

Supplementary Information

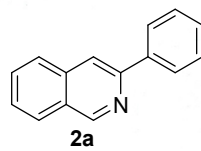
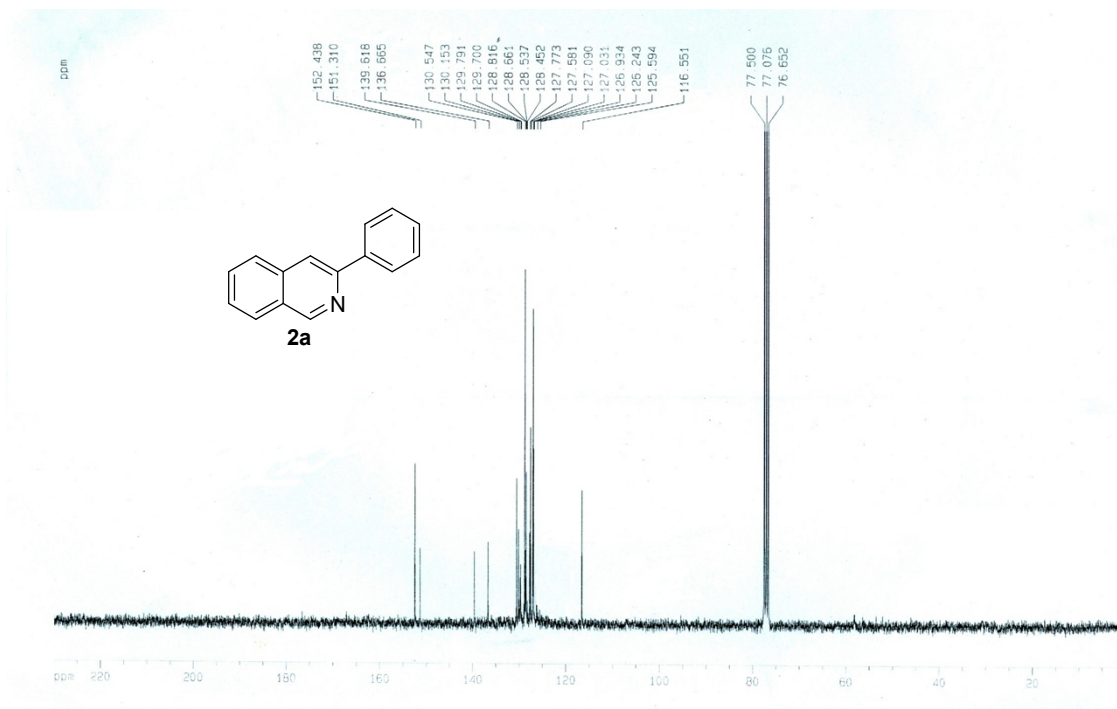
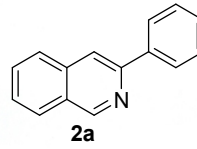
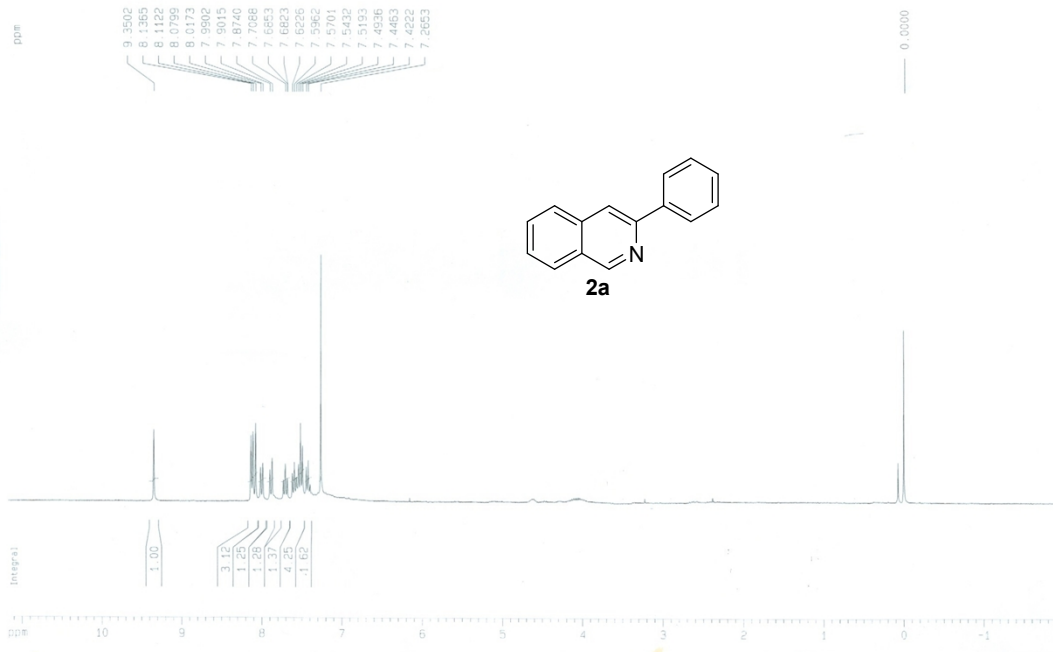
Efficient synthesis of isoquinolines and pyridines via copper(I)-catalyzed multi-component reaction

Kommoori Shekarrao, Partha Pratim Kaishap, Sanjib Gogoi,* Romesh C Boruah*

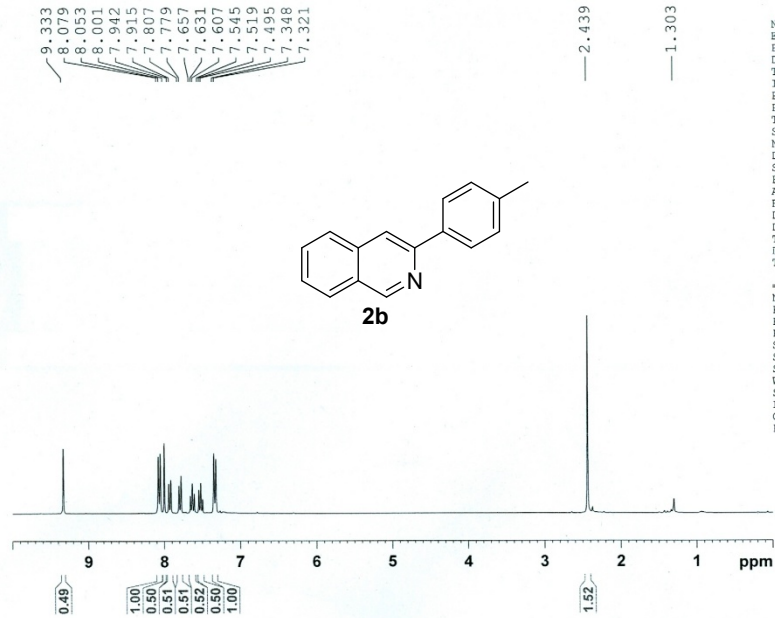
Medicinal Chemistry Division, CSIR-North East Institute of Science and Technology, Jorhat 785006, India Tel.: +91 3762372948; fax: +913762370011; Email: skgogoi@gmail.com; rc_boruah@yahoo.co.in

^1H NMR and ^{13}C NMR Spectra of compounds 2a-y

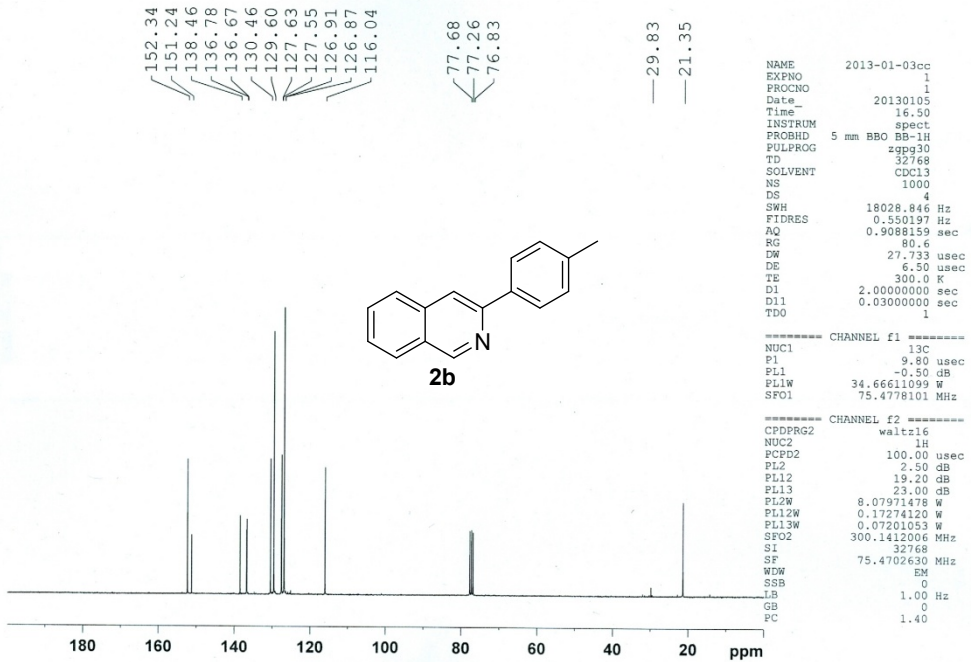
Name of Sample: 5-PHEN
Spectrum No: 10476



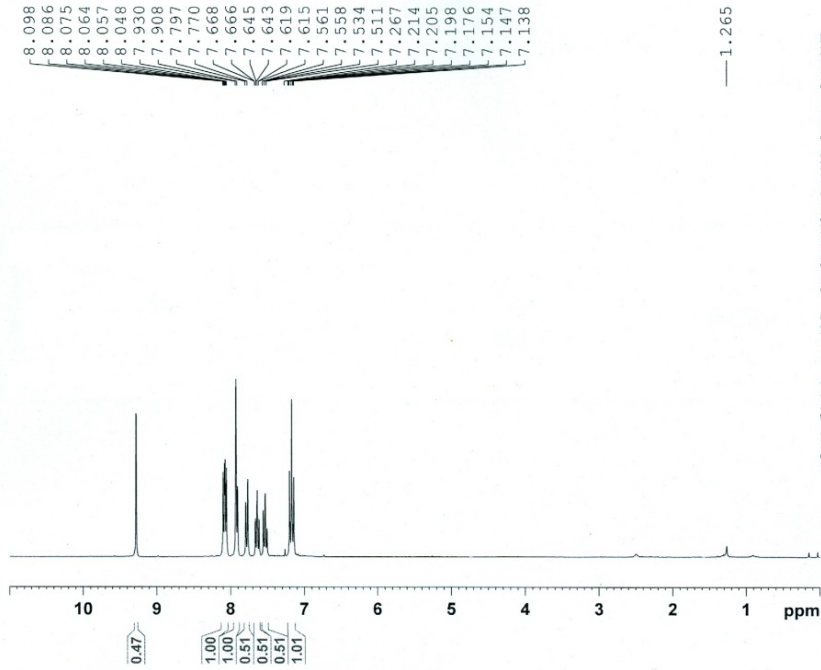
KS-1



KS-1

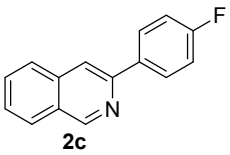


KS-2

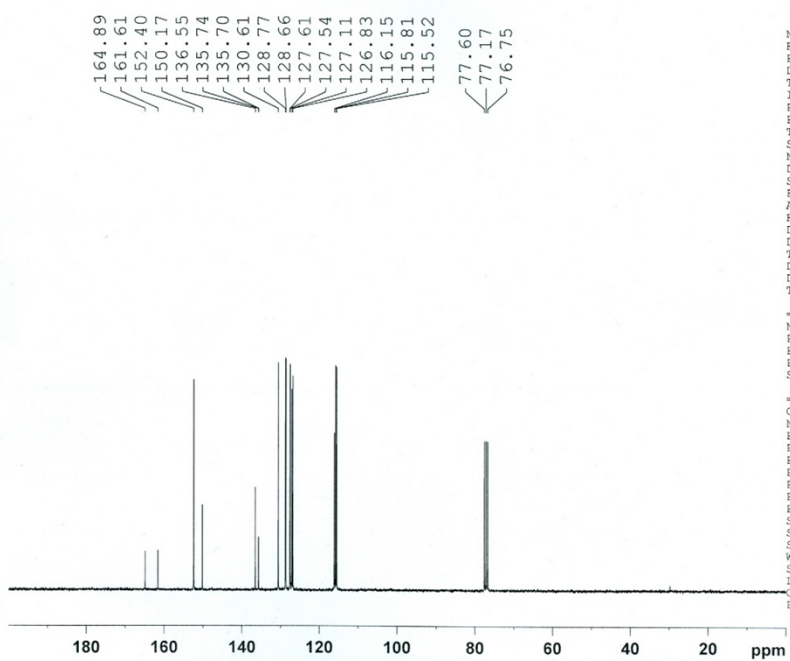


```
NAME      2013-01-03-d-d
EXPNO     1
PROCNO    1
Date_     20130105
Time      17.16
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD        32768
SOLVENT   CDCl3
NS        16
DS        2
SWH       6188.119 Hz
FIDRES    0.188846 Hz
AQ        2.6477044 sec
RG        40.3
DW        80.800 usec
DE        6.50 usec
TE        300.0 K
D1        1.00000000 sec
TDO       1
```

```
----- CHANNEL f1 -----
NUC1      1H
P1        14.75 usec
PL1       2.50 dB
PL1W      8.07971478 W
SFO1      300.1418535 MHz
SI        16384
SF        300.1400000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```



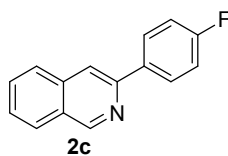
KS-2



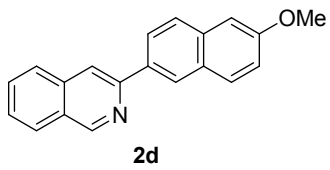
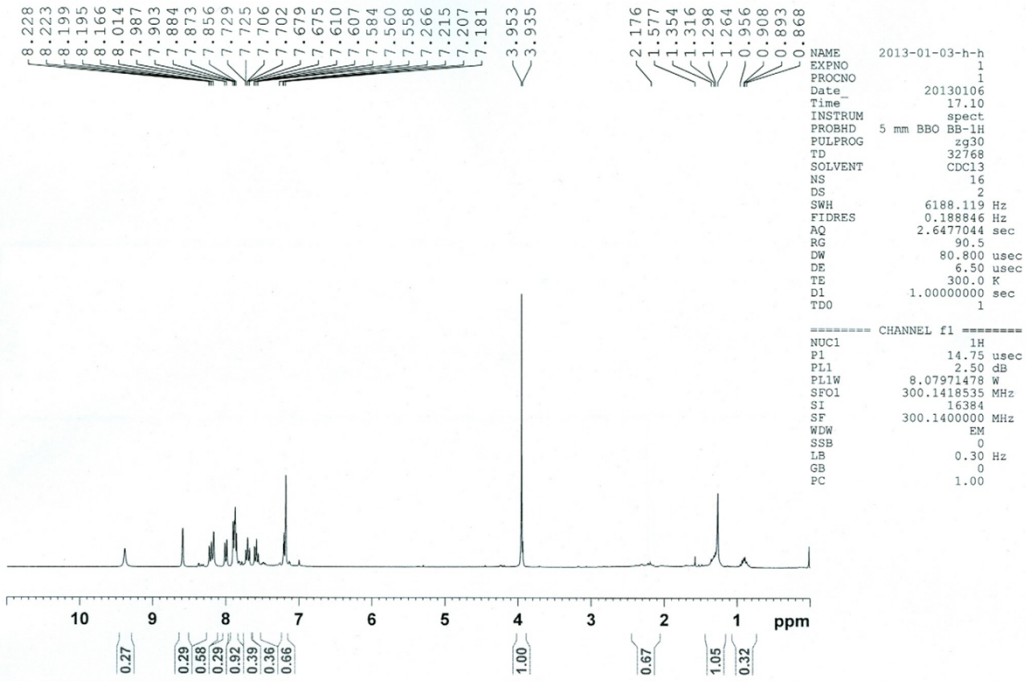
```
NAME      2013-01-03ddd
EXPNO     1
PROCNO    1
Date_     20130105
Time      17.41
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         496
DS         4
SWH        18028.846 Hz
FIDRES     0.550197 Hz
AQ         0.9088159 sec
RG         80.6
DW         27.733 usec
DE         6.50 usec
TE         300.0 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1
```

```
===== CHANNEL f1 =====
NUC1      13C
P1        9.80 usec
PL1       -0.50 dB
PL1W      34.6661099 W
SFO1      75.4778101 MHz
```

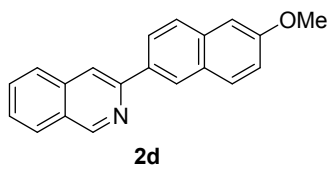
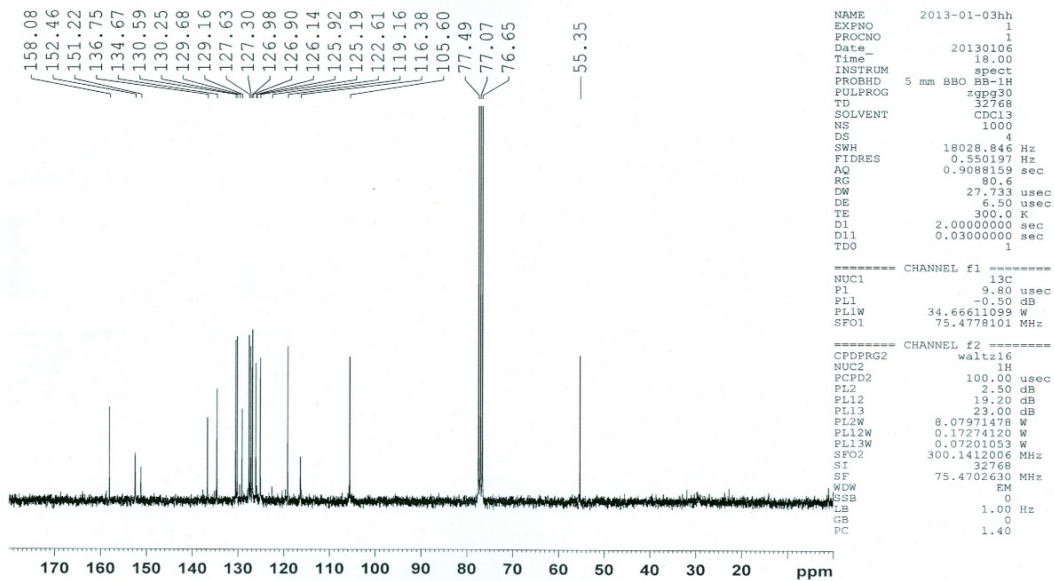
```
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     100.00 usec
PL2        2.50 dB
PL12      19.20 dB
PL13      23.00 dB
PL2W      8.07971478 W
PL12W     0.17274120 W
PL13W     0.07201053 W
SFO2      300.1412006 MHz
SI         32768
SF         75.4702630 MHz
WDW        EM
SSB        0
LB         1.00 Hz
CB         0
PC         1.40
```

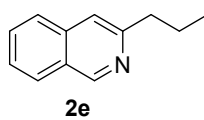
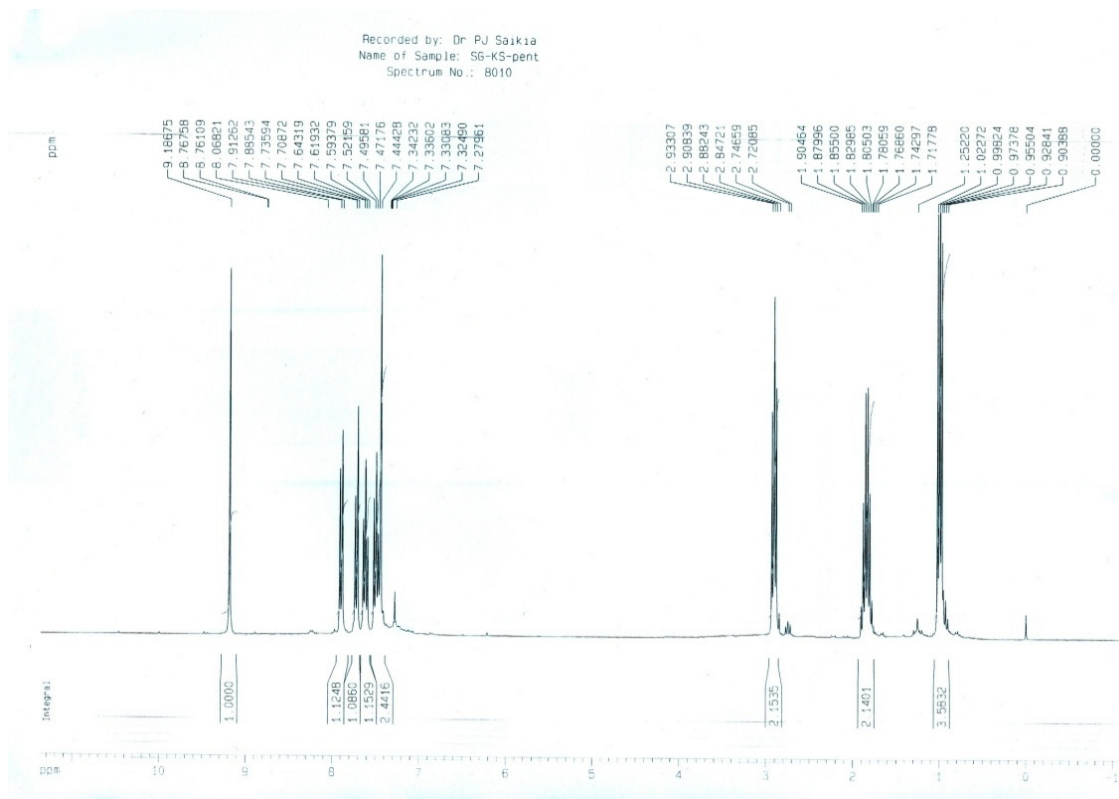


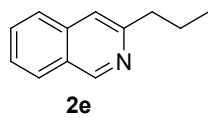
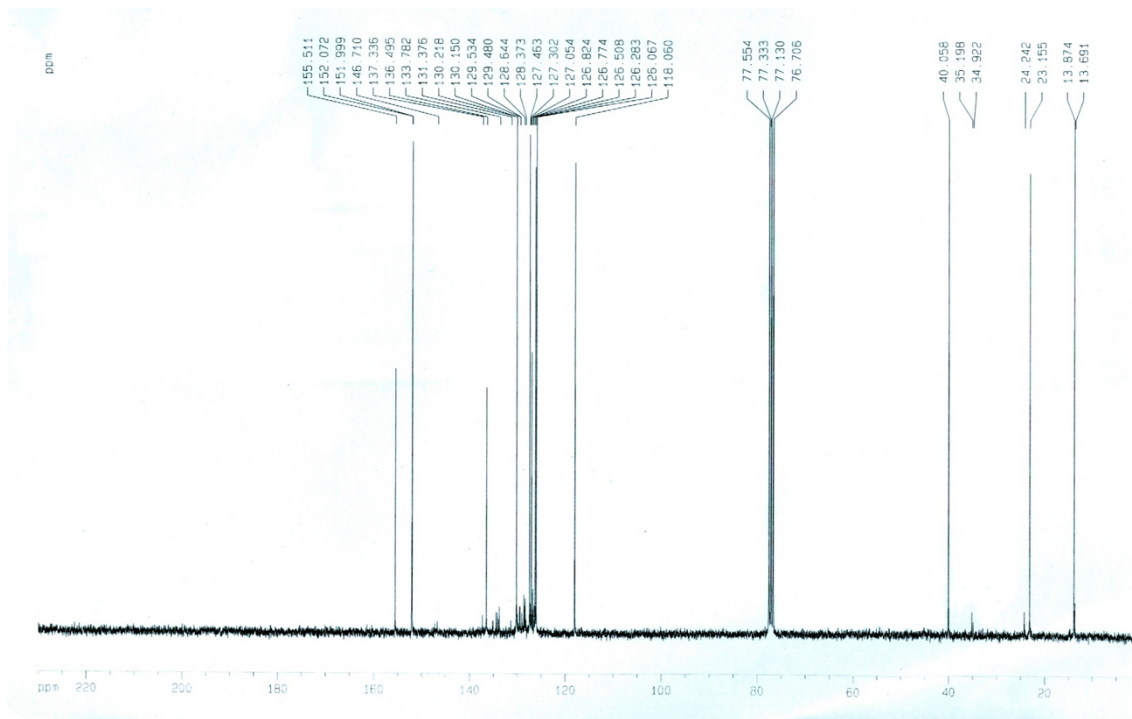
KS-4



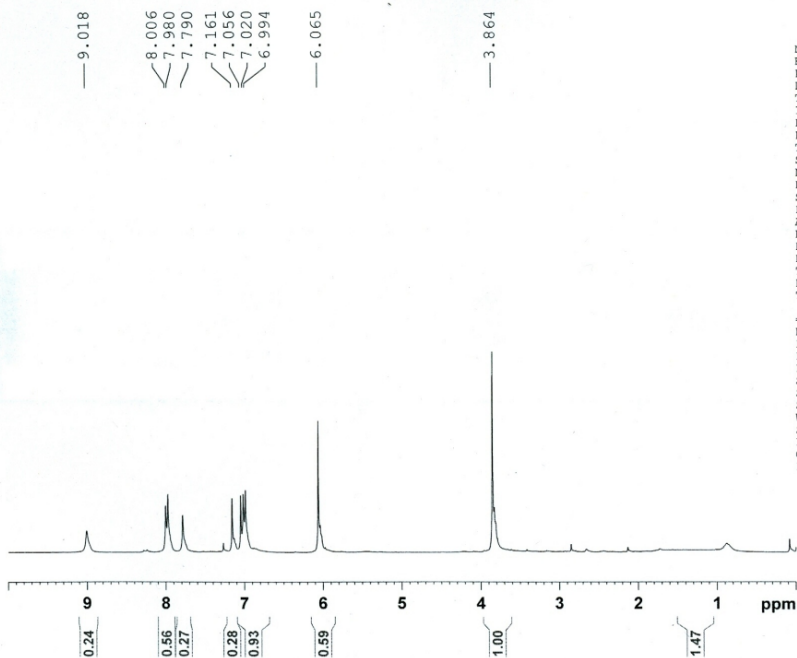
KS-4







KS-7

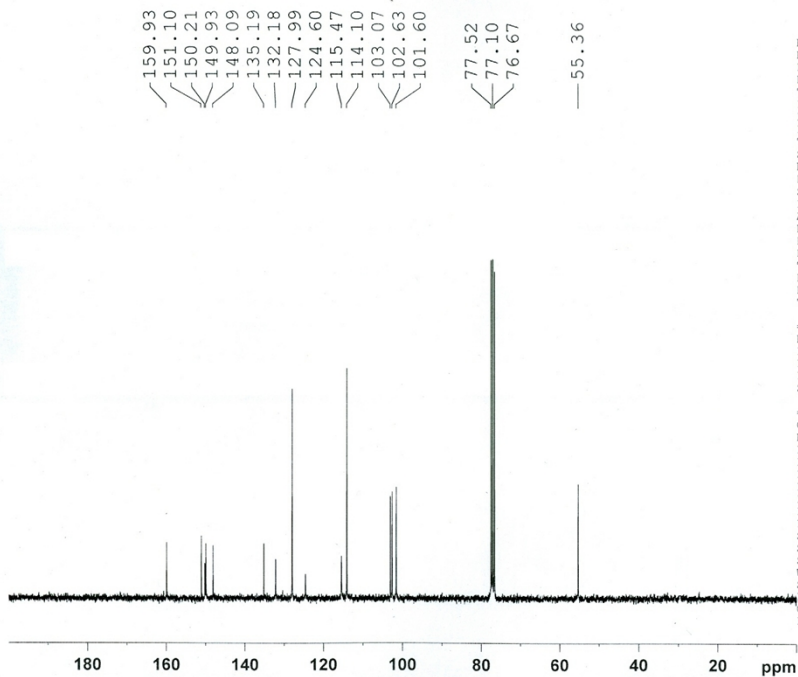
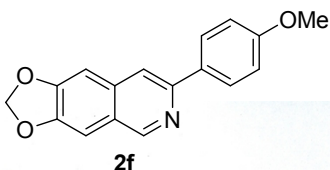


```

NAME      2013-01-03-a-a
EXPNO    1
PROCNO   1
Date_    20130103
Time     15.08
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zg30
TD       32768
SOLVENT  CDCl3
NS       16
DS       2
SWH      6188.119 Hz
FIDRES   0.188846 Hz
AQ       2.6477044 sec
RG       64
DW       80.800 usec
DE       6.50 usec
TE       300.0 K
D1       1.00000000 sec
TDO      1
  
```

```

===== CHANNEL f1 =====
NUC1     1H
P1       14.75 usec
PL1      2.50 dB
PL1W     8.07971478 W
SF01     300.1418535 MHz
SI       16384
SF       300.1400000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```



```

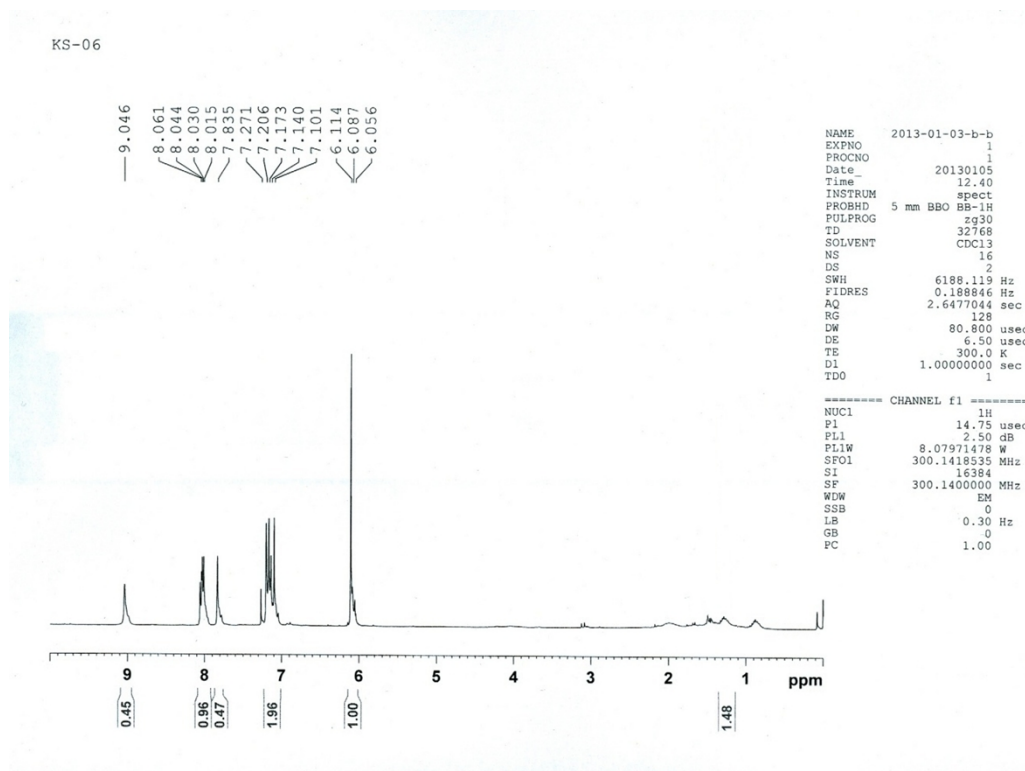
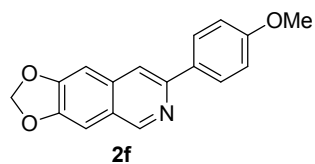
NAME      2013-01-03aa
EXPNO    1
PROCNO   1
Date_    20130103
Time     15.58
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
TD       32768
SOLVENT  CDCl3
NS       1000
DS       4
SWH      18028.846 Hz
FIDRES   0.550197 Hz
AQ       0.9088159 sec
RG       80.6
DW       27.733 usec
DE       6.50 usec
TE       300.0 K
D1       2.00000000 sec
D11      0.03000000 sec
TDO      1
  
```

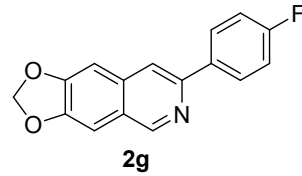
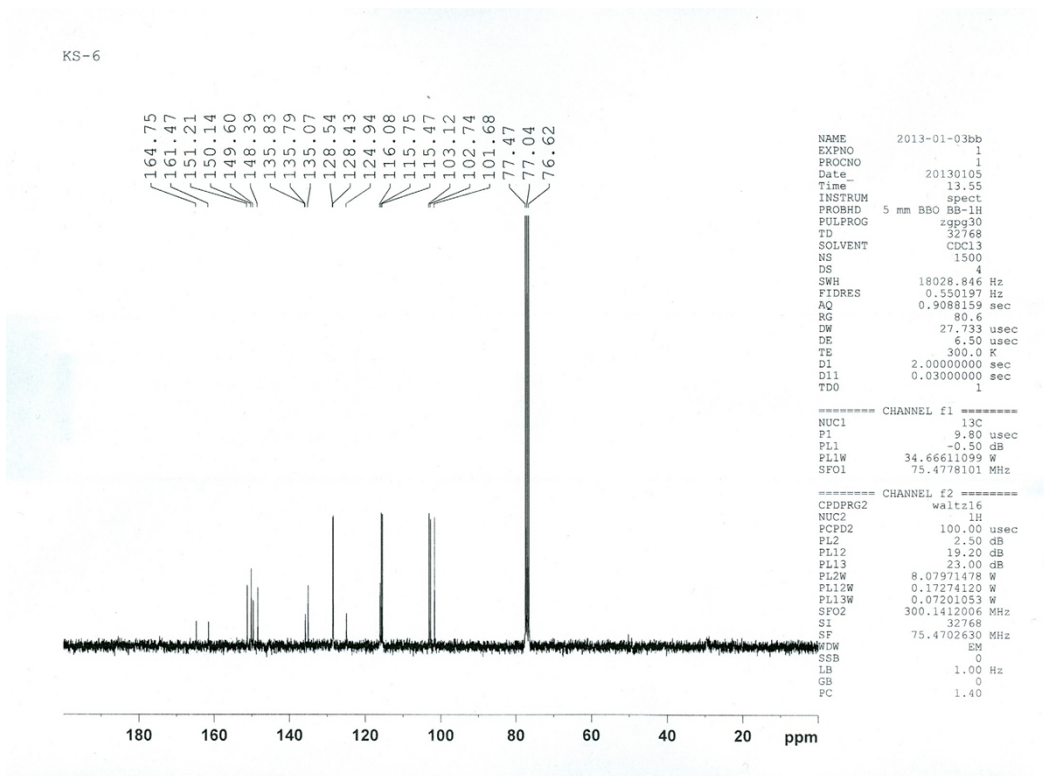
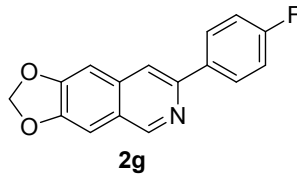
```

===== CHANNEL f1 =====
NUC1     13C
P1       9.80 usec
PL1      -0.50 dB
PL1W     34.66611099 W
SF01     75.4778101 MHz
  
```

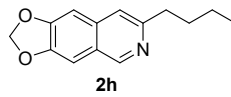
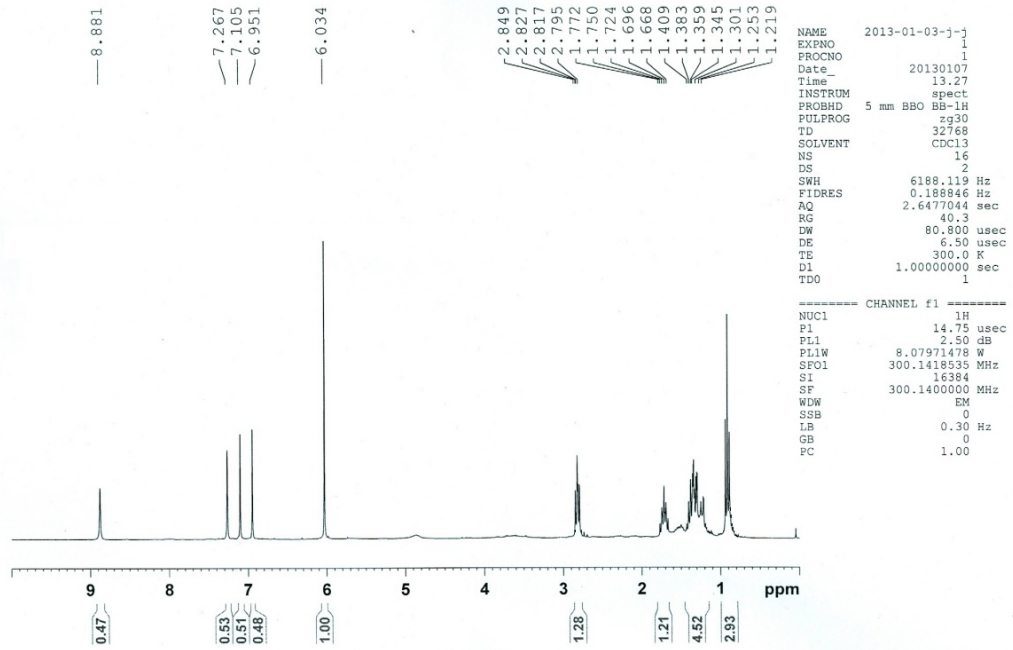
```

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    100.00 usec
PL2      2.50 dB
PL12     19.20 dB
PL13     23.00 dB
PL2W     8.07971478 W
PL12W    0.17274120 W
PL13W    0.07201053 W
SF02     300.1412006 MHz
SI       32768
SF       75.4702630 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```

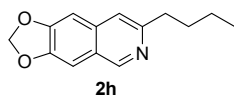
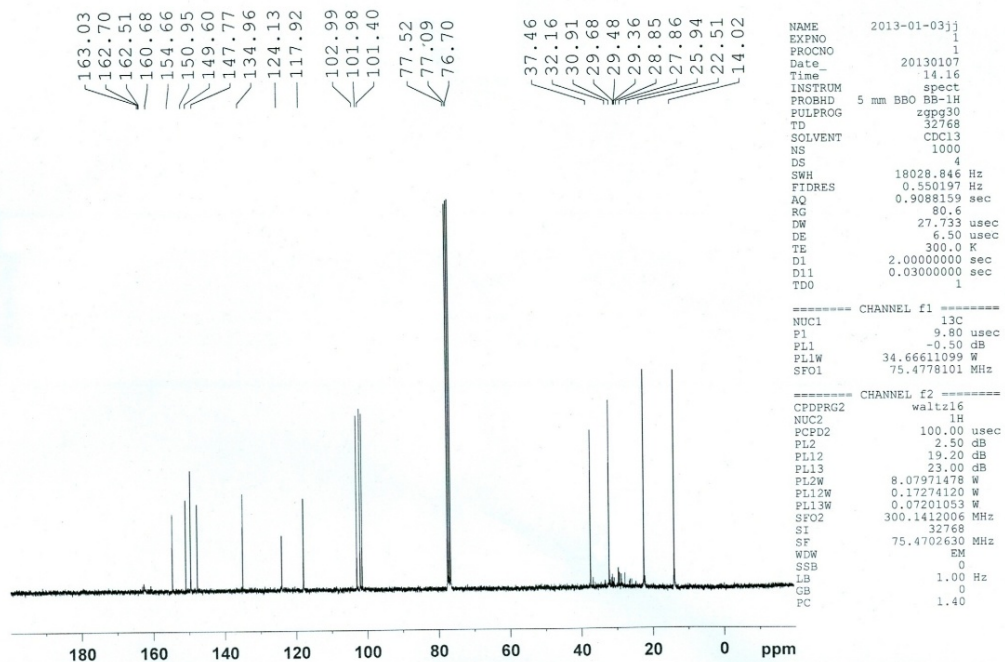


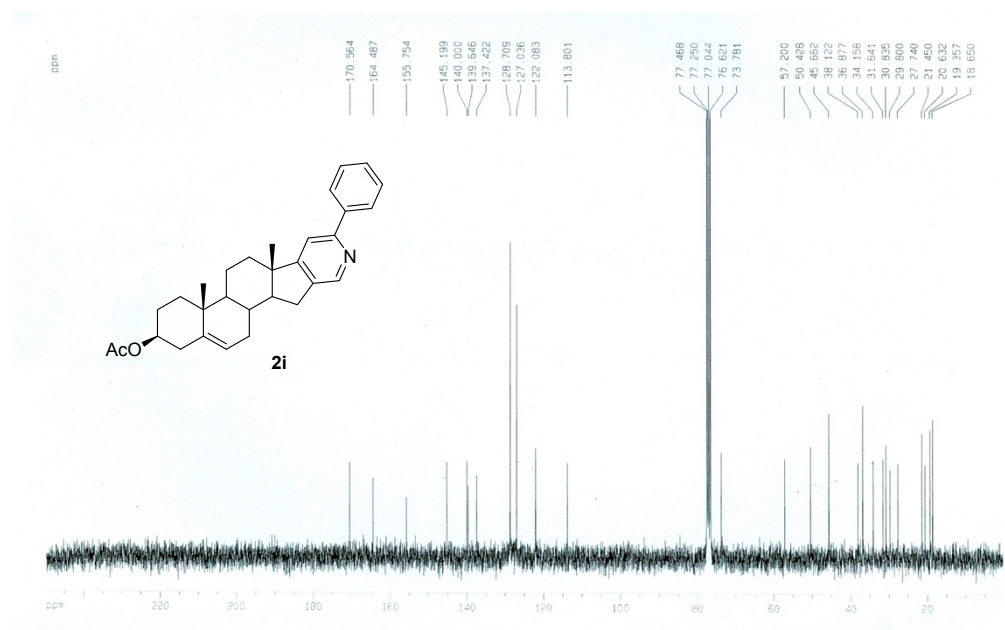
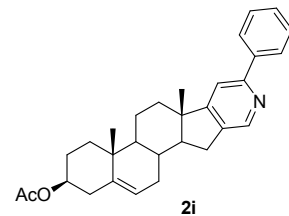
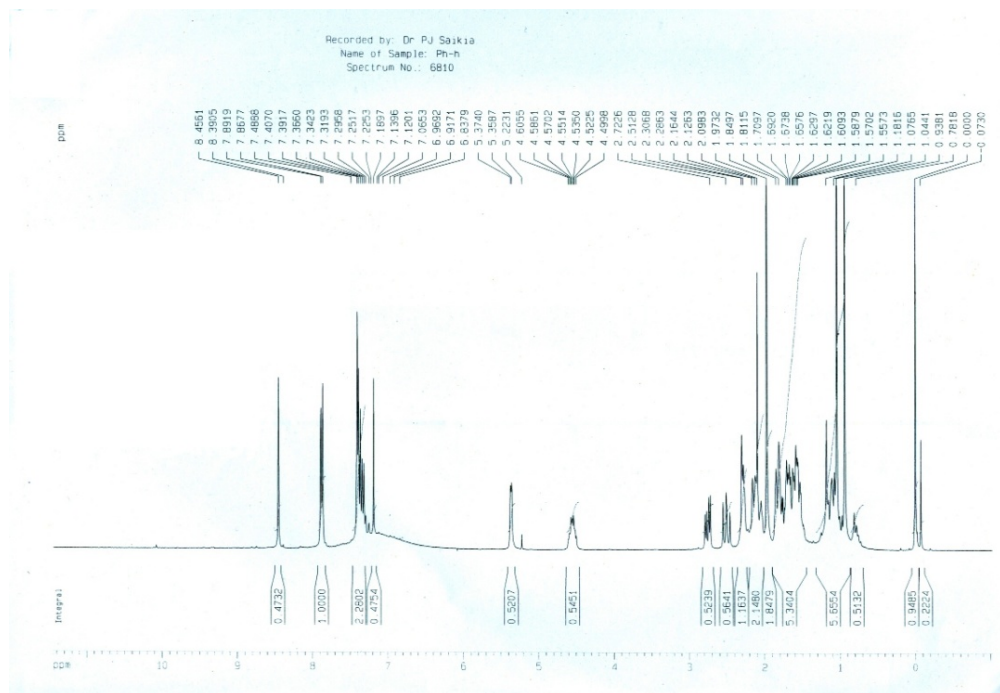


KS-9

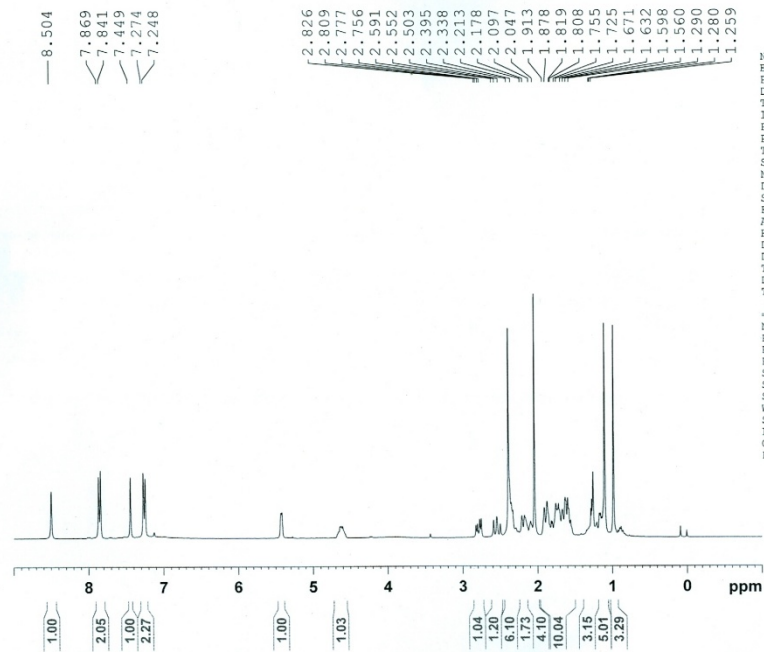


KS-9

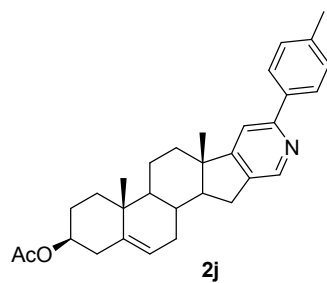




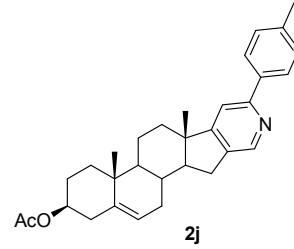
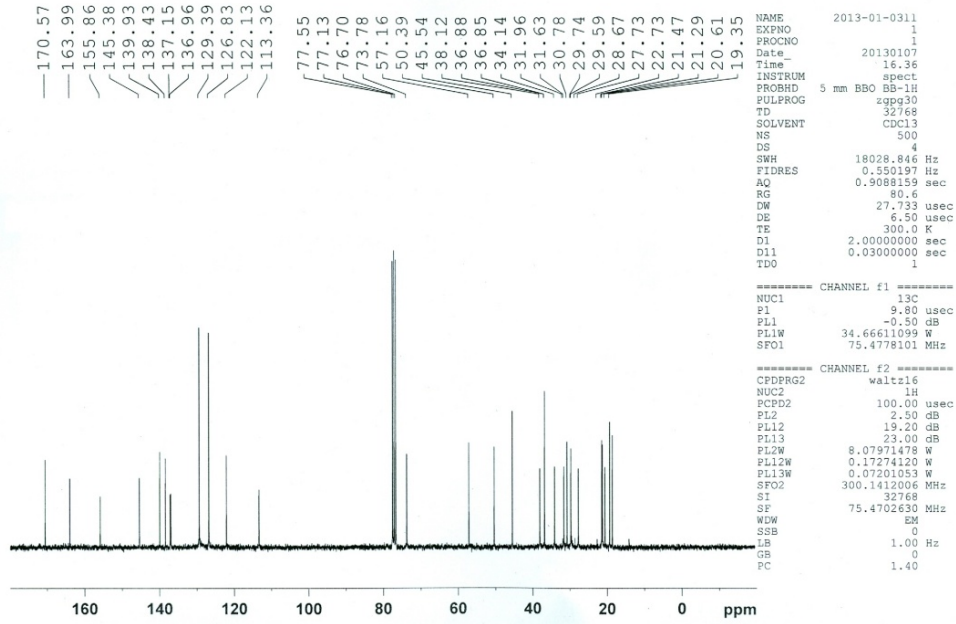
KS-11



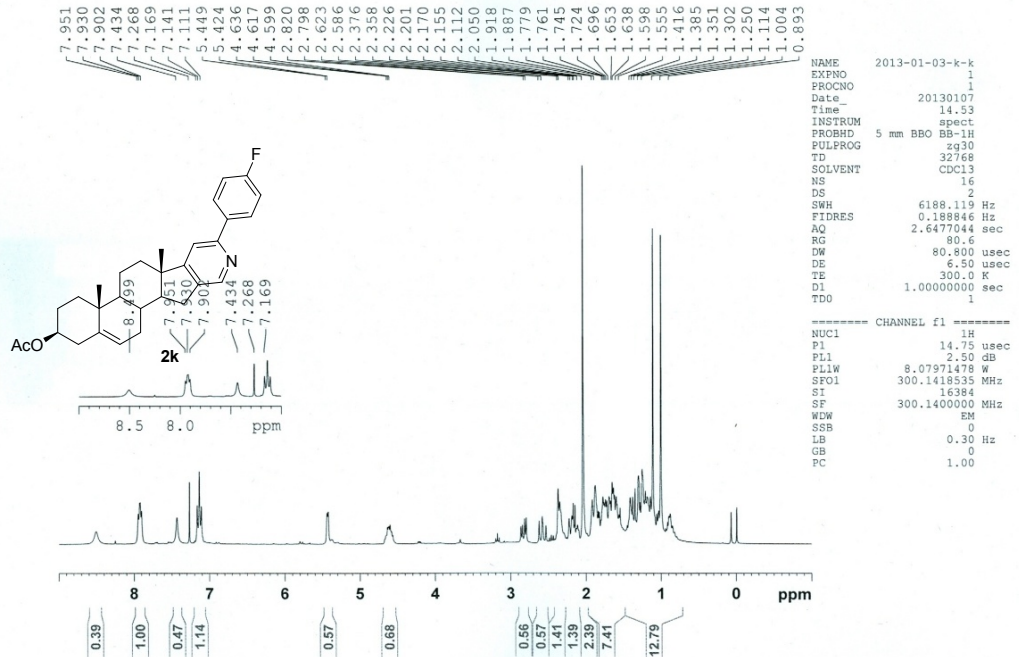
```
NAME      2013-01-03-1-1
EXPNO     1
PROCNO    1
Date_     20130107
Time      16.11
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD        32768
SOLVENT   CDCl3
NS        16
DS        2
SWH       6188.119 Hz
FIDRES    0.188846 Hz
AQ        2.6477044 sec
RG        36
DW        80.800 usec
DE        6.50 usec
TE        300.0 K
DL        1.0000000 sec
TDO       1
----- CHANNEL f1 -----
NUC1      1H
P1        14.75 usec
PL1       2.50 dB
PL1W      8.07971478 W
SFO1      300.1418535 MHz
SI        16384
SF        300.1400000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```



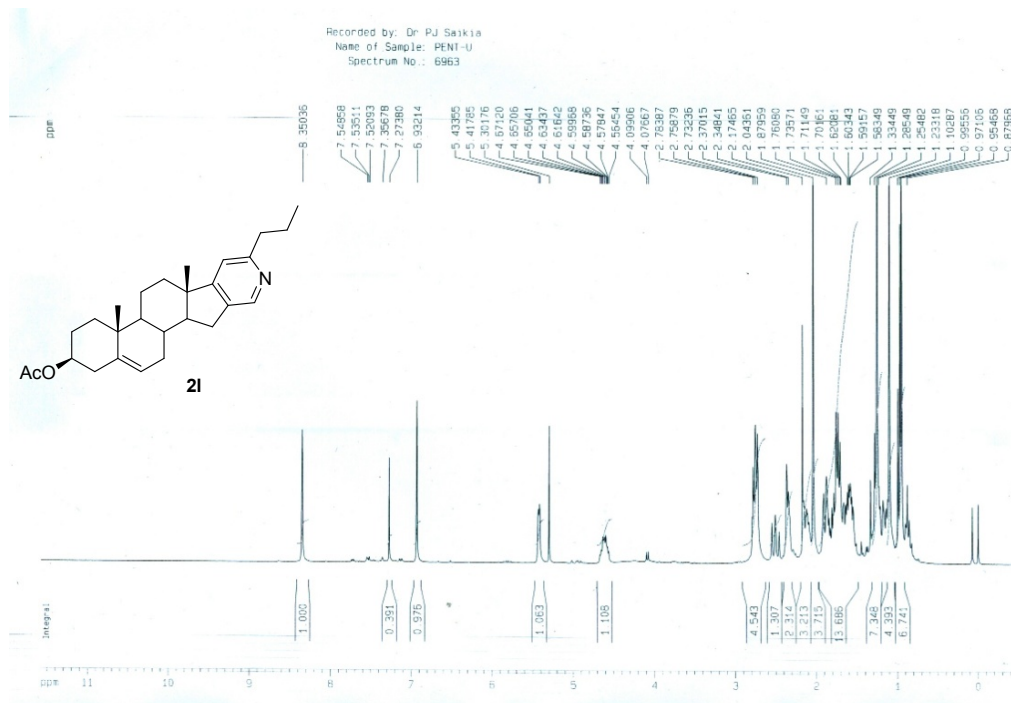
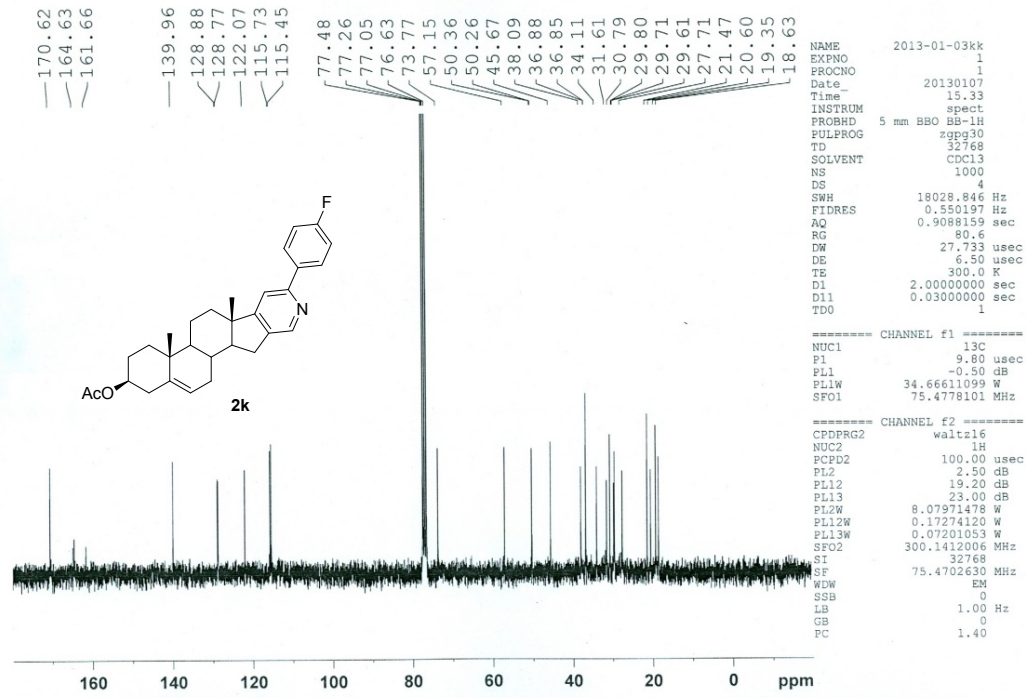
KS-11

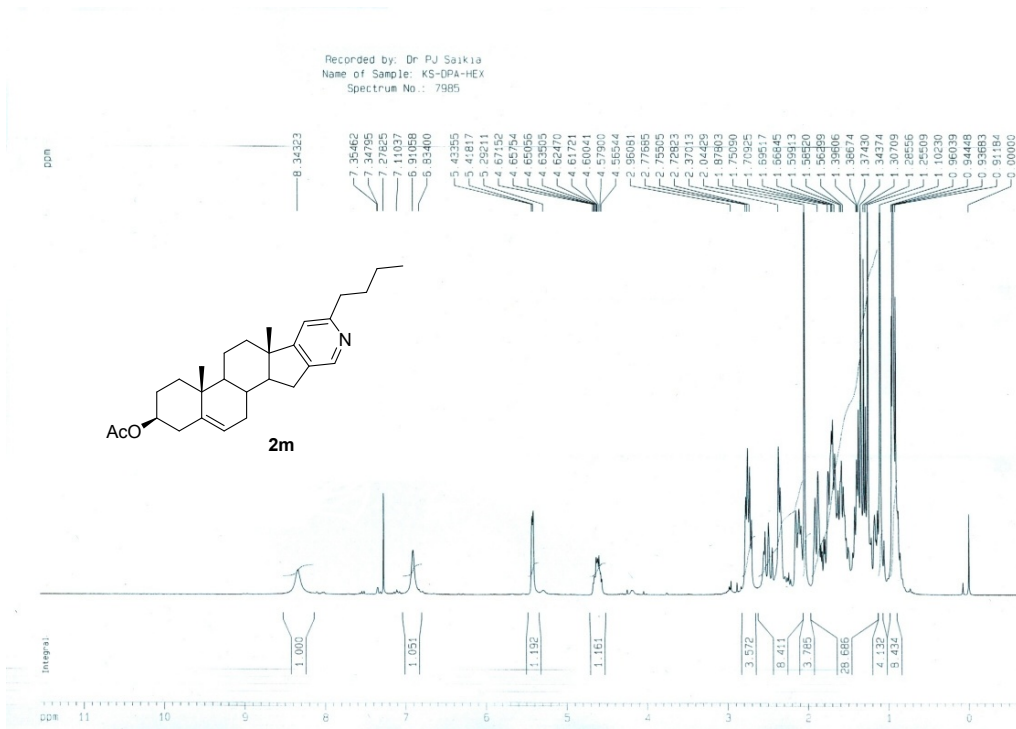
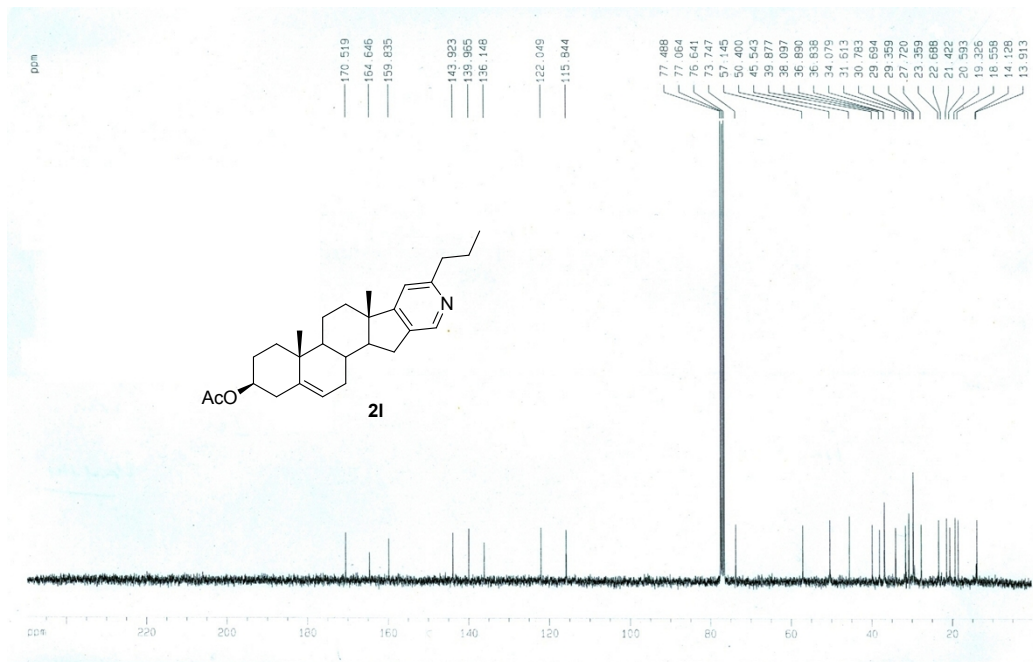


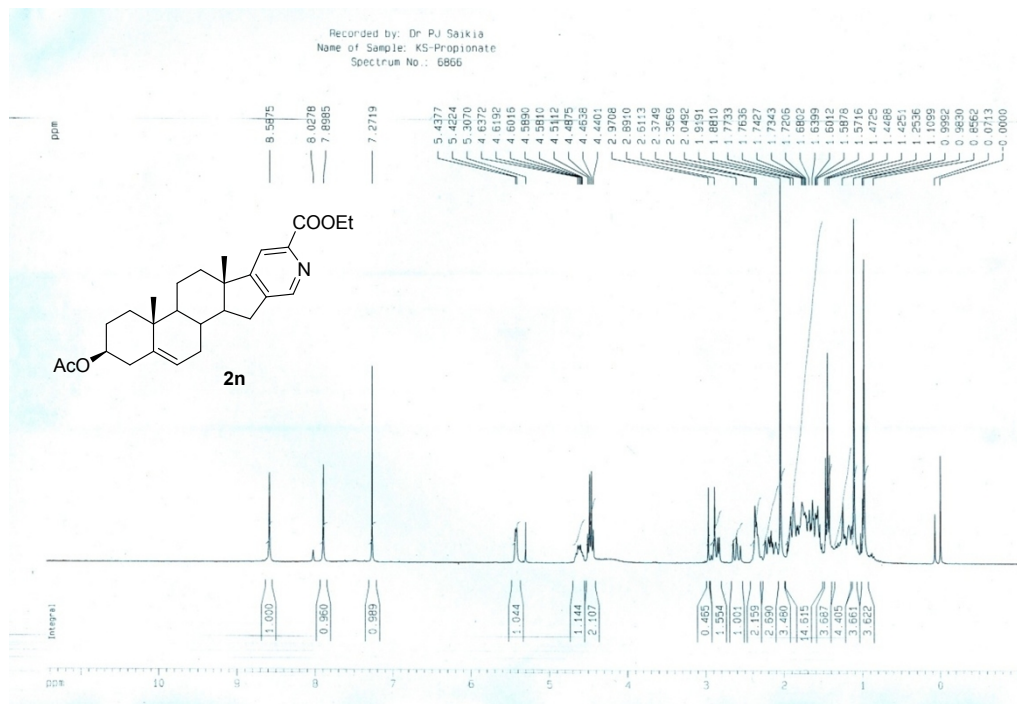
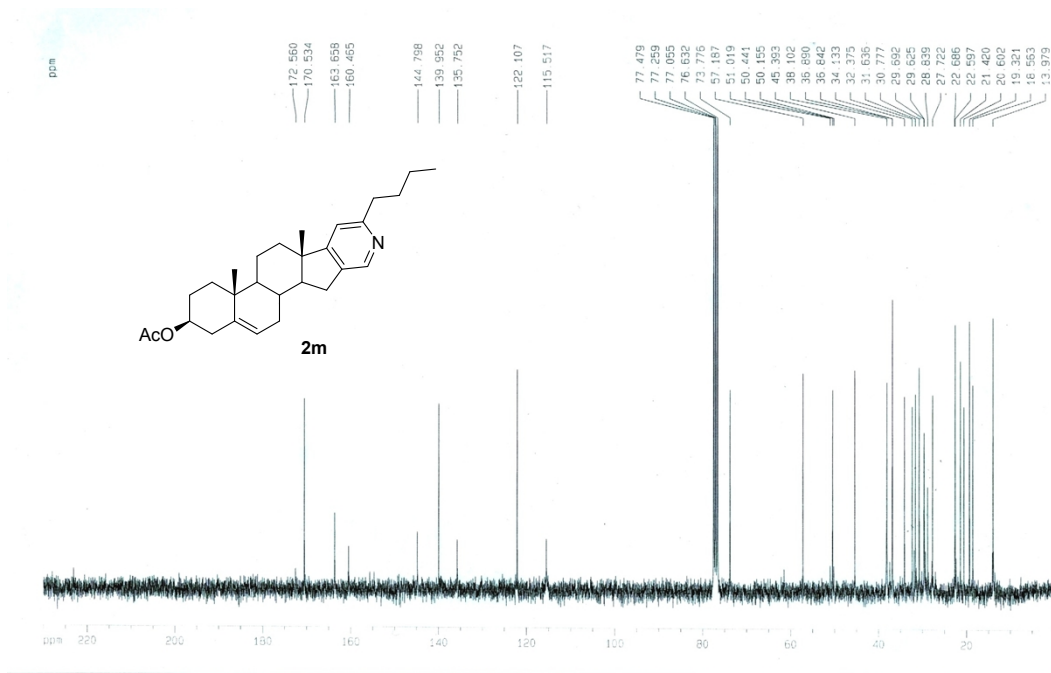
KS-12

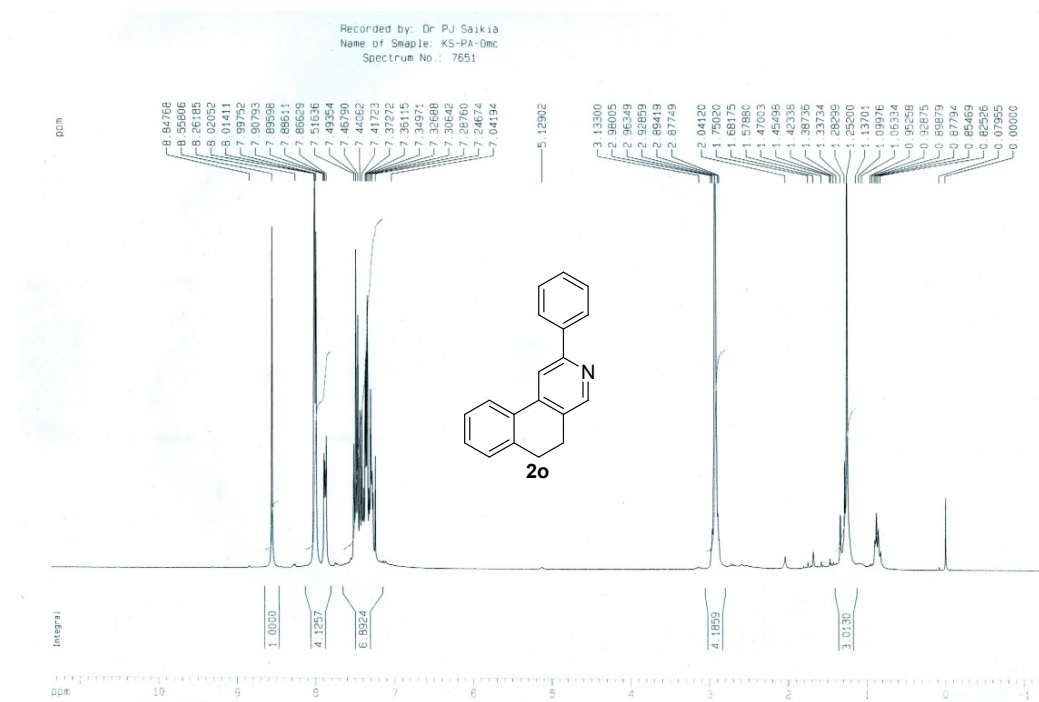
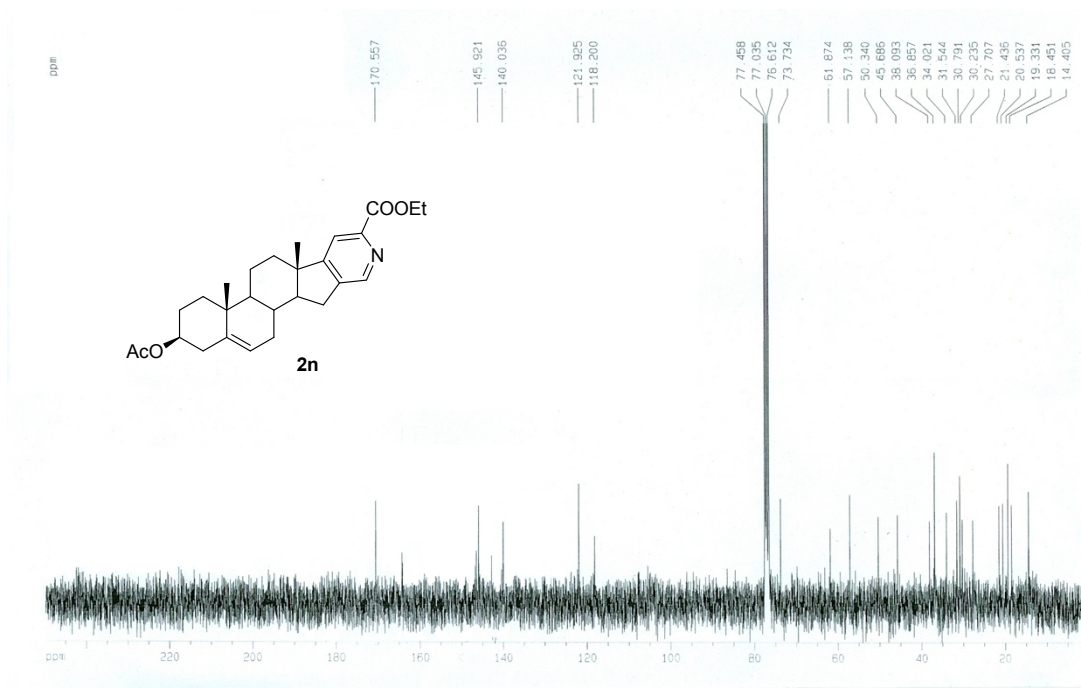


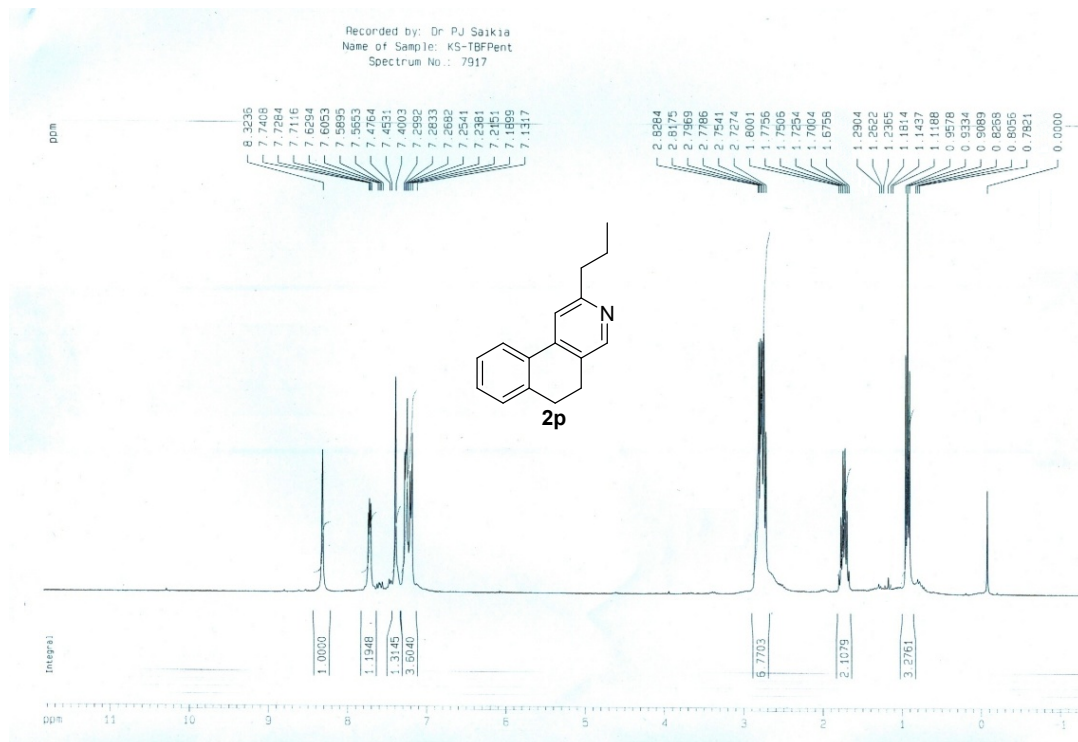
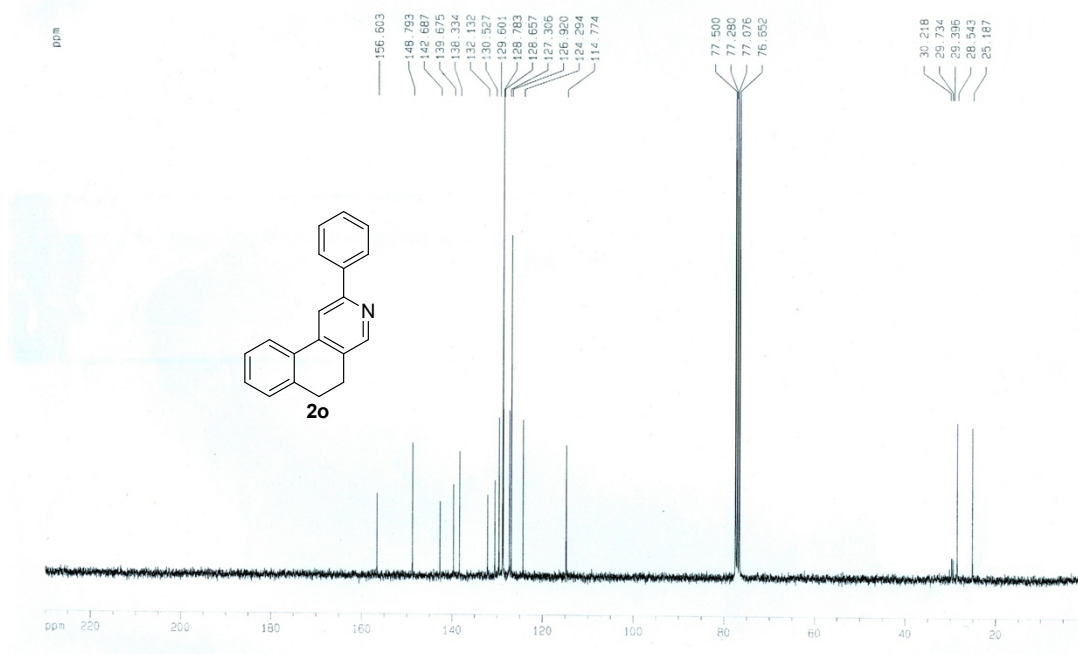
KS-12

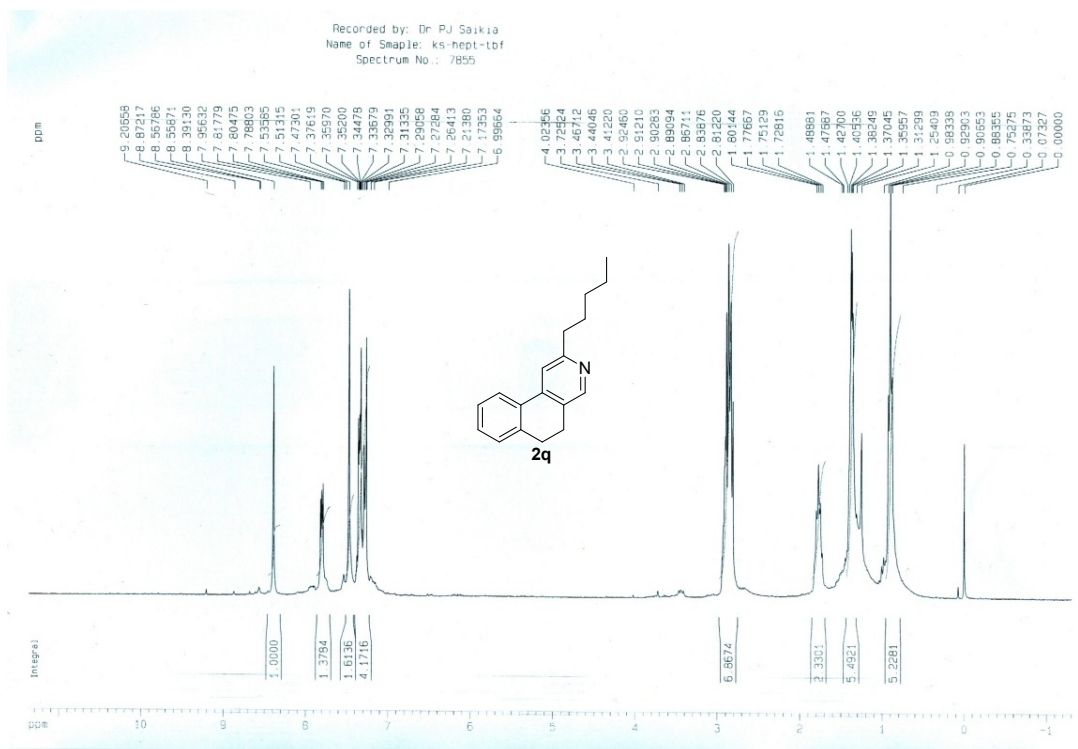
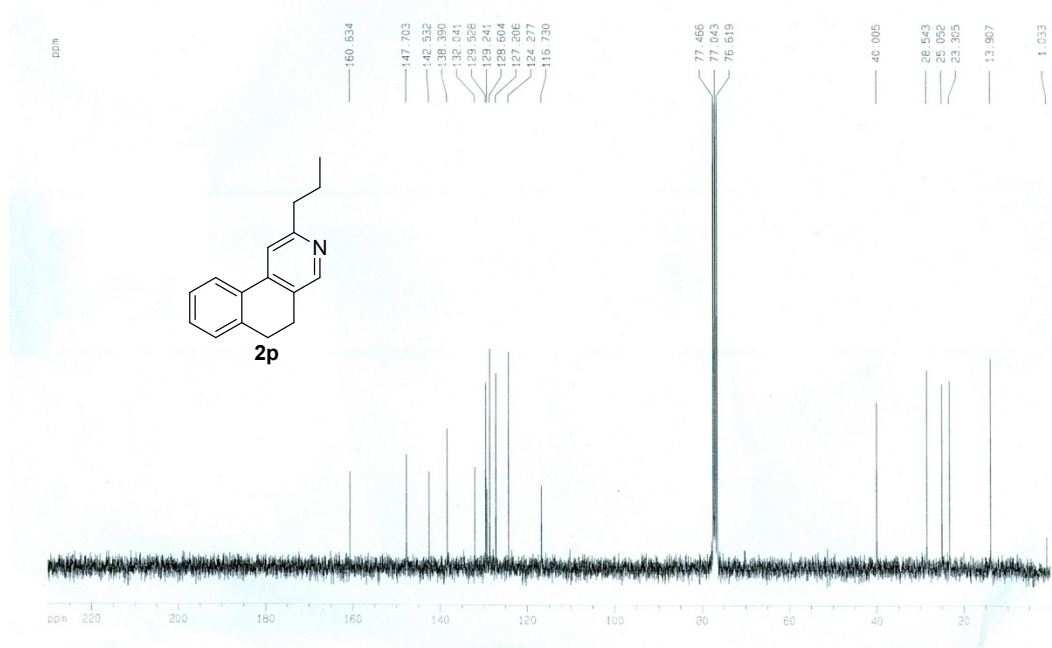


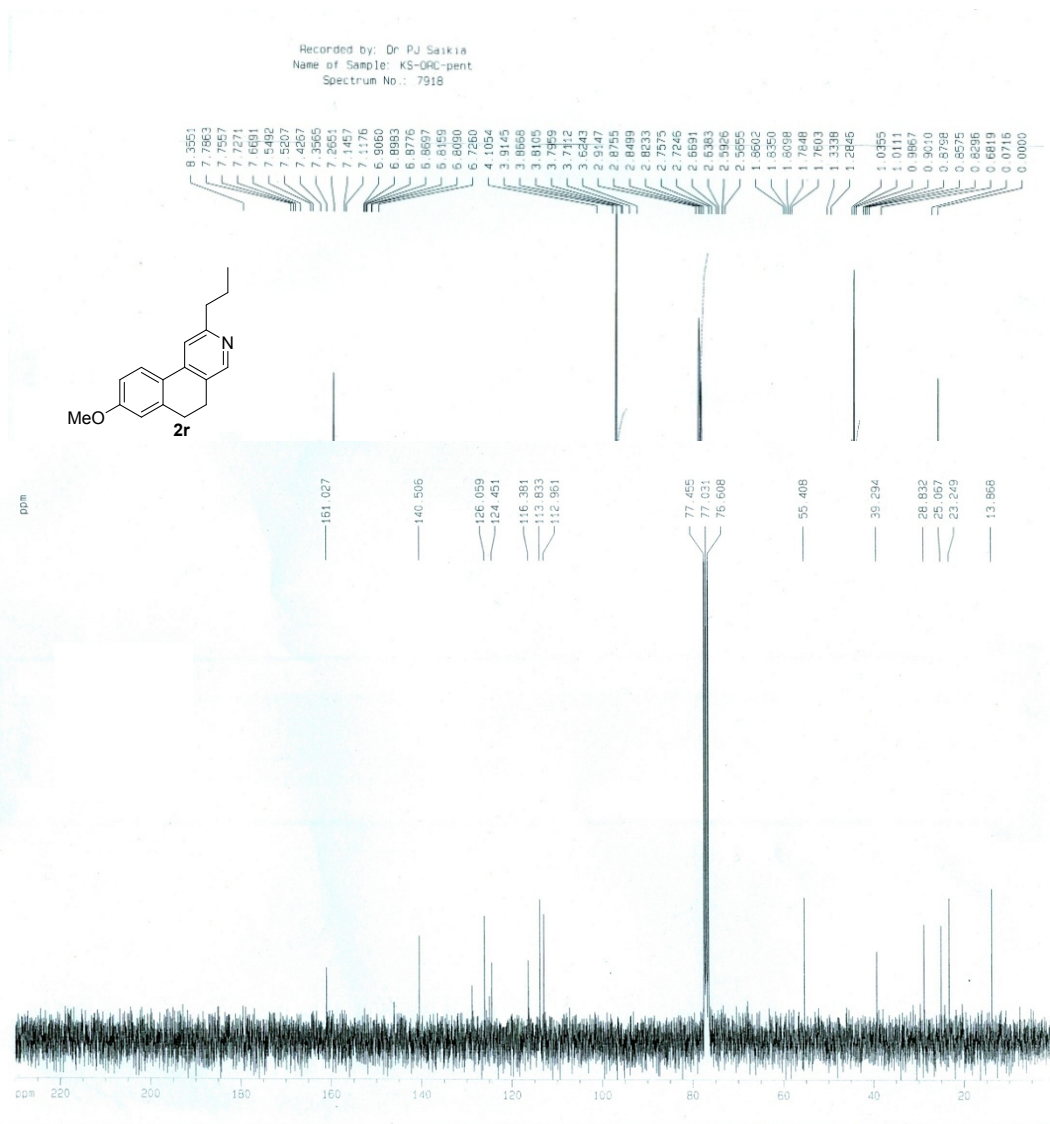
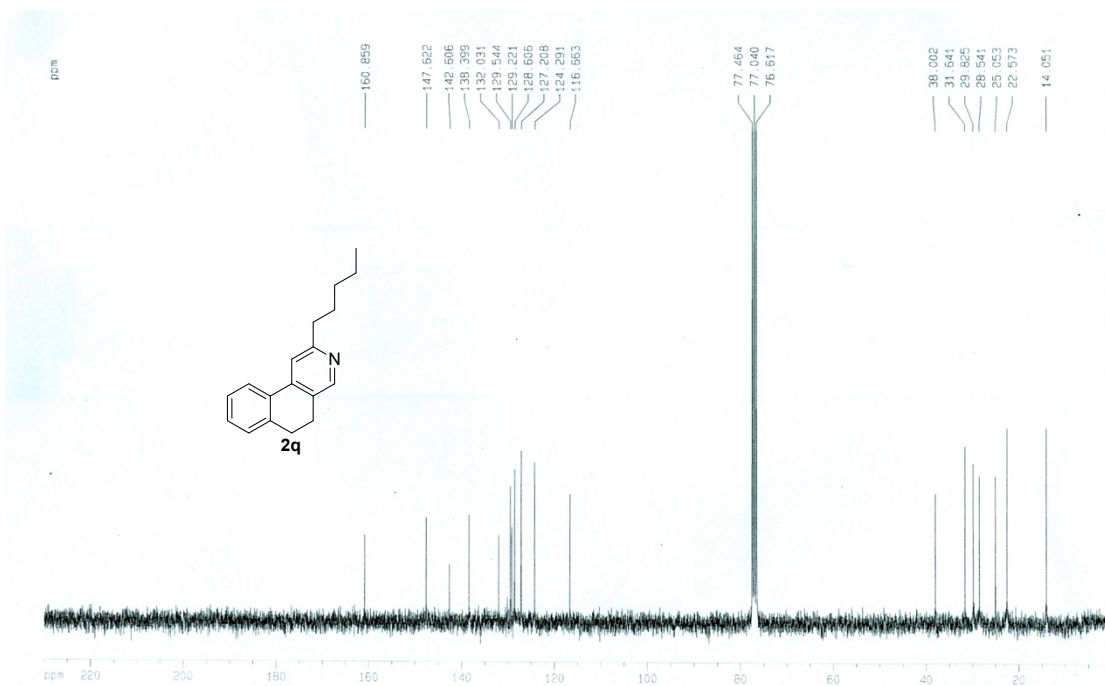


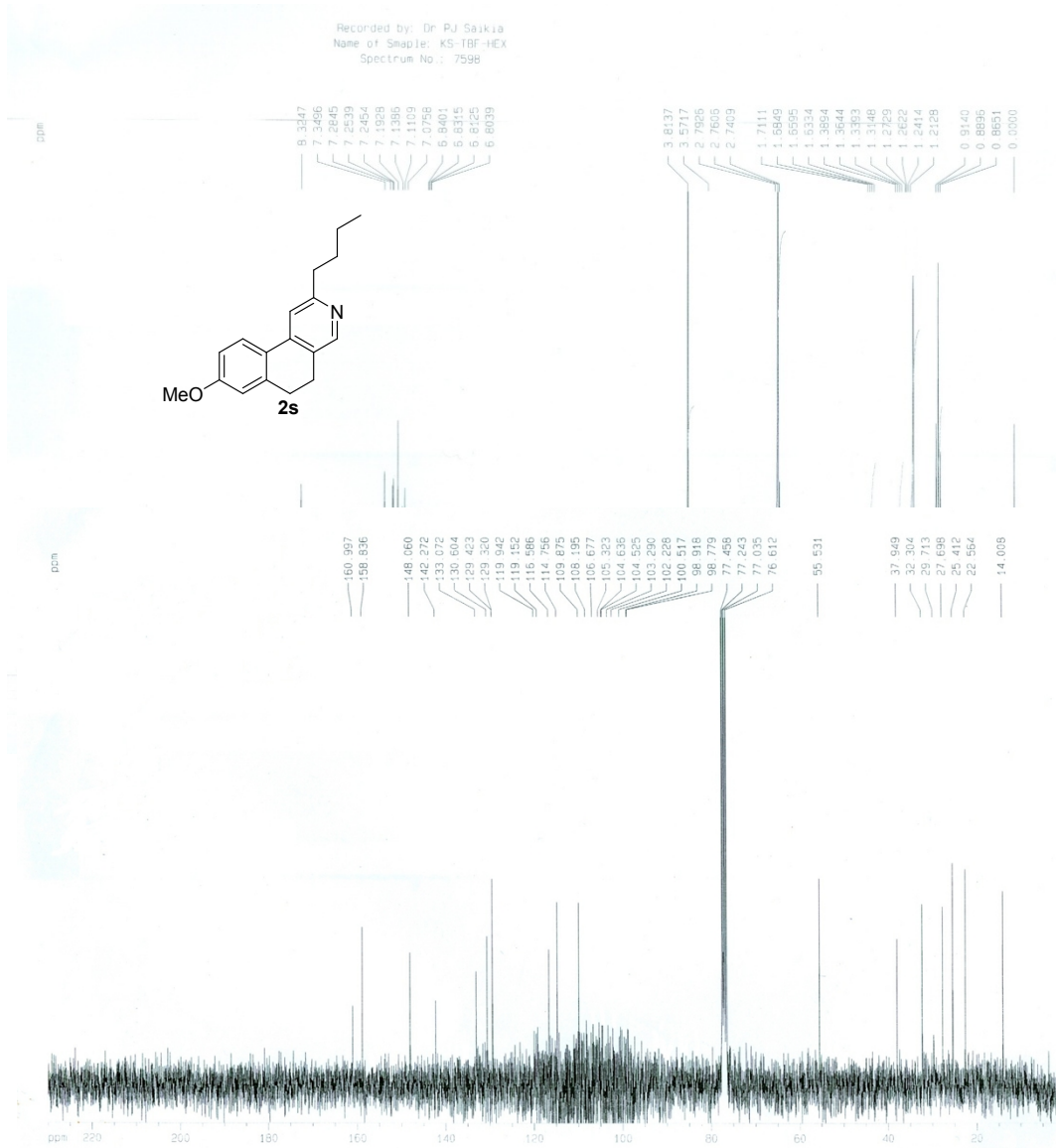
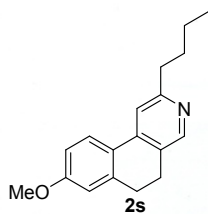
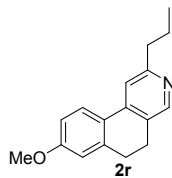


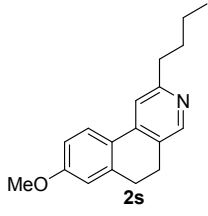




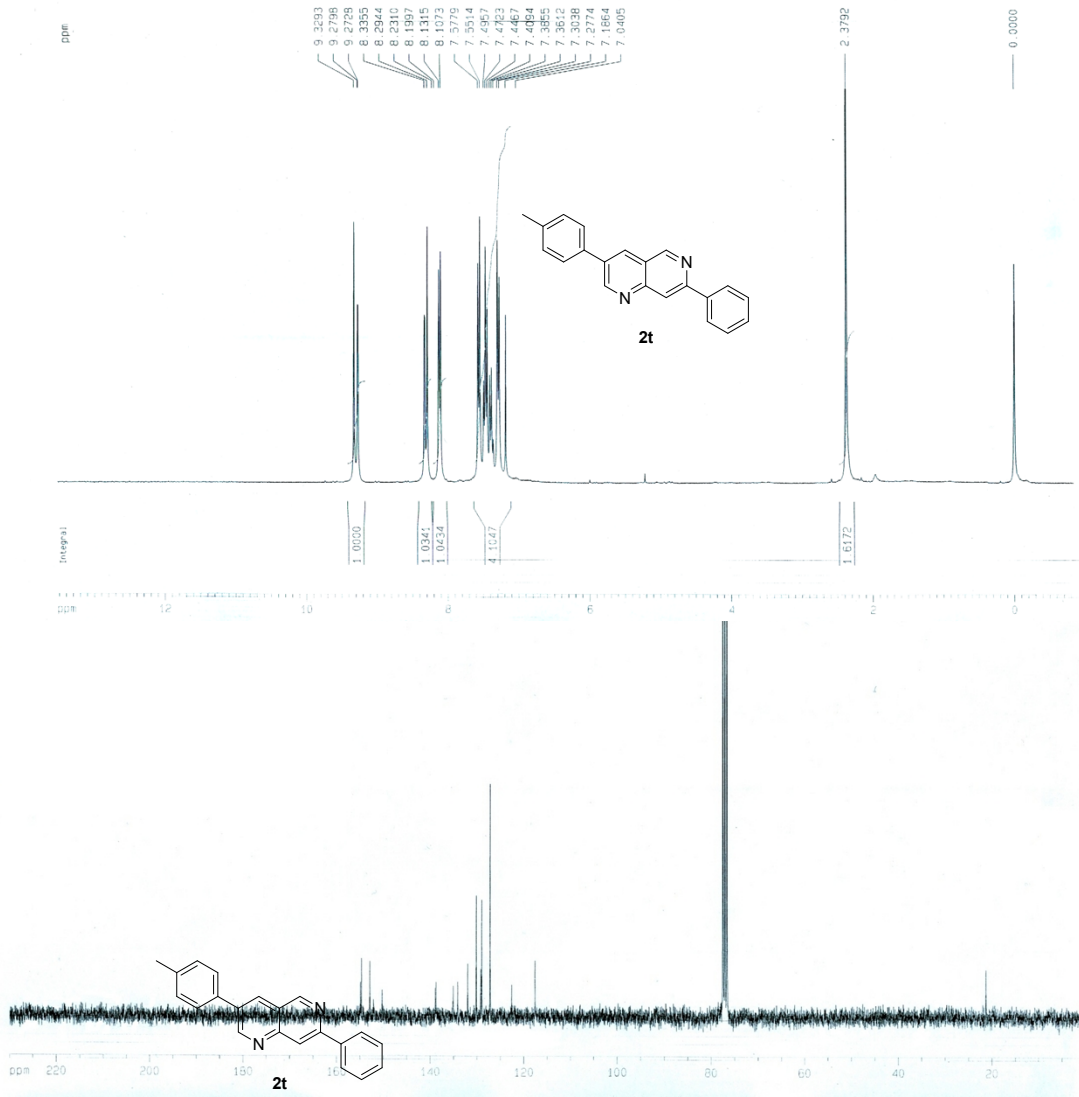






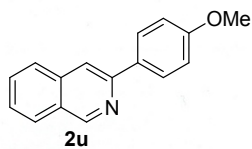


Recorded by: Dr. P.J. Saikia
 Name of Sample: PJ-PA
 Spectrum No: 8880



KS-3

9.301
8.100
8.069
7.976
7.937
7.832
7.806
7.682
7.679
7.659
7.654
7.632
7.628
7.561
7.558
7.535
7.511
7.508
7.055
7.026



3.870
3.841

```

NAME      2013-01-03-g-g
EXPNO     1
PROCNO    1
Date_     20130106
Time      11.21
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH       6188.119 Hz
FIDRES    0.188846 Hz
AQ         2.6477044 sec
RG         64
DW         80.800 usec
DE         6.50 usec
TE         300.0 K
D1         1.00000000 sec
TDO        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        14.75 usec
          dB
          W
          MHz
          MHz
          Hz
  
```

KS-3

160.10
152.29
150.99
136.75
132.22
130.50
128.22
127.57
127.41
126.76
126.70
115.43
114.18

77.54
77.12
76.69

55.42

```

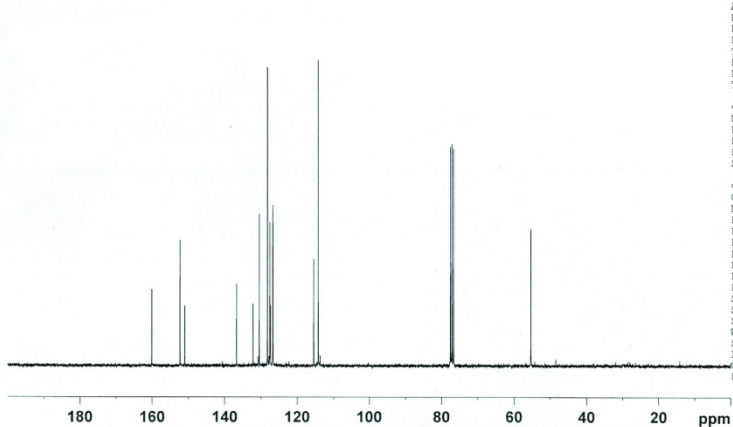
NAME      2013-01-03gg
EXPNO     1
PROCNO    1
Date_     20130106
Time      12.11
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         1000
DS         4
SWH       18028.846 Hz
FIDRES    0.550197 Hz
AQ         0.9088159 sec
RG         80.6
DW         27.733 usec
DE         6.50 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
  
```

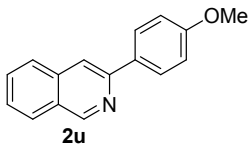
```

===== CHANNEL f1 =====
NUC1      13C
P1         9.80 usec
          -0.50 dB
          34.66611099 W
          75.4778101 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     100.00 usec
PL2       2.50 dB
PL12      19.20 dB
PL13      23.00 dB
PL2W      8.07971478 W
PL12W     0.17274120 W
PL13W     0.07201053 W
SFO2      300.1412006 MHz
SI         32768
SF         75.4702630 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



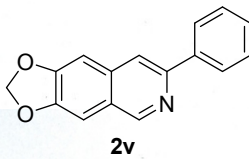


KS-5

8.995
8.065
8.042
7.785
7.506
7.481
7.454
7.411
7.387
7.361
7.083
7.075
6.971
6.960
5.955
5.945

```

NAME      2013-01-03-f-f
EXPNO     1
PROCNO    1
Date_     20130106
Time      10.54
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        6188.119 Hz
FIDRES    0.188846 Hz
AQ         2.6477044 sec
RG         32
DW         80.800 usec
DE         6.50 usec
TE         300.0 K
SI         1
  
```



KS-5

151.04
150.31
150.02
148.28
139.55
134.97
129.17
128.76
128.32
127.24
126.78
124.94
116.31
102.98
102.69
101.64
77.68
77.26
76.83

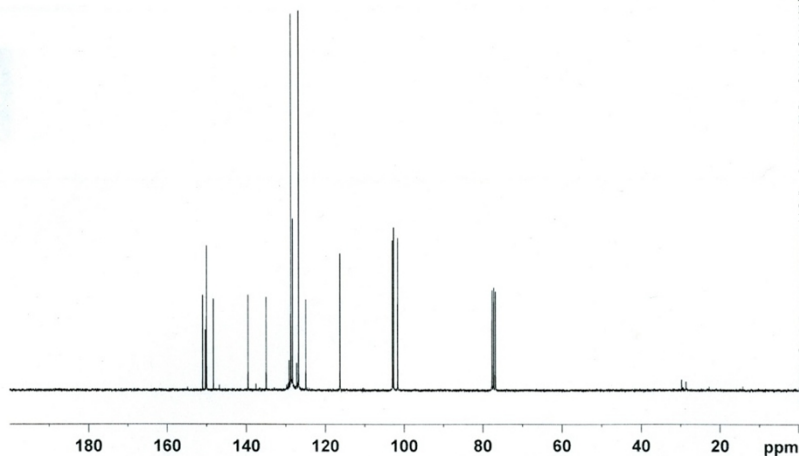
```

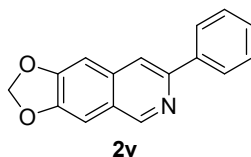
NAME      2013-01-03ff
EXPNO     1
PROCNO    1
Date_     20130106
Time      11.17
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         454
DS         4
SWH        18028.846 Hz
FIDRES    0.550197 Hz
AQ         0.9088159 sec
RG         80.6
DW         27.733 usec
DE         6.50 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
  
```

```

===== CHANNEL f1 =====
NUC1      13c
F1         9.80 usec
PL1       -0.50 dB
PL1W      34.66611099 W
SFO1      75.4778101 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     100.00 usec
PL2        2.50 dB
PL12      19.20 dB
PL13      23.00 dB
PL2W      8.07971478 W
PL12W     0.17274120 W
PL13W     0.07201053 W
SFO2      300.1412006 MHz
SI         32768
SF         75.4702630 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```





KS-8

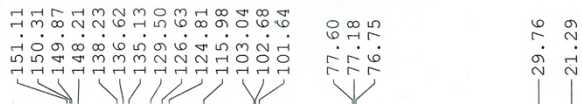


```

NAME      2013-01-03-e-e
EXPNO     1
PROCNO    1
Date_     20130105
Time      17.47
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD         32768
SOLVENT   CDC13
NS         16
DS         2
SWH        6188.119 Hz
FIDRES    0.188846 Hz
AQ         2.6477044 sec
RG         45.2
DE         80.800 usec
TE         300.0 K
D1         1.00000000 sec
TDO        1
  
```

----- CHANNEL f1 -----

KS-8



```

NAME      2013-01-03ee
EXPNO     1
PROCNO    1
Date_     20130105
Time      18.13
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD         32768
SOLVENT   CDC13
NS         500
DS         4
SWH        18028.846 Hz
FIDRES    0.550197 Hz
AQ         0.9088159 sec
RG         80.6
DE         27.733 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
  
```

----- CHANNEL f1 -----

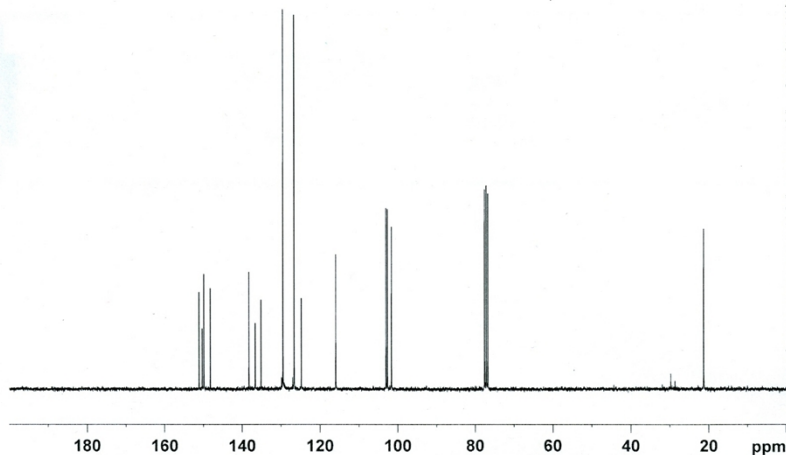
```

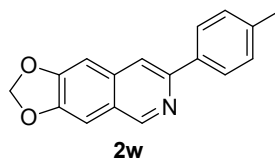
NUC1      13C
P1         9.80 usec
PL1        -0.50 dB
PL1W       34.66611099 W
SFO1      75.4778101 MHz
  
```

----- CHANNEL f2 -----

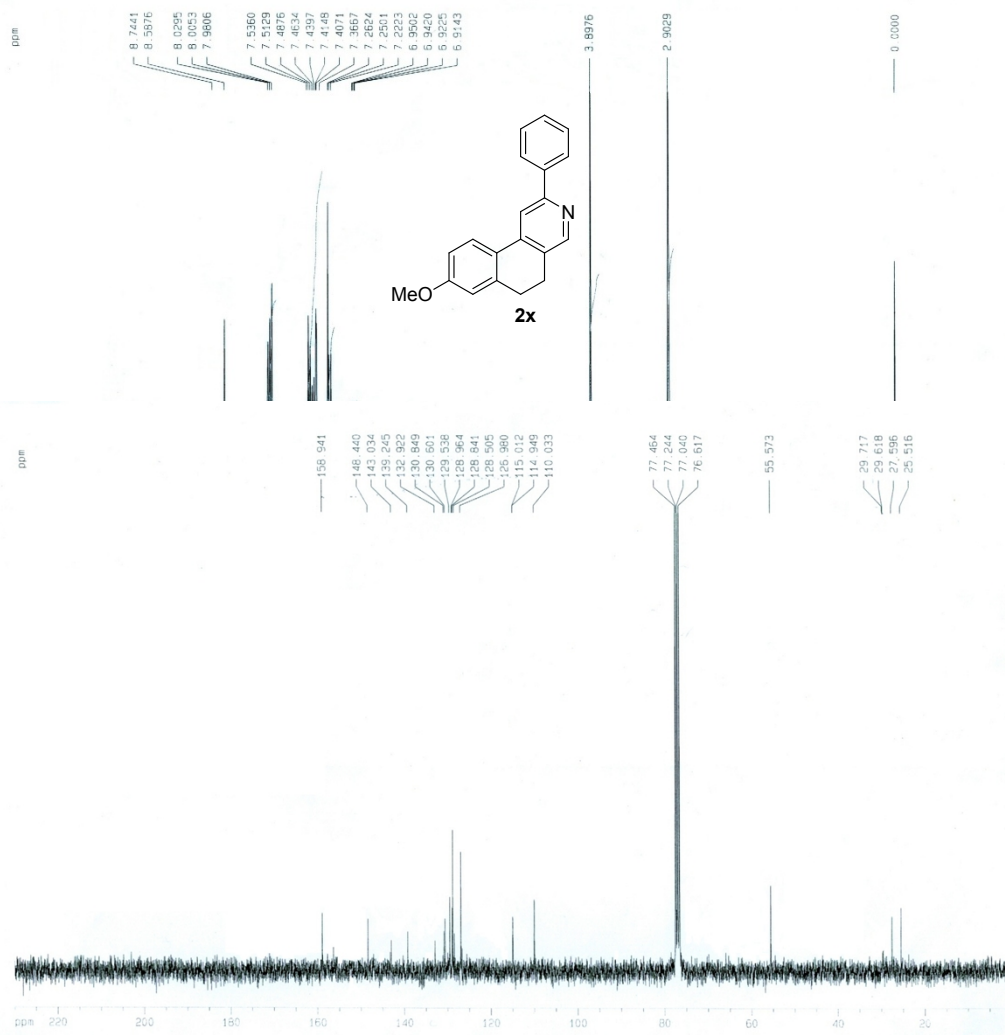
```

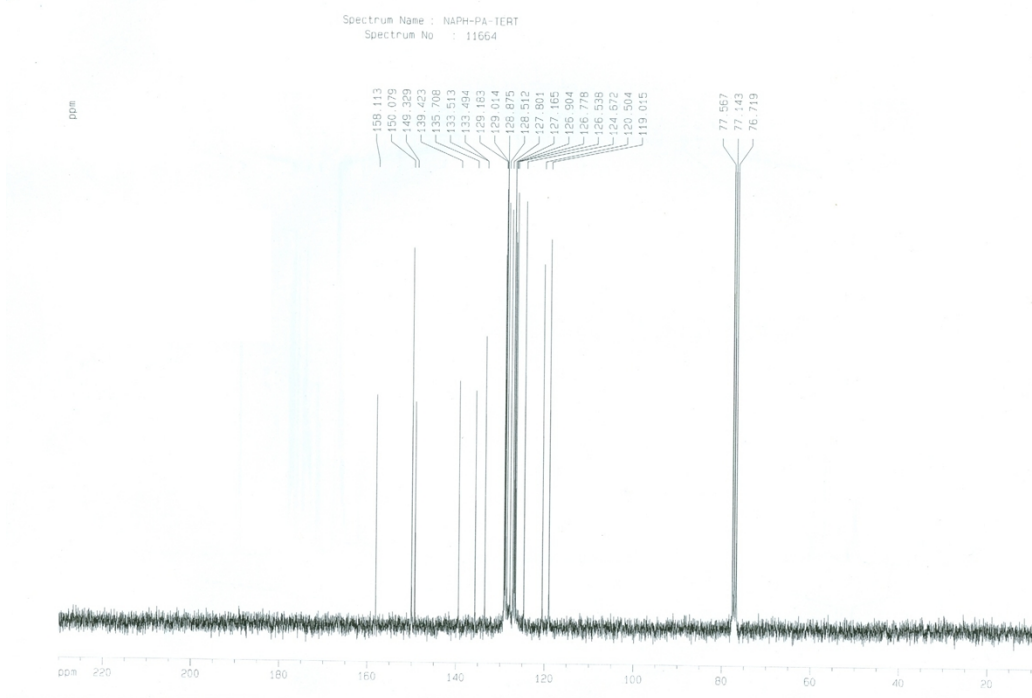
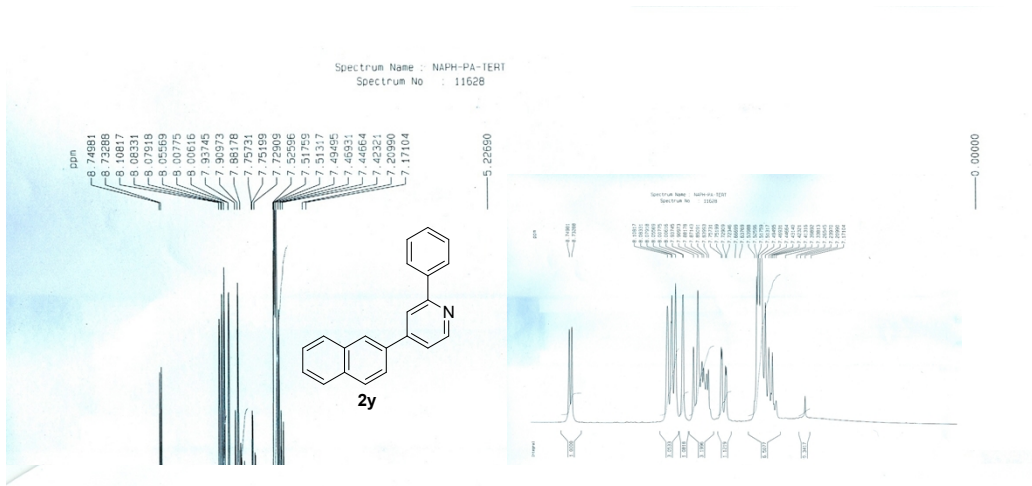
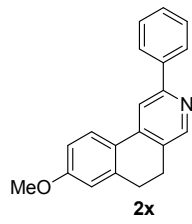
CPDPRG2   waltz16
NUC2       1H
PCPD2     100.00 usec
PL2        2.50 dB
PL12       19.20 dB
PL13       23.00 dB
PL2W       8.07971478 W
PL12W      0.17274120 W
PL13W      0.07201053 W
SFO2      300.1412006 MHz
SI         32768
SF         75.4702630 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

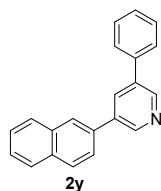




Recorded by: Dr. P.J. Saikia
 Name of Sample: Cul-cat
 Spectrum No.: 7412







MTT ASSAY PROTOCOL

Cellular viability in the presence of test compounds was determined by MTT-micro cultured tetrazolium assay. The cells seeded to flat bottomed 96 (1000 cells/100 μ l) well plates & cultured in the medium containing 10% serum and allowed to attach and recover for 24 hours in a hid chamber containing 5% CO₂. MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide; Sigma catalog No M2128) was dissolved in PBS at 5 mg/mL and filtered to sterilize. Different concentrations of compounds were added to the cells. After 48 hours, stock MTT solution (10 μ l) was added to the culture plate. Cells were again kept in CO₂ incubator for 2 hours. After incubation 100 μ L of DMSO was added and mixed. The absorbance was read at 562 nm in a plate reader. The results were represented as percentage of cytotoxicity/viability. All the experiments were carried out in triplicates. From the percentage of cytotoxicity the IC-50 values were calculated.

Media used was MEM (Catalog No M0643), DPBS (Catalog No D5652), 1X antibiotic solution of 100X, (Catalog No A5955), 1% Sodium pyruvate (Catalog No.S8636), 1% Non essential amino acids (Catalog No M7145), 10% fetal bovine ser (Catalog No F2442), DMSO (Catalog No D5879), Trypsin-EDTA solution (0.25%, 2.5 g porcine trypsin and 0.2 g EDTA) (Catalog No T4049).

Reference

- (1) S. Myadaraboina, M. Alla, V. Saddanapu, V. R. Bommena and A. Addlagatta, *Eur. J. Med. Chem.* 2010, 45, 5208.

