# Development of a Two-step Route to 3-PBC and βCCt, Two Agents Active Against Alcohol Self-Administration in Rodent and Primate Models

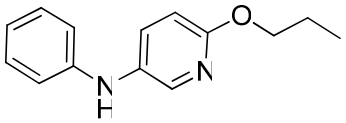
Ojas A. Namjoshi, Agnieszka Grzybkowska, German O. Fonseca, Michael L. Van Linn, Zh-jian Wang, Jeffrey R. Deschamps,[b] James M. Cook[a,]*

[a] *Department of Chemistry and Biochemistry, University of Wisconsin-Milwaukee, Milwaukee, WI 53211*
[b] *Laboratory for the Structure of Matter, Code 6030, Naval Research Laboratory, 4555 Overlook Avenue SW, Washington, DC*

## Supporting Information

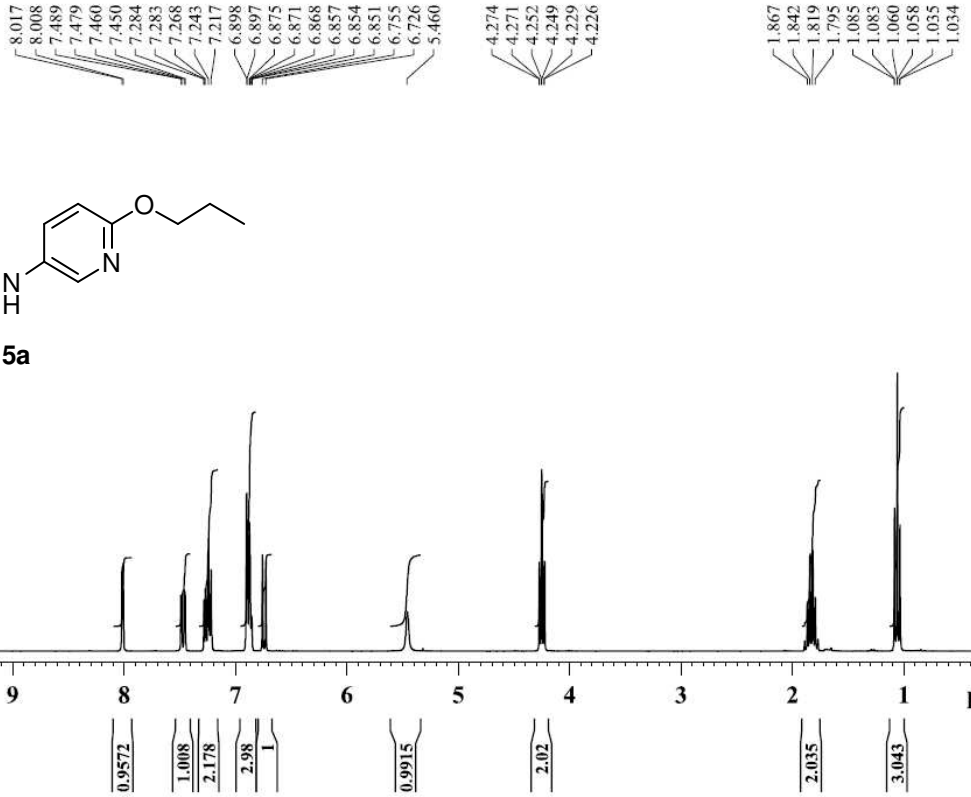
## Contents:

Copies of NMR spectra of intermediates and target compounds S2-S57
*N*-phenyl-6-propoxypyridin-3-amine (5a) S2
*N*-(2-chlorophenyl)-6-propoxypyridin-3-amine (5b) S4
*N*-(2-chlorophenyl)-6-methoxypyridin-3-amine (8a) S6
*N*-(2-chlorophenyl)-6-ethoxypyridin-3-amine (8b) S8
*N*-(2-chlorophenyl)-6-isopropoxypyridin-3-amine (8c) S10
6-butoxy-*N*-(2-chlorophenyl)pyridin-3-amine (8d) S12
*N*-(2-chlorophenyl)-6-isobutoxypyridin-3-amine (8e) S14
6-(*tert*-butoxy)-*N*-(2-chlorophenyl)pyridin-3-amine (8f) S16
6-(benzyloxy)-*N*-(2-chlorophenyl)pyridin-3-amine (8g) S18
*tert*-butyl 5-[(2-chlorophenyl)amino]picolinate (12) S20
3-propoxy-9*H*-pyrido[3,4-*b*]indole (1) S22
2-propoxy-5*H*-pyrido[3,2-*b*]indole (6) S24
3-methoxy-9*H*-pyrido[3,4-*b*]indole (9a) S26
2-methoxy-5*H*-pyrido[3,2-*b*]indole (10a) S28
3-ethoxy-9*H*-pyrido[3,4-*b*]indole (9b) S30
2-ethoxy-5*H*-pyrido[3,2-*b*]indole (10b) S32
3-isopropoxy-9*H*-pyrido[3,4-*b*]indole (9c) S34
2-isopropoxy-5*H*-pyrido[3,2-*b*]indole (10c) S36
3-butoxy-9*H*-pyrido[3,4-*b*]indole (19d) S38
2-butoxy-5*H*-pyrido[3,2-*b*]indole (10d) S40
3-isobutoxy-9*H*-pyrido[3,4-*b*]indole (9e) S42
2-isobutoxy-5*H*-pyrido[3,2-*b*]indole (10e) S44
3-(*tert*-butoxy)-9*H*-pyrido[3,4-*b*]indole (9f) S46
2-(*tert*-butoxy)-5*H*-pyrido[3,2-*b*]indole (10f) S48
3-(benzyloxy)-9*H*-pyrido[3,4-*b*]indole (9g) S50
2-(benzyloxy)-5*H*-pyrido[3,2-*b*]indole (10g) S52
*tert*-butyl 9*H*-pyrido[3,4-*b*]indole-3-carboxylate (2) S54
*tert*-butyl 5*H*-pyrido[3,2-*b*]indole-2-carboxylate (18) S56
X-ray diffraction data for compounds 1 and 6 S58-S73
Figure s1. ORTEP drawing for 1 S59
Figure s2. ORTEP drawing for 6 S59



***N*-phenyl-6-propoxypyridin-3-amine (5a)**

**Proton Spectrum**

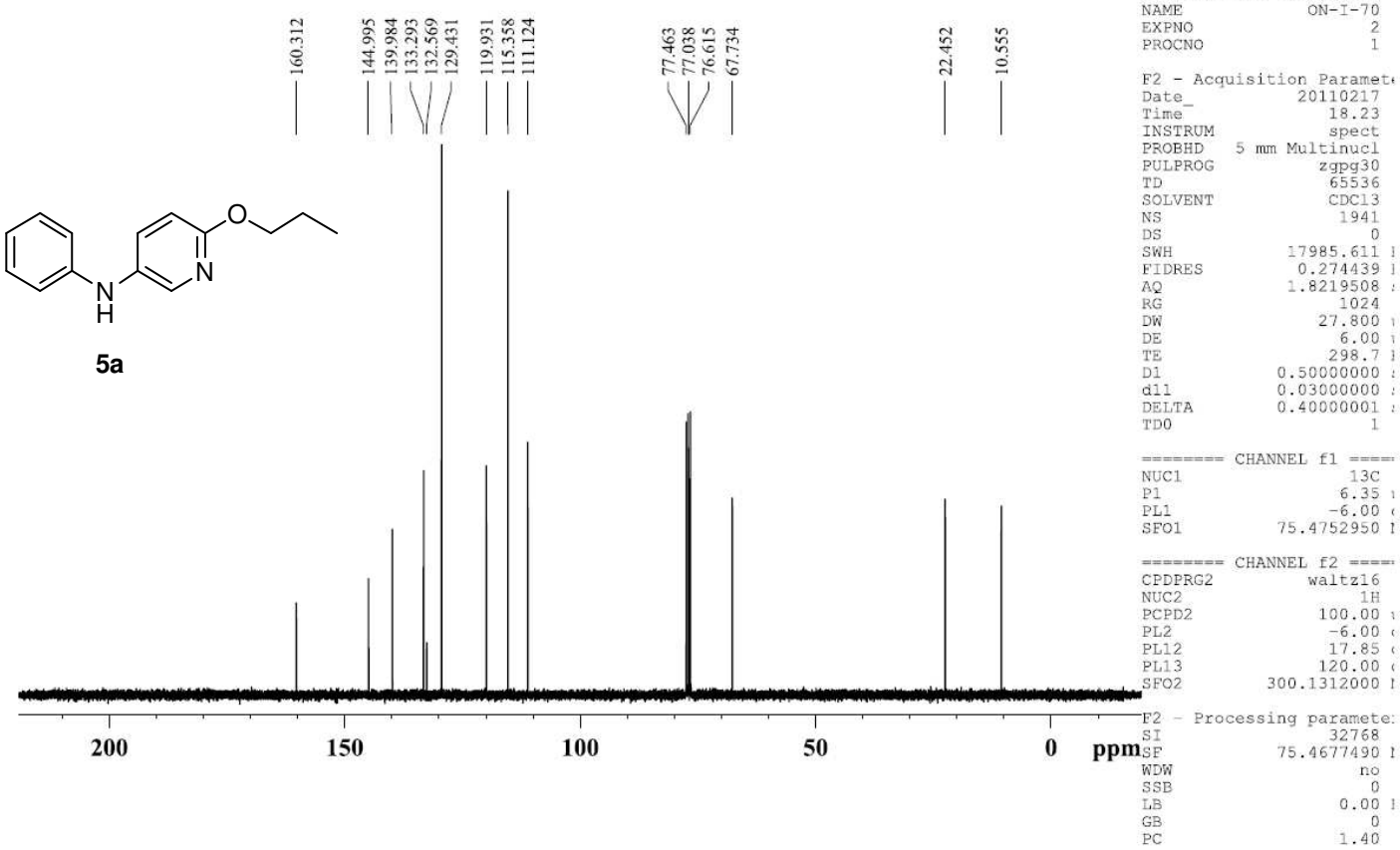





**5a**

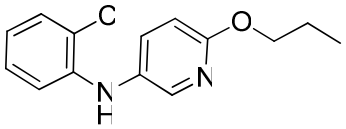
```
Current Data Parameters
NAME                  ON-I-70
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parame
Date_                20110217
Time                    17.06
INSTRUM                 spect
PROBHD    5 mm Multinucl
PULPROG                 zg30
TD                      32768
SOLVENT                 CDCl3
NS                         16
DS                          0
SWH                  6172.839
FIDRES               0.188380
AQ                   2.6542580
RG                       203.2
DW                      81.000
DE                        6.00
TE                       299.0
D1                1.00000000
TD0                         1

======== CHANNEL f1 ===
NUC1                       1H
P1                       9.00
PL1                     -6.00
SFO1             300.1318534

F2 - Processing paramet
SI                      32768
SF               300.1300000
WDW                        no
SSB                         0
LB                       0.00
GB                          0
PC                       1.00
```

**Carbon Spectrum**



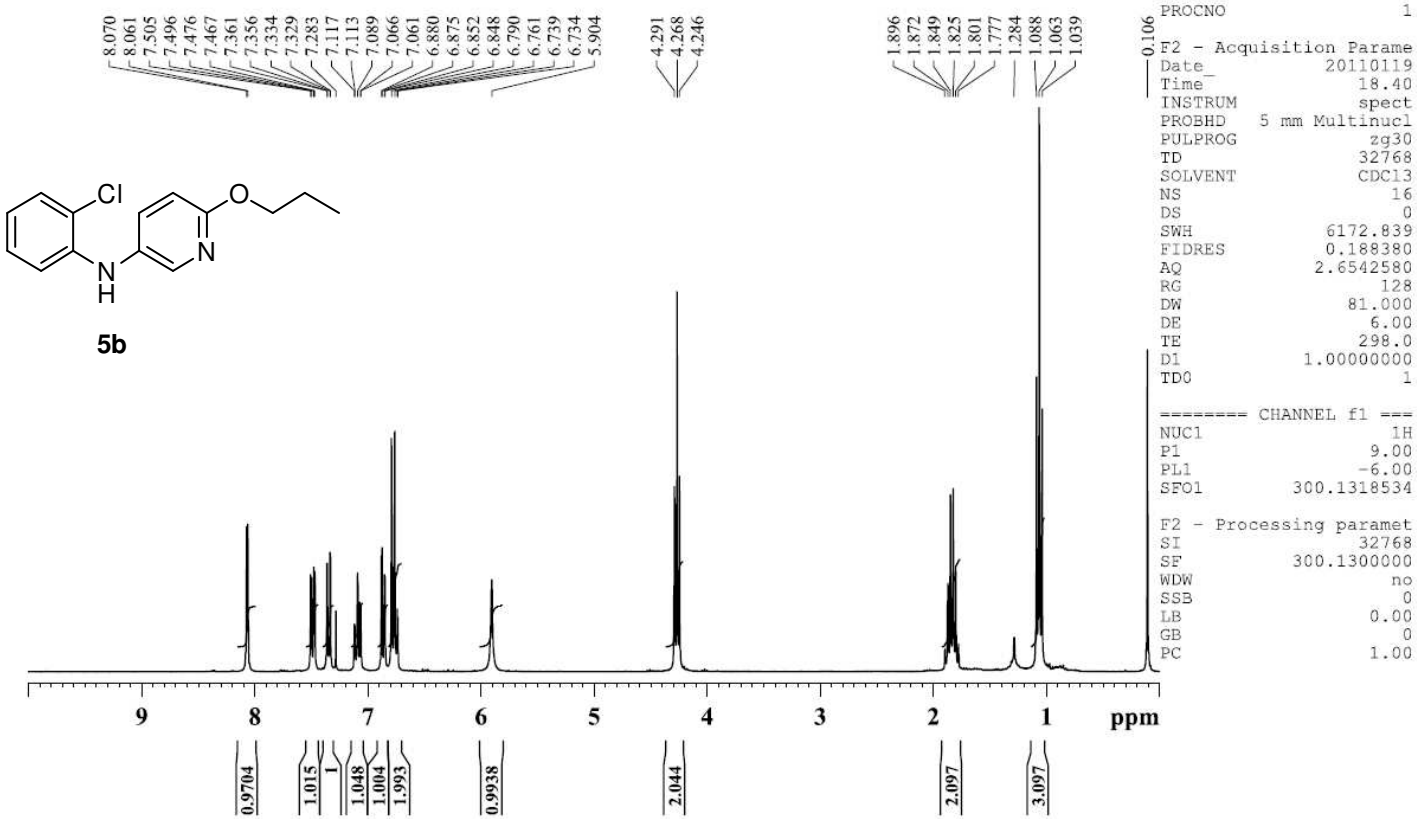

**5a**

```
Current Data Parameters
NAME                  ON-I-70
EXPNO                       2
PROCNO                      1

F2 - Acquisition Paramet
Date_                20110217
Time                    18.23
INSTRUM                 spect
PROBHD    5 mm Multinucl
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1941
DS                          0
SWH                 17985.611
FIDRES              0.274439
AQ                  1.8219508
RG                       1024
DW                     27.800
DE                       6.00
TE                      298.7
D1                0.50000000
d11               0.03000000
DELTA             0.40000001
TD0                         1

======== CHANNEL f1 =====
NUC1                      13C
P1                       6.35
PL1                     -6.00
SFO1               75.4752950

======== CHANNEL f2 =====
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  100.00
PL2                     -6.00
PL12                    17.85
PL13                   120.00
SFO2              300.1312000

F2 - Processing paramete
SI                       32768
SF                 75.4677490
WDW                         no
SSB                          0
LB                        0.00
GB                           0
PC                        1.40
```



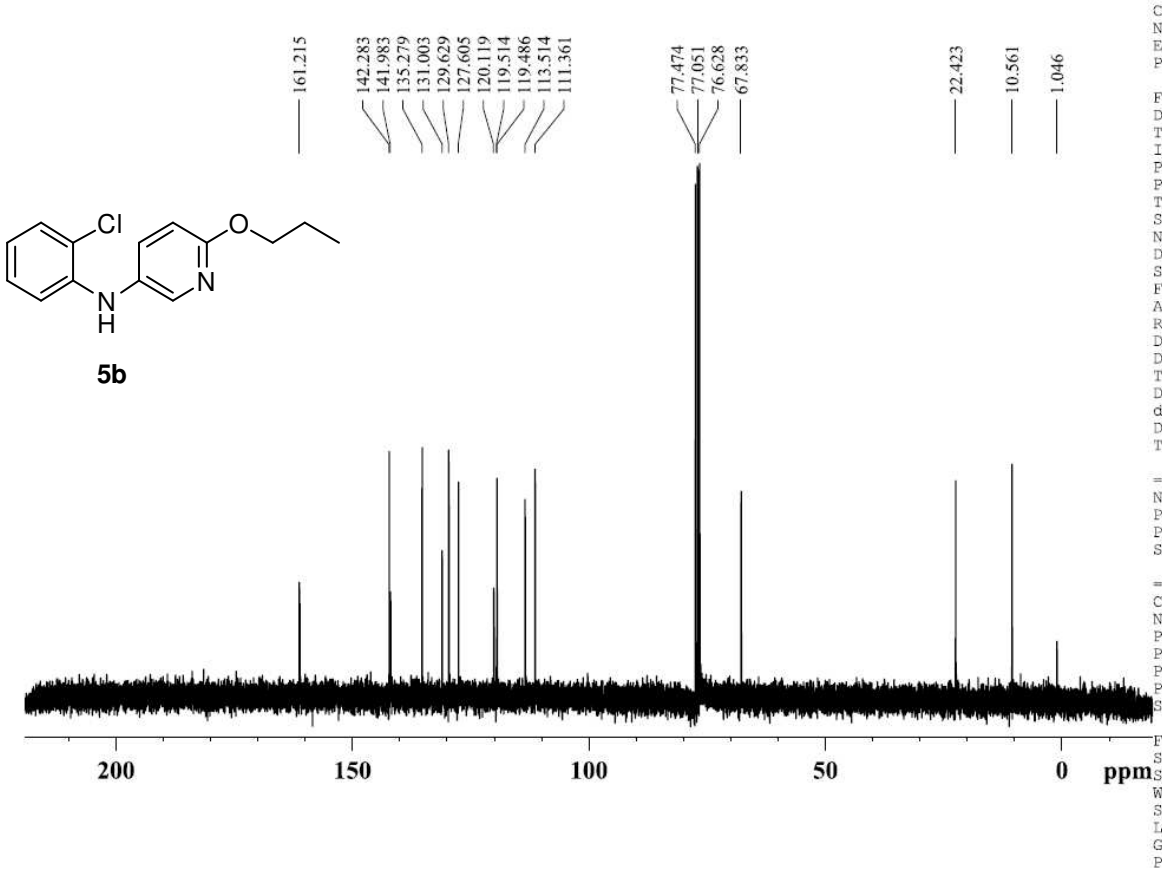

**_N_-(2-chlorophenyl)-6-propoxypyridin-3-amine (5b)**

**Proton Spectrum**



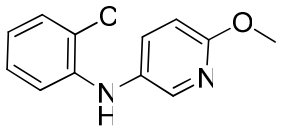

```
Current Data Parameters
NAME                  ON-II-51
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parame
Date_                 20110119
Time_                    18.40
INSTRUM                  spect
PROBHD     5 mm Multinucl
PULPROG                  zg30
TD                       32768
SOLVENT                  CDCl3
NS                          16
DS                           0
SWH                   6172.839
FIDRES                0.188380
AQ                    2.6542580
RG                         128
DW                      81.000
DE                        6.00
TE                       298.0
D1                  1.00000000
TD0                          1

======== CHANNEL f1 ===
NUC1                        1H
P1                        9.00
PL1                      -6.00
SFO1               300.1318534

F2 - Processing paramet
SI                       32768
SF                 300.1300000
WDW                         no
SSB                          0
LB                        0.00
GB                           0
PC                        1.00
```

**Carbon Spectrum**



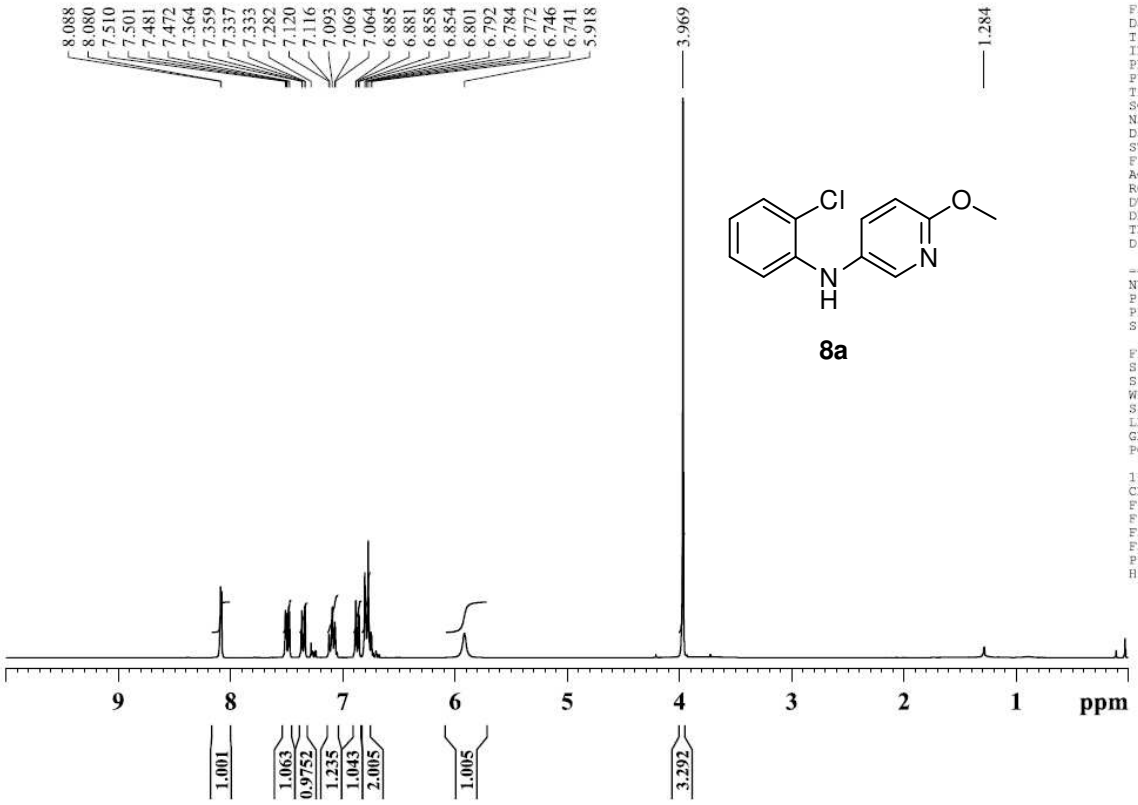

**5b**

```
Current Data Parameters
NAME                  ON-II-51
EXPNO                        2
PROCNO                       1

F2 - Acquisition Paramet
Date_                 20110119
Time                     20.08
INSTRUM                  spect
PROBHD    5 mm Multinucl
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1334
DS                           4
SWH                  17985.611
FIDRES                0.274439
AQ                    1.8219508
RG                        645.1
DW                       27.800
DE                        6.00
TE                       298.0
D1                   2.00000000
d11                  0.03000000
DELTA                1.89999998
TD0                          1

======== CHANNEL f1 =====
NUC1                       13C
P1                        6.35
PL1                      -6.00
SFO1                75.4752950

======== CHANNEL f2 =====
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   100.00
PL2                      -6.00
PL12                     17.85
PL13                     120.00
SFO2                300.1312000

F2 - Processing paramete
SI                        32768
SF                   75.4677490
WDW                         no
SSB                          0
LB                        0.00
GB                           0
PC                        1.40
```

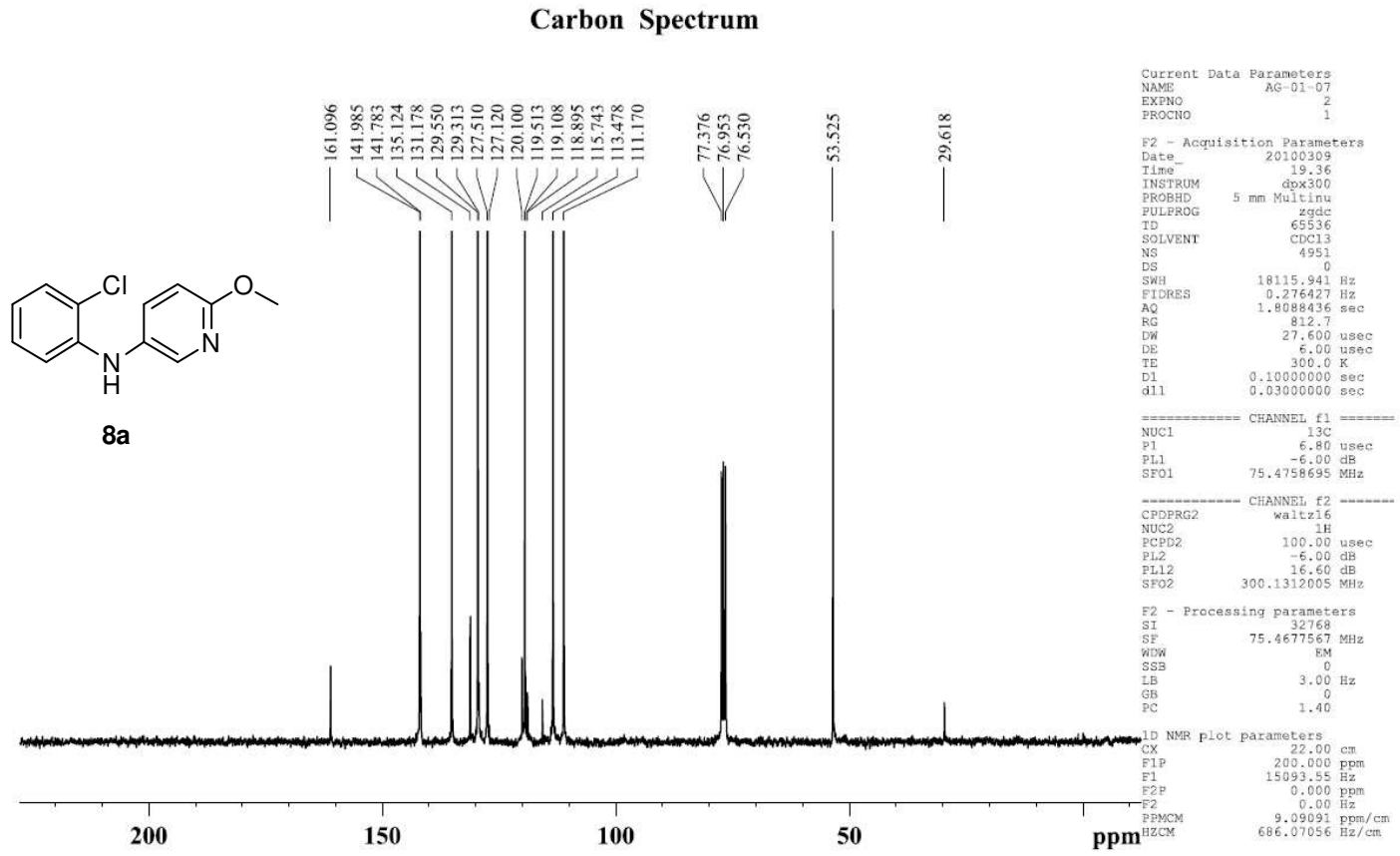


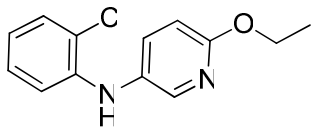
***N*-(2-chlorophenyl)-6-methoxypyridin-3-amine (8a)**

**Proton Spectrum**



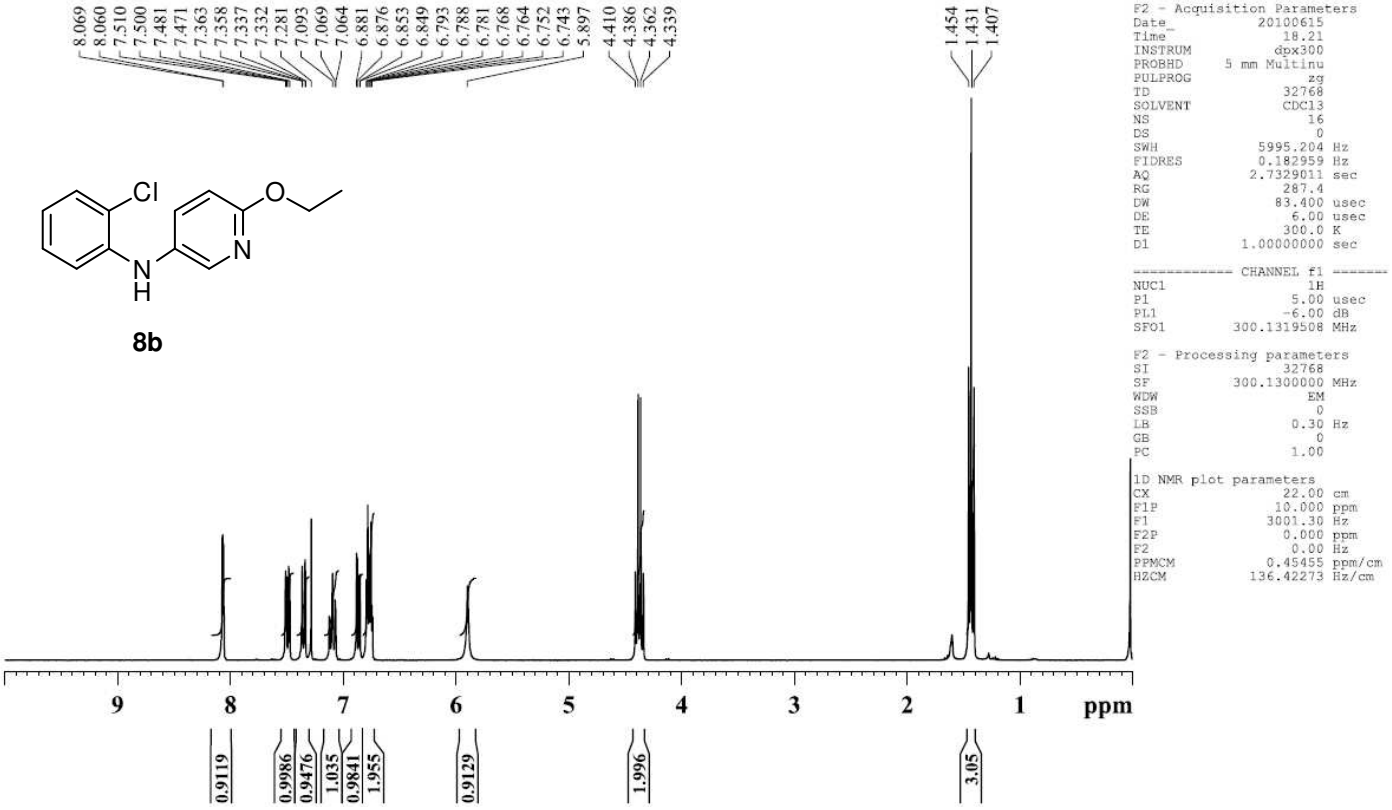

```
Current Data Parameters
NAME                  AG-01-07
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_               20100310
Time                    9.50
INSTRUM                dpx300
PROBHD      5 mm Multinu
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 5995.204 Hz
FIDRES              0.182959 Hz
AQ                  2.7329011 sec
RG                       114
DW                    83.400 usec
DE                     6.00 usec
TE                    300.0 K
D1                  1.00000000 sec

------------ CHANNEL f1 -------
NUC1                      1H
P1                     5.00 usec
PL1                   -6.00 dB
SFO1               300.1319508 MHz

F2 - Processing parameters
SI                     32768
SF                 300.1300000 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     22.00 cm
F1P                   10.000 ppm
F1                  3001.30 Hz
F2P                    0.000 ppm
F2                     0.00 Hz
PPMCM                 0.45455 ppm/cm
HZCM                136.42273 Hz/cm
```


Carbon Spectrum
161.096
141.985
141.783
135.124
131.178
129.550
129.313
127.510
127.120
120.100
119.513
119.108
118.895
115.743
113.478
111.170
77.376
76.953
76.530
53.525
29.618
Cl
O
N
N
H
8a
200
150
100
50
ppm
Current Data Parameters
NAME AG-01-07
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100309
Time 19.36
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 4951
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 812.7
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 200.000 ppm
F1 15093.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 9.09091 ppm/cm
HZCM 686.07056 Hz/cm

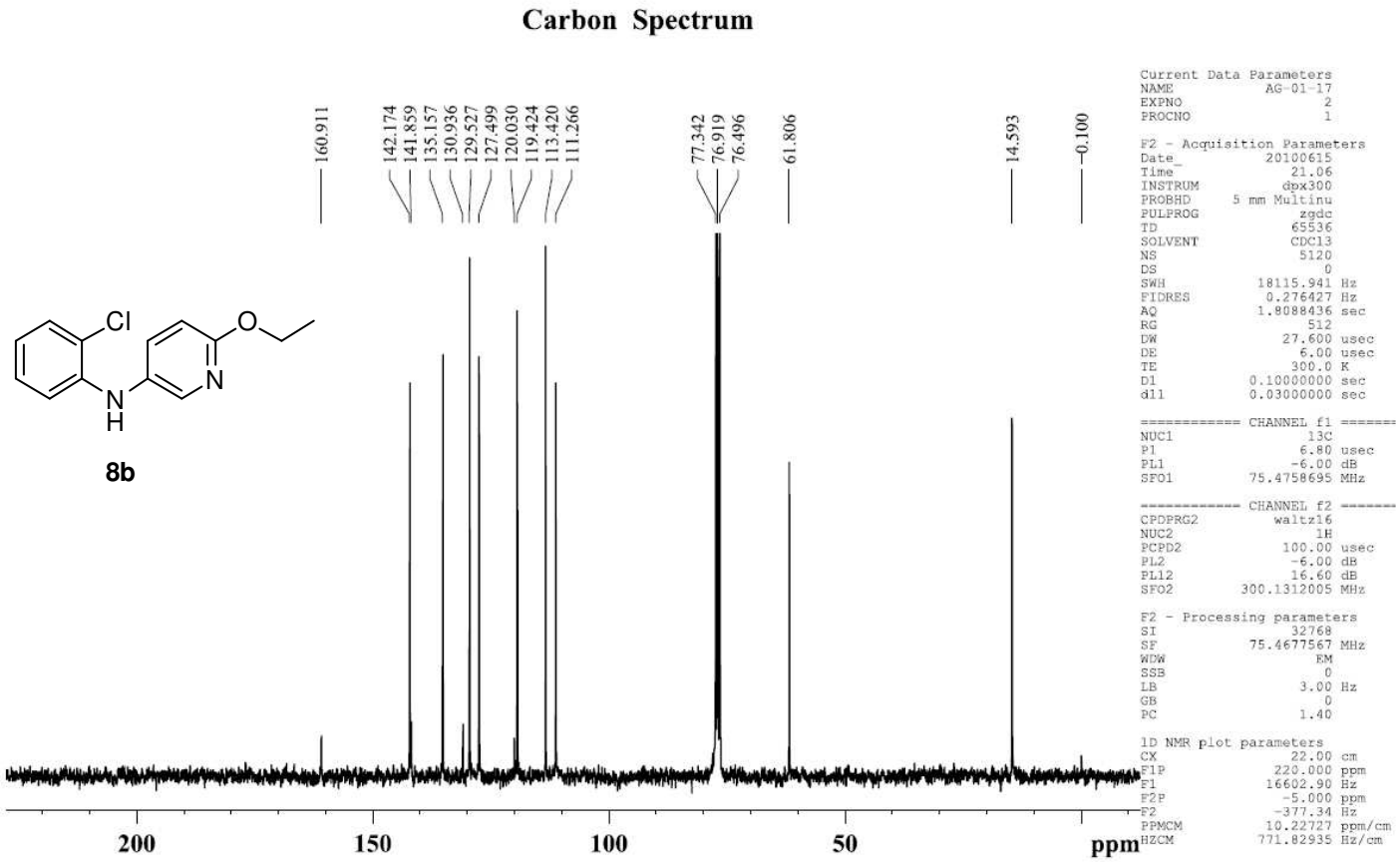


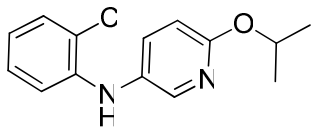
***N*-(2-chlorophenyl)-6-ethoxypyridin-3-amine (8b)**

**Proton Spectrum**



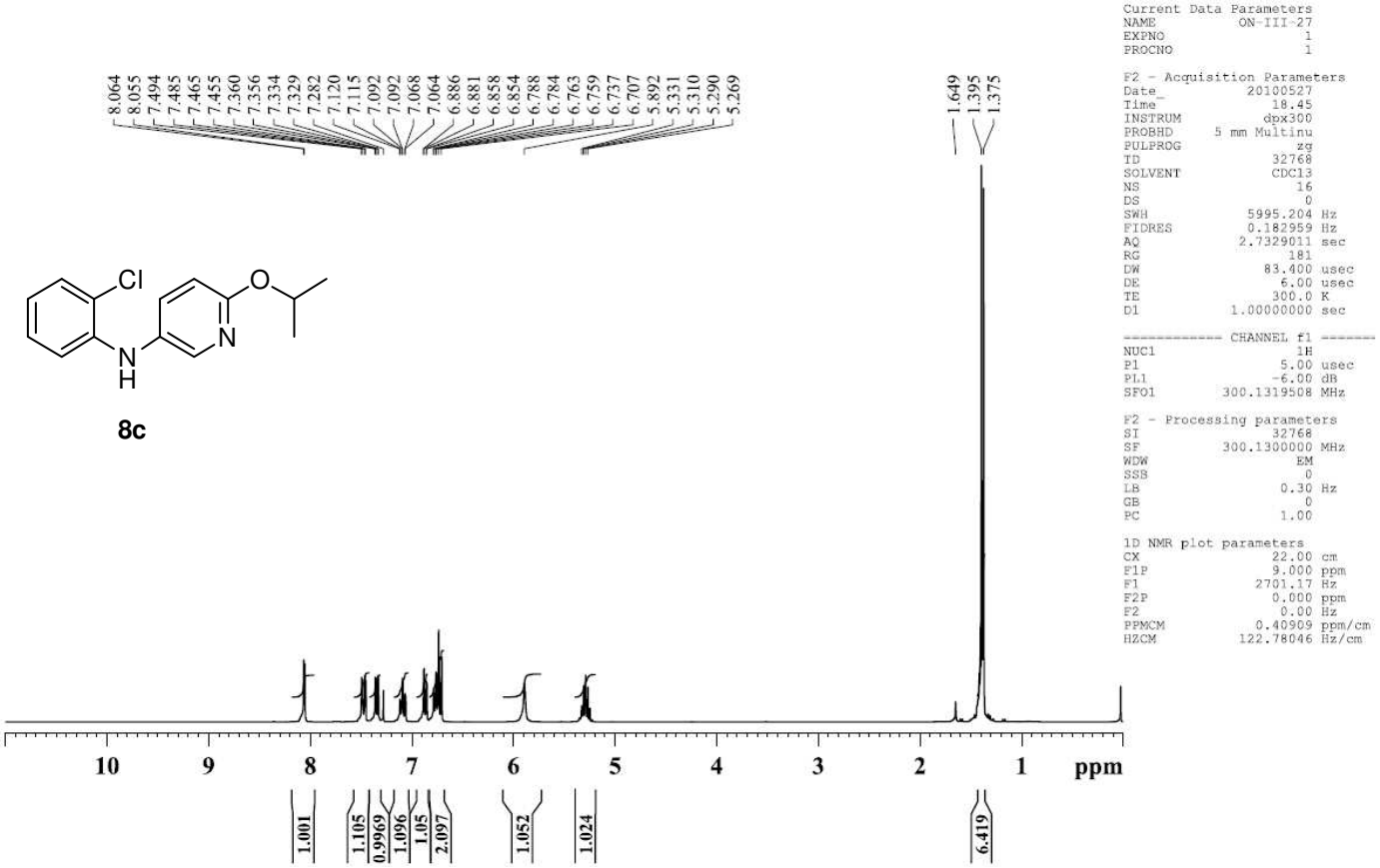

```
Current Data Parameters
NAME                  AG-01-17
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20100615
Time                   18.21
INSTRUM                dpx300
PROBHD     5 mm Multinu
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                5995.204 Hz
FIDRES             0.182959 Hz
AQ                 2.7329011 sec
RG                     287.4
DW                    83.400 usec
DE                     6.00 usec
TE                    300.0 K
D1                 1.00000000 sec

------------ CHANNEL f1 -------
NUC1                       1H
P1                       5.00 usec
PL1                     -6.00 dB
SFO1              300.1319508 MHz

F2 - Processing parameters
SI                     32768
SF                300.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     22.00 cm
F1P                   10.000 ppm
F1                  3001.30 Hz
F2P                    0.000 ppm
F2                     0.00 Hz
PPMCM                0.45455 ppm/cm
HZCM               136.42273 Hz/cm
```


Carbon Spectrum
160.911
142.174
141.859
135.157
130.936
129.527
127.499
120.030
119.424
113.420
111.266
77.342
76.919
76.496
61.806
14.593
-0.100
Cl
O
N
N
H
8b
200
150
100
50
ppm
Current Data Parameters
NAME AG-01-17
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100615
Time 21.06
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 5120
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 512
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
========== CHANNEL f1 =======
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
========== CHANNEL f2 =======
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm

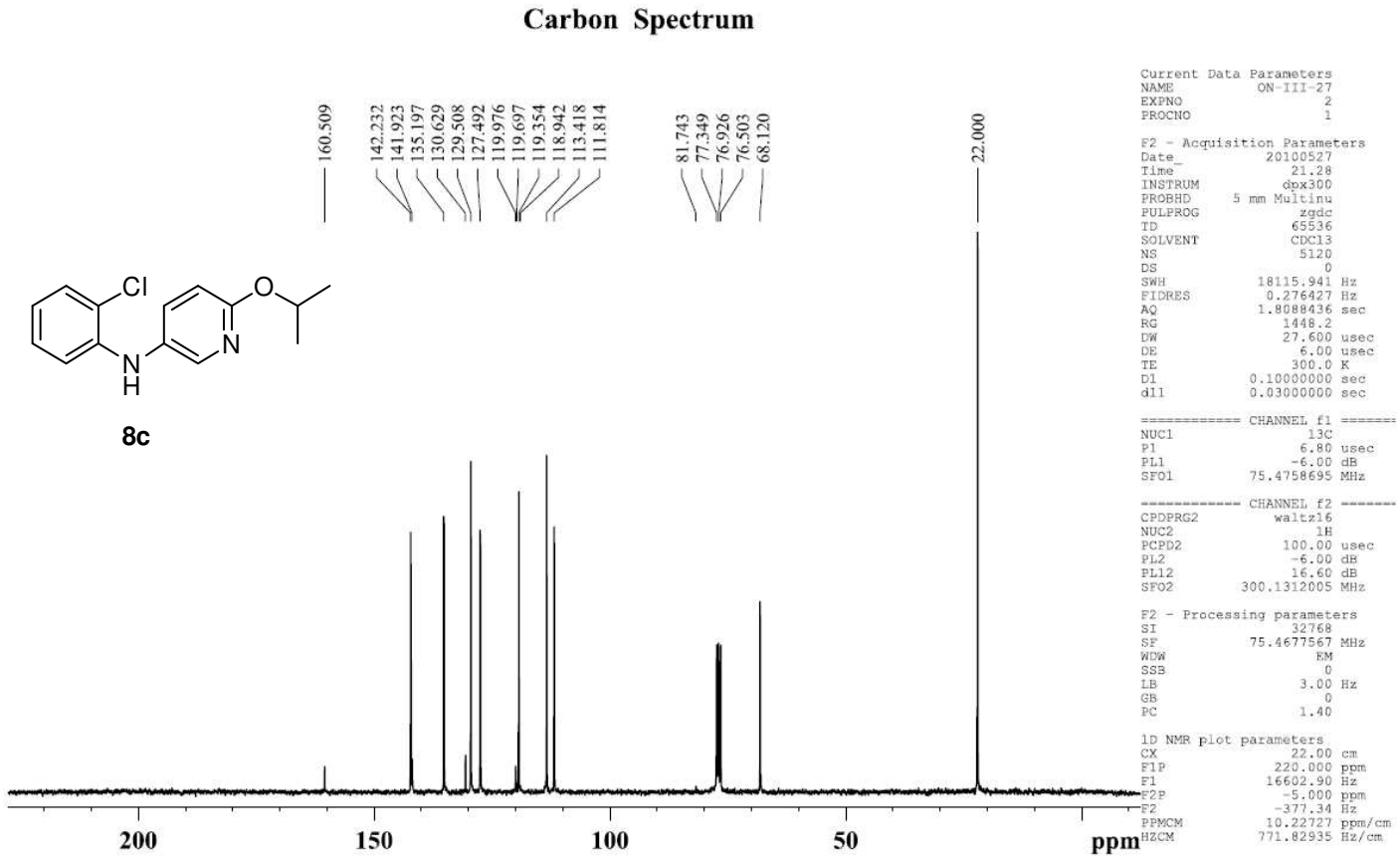


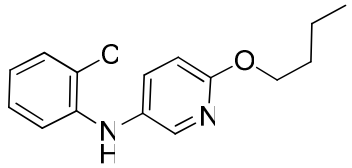
***N*-(2-chlorophenyl)-6-isopropoxypyridin-3-amine (8c)**

**Proton Spectrum**



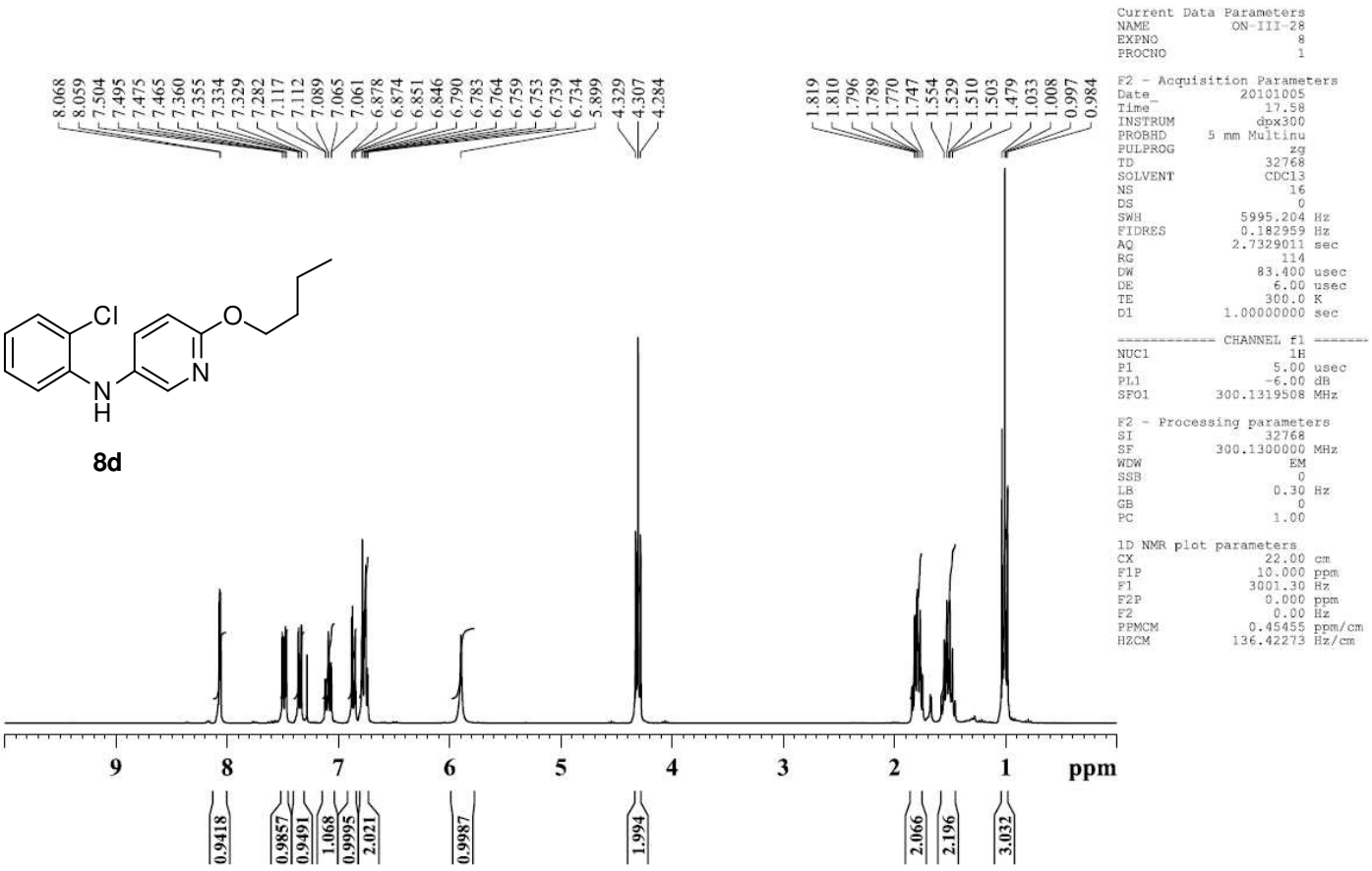

```
Current Data Parameters
NAME            ON-III-27
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100527
Time                18.45
INSTRUM           dpx300
PROBHD     5 mm Multinu
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      0
SWH              5995.204 Hz
FIDRES           0.182959 Hz
AQ               2.7329011 sec
RG                    181
DW                 83.400 usec
DE                  6.00 usec
TE                 300.0 K
D1              1.00000000 sec

------------ CHANNEL f1 -------
NUC1                   1H
P1                  5.00 usec
PL1                -6.00 dB
SFO1         300.1319508 MHz

F2 - Processing parameters
SI                  32768
SF           300.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  22.00 cm
F1P                 9.000 ppm
F1                2701.17 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM            0.40909 ppm/cm
HZCM           122.78046 Hz/cm
```


Carbon Spectrum
160.509
142.232
141.923
135.197
130.629
129.508
127.492
119.976
119.697
119.354
118.942
113.418
111.814
81.743
77.349
76.926
76.503
68.120
22.000
Cl
O
N
N
H
8c
200
150
100
50
ppm
Current Data Parameters
NAME ON-III-27
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100527
Time 21.28
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 5120
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 1448.2
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm

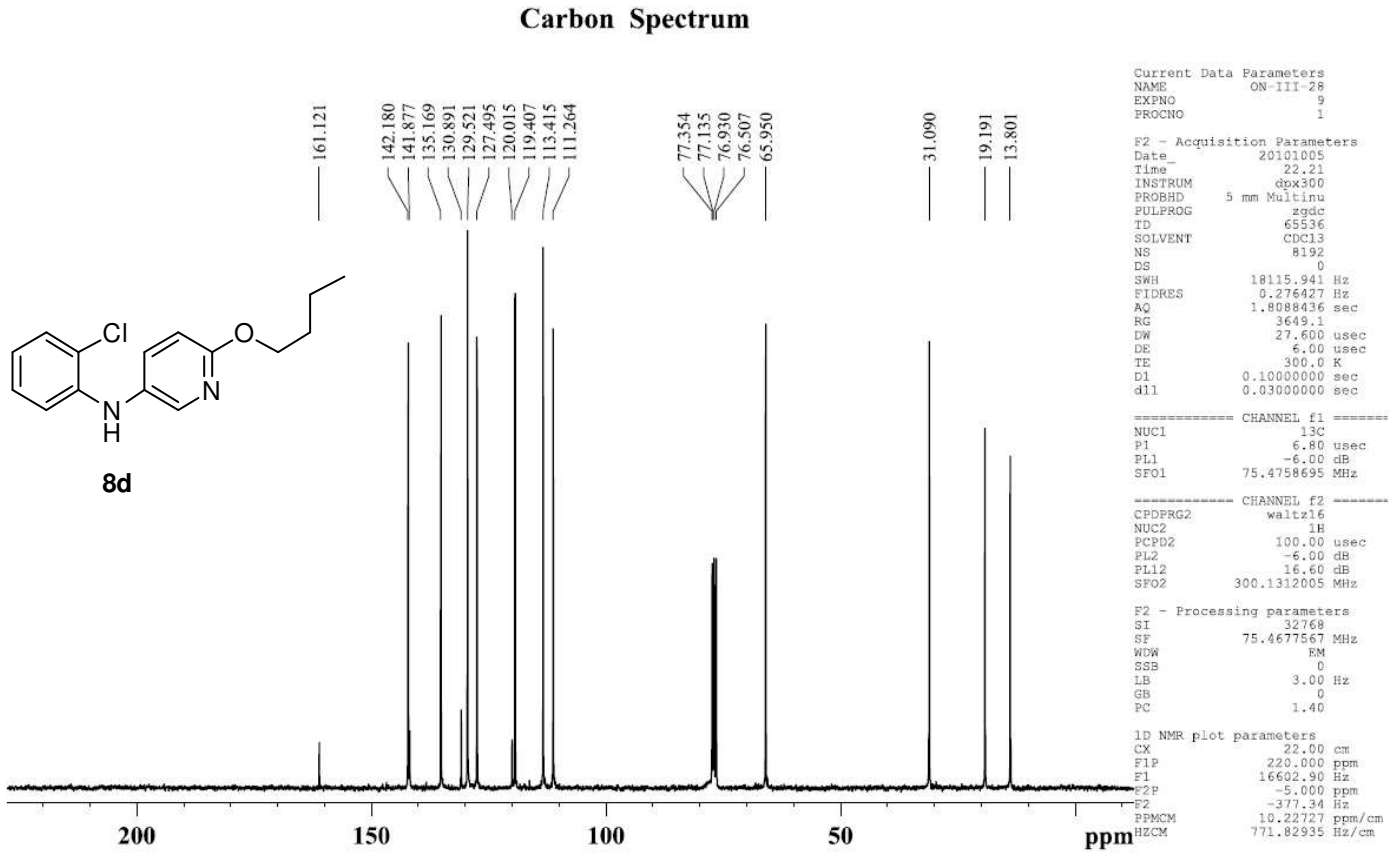


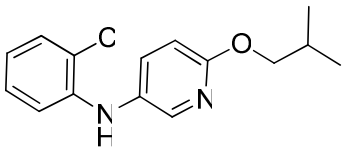

**6-butoxy-*N*-(2-chlorophenyl)pyridin-3-amine (8d)**

**Proton Spectrum**



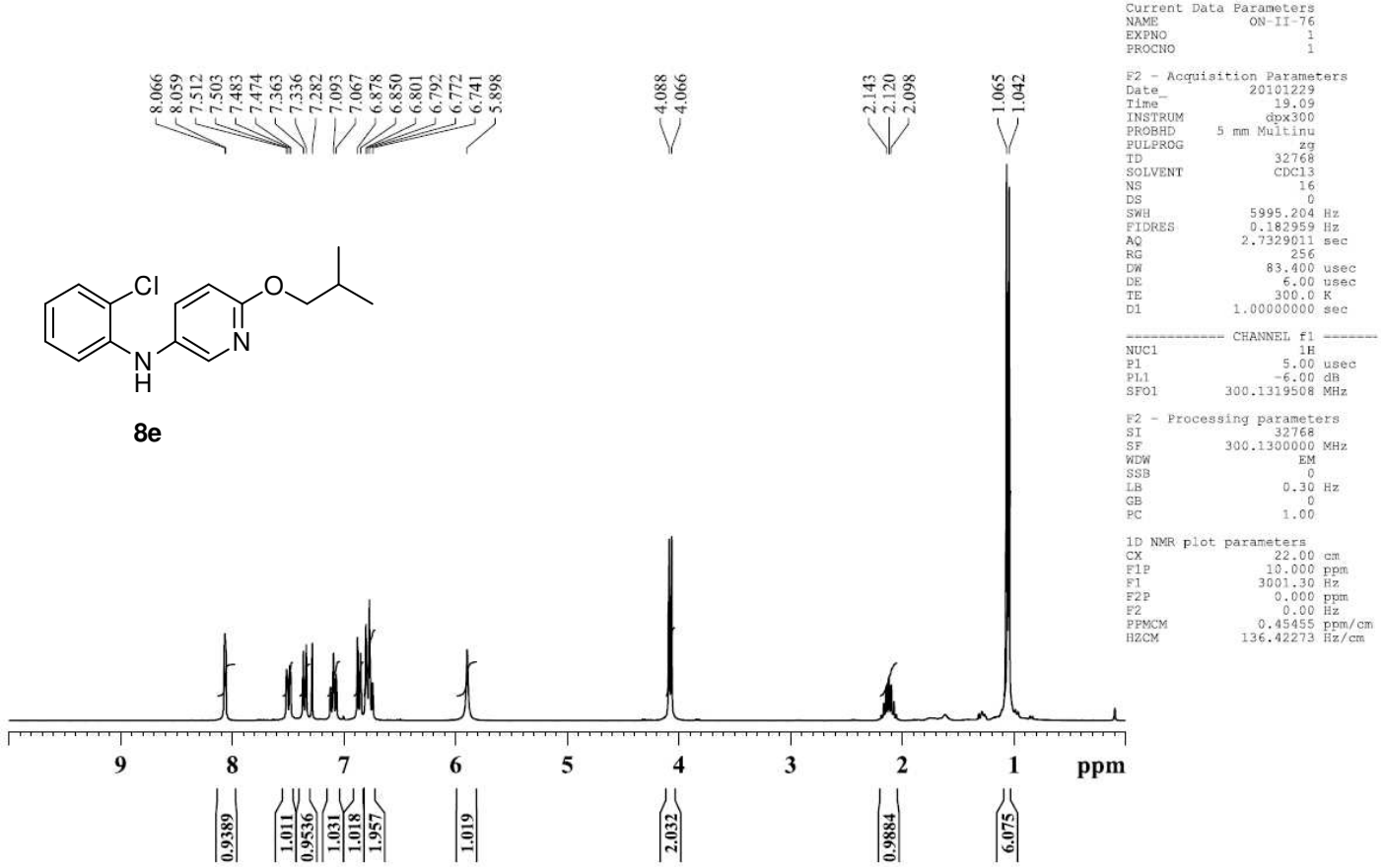

```
Current Data Parameters
NAME                 ON-III-28
EXPNO                        8
PROCNO                       1

F2 - Acquisition Parameters
Date_               20101005
Time                   17.58
INSTRUM                dpx300
PROBHD     5 mm Multinu
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 5995.204 Hz
FIDRES              0.182959 Hz
AQ                  2.7329011 sec
RG                       114
DW                    83.400 usec
DE                     6.00 usec
TE                    300.0 K
D1                 1.00000000 sec

============ CHANNEL f1 =======
NUC1                       1H
P1                      5.00 usec
PL1                    -6.00 dB
SFO1              300.1319508 MHz

F2 - Processing parameters
SI                     32768
SF                300.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     22.00 cm
F1P                    10.000 ppm
F1                   3001.30 Hz
F2P                     0.000 ppm
F2                      0.00 Hz
PPMCM                0.45455 ppm/cm
HZCM               136.42273 Hz/cm
```


Carbon Spectrum
161.121
142.180
141.877
135.169
130.891
129.521
127.495
120.015
119.407
113.415
111.264
77.354
77.135
76.930
76.507
65.950
31.090
19.191
13.801
Cl
O
N
N
H
8d
200
150
100
50
ppm
Current Data Parameters
NAME ON-III-28
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101005
Time 22.21
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 8192
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 3649.1
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm



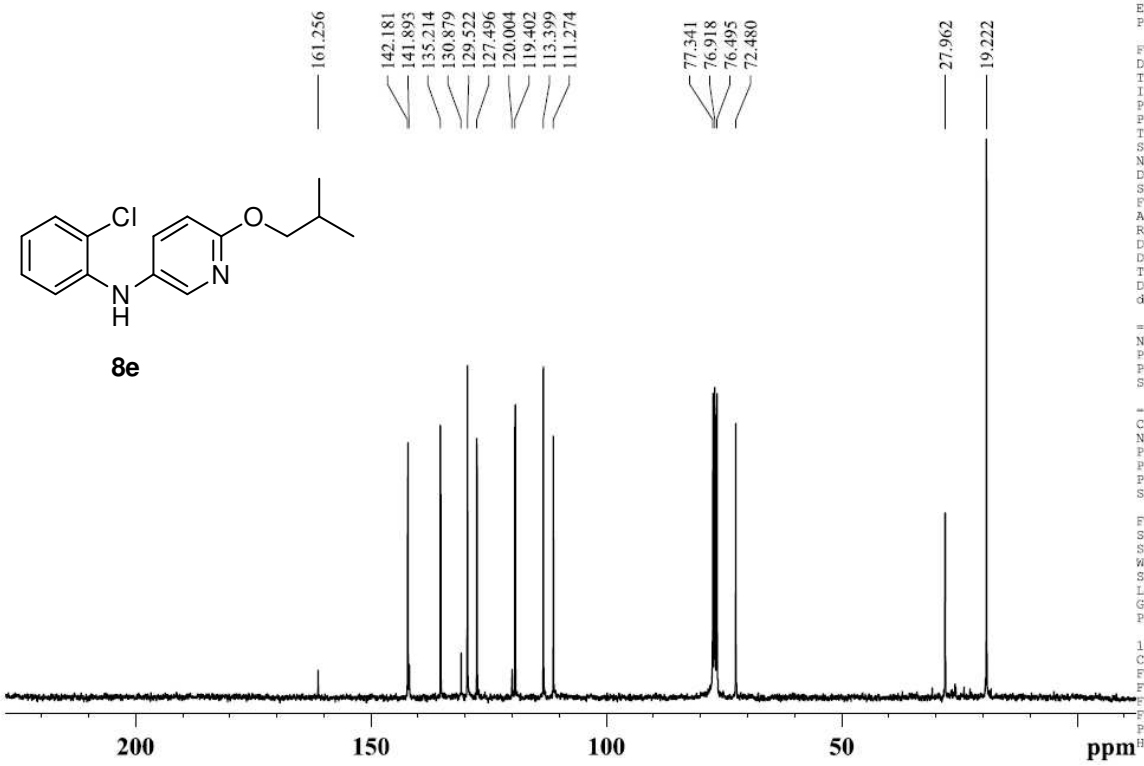

***N*-(2-chlorophenyl)-6-isobutoxypyridin-3-amine (8e)**

**Proton Spectrum**

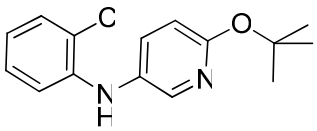



```
Current Data Parameters
NAME                  ON-II-76
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20101229
Time                   19.09
INSTRUM                dpx300
PROBHD     5 mm Multinu
PULPROG                    zg
TD                      32768
SOLVENT                CDCl3
NS                         16
DS                          0
SWH                 5995.204 Hz
FIDRES              0.182959 Hz
AQ                 2.7329011 sec
RG                        256
DW                     83.400 usec
DE                      6.00 usec
TE                     300.0 K
D1                  1.00000000 sec

------------ CHANNEL f1 -------
NUC1                       1H
P1                       5.00 usec
PL1                     -6.00 dB
SFO1              300.1319508 MHz

F2 - Processing parameters
SI                      32768
SF                300.1300000 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                      22.00 cm
F1P                    10.000 ppm
F1                   3001.30 Hz
F2P                     0.000 ppm
F2                      0.00 Hz
PPMCM                0.45455 ppm/cm
HZCM               136.42273 Hz/cm
```

## Carbon Spectrum

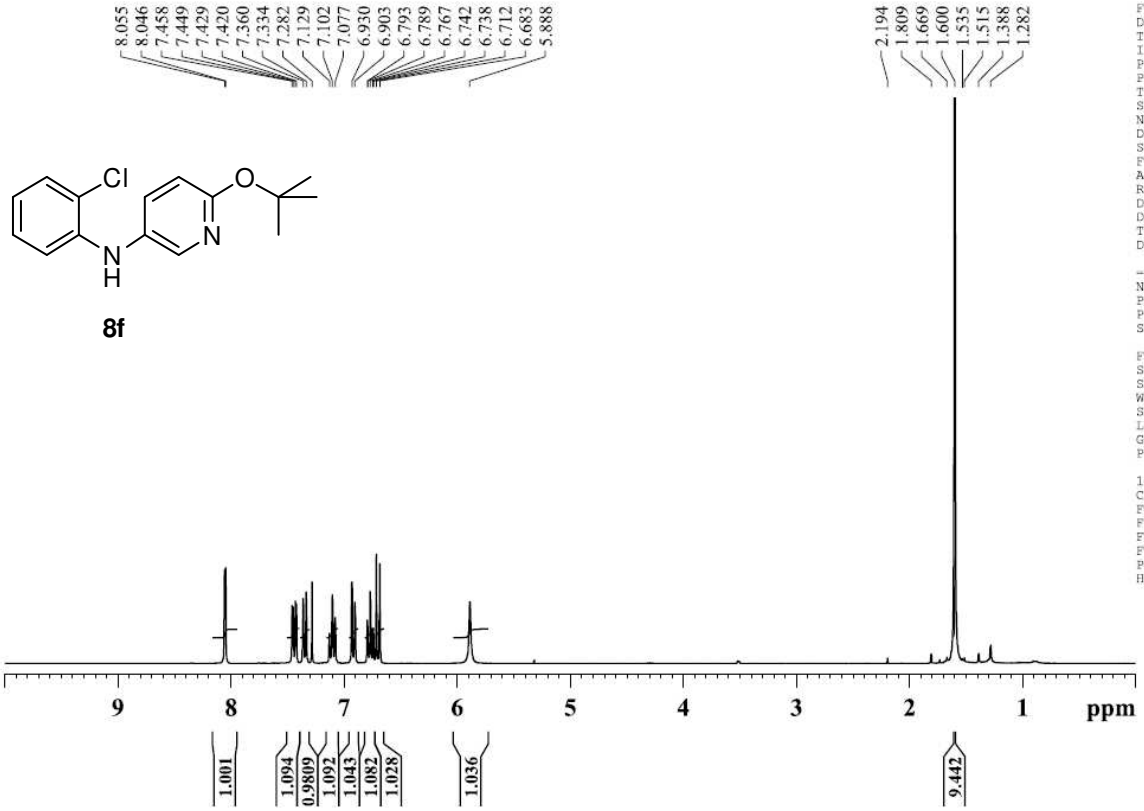



```
Current Data Parameters
NAME                  ON-II-76
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20101230
Time_                  0.37
INSTRUM              dpx300
PROBHD     5 mm Multinu
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                  10240
DS                      0
SWH             18115.941 Hz
FIDRES          0.276427 Hz
AQ              1.8088436 sec
RG                 1448.2
DW                27.600 usec
DE                 6.00 usec
TE                300.0 K
D1             0.10000000 sec
d11            0.03000000 sec

============ CHANNEL f1 =======
NUC1                  13C
P1                  6.80 usec
PL1                -6.00 dB
SFO1           75.4758695 MHz

============ CHANNEL f2 =======
CPDPRG2           waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                -6.00 dB
PL12               16.60 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                   32768
SF             75.4677567 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40

1D NMR plot parameters
CX                   22.00 cm
F1P                 220.000 ppm
F1                16602.90 Hz
F2P                -5.000 ppm
F2                -377.34 Hz
PPMCM             10.22727 ppm/cm
HZCM             771.82935 Hz/cm
```

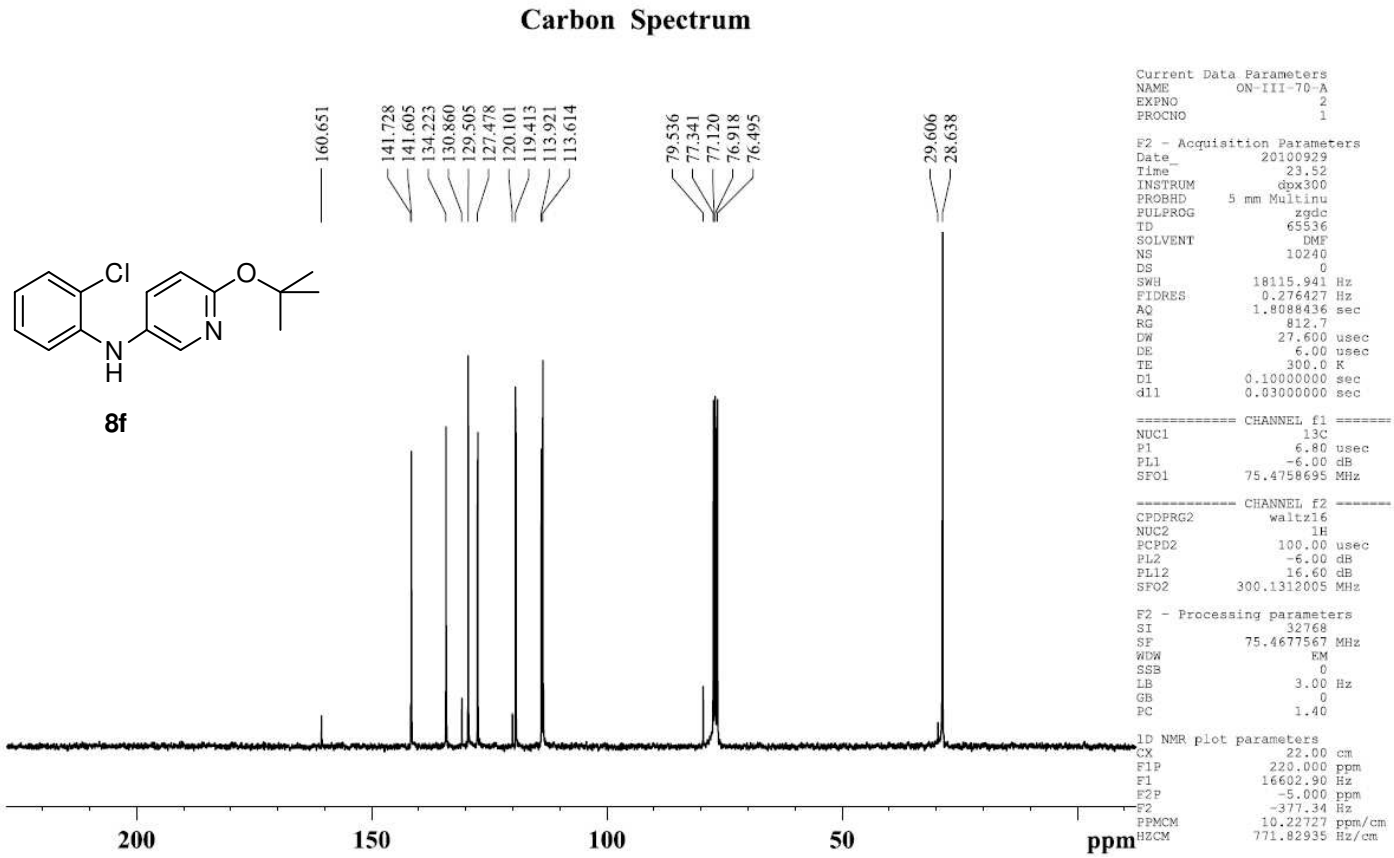


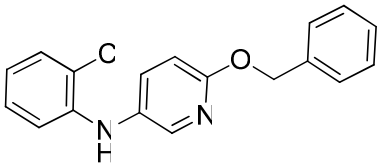

**6-(*tert*-butoxy)-*N*-(2-chlorophenyl)pyridin-3-amine (8f)**

## Proton Spectrum



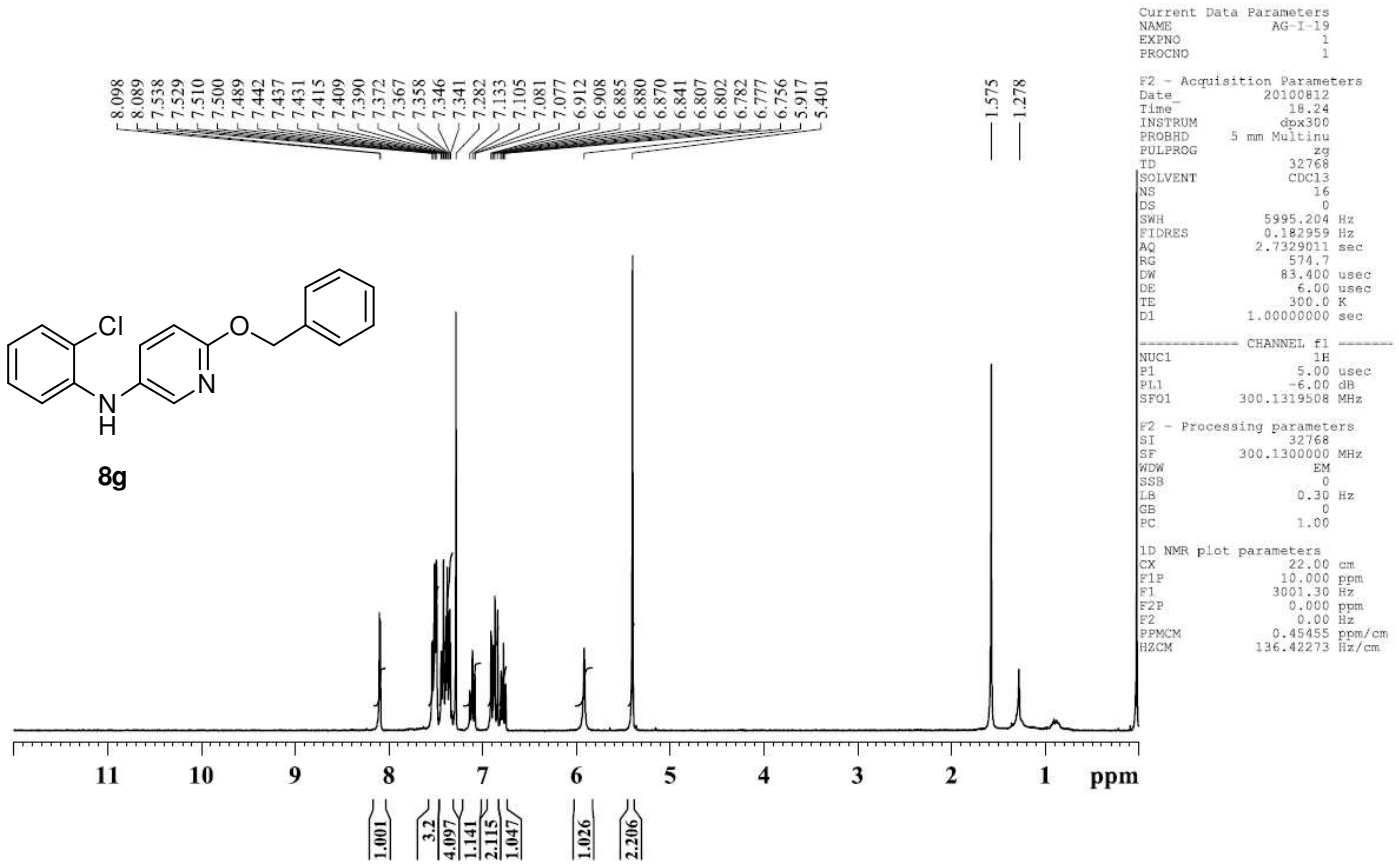

```
Current Data Parameters
NAME         ON-III-70-A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100929
Time              18.21
INSTRUM          dpx300
PROBHD     5 mm Multinu
PULPROG              zg
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.182959 Hz
AQ             2.7329011 sec
RG                228.1
DW                83.400 usec
DE                 6.00 usec
TE                300.0 K
D1            1.00000000 sec

------------ CHANNEL f1 -------
NUC1                 1H
P1                 5.00 usec
PL1               -6.00 dB
SFO1         300.1319508 MHz

F2 - Processing parameters
SI                32768
SF          300.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                22.00 cm
F1P               10.000 ppm
F1              3001.30 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM          0.45455 ppm/cm
HZCM         136.42273 Hz/cm
```


Carbon Spectrum
160.651
141.728
141.605
134.223
130.860
129.505
127.478
120.101
119.413
113.921
113.614
79.536
77.341
77.120
76.918
76.495
29.606
28.638
Cl
O
N
N
H
8f
200
150
100
50
ppm
Current Data Parameters
NAME ON-III-70-A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100929
Time 23.52
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT DMF
NS 10240
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 812.7
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm

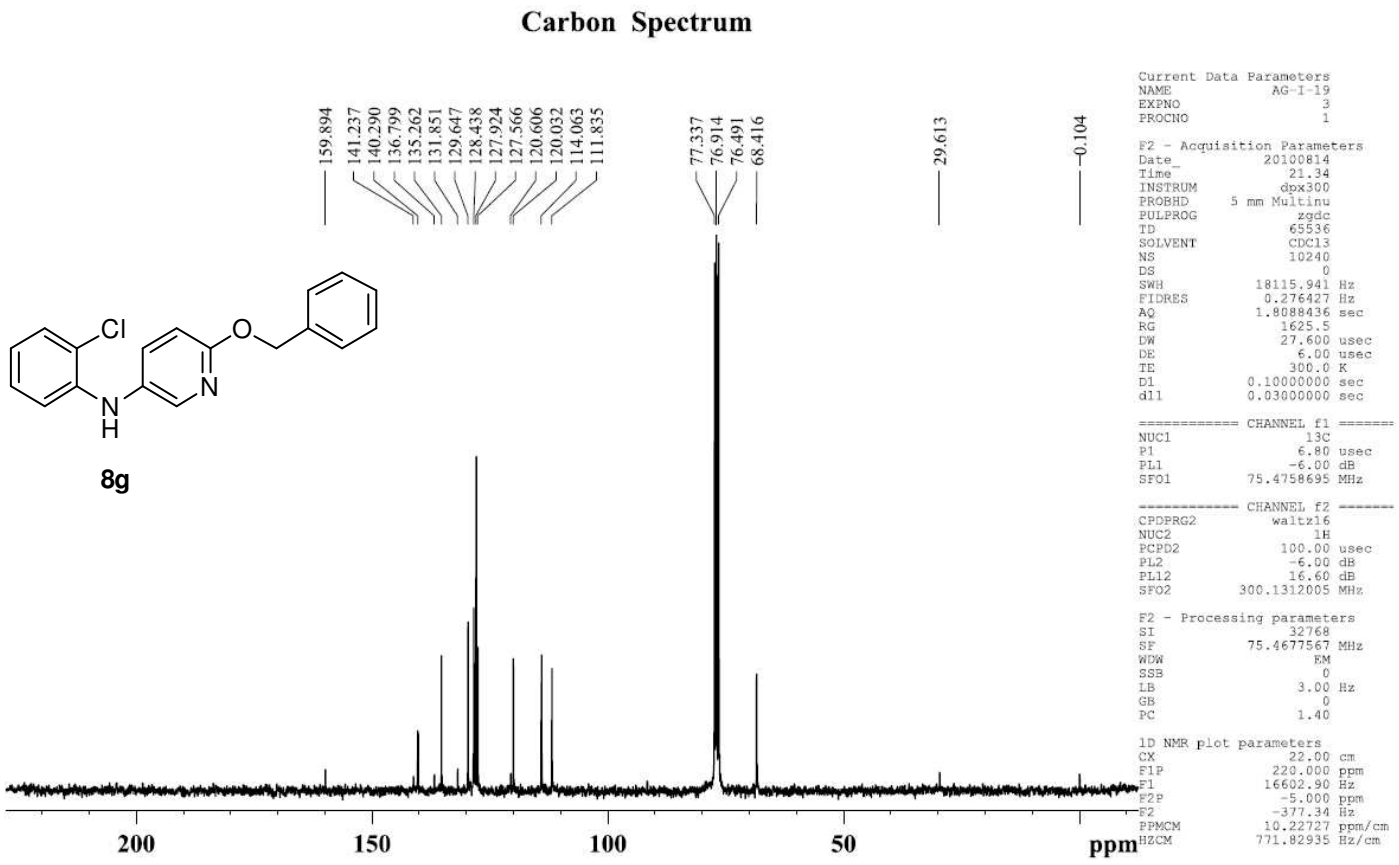


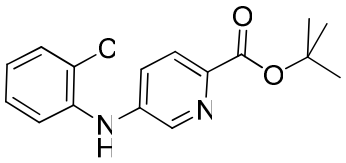

**6-(benzyloxy)-*N*-(2-chlorophenyl)pyridin-3-amine (8g)**

**Proton Spectrum**



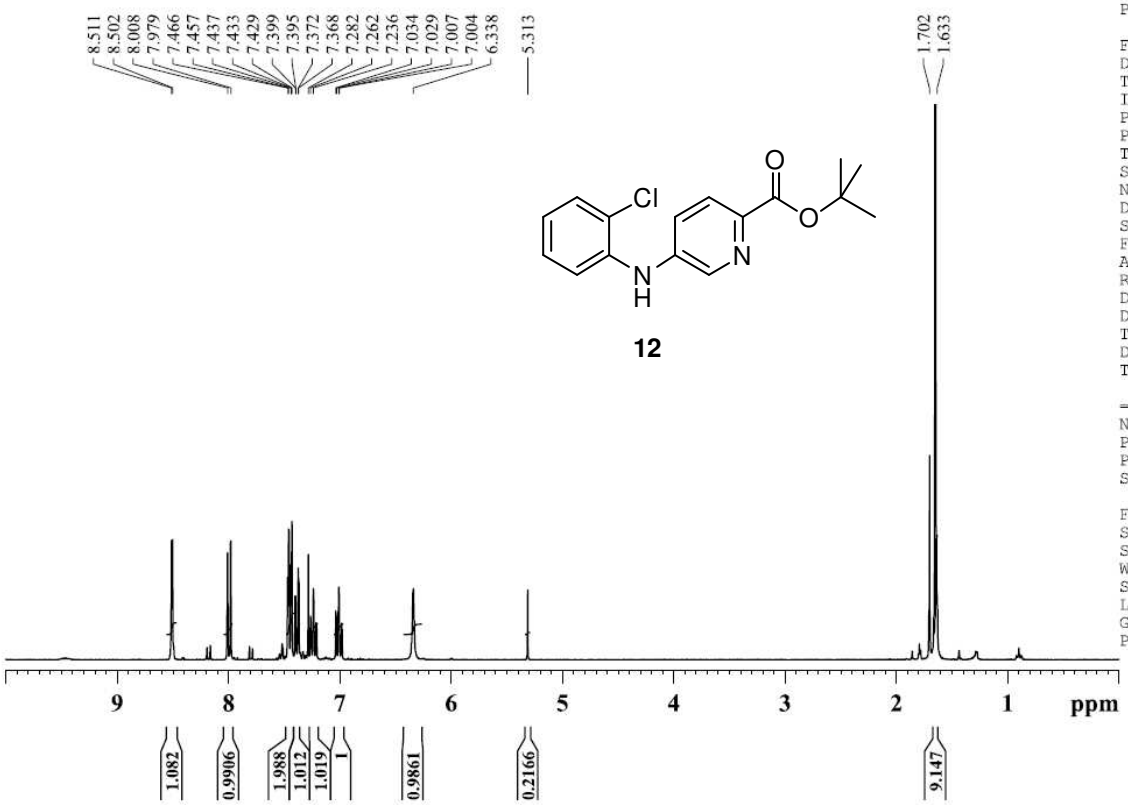

```
Current Data Parameters
NAME                  AG-I-19
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100812
Time                  18.24
INSTRUM               dpx300
PROBHD     5 mm Multinu
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                5995.204 Hz
FIDRES            0.182959 Hz
AQ                2.7329011 sec
RG                    574.7
DW                   83.400 usec
DE                    6.00 usec
TE                   300.0 K
D1                1.00000000 sec

========== CHANNEL f1 =======
NUC1                      1H
P1                     5.00 usec
PL1                   -6.00 dB
SFO1           300.1319508 MHz

F2 - Processing parameters
SI                     32768
SF               300.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     22.00 cm
F1P                   10.000 ppm
F1                  3001.30 Hz
F2P                    0.000 ppm
F2                     0.00 Hz
PPMCM                0.45455 ppm/cm
HZCM               136.42273 Hz/cm
```


Carbon Spectrum
159.894
141.237
140.290
136.799
135.262
131.851
129.647
128.438
127.924
127.566
120.606
120.032
114.063
111.835
77.337
76.914
76.491
68.416
29.613
-0.104
Cl
O
N
N
H
8g
200
150
100
50
ppm
Current Data Parameters
NAME AG-I-19
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100814
Time_ 21.34
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 10240
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 1625.5
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm



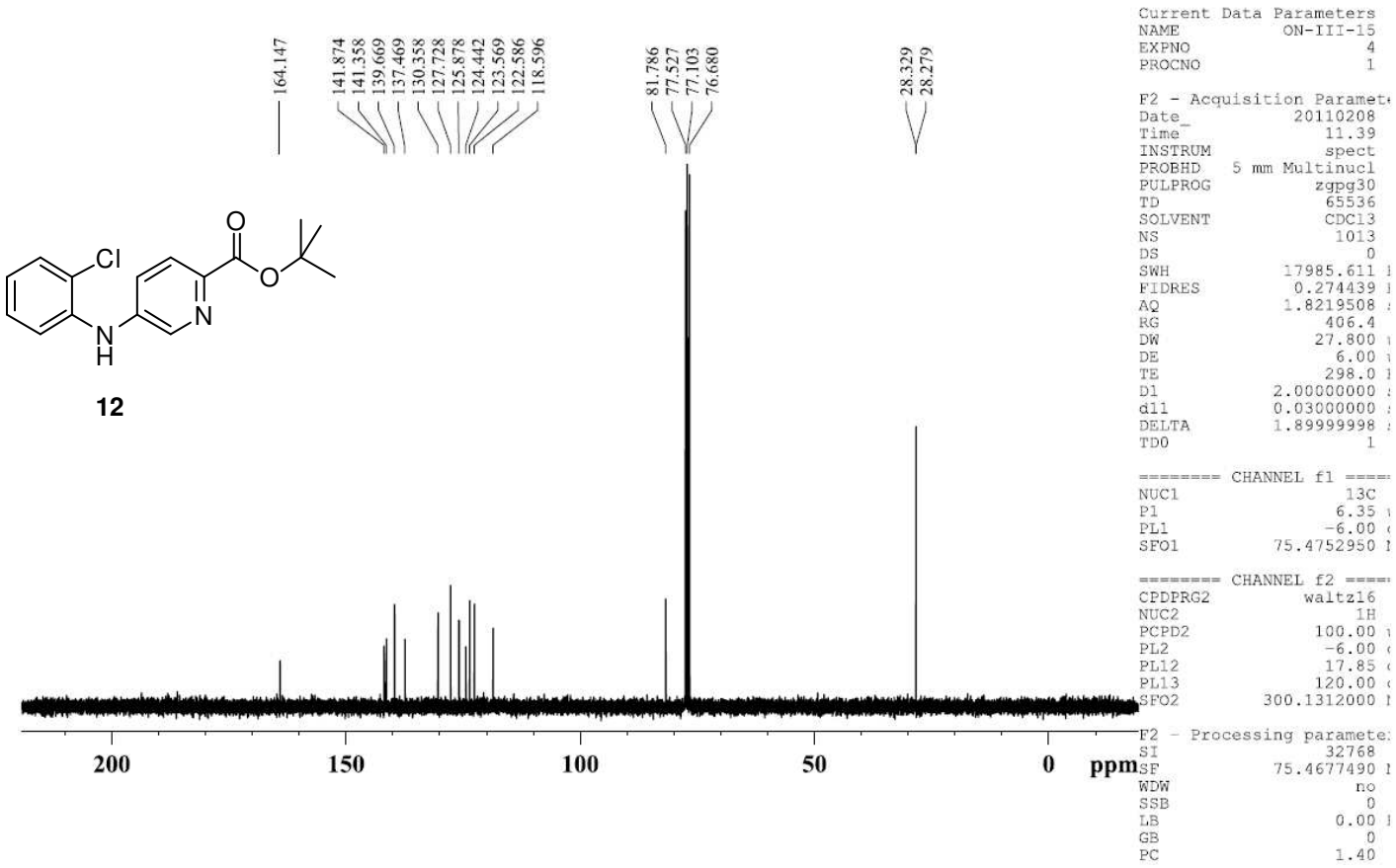
***tert*-butyl 5-[(2-chlorophenyl)amino]picolinate (12)**

**Proton Spectrum**



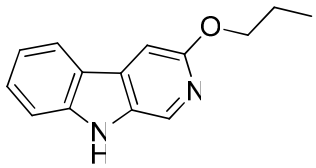

```
Current Data Parameters
NAME                  ON-III-15
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parame
Date_                  20110208
Time                      10.31
INSTRUM                   spect
PROBHD    5 mm Multinucl
PULPROG                    zg30
TD                        32768
SOLVENT                   CDCl3
NS                           16
DS                            0
SWH                    6172.839
FIDRES                 0.188380
AQ                     2.6542580
RG                          362
DW                       81.000
DE                         6.00
TE                        298.4
D1                   1.00000000
TD0                           1

======== CHANNEL f1 ===
NUC1                         1H
P1                         9.00
PL1                       -6.00
SFO1                300.1318534

F2 - Processing paramet
SI                        32768
SF                  300.1300000
WDW                          no
SSB                           0
LB                         0.00
GB                            0
PC                         1.00
```

**Carbon Spectrum**



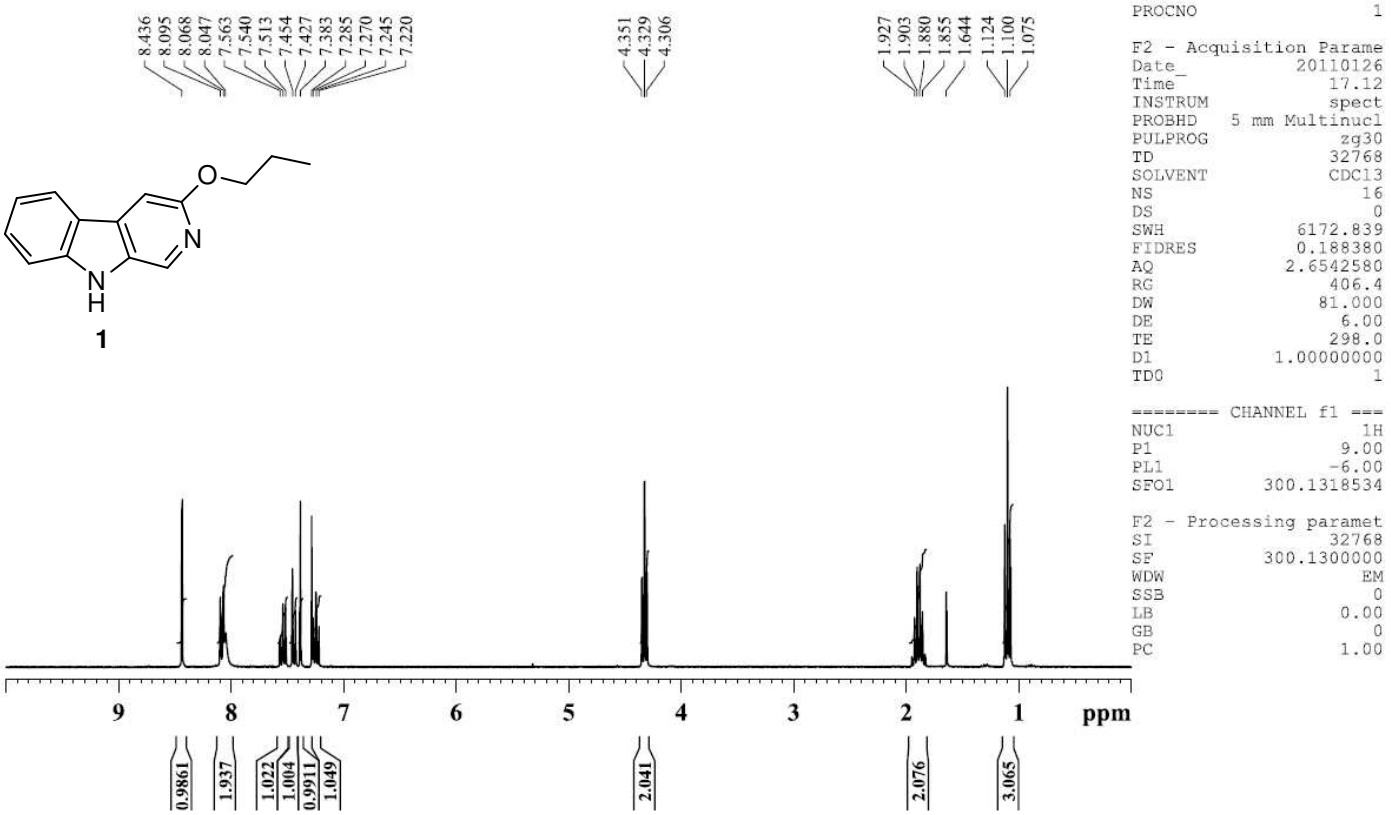

**12**

```
Current Data Parameters
NAME                 ON-III-15
EXPNO                        4
PROCNO                       1

F2 - Acquisition Paramet
Date_               20110208
Time                   11.39
INSTRUM                spect
PROBHD   5 mm Multinucl
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1013
DS                          0
SWH                 17985.611
FIDRES              0.274439
AQ                  1.8219508
RG                      406.4
DW                     27.800
DE                      6.00
TE                     298.0
D1                 2.00000000
d11                0.03000000
DELTA              1.89999998
TD0                          1

======== CHANNEL f1 =====
NUC1                       13C
P1                        6.35
PL1                      -6.00
SFO1               75.4752950

======== CHANNEL f2 =====
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   100.00
PL2                      -6.00
PL12                     17.85
PL13                    120.00
SFO2               300.1312000

F2 - Processing paramete
SI                       32768
SF                 75.4677490
WDW                         no
SSB                          0
LB                        0.00
GB                           0
PC                        1.40
```



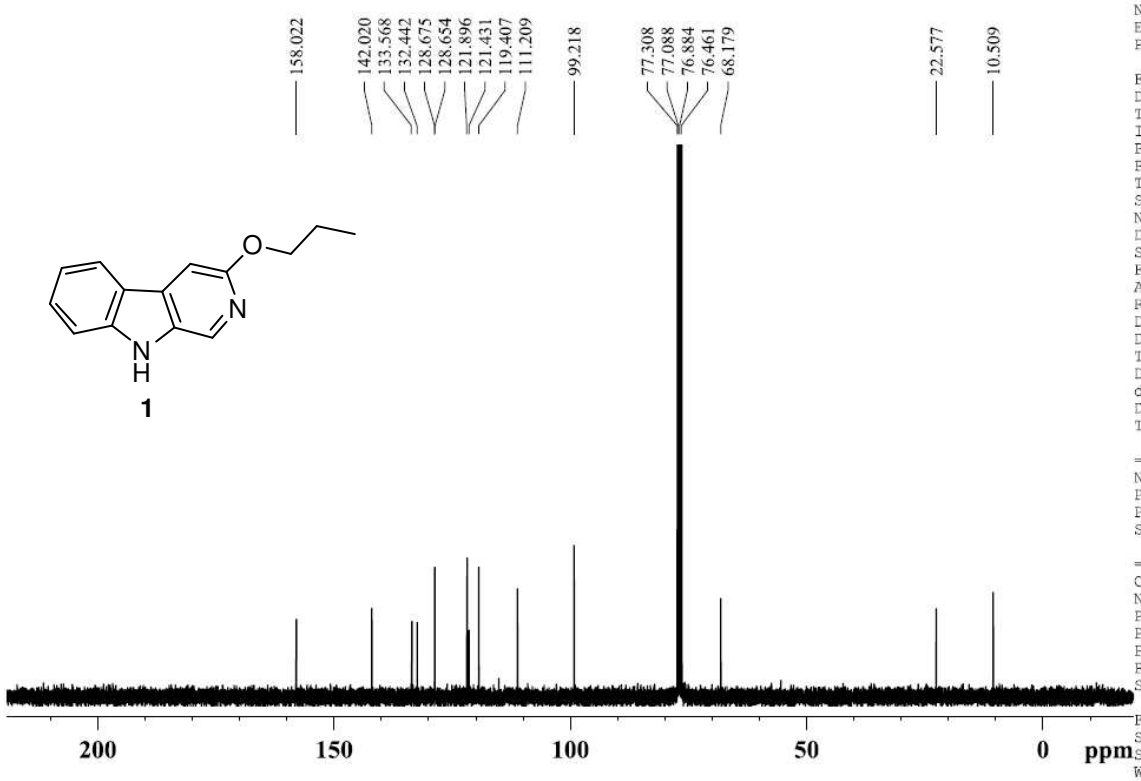
**3-propoxy-9*H*-pyrido[3,4-*b*]indole (1)**

**Proton Spectrum**



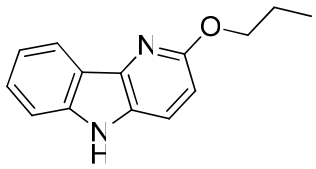

```
Current Data Parameters
NAME                  ON-I-91-B
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parame
Date_                  20110126
Time                      17.12
INSTRUM                   spect
PROBHD    5 mm Multinucl
PULPROG                   zg30
TD                       32768
SOLVENT                  CDCl3
NS                           16
DS                            0
SWH                    6172.839
FIDRES                 0.188380
AQ                     2.6542580
RG                         406.4
DW                        81.000
DE                          6.00
TE                         298.0
D1                  1.00000000
TD0                           1

======== CHANNEL f1 ===
NUC1                         1H
P1                         9.00
PL1                       -6.00
SFO1               300.1318534

F2 - Processing paramet
SI                       32768
SF                 300.1300000
WDW                         EM
SSB                          0
LB                        0.00
GB                           0
PC                        1.00
```

**Carbon Spectrum**



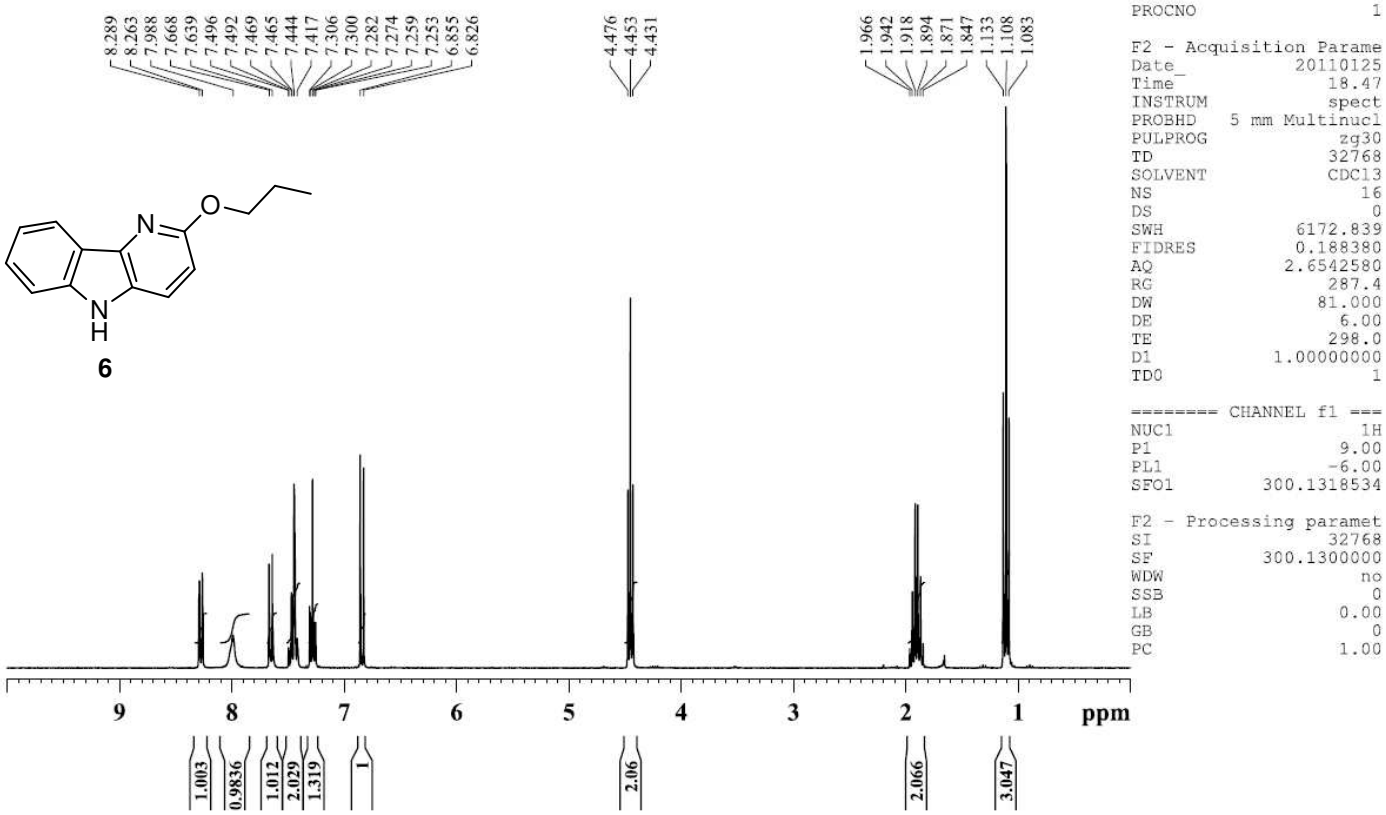

**1**

```
Current Data Parameters
NAME                 ON-I-91-B
EXPNO                        2
PROCNO                       1

F2 - Acquisition Paramet
Date_                 20110126
Time                     20.29
INSTRUM                  spect
PROBHD    5 mm Multinucl
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        3000
DS                           4
SWH                  17985.611
FIDRES                0.274439
AQ                    1.8219508
RG                       2896.3
DW                       27.800
DE                         6.00
TE                        298.0
D1                   2.00000000
d11                  0.03000000
DELTA                1.89999998
TD0                          1

======== CHANNEL f1 =====
NUC1                       13C
P1                        6.35
PL1                      -6.00
SFO1                75.4752950

======== CHANNEL f2 =====
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   100.00
PL2                      -6.00
PL12                     17.85
PL13                    120.00
SFO2                300.1312000

F2 - Processing paramete
SI                        32768
SF                  75.4677490
WDW                          no
SSB                           0
LB                         0.00
GB                            0
PC                         1.40
```



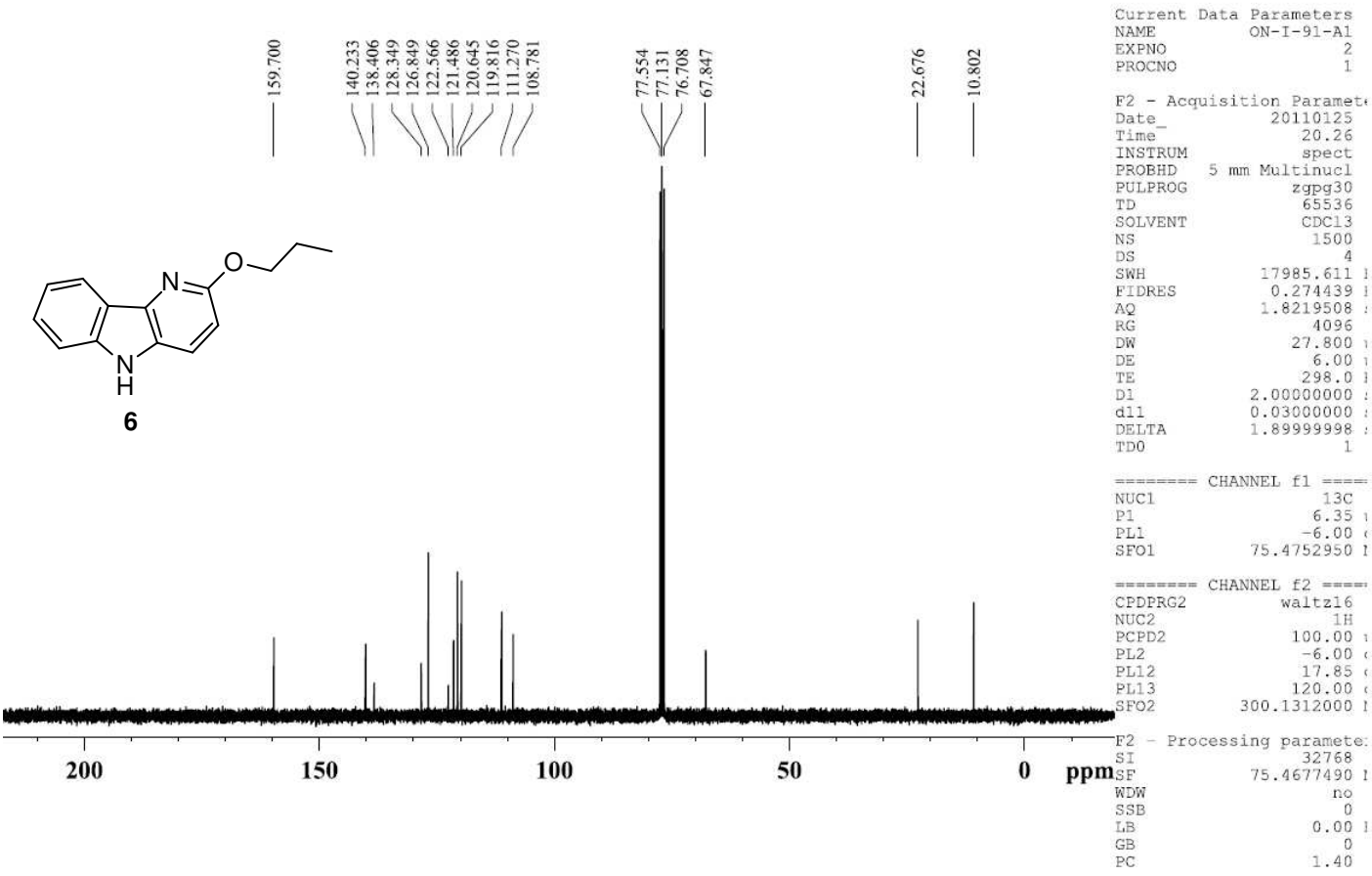
**2-propoxy-5*H*-pyrido[3,2-*b*]indole (6)**

**Proton Spectrum**

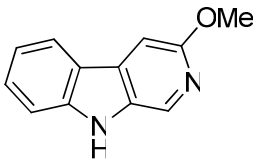



```
Current Data Parameters
NAME          ON-I-91-A1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parame
Date_           20110125
Time_              18.47
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             6172.839
FIDRES          0.188380
AQ              2.6542580
RG                 287.4
DW                81.000
DE                 6.00
TE                298.0
D1           1.00000000
TD0                    1

======== CHANNEL f1 ===
NUC1                  1H
P1                  9.00
PL1                -6.00
SFO1         300.1318534

F2 - Processing paramet
SI                 32768
SF          300.1300000
WDW                   no
SSB                    0
LB                  0.00
GB                     0
PC                  1.00
```

**Carbon Spectrum**

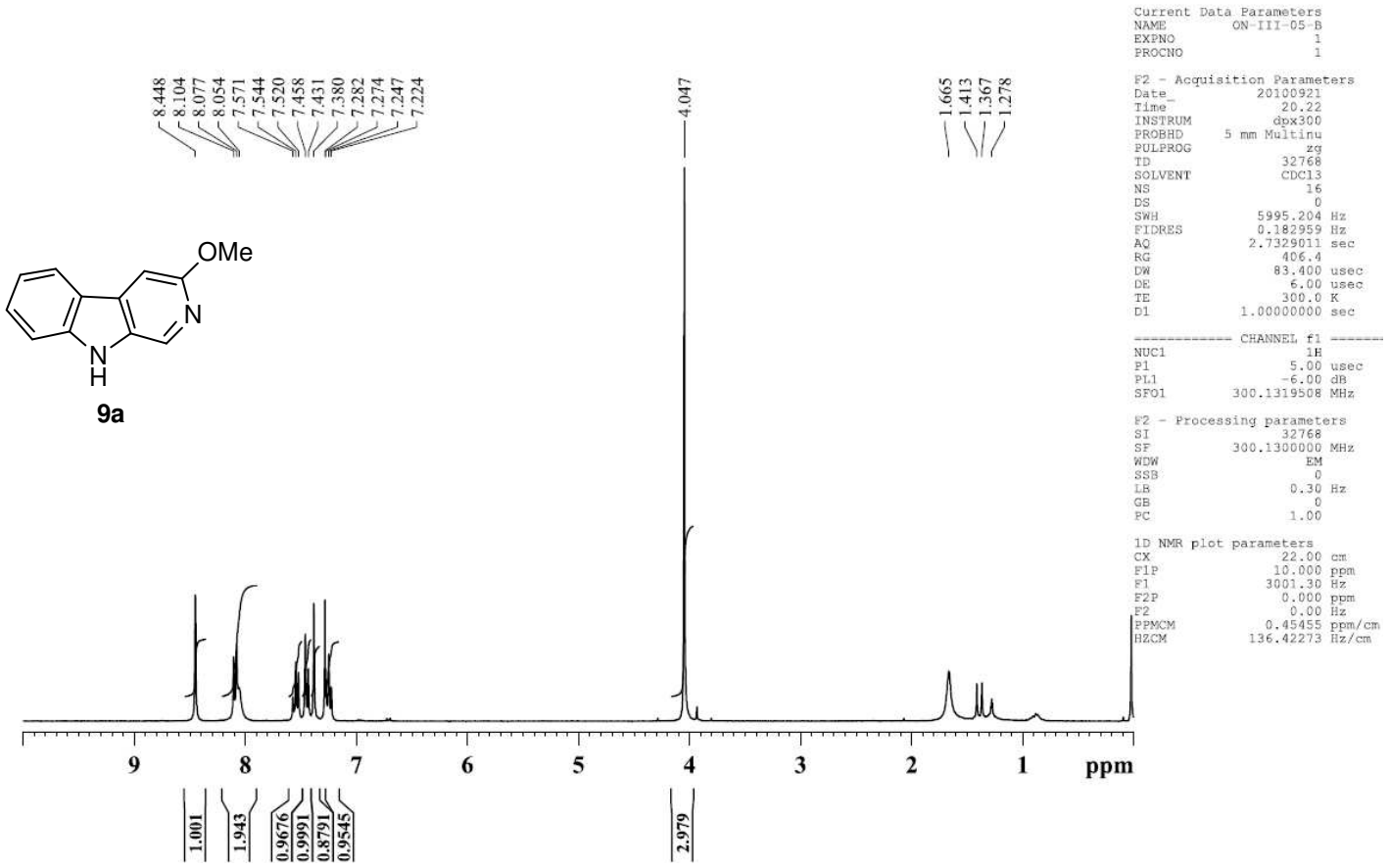


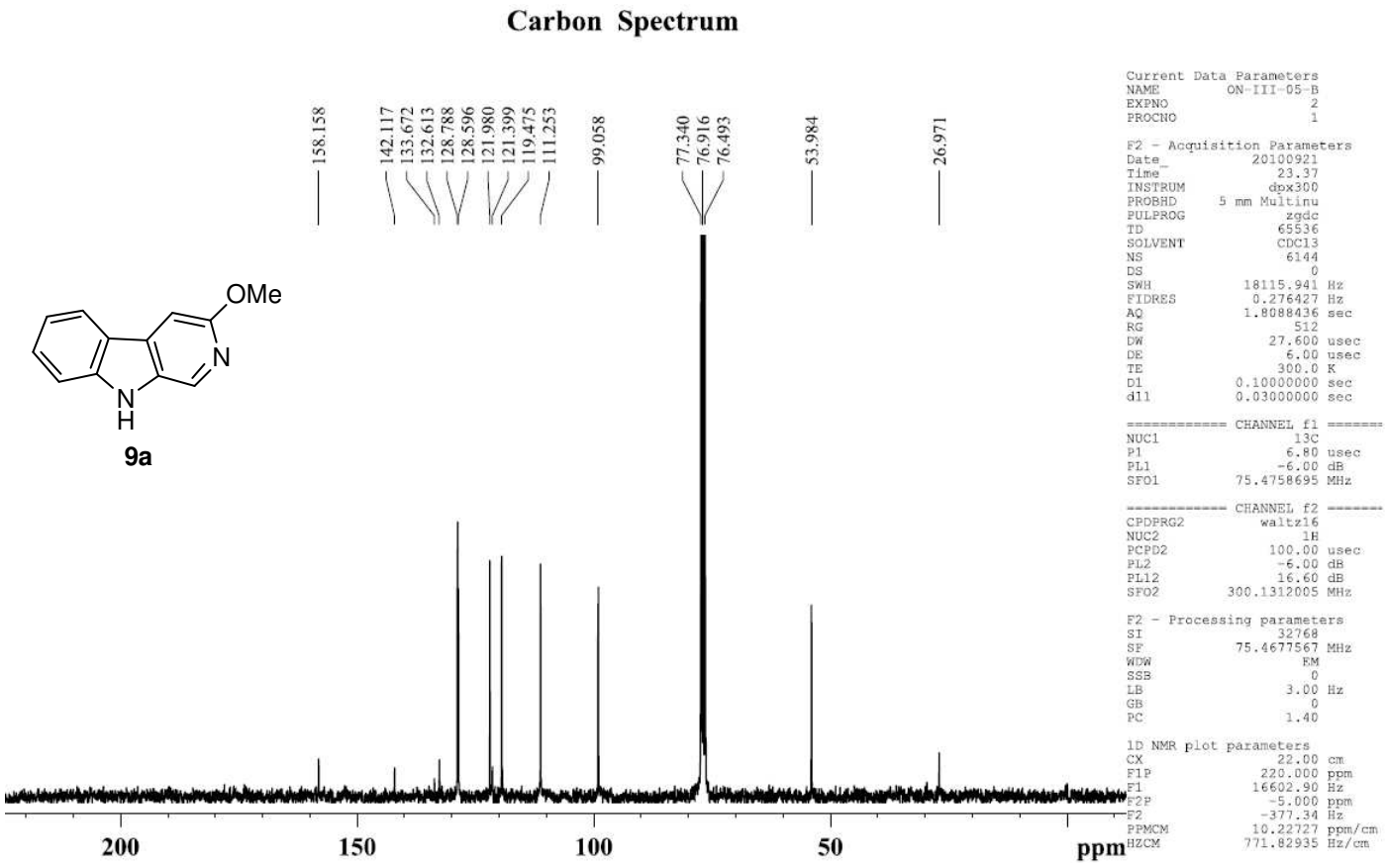

```
Current Data Parameters
NAME          ON-I-91-A1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Paramet
Date_           20110125
Time              20.26
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1500
DS                    4
SWH           17985.611
FIDRES         0.274439
AQ             1.8219508
RG                 4096
DW                27.800
DE                 6.00
TE                298.0
D1            2.00000000
d11           0.03000000
DELTA         1.89999998
TD0                    1

======== CHANNEL f1 ====
NUC1                13C
P1                 6.35
PL1               -6.00
SFO1          75.4752950

======== CHANNEL f2 ====
CPDPRG2         waltz16
NUC2                1H
PCPD2           100.00
PL2              -6.00
PL12             17.85
PL13            120.00
SFO2         300.1312000

F2 - Processing paramete
SI                 32768
SF            75.4677490
WDW                   no
SSB                    0
LB                  0.00
GB                     0
PC                  1.40
```

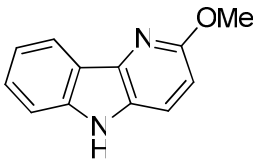



**3-methoxy-9*H*-pyrido[3,4-*b*]indole (9a)**

**Proton Spectrum**

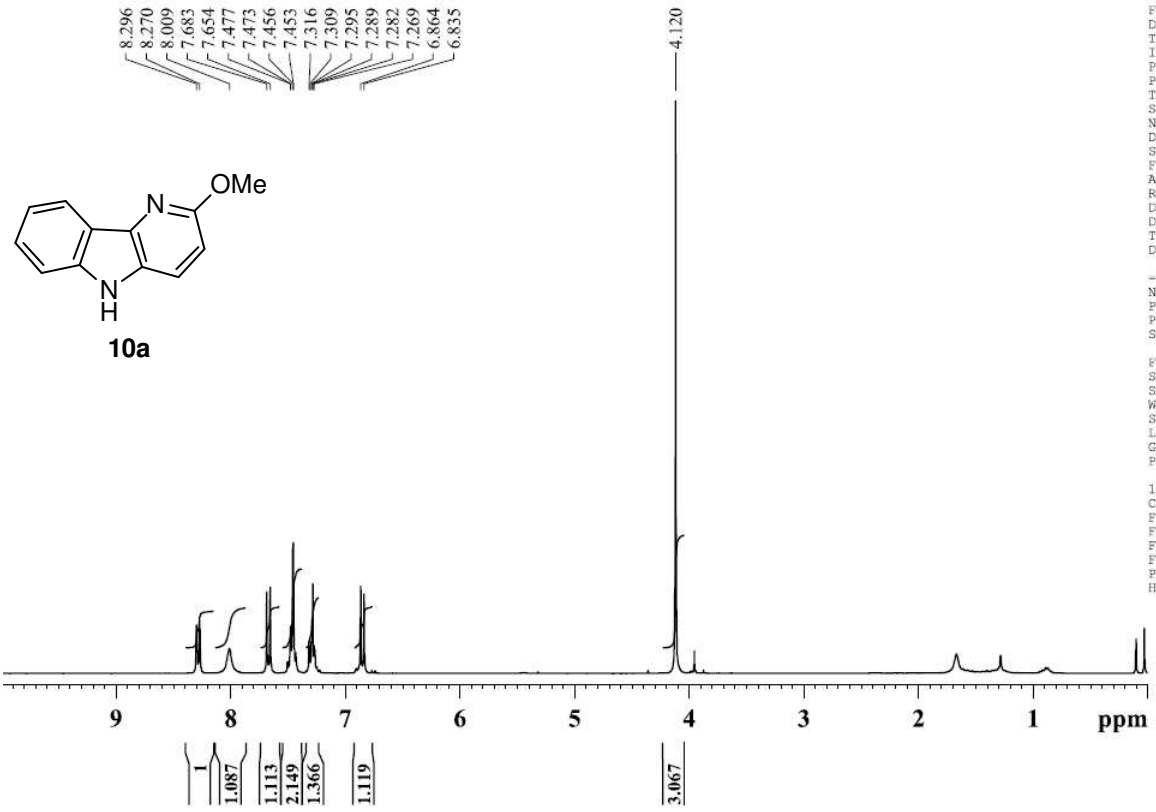



Carbon Spectrum
158.158
142.117
133.672
132.613
128.788
128.596
121.980
121.399
119.475
111.253
99.058
77.340
76.916
76.493
53.984
26.971
OMe
N
N
H
9a
200
150
100
50
ppm
Current Data Parameters
NAME ON-III-05-B
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100921
Time_ 23.37
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 6144
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 512
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm

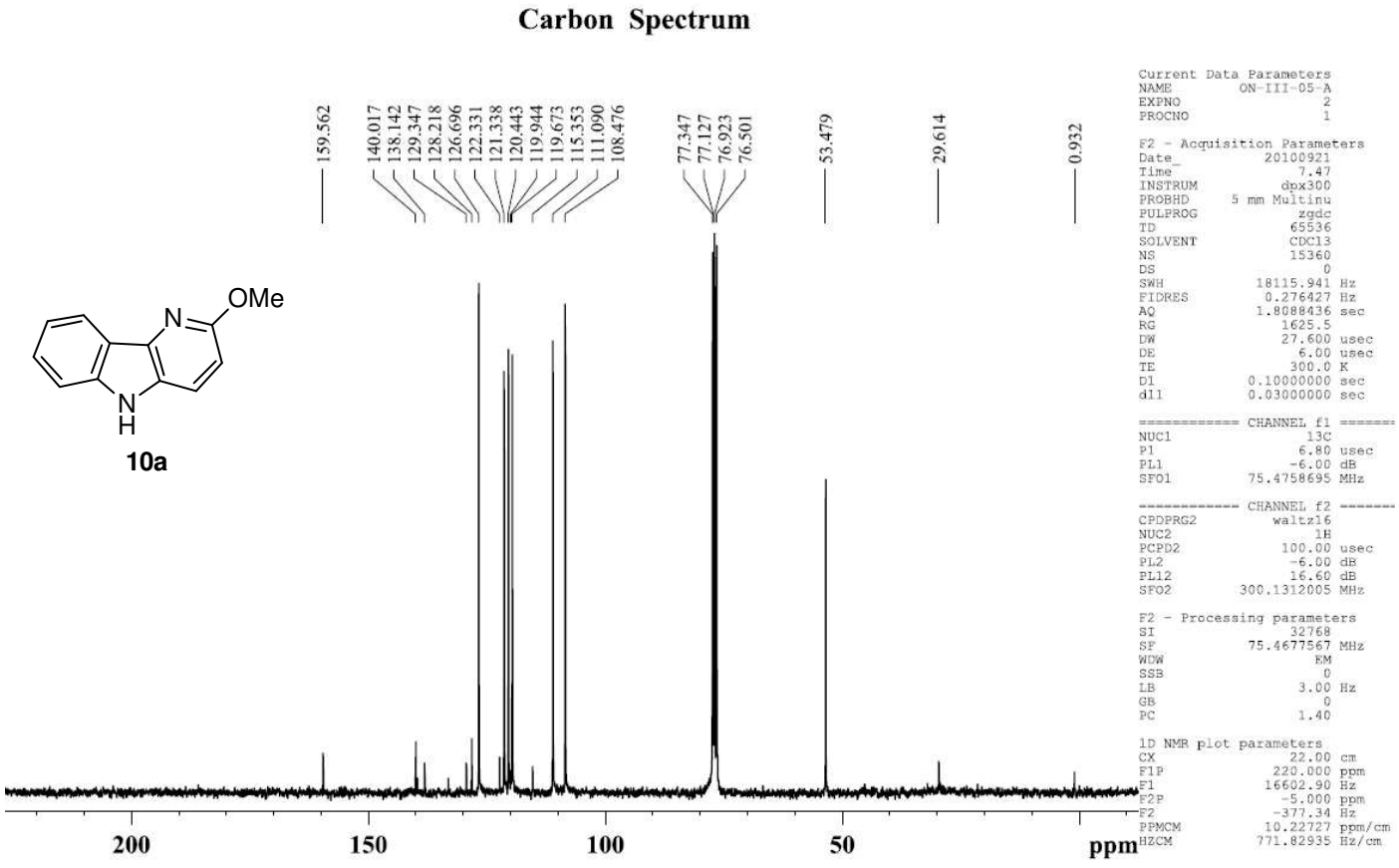


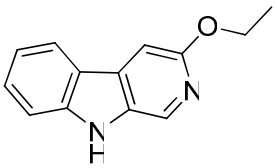

**2-methoxy-5*H*-pyrido[3,2-*b*]indole (10a)**

## Proton Spectrum



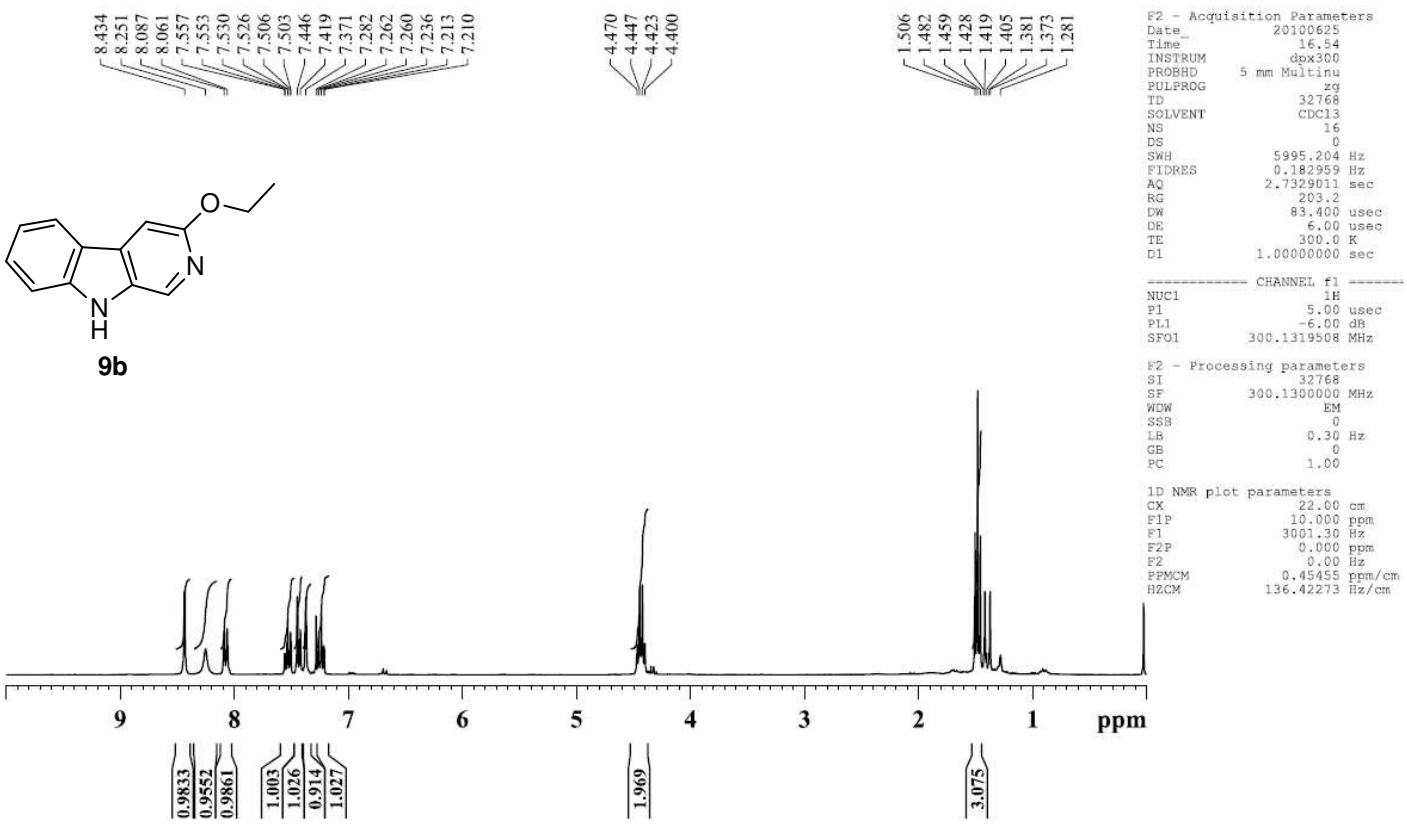

```
Current Data Parameters
NAME                  ON-III-05-A
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20100920
Time                        23.36
INSTRUM                   dpx300
PROBHD          5 mm Multinu
PULPROG                       zg
TD                         32768
SOLVENT                    CDCl3
NS                            16
DS                             0
SWH                     5995.204 Hz
FIDRES                  0.182959 Hz
AQ                     2.7329011 sec
RG                         287.4
DW                        83.400 usec
DE                         6.00 usec
TE                        300.0 K
D1                   1.00000000 sec

------------ CHANNEL f1 -------
NUC1                          1H
P1                         5.00 usec
PL1                       -6.00 dB
SFO1                300.1319508 MHz

F2 - Processing parameters
SI                         32768
SF                  300.1300000 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00

1D NMR plot parameters
CX                         22.00 cm
F1P                        10.000 ppm
F1                       3001.30 Hz
F2P                         0.000 ppm
F2                          0.00 Hz
PPMCM                    0.45455 ppm/cm
HZCM                   136.42273 Hz/cm
```


Carbon Spectrum
159.562
140.017
138.142
129.347
128.218
126.696
122.331
121.338
120.443
119.944
119.673
115.353
111.090
108.476
77.347
77.127
76.923
76.501
53.479
29.614
0.932
OMe
N
N
H
10a
200
150
100
50
ppm
Current Data Parameters
NAME ON-III-05-A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100921
Time 7.47
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 15360
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 1625.5
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm

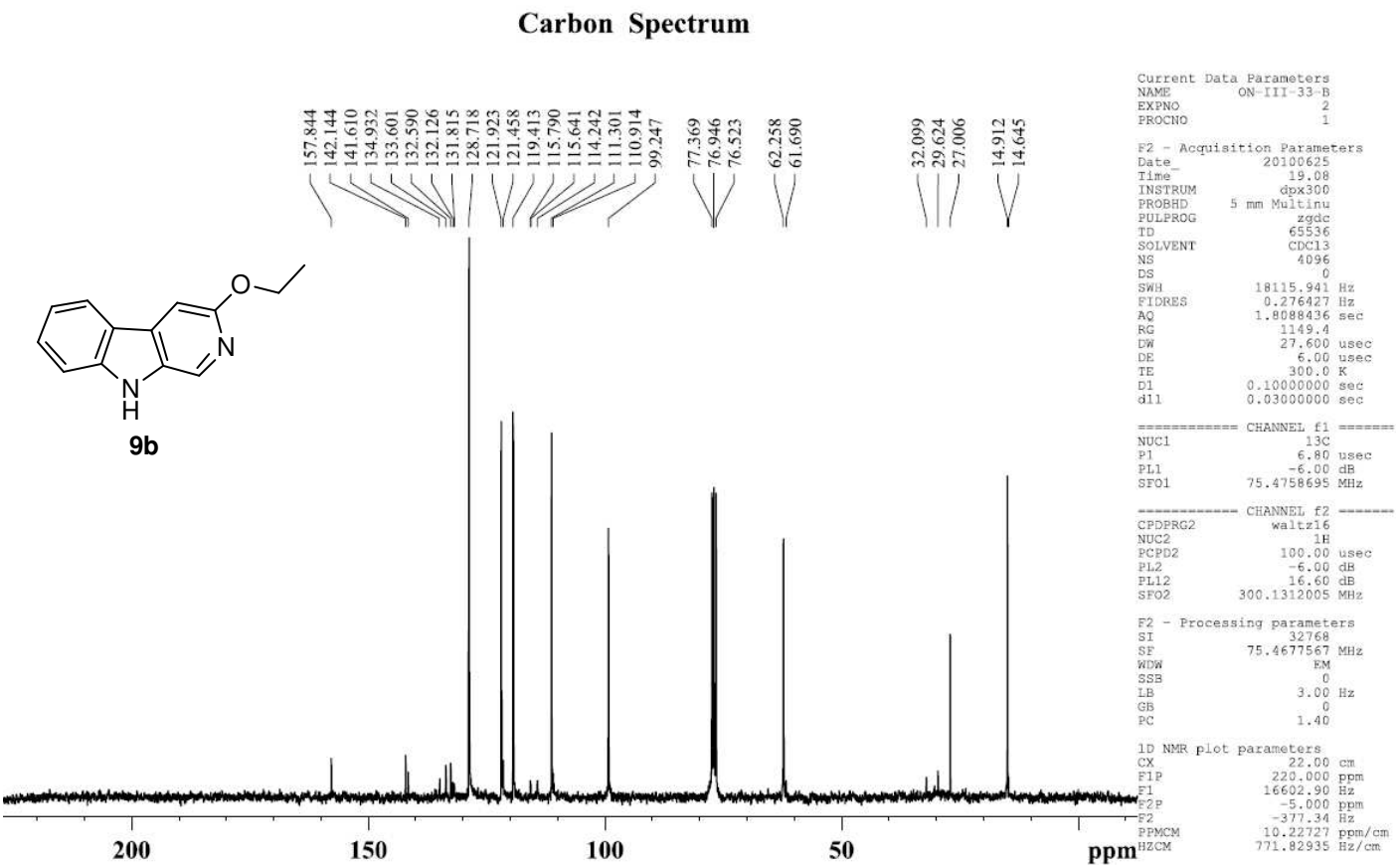


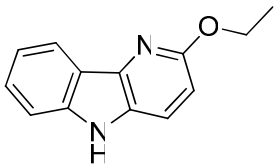
**3-ethoxy-9*H*-pyrido[3,4-*b*]indole (9b)**

## Proton Spectrum



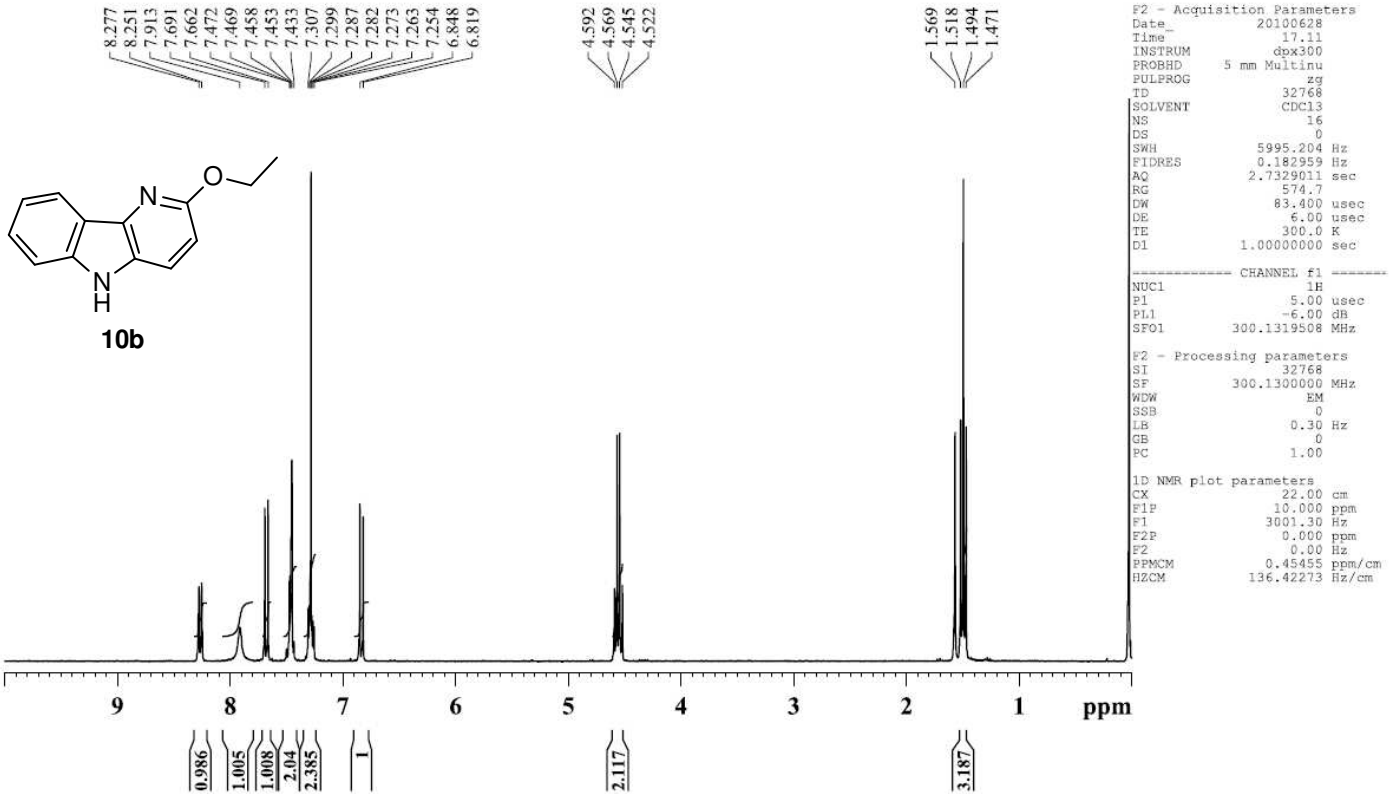

```
Current Data Parameters
NAME          ON-III-33-B
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100625
Time_               16.54
INSTRUM           dpx300
PROBHD     5 mm Multinu
PULPROG              zg
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.182959 Hz
AQ             2.7329011 sec
RG                203.2
DW                83.400 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec

------------ CHANNEL f1 -------
NUC1                  1H
P1                  5.00 usec
PL1                -6.00 dB
SFO1         300.1319508 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 22.00 cm
F1P                10.000 ppm
F1               3001.30 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM            0.45455 ppm/cm
HZCM           136.42273 Hz/cm
```


Carbon Spectrum
157.844
142.144
141.610
134.932
133.601
132.590
132.126
131.815
128.718
121.923
121.458
119.413
115.790
115.641
114.242
111.301
110.914
99.247
77.369
76.946
76.523
62.258
61.690
32.099
29.624
27.006
14.912
14.645
O
N
N
H
9b
200
150
100
50
ppm
Current Data Parameters
NAME ON-III-33-B
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100625
Time_ 19.08
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 4096
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 1149.4
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
========== CHANNEL f1 =======
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
========== CHANNEL f2 =======
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm

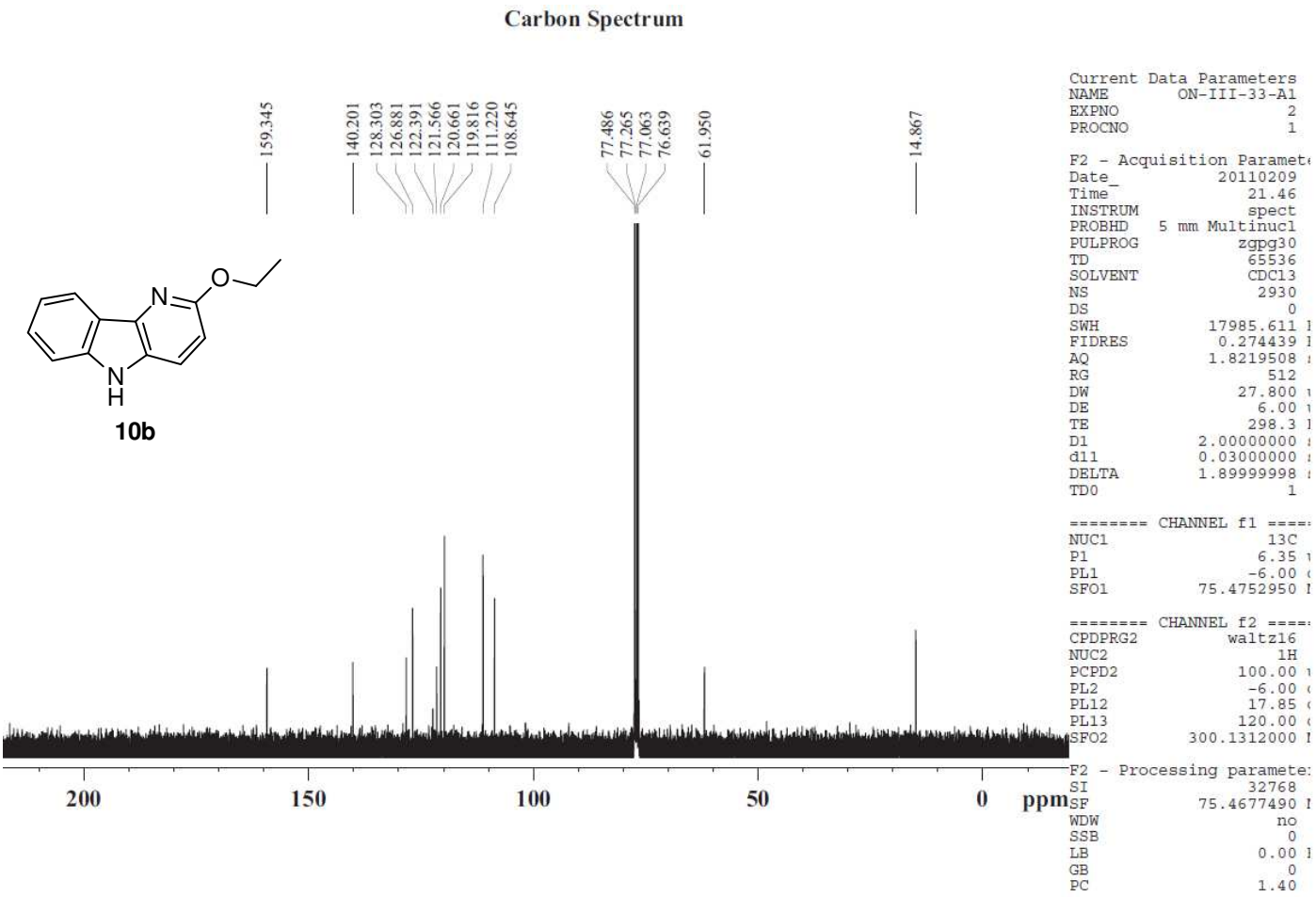


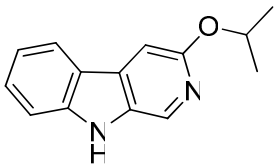
**2-Ethoxy-5*H*-pyrido[3,2-*b*]indole (10b)**

**Proton Spectrum**



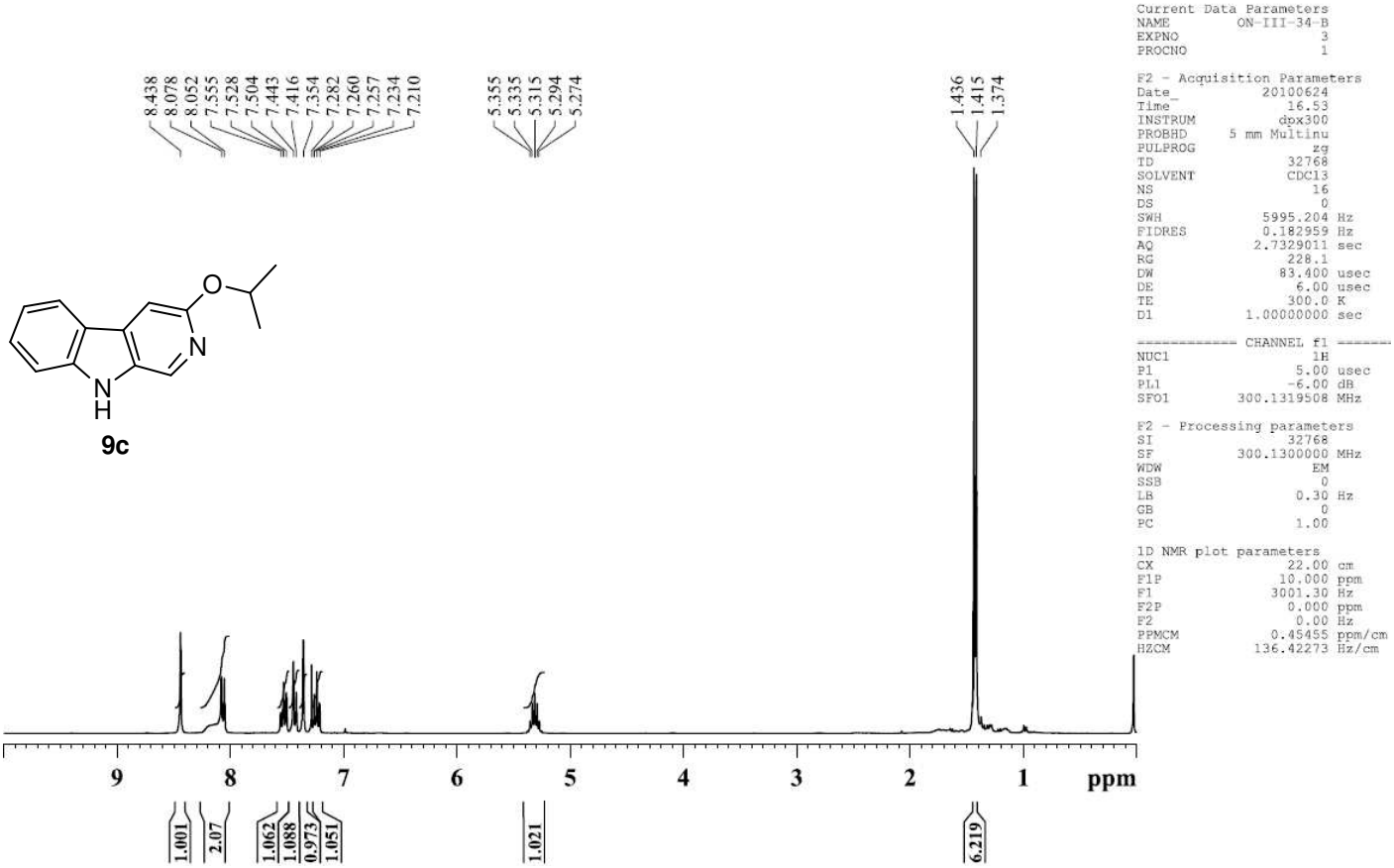

```
Current Data Parameters
NAME                  ON-III-33-A
EXPNO                           3
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20100628
Time                        17.11
INSTRUM                   dpx300
PROBHD           5 mm Multinu
PULPROG                         zg
TD                           32768
SOLVENT                     CDCl3
NS                             16
DS                              0
SWH                      5995.204 Hz
FIDRES                   0.182959 Hz
AQ                       2.7329011 sec
RG                           574.7
DW                          83.400 usec
DE                           6.00 usec
TE                          300.0 K
D1                       1.00000000 sec

------------ CHANNEL f1 -------
NUC1                           1H
P1                           5.00 usec
PL1                         -6.00 dB
SFO1                300.1319508 MHz

F2 - Processing parameters
SI                           32768
SF                  300.1300000 MHz
WDW                            EM
SSB                             0
LB                           0.30 Hz
GB                              0
PC                           1.00

1D NMR plot parameters
CX                          22.00 cm
F1P                         10.000 ppm
F1                        3001.30 Hz
F2P                          0.000 ppm
F2                           0.00 Hz
PPMCM                     0.45455 ppm/cm
HZCM                    136.42273 Hz/cm
```


Carbon Spectrum
159.345
140.201
128.303
126.881
122.391
121.566
120.661
119.816
111.220
108.645
77.486
77.265
77.063
76.639
61.950
14.867
N
O
N
H
10b
200
150
100
50
0
ppm
Current Data Parameters
NAME ON-III-33-A1
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20110209
Time 21.46
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2930
DS 0
SWH 17985.611
FIDRES 0.274439
AQ 1.8219508
RG 512
DW 27.800
DE 6.00
TE 298.3
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
======== CHANNEL f1 ====
NUC1 13C
P1 6.35
PL1 -6.00
SFO1 75.4752950
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00
PL2 -6.00
PL12 17.85
PL13 120.00
SFO2 300.1312000
F2 - Processing paramete
SI 32768
SF 75.4677490
WDW no
SSB 0
LB 0.00
GB 0
PC 1.40

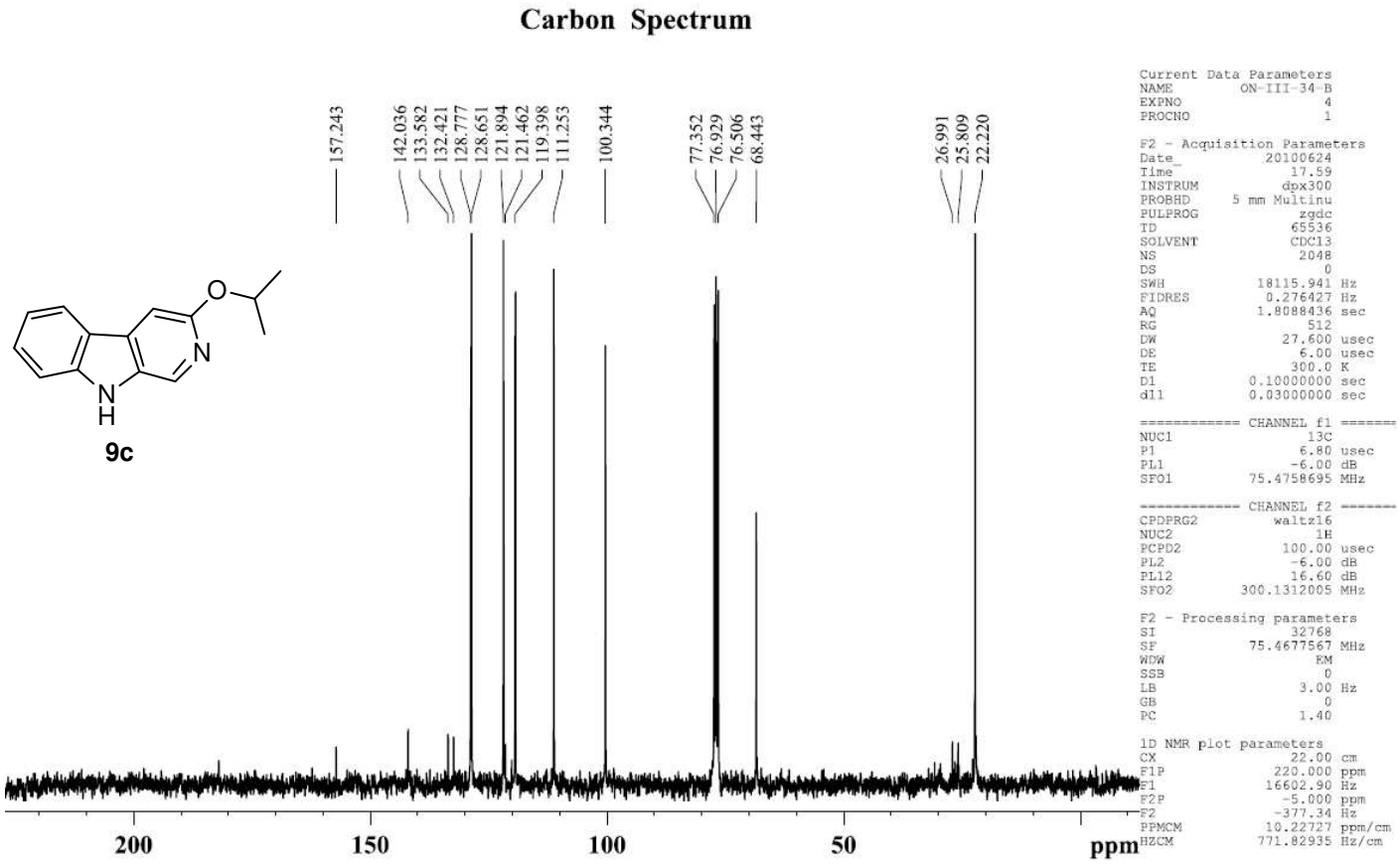


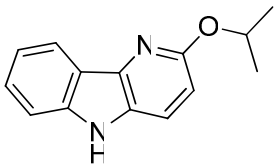
**3-isopropoxy-9*H*-pyrido[3,4-*b*]indole (9c)**

## Proton Spectrum



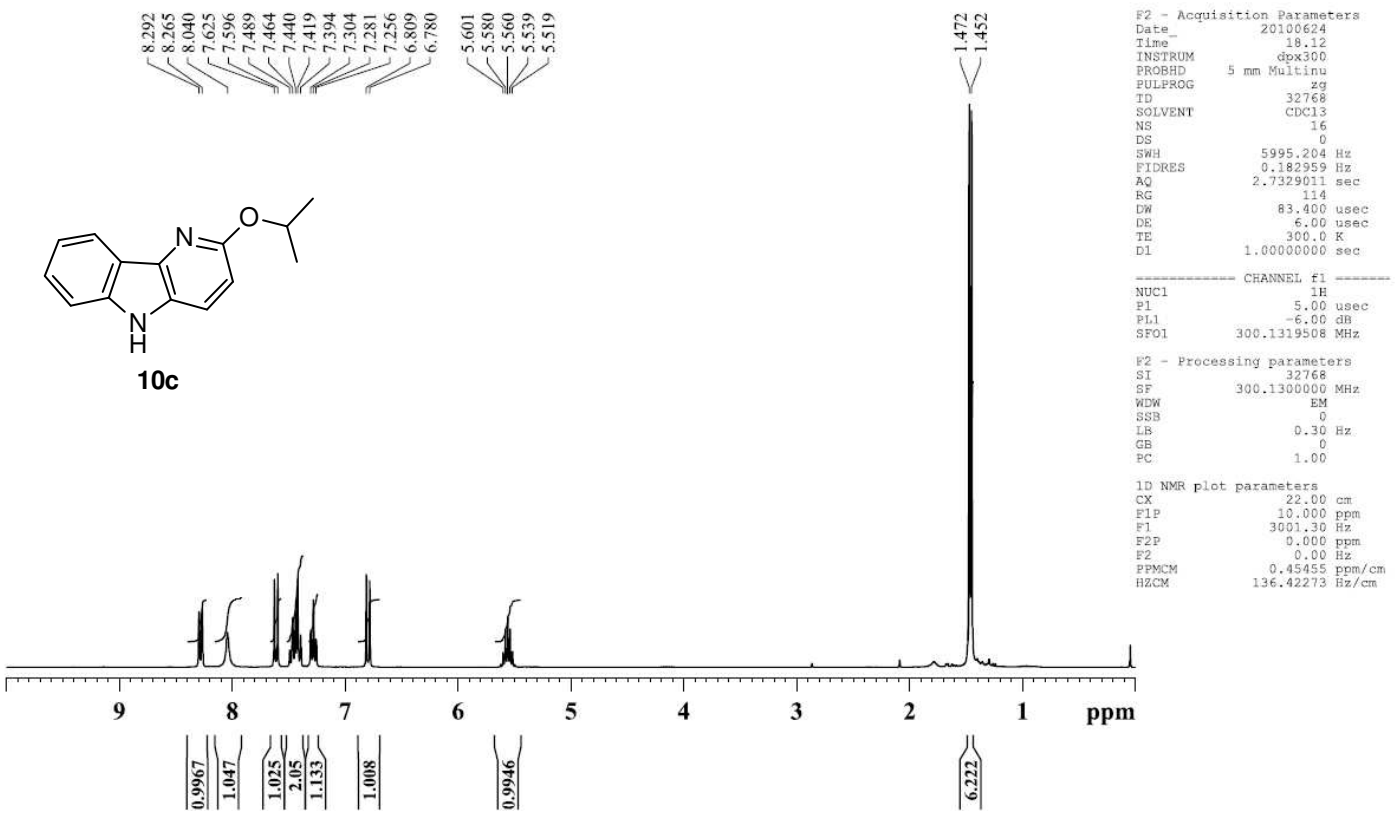

```
Current Data Parameters
NAME         ON-III-34-B
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100624
Time               16.53
INSTRUM          dpx300
PROBHD     5 mm Multinu
PULPROG              zg
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.182959 Hz
AQ             2.7329011 sec
RG                228.1
DW                83.400 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec

============ CHANNEL f1 =======
NUC1                  1H
P1                  5.00 usec
PL1                -6.00 dB
SFO1          300.1319508 MHz

F2 - Processing parameters
SI                 32768
SF            300.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 22.00 cm
F1P                10.000 ppm
F1               3001.30 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM            0.45455 ppm/cm
HZCM           136.42273 Hz/cm
```


Carbon Spectrum
157.243
142.036
133.582
132.421
128.777
128.651
121.894
121.462
119.398
111.253
100.344
77.352
76.929
76.506
68.443
26.991
25.809
22.220
O
N
N
H
9c
200
150
100
50
ppm
Current Data Parameters
NAME ON-III-34-B
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100624
Time 17.59
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 2048
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 512
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm

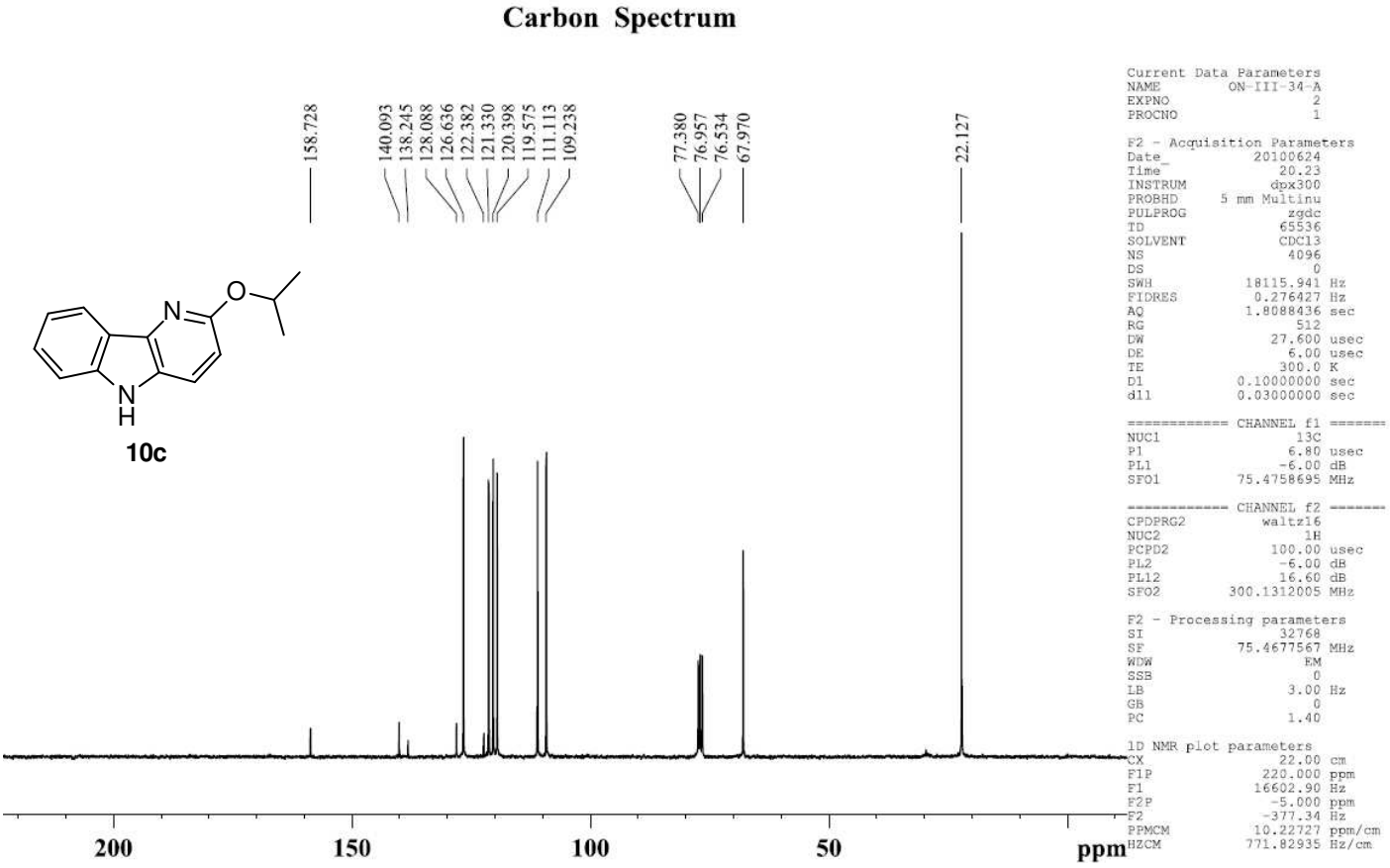


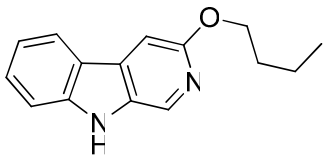
**2-isopropoxy-5*H*-pyrido[3,2-*b*]indole (10c)**

## Proton Spectrum



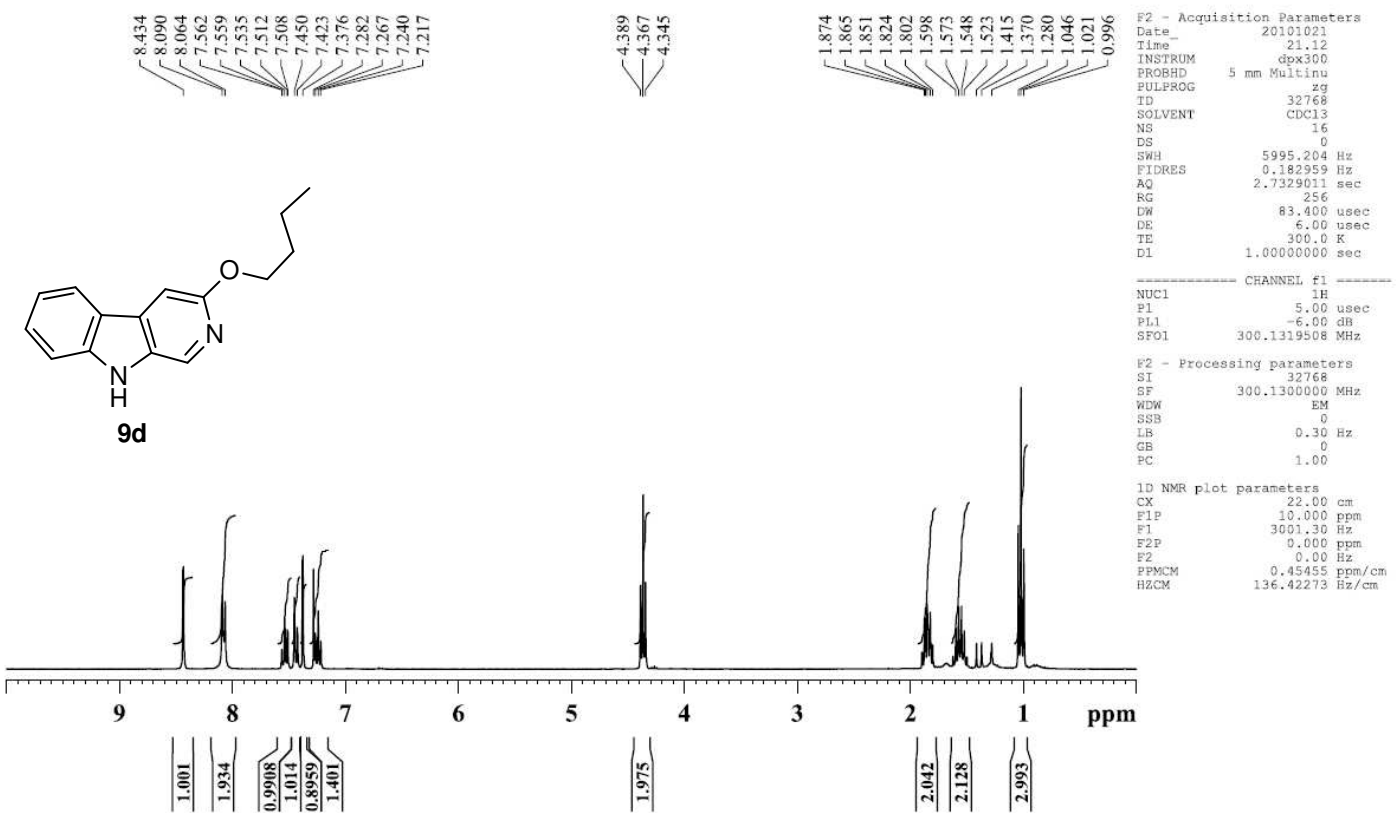

```
Current Data Parameters
NAME          ON-III-34-A
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_          20100624
Time              18.12
INSTRUM         dpx300
PROBHD     5 mm Multinu
PULPROG             zg
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.182959 Hz
AQ             2.7329011 sec
RG                  114
DW                83.400 usec
DE                 6.00 usec
TE                300.0 K
D1           1.00000000 sec

------------ CHANNEL f1 -------
NUC1                1H
P1                5.00 usec
PL1              -6.00 dB
SFO1        300.1319508 MHz

F2 - Processing parameters
SI                32768
SF          300.1300000 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00

1D NMR plot parameters
CX                22.00 cm
F1P               10.000 ppm
F1              3001.30 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM          0.45455 ppm/cm
HZCM         136.42273 Hz/cm
```


Carbon Spectrum
158.728
140.093
138.245
128.088
126.636
122.382
121.330
120.398
119.575
111.113
109.238
77.380
76.957
76.534
67.970
22.127
N
O
N
H
10c
200
150
100
50
ppm
Current Data Parameters
NAME ON-III-34-A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100624
Time 20.23
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 4096
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 512
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
========== CHANNEL f1 =======
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
========== CHANNEL f2 =======
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm



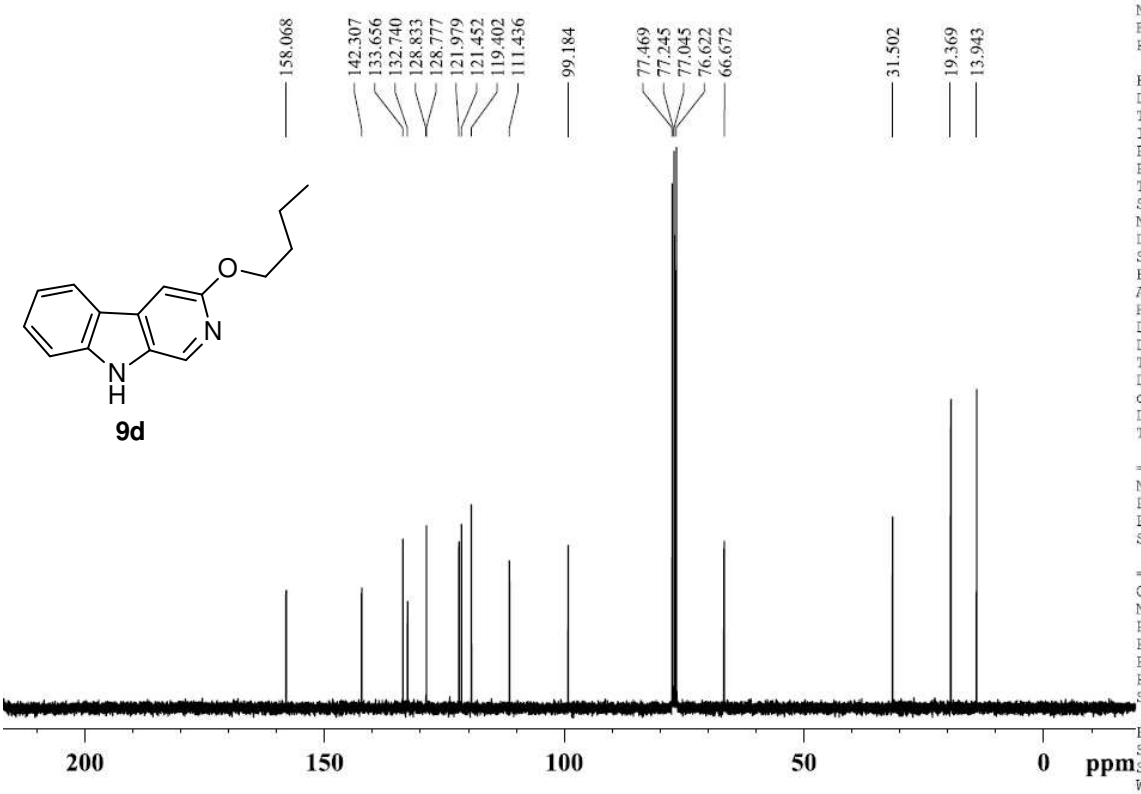
**3-butoxy-9*H*-pyrido[3,4-*b*]indole (9d)**

## Proton Spectrum

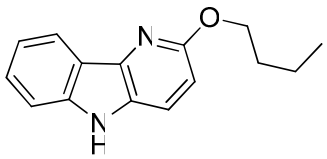



```
Current Data Parameters
NAME          ON-III-60-B
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20101021
Time_               21.12
INSTRUM           dpx300
PROBHD     5 mm Multinu
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH              5995.204 Hz
FIDRES           0.182959 Hz
AQ               2.7329011 sec
RG                   256
DW                 83.400 usec
DE                  6.00 usec
TE                 300.0 K
D1             1.00000000 sec

============ CHANNEL f1 =======
NUC1                   1H
P1                  5.00 usec
PL1                -6.00 dB
SFO1          300.1319508 MHz

F2 - Processing parameters
SI                 32768
SF            300.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 22.00 cm
F1P                10.000 ppm
F1               3001.30 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM            0.45455 ppm/cm
HZCM           136.42273 Hz/cm
```

## Carbon Spectrum

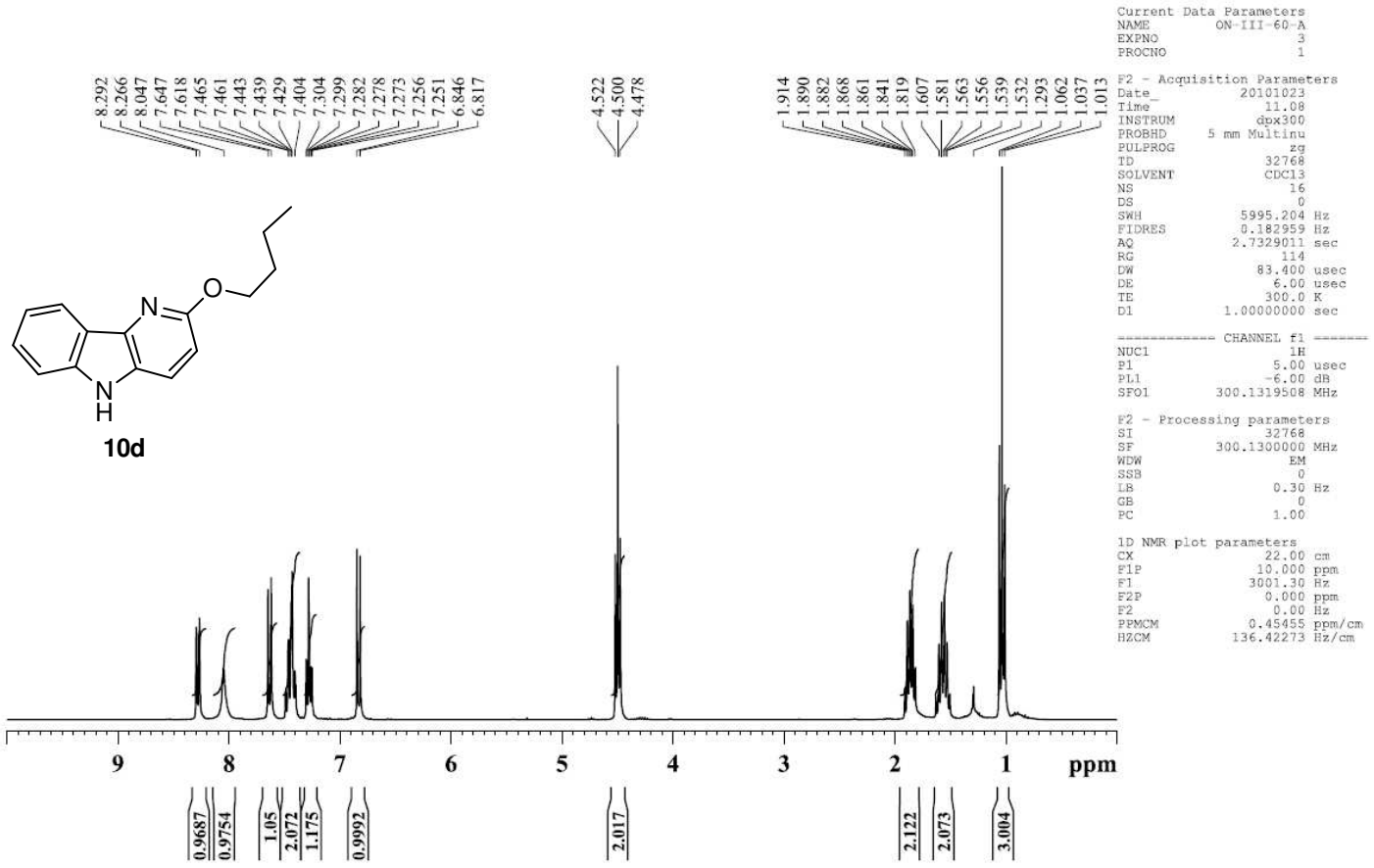



```
Current Data Parameters
NAME         ON-III-60-B
EXPNO                  2
PROCNO                 1

F2 - Acquisition Paramet
Date_           20110120
Time               19.20
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2000
DS                    4
SWH           17985.611
FIDRES         0.274439
AQ             1.8219508
RG                574.7
DW                27.800
DE                 6.00
TE                298.0
D1           2.00000000
d11          0.03000000
DELTA        1.89999998
TD0                   1

======== CHANNEL f1 ====
NUC1                 13C
P1                  6.35
PL1                -6.00
SFO1          75.4752950

======== CHANNEL f2 ====
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00
PL2                -6.00
PL12               17.85
PL13              120.00
SFO2         300.1312000

F2 - Processing paramete
SI                 32768
SF          75.4677490
WDW                   no
SSB                    0
LB                  0.00
GB                     0
PC                  1.40
```

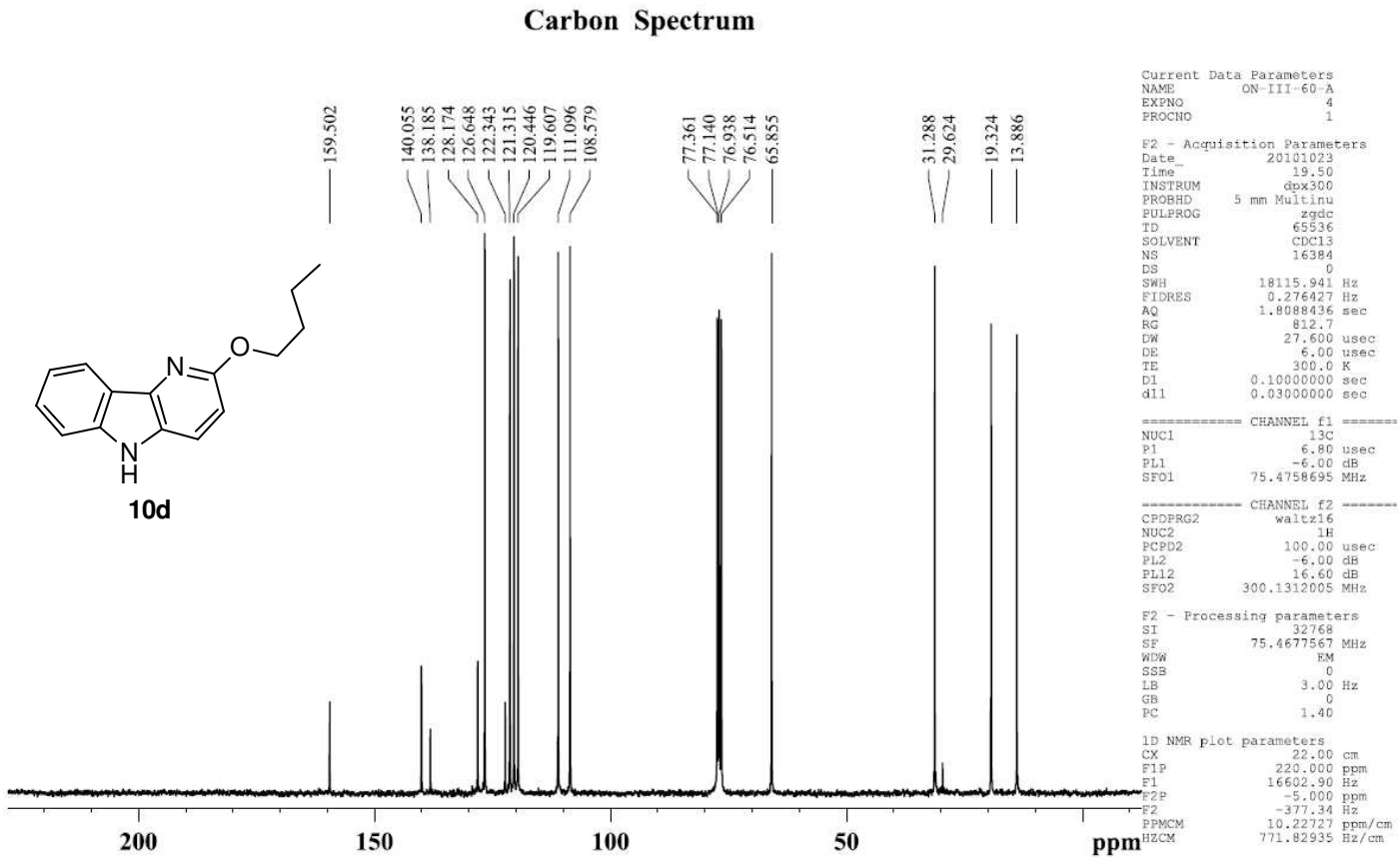


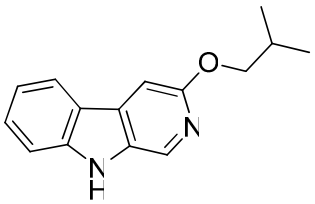
**2-butoxy-5*H*-pyrido[3,2-*b*]indole (10d)**

## Proton Spectrum



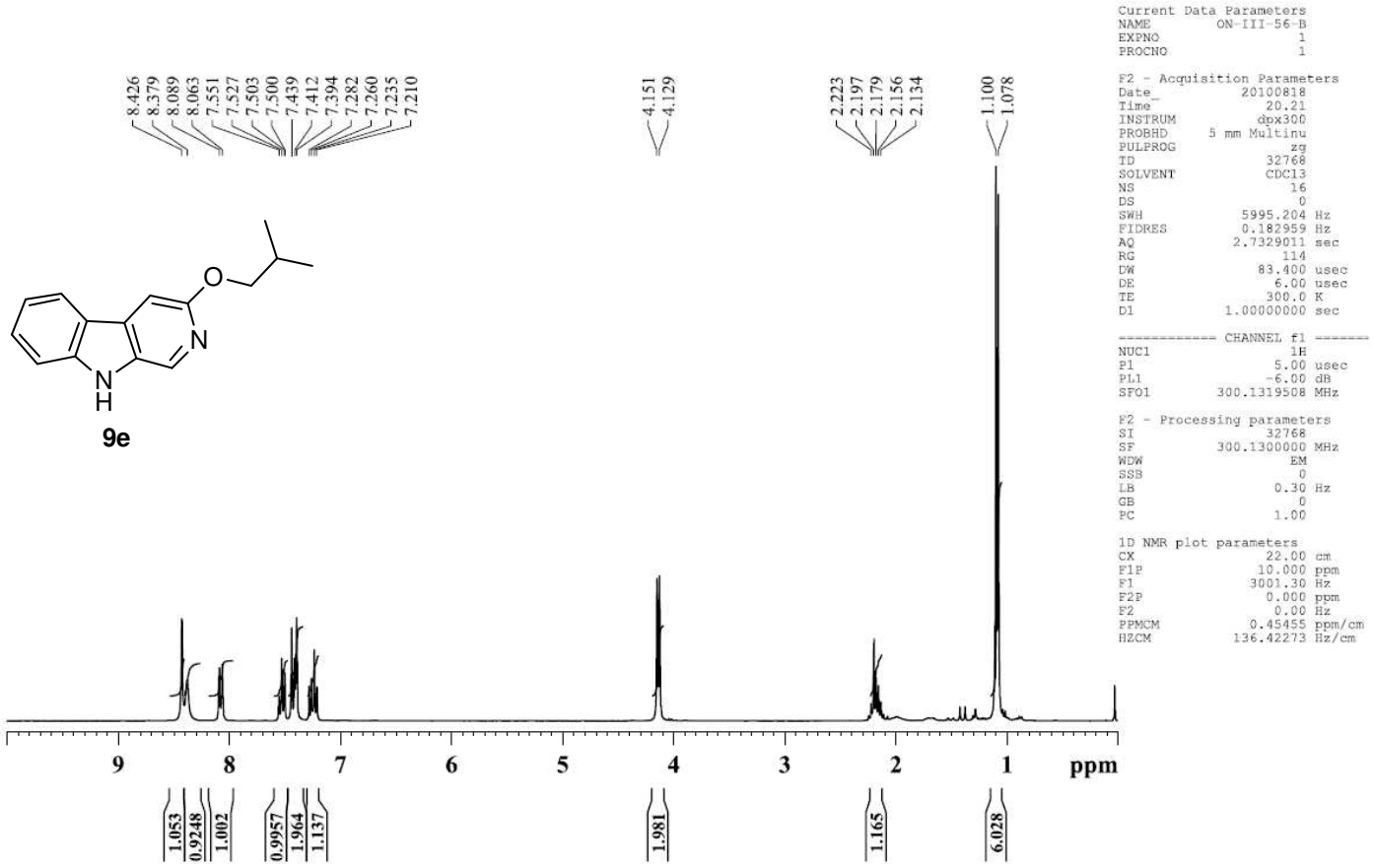

```
Current Data Parameters
NAME          ON-III-60-A
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_           20101023
Time              11.08
INSTRUM          dpx300
PROBHD     5 mm Multinu
PULPROG             zg
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.182959 Hz
AQ             2.7329011 sec
RG                  114
DW               83.400 usec
DE                6.00 usec
TE               300.0 K
D1            1.00000000 sec

============ CHANNEL f1 =======
NUC1                1H
P1                5.00 usec
PL1              -6.00 dB
SFO1        300.1319508 MHz

F2 - Processing parameters
SI                32768
SF          300.1300000 MHz
WDW                 EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                22.00 cm
F1P               10.000 ppm
F1              3001.30 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM          0.45455 ppm/cm
HZCM         136.42273 Hz/cm
```


Carbon Spectrum
159.502
140.055
138.185
128.174
126.648
122.343
121.315
120.446
119.607
111.096
108.579
77.361
77.140
76.938
76.514
65.855
31.288
29.624
19.324
13.886
N
O
N
H
10d
200
150
100
50
ppm
Current Data Parameters
NAME ON-III-60-A
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101023
Time 19.50
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 16384
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 812.7
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm

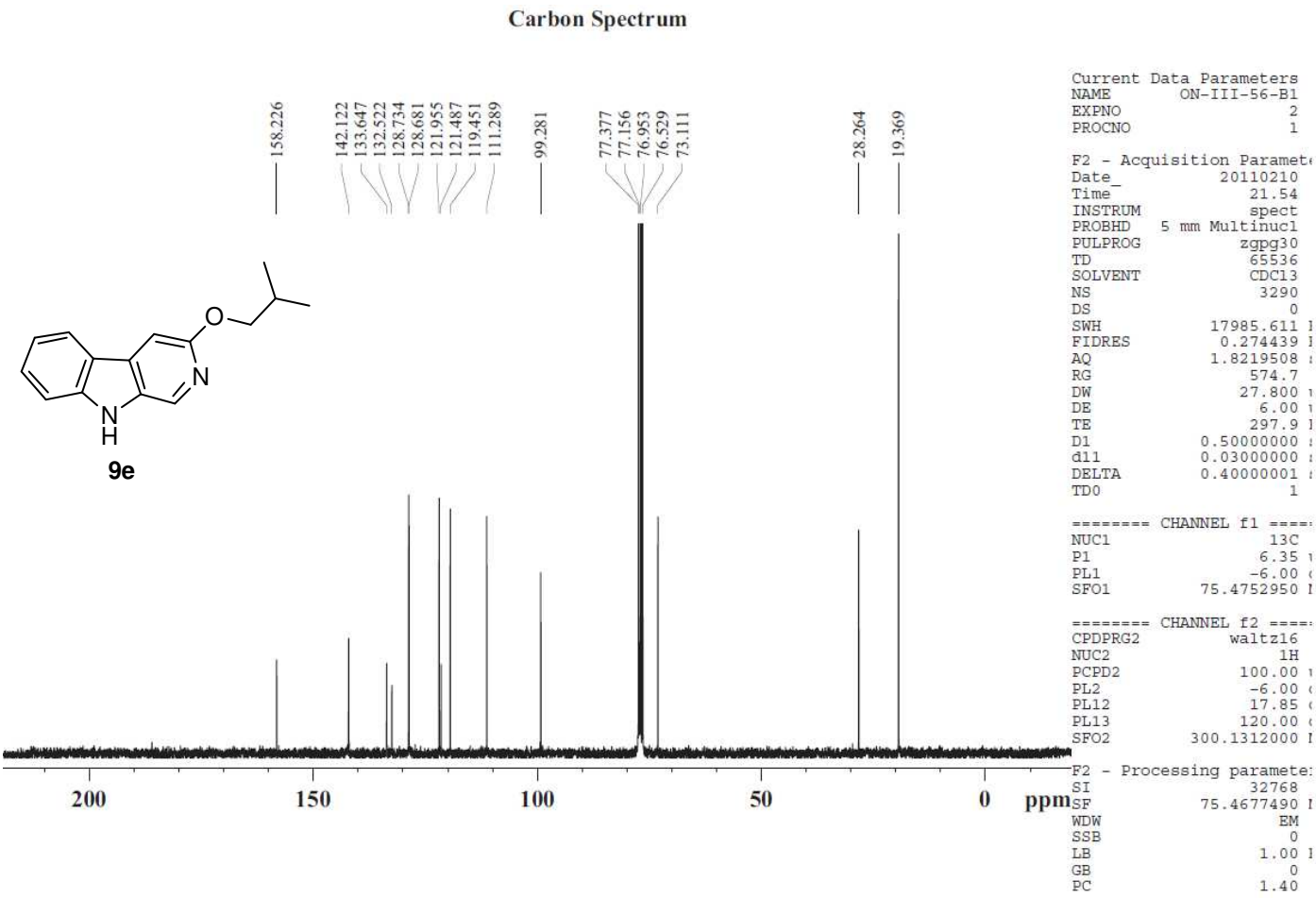


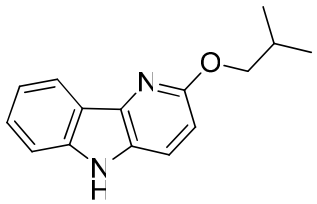
**3-isobutoxy-9*H*-pyrido[3,4-*b*]indole (9e)**

**Proton Spectrum**



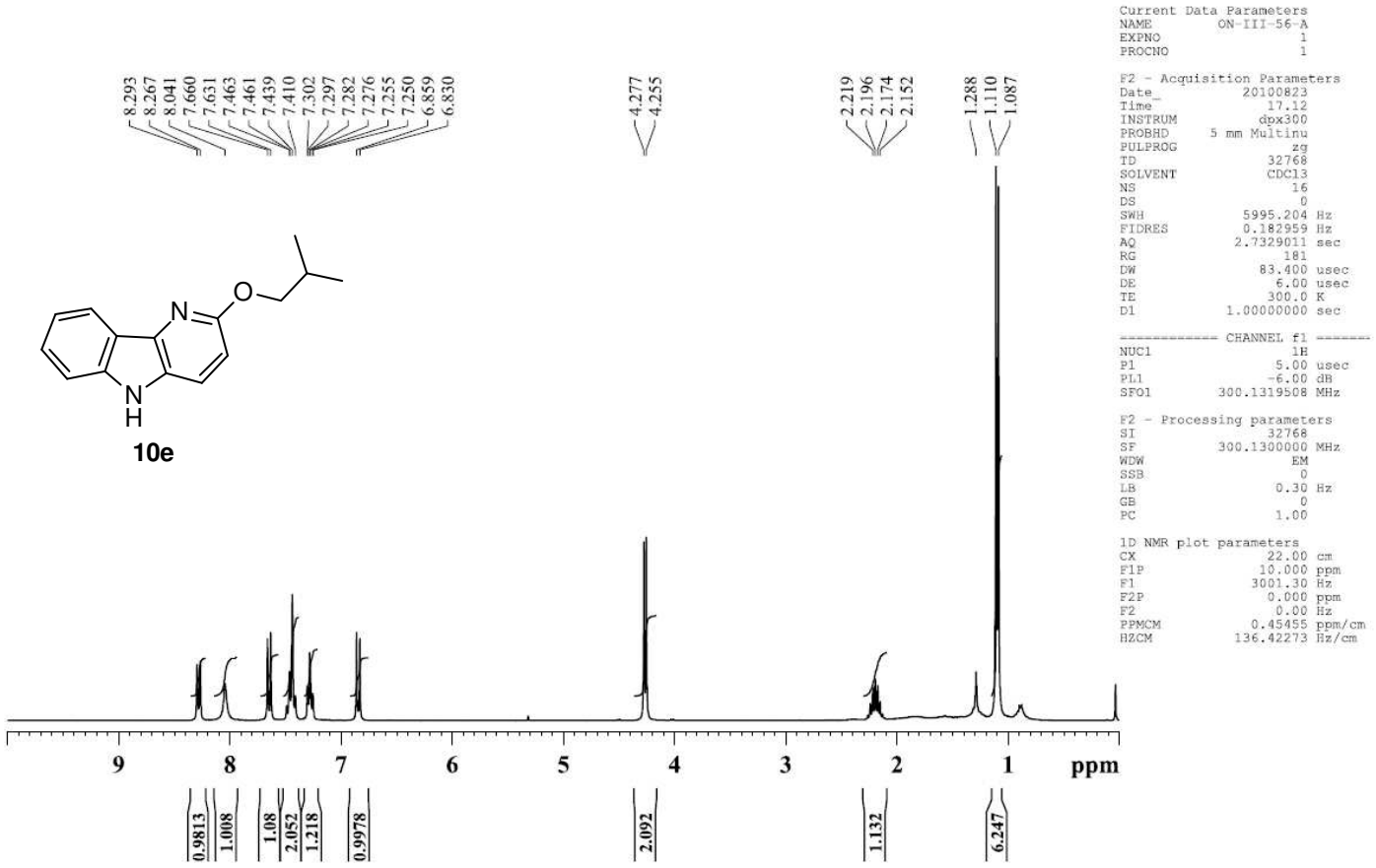

```
Current Data Parameters
NAME          ON-III-56-B
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100818
Time                20.21
INSTRUM           dpx300
PROBHD     5 mm Multinu
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             5995.204 Hz
FIDRES          0.182959 Hz
AQ              2.7329011 sec
RG                   114
DW                83.400 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec

------------ CHANNEL f1 -------
NUC1                  1H
P1                  5.00 usec
PL1                -6.00 dB
SFO1         300.1319508 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 22.00 cm
F1P                10.000 ppm
F1               3001.30 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM           0.45455 ppm/cm
HZCM          136.42273 Hz/cm
```


Carbon Spectrum
158.226
142.122
133.647
132.522
128.734
128.681
121.955
121.487
119.451
111.289
99.281
77.377
77.156
76.953
76.529
73.111
28.264
19.369
O
N
N
H
9e
200
150
100
50
0
ppm
Current Data Parameters
NAME ON-III-56-B1
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20110210
Time_ 21.54
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3290
DS 0
SWH 17985.611
FIDRES 0.274439
AQ 1.8219508
RG 574.7
DW 27.800
DE 6.00
TE 297.9
D1 0.50000000
d11 0.03000000
DELTA 0.40000001
TD0 1
======== CHANNEL f1 ====
NUC1 13C
P1 6.35
PL1 -6.00
SFO1 75.4752950
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00
PL2 -6.00
PL12 17.85
PL13 120.00
SFO2 300.1312000
F2 - Processing paramete
SI 32768
SF 75.4677490
WDW EM
SSB 0
LB 1.00
GB 0
PC 1.40

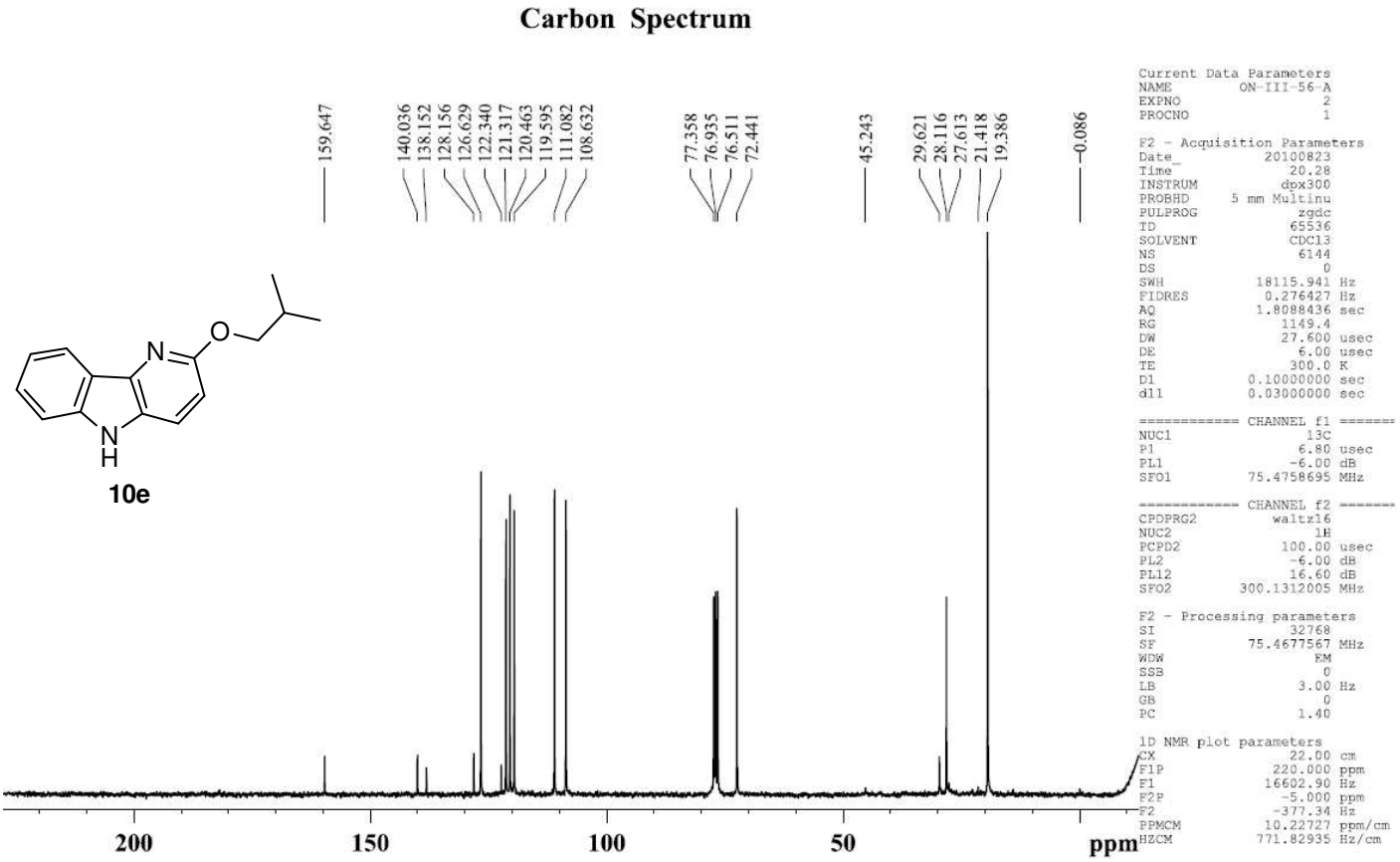


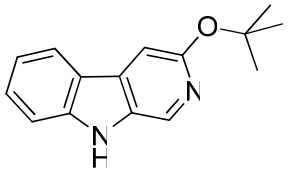
**2-isobutoxy-5*H*-pyrido[3,2-*b*]indole (10e)**

**Proton Spectrum**



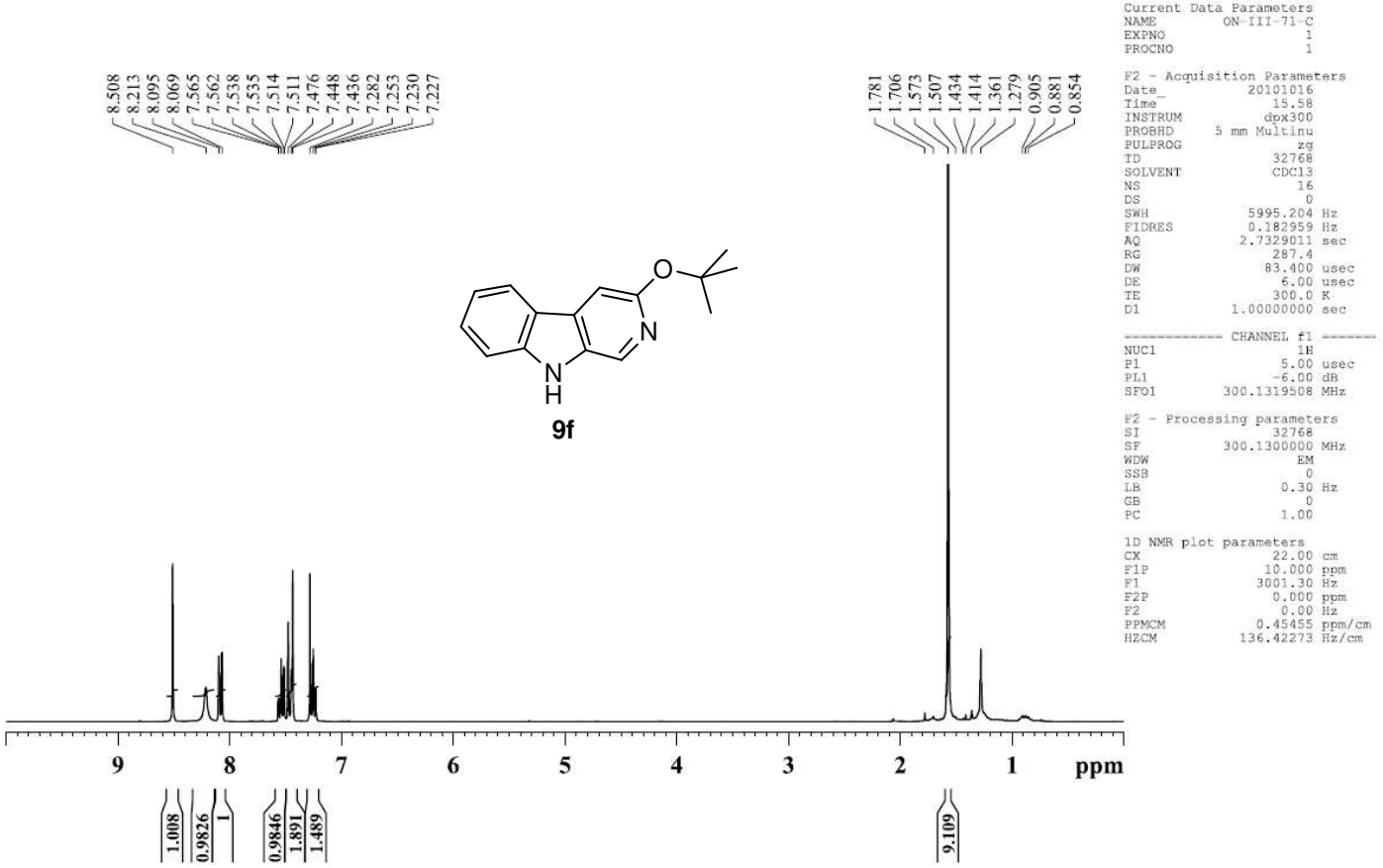

```
Current Data Parameters
NAME         ON-III-56-A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100823
Time              17.12
INSTRUM          dpx300
PROBHD     5 mm Multinu
PULPROG              zg
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.182959 Hz
AQ            2.7329011 sec
RG                  181
DW               83.400 usec
DE                6.00 usec
TE               300.0 K
D1            1.00000000 sec

------------ CHANNEL f1 -------
NUC1                1H
P1                5.00 usec
PL1              -6.00 dB
SFO1        300.1319508 MHz

F2 - Processing parameters
SI                32768
SF          300.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00

1D NMR plot parameters
CX               22.00 cm
F1P              10.000 ppm
F1             3001.30 Hz
F2P               0.000 ppm
F2                0.00 Hz
PPMCM          0.45455 ppm/cm
HZCM         136.42273 Hz/cm
```


Carbon Spectrum
159.647
140.036
138.152
128.156
126.629
122.340
121.317
120.463
119.595
111.082
108.632
77.358
76.935
76.511
72.441
45.243
29.621
28.116
27.613
21.418
19.386
0.086
N
O
N
H
10e
200
150
100
50
ppm
Current Data Parameters
NAME 0N-III-56-A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100823
Time 20.28
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 6144
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 1149.4
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm

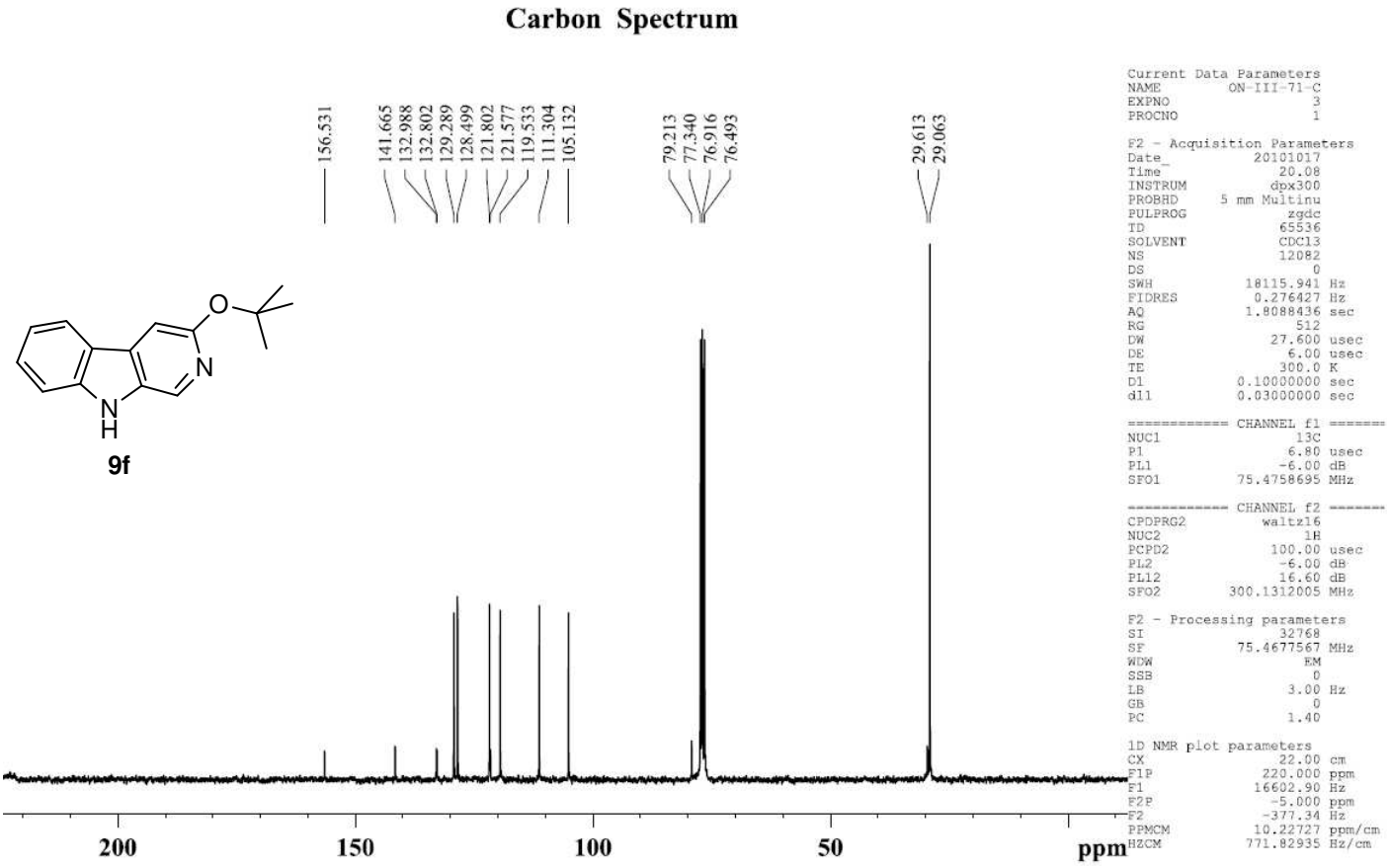


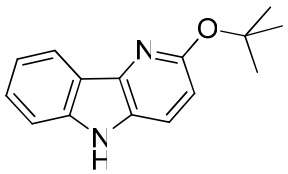
**3-(*tert*-butoxy)-9*H*-pyrido[3,4-*b*]indole (9f)**

**Proton Spectrum**



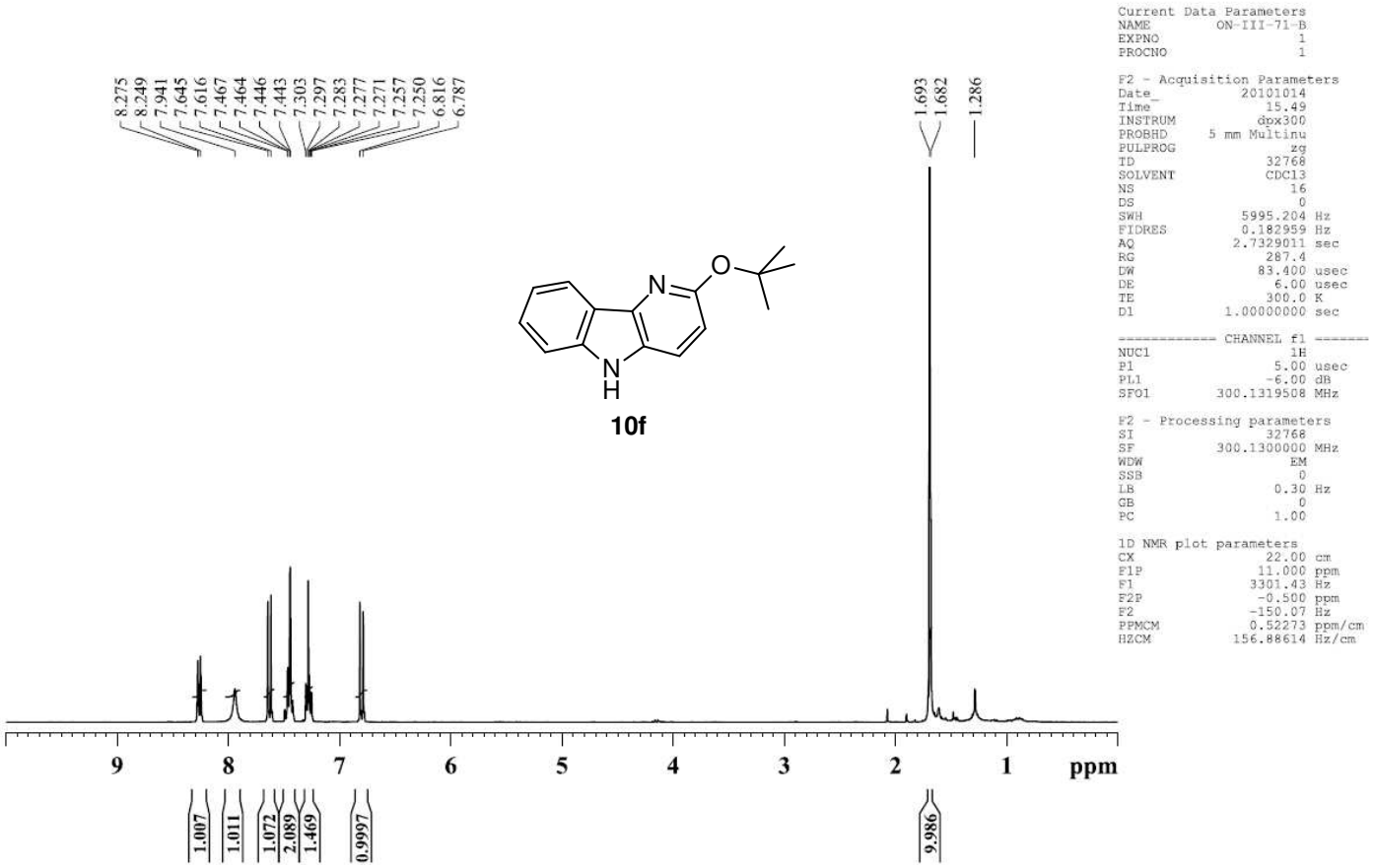

```
Current Data Parameters
NAME          ON-III-71-C
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_          20101016
Time              15.58
INSTRUM           dpx300
PROBHD     5 mm Multinu
PULPROG              zg
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.182959 Hz
AQ             2.7329011 sec
RG                287.4
DW               83.400 usec
DE                6.00 usec
TE                300.0 K
D1            1.00000000 sec

------------ CHANNEL f1 -------
NUC1                 1H
P1                5.00 usec
PL1              -6.00 dB
SFO1        300.1319508 MHz

F2 - Processing parameters
SI                32768
SF          300.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00

1D NMR plot parameters
CX               22.00 cm
F1P              10.000 ppm
F1             3001.30 Hz
F2P               0.000 ppm
F2                0.00 Hz
PPMCM          0.45455 ppm/cm
HZCM         136.42273 Hz/cm
```


Carbon Spectrum
156.531
141.665
132.988
132.802
129.289
128.499
121.802
121.577
119.533
111.304
105.132
79.213
77.340
76.916
76.493
29.613
29.063
O
N
N
H
9f
200
150
100
50
ppm
Current Data Parameters
NAME ON-III-71-C
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101017
Time 20.08
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 12082
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 512
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm

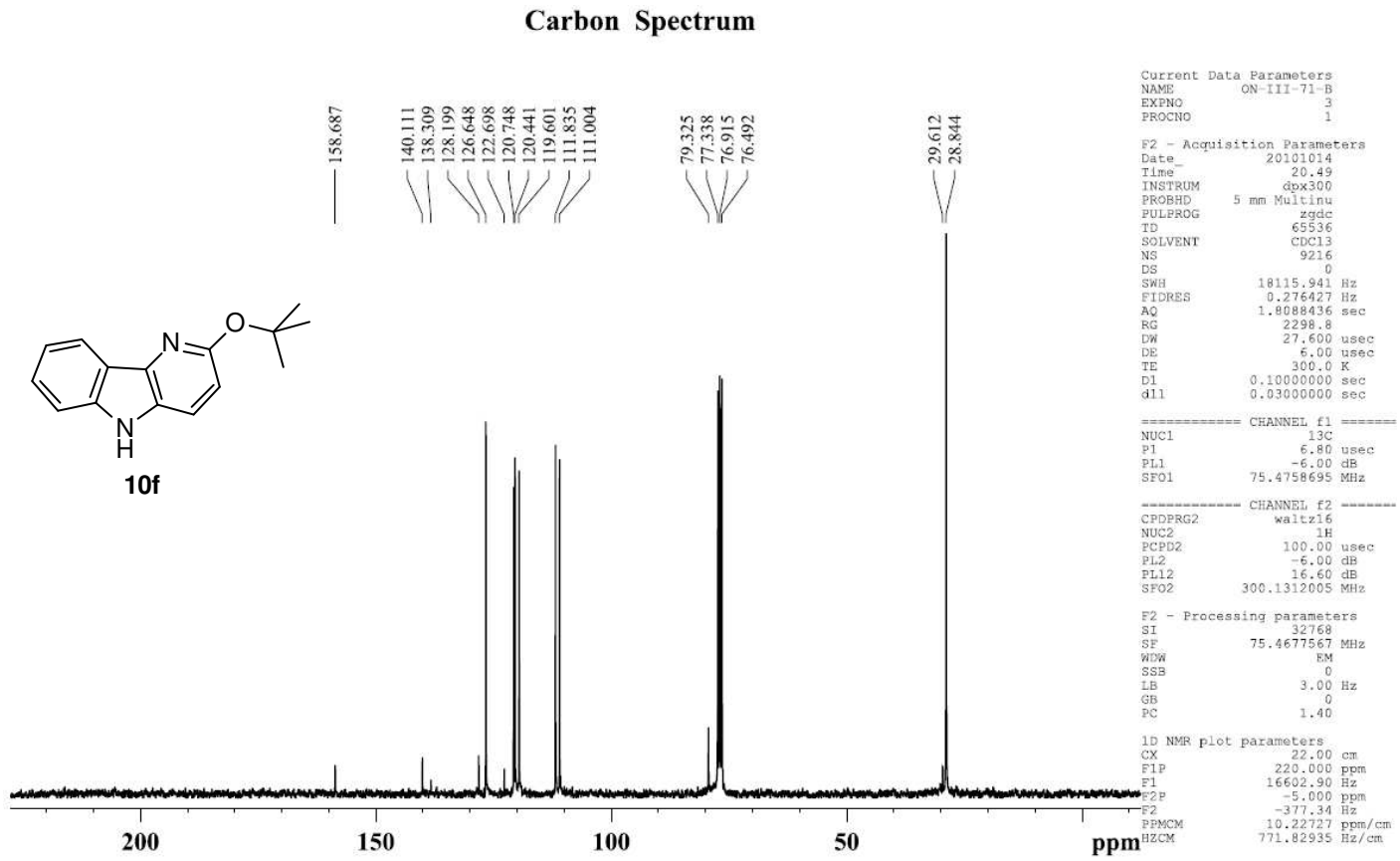


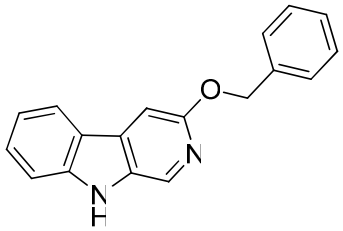
**2-(*tert*-butoxy)-5*H*-pyrido[3,2-*b*]indole (10f)**

**Proton Spectrum**



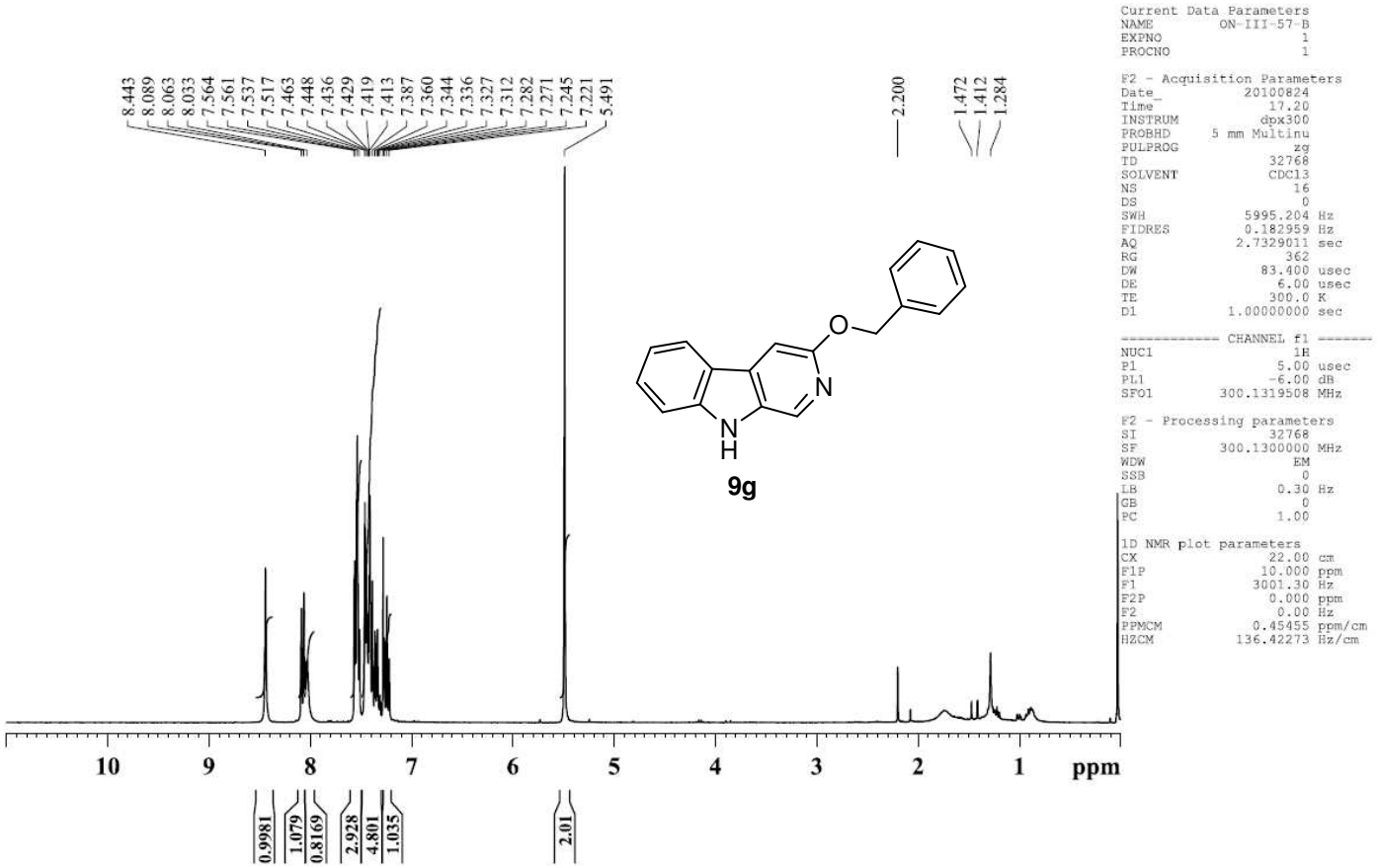

```
Current Data Parameters
NAME          ON-III-71-B
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_          20101014
Time              15.49
INSTRUM          dpx300
PROBHD     5 mm Multinu
PULPROG             zg
TD               32768
SOLVENT          CDCl3
NS                  16
DS                   0
SWH           5995.204 Hz
FIDRES        0.182959 Hz
AQ            2.7329011 sec
RG                287.4
DW               83.400 usec
DE                6.00 usec
TE               300.0 K
D1            1.00000000 sec

------------ CHANNEL f1 -------
NUC1                 1H
P1                 5.00 usec
PL1               -6.00 dB
SFO1         300.1319508 MHz

F2 - Processing parameters
SI               32768
SF           300.1300000 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00

1D NMR plot parameters
CX                22.00 cm
F1P               11.000 ppm
F1              3301.43 Hz
F2P               -0.500 ppm
F2              -150.07 Hz
PPMCM             0.52273 ppm/cm
HZCM            156.88614 Hz/cm
```


Carbon Spectrum
158.687
140.111
138.309
128.199
126.648
122.698
120.748
120.441
119.601
111.835
111.004
79.325
77.338
76.915
76.492
29.612
28.844
N
O
N
H
10f
200
150
100
50
ppm
Current Data Parameters
NAME ON-III-71-B
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101014
Time_ 20.49
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 9216
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 2298.8
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm

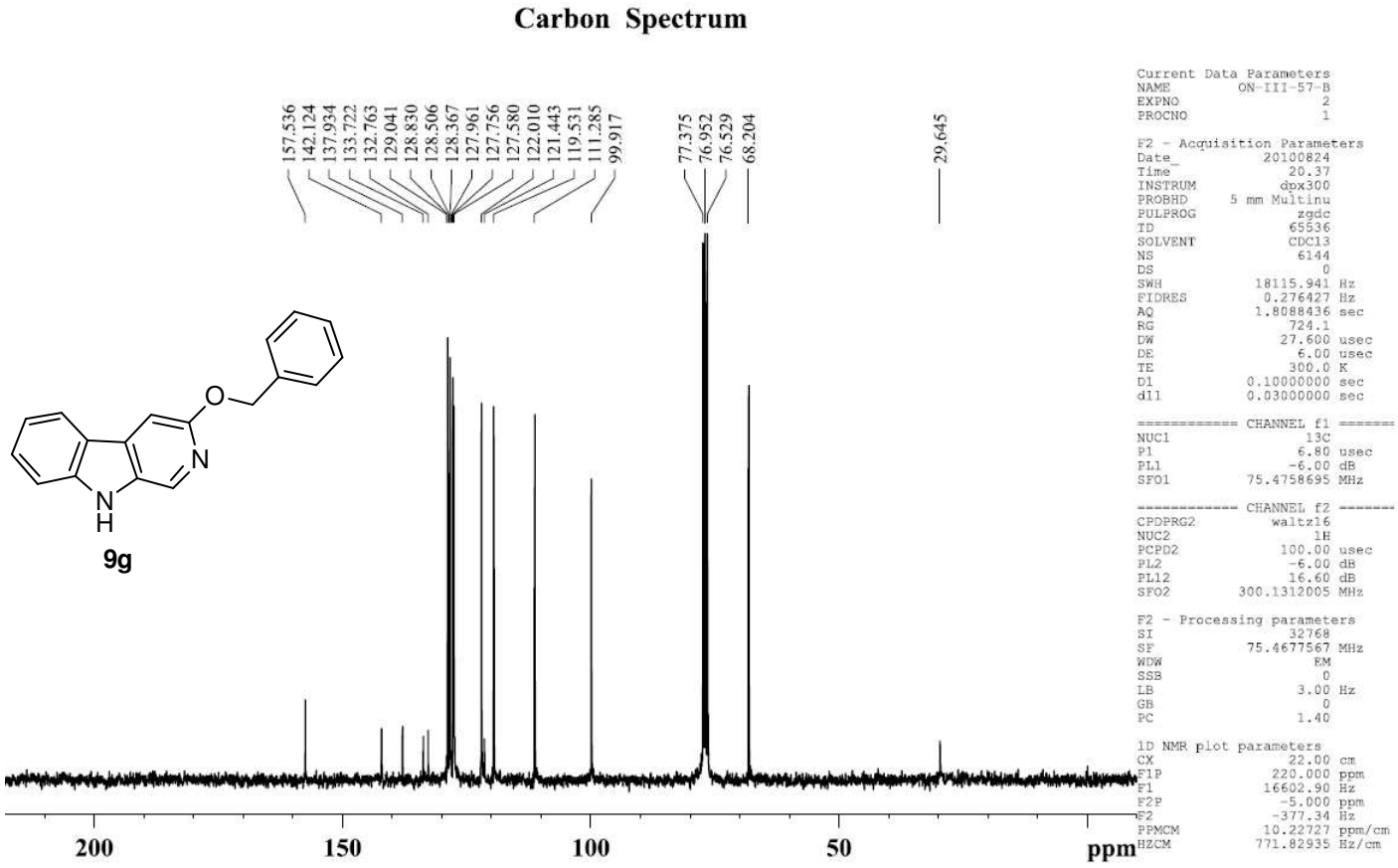


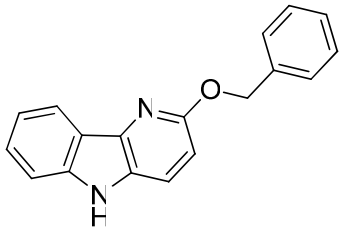
**3-(benzyloxy)-9*H*-pyrido[3,4-*b*]indole (9g)**

**Proton Spectrum**



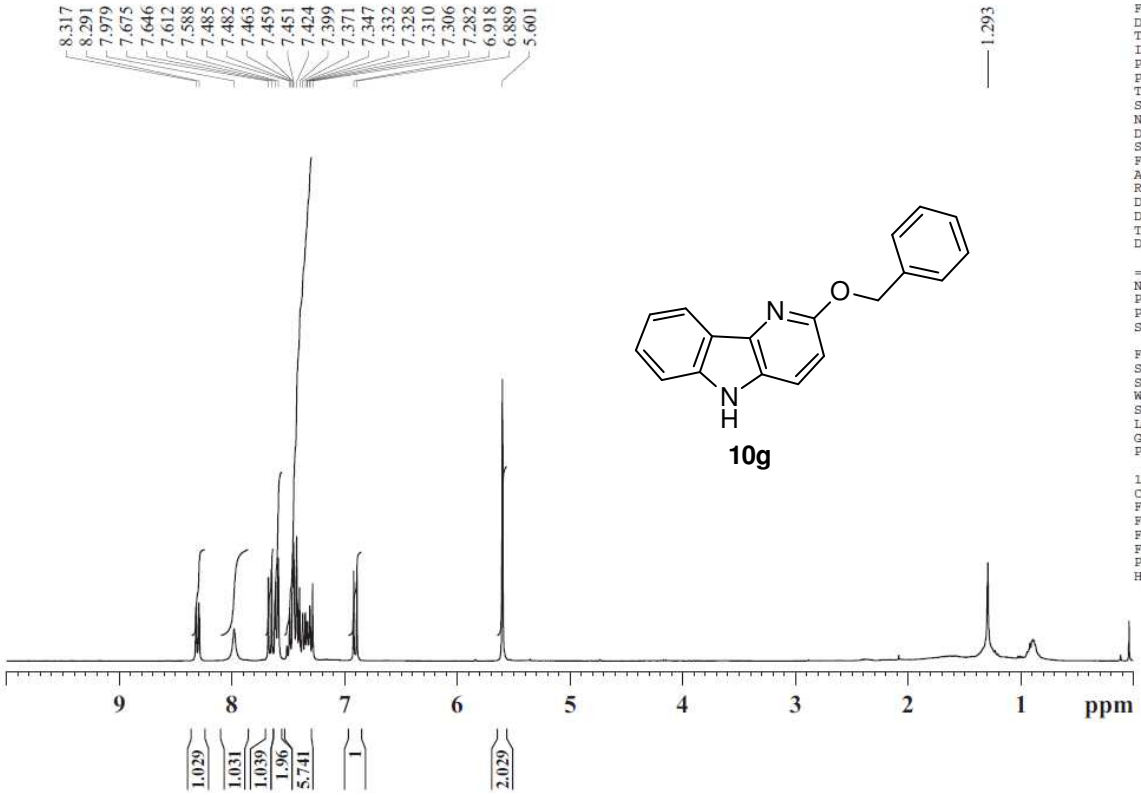

```
Current Data Parameters
NAME                  ON-III-57-B
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20100824
Time                        17.20
INSTRUM                   dpx300
PROBHD          5 mm Multinu
PULPROG                         zg
TD                           32768
SOLVENT                     CDCl3
NS                             16
DS                              0
SWH                   5995.204 Hz
FIDRES                0.182959 Hz
AQ                    2.7329011 sec
RG                            362
DW                       83.400 usec
DE                        6.00 usec
TE                        300.0 K
D1                    1.00000000 sec

------------ CHANNEL f1 -------
NUC1                          1H
P1                        5.00 usec
PL1                      -6.00 dB
SFO1                300.1319508 MHz

F2 - Processing parameters
SI                           32768
SF                  300.1300000 MHz
WDW                            EM
SSB                             0
LB                         0.30 Hz
GB                              0
PC                           1.00

1D NMR plot parameters
CX                          22.00 cm
F1P                        10.000 ppm
F1                       3001.30 Hz
F2P                         0.000 ppm
F2                          0.00 Hz
PPMCM                    0.45455 ppm/cm
HZCM                   136.42273 Hz/cm
```


Carbon Spectrum
157.536
142.124
137.934
133.722
132.763
129.041
128.830
128.506
128.367
127.961
127.756
127.580
122.010
121.443
119.531
111.285
99.917
77.375
76.952
76.529
68.204
29.645
O
N
N
H
9g
200
150
100
50
ppm
Current Data Parameters
NAME ON-III-57-B
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100824
Time 20.37
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 6144
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 724.1
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 6.80 usec
PL1 -6.00 dB
SFO1 75.4758695 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 16.60 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.22727 ppm/cm
HZCM 771.82935 Hz/cm



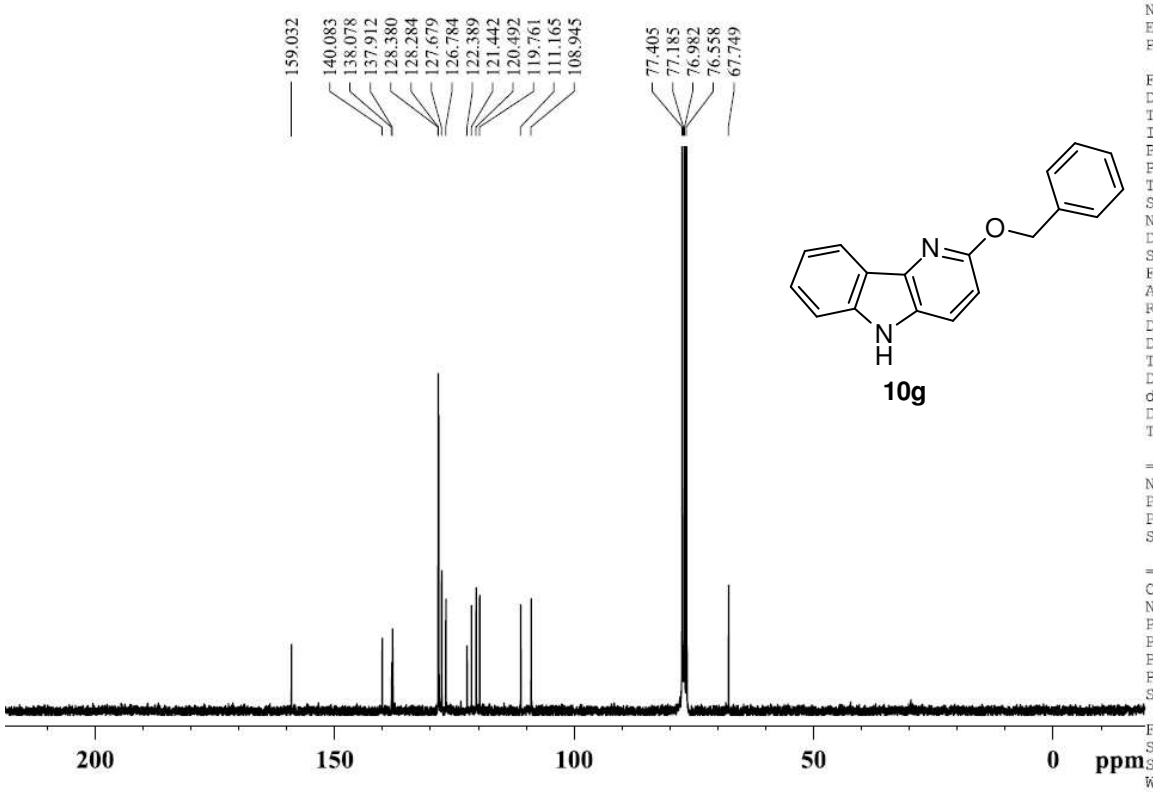
**2-(benzyloxy)-5*H*-pyrido[3,2-*b*]indole (10g)**

## Proton Spectrum




```
Current Data Parameters
NAME          ON-III-57-A
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100825
Time                17.24
INSTRUM           dpx300
PROBHD     5 mm Multinu
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             5995.204 Hz
FIDRES          0.182959 Hz
AQ              2.7329011 sec
RG                 228.1
DW                83.400 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec

============ CHANNEL f1 =======
NUC1                   1H
P1                   5.00 usec
PL1                 -6.00 dB
SFO1          300.1319508 MHz

F2 - Processing parameters
SI                 32768
SF            300.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 22.00 cm
F1P               10.000 ppm
F1              3001.30 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM           0.45455 ppm/cm
HZCM          136.42273 Hz/cm
```

**Carbon Spectrum**

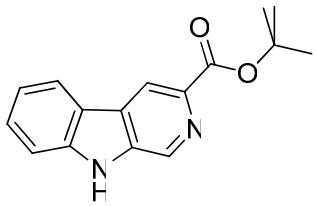






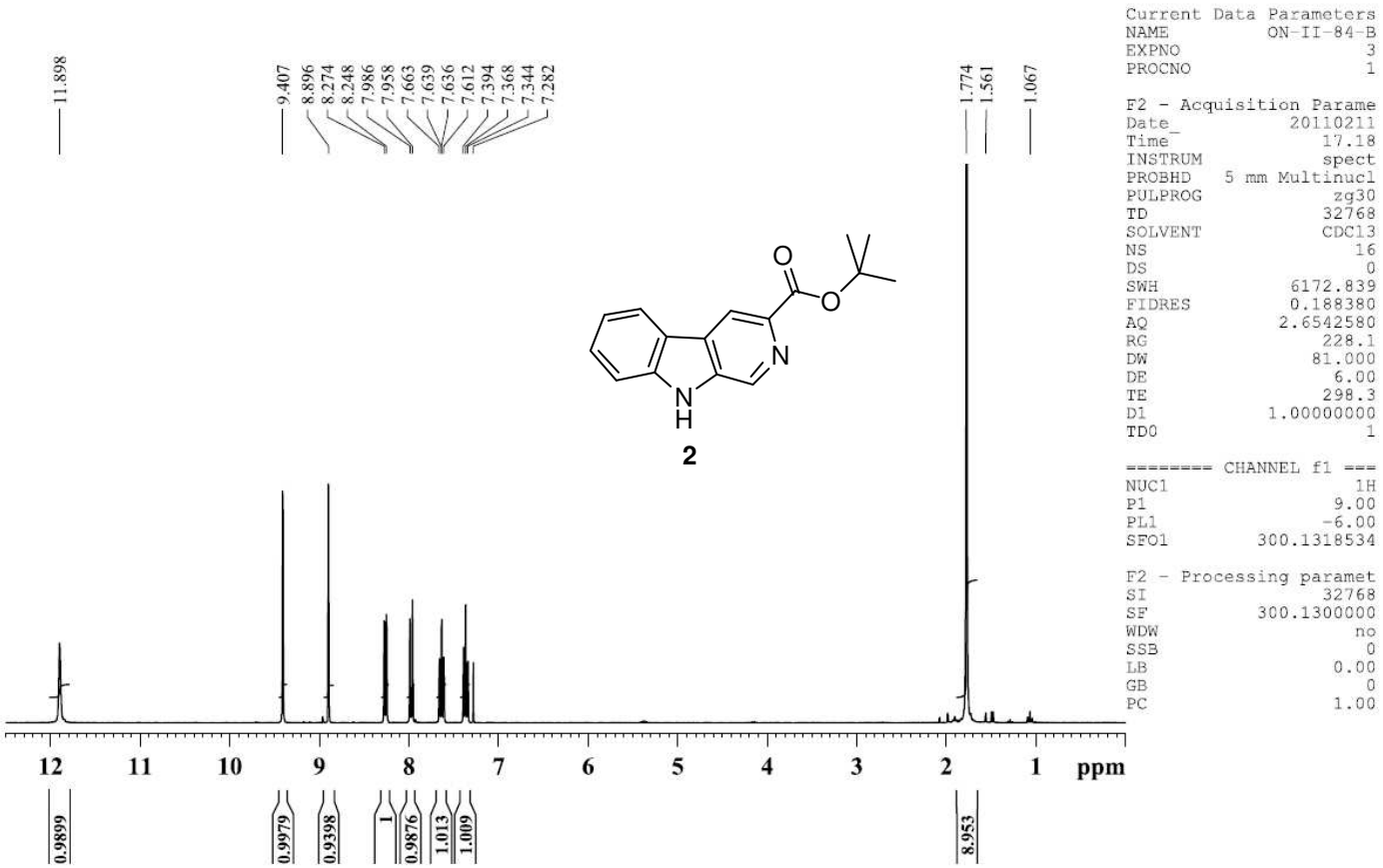
**10g**

```
Current Data Parameters
NAME          ON-III-57-A
EXPNO                   4
PROCNO                  1

F2 - Acquisition Paramet
Date_            20110121
Time                20.13
INSTRUM             spect
PROBHD   5 mm Multinucl
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    2894
DS                       4
SWH              17985.611
FIDRES           0.274439
AQ               1.8219508
RG                   724.1
DW                  27.800
DE                    6.00
TE                  298.0
D1             2.00000000
d11            0.03000000
DELTA          1.89999998
TD0                      1

======== CHANNEL f1 =====
NUC1                   13C
P1                    6.35
PL1                  -6.00
SFO1           75.4752950

======== CHANNEL f2 =====
CPDPRG2            waltz16
NUC2                   1H
PCPD2               100.00
PL2                  -6.00
PL12                 17.85
PL13                120.00
SFO2           300.1312000

F2 - Processing paramete
SI                    32768
SF             75.4677490
WDW                      EM
SSB         0
LB                    1.00
GB          0
PC                    1.40
```

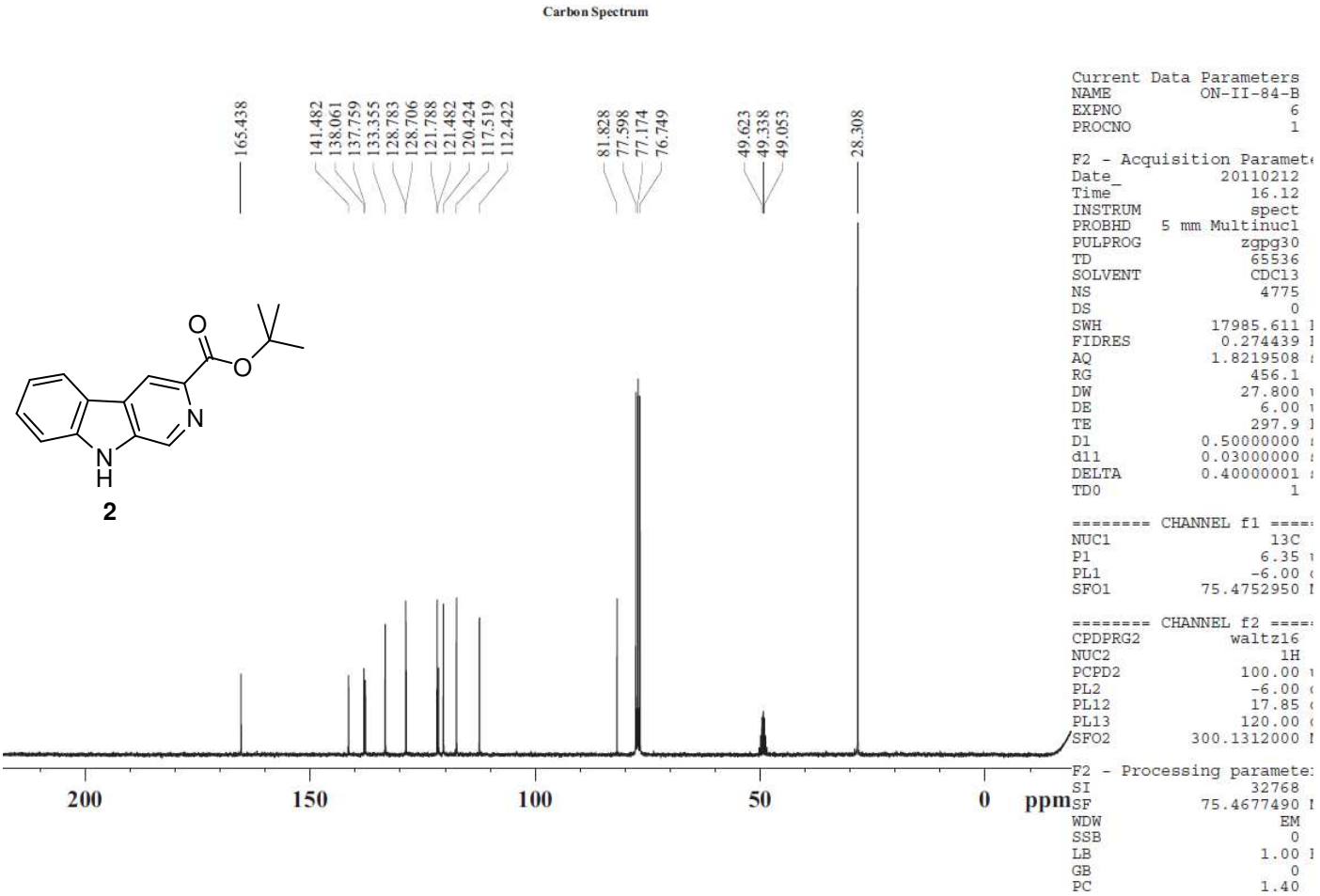


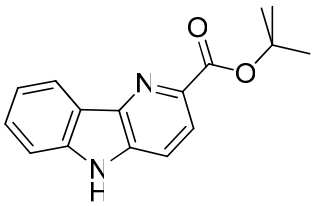
***tert*-butyl 9*H*-pyrido[3,4-*b*]indole-3-carboxylate (2)**

**Proton Spectrum**

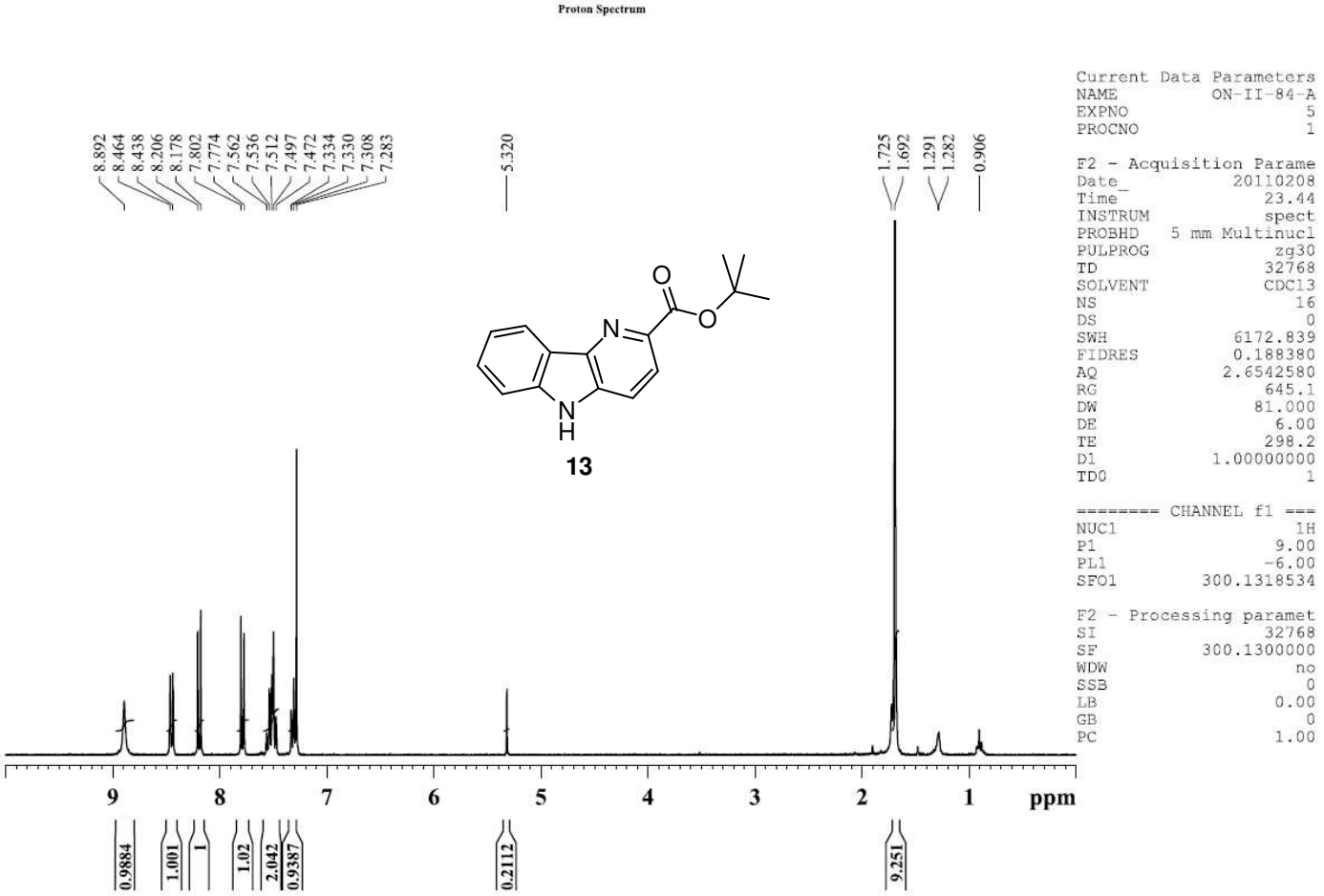


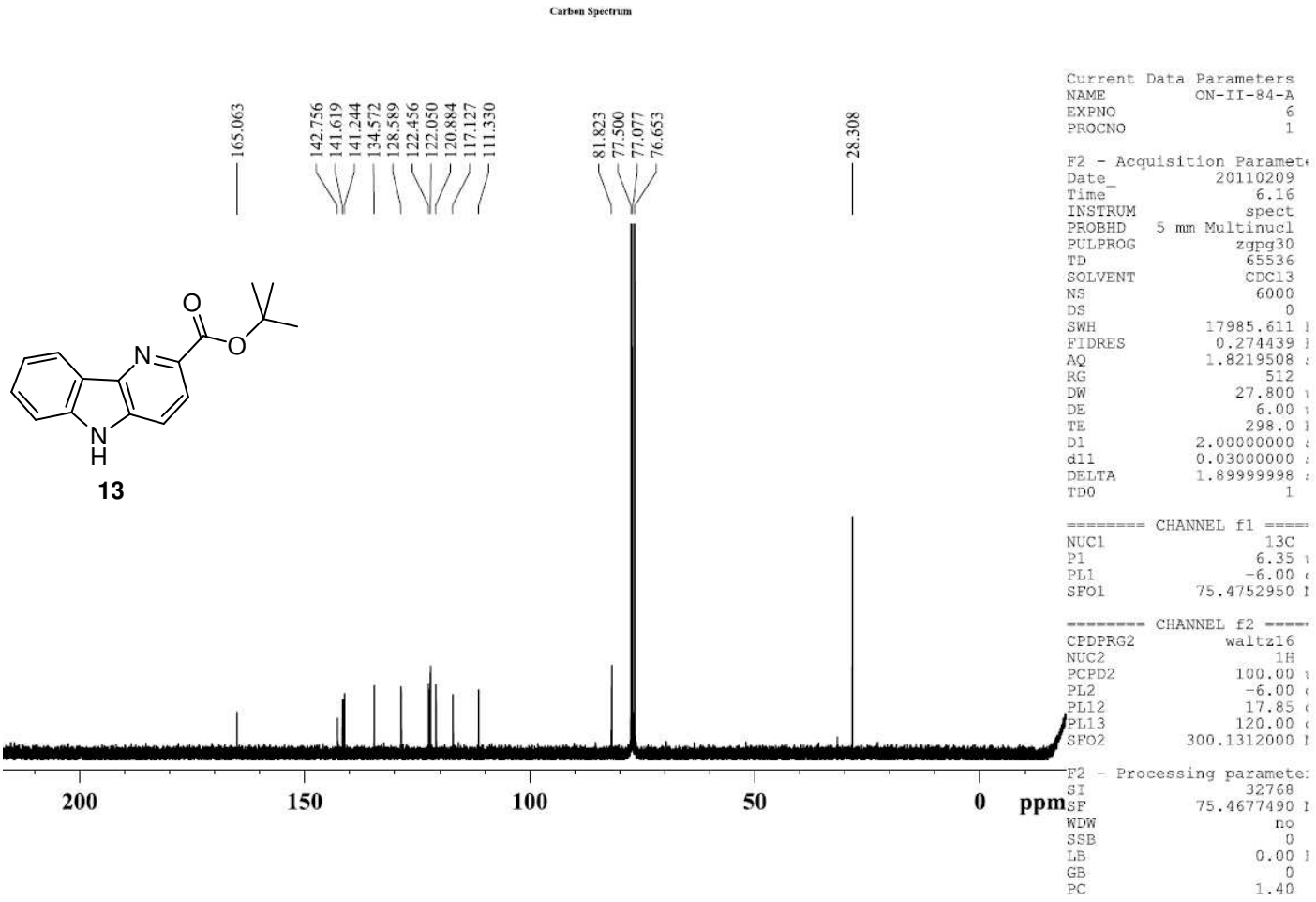

```
Current Data Parameters
NAME          ON-II-84-B
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parame
Date_           20110211
Time_              17.18
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             6172.839
FIDRES          0.188380
AQ              2.6542580
RG                 228.1
DW                81.000
DE                 6.00
TE                298.3
D1           1.00000000
TD0                    1

======== CHANNEL f1 ===
NUC1                  1H
P1                  9.00
PL1                -6.00
SFO1         300.1318534

F2 - Processing paramet
SI                 32768
SF          300.1300000
WDW                   no
SSB                    0
LB                  0.00
GB                     0
PC                  1.00
```


Carbon Spectrum
165.438
141.482
138.061
137.759
133.355
128.783
128.706
121.788
121.482
120.424
117.519
112.422
81.828
77.598
77.174
76.749
49.623
49.338
49.053
28.308
O
O
N
N
H
2
200
150
100
50
0
ppm
Current Data Parameters
NAME ON-II-84-B
EXPNO 6
PROCNO 1
F2 - Acquisition Paramet
Date_ 20110212
Time 16.12
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4775
DS 0
SWH 17985.611
FIDRES 0.274439
AQ 1.8219508
RG 456.1
DW 27.800
DE 6.00
TE 297.9
D1 0.50000000
d11 0.03000000
DELTA 0.40000001
TD0 1
======== CHANNEL f1 ====
NUC1 13C
P1 6.35
PL1 -6.00
SFO1 75.4752950
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00
PL2 -6.00
PL12 17.85
PL13 120.00
SFO2 300.1312000
F2 - Processing paramete
SI 32768
SF 75.4677490
WDW EM
SSB 0
LB 1.00
GB 0
PC 1.40



***tert*-butyl 5*H*-pyrido[3,2-*b*]indole-2-carboxylate (13)**




Carbon Spectrum
165.063
142.756
141.619
141.244
134.572
128.589
122.456
122.050
120.884
117.127
111.330
81.823
77.500
77.077
76.653
28.308
O
O
N
N
H
13
200
150
100
50
0
ppm
Current Data Parameters
NAME ON-II-84-A
EXPNO 6
PROCNO 1
F2 - Acquisition Paramet
Date_ 20110209
Time 6.16
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6000
DS 0
SWH 17985.611
FIDRES 0.274439
AQ 1.8219508
RG 512
DW 27.800
DE 6.00
TE 298.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
======== CHANNEL f1 ====
NUC1 13C
P1 6.35
PL1 -6.00
SFO1 75.4752950
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00
PL2 -6.00
PL12 17.85
PL13 120.00
SFO2 300.1312000
F2 - Processing paramete
SI 32768
SF 75.4677490
WDW no
SSB 0
LB 0.00
GB 0
PC 1.40

## X-ray diffraction data on compounds 1 and 6

Single-crystal X-ray diffraction data on compounds **1** and **6** were collected using MoKα radiation and a Bruker APEX 2 CCD area detector. Crystals were prepared for data collection by coating with high viscosity microscope oil. The oil-coated crystal was mounted on a micro-mesh mount (Mitergen, Inc.) and transferred to the diffractometer. The structures were solved by direct methods and refined by full-matrix least squares on $F^2$ values using the programs found in the SHELXTL suite (Bruker, SHELXTL v6.10, 2000, Bruker AXS Inc., Madison, WI).[1] Corrections were applied for Lorentz, polarization, and absorption effects. Parameters refined included atomic coordinates and anisotropic thermal parameters for all non-hydrogen atoms. Hydrogen atoms on carbons were included using a riding model [coordinate shifts of C applied to H atoms] with C-H distance set at 0.96 Å. Complete information on data collection and refinement is available in the supplemental material.

For compound **1** a 0.313 x 0.082 x 0.042 $mm^3$ crystal was prepared for data collection and a data set collected at 100 K. The crystal was orthorhombic in space group $P\ 2_12_12$, with unit cell dimensions a = 15.2022(11), b = 14.2864(9), and c = 11.7464(11) Å. Data was 100.0% complete to 25.00° θ with an average redundancy of 7.45. The final anisotropic full matrix least-squares refinement on $F^2$ with 304 variables converged at R1 = 5.27%, for the observed data and wR2 = 12.55% for all data.

For compound **6** a 0.651 x 0.287 x 0.015 $mm^3$ crystal was prepared for data collection and a data set collected at 100 K. The crystal was triclinic in space group $P\ 1$, with unit cell dimensions a = 5.1335(14), b = 10.319(3), c = 10.983(3) Å, α = 75.541(9)°, β = 84.199(10)°, and γ = 88.679(10)°. Data was 98.7% complete to 25.00° θ with an average redundancy of 2.01. The final anisotropic full matrix least-squares refinement on $F^2$ with 304 variables converged at R1 = 9.24%, for the observed data and wR2 = 24.69% for all data.

[1] Sheldrick, G.M. *Acta Cryst*. **2008**, *A64*, 112-122.

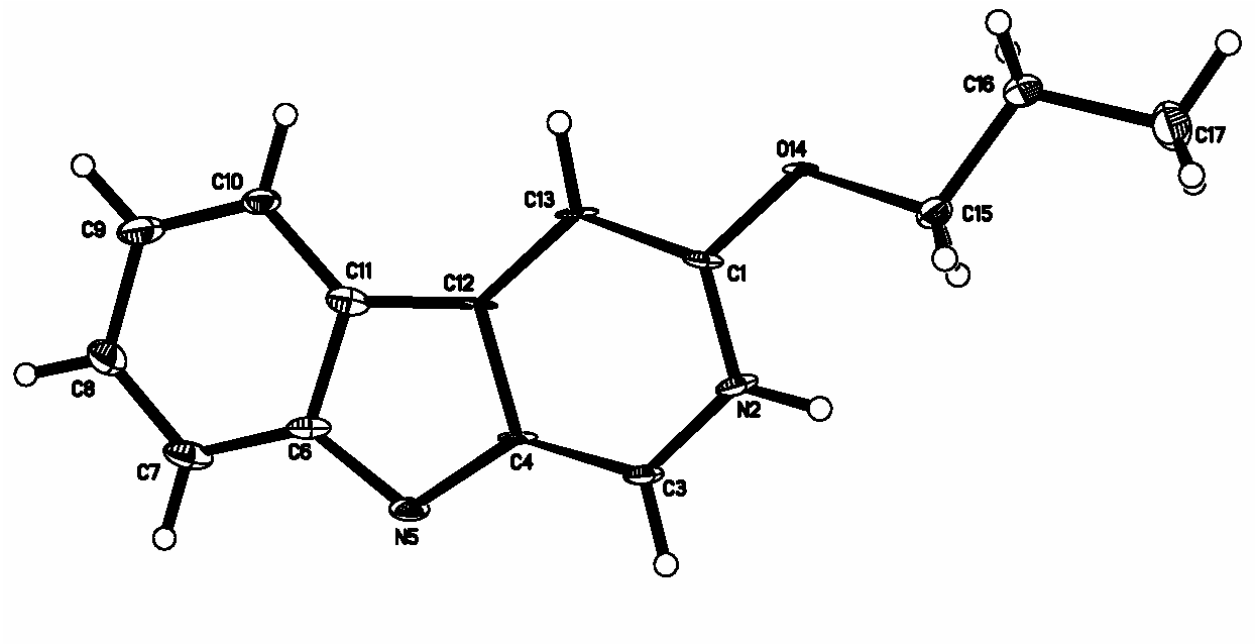



**Figure s1. ORTEP drawing for 1**

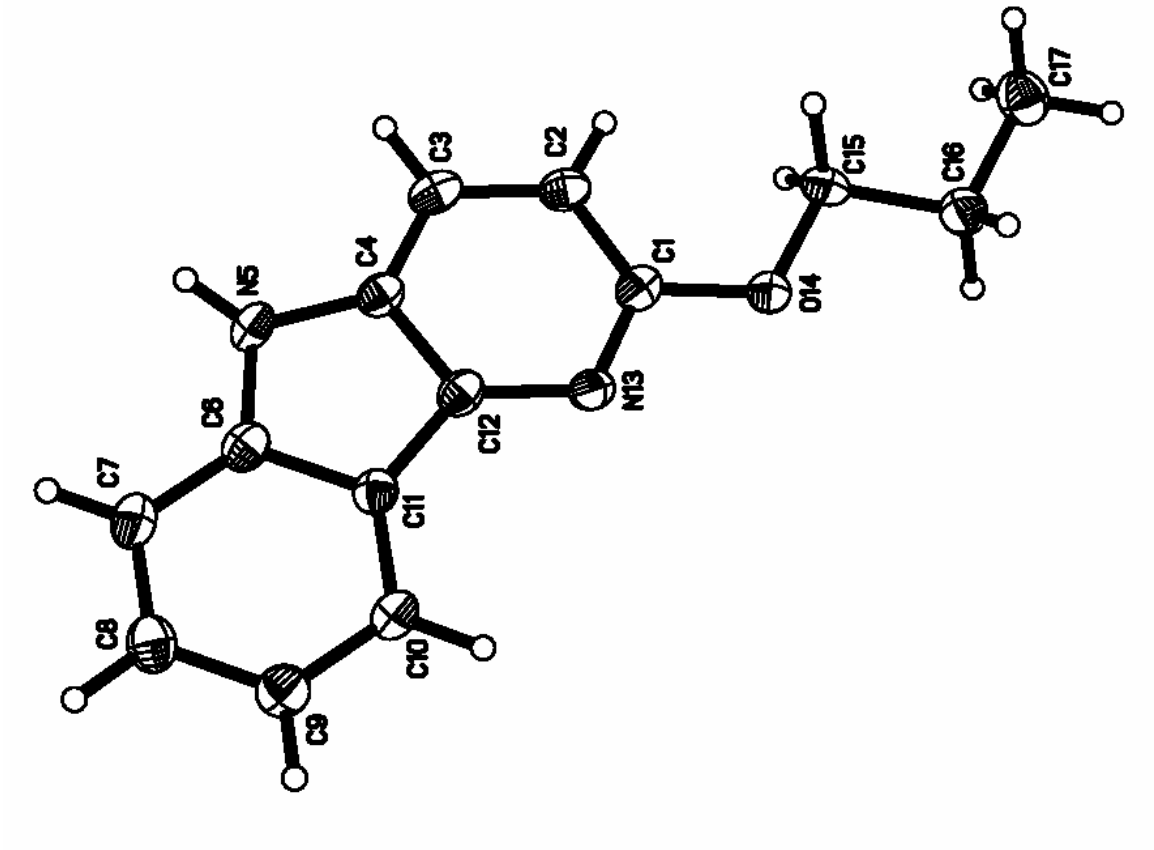



**Figure s2. ORTEP drawing for 6**

**Table s1.** Crystal data and structure refinement for **1**.

| | | |
|---|---|---|
| Empirical formula | $C_{14}H_{14}N_2O$ | |
| Formula weight | 212.16 | |
| Temperature | 100(2) °K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Orthorhombic | |
| Space group | $P\ 2_12_12$ | |
| Unit cell dimensions | a = 14.2022(11) Å | α= 90° |
| | b = 14.2864(9) Å | β= 90° |
| | c = 11.7464(11) Å | γ = 90° |
| Volume | 2383.3(3) $Å^3$ | |
| Z | 8 | |
| Density (calculated) | 1.183 $Mg/m^3$ | |
| Absorption coefficient | 0.078 $mm^{-1}$ | |
| F(000) | 848 | |
| Crystal size | 0.313 x 0.082 x 0.042 $mm^3$ | |
| θ range for data collection | 1.73 to 28.48° | |
| Index ranges | -18<=h<=19, -19<=k<=19, -15<=l<=15 | |
| Reflections collected | 25345 | |
| Independent reflections | 5989 [R(int) = 0.0736] | |
| Completeness to θ = 25.00° | 100.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.9967 and 0.9760 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 5989 / 12 / 304 | |
| Goodness-of-fit on $F^2$ | 1.027 | |
| Final R indices [I>2σ(I)] | R1 = 0.0527, wR2 = 0.1103 | |
| R indices (all data) | R1 = 0.0846, wR2 = 0.1255 | |
| Absolute structure parameter | 1.0(14) | |
| Extinction coefficient | 0.0046(7) | |
| Largest diff. peak and hole | 0.349 and -0.424 e.$Å^{-3}$ | |

**Table s2.** Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$ x $10^3$) for **1**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| C(1) | 6056(2) | 6232(2) | 5303(2) | 22(1) |
| C(2) | 6294(2) | 6119(2) | 4151(2) | 24(1) |
| C(3) | 5599(2) | 6074(2) | 3346(2) | 26(1) |
| C(4) | 4682(2) | 6142(2) | 3723(2) | 22(1) |
| N(5) | 3842(1) | 6113(1) | 3142(2) | 24(1) |
| C(6) | 3116(2) | 6180(2) | 3917(2) | 23(1) |
| C(7) | 2153(2) | 6159(2) | 3721(2) | 27(1) |
| C(8) | 1562(2) | 6274(2) | 4650(2) | 29(1) |
| C(9) | 1928(2) | 6401(2) | 5752(2) | 27(1) |
| C(10) | 2883(2) | 6403(2) | 5944(2) | 23(1) |
| C(11) | 3493(2) | 6293(2) | 5023(2) | 20(1) |
| C(12) | 4498(2) | 6254(2) | 4894(2) | 22(1) |
| N(13) | 5184(1) | 6301(1) | 5688(1) | 21(1) |
| O(14) | 6715(1) | 6267(1) | 6152(1) | 23(1) |
| C(15) | 7685(1) | 6234(2) | 5804(2) | 24(1) |
| C(16) | 8296(2) | 6225(2) | 6851(2) | 27(1) |
| C(17) | 9344(1) | 6238(1) | 6484(2) | 33(1) |
| C(1') | 3209(1) | 4962(1) | 10346(1) | 23(1) |
| C(2') | 3182(1) | 4694(1) | 9212(1) | 25(1) |
| C(3') | 3684(2) | 5155(2) | 8388(2) | 25(1) |
| C(4') | 4237(2) | 5889(2) | 8738(2) | 21(1) |
| N(5') | 4840(1) | 6461(1) | 8145(2) | 23(1) |
| C(6') | 5249(2) | 7077(2) | 8892(2) | 24(1) |
| C(7') | 5925(2) | 7750(2) | 8684(2) | 34(1) |
| C(8') | 6213(2) | 8302(2) | 9580(2) | 40(1) |
| C(9') | 5849(2) | 8178(2) | 10675(2) | 37(1) |
| C(10') | 5189(2) | 7494(2) | 10895(2) | 28(1) |
| C(11') | 4889(2) | 6922(2) | 9999(2) | 22(1) |
| C(12') | 4248(2) | 6150(2) | 9897(2) | 21(1) |
| N(13') | 3747(1) | 5691(1) | 10705(1) | 21(1) |
| O(14') | 2762(1) | 4534(1) | 11205(1) | 27(1) |
| C(15') | 2234(2) | 3708(2) | 10893(2) | 31(1) |
| C(16') | 1904(2) | 3226(2) | 11948(2) | 38(1) |
| C(17') | 1210(2) | 3786(2) | 12659(2) | 49(1) |

**Table s3.** Bond lengths [Å] and angles [°] for **1**.

| | | | |
|---|---|---|---|
| C(1)-N(13) | 1.322(3) | C(1)-O(14) | 1.369(3) |
| C(1)-C(2) | 1.404(3) | C(2)-C(3) | 1.369(3) |
| C(2)-H(2A) | 0.9500 | C(3)-C(4) | 1.379(3) |
| C(3)-H(3A) | 0.9500 | C(4)-N(5) | 1.375(3) |
| C(4)-C(12) | 1.409(3) | N(5)-C(6) | 1.378(3) |
| N(5)-H(5A) | 0.8800 | C(6)-C(7) | 1.387(3) |
| C(6)-C(11) | 1.415(3) | C(7)-C(8) | 1.386(3) |
| C(7)-H(7A) | 0.9500 | C(8)-C(9) | 1.407(3) |
| C(8)-H(8A) | 0.9500 | C(9)-C(10) | 1.375(3) |
| C(9)-H(9A) | 0.9500 | C(10)-C(11) | 1.396(3) |
| C(10)-H(10A) | 0.9500 | C(11)-C(12) | 1.437(3) |
| C(12)-N(13) | 1.350(3) | O(14)-C(15) | 1.437(2) |
| C(15)-C(16) | 1.505(3) | C(15)-H(15A) | 0.9900 |
| C(15)-H(15B) | 0.9900 | C(16)-C(17) | 1.550(3) |
| C(16)-H(16A) | 0.9900 | C(16)-H(16B) | 0.9900 |
| C(17)-H(17A) | 0.9800 | C(17)-H(17B) | 0.9800 |
| C(17)-H(17C) | 0.9800 | C(1')-O(14') | 1.3400(19) |
| C(1')-N(13') | 1.358(2) | C(1')-C(2') | 1.3869 |
| C(2')-C(3') | 1.372(3) | C(2')-H(2'A) | 0.9500 |
| C(3')-C(4') | 1.373(3) | C(3')-H(3'A) | 0.9500 |
| C(4')-N(5') | 1.373(3) | C(4')-C(12') | 1.412(3) |
| N(5')-C(6') | 1.372(3) | N(5')-H(5'A) | 0.8800 |
| C(6')-C(7') | 1.381(3) | C(6')-C(11') | 1.415(3) |
| C(7')-C(8') | 1.377(4) | C(7')-H(7'A) | 0.9500 |
| C(8')-C(9') | 1.398(3) | C(8')-H(8'A) | 0.9500 |
| C(9')-C(10') | 1.379(3) | C(9')-H(9'A) | 0.9500 |
| C(10')-C(11') | 1.398(3) | C(10')-H(10B) | 0.9500 |
| C(11')-C(12') | 1.434(3) | C(12')-N(13') | 1.356(3) |
| O(14')-C(15') | 1.445(3) | C(15')-C(16') | 1.493(3) |
| C(15')-H(15C) | 0.9900 | C(15')-H(15D) | 0.9900 |
| C(16')-C(17') | 1.520(4) | C(16')-H(16C) | 0.9900 |
| C(16')-H(16D) | 0.9900 | C(17')-H(17D) | 0.9800 |
| C(17')-H(17E) | 0.9800 | C(17')-H(17F) | 0.9800 |
| N(13)-C(1)-O(14) | 112.90(17) | N(13)-C(1)-C(2) | 124.3(2) |
| O(14)-C(1)-C(2) | 122.8(2) | C(3)-C(2)-C(1) | 119.8(2) |
| C(3)-C(2)-H(2A) | 120.1 | C(1)-C(2)-H(2A) | 120.1 |
| C(2)-C(3)-C(4) | 117.2(2) | C(2)-C(3)-H(3A) | 121.4 |
| C(4)-C(3)-H(3A) | 121.4 | N(5)-C(4)-C(3) | 131.15(19) |
| N(5)-C(4)-C(12) | 109.11(19) | C(3)-C(4)-C(12) | 119.7(2) |
| C(4)-N(5)-C(6) | 108.62(17) | C(4)-N(5)-H(5A) | 125.7 |
| C(6)-N(5)-H(5A) | 125.7 | N(5)-C(6)-C(7) | 128.8(2) |
| N(5)-C(6)-C(11) | 109.36(19) | C(7)-C(6)-C(11) | 121.8(2) |
| C(8)-C(7)-C(6) | 117.7(2) | C(8)-C(7)-H(7A) | 121.1 |
| C(6)-C(7)-H(7A) | 121.1 | C(7)-C(8)-C(9) | 121.0(2) |
| C(7)-C(8)-H(8A) | 119.5 | C(9)-C(8)-H(8A) | 119.5 |
| C(10)-C(9)-C(8) | 121.1(2) | C(10)-C(9)-H(9A) | 119.5 |
| C(8)-C(9)-H(9A) | 119.5 | C(9)-C(10)-C(11) | 119.0(2) |

**Table s3.** (continued)

| | | | |
|---|---|---|---|
| C(9)-C(10)-H(10A) | 120.5 | C(11)-C(10)-H(10A) | 120.5 |
| C(10)-C(11)-C(6) | 119.4(2) | C(10)-C(11)-C(12) | 134.7(2) |
| C(6)-C(11)-C(12) | 105.96(18) | N(13)-C(12)-C(4) | 123.1(2) |
| N(13)-C(12)-C(11) | 129.96(19) | C(4)-C(12)-C(11) | 106.90(19) |
| C(1)-N(13)-C(12) | 115.82(18) | C(1)-O(14)-C(15) | 116.55(16) |
| O(14)-C(15)-C(16) | 108.65(17) | O(14)-C(15)-H(15A) | 110.0 |
| C(16)-C(15)-H(15A) | 110.0 | O(14)-C(15)-H(15B) | 110.0 |
| C(16)-C(15)-H(15B) | 110.0 | H(15A)-C(15)-H(15B) | 108.3 |
| C(15)-C(16)-C(17) | 109.05(17) | C(15)-C(16)-H(16A) | 109.9 |
| C(17)-C(16)-H(16A) | 109.9 | C(15)-C(16)-H(16B) | 109.9 |
| C(17)-C(16)-H(16B) | 109.9 | H(16A)-C(16)-H(16B) | 108.3 |
| C(16)-C(17)-H(17A) | 109.5 | C(16)-C(17)-H(17B) | 109.5 |
| H(17A)-C(17)-H(17B) | 109.5 | C(16)-C(17)-H(17C) | 109.5 |
| H(17A)-C(17)-H(17C) | 109.5 | H(17B)-C(17)-H(17C) | 109.5 |
| O(14')-C(1')-N(13') | 112.53(14) | O(14')-C(1')-C(2') | 125.69(11) |
| N(13')-C(1')-C(2') | 121.73(10) | C(3')-C(2')-C(1') | 122.03(11) |
| C(3')-C(2')-H(2'A) | 119.0 | C(1')-C(2')-H(2'A) | 119.0 |
| C(2')-C(3')-C(4') | 116.95(19) | C(2')-C(3')-H(3'A) | 121.5 |
| C(4')-C(3')-H(3'A) | 121.5 | C(3')-C(4')-N(5') | 131.2(2) |
| C(3')-C(4')-C(12') | 119.8(2) | N(5')-C(4')-C(12') | 108.99(19) |
| C(6')-N(5')-C(4') | 108.70(18) | C(6')-N(5')-H(5'A) | 125.6 |
| C(4')-N(5')-H(5'A) | 125.6 | N(5')-C(6')-C(7') | 128.9(2) |
| N(5')-C(6')-C(11') | 109.54(19) | C(7')-C(6')-C(11') | 121.6(2) |
| C(8')-C(7')-C(6') | 118.0(2) | C(8')-C(7')-H(7'A) | 121.0 |
| C(6')-C(7')-H(7'A) | 121.0 | C(7')-C(8')-C(9') | 121.4(2) |
| C(7')-C(8')-H(8'A) | 119.3 | C(9')-C(8')-H(8'A) | 119.3 |
| C(10')-C(9')-C(8') | 121.0(2) | C(10')-C(9')-H(9'A) | 119.5 |
| C(8')-C(9')-H(9'A) | 119.5 | C(9')-C(10')-C(11') | 118.7(2) |
| C(9')-C(10')-H(10B) | 120.7 | C(11')-C(10')-H(10B) | 120.7 |
| C(10')-C(11')-C(6') | 119.3(2) | C(10')-C(11')-C(12') | 134.8(2) |
| C(6')-C(11')-C(12') | 105.85(18) | N(13')-C(12')-C(4') | 122.7(2) |
| N(13')-C(12')-C(11') | 130.32(19) | C(4')-C(12')-C(11') | 106.90(18) |
| C(12')-N(13')-C(1') | 116.72(16) | C(1')-O(14')-C(15') | 115.34(15) |
| O(14')-C(15')-C(16') | 109.16(18) | O(14')-C(15')-H(15C) | 109.8 |
| C(16')-C(15')-H(15C) | 109.8 | O(14')-C(15')-H(15D) | 109.8 |
| C(16')-C(15')-H(15D) | 109.8 | H(15C)-C(15')-H(15D) | 108.3 |
| C(15')-C(16')-C(17') | 114.7(2) | C(15')-C(16')-H(16C) | 108.6 |
| C(17')-C(16')-H(16C) | 108.6 | C(15')-C(16')-H(16D) | 108.6 |
| C(17')-C(16')-H(16D) | 108.6 | H(16C)-C(16')-H(16D) | 107.6 |
| C(16')-C(17')-H(17D) | 109.5 | C(16')-C(17')-H(17E) | 109.5 |
| H(17D)-C(17')-H(17E) | 109.5 | C(16')-C(17')-H(17F) | 109.5 |
| H(17D)-C(17')-H(17F) | 109.5 | H(17E)-C(17')-H(17F) | 109.5 |

**Table s4.** Anisotropic displacement parameters ($Å^2$ x $10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [ $h^2 a^{*2} U^{11}$ + ... + 2 h k a* b* $U^{12}$ ]

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| C(1) | 28(1) | 18(1) | 20(1) | -1(1) | 1(1) | 1(1) |
| C(2) | 26(1) | 25(1) | 22(1) | 0(1) | 6(1) | 2(1) |
| C(3) | 34(1) | 24(1) | 20(1) | 1(1) | 6(1) | 2(1) |
| C(4) | 27(1) | 19(1) | 19(1) | 1(1) | 1(1) | 1(1) |
| N(5) | 28(1) | 26(1) | 16(1) | 1(1) | -2(1) | 4(1) |
| C(6) | 29(1) | 19(1) | 22(1) | 1(1) | -1(1) | 3(1) |
| C(7) | 30(1) | 26(1) | 24(1) | 2(1) | -6(1) | 2(1) |
| C(8) | 26(1) | 29(1) | 32(1) | 1(1) | -4(1) | 4(1) |
| C(9) | 28(1) | 27(1) | 27(1) | -1(1) | 2(1) | 5(1) |
| C(10) | 28(1) | 24(1) | 19(1) | 0(1) | -1(1) | 3(1) |
| C(11) | 22(1) | 18(1) | 21(1) | 3(1) | -1(1) | 1(1) |
| C(12) | 27(1) | 19(1) | 20(1) | 2(1) | -1(1) | 2(1) |
| N(13) | 24(1) | 21(1) | 19(1) | 1(1) | 2(1) | -2(1) |
| O(14) | 20(1) | 31(1) | 20(1) | 1(1) | 1(1) | -2(1) |
| C(15) | 19(1) | 25(1) | 26(1) | 1(1) | 6(1) | -2(1) |
| C(16) | 26(1) | 30(1) | 26(1) | -2(1) | 2(1) | -2(1) |
| C(17) | 26(1) | 37(1) | 38(1) | -2(1) | 0(1) | 2(1) |
| C(1') | 27(1) | 21(1) | 21(1) | 3(1) | -4(1) | -2(1) |
| C(2') | 30(1) | 23(1) | 23(1) | -3(1) | -7(1) | 0(1) |
| C(3') | 31(1) | 25(1) | 19(1) | -3(1) | -3(1) | 4(1) |
| C(4') | 23(1) | 22(1) | 19(1) | 1(1) | 1(1) | 5(1) |
| N(5') | 26(1) | 27(1) | 17(1) | 2(1) | 2(1) | 3(1) |
| C(6') | 25(1) | 27(1) | 19(1) | 4(1) | -1(1) | 1(1) |
| C(7') | 34(2) | 40(1) | 30(1) | 8(1) | 4(1) | -8(1) |
| C(8') | 44(2) | 39(2) | 37(2) | 9(1) | 2(1) | -18(1) |
| C(9') | 46(2) | 37(2) | 28(1) | 0(1) | -2(1) | -16(1) |
| C(10') | 34(1) | 29(1) | 21(1) | 1(1) | 0(1) | -4(1) |
| C(11') | 23(1) | 23(1) | 20(1) | 0(1) | 1(1) | -1(1) |
| C(12') | 21(1) | 23(1) | 18(1) | -1(1) | 2(1) | 3(1) |
| N(13') | 24(1) | 21(1) | 18(1) | 0(1) | 0(1) | -2(1) |
| O(14') | 34(1) | 28(1) | 20(1) | 3(1) | -3(1) | -12(1) |
| C(15') | 37(1) | 28(1) | 29(1) | 4(1) | -11(1) | -15(1) |
| C(16') | 44(2) | 40(2) | 31(1) | 7(1) | -11(1) | -21(1) |
| C(17') | 49(2) | 57(2) | 42(2) | 3(2) | 2(1) | -22(2) |

**Table s5.** Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (Å$^2$ x $10^3$) for **1**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 6936 | 6075 | 3931 | 29 |
| H(3A) | 5742 | 5998 | 2562 | 31 |
| H(5A) | 3778 | 6060 | 2400 | 28 |
| H(7A) | 1908 | 6070 | 2977 | 32 |
| H(8A) | 899 | 6266 | 4540 | 35 |
| H(9A) | 1508 | 6488 | 6373 | 33 |
| H(10A) | 3123 | 6478 | 6693 | 28 |
| H(15A) | 7836 | 6787 | 5330 | 28 |
| H(15B) | 7801 | 5663 | 5346 | 28 |
| H(16A) | 8165 | 5656 | 7306 | 33 |
| H(16B) | 8156 | 6780 | 7328 | 33 |
| H(17A) | 9746 | 6245 | 7163 | 50 |
| H(17B) | 9467 | 6799 | 6028 | 50 |
| H(17C) | 9482 | 5679 | 6031 | 50 |
| H(2'A) | 2803 | 4174 | 8999 | 30 |
| H(3'A) | 3651 | 4975 | 7610 | 30 |
| H(5'A) | 4946 | 6437 | 7407 | 28 |
| H(7'A) | 6184 | 7831 | 7944 | 41 |
| H(8'A) | 6669 | 8777 | 9451 | 48 |
| H(9'A) | 6059 | 8570 | 11277 | 44 |
| H(10B) | 4942 | 7412 | 11640 | 33 |
| H(15C) | 2637 | 3280 | 10444 | 38 |
| H(15D) | 1686 | 3886 | 10419 | 38 |
| H(16C) | 2459 | 3078 | 12425 | 46 |
| H(16D) | 1605 | 2627 | 11730 | 46 |
| H(17D) | 992 | 3404 | 13300 | 74 |
| H(17E) | 670 | 3965 | 12187 | 74 |
| H(17F) | 1519 | 4351 | 12950 | 74 |

**Table s6.** Torsion angles [°] for **1**.

| | | | |
|---|---|---|---|
| N(13)-C(1)-C(2)-C(3) | -0.1(4) | O(14)-C(1)-C(2)-C(3) | 178.9(2) |
| C(1)-C(2)-C(3)-C(4) | 0.0(3) | C(2)-C(3)-C(4)-N(5) | -179.3(2) |
| C(2)-C(3)-C(4)-C(12) | 0.0(3) | C(3)-C(4)-N(5)-C(6) | 177.9(2) |
| C(12)-C(4)-N(5)-C(6) | -1.5(2) | C(4)-N(5)-C(6)-C(7) | -178.4(2) |
| C(4)-N(5)-C(6)-C(11) | 2.4(2) | N(5)-C(6)-C(7)-C(8) | -177.8(2) |
| C(11)-C(6)-C(7)-C(8) | 1.3(4) | C(6)-C(7)-C(8)-C(9) | -0.3(3) |
| C(7)-C(8)-C(9)-C(10) | -0.9(4) | C(8)-C(9)-C(10)-C(11) | 1.2(3) |
| C(9)-C(10)-C(11)-C(6) | -0.2(3) | C(9)-C(10)-C(11)-C(12) | -179.5(2) |
| N(5)-C(6)-C(11)-C(10) | 178.2(2) | C(7)-C(6)-C(11)-C(10) | -1.1(3) |
| N(5)-C(6)-C(11)-C(12) | -2.3(3) | C(7)-C(6)-C(11)-C(12) | 178.5(2) |
| N(5)-C(4)-C(12)-N(13) | 179.5(2) | C(3)-C(4)-C(12)-N(13) | 0.1(4) |
| N(5)-C(4)-C(12)-C(11) | 0.0(3) | C(3)-C(4)-C(12)-C(11) | -179.4(2) |
| C(10)-C(11)-C(12)-N(13) | 1.3(5) | C(6)-C(11)-C(12)-N(13) | -178.1(2) |
| C(10)-C(11)-C(12)-C(4) | -179.3(2) | C(6)-C(11)-C(12)-C(4) | 1.4(3) |
| O(14)-C(1)-N(13)-C(12) | -178.92(19) | C(2)-C(1)-N(13)-C(12) | 0.2(3) |
| C(4)-C(12)-N(13)-C(1) | -0.2(3) | C(11)-C(12)-N(13)-C(1) | 179.1(2) |
| N(13)-C(1)-O(14)-C(15) | -177.65(19) | C(2)-C(1)-O(14)-C(15) | 3.2(3) |
| C(1)-O(14)-C(15)-C(16) | -176.81(18) | O(14)-C(15)-C(16)-C(17) | -177.24(18) |
| O(14')-C(1')-C(2')-C(3') | -178.0(2) | N(13')-C(1')-C(2')-C(3') | -0.92(18) |
| C(1')-C(2')-C(3')-C(4') | 1.4(3) | C(2')-C(3')-C(4')-N(5') | 177.4(2) |
| C(2')-C(3')-C(4')-C(12') | -1.6(3) | C(3')-C(4')-N(5')-C(6') | -178.3(2) |
| C(12')-C(4')-N(5')-C(6') | 0.8(2) | C(4')-N(5')-C(6')-C(7') | 177.1(2) |
| C(4')-N(5')-C(6')-C(11') | -1.5(3) | N(5')-C(6')-C(7')-C(8') | 178.6(2) |
| C(11')-C(6')-C(7')-C(8') | -2.9(4) | C(6')-C(7')-C(8')-C(9') | 1.2(4) |
| C(7')-C(8')-C(9')-C(10') | 0.2(4) | C(8')-C(9')-C(10')-C(11') | 0.1(4) |
| C(9')-C(10')-C(11')-C(6') | -1.8(3) | C(9')-C(10')-C(11')-C(12') | 178.7(3) |
| N(5')-C(6')-C(11')-C(10') | -178.0(2) | C(7')-C(6')-C(11')-C(10') | 3.2(3) |
| N(5')-C(6')-C(11')-C(12') | 1.6(3) | C(7')-C(6')-C(11')-C(12') | -177.1(2) |
| C(3')-C(4')-C(12')-N(13') | 1.6(3) | N(5')-C(4')-C(12')-N(13') | -177.6(2) |
| C(3')-C(4')-C(12')-C(11') | 179.4(2) | N(5')-C(4')-C(12')-C(11') | 0.2(2) |
| C(10')-C(11')-C(12')-N(13') | -3.9(4) | C(6')-C(11')-C(12')-N(13') | 176.5(2) |
| C(10')-C(11')-C(12')-C(4') | 178.4(3) | C(6')-C(11')-C(12')-C(4') | -1.1(2) |
| C(4')-C(12')-N(13')-C(1') | -1.0(3) | C(11')-C(12')-N(13')-C(1') | -178.4(2) |
| O(14')-C(1')-N(13')-C(12') | 178.16(17) | C(2')-C(1')-N(13')-C(12') | 0.7(2) |
| N(13')-C(1')-O(14')-C(15') | -175.48(17) | C(2')-C(1')-O(14')-C(15') | 1.9(2) |
| C(1')-O(14')-C(15')-C(16') | 171.2(2) | O(14')-C(15')-C(16')-C(17') | 64.5(3) |

**Table s7.** Crystal data and structure refinement for **6**.

| | | |
|---|---|---|
| Empirical formula | C14 H14 N2 O | |
| Formula weight | 226.27 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P 1 | |
| Unit cell dimensions | a = 5.1335(14) Å | α= 75.541(9)° |
| | b = 10.319(3) Å | β= 84.199(10)° |
| | c = 10.983(3) Å | γ = 88.679(10)° |
| Volume | 560.4(3) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.341 $Mg/m^3$ | |
| Absorption coefficient | 0.086 $mm^{-1}$ | |
| F(000) | 240 | |
| Crystal size | 0.651 x 0.287 x 0.015 $mm^3$ | |
| θ range for data collection | 1.92 to 28.33° | |
| Index ranges | -6<=h<=6, -13<=k<=13, -14<=l<=14 | |
| Reflections collected | 5612 | |
| Independent reflections | 4441 [R(int) = 0.0573] | |
| Completeness to θ = 25.00° | 98.7 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.9987 and 0.9460 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 4441 / 231 / 309 | |
| Goodness-of-fit on $F^2$ | 1.085 | |
| Final R indices [I>2σ(I)] | R1 = 0.0924, wR2 = 0.2292 | |
| R indices (all data) | R1 = 0.1124, wR2 = 0.2469 | |
| Absolute structure parameter | 0(2) | |
| Largest diff. peak and hole | 0.966 and -0.469 $e.Å^{-3}$ | |

**Table s8.** Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$ x $10^3$) for **6**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| C(1) | 134(8) | 2903(4) | 1022(4) | 10(1) |
| N(2) | 22(7) | 3063(4) | 2190(3) | 13(1) |
| C(3) | 1574(9) | 2311(4) | 3003(4) | 12(1) |
| C(4) | 3287(8) | 1408(4) | 2624(4) | 11(1) |
| N(5) | 5113(8) | 552(4) | 3272(4) | 15(1) |
| C(6) | 6385(8) | -146(4) | 2472(4) | 12(1) |
| C(7) | 8424(9) | -1057(5) | 2684(5) | 17(1) |
| C(8) | 9355(10) | -1620(5) | 1719(5) | 19(1) |
| C(9) | 8327(10) | -1276(5) | 527(5) | 19(1) |
| C(10) | 6319(9) | -362(4) | 316(4) | 14(1) |
| C(11) | 5350(8) | 229(4) | 1291(4) | 13(1) |
| C(12) | 3399(8) | 1203(4) | 1359(4) | 9(1) |
| C(13) | 1737(8) | 1994(4) | 552(4) | 11(1) |
| O(14) | -1359(6) | 3720(3) | 199(3) | 11(1) |
| C(15) | -3250(9) | 4564(4) | 679(4) | 14(1) |
| C(16) | -4623(10) | 5348(5) | -428(4) | 17(1) |
| C(17) | -6654(11) | 6281(5) | -18(6) | 25(1) |
| C(1') | -4838(8) | 1932(4) | 6242(4) | 12(1) |
| N(2') | -4984(7) | 1776(4) | 7478(3) | 13(1) |
| C(3') | -3432(9) | 2542(4) | 7950(4) | 12(1) |
| C(4') | -1716(9) | 3445(4) | 7155(4) | 12(1) |
| N(5') | 78(7) | 4301(4) | 7430(3) | 13(1) |
| C(6') | 1377(9) | 5012(4) | 6309(4) | 13(1) |
| C(7') | 3420(9) | 5931(5) | 6129(4) | 17(1) |
| C(8') | 4431(10) | 6476(5) | 4892(5) | 18(1) |
| C(9') | 3490(10) | 6146(5) | 3863(5) | 19(1) |
| C(10') | 1455(9) | 5213(4) | 4051(4) | 13(1) |
| C(11') | 426(8) | 4633(4) | 5293(4) | 12(1) |
| C(12') | -1583(8) | 3645(4) | 5812(4) | 8(1) |
| C(13') | -3218(8) | 2854(4) | 5351(4) | 12(1) |
| O(14') | -6327(6) | 1126(3) | 5785(3) | 12(1) |
| C(15') | -8194(9) | 266(4) | 6678(4) | 13(1) |
| C(16') | -9644(10) | -517(5) | 5949(5) | 18(1) |
| C(17') | -11542(12) | -1499(5) | 6855(5) | 26(1) |

**Table s9.** Bond lengths [Å] and angles [°] for **6**.

| | | | |
|---|---|---|---|
| C(1)-N(2) | 1.330(5) | C(1)-O(14) | 1.358(5) |
| C(1)-C(13) | 1.393(5) | N(2)-C(3) | 1.343(6) |
| N(2)-H(2A) | 0.8800 | C(3)-C(4) | 1.377(6) |
| C(3)-H(3A) | 0.9500 | C(4)-N(5) | 1.396(6) |
| C(4)-C(12) | 1.452(6) | N(5)-C(6) | 1.377(6) |
| C(6)-C(7) | 1.389(6) | C(6)-C(11) | 1.412(6) |
| C(7)-C(8) | 1.371(7) | C(7)-H(7A) | 0.9500 |
| C(8)-C(9) | 1.420(7) | C(8)-H(8A) | 0.9500 |
| C(9)-C(10) | 1.379(7) | C(9)-H(9A) | 0.9500 |
| C(10)-C(11) | 1.403(6) | C(10)-H(10A) | 0.9500 |
| C(11)-C(12) | 1.412(6) | C(12)-C(13) | 1.393(6) |
| C(13)-H(13A) | 0.9500 | O(14)-C(15) | 1.438(5) |
| C(15)-C(16) | 1.512(7) | C(15)-H(15D) | 0.9900 |
| C(15)-H(15E) | 0.9900 | C(16)-C(17) | 1.514(6) |
| C(16)-H(16C) | 0.9900 | C(16)-H(16D) | 0.9900 |
| C(17)-H(17C) | 0.9800 | C(17)-H(17D) | 0.9800 |
| C(17)-H(17E) | 0.9800 | C(1')-N(2') | 1.321(5) |
| C(1')-O(14') | 1.357(5) | C(1')-C(13') | 1.401(6) |
| N(2')-C(3') | 1.358(6) | N(2')-H(2'A) | 0.8800 |
| C(3')-C(4') | 1.372(6) | C(3')-H(3'A) | 0.9500 |
| C(4')-N(5') | 1.395(6) | C(4')-C(12') | 1.432(6) |
| N(5')-C(6') | 1.380(5) | C(6')-C(7') | 1.396(7) |
| C(6')-C(11') | 1.405(6) | C(7')-C(8') | 1.386(6) |
| C(7')-H(7'A) | 0.9500 | C(8')-C(9') | 1.392(7) |
| C(8')-H(8'A) | 0.9500 | C(9')-C(10') | 1.401(7) |
| C(9')-H(9'A) | 0.9500 | C(10')-C(11') | 1.399(6) |
| C(10')-H(10B) | 0.9500 | C(11')-C(12') | 1.438(6) |
| C(12')-C(13') | 1.396(6) | C(13')-H(13B) | 0.9500 |
| O(14')-C(15') | 1.443(5) | C(15')-C(16') | 1.523(6) |
| C(15')-H(15A) | 0.9900 | C(15')-H(15B) | 0.9900 |
| C(16')-C(17') | 1.520(7) | C(16')-H(16A) | 0.9900 |
| C(16')-H(16B) | 0.9900 | C(17')-H(17A) | 0.9800 |
| C(17')-H(17B) | 0.9800 | C(17')-H(17F) | 0.9800 |
| N(2)-C(1)-O(14) | 117.8(4) | N(2)-C(1)-C(13) | 125.3(4) |
| O(14)-C(1)-C(13) | 116.8(4) | C(1)-N(2)-C(3) | 118.8(4) |
| C(1)-N(2)-H(2A) | 120.6 | C(3)-N(2)-H(2A) | 120.6 |
| N(2)-C(3)-C(4) | 120.5(4) | N(2)-C(3)-H(3A) | 119.8 |
| C(4)-C(3)-H(3A) | 119.8 | C(3)-C(4)-N(5) | 131.1(4) |
| C(3)-C(4)-C(12) | 121.4(4) | N(5)-C(4)-C(12) | 107.6(3) |
| C(6)-N(5)-C(4) | 108.9(4) | N(5)-C(6)-C(7) | 129.3(4) |
| N(5)-C(6)-C(11) | 109.2(4) | C(7)-C(6)-C(11) | 121.5(4) |
| C(8)-C(7)-C(6) | 117.8(5) | C(8)-C(7)-H(7A) | 121.1 |
| C(6)-C(7)-H(7A) | 121.1 | C(7)-C(8)-C(9) | 121.9(5) |
| C(7)-C(8)-H(8A) | 119.0 | C(9)-C(8)-H(8A) | 119.0 |
| C(10)-C(9)-C(8) | 120.1(4) | C(10)-C(9)-H(9A) | 120.0 |
| C(8)-C(9)-H(9A) | 120.0 | C(9)-C(10)-C(11) | 118.8(5) |
| C(9)-C(10)-H(10A) | 120.6 | C(11)-C(10)-H(10A) | 120.6 |

**Table s9.** (continued)

| | | | |
|---|---|---|---|
| C(10)-C(11)-C(12) | 132.3(4) | C(10)-C(11)-C(6) | 119.9(4) |
| C(12)-C(11)-C(6) | 107.9(4) | C(13)-C(12)-C(11) | 137.4(4) |
| C(13)-C(12)-C(4) | 116.2(4) | C(11)-C(12)-C(4) | 106.4(4) |
| C(12)-C(13)-C(1) | 117.8(4) | C(12)-C(13)-H(13A) | 121.1 |
| C(1)-C(13)-H(13A) | 121.1 | C(1)-O(14)-C(15) | 118.4(3) |
| O(14)-C(15)-C(16) | 107.1(4) | O(14)-C(15)-H(15D) | 110.3 |
| C(16)-C(15)-H(15D) | 110.3 | O(14)-C(15)-H(15E) | 110.3 |
| C(16)-C(15)-H(15E) | 110.3 | H(15D)-C(15)-H(15E) | 108.6 |
| C(15)-C(16)-C(17) | 111.1(4) | C(15)-C(16)-H(16C) | 109.4 |
| C(17)-C(16)-H(16C) | 109.4 | C(15)-C(16)-H(16D) | 109.4 |
| C(17)-C(16)-H(16D) | 109.4 | H(16C)-C(16)-H(16D) | 108.0 |
| C(16)-C(17)-H(17C) | 109.5 | C(16)-C(17)-H(17D) | 109.5 |
| H(17C)-C(17)-H(17D) | 109.5 | C(16)-C(17)-H(17E) | 109.5 |
| H(17C)-C(17)-H(17E) | 109.5 | H(17D)-C(17)-H(17E) | 109.5 |
| N(2')-C(1')-O(14') | 118.3(4) | N(2')-C(1')-C(13') | 125.1(4) |
| O(14')-C(1')-C(13') | 116.6(4) | C(1')-N(2')-C(3') | 118.8(4) |
| C(1')-N(2')-H(2'A) | 120.6 | C(3')-N(2')-H(2'A) | 120.6 |
| N(2')-C(3')-C(4') | 120.4(4) | N(2')-C(3')-H(3'A) | 119.8 |
| C(4')-C(3')-H(3'A) | 119.8 | C(3')-C(4')-N(5') | 130.0(4) |
| C(3')-C(4')-C(12') | 121.3(4) | N(5')-C(4')-C(12') | 108.7(4) |
| C(6')-N(5')-C(4') | 108.4(4) | N(5')-C(6')-C(7') | 128.5(4) |
| N(5')-C(6')-C(11') | 109.6(4) | C(7')-C(6')-C(11') | 121.9(4) |
| C(8')-C(7')-C(6') | 116.6(5) | C(8')-C(7')-H(7'A) | 121.7 |
| C(6')-C(7')-H(7'A) | 121.7 | C(7')-C(8')-C(9') | 122.8(5) |
| C(7')-C(8')-H(8'A) | 118.6 | C(9')-C(8')-H(8'A) | 118.6 |
| C(8')-C(9')-C(10') | 120.2(4) | C(8')-C(9')-H(9'A) | 119.9 |
| C(10')-C(9')-H(9'A) | 119.9 | C(11')-C(10')-C(9') | 118.1(4) |
| C(11')-C(10')-H(10B) | 121.0 | C(9')-C(10')-H(10B) | 121.0 |
| C(10')-C(11')-C(6') | 120.3(4) | C(10')-C(11')-C(12') | 132.3(4) |
| C(6')-C(11')-C(12') | 107.4(4) | C(13')-C(12')-C(4') | 117.1(4) |
| C(13')-C(12')-C(11') | 136.9(4) | C(4')-C(12')-C(11') | 106.0(4) |
| C(12')-C(13')-C(1') | 117.2(4) | C(12')-C(13')-H(13B) | 121.4 |
| C(1')-C(13')-H(13B) | 121.4 | C(1')-O(14')-C(15') | 117.1(3) |
| O(14')-C(15')-C(16') | 107.5(3) | O(14')-C(15')-H(15A) | 110.2 |
| C(16')-C(15')-H(15A) | 110.2 | O(14')-C(15')-H(15B) | 110.2 |
| C(16')-C(15')-H(15B) | 110.2 | H(15A)-C(15')-H(15B) | 108.5 |
| C(17')-C(16')-C(15') | 109.9(4) | C(17')-C(16')-H(16A) | 109.7 |
| C(15')-C(16')-H(16A) | 109.7 | C(17')-C(16')-H(16B) | 109.7 |
| C(15')-C(16')-H(16B) | 109.7 | H(16A)-C(16')-H(16B) | 108.2 |
| C(16')-C(17')-H(17A) | 109.5 | C(16')-C(17')-H(17B) | 109.5 |
| H(17A)-C(17')-H(17B) | 109.5 | C(16')-C(17')-H(17F) | 109.5 |
| H(17A)-C(17')-H(17F) | 109.5 | H(17B)-C(17')-H(17F) | 109.5 |

**Table s10.** Anisotropic displacement parameters ($Å^2$ x $10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^3$ [ $h^3$ $a^{*2}U^{11}$ + ... + 2 h k a* b* $U^{12}$ ]

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| C(1) | 8(2) | 18(2) | 4(2) | -2(1) | -2(1) | -2(2) |
| N(2) | 12(2) | 22(2) | 7(2) | -8(1) | -1(1) | -1(1) |
| C(3) | 13(2) | 20(2) | 5(2) | -5(2) | -2(2) | 1(2) |
| C(4) | 12(2) | 16(1) | 7(1) | -4(1) | -4(1) | 0(1) |
| N(5) | 14(2) | 24(2) | 8(2) | -7(1) | -6(1) | 4(1) |
| C(6) | 11(2) | 21(2) | 6(2) | -3(2) | -2(2) | -3(2) |
| C(7) | 13(2) | 27(2) | 11(2) | -1(2) | -4(2) | 0(2) |
| C(8) | 21(2) | 19(2) | 17(2) | -3(2) | -8(2) | 2(2) |
| C(9) | 20(2) | 28(2) | 11(2) | -8(2) | -2(2) | 2(2) |
| C(10) | 18(2) | 16(2) | 7(2) | -3(2) | -1(2) | -1(2) |
| C(11) | 9(2) | 19(2) | 9(2) | -1(2) | -1(2) | -3(2) |
| C(12) | 11(2) | 10(1) | 5(1) | 0(1) | -3(1) | -2(1) |
| C(13) | 12(2) | 20(2) | 3(2) | -4(2) | -1(2) | -2(2) |
| O(14) | 13(1) | 17(1) | 7(1) | -6(1) | -5(1) | 2(1) |
| C(15) | 12(2) | 21(2) | 11(2) | -7(2) | -1(2) | 3(2) |
| C(16) | 19(2) | 23(2) | 9(2) | -5(2) | -1(2) | 5(2) |
| C(17) | 24(2) | 24(2) | 29(3) | -12(2) | -11(2) | 8(2) |
| C(1') | 11(2) | 21(2) | 6(2) | -5(2) | -2(2) | 2(2) |
| N(2') | 12(2) | 21(2) | 7(2) | -4(1) | -4(1) | 0(1) |
| C(3') | 15(2) | 18(2) | 5(2) | -5(2) | -2(2) | -1(2) |
| C(4') | 13(2) | 15(2) | 9(2) | -4(2) | -3(2) | -2(2) |
| N(5') | 16(2) | 20(2) | 6(2) | -6(1) | -1(1) | -3(1) |
| C(6') | 12(2) | 21(2) | 8(2) | -8(2) | -2(2) | 2(2) |
| C(7') | 17(2) | 24(2) | 10(2) | -6(2) | -5(2) | -1(2) |
| C(8') | 22(2) | 21(2) | 12(2) | -3(2) | -2(2) | 0(2) |
| C(9') | 16(2) | 30(2) | 11(2) | -3(2) | -2(2) | 1(2) |
| C(10') | 14(2) | 21(2) | 6(2) | -6(2) | -2(2) | 2(2) |
| C(11') | 9(2) | 22(2) | 4(2) | -4(2) | -3(2) | 2(2) |
| C(12') | 11(2) | 7(2) | 7(2) | -4(1) | -4(1) | 3(1) |
| C(13') | 13(2) | 16(1) | 7(1) | -6(1) | 0(1) | 1(1) |
| O(14') | 12(2) | 21(2) | 4(1) | -4(1) | -4(1) | -2(1) |
| C(15') | 11(2) | 22(2) | 8(2) | -5(2) | -3(2) | -2(2) |
| C(16') | 19(2) | 24(2) | 12(2) | -7(2) | -3(2) | -5(2) |
| C(17') | 33(3) | 22(2) | 24(2) | -11(2) | 3(2) | -10(2) |

**Table s11.** Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$ x $10^3$) for **6**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | -1050 | 3652 | 2427 | 16 |
| H(3A) | 1490 | 2402 | 3846 | 15 |
| H(7A) | 9151 | -1284 | 3472 | 21 |
| H(8A) | 10727 | -2258 | 1852 | 23 |
| H(9A) | 9025 | -1676 | -126 | 23 |
| H(10A) | 5604 | -136 | -475 | 16 |
| H(13A) | 1697 | 1917 | -290 | 14 |
| H(15D) | -2368 | 5180 | 1069 | 17 |
| H(15E) | -4528 | 4015 | 1328 | 17 |
| H(16C) | -5483 | 4720 | -812 | 20 |
| H(16D) | -3318 | 5877 | -1077 | 20 |
| H(17C) | -7595 | 6731 | -740 | 37 |
| H(17D) | -5787 | 6951 | 297 | 37 |
| H(17E) | -7897 | 5764 | 655 | 37 |
| H(2'A) | -6068 | 1187 | 7987 | 16 |
| H(3'A) | -3535 | 2452 | 8836 | 15 |
| H(7'A) | 4084 | 6171 | 6820 | 20 |
| H(8'A) | 5826 | 7103 | 4740 | 22 |
| H(9'A) | 4231 | 6553 | 3031 | 23 |
| H(10B) | 792 | 4982 | 3356 | 16 |
| H(13B) | -3230 | 2938 | 4471 | 14 |
| H(15A) | -9442 | 807 | 7092 | 16 |
| H(15B) | -7279 | -355 | 7338 | 16 |
| H(16A) | -10618 | 109 | 5317 | 21 |
| H(16B) | -8372 | -1009 | 5495 | 21 |
| H(17A) | -12678 | -1886 | 6371 | 38 |
| H(17B) | -12615 | -1030 | 7399 | 38 |
| H(17F) | -10556 | -2214 | 7378 | 38 |

**Table s12.** Torsion angles [°] for **6**.

| | | | |
|---|---|---|---|
| O(14)-C(1)-N(2)-C(3) | -176.9(4) | C(13)-C(1)-N(2)-C(3) | 0.6(6) |
| C(1)-N(2)-C(3)-C(4) | 1.2(6) | N(2)-C(3)-C(4)-N(5) | 178.2(4) |
| N(2)-C(3)-C(4)-C(12) | -2.4(6) | C(3)-C(4)-N(5)-C(6) | -179.2(4) |
| C(12)-C(4)-N(5)-C(6) | 1.4(5) | C(4)-N(5)-C(6)-C(7) | 176.8(4) |
| C(4)-N(5)-C(6)-C(11) | -1.3(5) | N(5)-C(6)-C(7)-C(8) | -180.0(5) |
| C(11)-C(6)-C(7)-C(8) | -2.1(6) | C(6)-C(7)-C(8)-C(9) | 1.2(7) |
| C(7)-C(8)-C(9)-C(10) | -0.6(7) | C(8)-C(9)-C(10)-C(11) | 0.9(7) |
| C(9)-C(10)-C(11)-C(12) | 178.1(5) | C(9)-C(10)-C(11)-C(6) | -1.8(6) |
| N(5)-C(6)-C(11)-C(10) | -179.3(4) | C(7)-C(6)-C(11)-C(10) | 2.4(6) |
| N(5)-C(6)-C(11)-C(12) | 0.8(5) | C(7)-C(6)-C(11)-C(12) | -177.5(4) |
| C(10)-C(11)-C(12)-C(13) | -2.6(9) | C(6)-C(11)-C(12)-C(13) | 177.3(5) |
| C(10)-C(11)-C(12)-C(4) | -179.8(4) | C(6)-C(11)-C(12)-C(4) | 0.1(5) |
| C(3)-C(4)-C(12)-C(13) | 1.7(6) | N(5)-C(4)-C(12)-C(13) | -178.8(4) |
| C(3)-C(4)-C(12)-C(11) | 179.7(4) | N(5)-C(4)-C(12)-C(11) | -0.9(5) |
| C(11)-C(12)-C(13)-C(1) | -177.0(5) | C(4)-C(12)-C(13)-C(1) | 0.1(6) |
| N(2)-C(1)-C(13)-C(12) | -1.3(6) | O(14)-C(1)-C(13)-C(12) | 176.2(4) |
| N(2)-C(1)-O(14)-C(15) | -9.2(5) | C(13)-C(1)-O(14)-C(15) | 173.1(4) |
| C(1)-O(14)-C(15)-C(16) | -179.7(4) | O(14)-C(15)-C(16)-C(17) | -179.6(4) |
| O(14')-C(1')-N(2')-C(3') | 177.6(4) | C(13')-C(1')-N(2')-C(3') | -1.2(6) |
| C(1')-N(2')-C(3')-C(4') | -1.0(6) | N(2')-C(3')-C(4')-N(5') | -178.4(4) |
| N(2')-C(3')-C(4')-C(12') | 2.5(6) | C(3')-C(4')-N(5')-C(6') | 179.6(5) |
| C(12')-C(4')-N(5')-C(6') | -1.3(5) | C(4')-N(5')-C(6')-C(7') | -176.6(4) |
| C(4')-N(5')-C(6')-C(11') | 0.4(5) | N(5')-C(6')-C(7')-C(8') | 178.1(5) |
| C(11')-C(6')-C(7')-C(8') | 1.4(6) | C(6')-C(7')-C(8')-C(9') | 0.2(7) |
| C(7')-C(8')-C(9')-C(10') | -0.7(8) | C(8')-C(9')-C(10')-C(11') | -0.2(7) |
| C(9')-C(10')-C(11')-C(6') | 1.8(6) | C(9')-C(10')-C(11')-C(12') | -178.5(4) |
| N(5')-C(6')-C(11')-C(10') | -179.7(4) | C(7')-C(6')-C(11')-C(10') | -2.4(6) |
| N(5')-C(6')-C(11')-C(12') | 0.6(5) | C(7')-C(6')-C(11')-C(12') | 177.8(4) |
| C(3')-C(4')-C(12')-C(13') | -1.8(6) | N(5')-C(4')-C(12')-C(13') | 178.9(4) |
| C(3')-C(4')-C(12')-C(11') | -179.2(4) | N(5')-C(4')-C(12')-C(11') | 1.6(5) |
| C(10')-C(11')-C(12')-C(13') | 2.4(9) | C(6')-C(11')-C(12')-C(13') | -177.8(5) |
| C(10')-C(11')-C(12')-C(4') | 178.9(5) | C(6')-C(11')-C(12')-C(4') | -1.3(5) |
| C(4')-C(12')-C(13')-C(1') | -0.2(6) | C(11')-C(12')-C(13')-C(1') | 176.1(5) |
| N(2')-C(1')-C(13')-C(12') | 1.7(6) | O(14')-C(1')-C(13')-C(12') | -177.0(4) |
| N(2')-C(1')-O(14')-C(15') | 7.2(5) | C(13')-C(1')-O(14')-C(15') | -174.0(4) |
| C(1')-O(14')-C(15')-C(16') | 179.1(4) | O(14')-C(15')-C(16')-C(17') | 176.9(4) |