13      20.00 dB
SFO2     400.1316005 MHz

F2 - Processing parameters
SI        32768
SF        100.6127690 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
    
```

**4-Methyl -4'-(N, N-Dimethylamino) biphenyl (3j)**



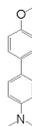
Current Data Parameters  
 Name: Liud  
 ExpNO: 124  
 PROCNO: 1

F2 - Acquisition Parameters  
 Date\_: 20090323  
 Time: 11:28  
 Time2: 11:40  
 Date2: 20090323  
 PROBRD: 5 mm BBO  
 PULPROG: zgpg30  
 TD: 65536  
 SOLVENT: CDCl3  
 NS: 16  
 DS: 2  
 SWH: 5630.631 Hz  
 FIDRES: 0.085917 Hz  
 AQ: 5.8196468 sec  
 RG: 1625.5  
 DM: 88.800 usec  
 DE: 29.00 usec  
 TE: 299.2 K  
 D1: 1.00000000 sec  
 MCREST: 0.00000000 sec  
 KCMRR: 0.01500000 sec

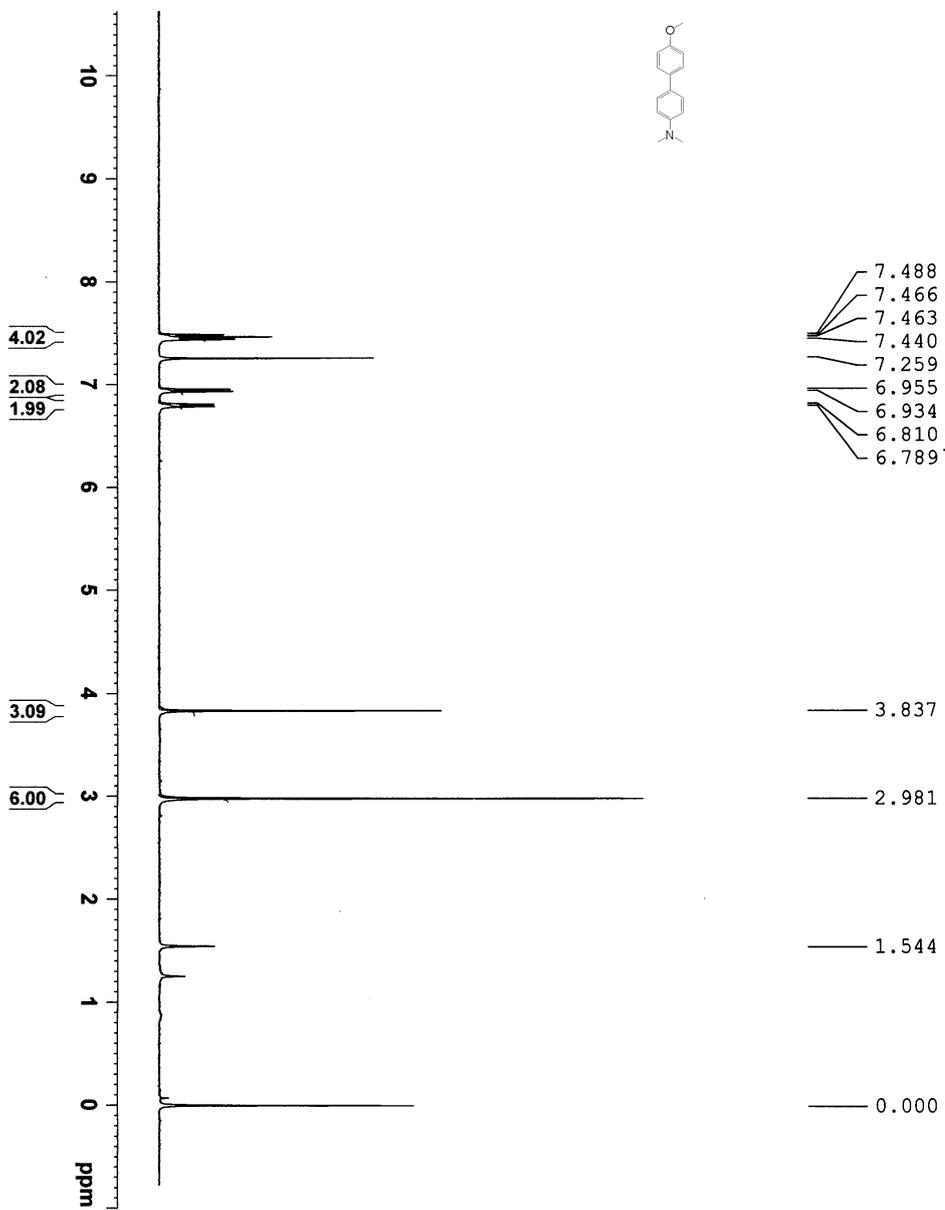
===== CHANNEL f1 =====  
 NUC1: 1H  
 P1: 8.70 usec  
 PL1: -3.00 dB  
 SFO1: 400.1325123 MHz

F2 - Processing parameters  
 SI: 32768  
 SF: 400.1300106 MHz  
 WBW: EM  
 SSB: 0  
 LB: 0.30 Hz  
 GB: 0  
 PC: 1.00

4-Methoxy-4'- (N, N-dimethylamino) biphenyl (3k)



1j1b4



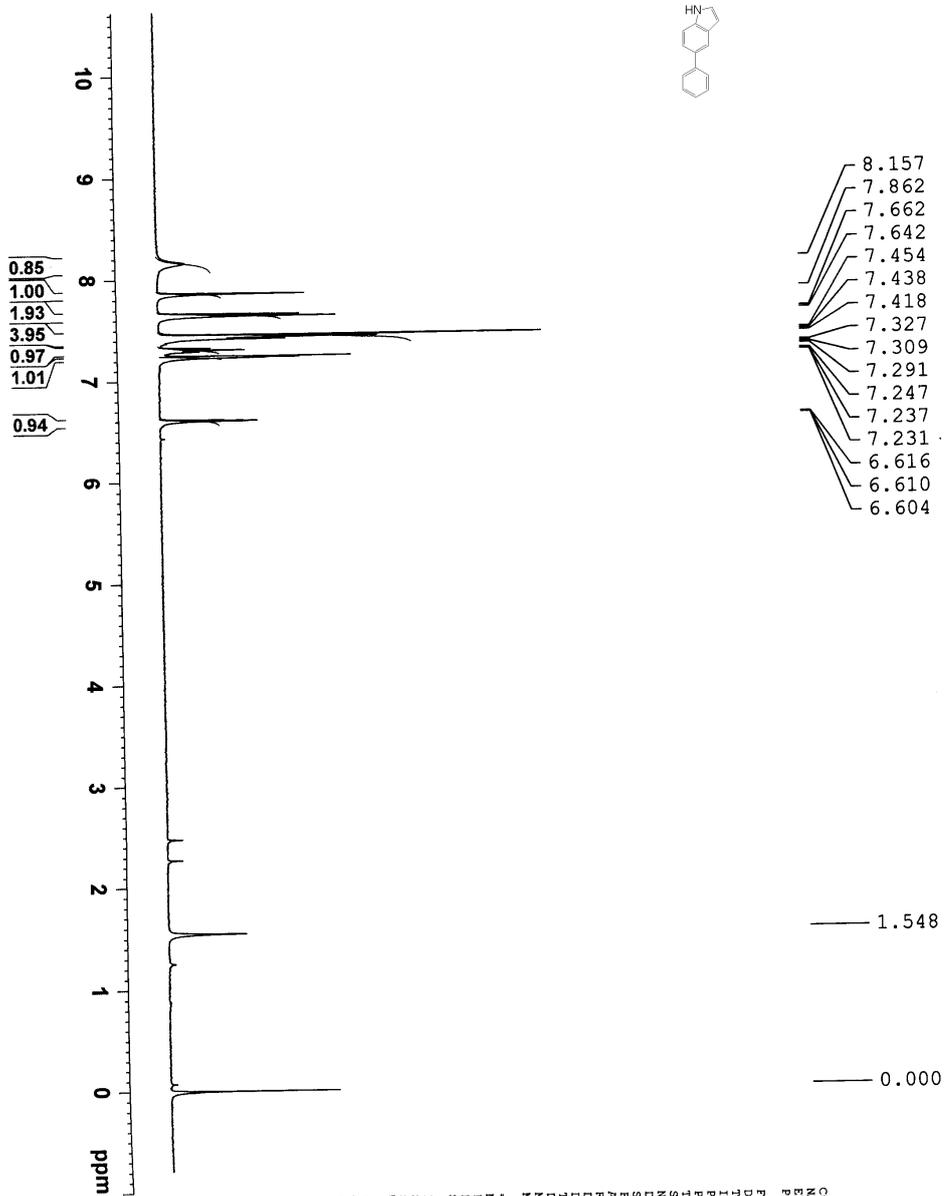
```

Current Data Parameters
NAME          1j1b4
EXPNO         231
PROCNO        1
===== Acquisition Parameters =====
Date_         20091106
Time         11:29
INSTRUM      av400
PROBHD       5 mm BBO BB-1H
PULPROG      zg30
SOLVENT      CDCl3
NS           8
DS           2
SF           5638.631 Hz
AQ           0.00000000 sec
RG           1824.6
DM           88.800 usec
DE           2.00 usec
TE           29.97
D1           1.00000000 sec
MKREST       0.00000000 sec
MKMKR        0.01500000 sec
===== CHANNEL f1 =====
NUC1          1H
P1            8.70 usec
PL1           -2.00 dB
SFO1         400.1325123 MHz
===== Processing parameters =====
SI           32768
SF           400.1300250 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
    
```

5-phenyl-1H-indole (4a)



1j1b1



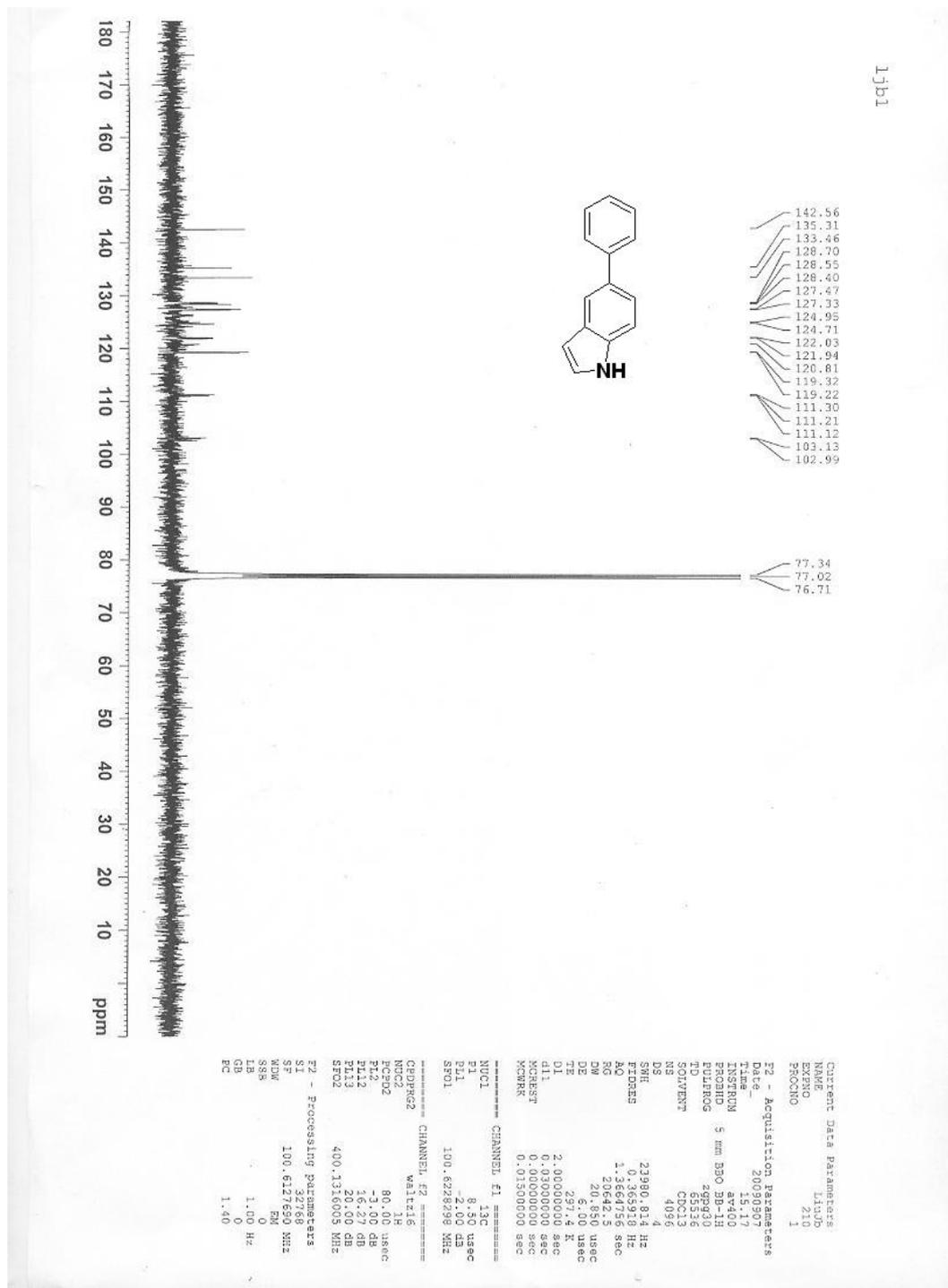
Current Data Parameters  
 Name: 1j1b1  
 ExpNo: 227  
 ProcNo: 1

F2 - Acquisition Parameters  
 Date\_: 20091106  
 Time: 11:18  
 Instrument: 5 mm BBO BB-4H  
 PULPROG: zg30  
 TD: 65536  
 SOLVENT: CDCl3  
 NS: 2  
 DS: 2  
 SWH: 5630.631 Hz  
 FIDRES: 0.085910 Hz  
 AQ: 5.231170 sec  
 T1: 1.494 sec  
 T2: 149.4 sec  
 DE: 88.800 usec  
 TE: 300.2 K  
 MCREST: 1.0000000 sec  
 MCRRK: 0.01500000 sec

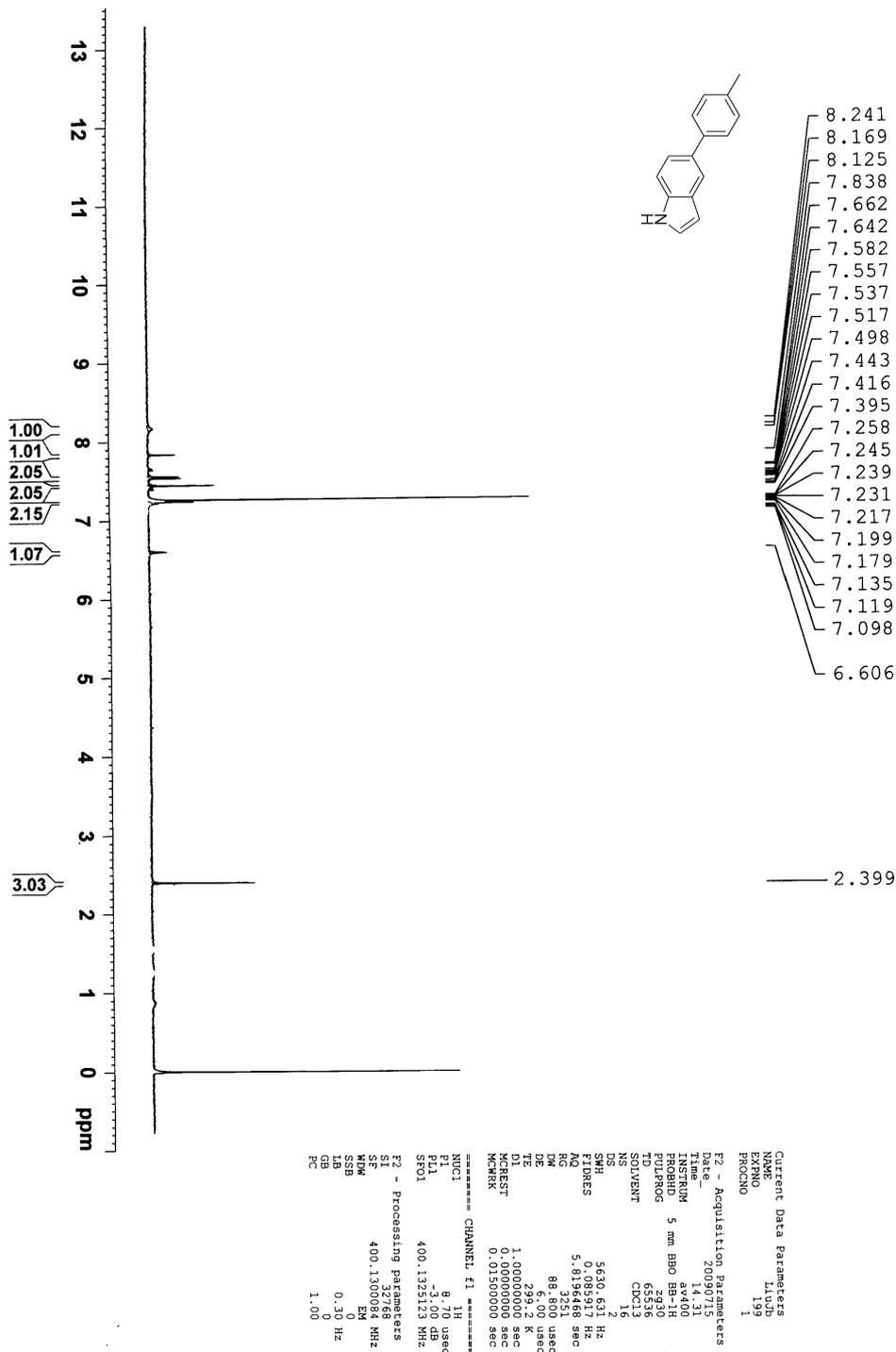
----- CHANNEL f1 -----  
 NUC1: 1H  
 P1: 8.70 usec  
 PL1: -3.00 dB  
 SFO1: 400.132320 MHz

F2 - Processing parameters  
 SI: 32768  
 SF: 400.1300126 MHz  
 SFO: 400.1300126 MHz  
 LB: 0  
 GB: 0.30 Hz  
 PC: 1.00

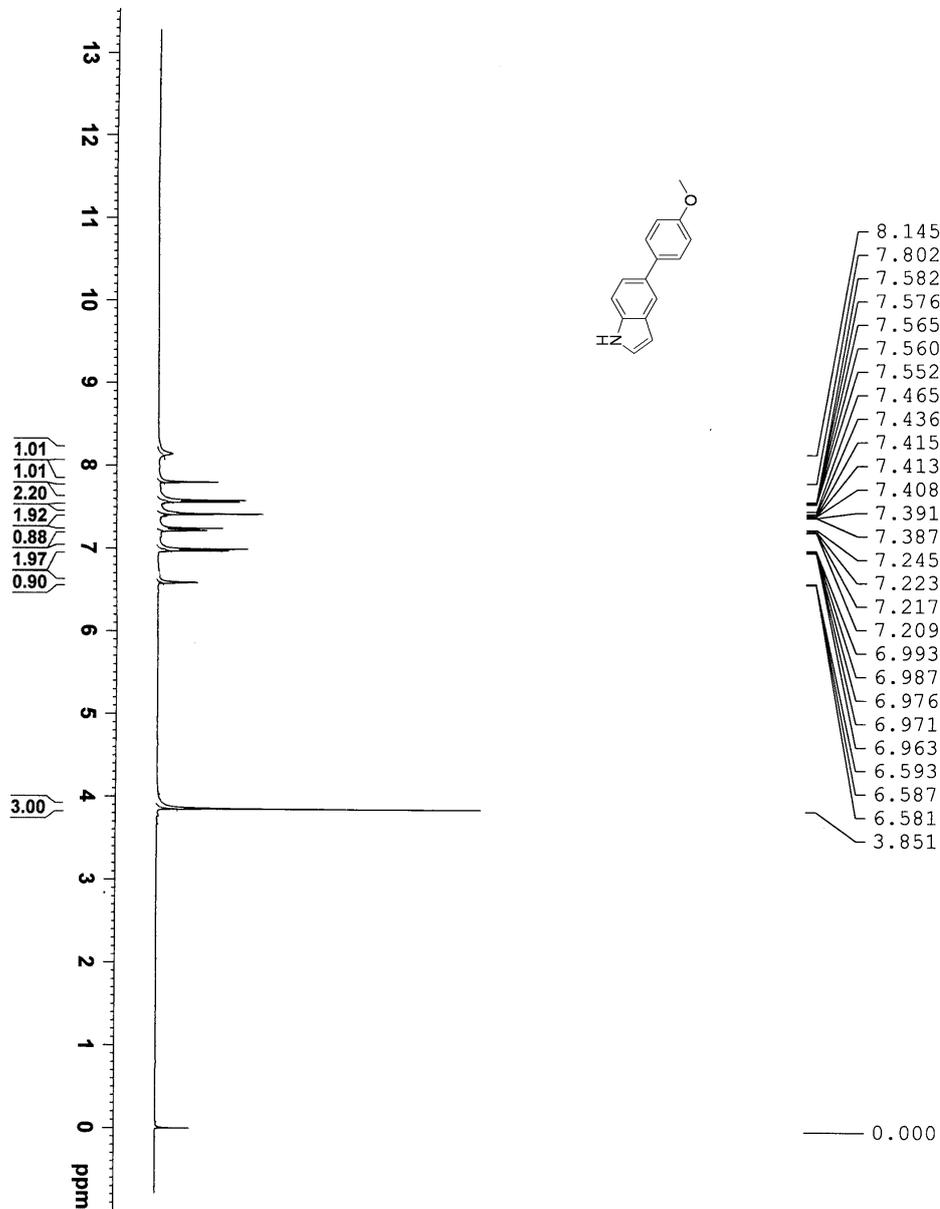
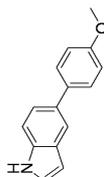
### 5-phenyl-1H-indole (4a)



**5-*p*-tolyl-1H-indole (4b)**



### 5-(4-methoxyphenyl)-1H-indole (4c)



```

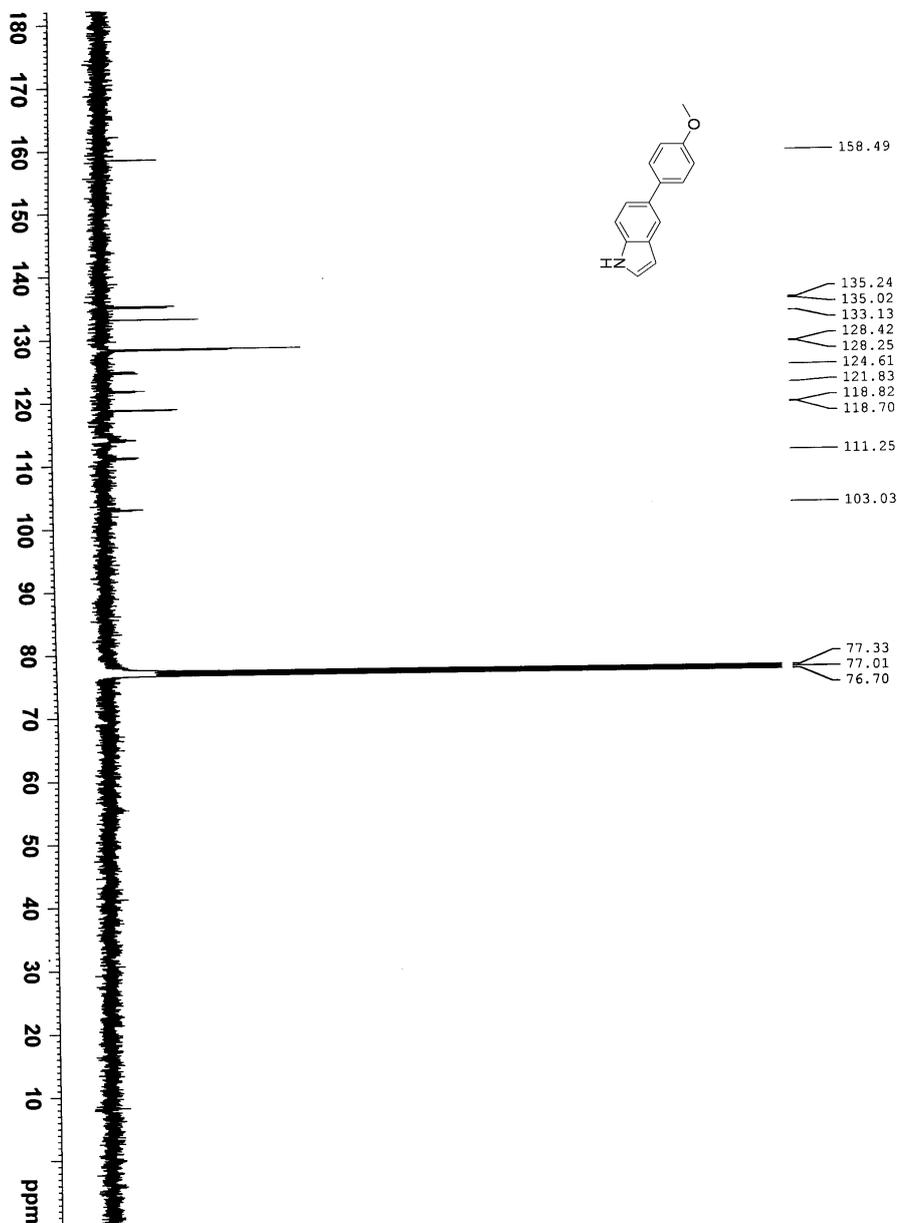
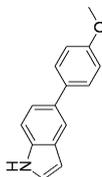
Current Data Parameters
NAME      Liubd
EXPNO     189
PROCNO    1

F2 - Acquisition Parameters
Date_     20090712
Time      10.08
INSTRUM   spect
PROBHD    5 mm BBO
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
DS        2
AQ        1.000000 sec
FIDRES    0.089917 Hz
AQ        5.8196468 sec
RG        655.36
DE        88.500 usec
TE        299.0 K
AQRSTRT   1.000000 sec
MCRSTRT   0.01500000 sec

===== CHANNEL f1 =====
NUC1      13
P1        8.70 usec
PL1       -3.00 dB
SFO1      400.1325123 MHz

F2 - Processing parameters
SI        32768
SF        400.1300125 MHz
MDM       64
GB        0
PC        1.00
    
```

### 5-(4-methoxyphenyl)-1H-indole (4c)



```

Current Data Parameters
NAME          LIND
EXPNO        195
PROCNO       1

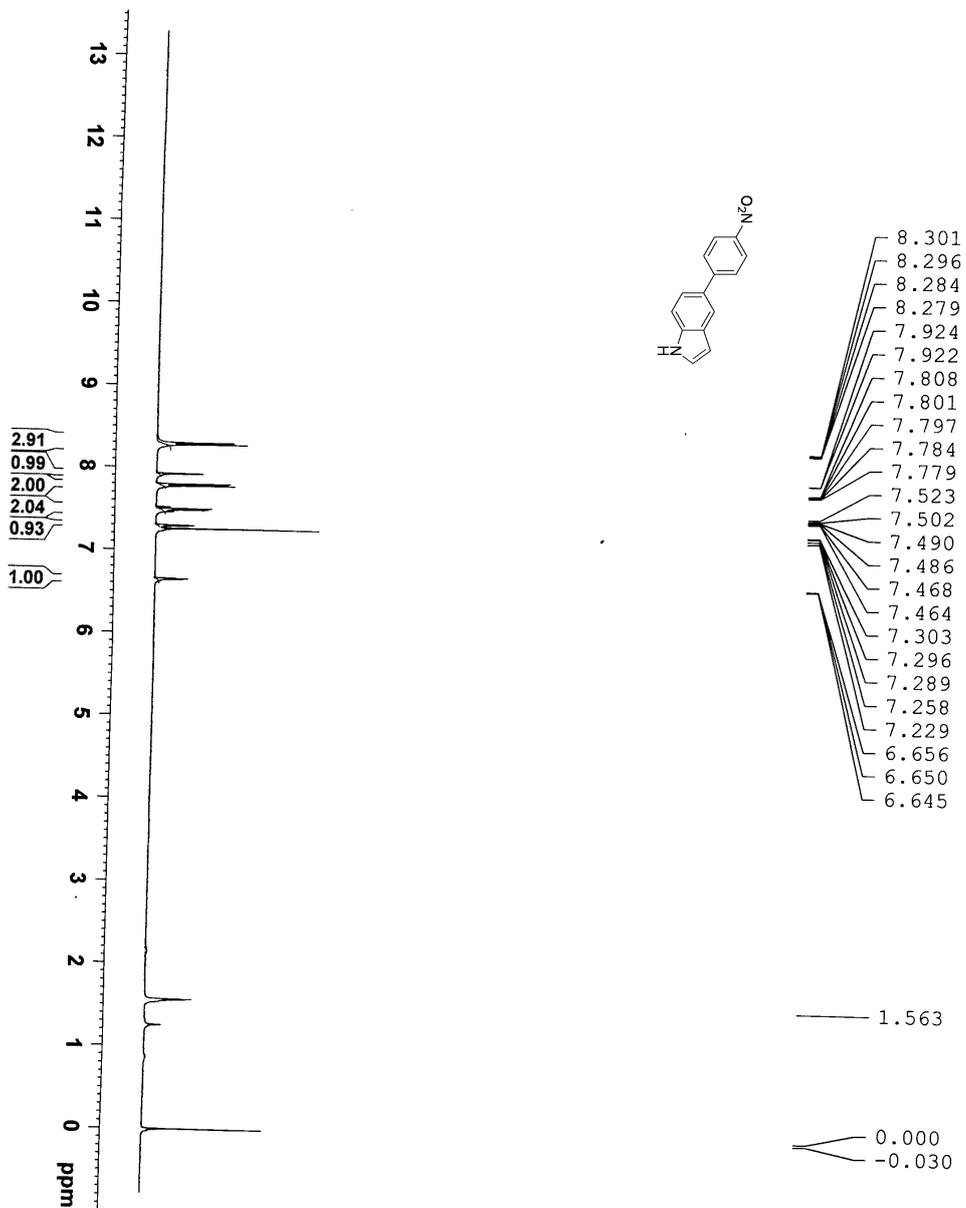
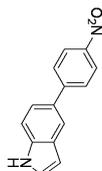
F2 - Acquisition Parameters
Date_        20090714
Time         11.49
INSTRUM     av400
PROBHD      5 mm BBO BB-1H
PULPROG     zgpg30
TD           65536
SOLVENT     CDCl3
NS           3072
DS           4
SWH          23980.814 Hz
FIDRES       0.363918 Hz
AQ           1.369278 sec
RG           399
SFO1         20.850 usec
DM           6.00 usec
TE           299.2 K
D1           2.00000000 sec
d11          0.03000000 sec
MCREST      0.00000000 sec
MCWRK       0.01500000 sec

===== CHANNEL f1 =====
NUC1         13C usec
P1          8.100 usec
PL1         -4.00 dB
SFO1        100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2         1H
PCPD2       80.00 usec
PL2         -3.00 dB
PL12        16.27 dB
PL13        20.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SF           32768
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
    
```

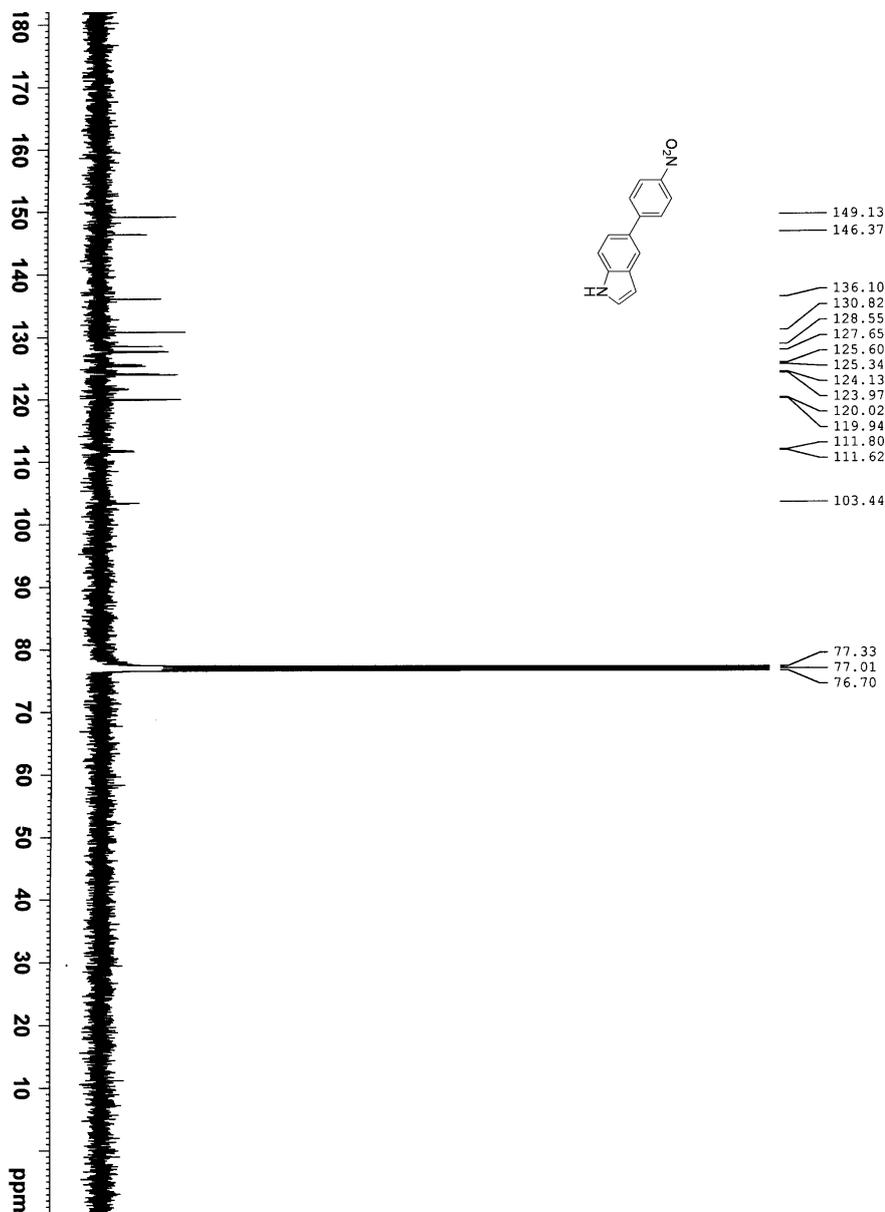
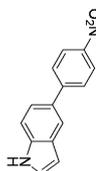
### 5-(4-nitrophenyl)-1H-indole (4d)



```

Current Data Parameters
NAME          1
EXPNO        191
PROCNO       1
F2 - Acquisition Parameters
Date_         20090520
Time          20.16
INSTRUM      5 mm BBO BB-1H
PROBHD       5 mm BBO BB-1H
PULPROG      zgpg30
TD            65536
SOLVENT      CDCl3
NS            16
DS            4
SWH           5630.631 Hz
AQ            0.085911 Hz
RG            3251
DE            88.800 usec
TE            298.6 K usec
D1            1.00000000 sec
MKRGST       0.00000000 sec
MKRMN        0.01500000 sec
===== CHANNEL f1 =====
NUC1          1H
P1            8.70 usec
PL1           -2.00 dB
SFO1          400.1325123 MHz
F2 - Processing parameters
SI            32768
SF            400.130000 MHz
WDW           EM
SSB           0
GB            0
PC            1.00
  
```

### 5-(4-nitrophenyl)-1H-indole (4d)



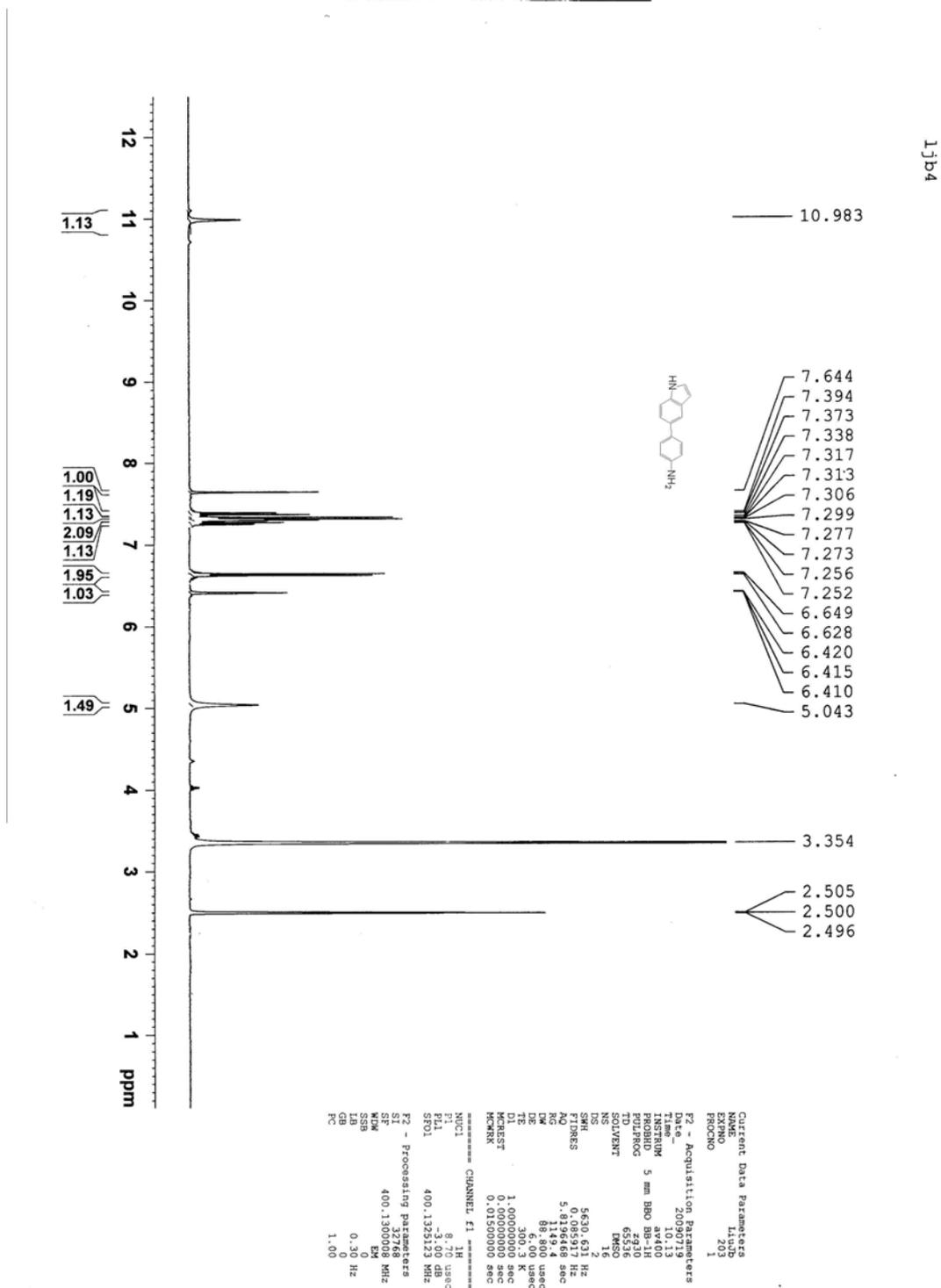
149.13  
 146.37  
 136.10  
 130.82  
 128.55  
 127.65  
 125.60  
 125.34  
 124.13  
 123.97  
 120.02  
 119.94  
 111.80  
 111.62  
 103.44

77.33  
 77.01  
 76.70

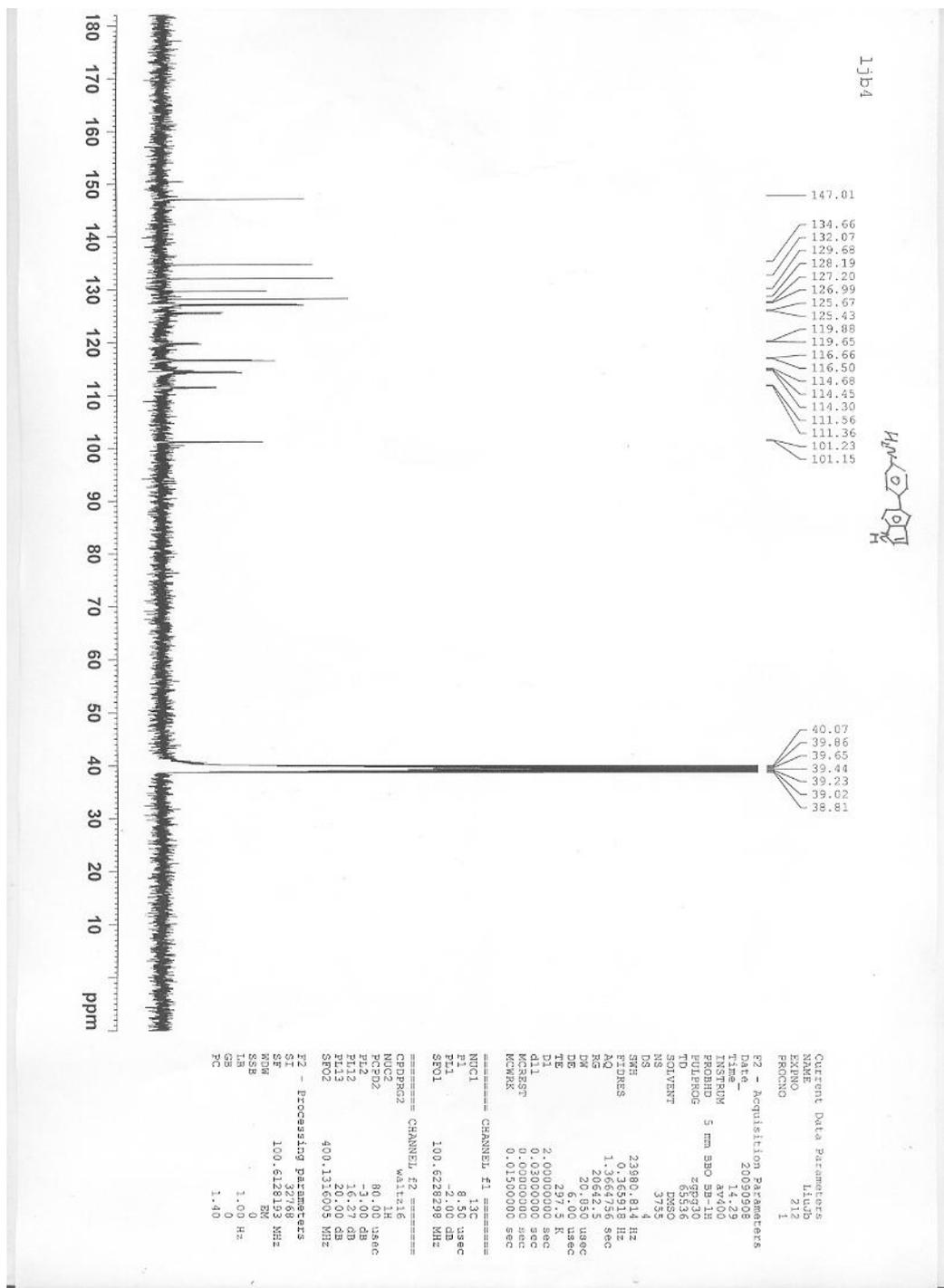
```

Current Data Parameters
NAME          L1udb
EXPNO        192
PROCNO       1
=====
F2 - Acquisition Parameters
Date_        20090713
Time        20:12
INSTRUM     spect
PROBHD      5 mm BBO BB-1H
PULPROG     zgpg30
TD           65536
SOLVENT     CDCl3
NS           3072
DS           4
SWH          23980.814 Hz
FIDRES       0.365918 Hz
AQ           1.3664756 sec
RG           919.72
AQ           1.3664756 sec
RG           919.72
DE           20.850 usec
DM           6.00
TE           298.6 K
D1           2.00000000 sec
d11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec
=====
CHANNEL F1 =====
NUC1         13C
P1           8.50 usec
PL1          2.00 dB
SFO1         100.6228238 MHz
=====
CHANNEL F2 =====
CPDPRG2     waltz16
NUC2         1H
PCPD2       80.00 usec
PL2         -3.00 dB
PL12        16.27 dB
PL13        20.00 dB
SFO2        400.1316005 MHz
=====
F2 - Processing parameters
SI           32768
SF           100.6127690 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
    
```

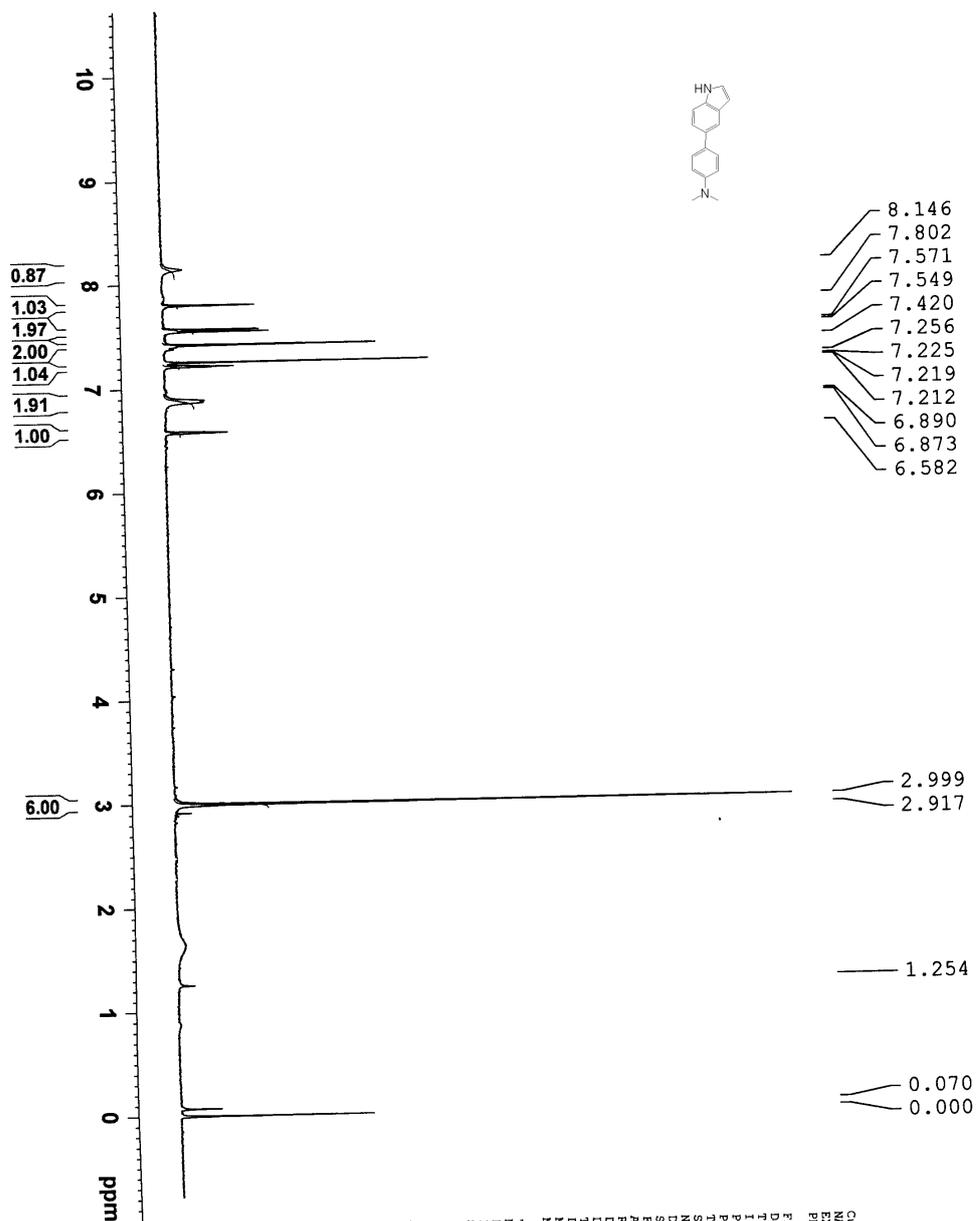
5-(4-aminophenyl)-1H-indole (4e)



5-(4-aminophenyl)-1H-indole (4e)



5-(4-*N,N*-dimethylaminophenyl)-1H-indole (4f)



```

Current Data Parameters
NAME      L14Jb
EXPNO     228
PROCNO    1

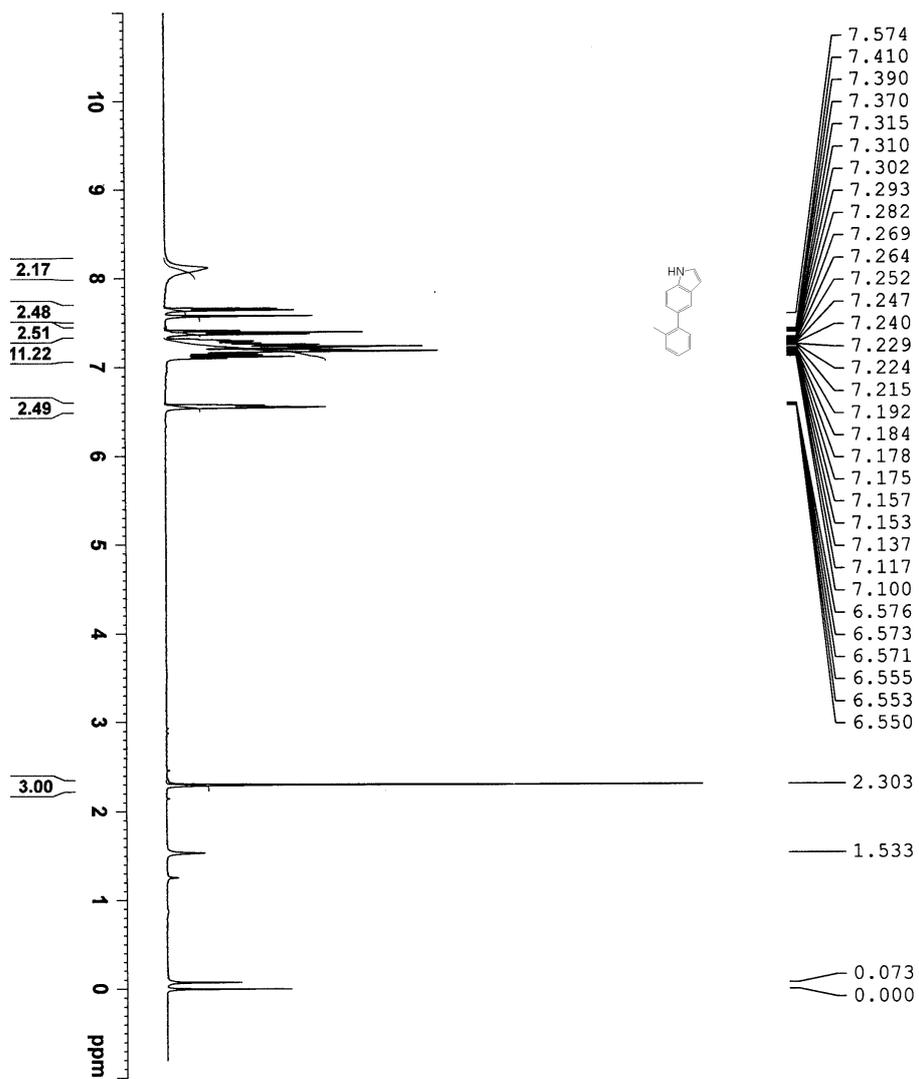
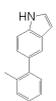
F2 - Acquisition Parameters
Date_     20091106
Time      11:23
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         2
DS         2
SWH        5630.631 Hz
FIDRES     0.085917 Hz
AQ         5.8159468 sec
RG         88.600 usec
DE         6.00 usec
TE         294.3 K
D1         1.00000000 sec
MCNST     0.10500000 sec
HOMR      0.01500000 sec

===== CHANNEL f1 =====
NUC1      13C
P1        8.70 usec
PL1       -3.00 dB
SFO1     400.1325123 MHz

F2 - Processing parameters
SI        32768
SF        400.1300998 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

1jfb2

5-(2-Methylphenyl)-1H-indole (4g) <sup>7</sup>



1j63

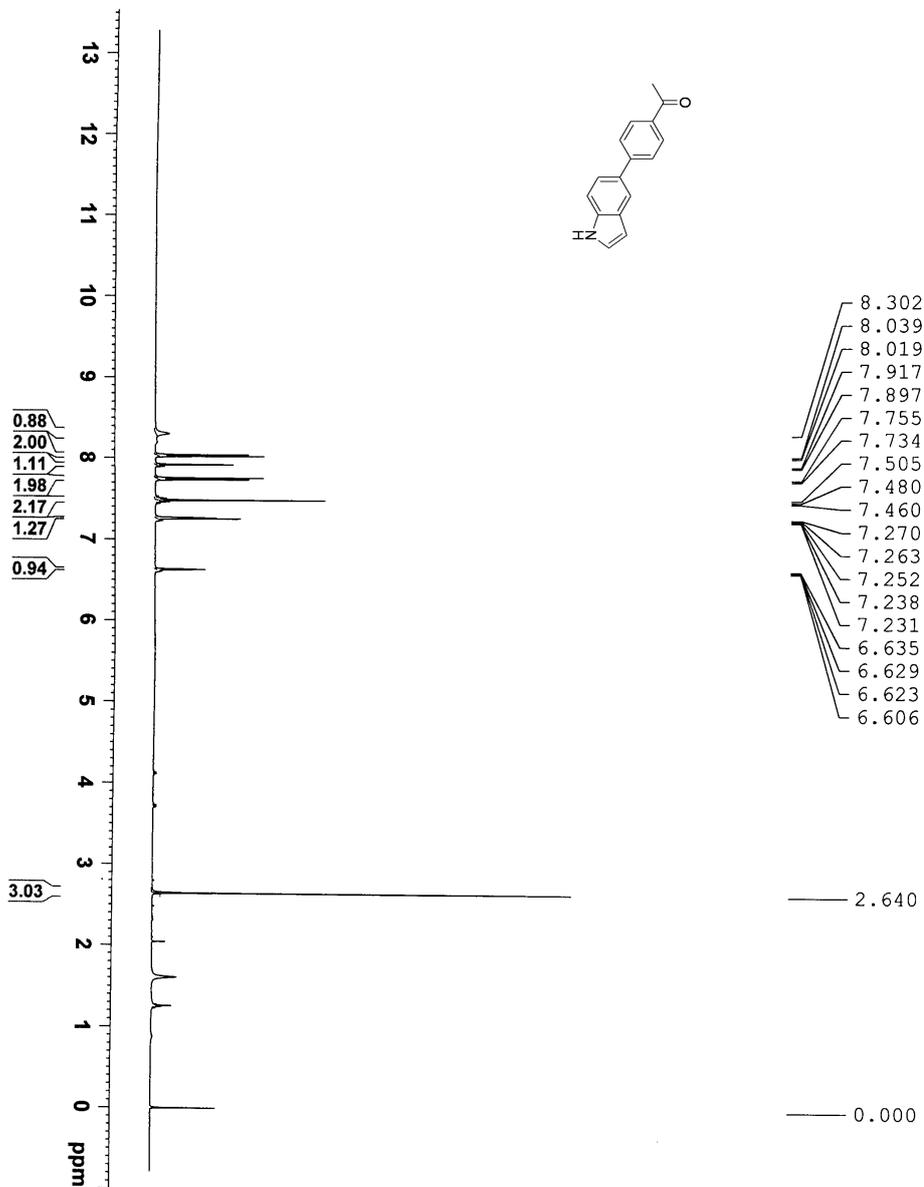
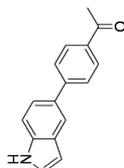
Current Data Parameters  
 NAME: L1ub  
 EXPNO: 229  
 PROCNO: 1

F2 - Acquisition Parameters  
 Date\_: 20091106  
 Time: 12.00  
 INSTRUM: av400  
 PROBHD: 5 mm BBO BB-1H  
 PULPROG: zgpg30  
 SOLVENT: CDCl3  
 NS: 8  
 DS: 2  
 SWH: 5630.637 Hz  
 FIDRES: 0.1085917 Hz  
 AQ: 5.8196468 sec  
 RG: 643.1  
 DE: 8.000000 usec  
 TE: 294.7 K  
 D1: 1.0000000 sec  
 KICK: 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1: 13C  
 P1: 8.70 usec  
 PL1: -3.00 dB  
 SFO1: 400.1325123 MHz

F2 - Processing parameters  
 SI: 32768  
 SF: 400.1300213 MHz  
 DS: 4  
 SSB: 0  
 LB: 0.30 Hz  
 GB: 0  
 PC: 1.00

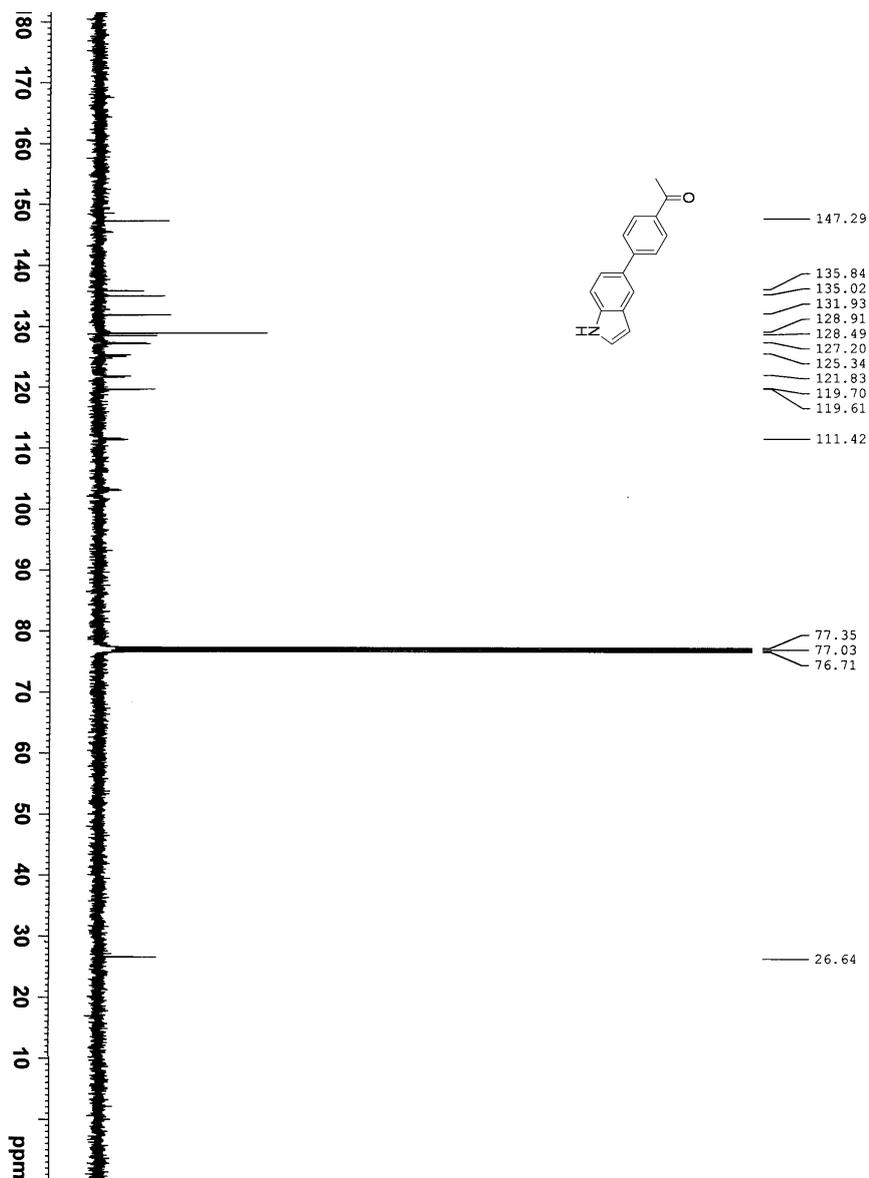
### 5-(4-Acetylphenyl)-1H-indole (4h)



```

Current Data Parameters
NAME      4h
EXPNO    133
PROCNO   1
F2 - Acquisition Parameters
Date_     20090909
Time      9.08
INSTRUM   av400
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         4
SWH        5630.611 Hz
FIDRES     0.085917 Hz
AQ          5.8196468 sec
RG          32768
AQ          1290.72 usec
DE          6.00 usec
TE          298.9 K
D1          1.0000000 sec
DELTA      0.0150000 sec
MCWPRG    0.0150000 sec
===== CHANNEL f1 =====
NUC1       13C
P1         8.19 usec
PL1        -3.00 dB
SFO1       400.1325123 MHz
F2 - Processing parameters
SI         32768
SF         400.1300117 MHz
WDW        EM
SSB        0
GB         0
PC         1.00
  
```

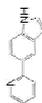
### 5-(4-Acetylphenyl)-1H-indole (4h)



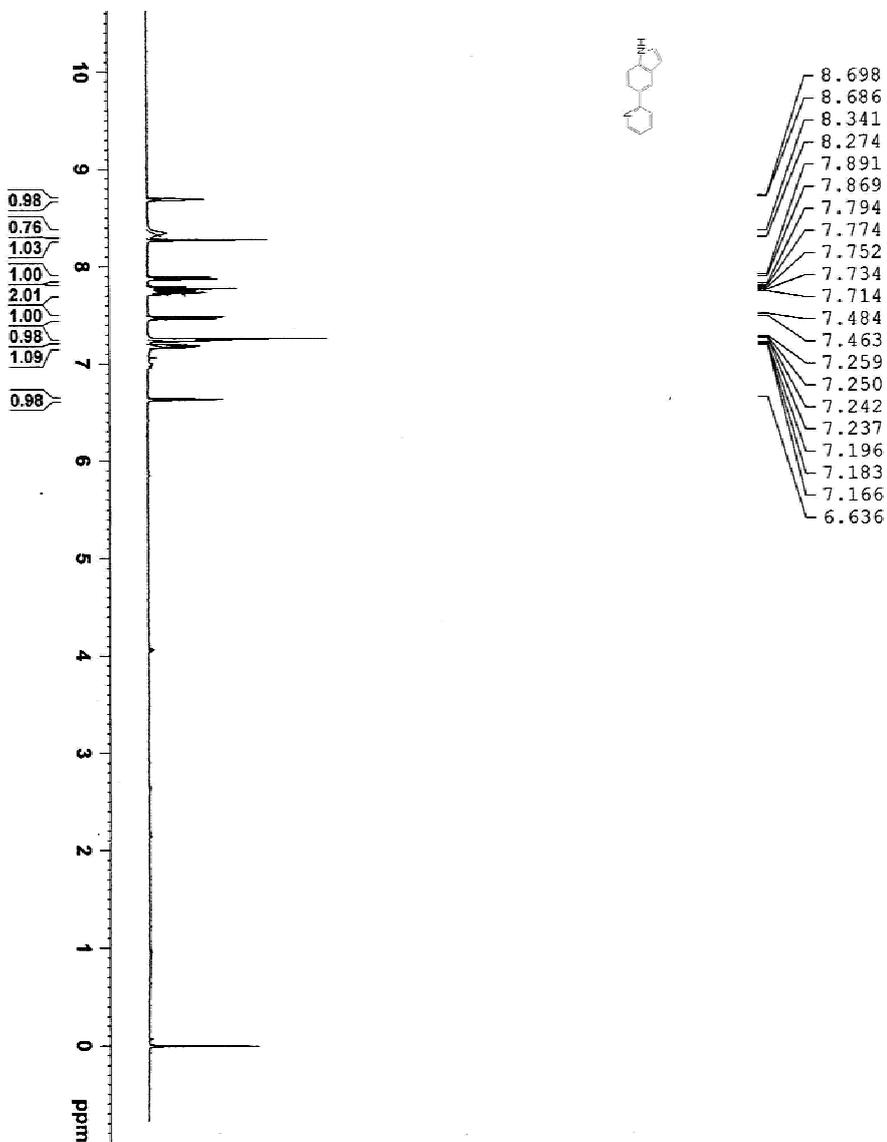
```

Current Data Parameters
NAME          1h13
EXPNO        1194
PROCNO       1
-----
F2 - Acquisition Parameters
Date_        20090714
Time         9.53
INSTRUM     aw400
PROBHD      5 mm BBO BB-1H
PULPROG     zgpg30
TD           65536
SOLVENT     CDCl3
NS           625
DS           4
SWH          23980.814 Hz
FIDRES      0.365918 Hz
AQ           1.3664756 sec
RG           6502
AQ           20.850 usec
DE           29.0 K
TE           2.00000000 sec
d11          0.03000000 sec
MCREST      0.00000000 sec
MCWRR       0.01500000 sec
-----
===== CHANNEL f1 =====
NUC1         13C
P1           8.50 usec
PL1         -2.00 dB
SFO1        100.6282298 MHz
===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2         1H
P2           80.00 usec
PL2         0.00 dB
SFO2        400.1316005 MHz
-----
F2 - Processing parameters
SI           32768
SF           100.6127690 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

5-(pyridin-2-yl)-1H-indole (4i)



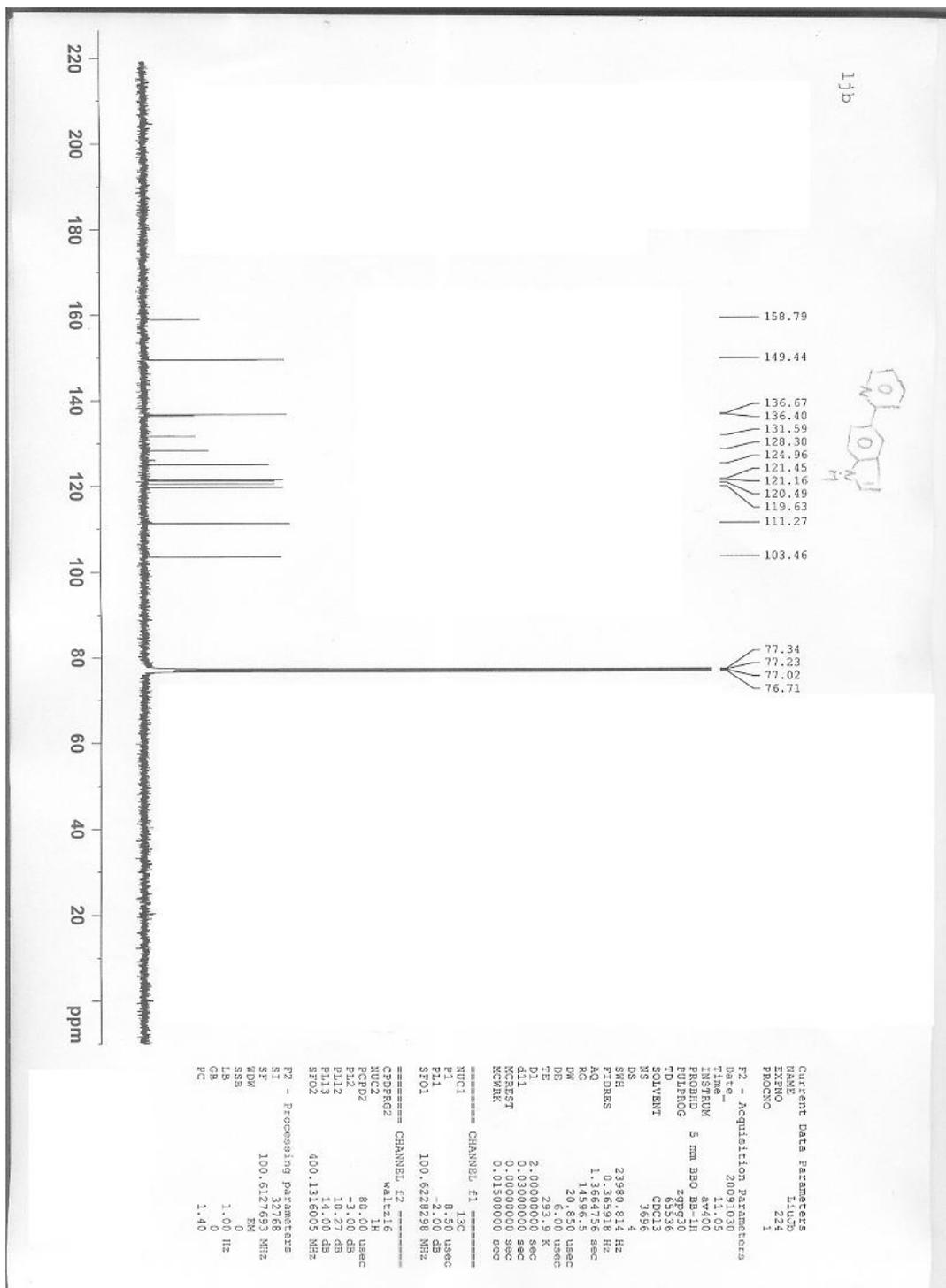
1.jb



- 8.698
- 8.686
- 8.341
- 8.274
- 7.891
- 7.869
- 7.794
- 7.774
- 7.752
- 7.734
- 7.714
- 7.484
- 7.463
- 7.259
- 7.250
- 7.242
- 7.237
- 7.196
- 7.183
- 7.166
- 6.636

CHANNEL: F1  
 P1 4.70 usec  
 P2 1.00 usec  
 SFO1 400.325123 MHz  
 P2 - Processing parameters  
 S 32768  
 SF 400.300091 MHz  
 WDM EN  
 USB 0.30 Hz  
 CB 0  
 PC 1.00  
 Acquisition Parameters  
 Date\_ 20090909  
 Time 9.00  
 INSTRUM av400  
 PULPROG zgpg30  
 PROCNO 5  
 F2 - Acquisition Parameters  
 Date\_ 20090909  
 Time 9.00  
 INSTRUM 5 mm BBO BB5-1H  
 PULPROG zgpg30  
 PROCNO 65536  
 TD 65536  
 SFO1 400.13  
 SOLVENT CDCl3  
 DS 2  
 DE 2.00  
 NS 2  
 SFO1 5130.631 Hz  
 SWH 0.065917 Hz  
 FIDRES 5.912546 sec  
 AQ 0.025466 sec  
 RG 88.800 usec  
 DW 88.800 usec  
 DE 6.00 usec  
 TE 300.2 K  
 DI 1.00000000 sec  
 MEASUREMENT 0.07000000 sec  
 MEMORY 0.01500000 sec

5-(pyridin-2-yl)-1H-indole (4i)



### 5-(thiophen-2-yl)-1H-indole (4j)

