Supporting Information

C-H Activation Guided by Aromatic N-H Ketimines: Synthesis of Functionalized Isoquinolines Using Benzyl Azides and Alkynes

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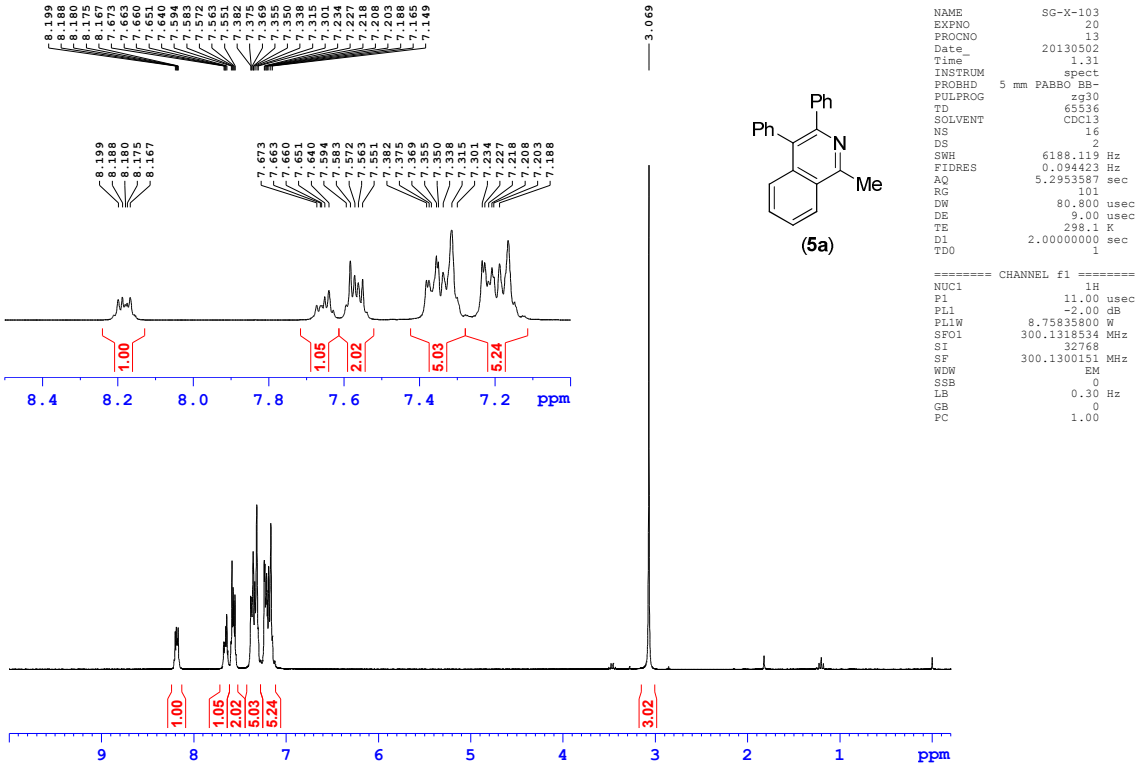
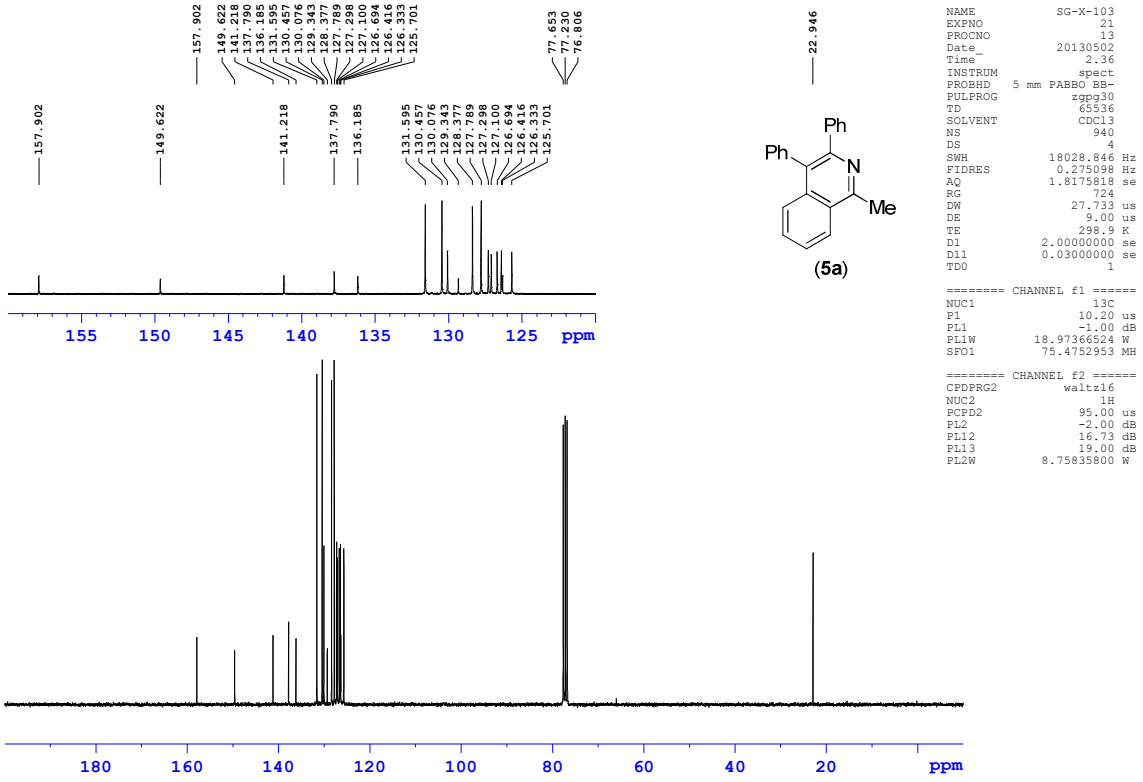



```
NAME            SG-X-103
EXPNO                20
PROCNO               13
Date_          20130502
Time_              1.31
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           6188.119 Hz
FIDRES          0.094423 Hz
AQ            5.2953587 sec
RG                  101
DW               80.800 usec
DE                9.00 usec
TE                298.1 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                1H
P1                11.00 usec
PL1               -2.00 dB
PL1W         8.75835800 W
SFO1        300.1318534 MHz
SI                32768
SF          300.1300151 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

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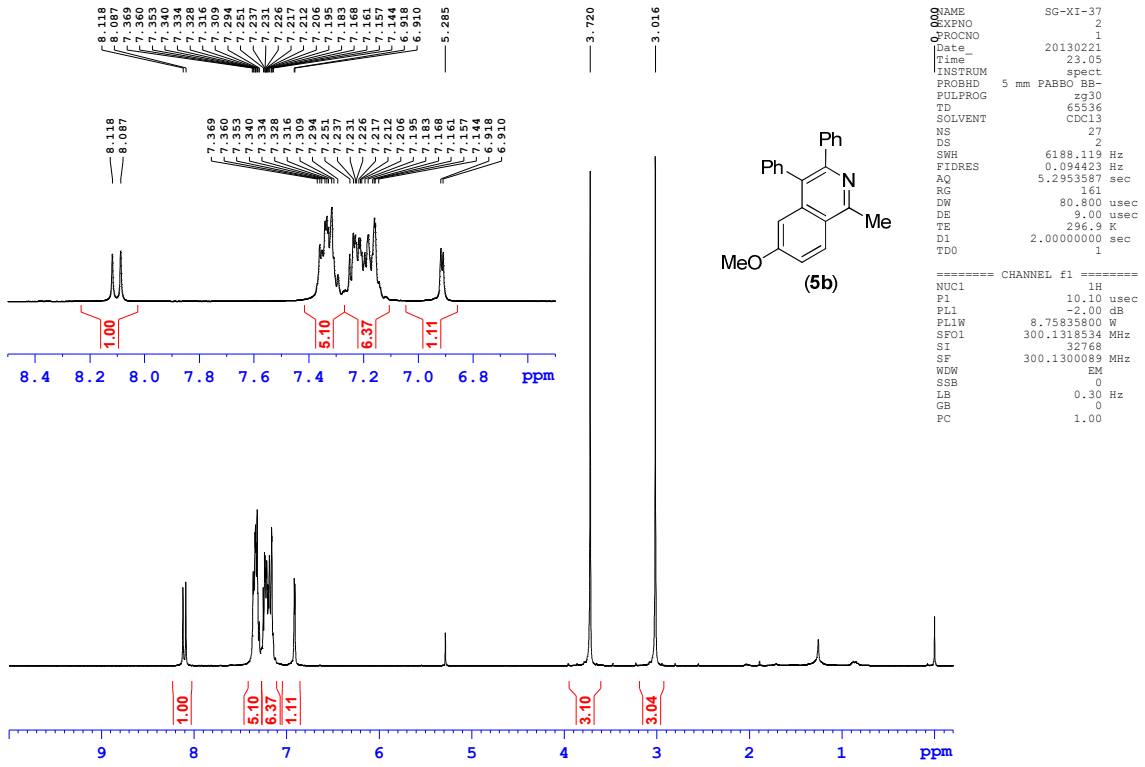
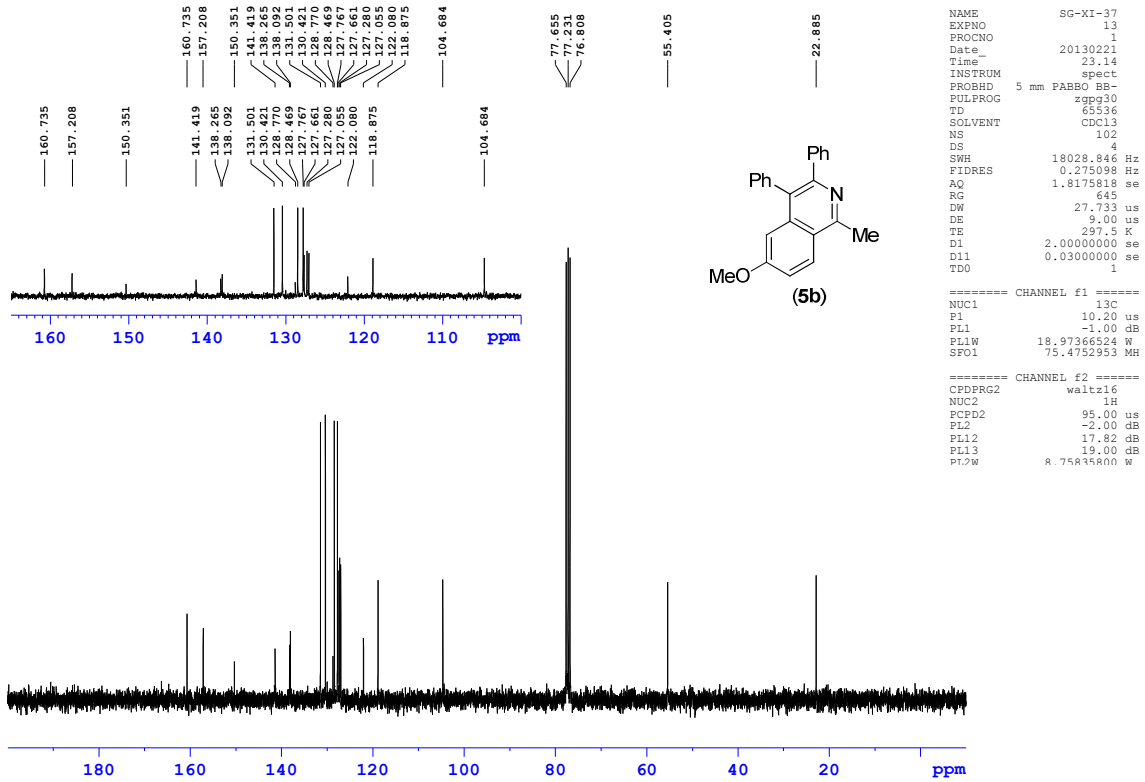
NAME            SG-X-103
EXPNO                21
PROCNO               13
Date_          20130502
Time_              2.36
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  940
DS                    4
SWH          18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 se
RG                  724
DW               27.733 us
DE                9.00 us
TE                298.9 K
D1           2.00000000 se
D11          0.03000000 se
TD0                   1

======== CHANNEL f1 ======
NUC1               13C
P1               10.20 us
PL1              -1.00 dB
PL1W        18.97366524 W
SFO1        75.4752953 MH

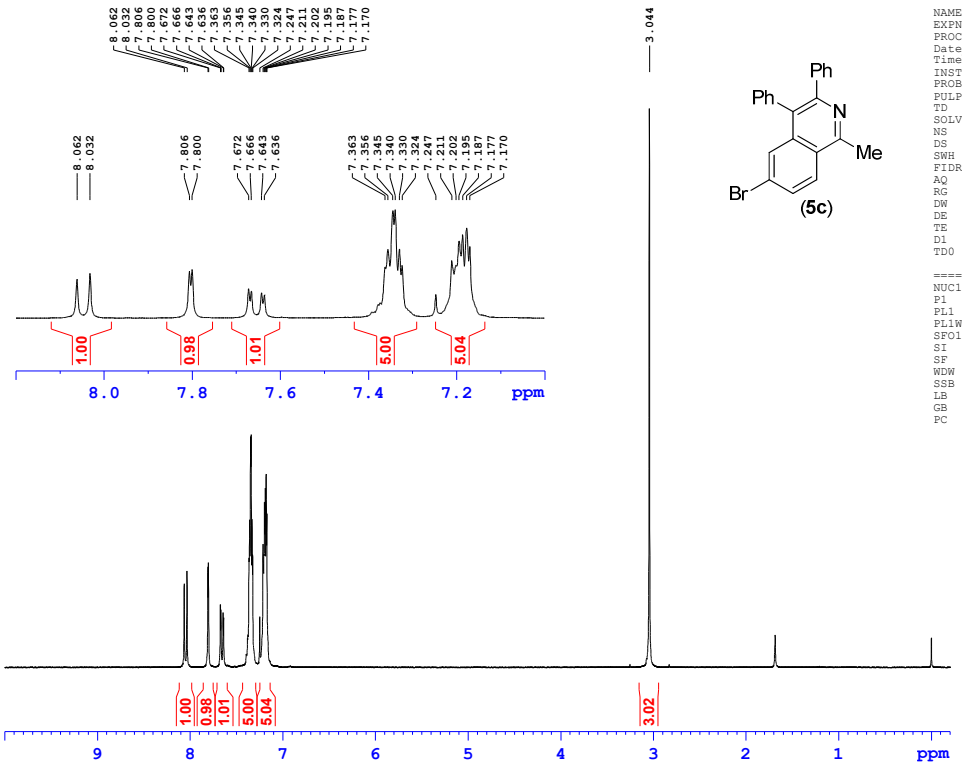
======== CHANNEL f2 ======
CPDPRG2         waltz16
NUC2                1H
PCPD2            95.00 us
PL2              -2.00 dB
PL12             16.73 dB
PL13             19.00 dB
PL2W         8.75835800 W
```

6-Methoxy-1-methyl-3,4-diphenylisoquinoline (5b):



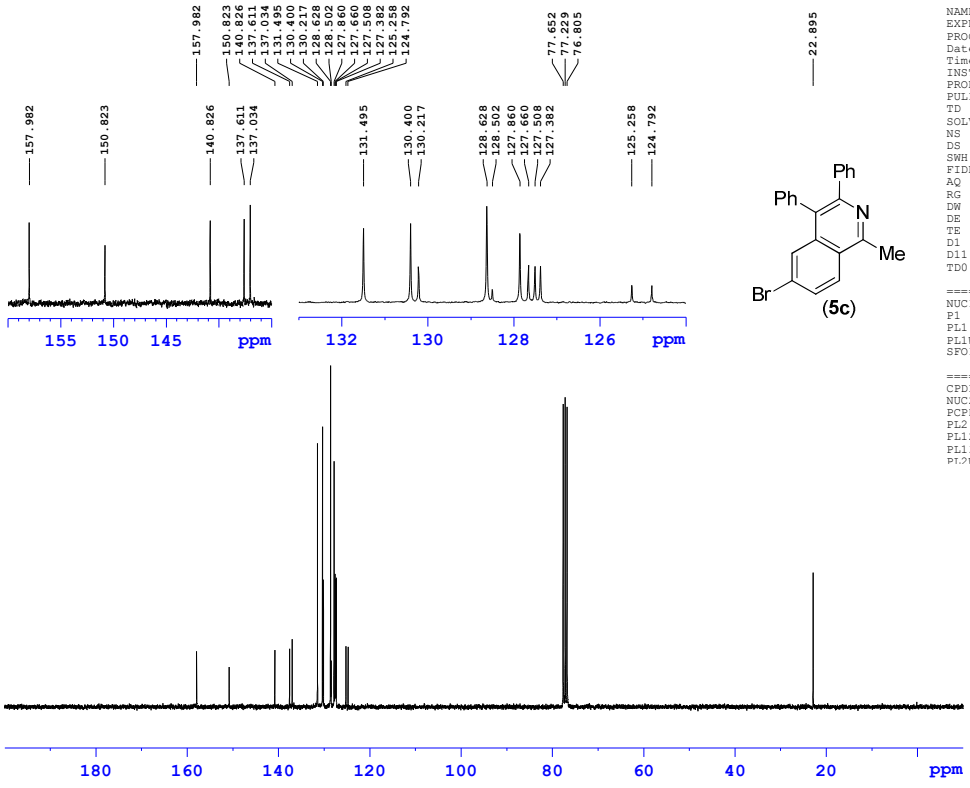


6-Bromo-1-methyl-3,4-diphenylisoquinoline (5c):




```
NAME            SG-XI-41
EXPNO                20
PROCNO                1
Date_          20130503
Time_              4.04
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH           6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                  144
DW               80.800 usec
DE                9.00 usec
TE               298.1 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1               11.00 usec
PL1              -2.00 dB
PL1W          8.75835800 W
SFO1        300.1318534 MHz
SI                 32768
SF          300.1300098 MHz
WDW                  EM
SSB                   0
LB               0.30 Hz
GB                    0
PC                 1.00
```

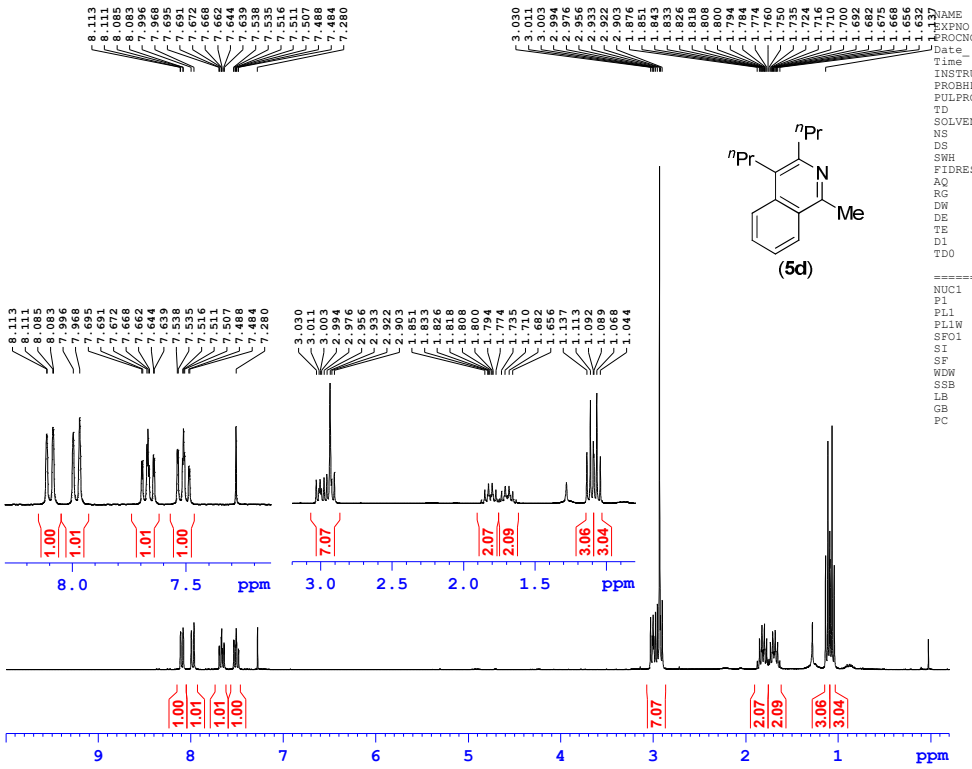



```
NAME            SG-XI-41
EXPNO                21
PROCNO                1
Date_          20130503
Time_              5.15
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH          18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 se
RG                  912
DW               27.733 us
DE                9.00 us
TE               298.9 K
D1            2.00000000 se
D11           0.03000000 se
TD0                   1

======== CHANNEL f1 ======
NUC1                13C
P1               10.20 us
PL1              -1.00 dB
PL1W         18.97366524 W
SFO1         75.4752953 MH

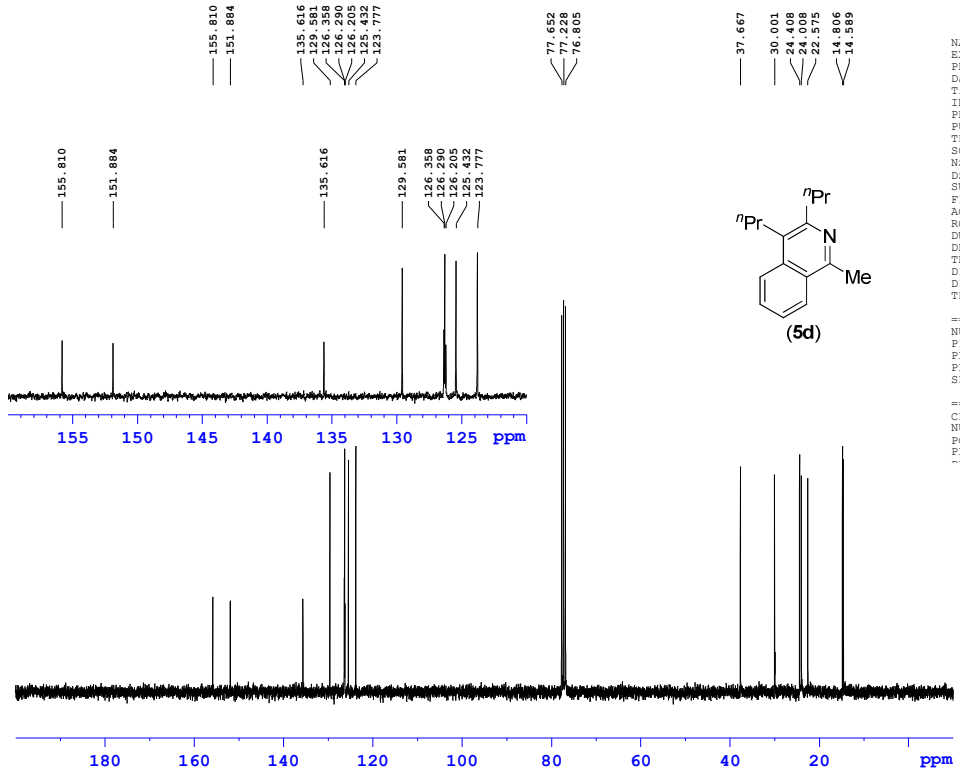
======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                 1H
PCPD2             95.00 us
PL2               -2.00 dB
PL12              16.73 dB
PL13              19.00 dB
PL2W          8.75835800 W
```

1-Methyl -3,4-dipropylisoquinoline (5d):



NAME KYJ-1-109
EXPNO 2
PROCNO 1
Date_ 20130604
Time 19.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 101
DW 80.800 usec
DE 9.00 usec
TE 298.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
PL1W 8.75835800 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300001 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

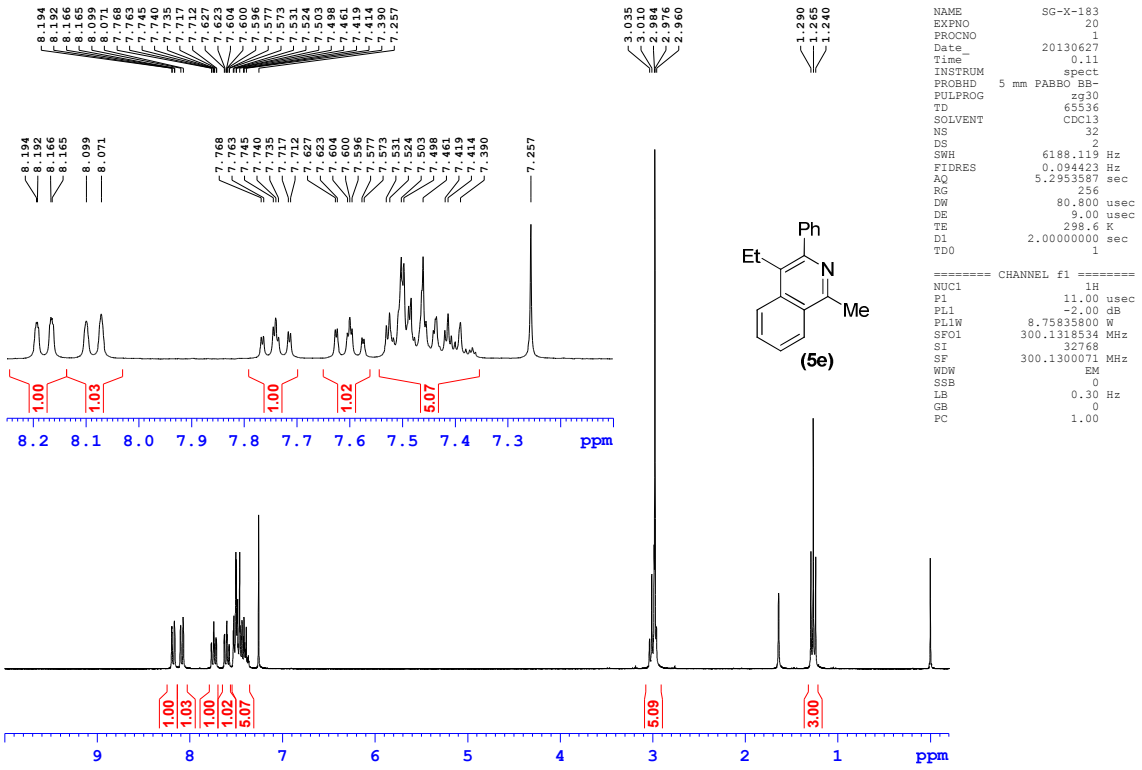


NAME KYJ-1-109
EXPNO 14
PROCNO 1
Date_ 20130604
Time 19.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 326
DS 2
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 se
RG 12.7
DW 27.733 us
DE 6.50 us
TE 299.4 K
D1 1.50000000 se
D11 0.03000000 se
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 10.20 us
PL1 -1.00 dB
PL1W 18.97366524 W
SFO1 75.4752953 MH

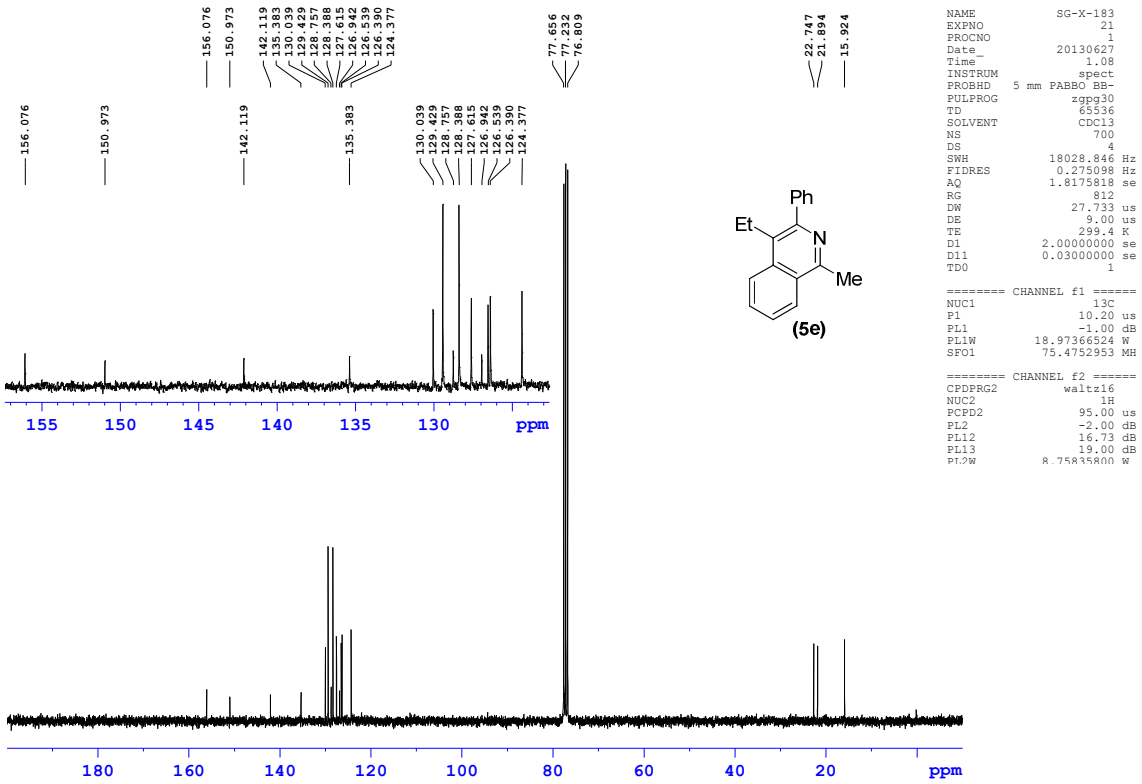
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 us
PL2 -2.00 dB

4-Ethyl-1-methyl-3-phenylisoquinoline (5e):




```
NAME            SG-X-183
EXPNO                20
PROCNO                1
Date_          20130627
Time               0.11
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH           6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                  256
DW               80.800 usec
DE                9.00 usec
TE                298.6 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                11.00 usec
PL1               -2.00 dB
PL1W         8.75835800 W
SFO1        300.1318534 MHz
SI                32768
SF          300.1300071 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

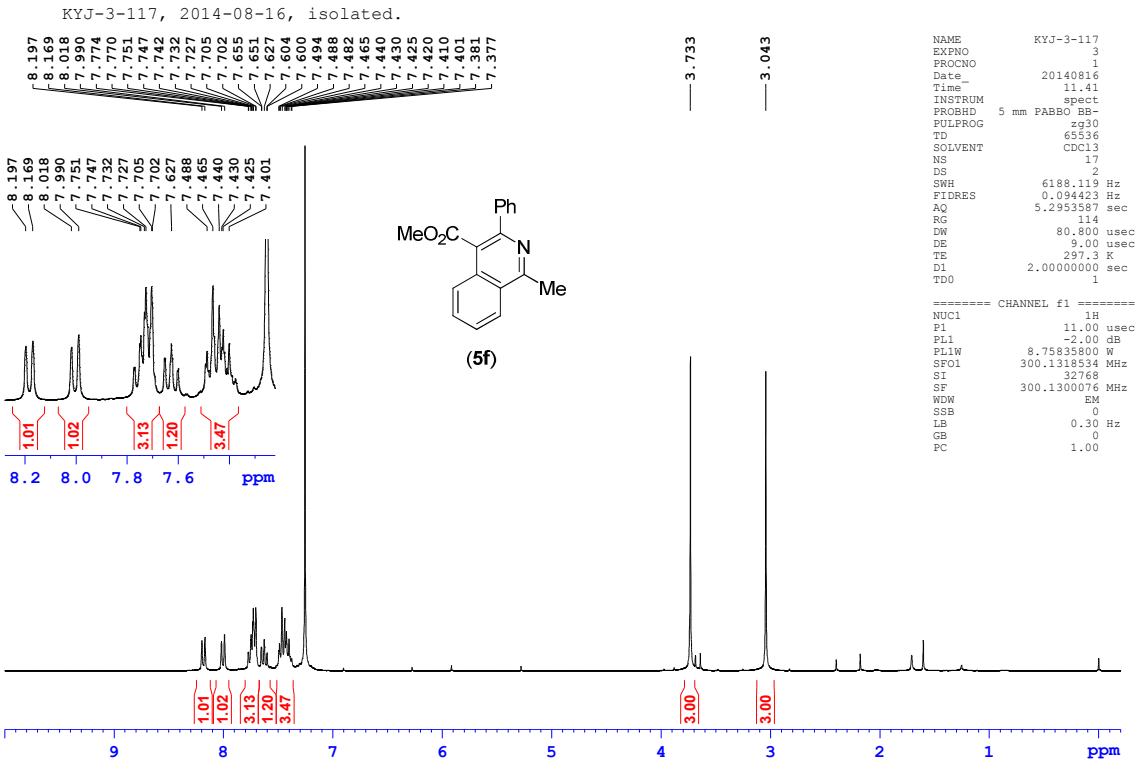


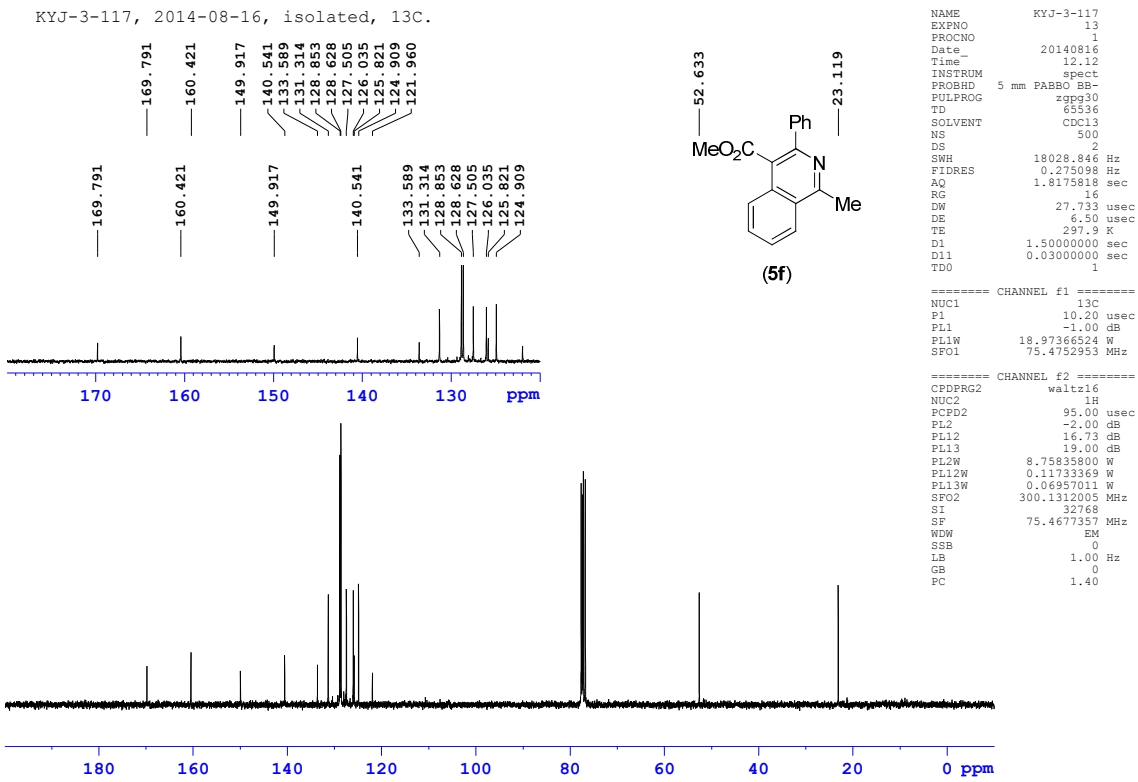

```
NAME            SG-X-183
EXPNO                21
PROCNO                1
Date_          20130627
Time               1.08
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  700
DS                    4
SWH          18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 se
RG                  812
DW               27.733 us
DE                9.00 us
TE                299.4 K
D1           2.00000000 se
D11          0.03000000 se
TD0                   1

======== CHANNEL f1 ======
NUC1                13C
P1               10.20 us
PL1              -1.00 dB
PL1W        18.97366524 W
SFO1        75.4752953 MH

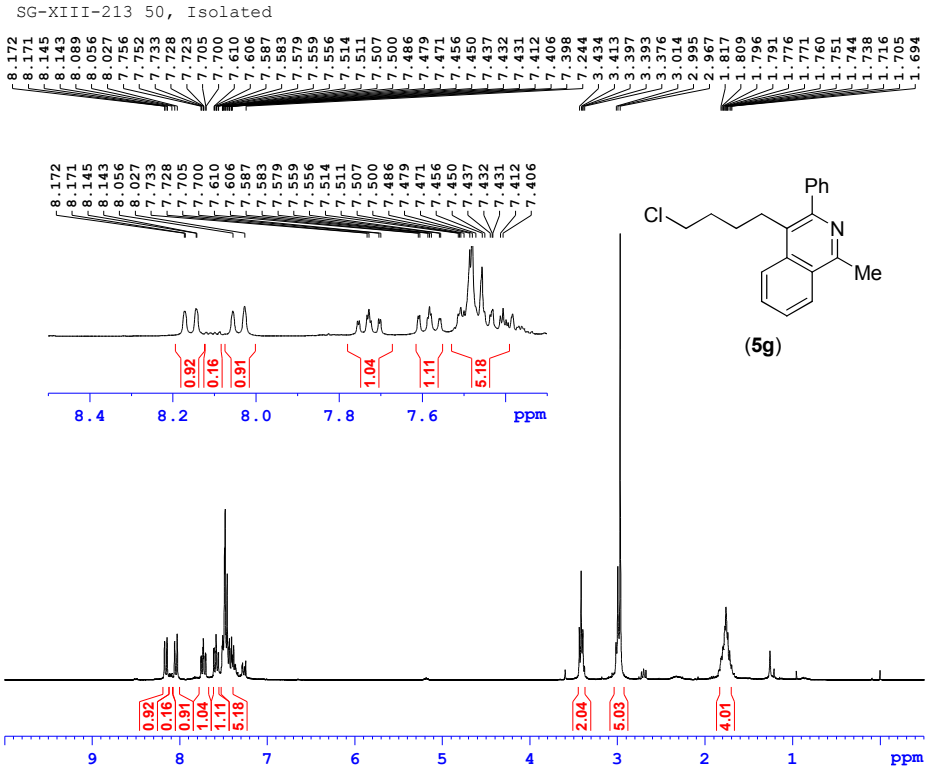
======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                 1H
PCPD2            95.00 us
PL2              -2.00 dB
PL12             16.73 dB
PL13             19.00 dB
PL2W         8.75835800 W
```

Methyl 1-methyl-3-phenylisoquinoline-4-carboxylate (5f):



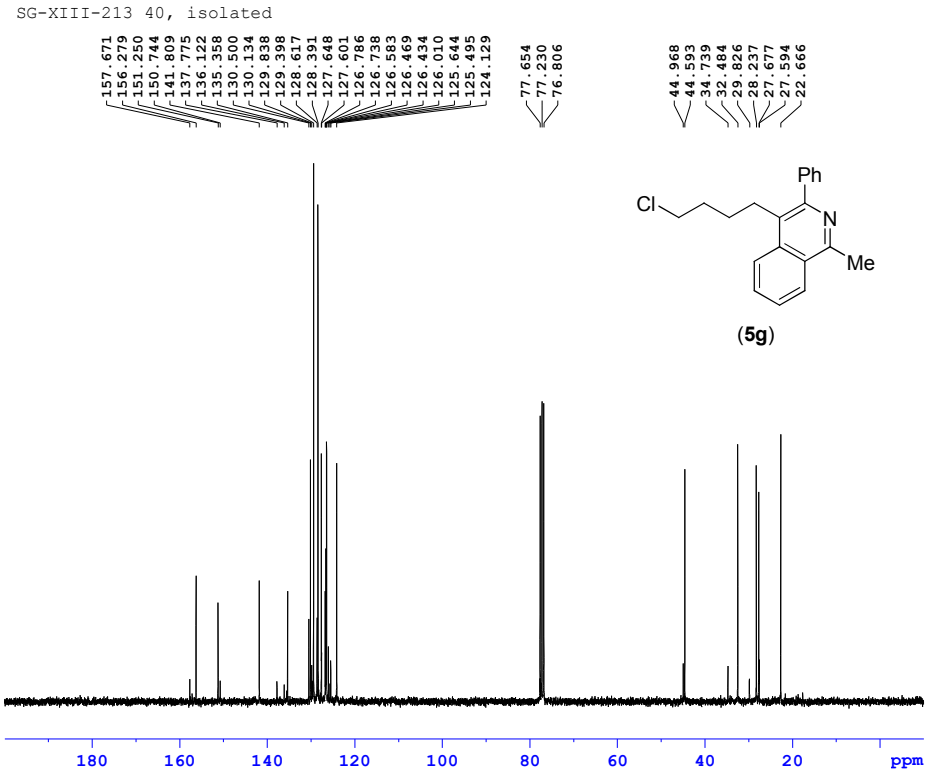


4-(4-Chlorobutyl)-1-methyl-3-phenylisoquinoline (5g):




```
NAME          SG-XIII-213
EXPNO              50
PROCNO              1
Date_          20140828
Time_              1.43
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD                65536
SOLVENT           CDCl3
NS                  32
DS                   2
SWH           6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                50.8
DW               80.800 usec
DE                9.00 usec
TE               297.6 K
D1           2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               1H
P1               11.00 usec
PL1              -2.00 dB
PL1W          8.75835800 W
SFO1        300.1318534 MHz
SI                32768
SF          300.1300109 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```

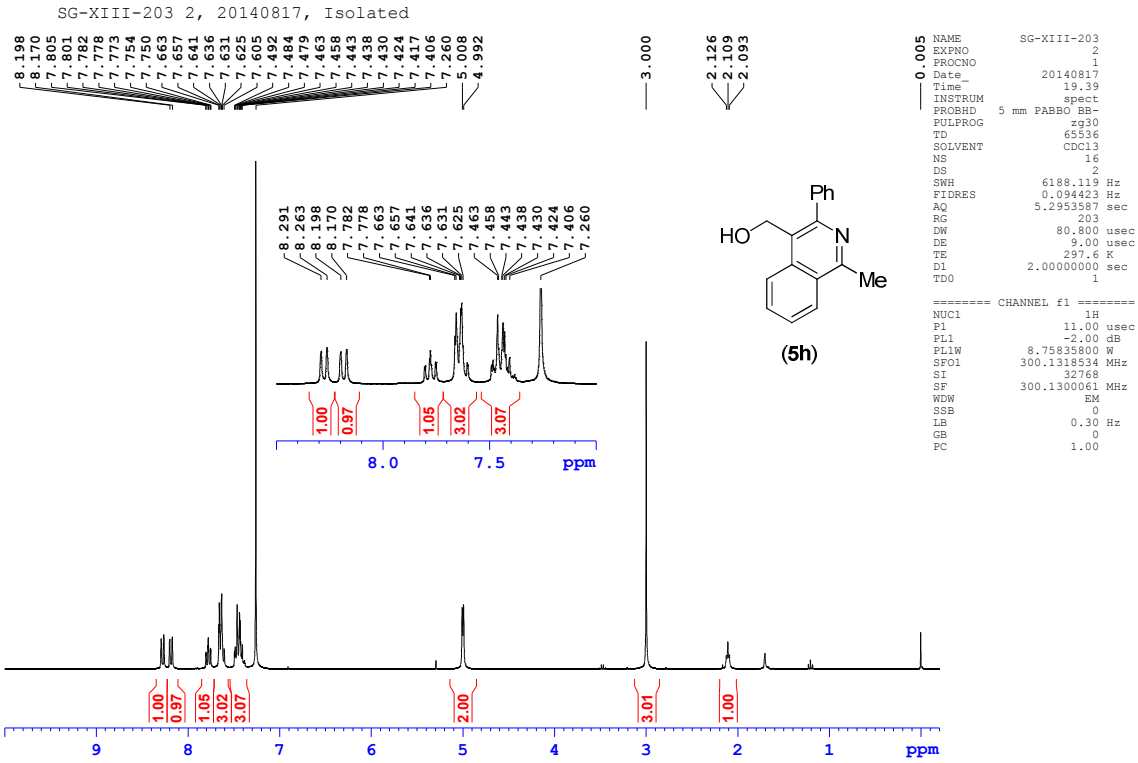


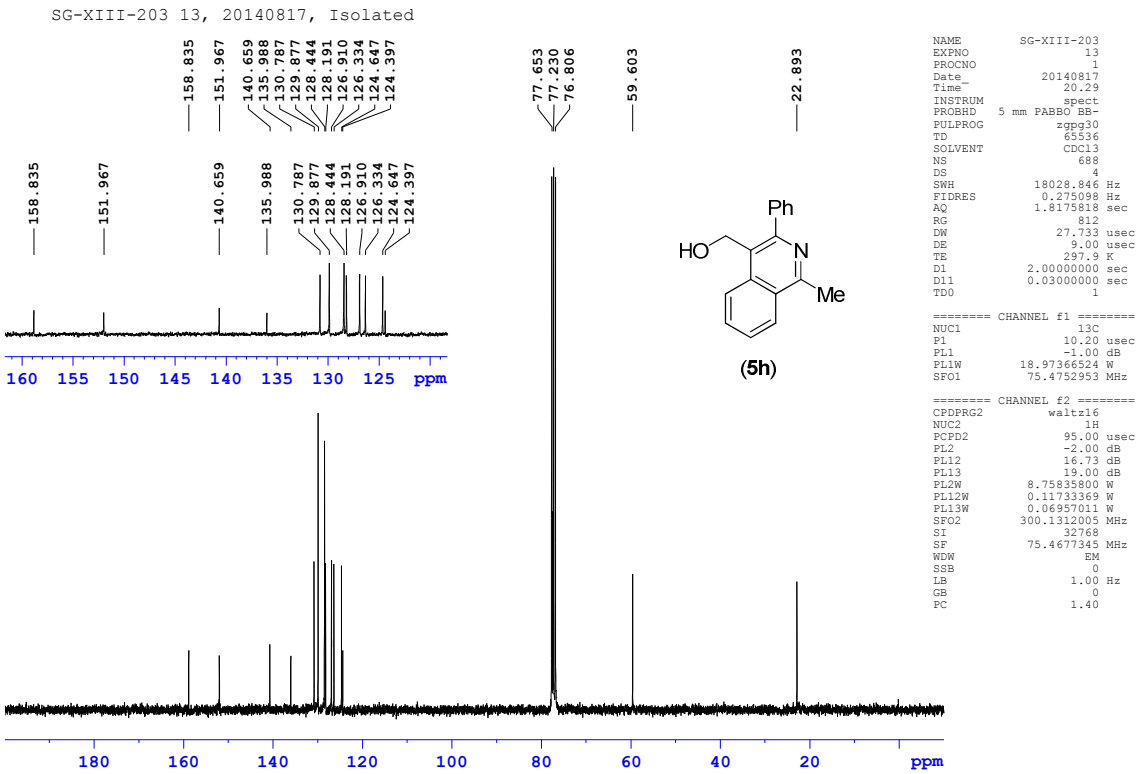

```
NAME          SG-XIII-213
EXPNO              41
PROCNO              1
Date_          20140827
Time_             14.23
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                 280
DS                   4
SWH          18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 sec
RG                724
DW               27.733 usec
DE                9.00 usec
TE               297.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1              13C
P1               10.20 usec
PL1              -1.00 dB
PL1W         18.97366524 W
SFO1         75.4752953 MHz

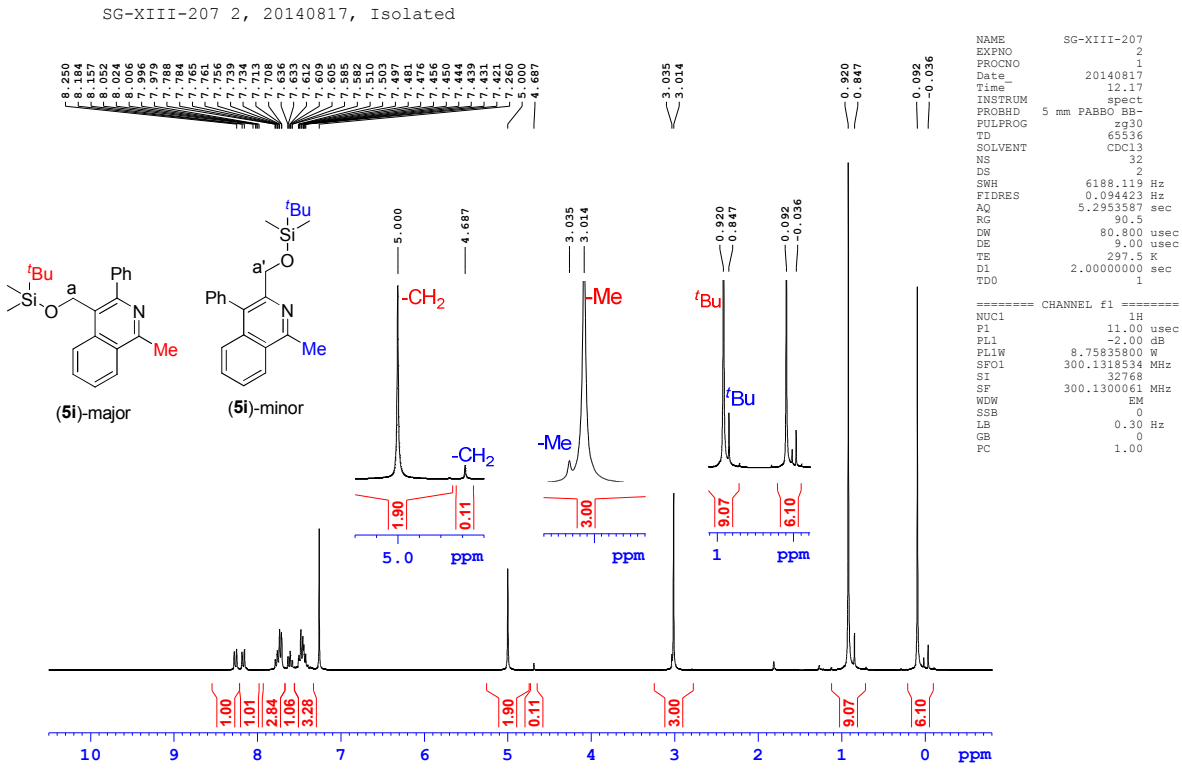
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2               1H
PCPD2            95.00 usec
PL2              -2.00 dB
PL12             16.73 dB
PL13             19.00 dB
PL2W          8.75835800 W
PL12W         0.11733369 W
PL13W         0.06957011 W
SFO2        300.1312005 MHz
SI                32768
SF           75.4677419 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

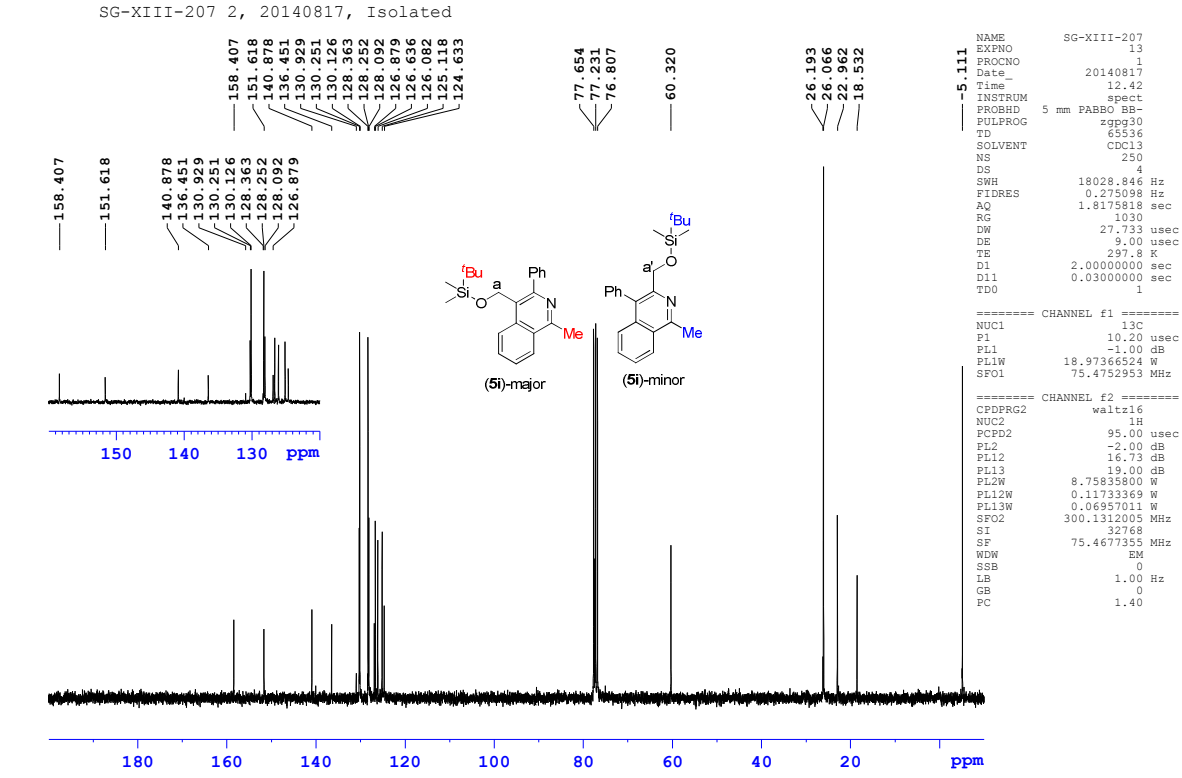
(1-Methyl-3-phenylisoquinoline-4-yl)methanol (5h):



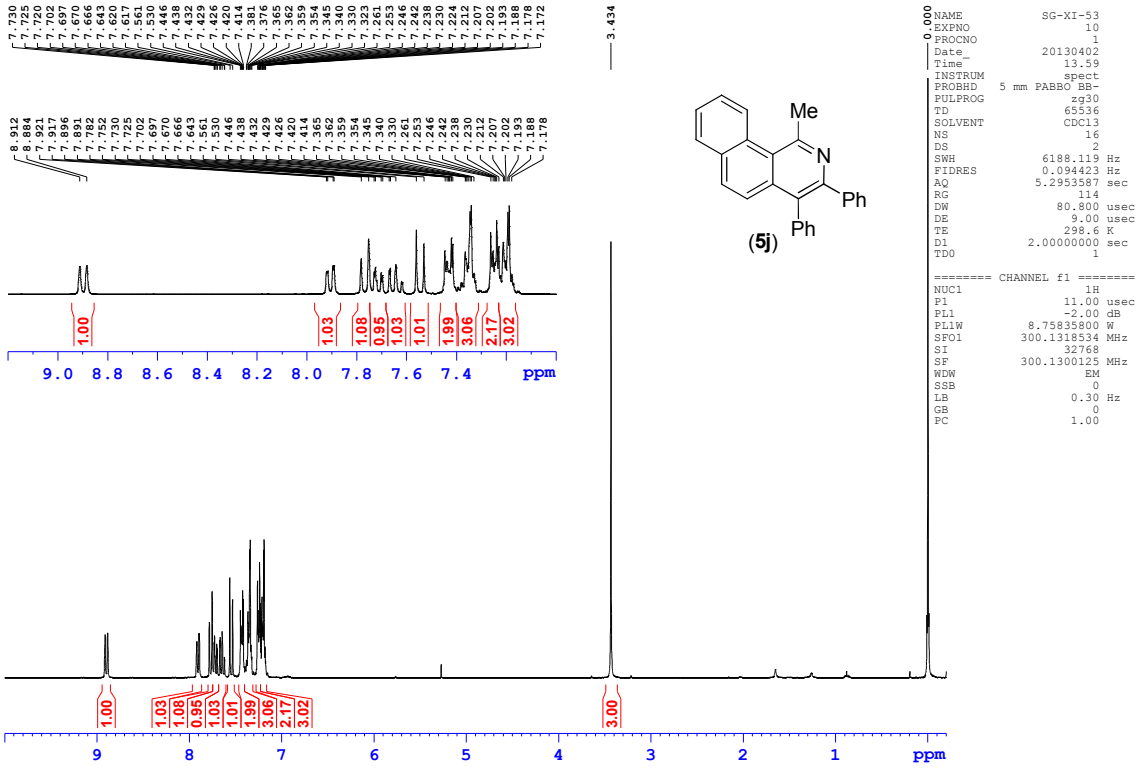


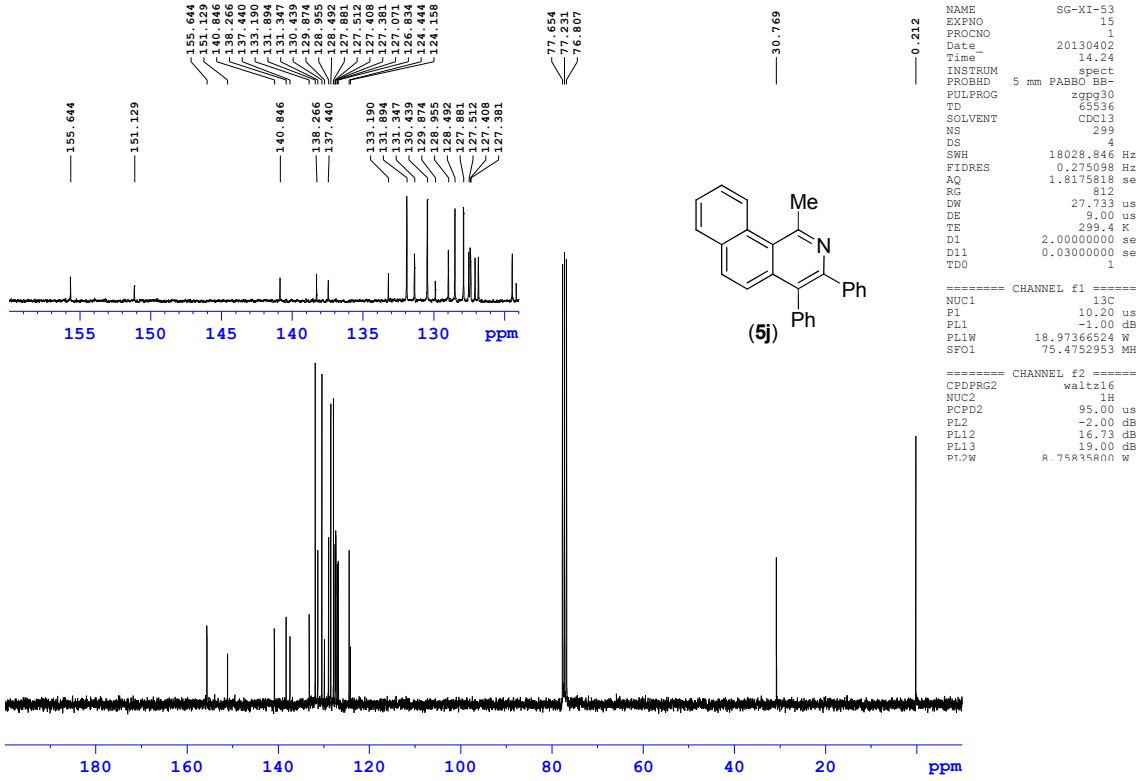
4-((tert-butyldimethylsilyloxy)methyl)-1-methyl-3-phenylisoquinoline (5i):



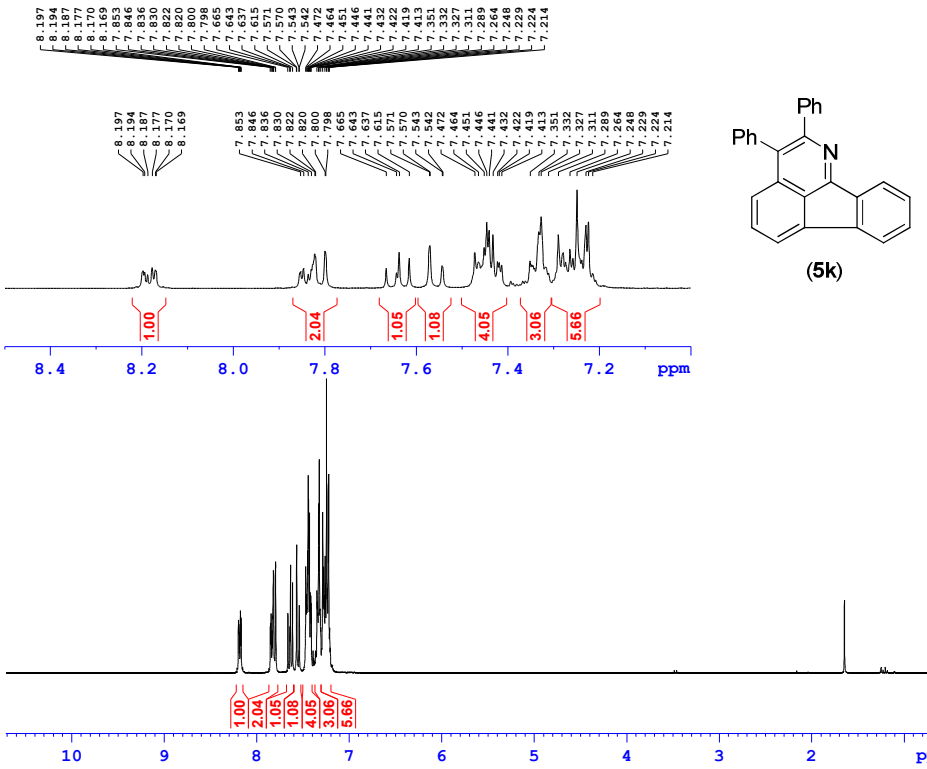


1-Methyl-3,4-diphenylbenzo[h]isoquinoline (5j):





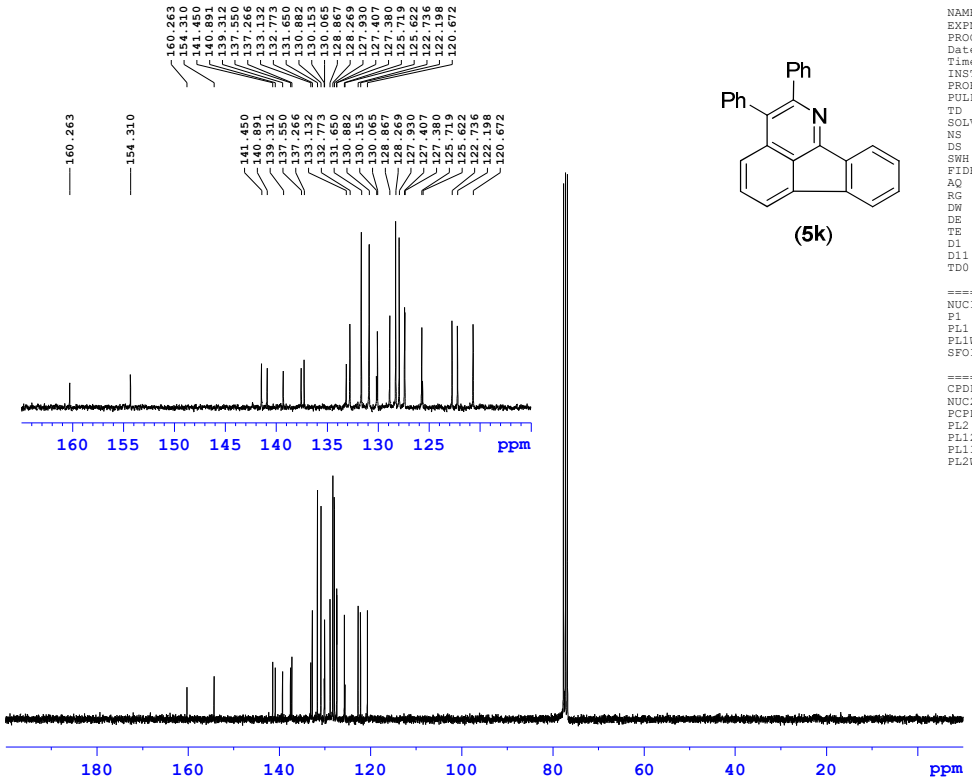
2,3-Diphenylindeno[1,2,3-*ij*]isoquinoline (5k):



(5k)

```
NAME            SG-X-283
EXPNO                20
PROCNO               13
Date_          20130502
Time                0.06
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH             6188.119 Hz
FIDRES             0.094423 Hz
AQ              5.2953587 sec
RG                   203
DW                80.800 usec
DE                 9.00 usec
TE                298.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 1H
P1                11.00 usec
PL1               -2.00 dB
PL1W           8.75835800 W
SFO1         300.1318534 MHz
SI                 32768
SF           300.1300098 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



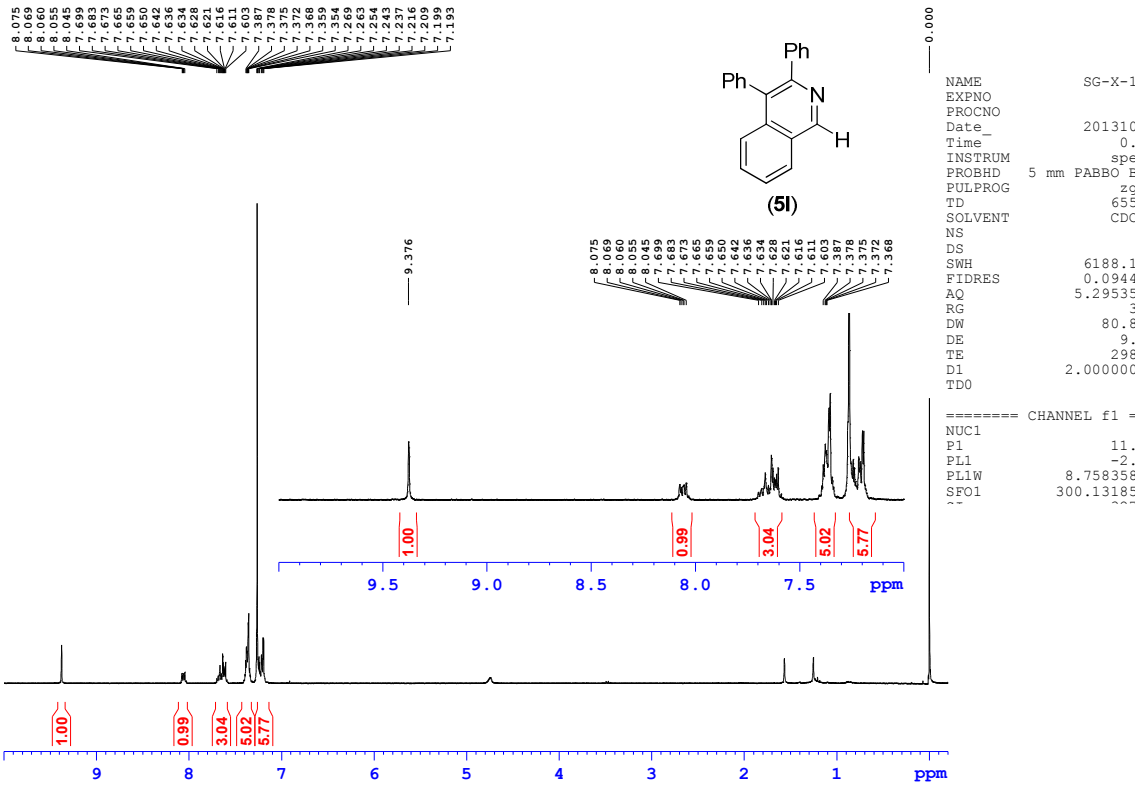
(5k)

```
NAME            SG-X-283
EXPNO                21
PROCNO               13
Date_          20130502
Time                1.16
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            18028.846 Hz
FIDRES             0.275098 Hz
AQ              1.8175818 se
RG                  1030
DW                27.733 us
DE                 9.00 us
TE                298.9 K
D1           2.00000000 se
D11          0.03000000 se
TD0                    1

======== CHANNEL f1 ======
NUC1                13C
P1                10.20 us
PL1               -1.00 dB
PL1W          18.97366524 W
SFO1          75.4752953 MH

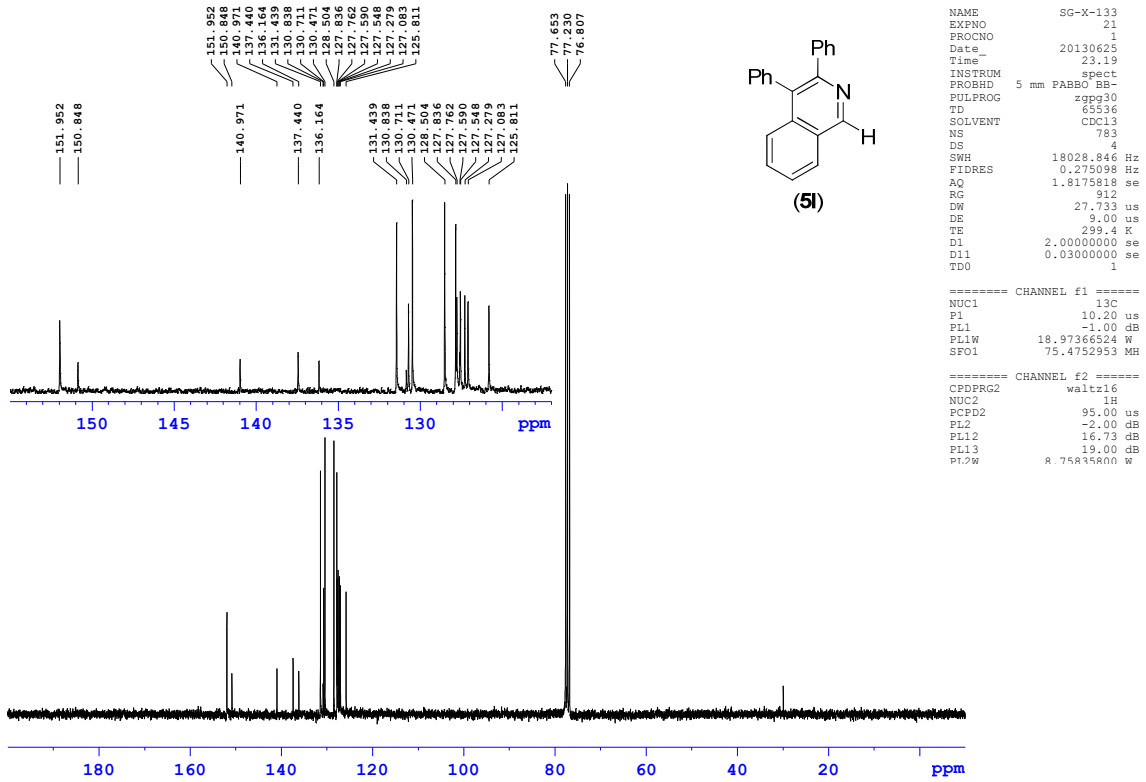
======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                 1H
PCPD2             95.00 us
PL2               -2.00 dB
PL12              16.73 dB
PL13              19.00 dB
PL2W           8.75835800 W
```

3,4-diphenylisoquinoline (5l):




```
NAME            SG-X-1
EXPNO
PROCNO
Date_           20131(
Time                0.
INSTRUM           spe
PROBHD   5 mm PABBO B
PULPROG             zg
TD                 65
SOLVENT           CDC
NS
DS
SWH            6188.1
FIDRES         0.0944
AQ             5.2953
RG                  3
DW                80.8
DE                 9.
TE                29
D1          2.000000
TD0

======== CHANNEL f1 =
NUC1
P1                11.
PL1               -2.
PL1W        8.758358
SFO1      300.13185
```

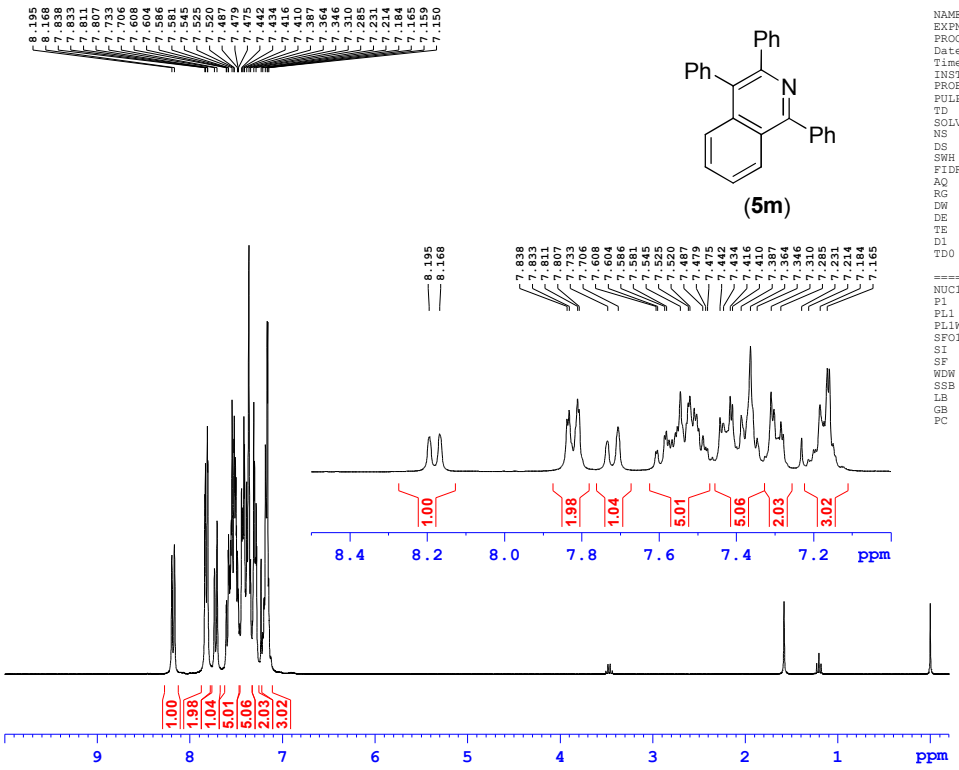



```
NAME            SG-X-133
EXPNO                 21
PROCNO                 1
Date_           20130625
Time               23.19
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  783
DS                    4
SWH          18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 se
RG                  912
DW               27.733 us
DE                9.00 us
TE               299.4 K
D1          2.00000000 se
D11         0.03000000 se
TD0                   1

======== CHANNEL f1 ======
NUC1                 13C
P1                10.20 us
PL1               -1.00 dB
PL1W        18.97366524 W
SFO1        75.4752953 MH

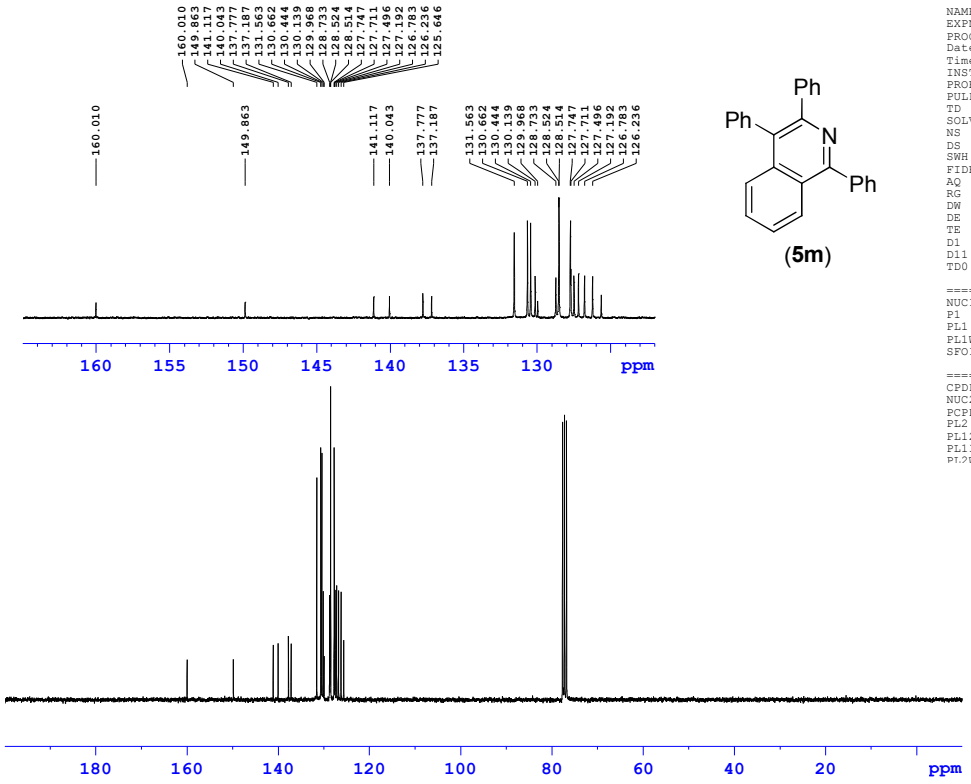
======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                 1H
PCPD2             95.00 us
PL2               -2.00 dB
PL12              16.73 dB
PL13              19.00 dB
PL2W        8.75835800 W
```

1,3,4-Triphenylisoquinoline (5m):




```
NAME            SG-X-247
EXPNO                20
PROCNO                1
Date_          20130503
Time               2.30
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH           6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                  128
DW               80.800 usec
DE                9.00 usec
TE               298.0 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                11.00 usec
PL1               -2.00 dB
PL1W         8.75835800 W
SFO1        300.1318534 MHz
SI                32768
SF          300.1300144 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

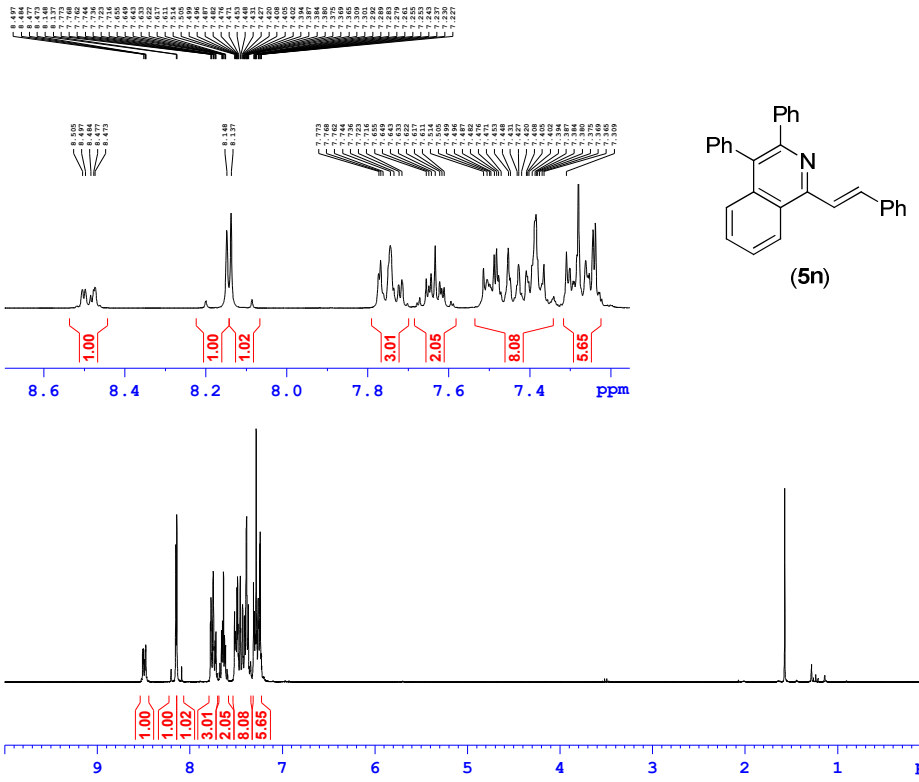



```
NAME            SG-X-247
EXPNO                21
PROCNO                1
Date_          20130503
Time               3.41
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH          18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 se
RG                  724
DW               27.733 us
DE                9.00 us
TE               299.0 K
D1            2.00000000 se
D11           0.03000000 se
TD0                   1

======== CHANNEL f1 ======
NUC1                13C
P1                10.20 us
PL1               -1.00 dB
PL1W        18.97366524 W
SFO1         75.4752953 MH

======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                1H
PCPD2             95.00 us
PL2               -2.00 dB
PL12              16.73 dB
PL13              19.00 dB
PL2W         8.75835800 W
```

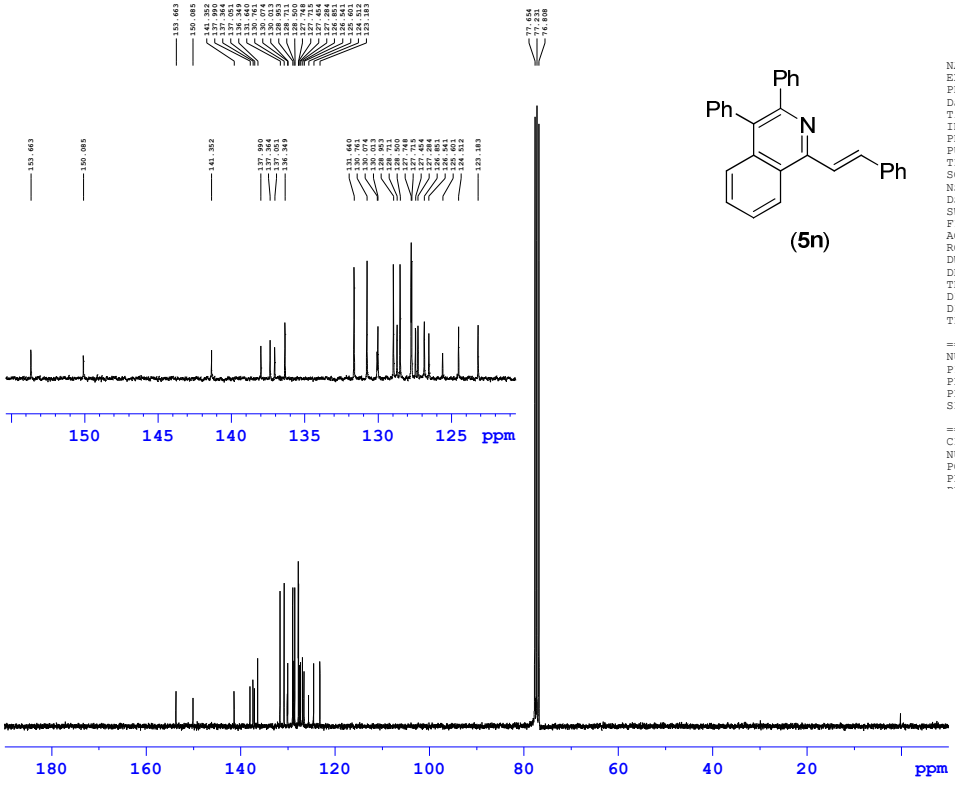
(*E*)-3,4-diphenyl-1-styrylisoquinoline (5n):



(5n)

```
NAME            SG-X-257
EXPNO                 20
PROCNO                 1
Date_           20130509
Time                0.11
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    23
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 se
RG                   256
DW                80.800 us
DE                 9.00 us
TE                298.3 K
D1             2.00000000 se
TD0                    1

======== CHANNEL f1 ======
NUC1                  1H
P1                 11.00 us
PL1                -2.00 dB
PL1W         8.75835800 W
SFO1       300.1318534 MH
SI                 32768
SF         300.1300001 MH
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



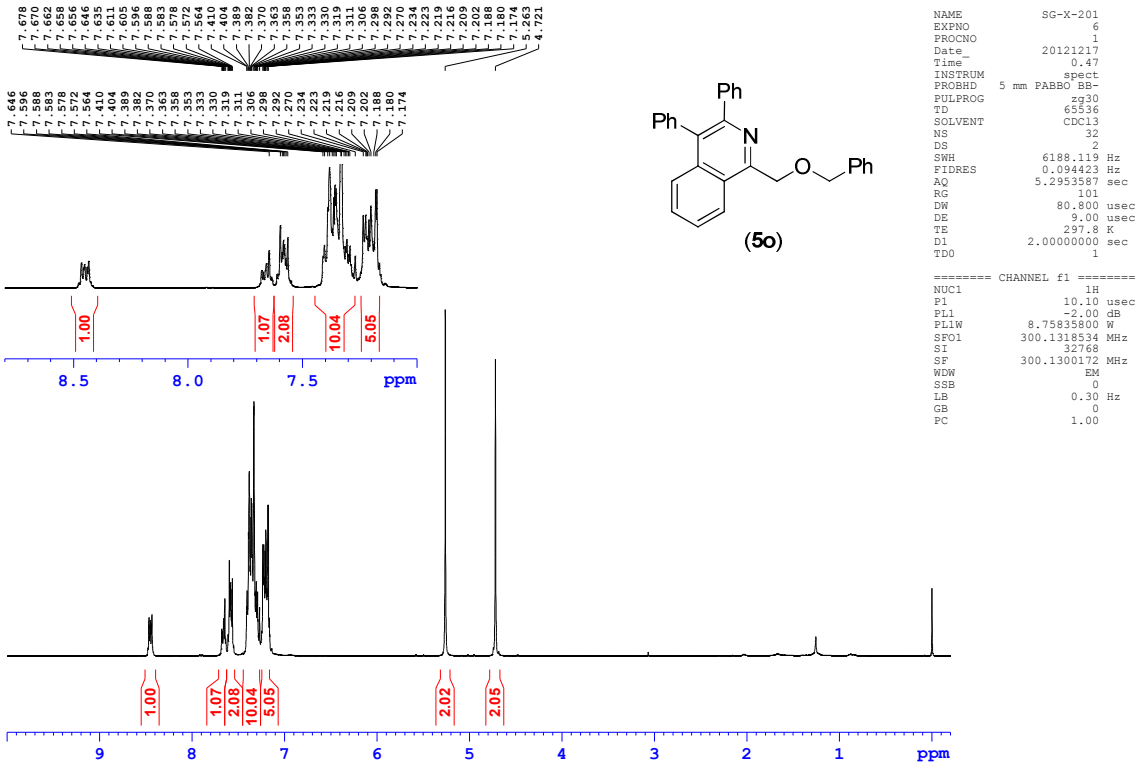
(5n)

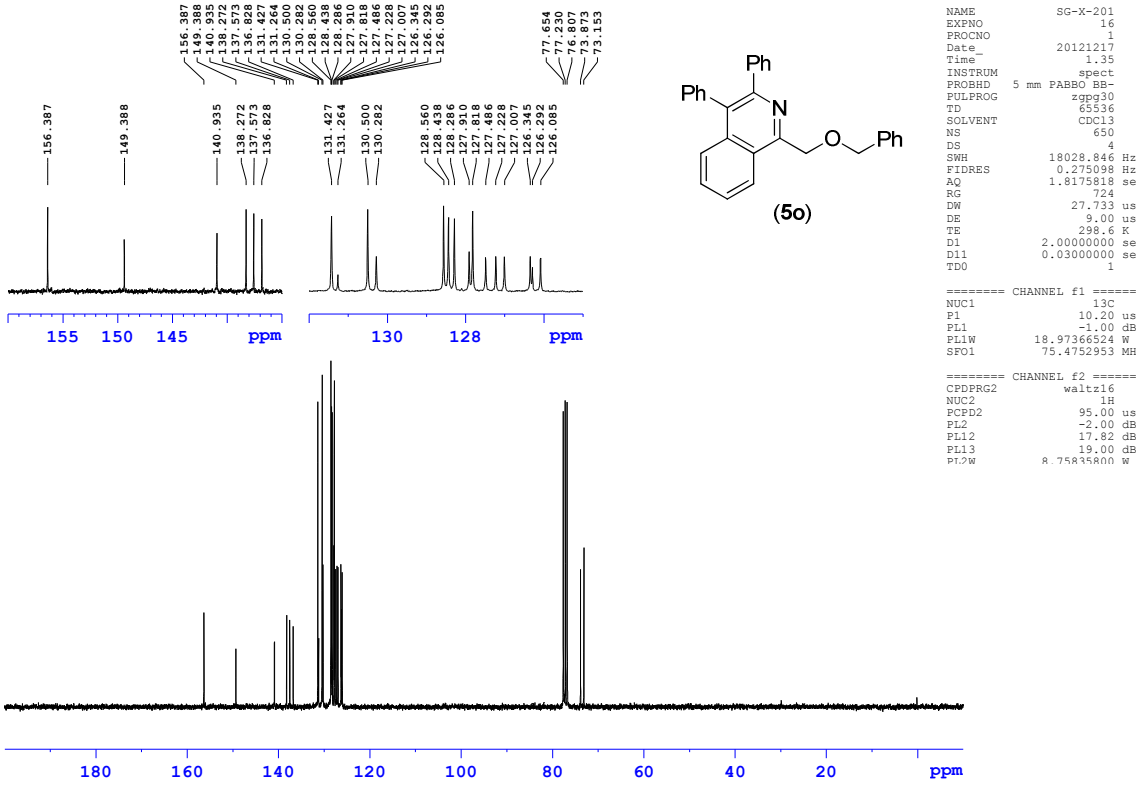
```
NAME            SG-X-257
EXPNO                 28
PROCNO                 1
Date_           20130509
Time                3.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2443
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175818 se
RG                  2050
DW                27.733 us
DE                 9.00 us
TE                299.2 K
D1             2.00000000 se
D11            0.03000000 se
TD0                    1

======== CHANNEL f1 ======
NUC1                  13C
P1                 10.20 us
PL1                -1.00 dB
PL1W         18.97366524 W
SFO1         75.4752953 MH

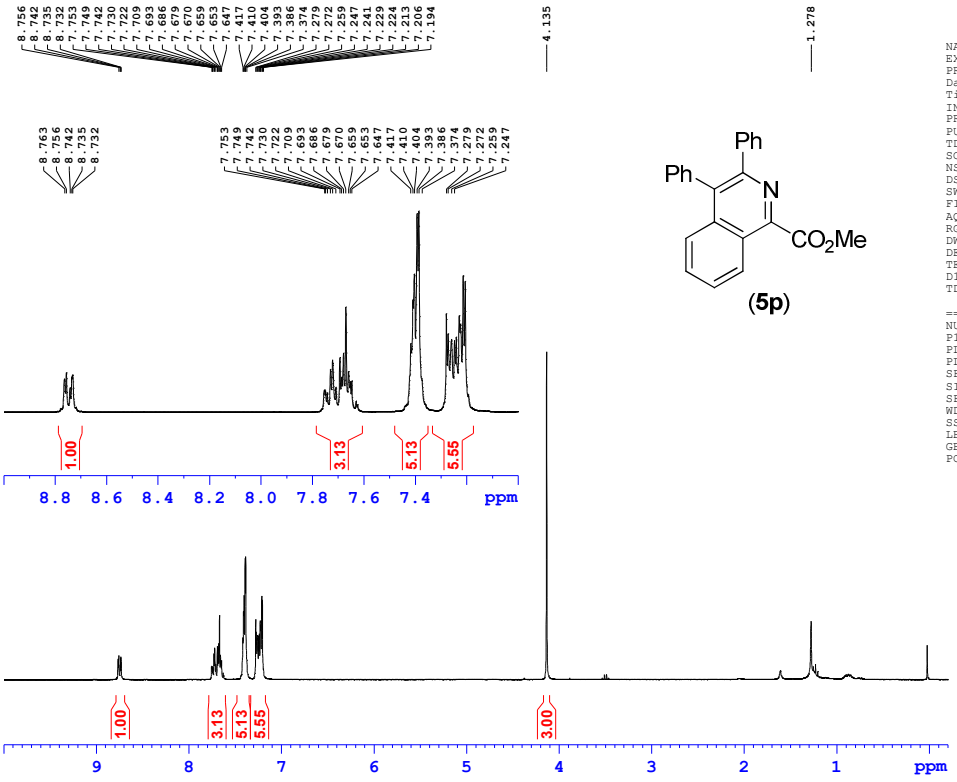
======== CHANNEL f2 ======
CPDPRG2           waltz16
NUC2                  1H
PCPD2              95.00 us
PL2                -2.00 dB
```

1-(benzyloxymethyl)-3,4-diphenylisoquinoline (5o):



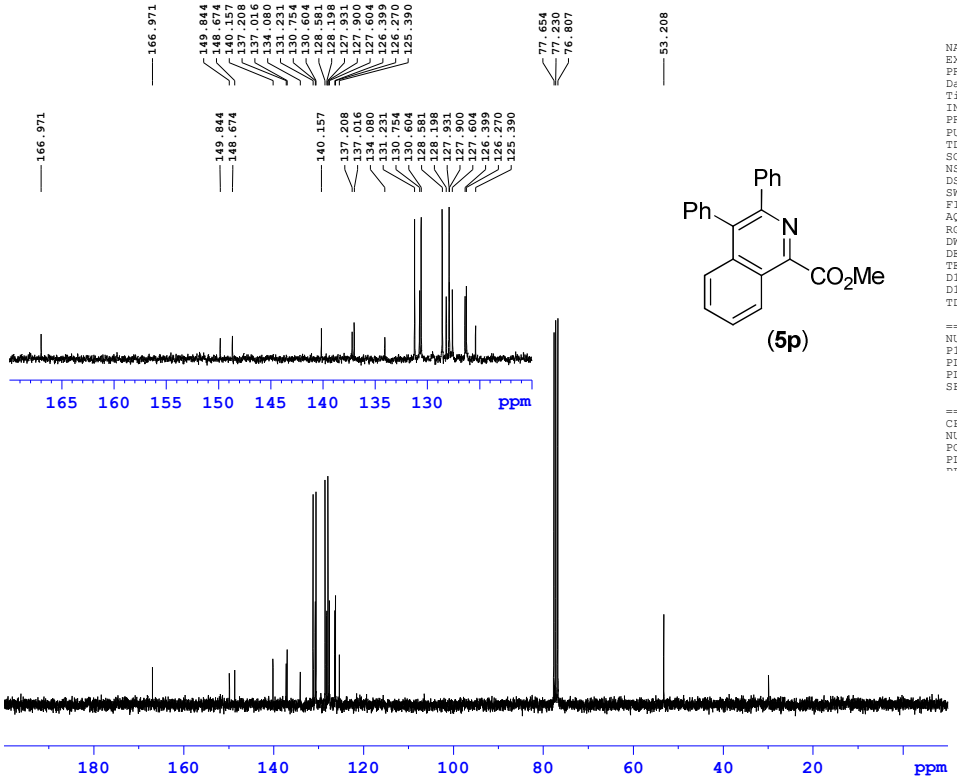


Methyl-3,4-diphenylisoquinoline-1-carboxylate (5p):




```
NAME           KYJ-1-107
EXPNO                  3
PROCNO                 1
Date_           20130604
Time               15.07
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 se
RG                   181
DW                80.800 us
DE                 9.00 us
TE                298.3 K
D1             2.00000000 se
TD0                    1

======== CHANNEL f1 ======
NUC1                  1H
P1                 11.00 us
PL1                -2.00 dB
PL1W         8.75835800 W
SFO1        300.1318534 MH
SI                 32768
SF          300.1300001 MH
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

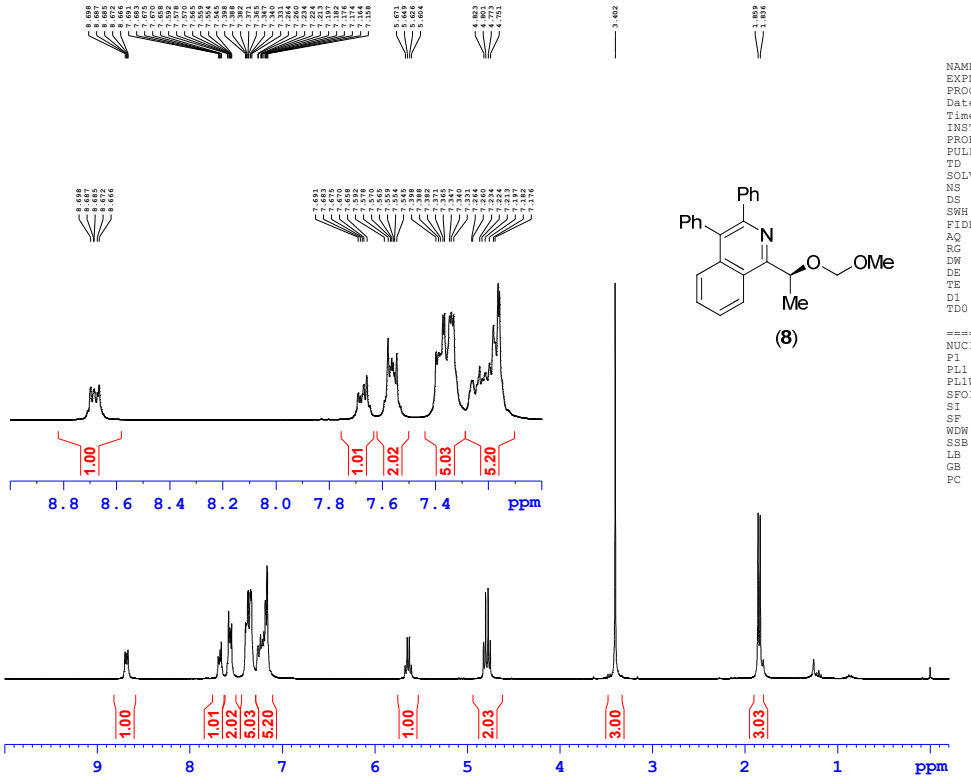



```
NAME           KYJ-1-107
EXPNO                 13
PROCNO                 1
Date_           20130604
Time               15.34
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   443
DS                     2
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175818 se
RG                    16
DW                27.733 us
DE                 6.50 us
TE                299.2 K
D1             1.50000000 se
D11            0.03000000 se
TD0                    1

======== CHANNEL f1 ======
NUC1                 13C
P1                 10.20 us
PL1                -1.00 dB
PL1W         18.97366524 W
SFO1         75.4752953 MH

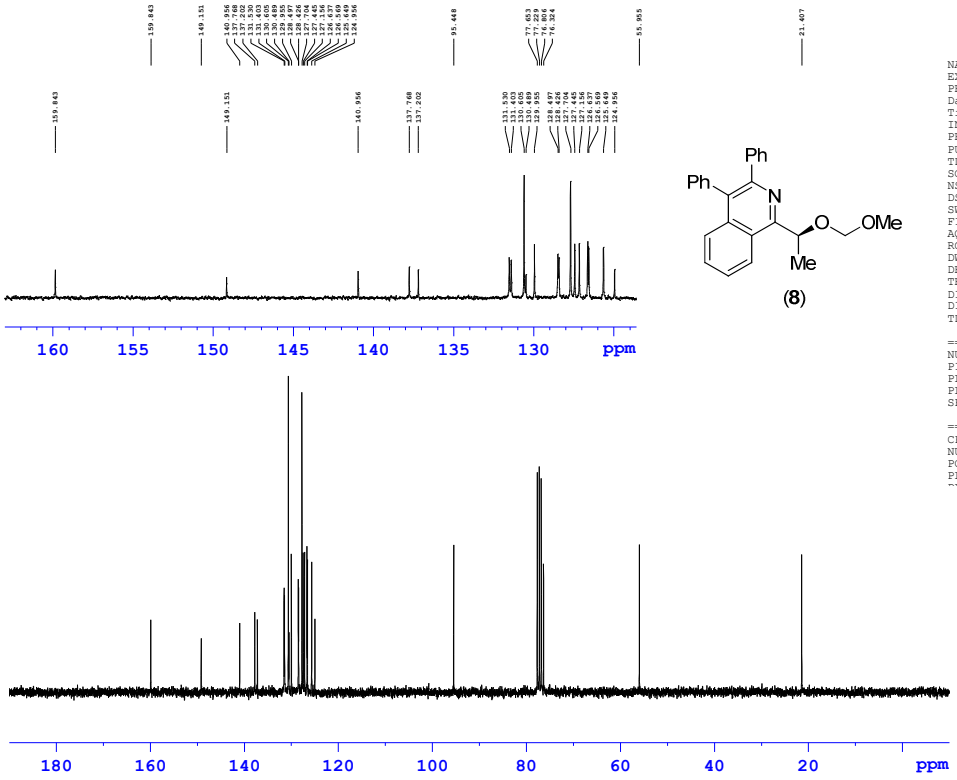
======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                  1H
PCPD2              95.00 us
PL2                -2.00 dB
```

(*S*)-1-(1-(methoxymethoxy)ethyl)-3,4-diphenylisoquinoline (8):




```
NAME            SG-XII-35
EXPNO                  20
PROCNO                  1
Date_            20130801
Time                21.41
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH           6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 se
RG                  80.6
DW                80.800 us
DE                 9.00 us
TE                298.5 K
D1            2.00000000 se
TD0                    1

======== CHANNEL f1 ======
NUC1                  1H
P1                11.00 us
PL1               -2.00 dB
PL1W         8.75835800 W
SFO1        300.1318534 MH
SI                 32768
SF          300.1300141 MH
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

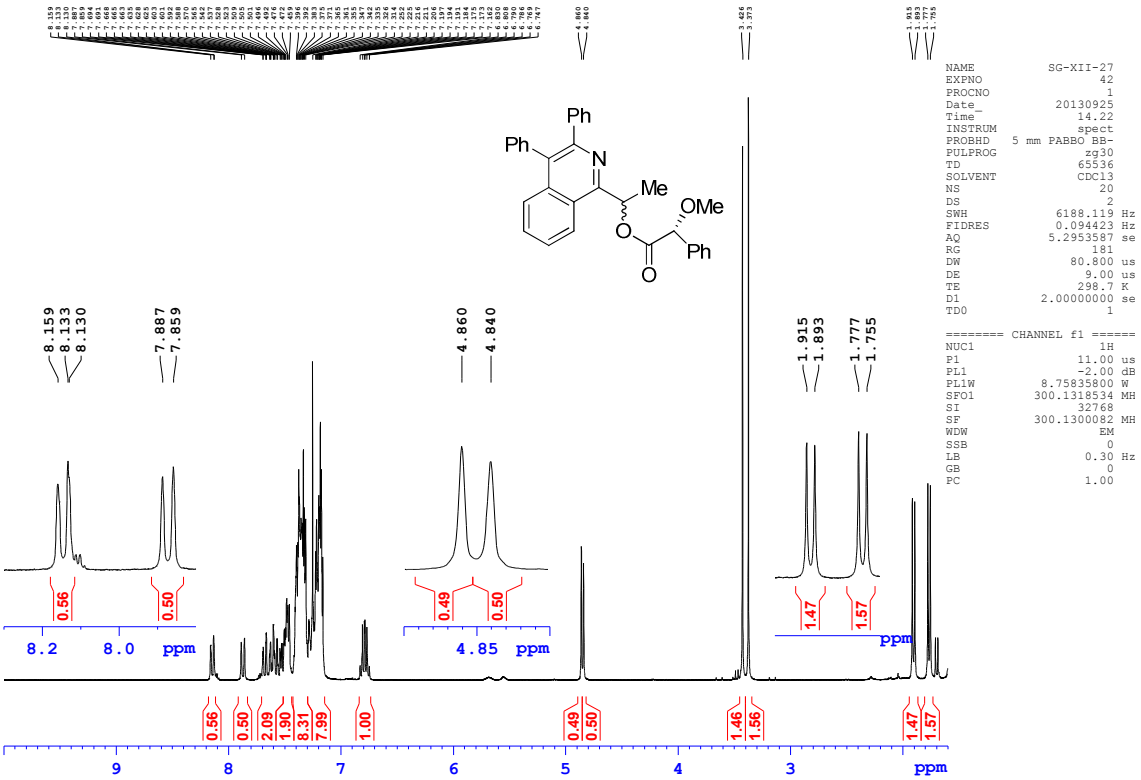



```
NAME            SG-XII-35
EXPNO                  21
PROCNO                  1
Date_            20130801
Time                21.55
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   160
DS                     4
SWH          18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175818 se
RG                  1150
DW                27.733 us
DE                 9.00 us
TE                299.2 K
D1            2.00000000 se
D11           0.03000000 se
TD0                    1

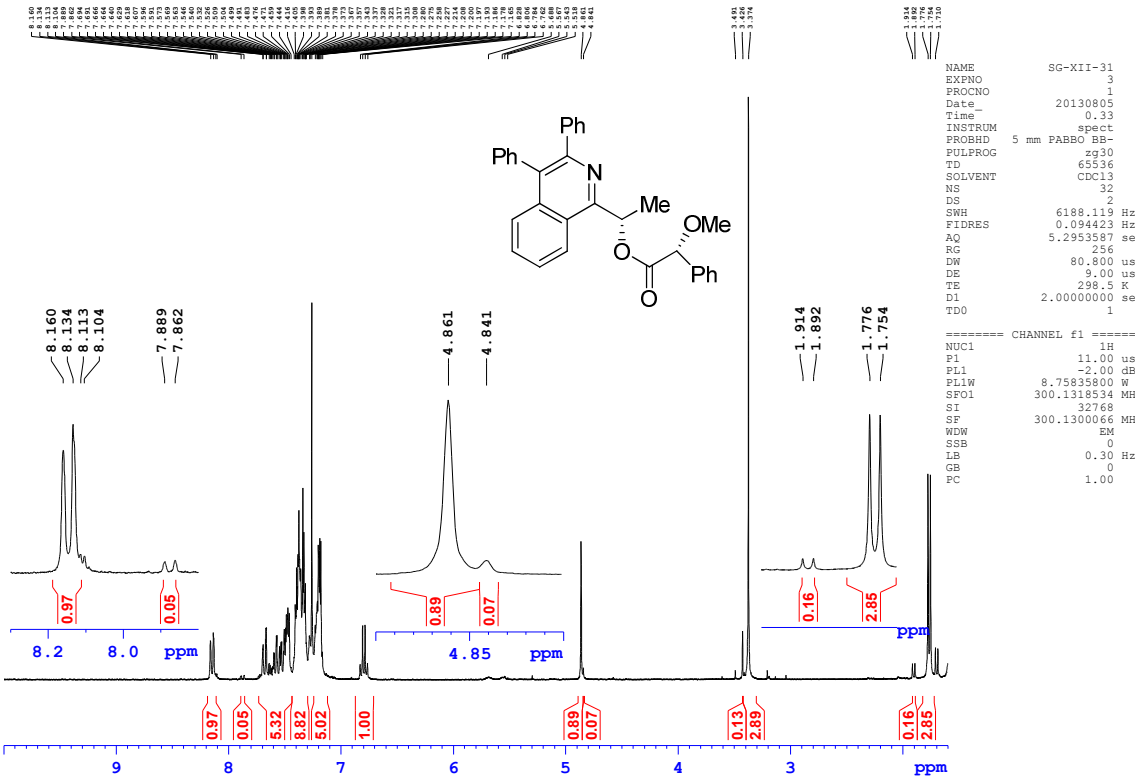
======== CHANNEL f1 ======
NUC1                 13C
P1                10.20 us
PL1               -1.00 dB
PL1W        18.97366524 W
SFO1         75.4752953 MH

======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                  1H
PCPD2             95.00 us
PL2               -2.00 dB
```

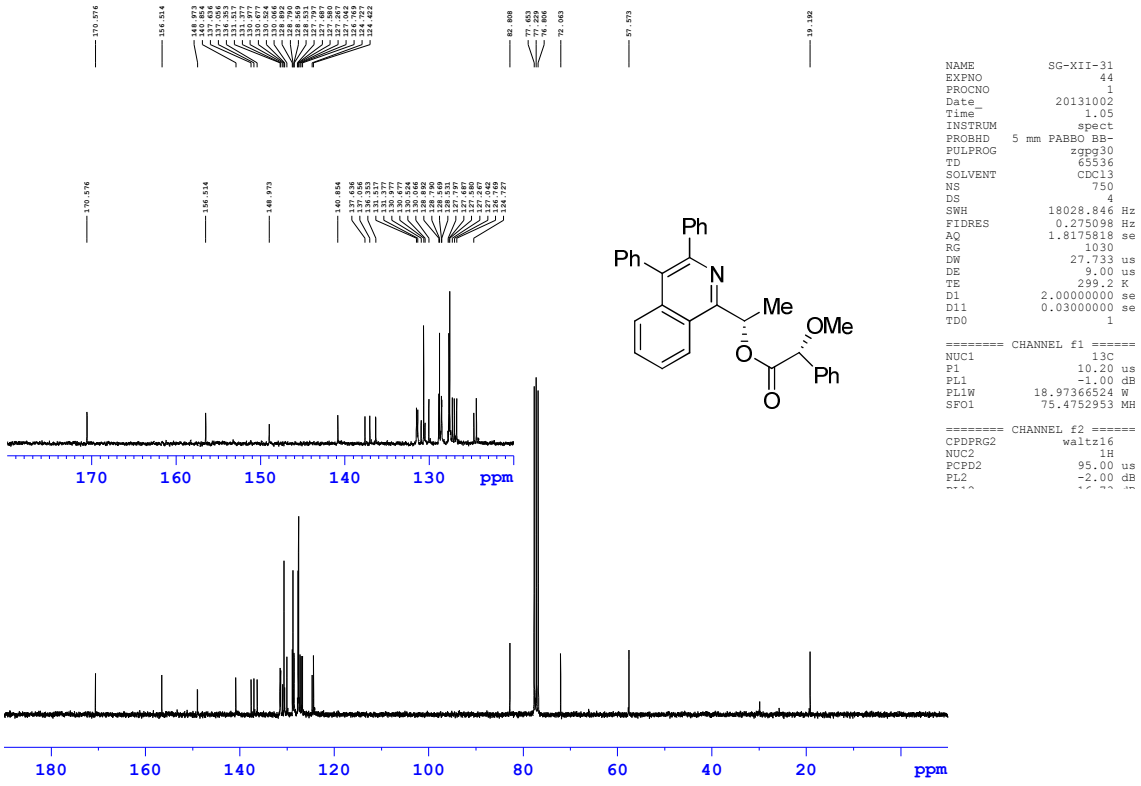
^{1}H NMR of (*R*)-1-(3,4-diphenylisoquinolin-1-yl)ethyl 2-methoxy-2-phenylacetate:



^{1}H NMR of (*R*)-((*S*)-1-(3,4-diphenylisoquinolin-1-yl)ethyl) 2-methoxy-2-phenylacetate:

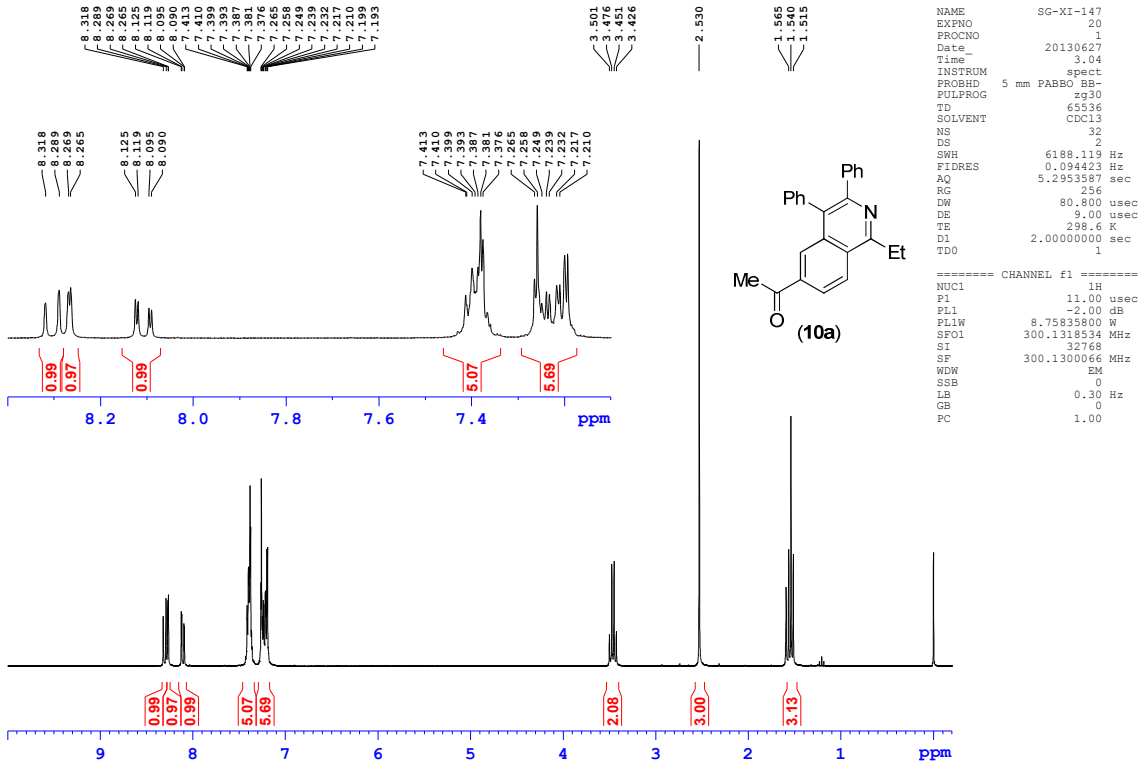


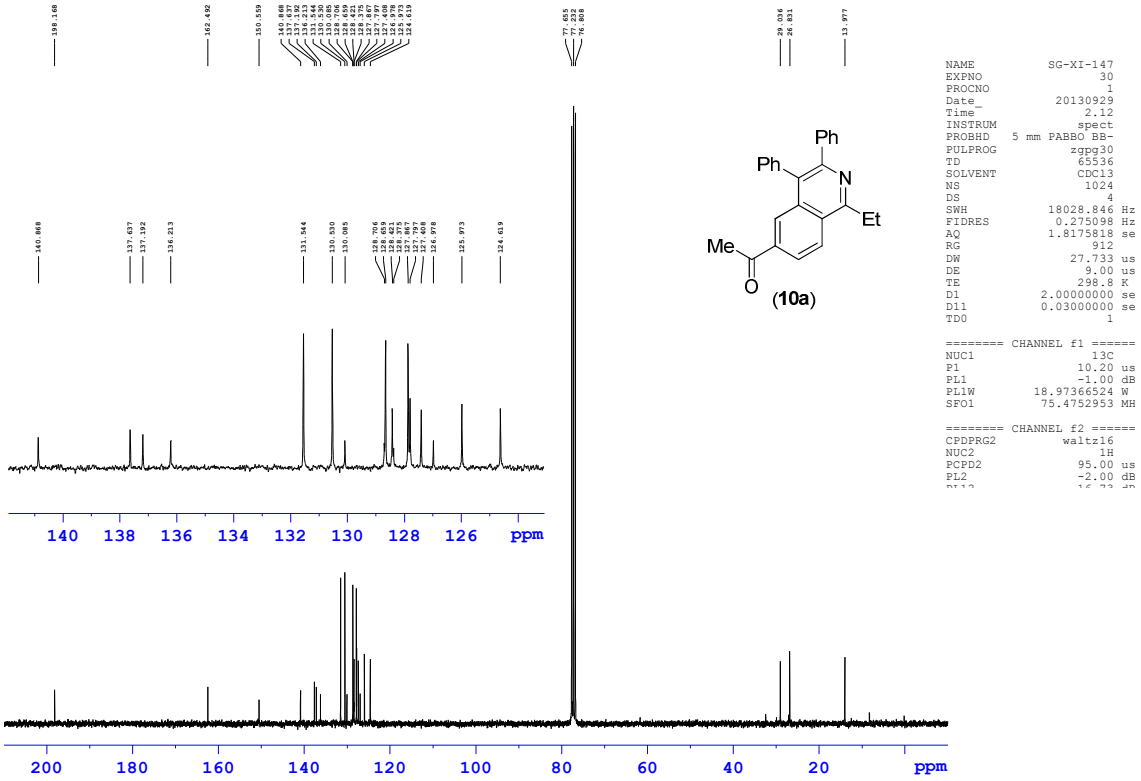
^{13}C NMR of (*R*)-((*S*)-1-(3,4-diphenylisoquinolin-1-yl)ethyl) 2-methoxy-2-phenylacetate:



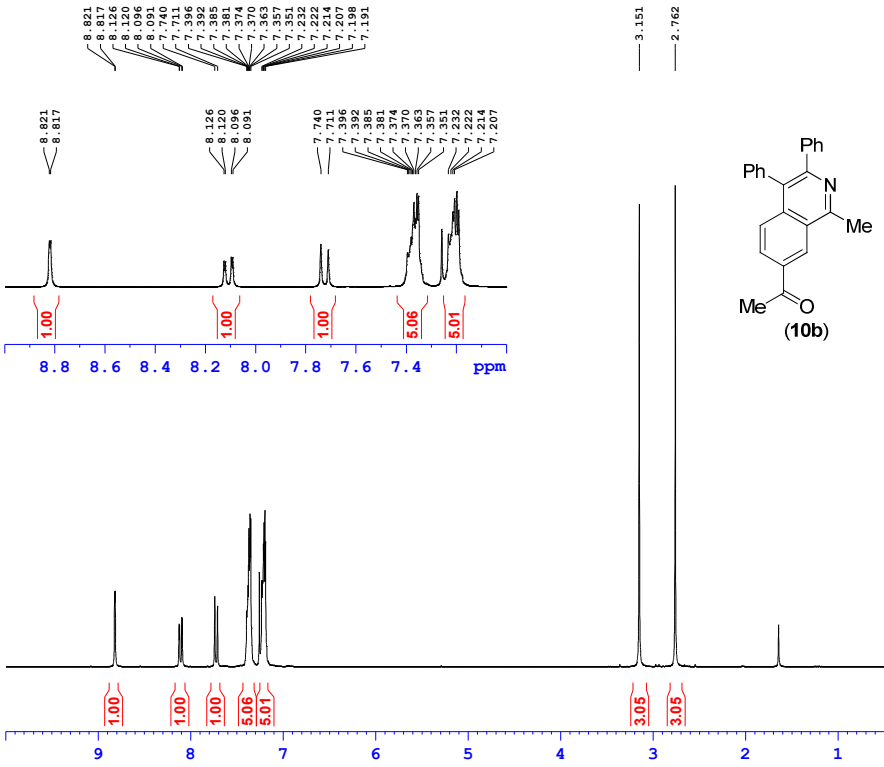
[Note: We envisioned that the formation of minor isomer (about 5%) from ^{1}H NMR analysis could be originated from the purity of (*R*)-2-methoxy-2-phenylacetic acid. To determine the correct enantiomeric excess value for **8**, we tested the ester formation from commercially available (*S*)-(+)-4-phenyl-2-butanol (Aldrich, 99% *ee*) and (*R*)-2-methoxy-2-phenylacetic at same reaction conditions. ^{1}H NMR analysis of the formed ester also shown the formation of two isomers is about 95:5 ratio. By the analogy, we conclude that the enantiomeric excess (*ee*) of **8** is >98%.]

1-(1-ethyl-3,4-diphenylisoquinolin-6-yl)ethanone (10a):



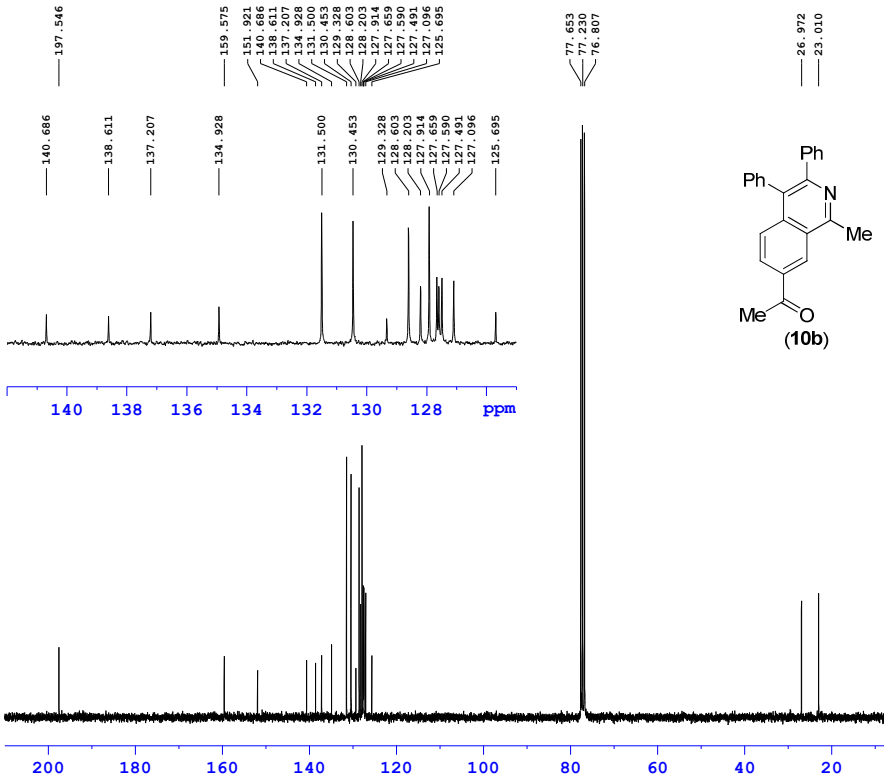


1-(1-methyl-3,4-diphenylisoquinolin-7-yl)ethanone (10b):




```
NAME            SG-XI-67
EXPNO                20
PROCNO                1
Date_          20130503
Time               0.02
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH           6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                  203
DW               80.800 usec
DE                9.00 usec
TE               298.1 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                1H
P1              11.00 usec
PL1             -2.00 dB
PL1W         8.75835800 W
SFO1        300.1318534 MHz
SI                32768
SF          300.1300065 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```

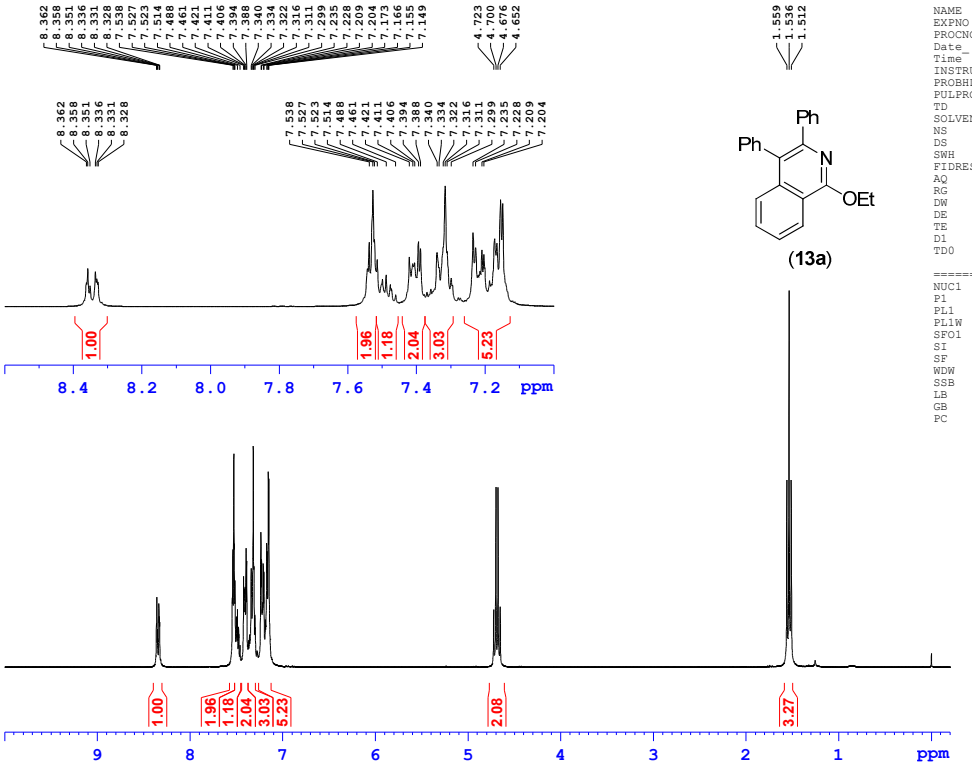



```
NAME            SG-XI-67
EXPNO                21
PROCNO                1
Date_          20130503
Time               1.12
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH          18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 se
RG                  912
DW               27.733 us
DE                9.00 us
TE               299.1 K
D1            2.00000000 se
D11           0.03000000 se
TD0                   1

======== CHANNEL f1 ======
NUC1                13C
P1              10.20 us
PL1             -1.00 dB
PL1W        18.97366524 W
SFO1         75.4752953 MH

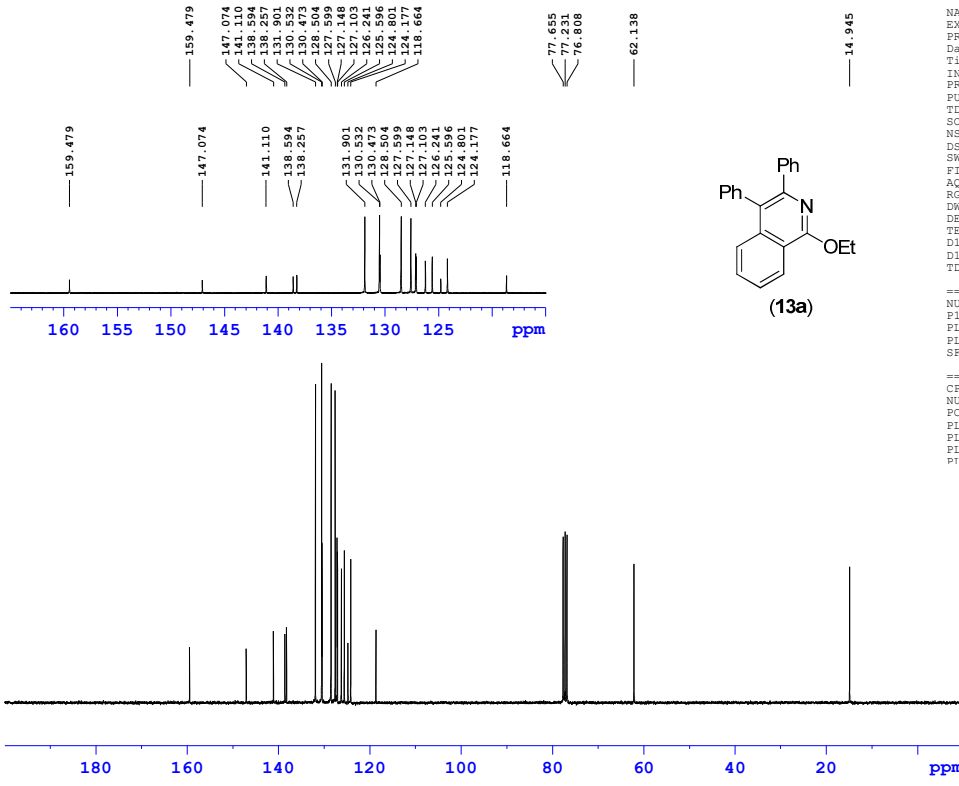
======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                1H
PCPD2           95.00 us
PL2             -2.00 dB
PL12            16.73 dB
PL13            19.00 dB
PL2W         8.75835800 W
```

1-Ethoxy-3,4-diphenylisoquinoline (13a):




```
NAME            SG-XI-117
EXPNO                20
PROCNO                1
Date_          20130620
Time               0.01
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH           6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                 50.8
DW               80.800 usec
DE                9.00 usec
TE               298.9 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                11.00 usec
PL1               -2.00 dB
PL1W        8.75835800 W
SFO1       300.1318534 MHz
SI               32768
SF         300.1300238 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

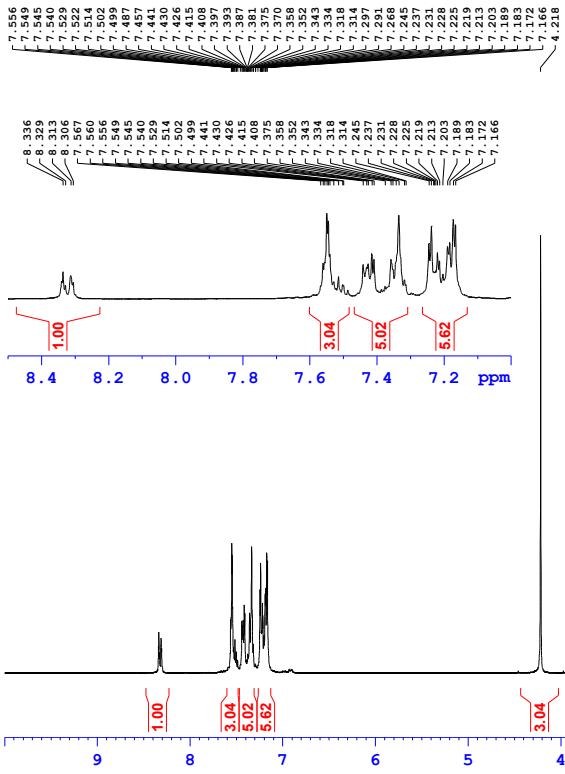


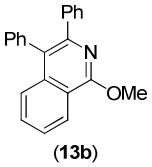

```
NAME            SG-XI-117
EXPNO                21
PROCNO                1
Date_          20130620
Time               1.12
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH          18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 se
RG                 1150
DW               27.733 us
DE                9.00 us
TE               299.4 K
D1           2.00000000 se
D11          0.03000000 se
TD0                   1

======== CHANNEL f1 ======
NUC1                13C
P1               10.20 us
PL1              -1.00 dB
PL1W       18.97366524 W
SFO1       75.4752953 MH

======== CHANNEL f2 ======
CPDPRG2         waltz16
NUC2                 1H
PCPD2            95.00 us
PL2              -2.00 dB
PL12             16.73 dB
PL13             19.00 dB
PL2W        8.75835800 W
```

1-Methoxy-3,4-diphenylisoquinoline (13b):

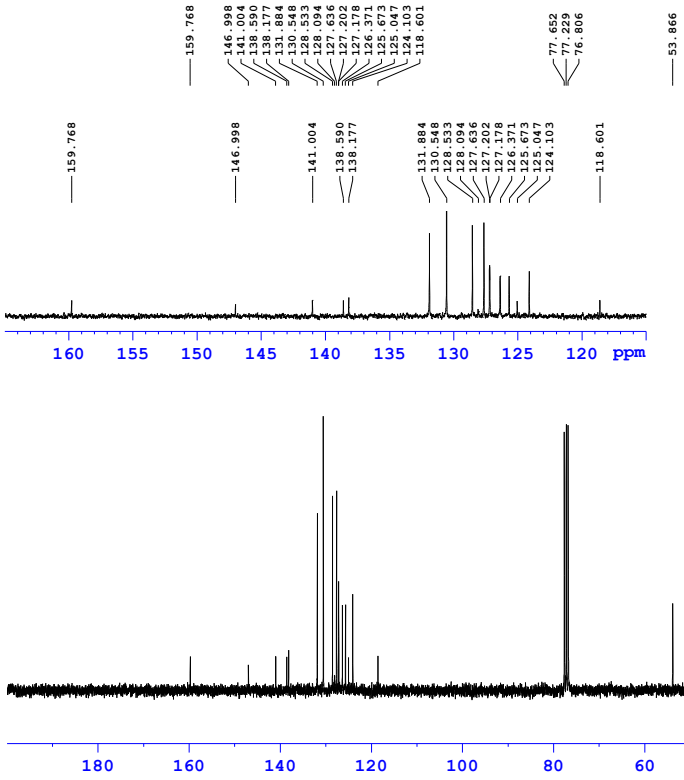


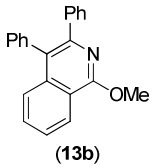


(13b)

```
NAME            SG-XI-81
EXPNO                3
PROCNO               1
Date_         20130322
Time             11.08
INSTRUM          spect
PROBHD  5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  32
DS                   2
SWH           6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                 161
DW              80.800 usec
DE               9.00 usec
TE              297.8 K
D1           2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               10.10 usec
PL1              -2.00 dB
PL1W          8.75835800 W
SFO1        300.1318534 MHz
SI                32768
SF          300.1300129 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```





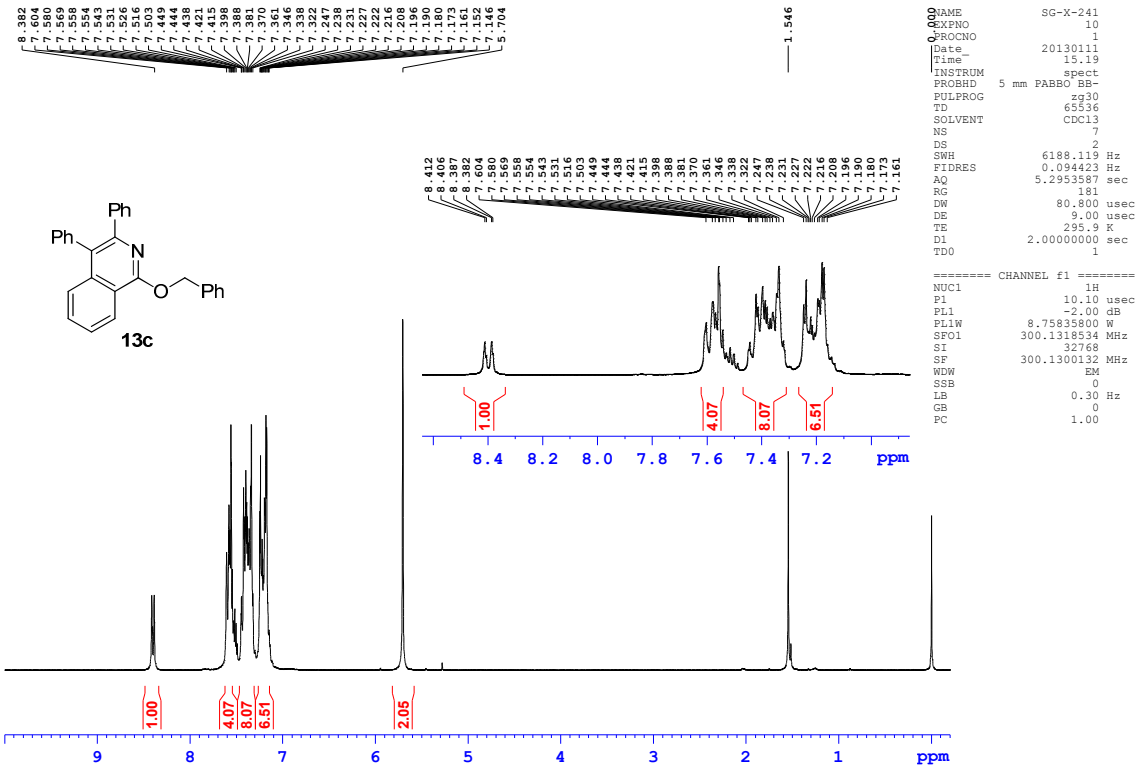
(13b)

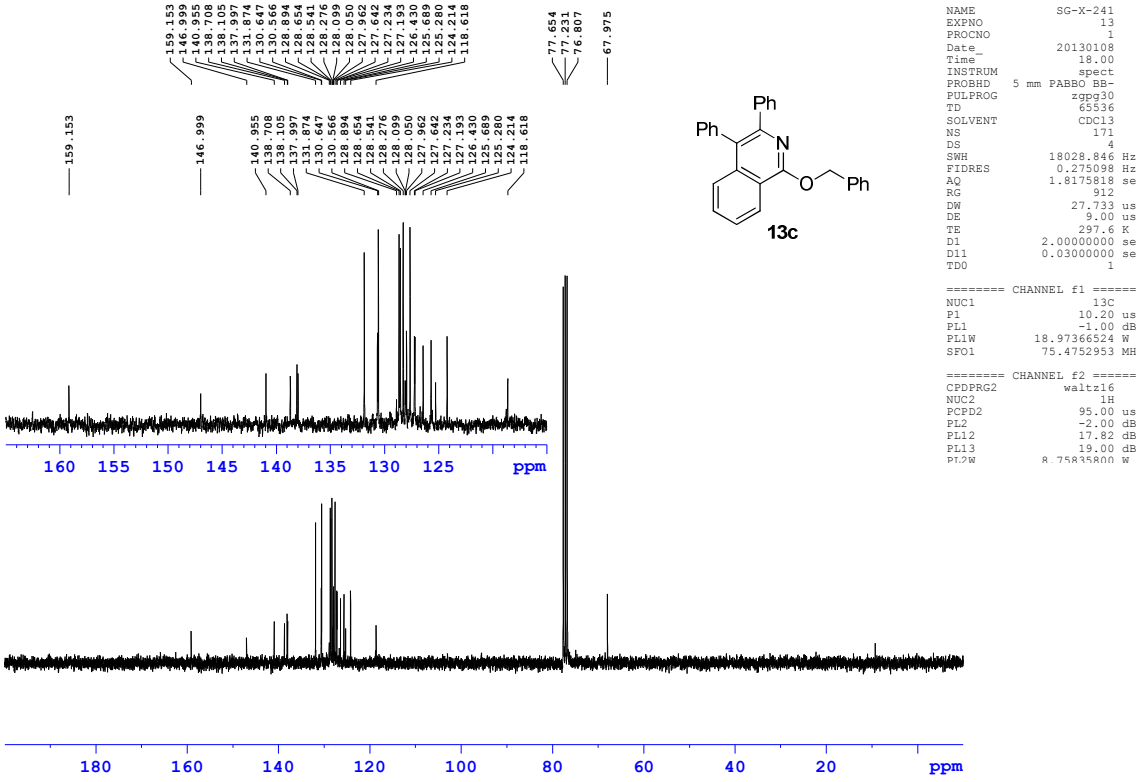
```
NAME            SG-XI-81
EXPNO               13
PROCNO               1
Date_         20130322
Time             11.22
INSTRUM          spect
PROBHD  5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 126
DS                   4
SWH          18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 se
RG                 724
DW              27.733 us
DE               9.00 us
TE              298.3 K
D1           2.00000000 se
D11          0.03000000 se
TD0                  1

======== CHANNEL f1 ======
NUC1                13C
P1               10.20 us
PL1              -1.00 dB
PL1W        18.97366524 W
SFO1         75.4752953 MH

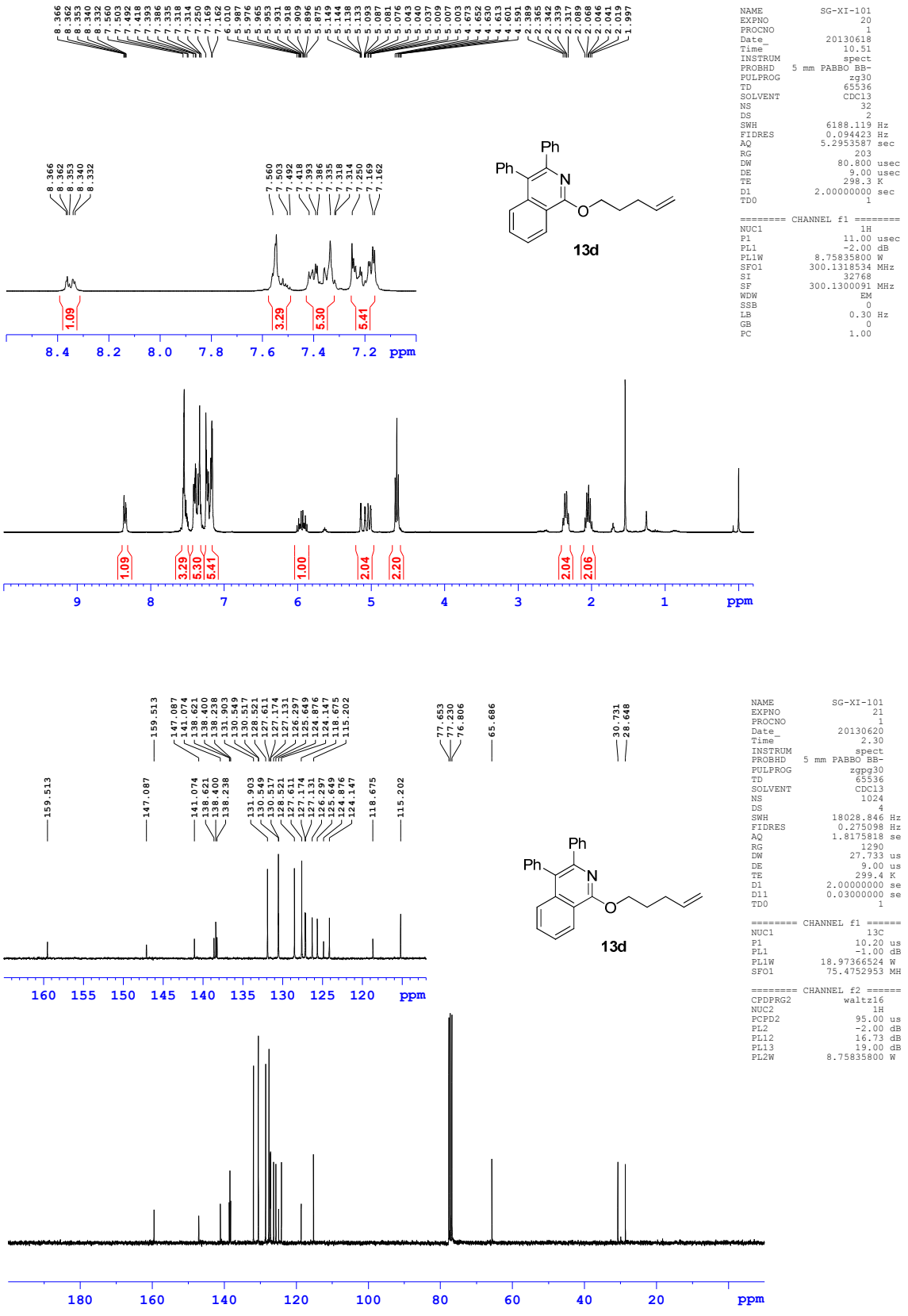
======== CHANNEL f2 ======
CPDPRG2         waltz16
NUC2                1H
PCPD2            95.00 us
PL2              -2.00 dB
PL12             17.82 dB
PL13             19.00 dB
PL2W          8.75835800 W
```

1-(Benzyloxy)-3,4-diphenylisoquinoline (13c):





1-(pent-4-enyloxy)-3,4-diphenylisoquinoline (13d):




```
NAME            SG-XI-101
EXPNO                  20
PROCNO                  1
Date_            20130618
Time                10.51
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     32
DS                      2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                    203
DW                80.800 usec
DE                 9.00 usec
TE                298.3 K
D1             2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 11.00 usec
PL1                -2.00 dB
PL1W          8.75835800 W
SFO1         300.1318534 MHz
SI                  32768
SF           300.1300091 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```

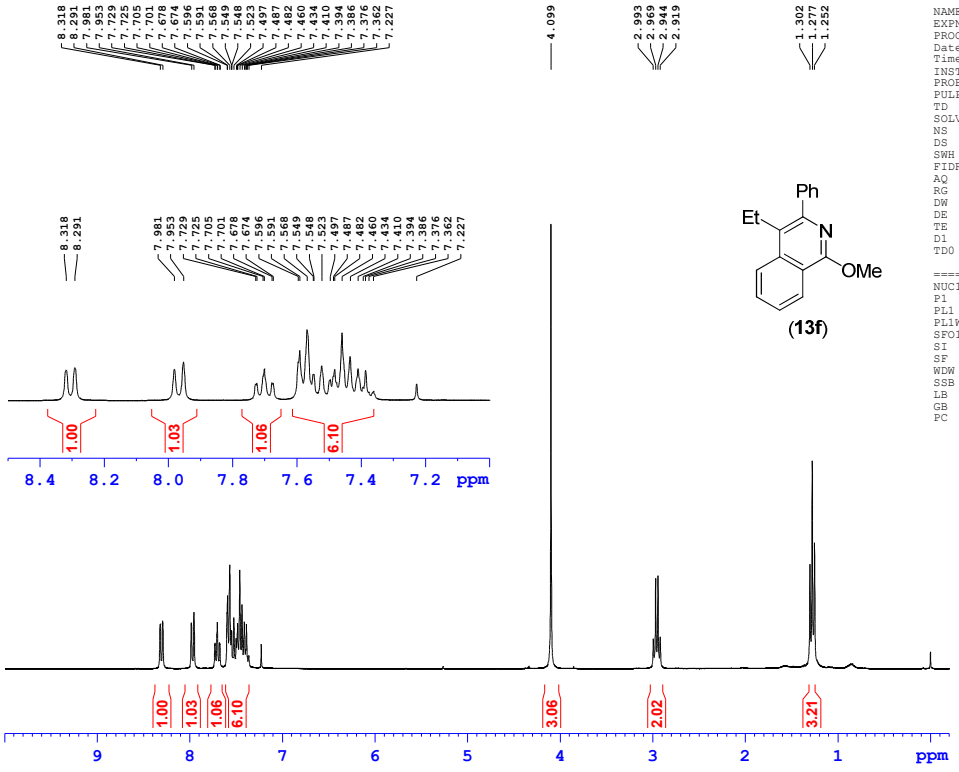


```
NAME            SG-XI-101
EXPNO                  21
PROCNO                  1
Date_            20130620
Time                 2.30
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175818 se
RG                   1290
DW                27.733 us
DE                 9.00 us
TE                299.4 K
D1             2.00000000 se
D11            0.03000000 se
TD0                     1

======== CHANNEL f1 ======
NUC1                  13C
P1                 10.20 us
PL1                -1.00 dB
PL1W          18.97366524 W
SFO1           75.4752953 MH

======== CHANNEL f2 ======
CPDPRG2            waltz16
NUC2                   1H
PCPD2              95.00 us
PL2                -2.00 dB
PL12               16.73 dB
PL13               19.00 dB
PL2W          8.75835800 W
```

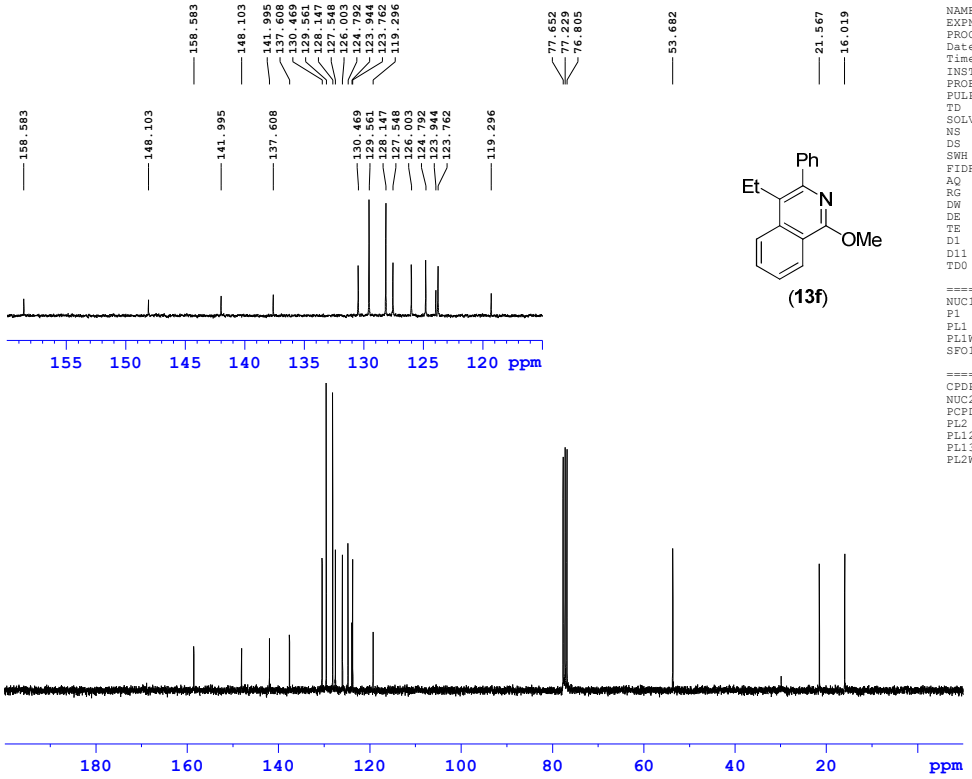
4-Ethyl-1-methoxy-3-phenylisoquinoline (13f):



(13f)

```
NAME            SG-XI-99
EXPNO                5
PROCNO               1
Date_         20130420
Time_            15.56
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  32
DS                   2
SWH           6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                 101
DW              80.800 usec
DE               9.00 usec
TE              296.7 K
D1            2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1                11.00 usec
PL1               -2.00 dB
PL1W         8.75835800 W
SFO1        300.1318534 MHz
SI                32768
SF          300.1300160 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



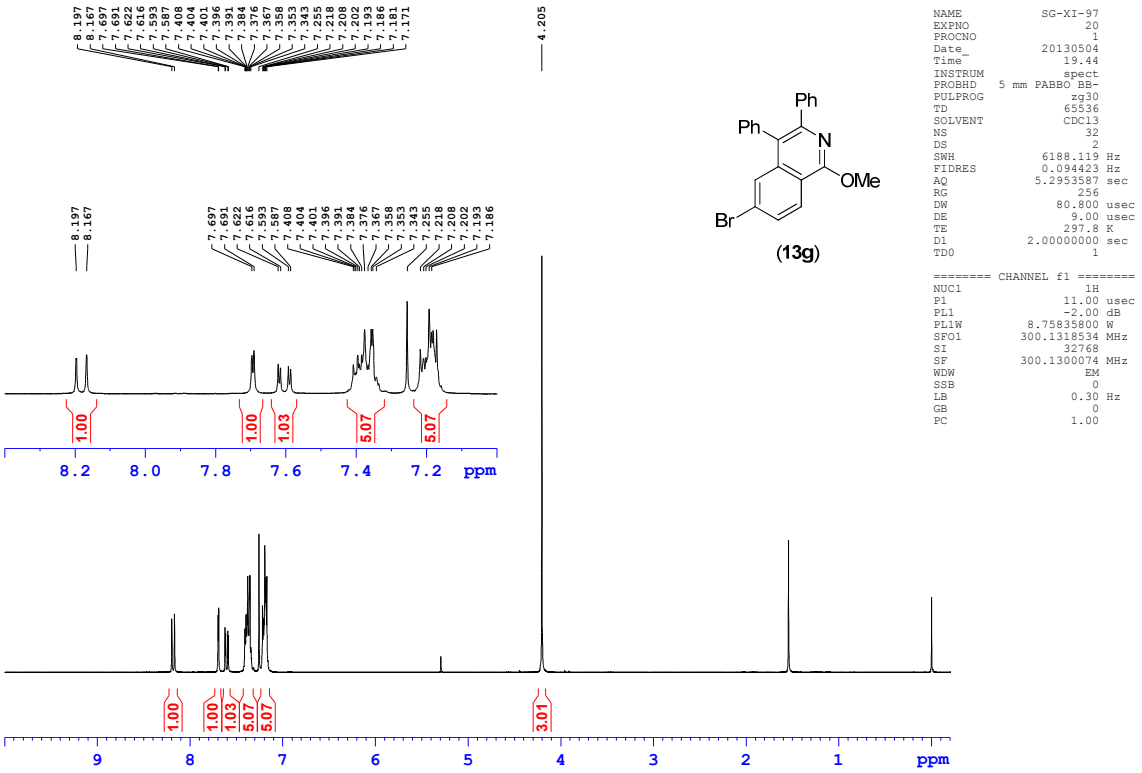
(13f)

```
NAME            SG-XI-99
EXPNO               13
PROCNO               1
Date_         20130420
Time_            16.14
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 200
DS                   4
SWH          18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 se
RG                 812
DW              27.733 us
DE               9.00 us
TE              297.4 K
D1            2.00000000 se
D11           0.03000000 se
TD0                  1

======== CHANNEL f1 ======
NUC1               13C
P1               10.20 us
PL1              -1.00 dB
PL1W        18.97366524 W
SFO1         75.4752953 MH

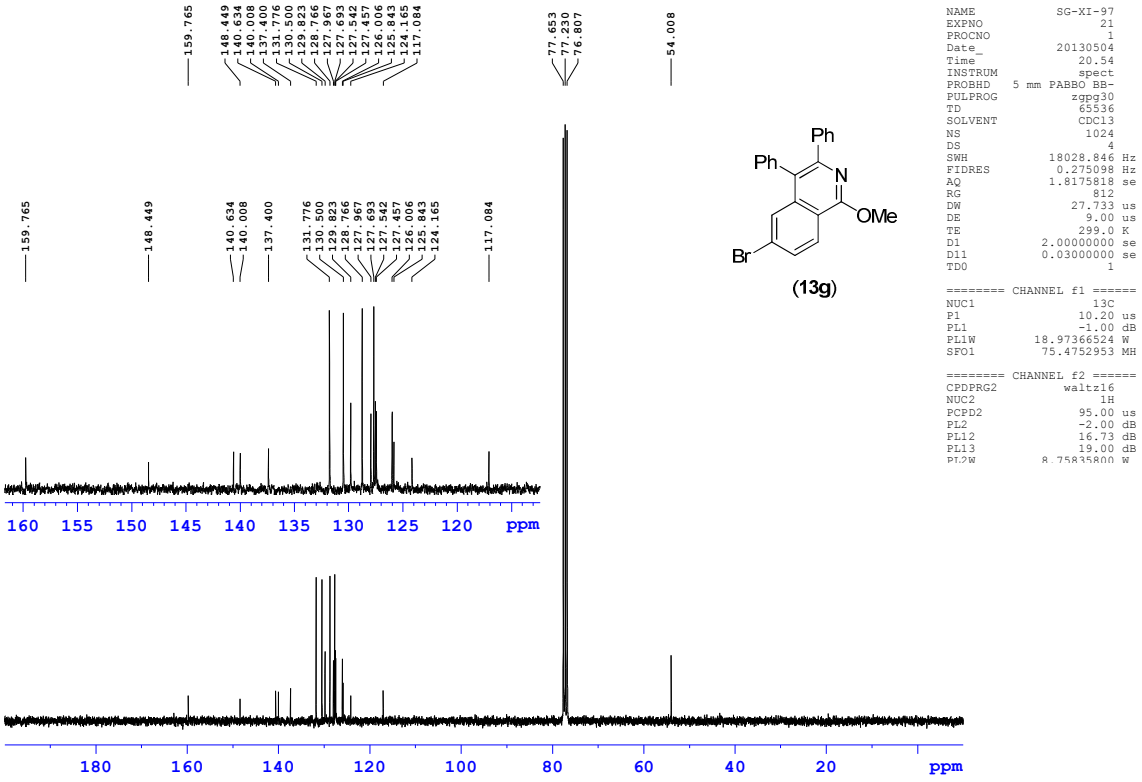
======== CHANNEL f2 ======
CPDPRG2         waltz16
NUC2               1H
PCPD2            95.00 us
PL2              -2.00 dB
PL12             16.73 dB
PL13             19.00 dB
PL2W         8.75835800 W
```

6-Bromo-1-methoxy-3,4-diphenylisoquinoline (13g):




```
NAME            SG-XI-97
EXPNO                20
PROCNO                1
Date_            20130504
Time                19.44
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     32
DS                      2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                    256
DW                80.800 usec
DE                 9.00 usec
TE                297.8 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.00 usec
PL1                -2.00 dB
PL1W          8.75835800 W
SFO1         300.1318534 MHz
SI                 32768
SF           300.1300074 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

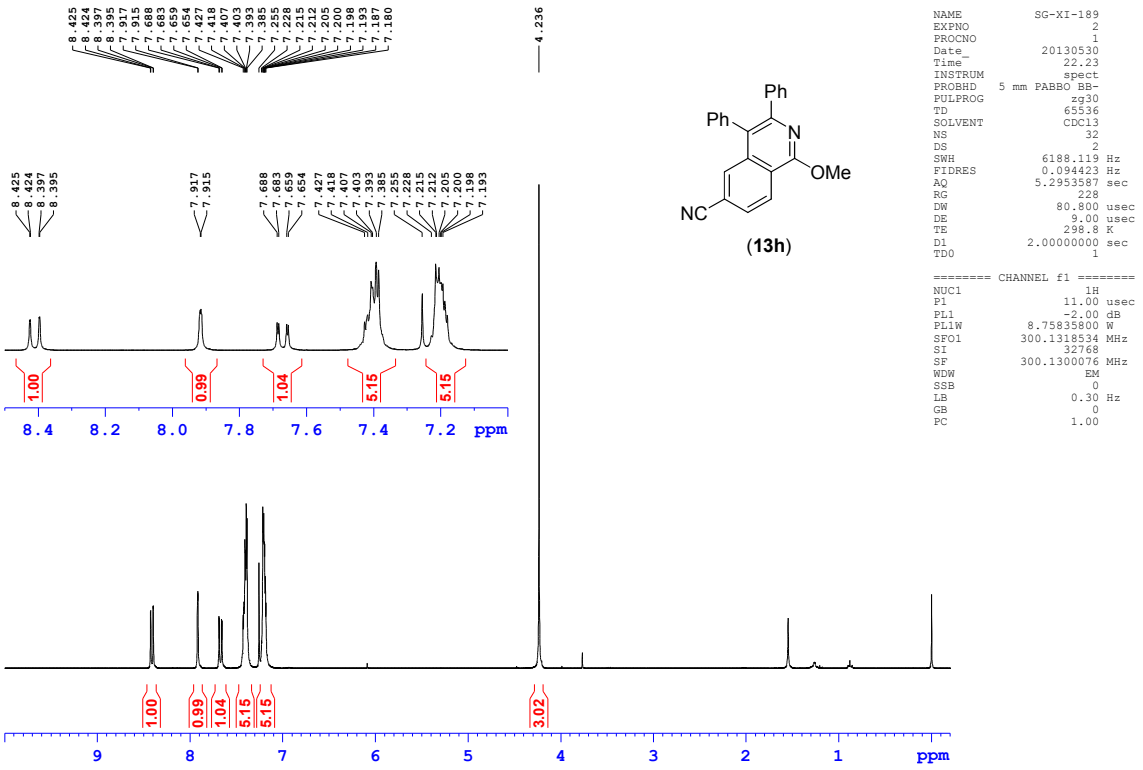



```
NAME            SG-XI-97
EXPNO                21
PROCNO                1
Date_            20130504
Time                20.54
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175818 se
RG                    812
DW                27.733 us
DE                 9.00 us
TE                299.0 K
D1             2.00000000 se
D11            0.03000000 se
TD0                    1

======== CHANNEL f1 ======
NUC1                 13C
P1                 10.20 us
PL1                -1.00 dB
PL1W          18.97366524 W
SFO1           75.4752953 MH

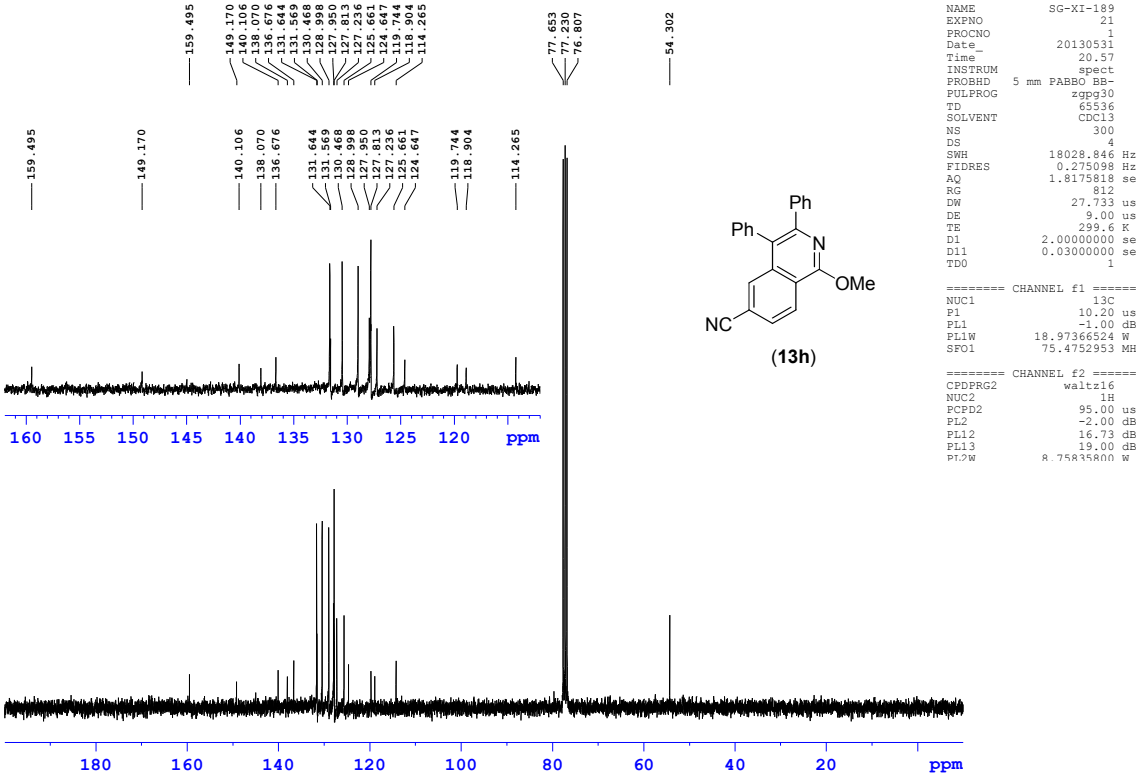
======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                  1H
PCPD2              95.00 us
PL2                -2.00 dB
PL12               16.73 dB
PL13               19.00 dB
PL2W          8.75835800 W
```

1-Methoxy-3,4-diphenylisoquinoline-6-carbonitrile (13h):




```
NAME            SG-XI-189
EXPNO                   2
PROCNO                  1
Date_            20130530
Time                22.23
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     32
DS                      2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                    228
DW                 80.800 usec
DE                  9.00 usec
TE                298.8 K
D1             2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 11.00 usec
PL1                -2.00 dB
PL1W          8.75835800 W
SFO1         300.1318534 MHz
SI                  32768
SF           300.1300076 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```



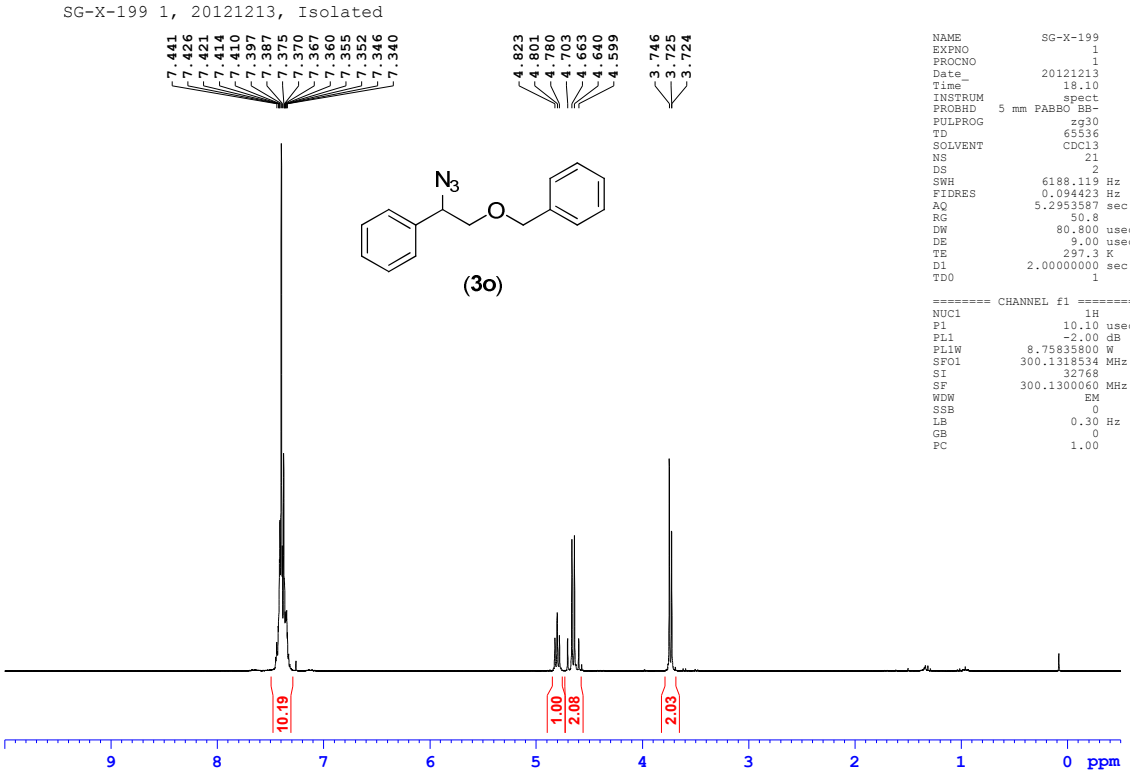

```
NAME            SG-XI-189
EXPNO                  21
PROCNO                  1
Date_            20130531
Time                20.57
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    300
DS                      4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175818 se
RG                    812
DW                 27.733 us
DE                  9.00 us
TE                299.6 K
D1             2.00000000 se
D11            0.03000000 se
TD0                     1

======== CHANNEL f1 ======
NUC1                  13C
P1                 10.20 us
PL1                -1.00 dB
PL1W          18.97366524 W
SFO1          75.4752953 MH

======== CHANNEL f2 ======
CPDPRG2           waltz16
NUC2                   1H
PCPD2              95.00 us
PL2                -2.00 dB
PL12               16.73 dB
PL13               19.00 dB
PL2W          8.75835800 W
```

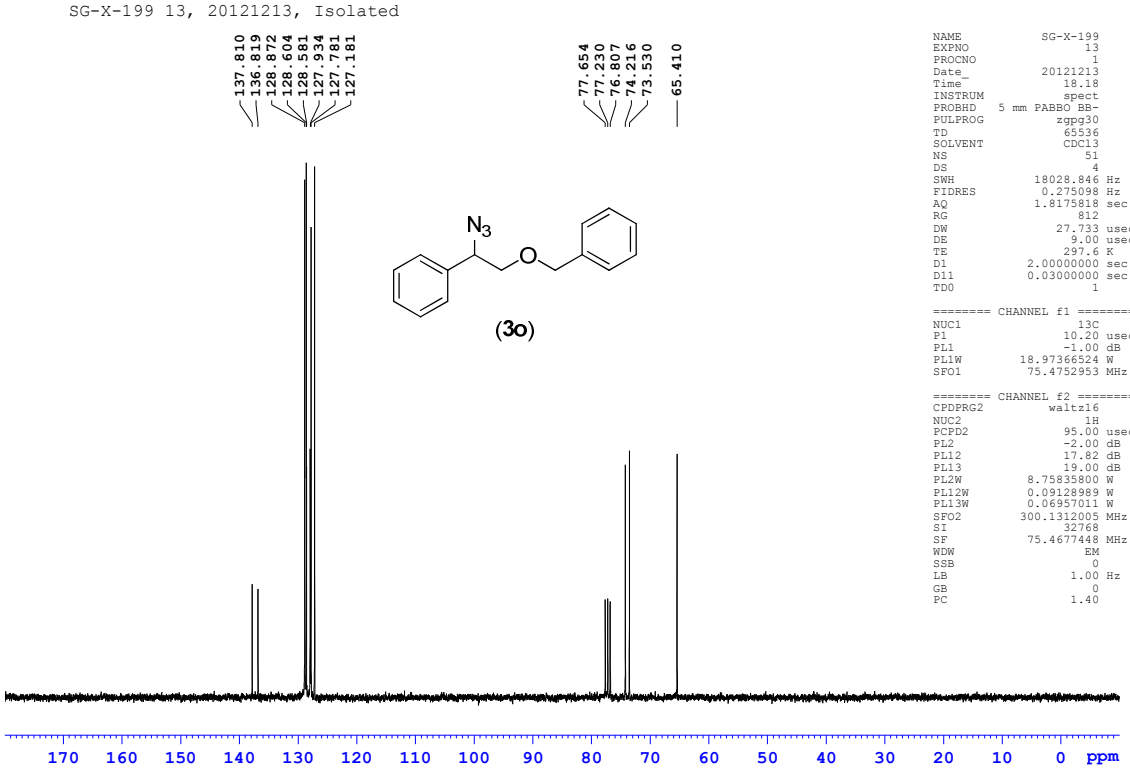
2. ^{1}H and ^{13}C NMR data of isoquinolines:

(1-azido-2-(benzyloxy)ethyl)benzene (3o):




```
NAME            SG-X-199
EXPNO                1
PROCNO               1
Date_         20121213
Time              18.10
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  21
DS                   2
SWH           6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                50.8
DW               80.800 usec
DE                9.00 usec
TE               297.3 K
D1            2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1                10.10 usec
PL1               -2.00 dB
PL1W         8.75835800 W
SFO1        300.1318534 MHz
SI               32768
SF          300.1300060 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

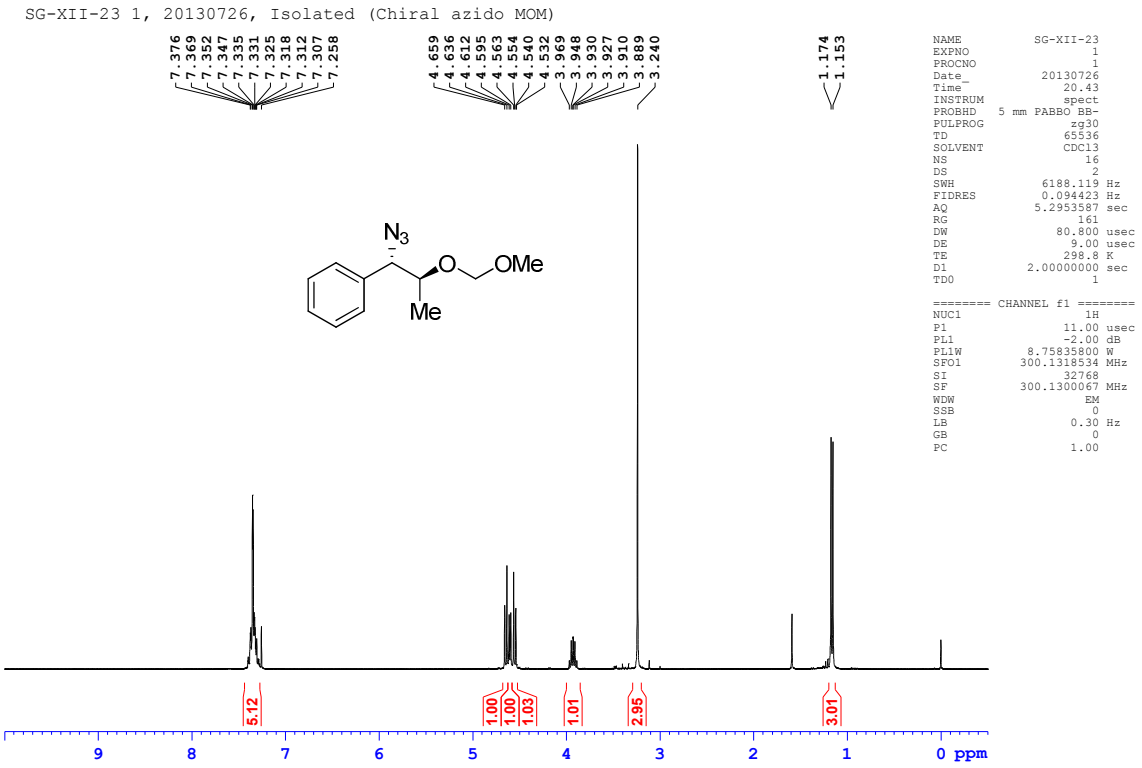


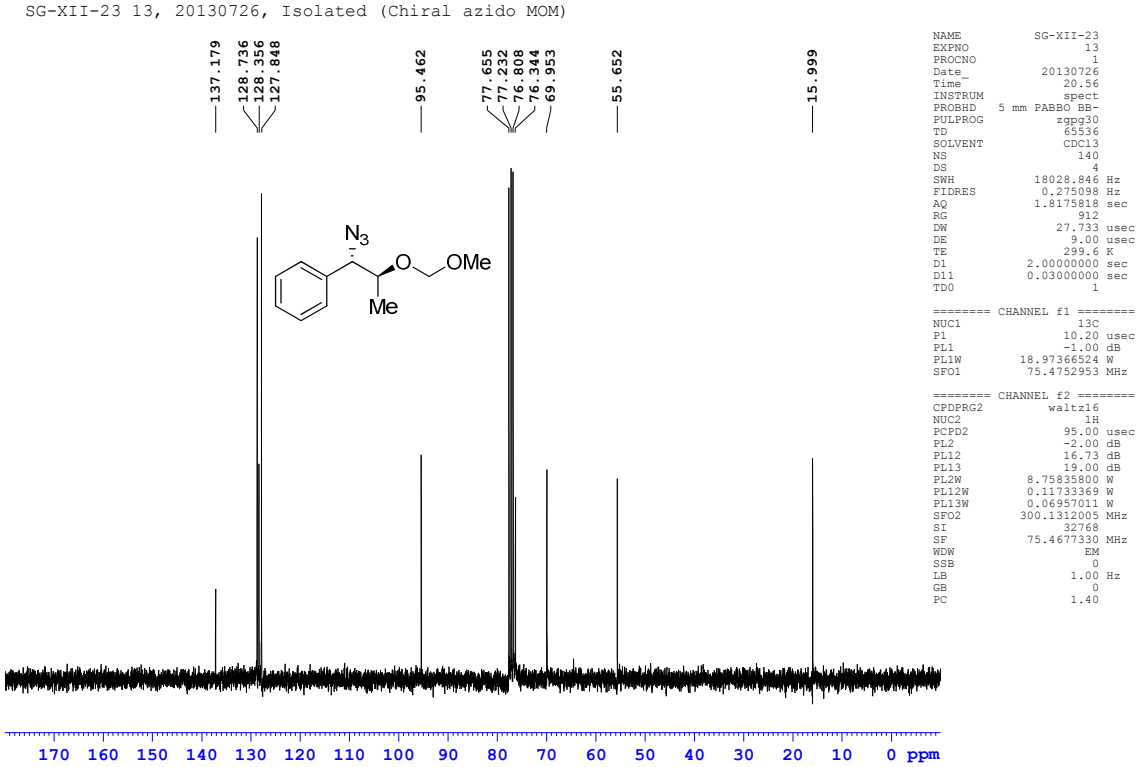

```
NAME            SG-X-199
EXPNO               13
PROCNO               1
Date_         20121213
Time              18.18
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                  51
DS                   4
SWH          18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 sec
RG                 812
DW               27.733 usec
DE                9.00 usec
TE               297.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.20 usec
PL1               -1.00 dB
PL1W        18.97366524 W
SFO1         75.4752953 MHz

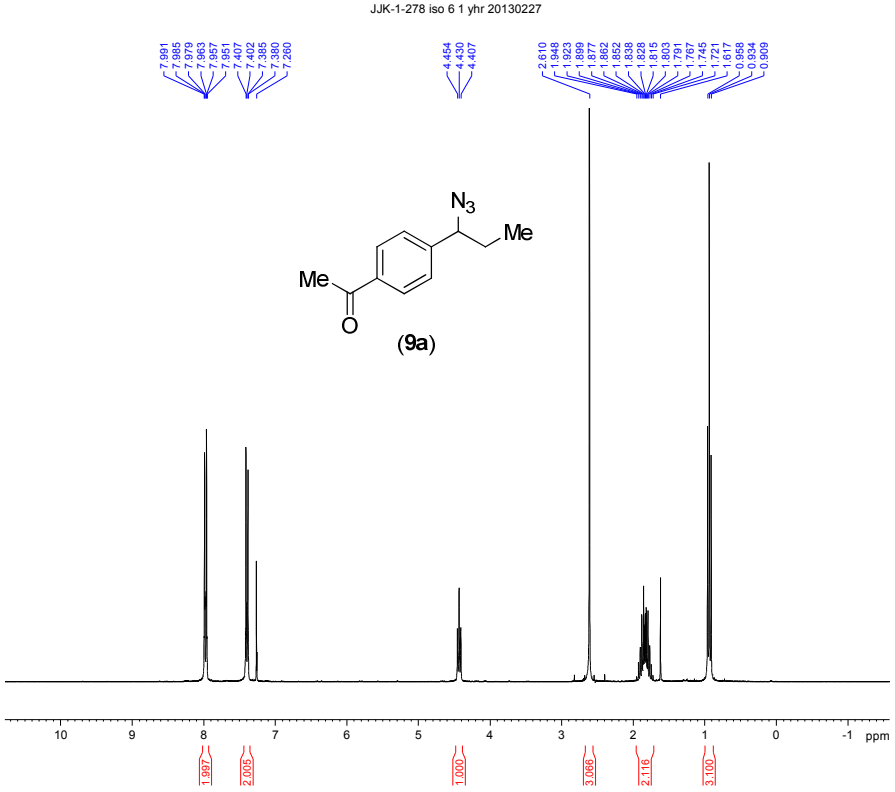
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             95.00 usec
PL2               -2.00 dB
PL12              17.82 dB
PL13              19.00 dB
PL2W         8.75835800 W
PL12W        0.09128989 W
PL13W        0.06957011 W
SFO2        300.1312005 MHz
SI               32768
SF           75.4677448 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

((1*R*,2*S*)-1-azido-2-(methoxymethoxy)propyl)benzene:



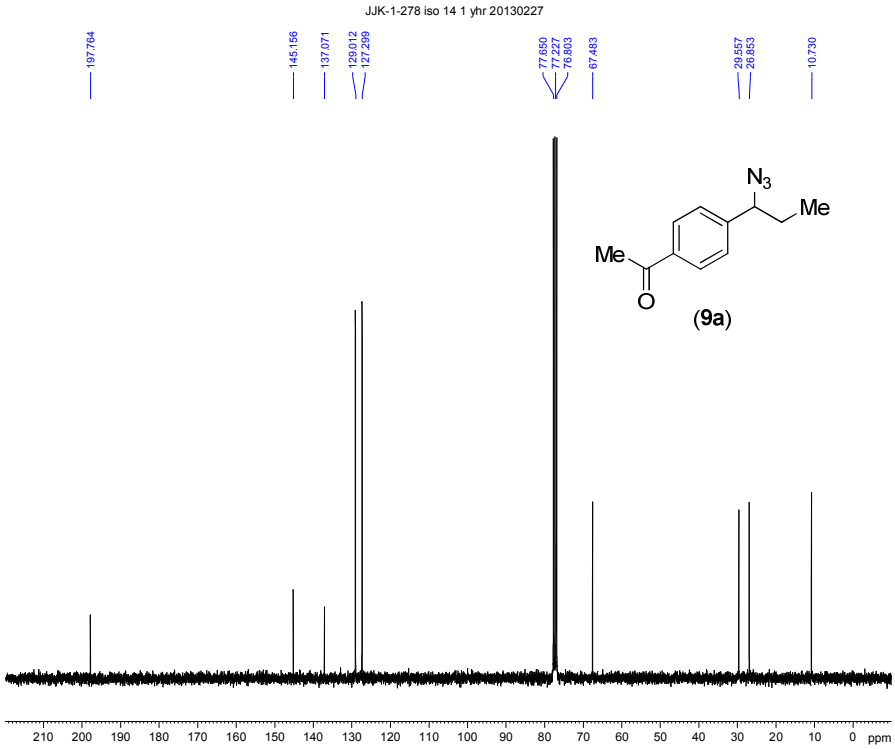


1-(4-(1-azidopropyl)phenyl)ethanone (9a):




```
NAME        JJK-1-278 iso
EXPNO                   6
PROCNO                  1
Date_            20130227
Time                9.20
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   203
DW                80.800 usec
DE                 9.00 usec
TE                296.9 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.10 usec
PL1                -2.00 dB
PL1W          8.75835800 W
SFO1         300.1318534 MHz
SI                 32768
SF           300.1300064 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

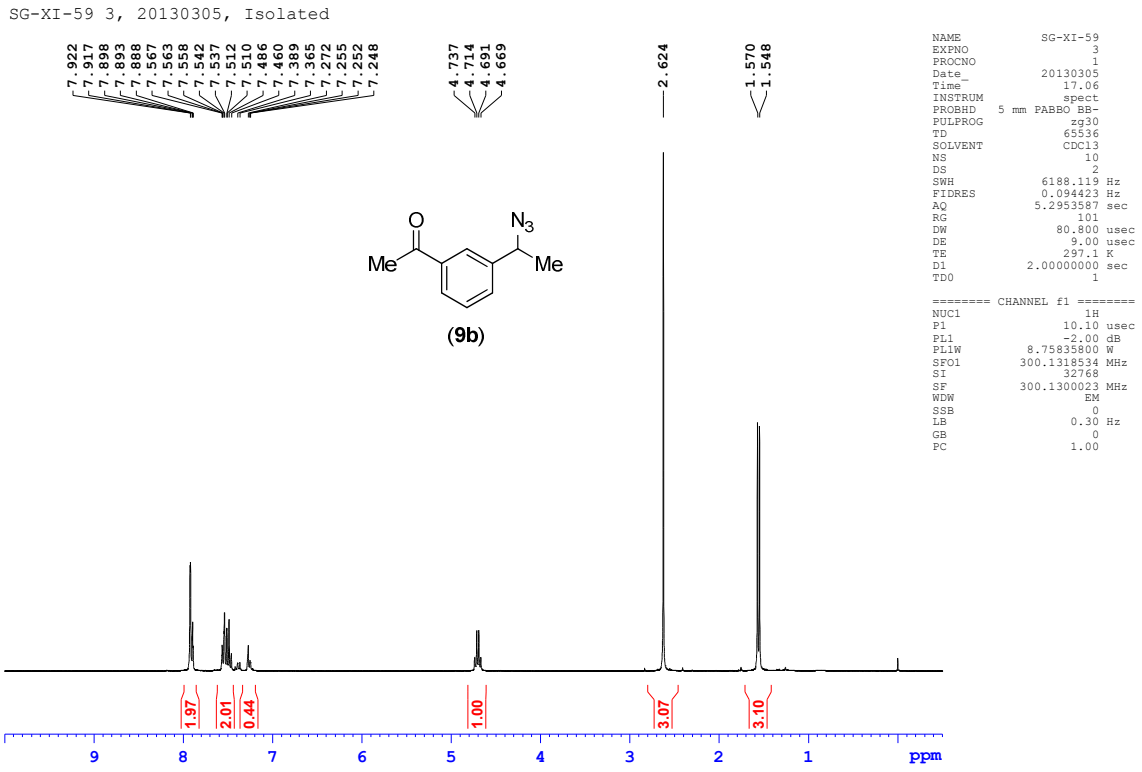


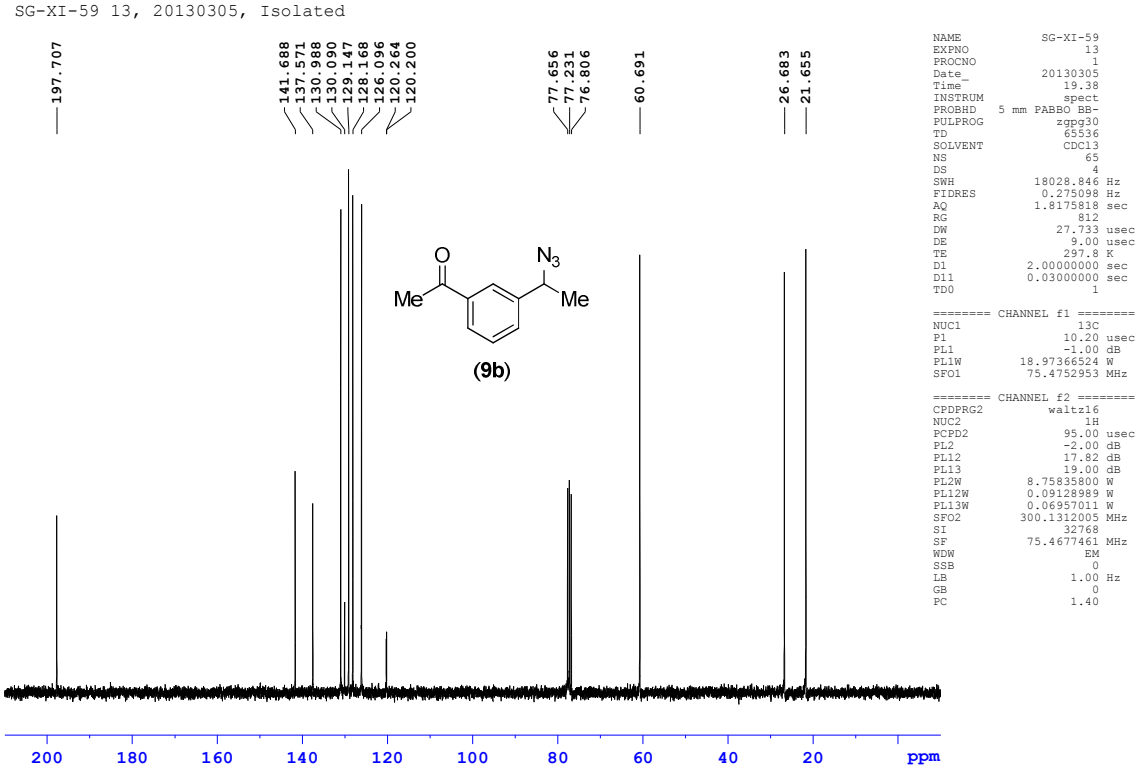

```
NAME        JJK-1-278 iso
EXPNO                  14
PROCNO                  1
Date_            20130227
Time                9.29
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   477
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175818 sec
RG                   812
DW                27.733 usec
DE                 9.00 usec
TE                297.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.20 usec
PL1                -1.00 dB
PL1W          18.97366524 W
SFO1          75.4752953 MHz

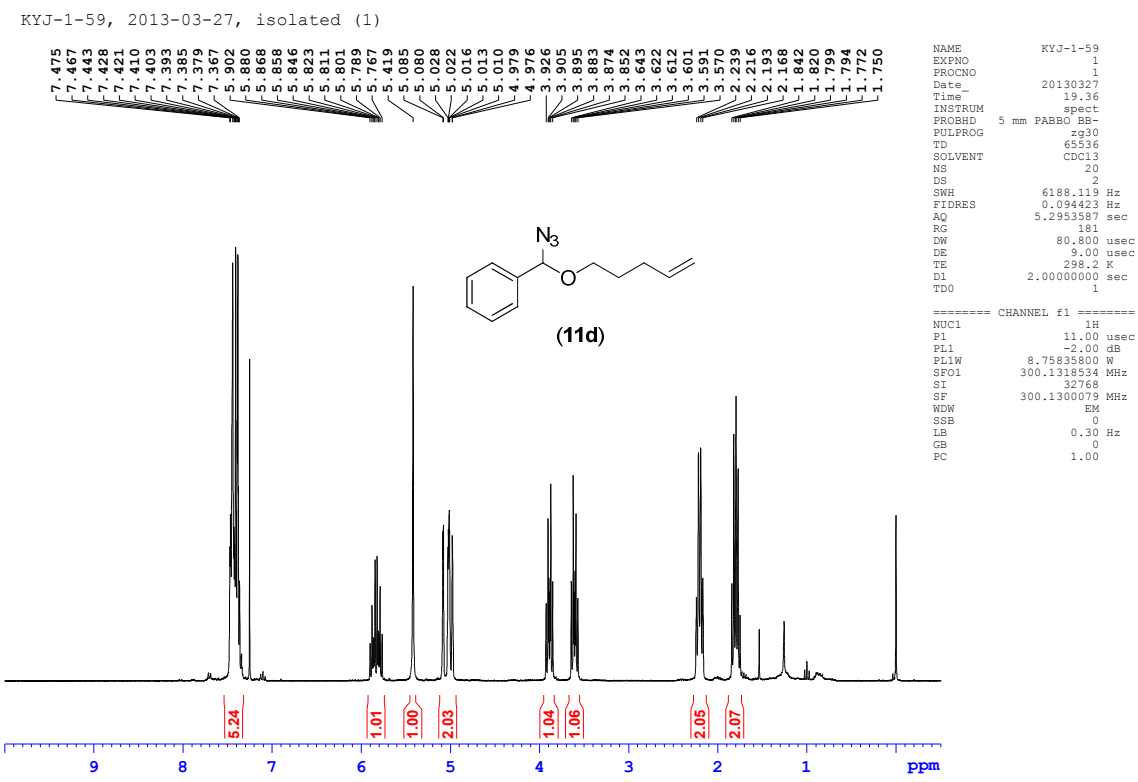
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              95.00 usec
PL2                -2.00 dB
PL12               17.82 dB
PL13               19.00 dB
PL2W          8.75835800 W
```

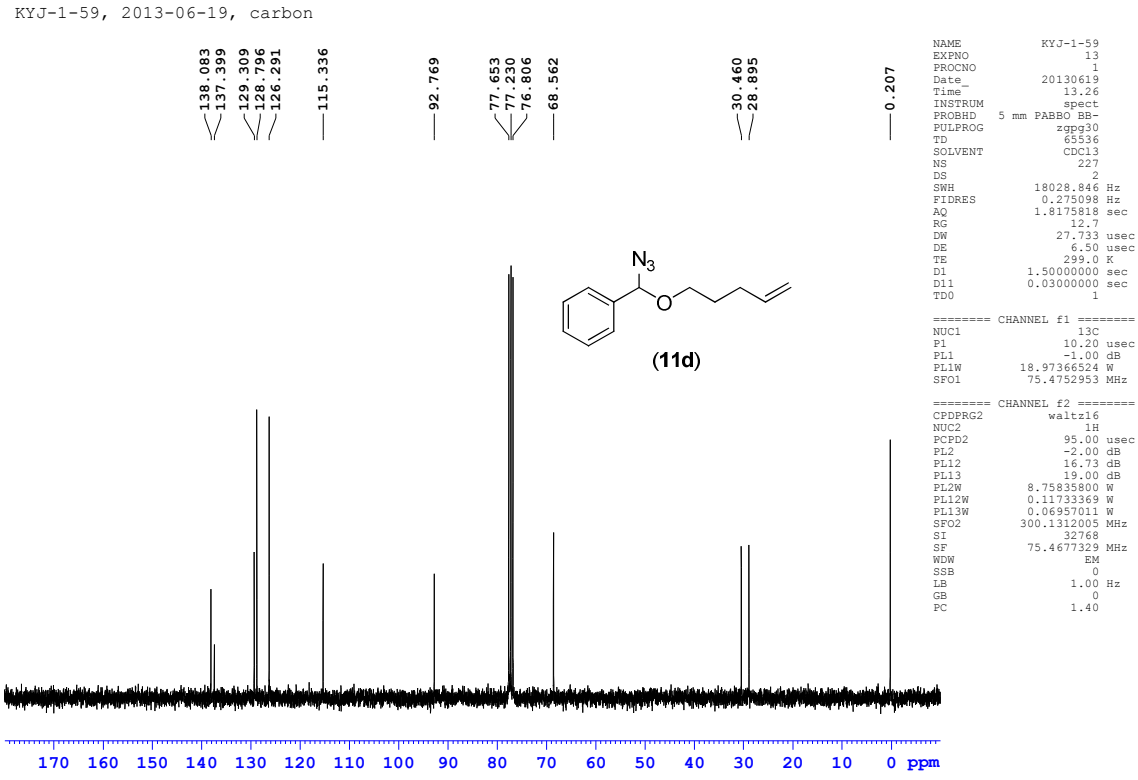
1-(3-(1-azidoethyl)phenyl)ethanone (9b):



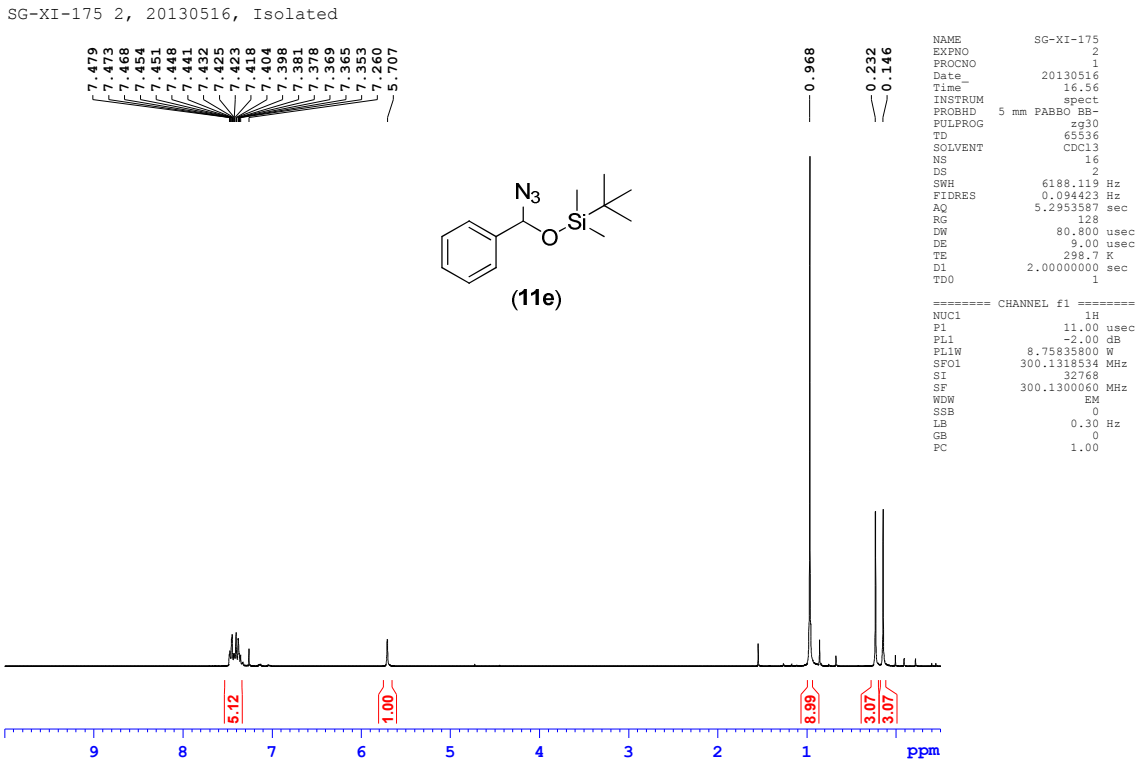


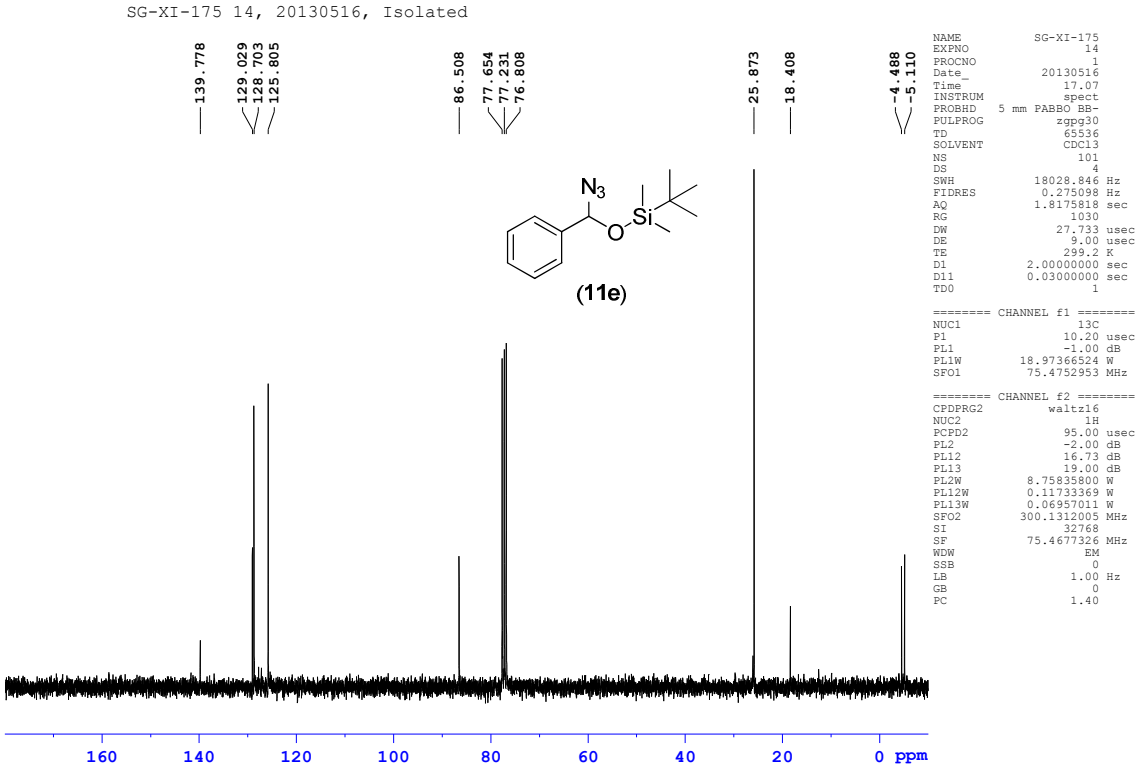
(Azido(pent-4-enyloxy)methyl)benzene (11d):



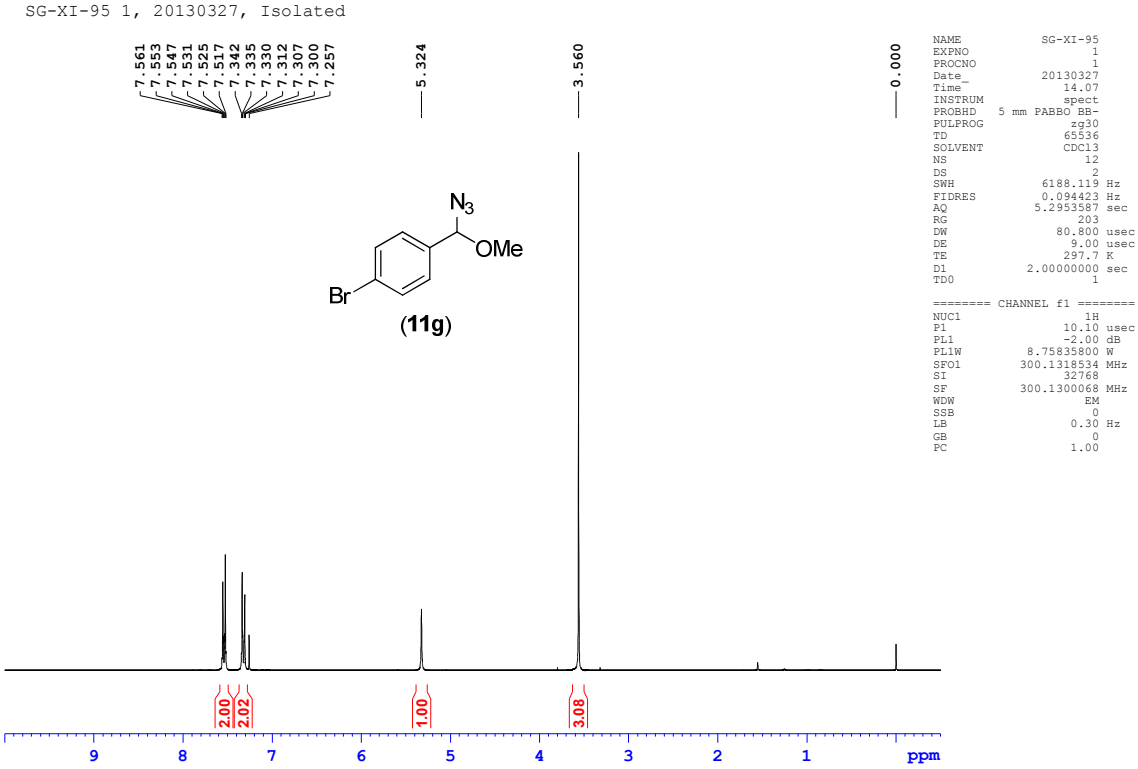


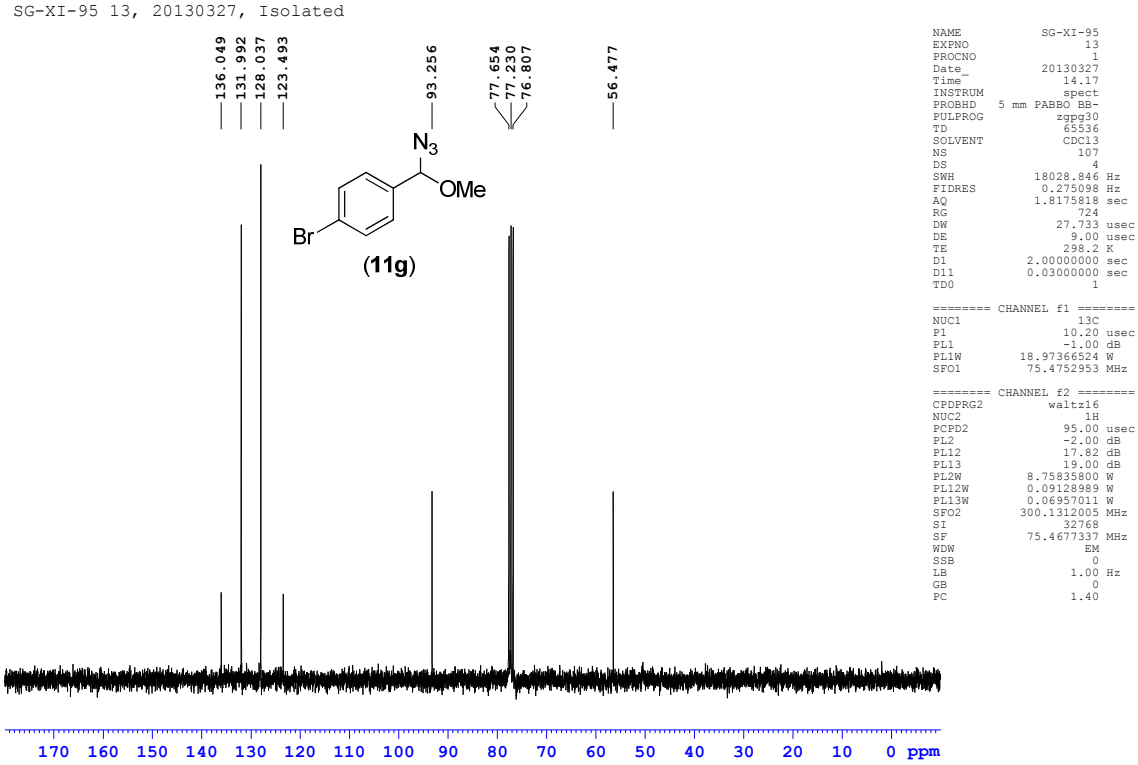
(Azido(phenyl)methoxy)(*tert*-butyl)dimethylsilane (11e):





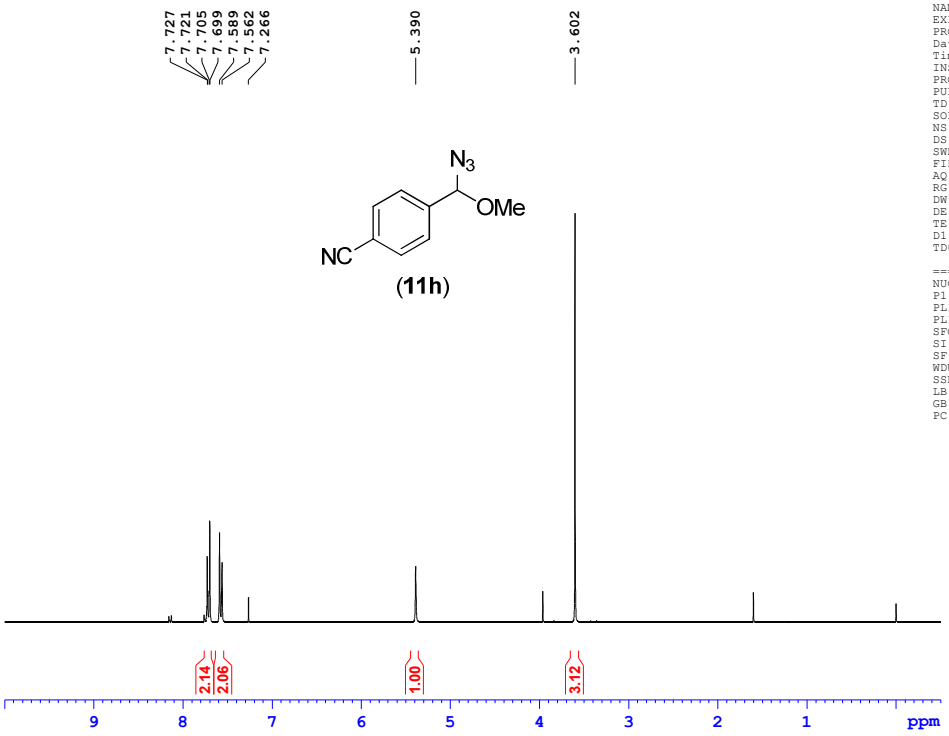
1-(Azido(methoxy)methyl)-4-bromobenzene (11g):





1-(Azido(methoxy)methyl)-4-benzonitrile (11h):

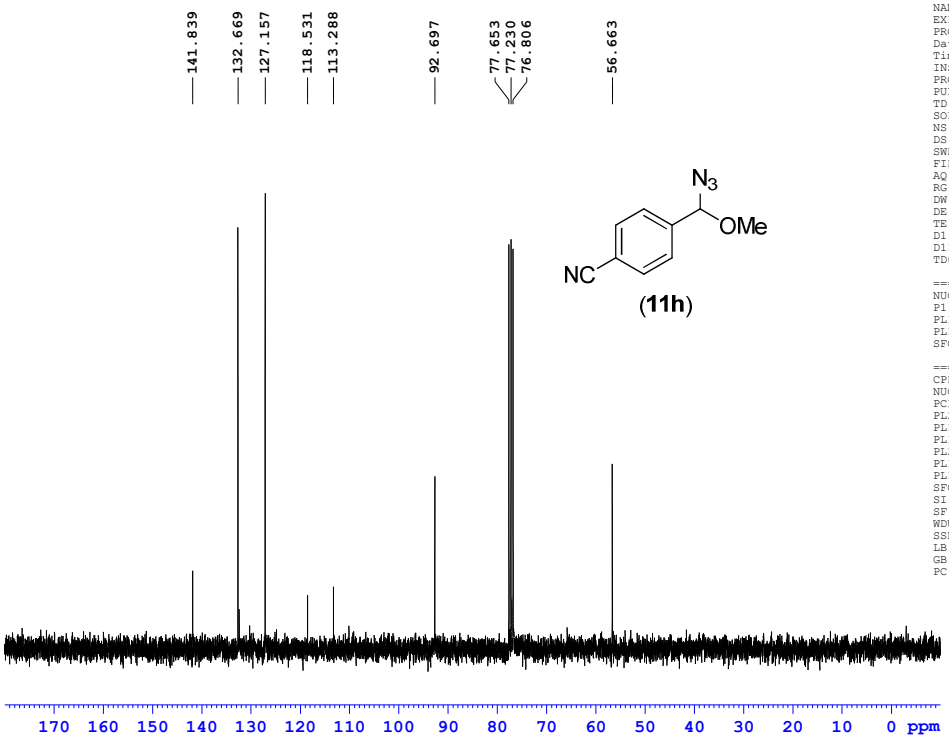
SG-XI-185, 10, 20130527, Isolated (2 nd column)




```
NAME           SG-XI-185
EXPNO                 10
PROCNO                 1
Date_           20130527
Time_              17.29
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   181
DW                80.800 usec
DE                 9.00 usec
TE                298.2 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.00 usec
PL1                -2.00 dB
PL1W          8.75835800 W
SFO1        300.1318534 MHz
SI                 32768
SF          300.1300040 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

SG-XI-185, 16, 20130527, Isolated (2 nd column)



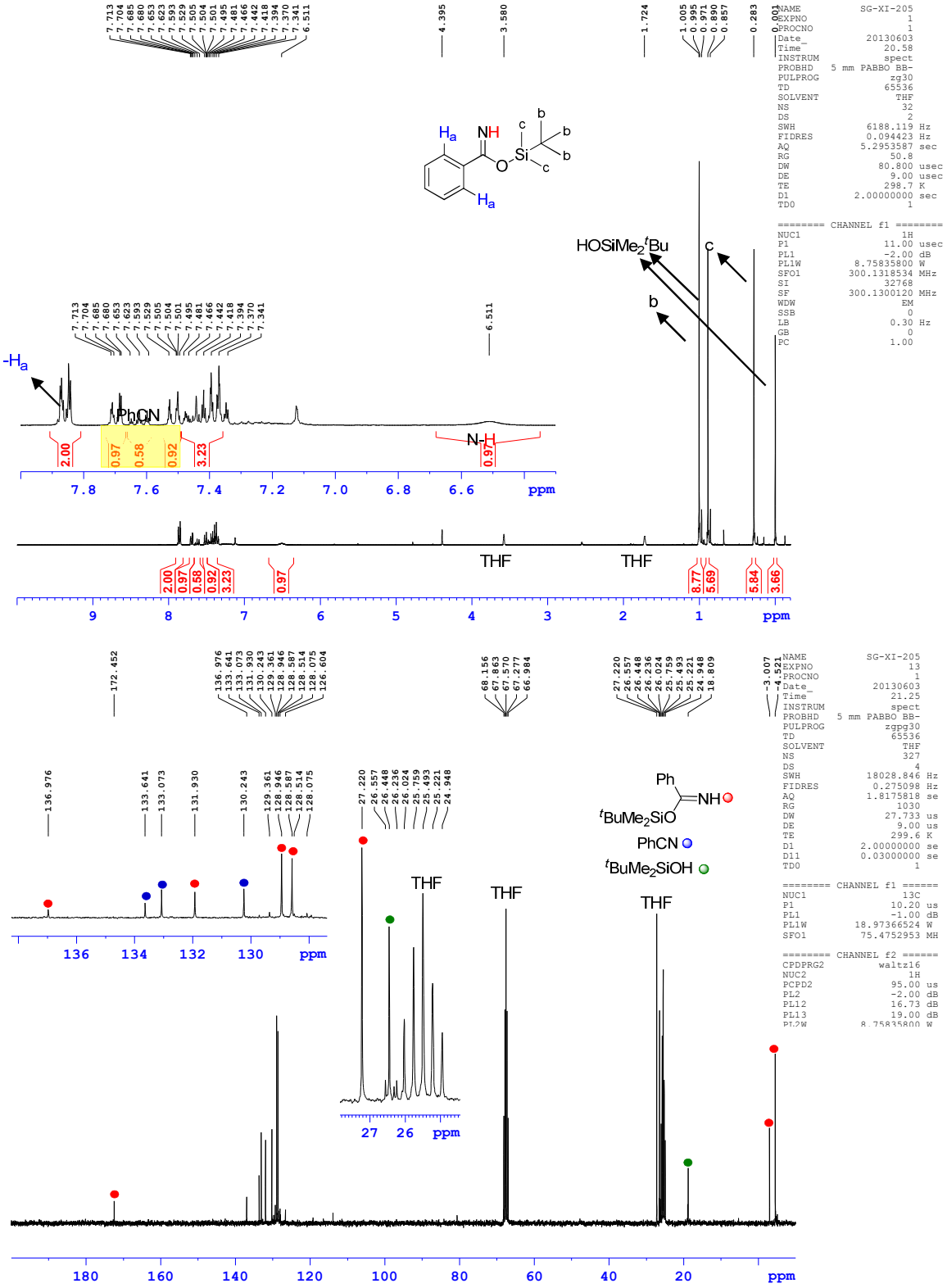

```
NAME           SG-XI-185
EXPNO                 16
PROCNO                 1
Date_           20130527
Time_              17.35
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    45
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175818 sec
RG                   724
DW                27.733 usec
DE                 9.00 usec
TE                298.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.20 usec
PL1                -1.00 dB
PL1W         18.97366524 W
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              95.00 usec
PL2                -2.00 dB
PL12               16.73 dB
PL13               19.00 dB
PL2W          8.75835800 W
PL12W         0.11733369 W
PL13W         0.06957011 W
SFO2        300.1312005 MHz
SI                 32768
SF          75.4677345 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

3. ^{1}H and ^{13}C NMR data of crude imidates:

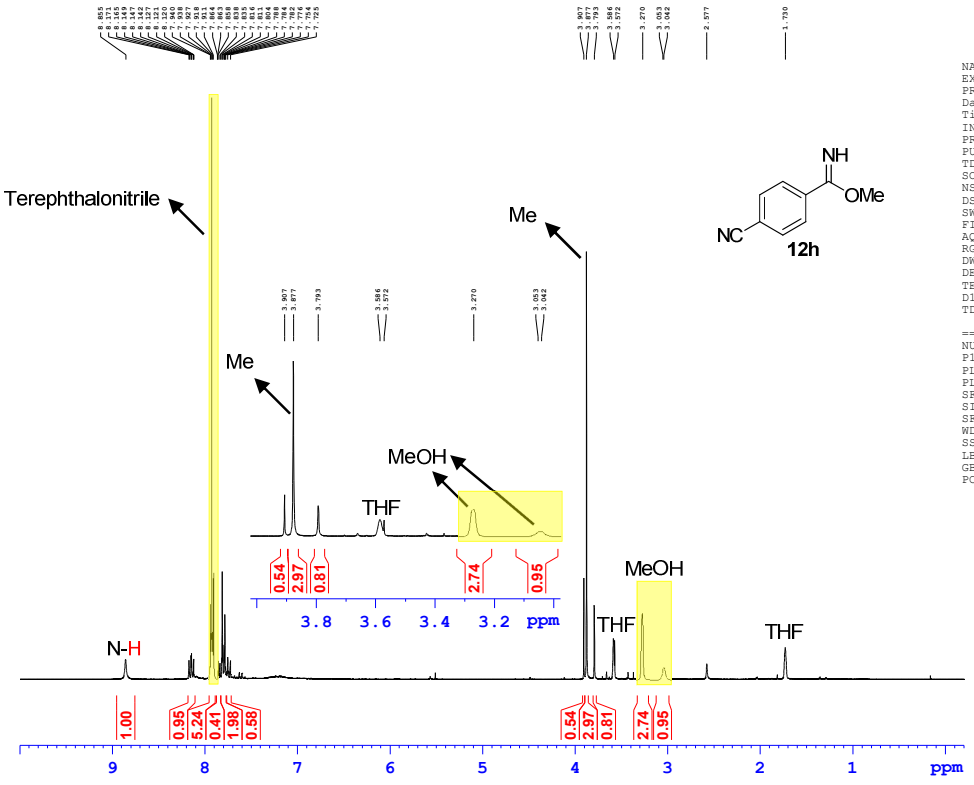
a) *tert*-Butyldimethylsilyl benzimidate in THF-d_8 (12e):



NAME	SG-XI-205
EXPNO	1
PROCNO	1
Date_	20130603
Time	20.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	THF
NS	32
DS	2
SWH	6188.119 Hz
FIDRES	0.094423 Hz
AQ	5.2953587 sec
RG	50.8
DW	80.800 usec
DE	9.00 usec
TE	298.7 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	11.00 usec
PL1	-2.00 dB
PL1W	8.75835800 W
SFO1	300.1318534 MHz
SI	32768
SF	300.1300120 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

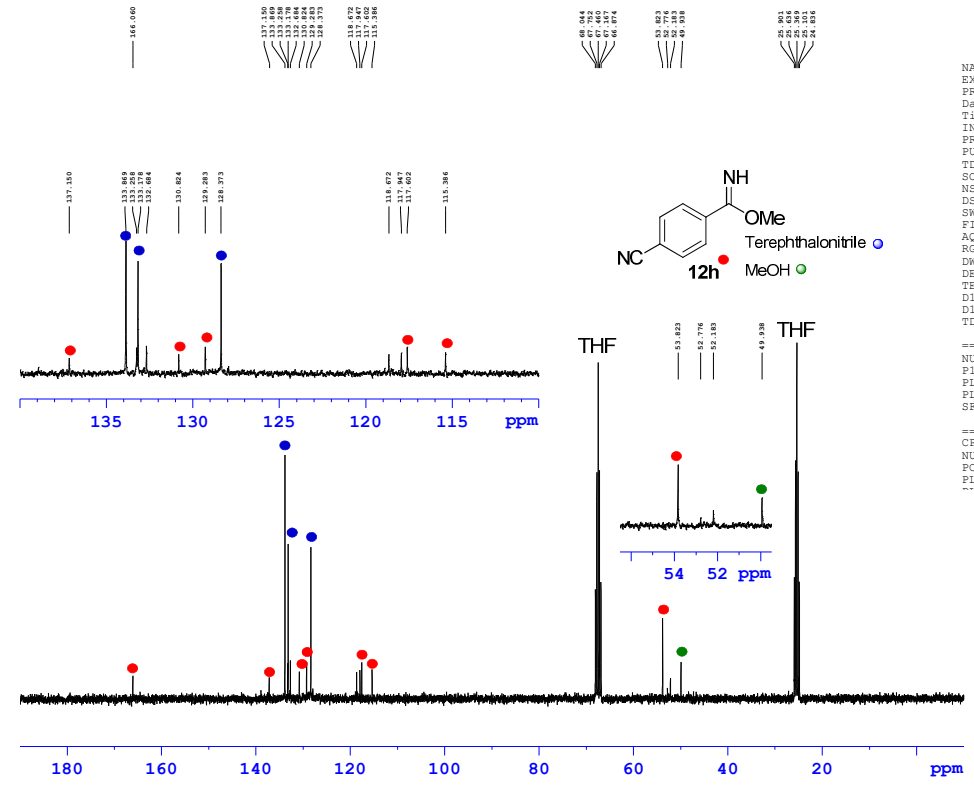
NAME	SG-XI-205
EXPNO	13
PROCNO	1
Date_	20130603
Time	21.25
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	THF
NS	327
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 se
RG	1030
DW	27.733 us
DE	9.00 us
TE	299.6 K
D1	2.00000000 se
D11	0.03000000 se
TD0	1
======== CHANNEL f1 ======	
NUC1	13C
P1	10.20 us
PL1	-1.00 dB
PL1W	18.97366524 W
SFO1	75.4752953 MH
======== CHANNEL f2 ======	
CPDPRG2	waltz16
NUC2	1H
PCPD2	95.00 us
PL2	-2.00 dB
PL12	16.73 dB
PL13	19.00 dB
PL2W	8.75835800 W

b) Methyl 4-cyanobenzimidate in THF-d_8 (12h):




```
NAME            SG-XI-199
EXPNO                   2
PROCNO                  1
Date_            20130601
Time                23.12
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT               THF
NS                     16
DS                      2
SWH             6188.119 Hz
FIDRES             0.094423 Hz
AQ              5.2953587 se
RG                    114
DW                 80.800 us
DE                  9.00 us
TE                298.9 K
D1             2.00000000 se
TD0                     1

======== CHANNEL f1 ======
NUC1                   1H
P1                 11.00 us
PL1                -2.00 dB
PL1W         8.75835800 W
SFO1         300.1318534 MH
SI                  32768
SF           300.1294507 MH
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```



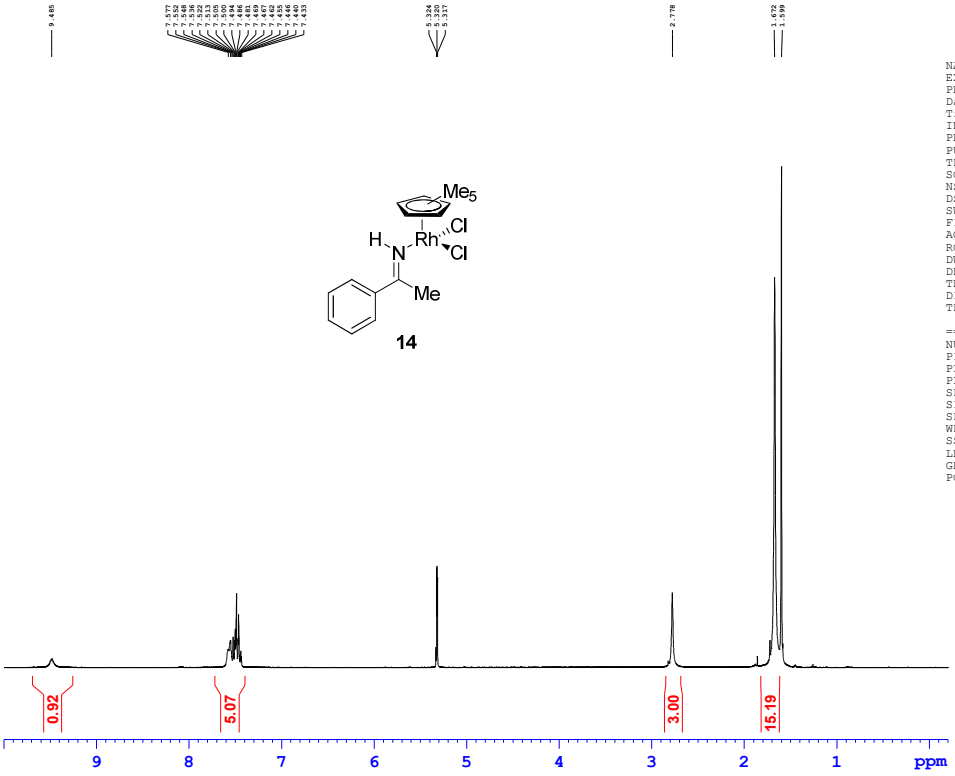

```
NAME            SG-XI-199
EXPNO                  13
PROCNO                  1
Date_            20130601
Time                23.22
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT               THF
NS                    136
DS                      4
SWH            18028.846 Hz
FIDRES             0.275098 Hz
AQ              1.8175818 se
RG                   1030
DW                 27.733 us
DE                  9.00 us
TE                299.5 K
D1             2.00000000 se
D11            0.03000000 se
TD0                     1

======== CHANNEL f1 ======
NUC1                  13C
P1                 10.20 us
PL1                -1.00 dB
PL1W         18.97366524 W
SFO1          75.4752953 MH

======== CHANNEL f2 ======
CPDPRG2           waltz16
NUC2                   1H
PCPD2              95.00 us
PL2                -2.00 dB
```

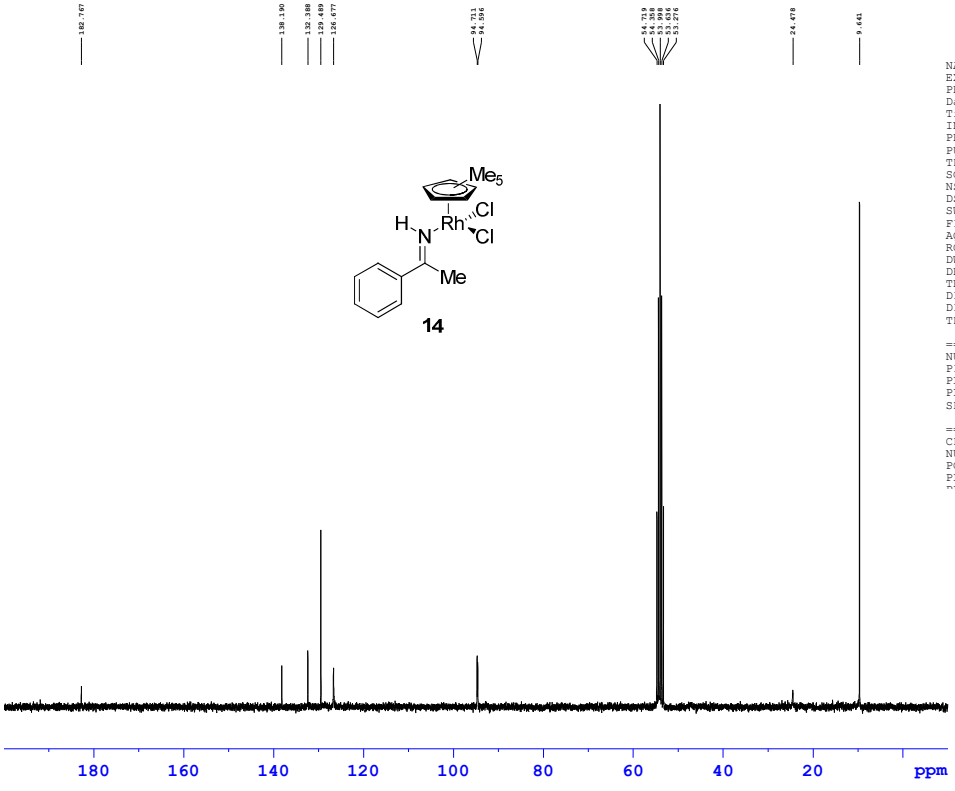
4. ^{1}H and ^{13}C NMR data of 14 and 15:

a) Rh-imine complex 14 (in CD_2Cl_2):




```
NAME           SG-XII-61
EXPNO                  2
PROCNO                 1
Date_           20130826
Time               20.48
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT          CD2Cl2
NS                    32
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 se
RG                   287
DW                80.800 us
DE                 9.00 us
TE                299.0 K
D1             2.00000000 se
TD0                    1

======== CHANNEL f1 ======
NUC1                  1H
P1                 11.00 us
PL1                -2.00 dB
PL1W         8.75835800 W
SFO1        300.1318534 MH
SI                 32768
SF          300.1300102 MH
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

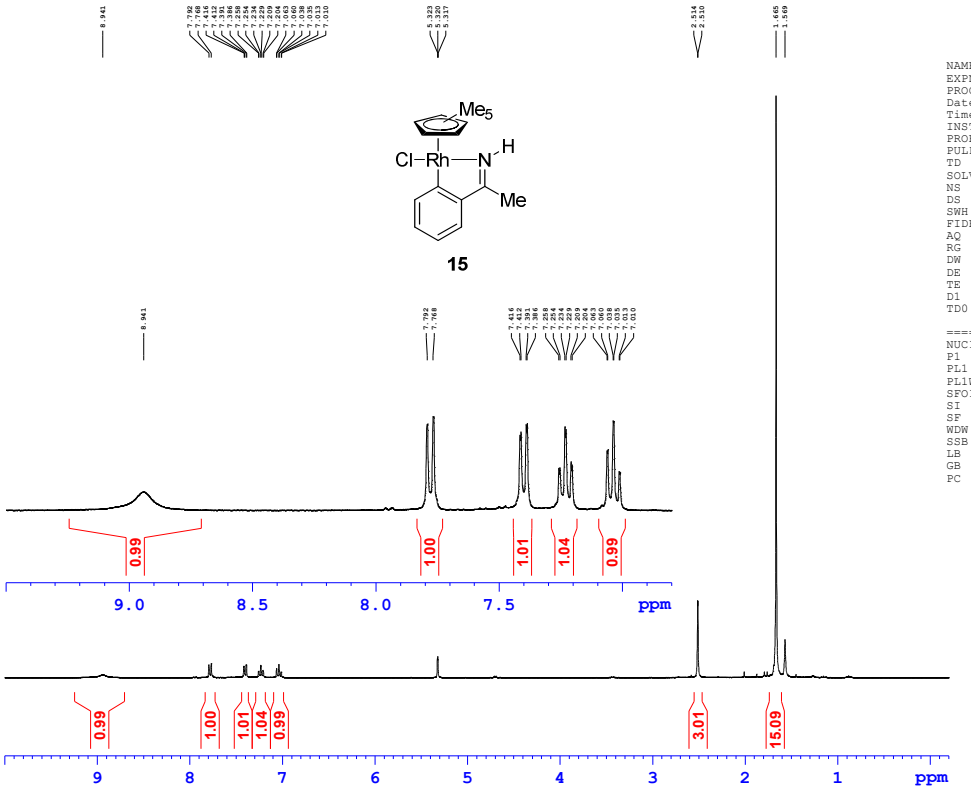



```
NAME           SG-XI-249
EXPNO                 13
PROCNO                 1
Date_           20130701
Time               4.06
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT          CD2Cl2
NS                  1024
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175818 se
RG                  1030
DW                27.733 us
DE                 9.00 us
TE                299.3 K
D1             2.00000000 se
D11            0.03000000 se
TD0                    1

======== CHANNEL f1 ======
NUC1                 13C
P1                 10.20 us
PL1                -1.00 dB
PL1W        18.97366524 W
SFO1         75.4752953 MH

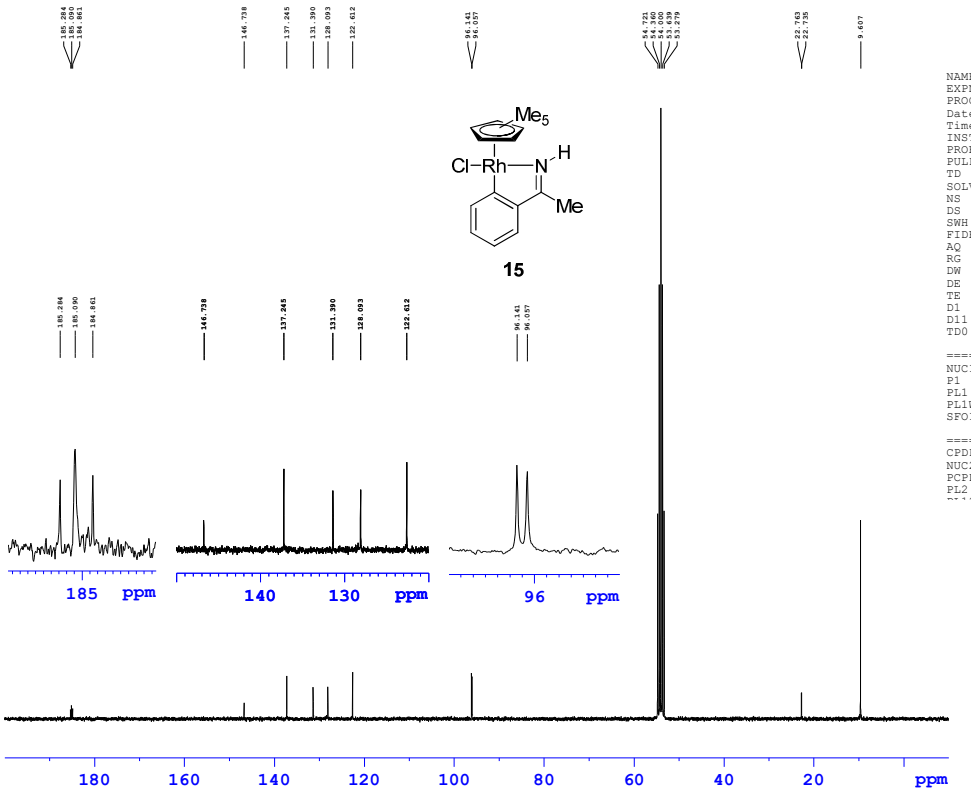
======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                  1H
PCPD2              95.00 us
PL2                -2.00 dB
```

b) Rhodacycle complex 15 (in CD_2Cl_2):




```
NAME           SG-XII-49
EXPNO                  1
PROCNO                 1
Date_           20130901
Time_              11.56
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    32
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 se
RG                   256
DW                80.800 us
DE                 9.00 us
TE                298.9 K
D1              2.00000000 se
TD0                    1

======== CHANNEL f1 ======
NUC1                  1H
P1                11.00 us
PL1               -2.00 dB
PL1W         8.75835800 W
SFO1        300.1318534 MH
SI                 32768
SF          300.1300103 MH
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```




```
NAME           SG-XII-49
EXPNO                 13
PROCNO                 1
Date_           20130901
Time_              16.11
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT           CD2Cl2
NS                  3800
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175818 se
RG                   912
DW                27.733 us
DE                 9.00 us
TE                299.4 K
D1              2.00000000 se
D11             0.03000000 se
TD0                    1

======== CHANNEL f1 ======
NUC1                 13C
P1                10.20 us
PL1               -1.00 dB
PL1W        18.97366524 W
SFO1        75.4752953 MH

======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                  1H
PCPD2             95.00 us
PL2               -2.00 dB
```

5. Crystal structures of Rh-imine complexes:

a) Crystal structures of Rh-imine complexes 14:

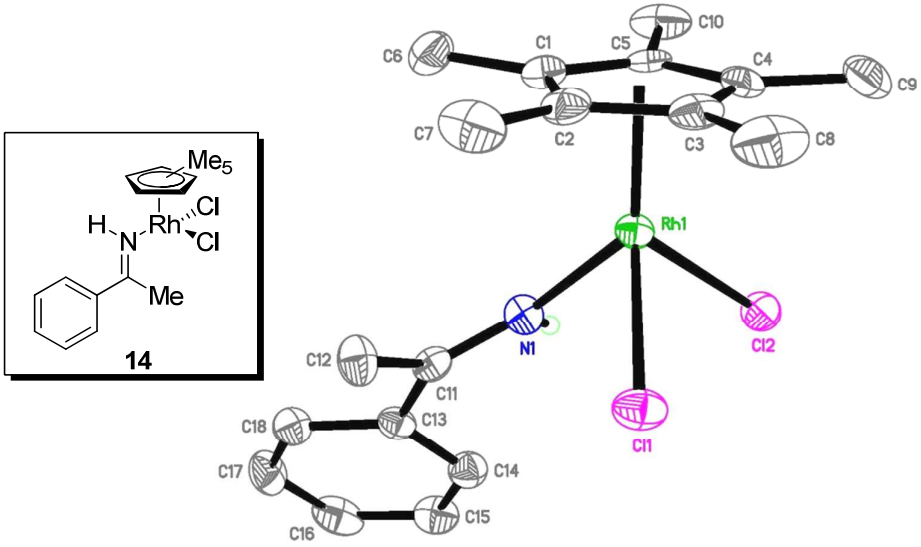


Figure 1. ORTEP drawing of Rh-imine complex **14**·H_2O with 40% atomic displacement parameters. (The lattice water is omitted for clarity.)

X-ray Structure Determination of Rh-imine complex 14.

An orange crystal of Rh-imine complex **14**.H_2O, shaped as a block of approximate dimensions 0.19 × 0.14 × 0.10 mm, was used for crystal- and intensity data collection. The structure was solved by direct methods. All non-hydrogen atoms were refined anisotropically. The N-H and O-H hydrogen atoms were located and refined freely, and the remaining hydrogen atoms were generated in idealized positions and a riding model. Details on crystal data, intensity collection, and refinement details are given in Table 1. Atomic coordinates and equivalent isotropic displacement parameters are given in Table 2. Bond lengths and bond angels are presented in Table 3. Anisotropic displacement parameters for Rh-imine complex **14**.H_2O are presented in Table 4.

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

Identification code	rhncr	
Empirical formula	$C_{18}H_{26}Cl_2NORh$	
Formula weight	446.21	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 7.4410(4) Å	α = 90°.
	b = 15.3649(8) Å	β = 95.9690(10)°.
	c = 16.7791(9) Å	γ = 90°.
Volume	1907.96(18) Å^3	
Z	4	
Density (calculated)	1.553 Mg/m^3	
Absorption coefficient	1.179 mm^{-1}	
F(000)	912	
Crystal size	0.19 × 0.14 × 0.10 mm^3	
θ range for data collection	1.80–28.33°.	
Index ranges	$-9 \le h \le 7$, $-20 \le k \le 15$, $-22 \le l \le 22$	
Reflections collected	13793	
Independent reflections	4677 [R(int) = 0.0628]	
Completeness to θ = 28.33°	98.4%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8912 and 0.8071	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	4677/0/225	
Goodness-of-fit on F^2	0.963	
Final R indices [$I > 2\sigma(I)$]	$R1$ = 0.0397, $wR2$ = 0.0692	
R indices (all data)	$R1$ = 0.0889, $wR2$ = 0.0880	
Largest diff. peak and hole	1.546 and −0.674 e·Å^{-3}	

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

	x	y	z	U(eq)
Rh(1)	3368(1)	8061(1)	3432(1)	23(1)
Cl(1)	6286(1)	8779(1)	3562(1)	36(1)
Cl(2)	4421(1)	6960(1)	2547(1)	31(1)
N(1)	4460(5)	7171(2)	4294(2)	28(1)
C(1)	876(6)	8320(2)	3930(2)	29(1)
C(2)	1776(6)	9117(2)	3810(2)	33(1)
C(3)	1934(5)	9200(2)	2963(3)	33(1)
C(4)	1156(6)	8450(3)	2576(2)	34(1)
C(5)	521(5)	7897(2)	3177(2)	27(1)
C(6)	371(6)	7982(3)	4717(2)	43(1)
C(7)	2339(7)	9803(3)	4417(3)	50(1)
C(8)	2701(7)	9972(3)	2571(3)	59(2)
C(9)	1026(7)	8258(3)	1693(2)	51(1)
C(10)	-527(6)	7072(2)	3018(3)	46(1)
C(11)	5273(5)	7192(2)	5005(2)	27(1)
C(12)	5350(6)	8020(2)	5470(2)	36(1)
C(13)	6129(5)	6391(2)	5377(2)	27(1)
C(14)	6906(6)	5780(2)	4909(2)	33(1)
C(15)	7653(6)	5025(3)	5248(3)	38(1)
C(16)	7635(6)	4883(3)	6063(3)	44(1)
C(17)	6880(6)	5481(3)	6521(2)	39(1)
C(18)	6142(6)	6243(2)	6194(2)	31(1)
O(1)	1605(6)	5666(3)	1539(2)	62(1)

Table 3. Bond lengths [Å] and angles [°] for RHNCR.

Rh1–N1	2.092(3)
Rh(1)-C(5)	2.132(4)
Rh(1)-C(2)	2.143(4)
Rh(1)-C(1)	2.149(4)
Rh(1)-C(4)	2.153(4)
Rh(1)-C(3)	2.155(4)
Rh1–Cl1	2.4251(11)
Rh1–Cl2	2.4347(10)
N1–C11	1.280(5)
N1–H1N	0.74(3)
C(1)-C(5)	1.420(5)
C(1)-C(2)	1.421(5)
C(1)-C(6)	1.503(5)
C(2)-C(3)	1.444(5)
C(2)-C(7)	1.495(5)
C(3)-C(4)	1.417(5)
C(3)-C(8)	1.497(5)
C(4)-C(5)	1.436(5)
C(4)-C(9)	1.504(6)
C(5)-C(10)	1.498(5)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.490(5)

C(11)-C(13)	1.493(5)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.388(5)
C(13)-C(18)	1.390(5)
C(14)-C(15)	1.384(5)
C(14)-H(14)	0.9500
C(15)-C(16)	1.385(6)
C(15)-H(15)	0.9500
C(16)-C(17)	1.357(6)
C(16)-H(16)	0.9500
C(17)-C(18)	1.382(5)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
O(1)-H(1O)	0.85(5)
O(1)-H(2O)	0.81(5)
N(1)-Rh(1)-C(5)	111.54(14)
N(1)-Rh(1)-C(2)	118.48(15)
C(5)-Rh(1)-C(2)	65.23(15)
N(1)-Rh(1)-C(1)	98.09(14)
C(5)-Rh(1)-C(1)	38.75(14)
C(2)-Rh(1)-C(1)	38.66(14)
N(1)-Rh(1)-C(4)	149.00(15)
C(5)-Rh(1)-C(4)	39.16(15)
C(2)-Rh(1)-C(4)	65.16(15)
C(1)-Rh(1)-C(4)	64.99(16)
N(1)-Rh(1)-C(3)	157.67(15)
C(5)-Rh(1)-C(3)	65.13(15)
C(2)-Rh(1)-C(3)	39.26(15)
C(1)-Rh(1)-C(3)	65.01(15)
C(4)-Rh(1)-C(3)	38.40(15)
N1–Rh1–Cl1	87.45(10)
C(5)-Rh(1)-Cl(1)	159.02(10)
C(2)-Rh(1)-Cl(1)	98.42(12)
C(1)-Rh(1)-Cl(1)	133.00(11)
C(4)-Rh(1)-Cl(1)	123.30(12)
C(3)-Rh(1)-Cl(1)	93.91(11)

N1–Rh1–Cl2	80.85(10)
C(5)-Rh(1)-Cl(2)	99.85(10)
C(2)-Rh(1)-Cl(2)	158.38(11)
C(1)-Rh(1)-Cl(2)	135.32(11)
C(4)-Rh(1)-Cl(2)	93.32(11)
C(3)-Rh(1)-Cl(2)	121.34(12)
Cl1–Rh1–Cl2	91.68(4)
C11–N1–Rh1	137.7(3)
C(11)-N(1)-H(1N)	110(3)
Rh(1)-N(1)-H(1N)	111(3)
C(5)-C(1)-C(2)	108.4(3)
C(5)-C(1)-C(6)	125.7(4)
C(2)-C(1)-C(6)	126.0(4)
C(5)-C(1)-Rh(1)	70.0(2)
C(2)-C(1)-Rh(1)	70.4(2)
C(6)-C(1)-Rh(1)	125.6(3)
C(1)-C(2)-C(3)	107.7(3)
C(1)-C(2)-C(7)	127.9(4)
C(3)-C(2)-C(7)	124.2(4)
C(1)-C(2)-Rh(1)	70.9(2)
C(3)-C(2)-Rh(1)	70.8(2)
C(7)-C(2)-Rh(1)	127.7(3)
C(4)-C(3)-C(2)	107.9(3)
C(4)-C(3)-C(8)	126.8(4)
C(2)-C(3)-C(8)	125.2(4)
C(4)-C(3)-Rh(1)	70.7(2)
C(2)-C(3)-Rh(1)	69.9(2)
C(8)-C(3)-Rh(1)	127.3(3)
C(3)-C(4)-C(5)	108.0(3)
C(3)-C(4)-C(9)	126.3(4)
C(5)-C(4)-C(9)	125.7(4)
C(3)-C(4)-Rh(1)	70.9(2)
C(5)-C(4)-Rh(1)	69.6(2)
C(9)-C(4)-Rh(1)	124.7(3)
C(1)-C(5)-C(4)	108.0(3)
C(1)-C(5)-C(10)	126.2(4)
C(4)-C(5)-C(10)	125.4(4)
C(1)-C(5)-Rh(1)	71.3(2)

C(4)-C(5)-Rh(1)	71.2(2)
C(10)-C(5)-Rh(1)	128.7(3)
C(1)-C(6)-H(6A)	109.5
C(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(3)-C(8)-H(8A)	109.5
C(3)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(3)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(4)-C(9)-H(9A)	109.5
C(4)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(4)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(1)-C(11)-C(12)	119.9(4)
N(1)-C(11)-C(13)	120.6(3)
C(12)-C(11)-C(13)	119.6(3)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5

C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	119.2(4)
C(14)-C(13)-C(11)	120.4(3)
C(18)-C(13)-C(11)	120.4(3)
C(15)-C(14)-C(13)	120.5(4)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
C(14)-C(15)-C(16)	119.6(4)
C(14)-C(15)-H(15)	120.2
C(16)-C(15)-H(15)	120.2
C(17)-C(16)-C(15)	120.0(4)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	121.3(4)
C(16)-C(17)-H(17)	119.4
C(18)-C(17)-H(17)	119.4
C(17)-C(18)-C(13)	119.5(4)
C(17)-C(18)-H(18)	120.3
C(13)-C(18)-H(18)	120.3
H(1O)-O(1)-H(2O)	106(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for RHNCR. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	22(1)	19(1)	27(1)	1(1)	1(1)	1(1)
Cl(1)	27(1)	31(1)	50(1)	6(1)	1(1)	-5(1)
Cl(2)	33(1)	29(1)	32(1)	-5(1)	3(1)	5(1)
N(1)	33(2)	22(2)	30(2)	0(2)	2(2)	1(2)
C(1)	22(2)	28(2)	39(2)	-1(2)	4(2)	4(2)
C(2)	26(2)	29(2)	43(3)	-6(2)	5(2)	9(2)
C(3)	24(2)	21(2)	53(3)	12(2)	7(2)	10(2)
C(4)	23(2)	42(3)	35(2)	2(2)	-4(2)	13(2)
C(5)	12(2)	30(2)	40(2)	-1(2)	4(2)	7(2)
C(6)	38(3)	56(3)	39(3)	7(2)	14(2)	6(2)
C(7)	46(3)	32(3)	70(3)	-23(2)	-8(3)	9(2)
C(8)	43(3)	38(3)	97(4)	36(3)	16(3)	11(2)
C(9)	44(3)	70(3)	37(3)	-1(2)	-9(2)	25(2)
C(10)	26(3)	34(3)	77(4)	-15(2)	-2(2)	1(2)
C(11)	24(2)	26(2)	31(2)	1(2)	9(2)	-2(2)
C(12)	48(3)	29(2)	29(2)	1(2)	1(2)	3(2)
C(13)	22(2)	25(2)	31(2)	2(2)	0(2)	-4(2)
C(14)	30(3)	33(2)	35(2)	2(2)	4(2)	2(2)
C(15)	35(3)	28(2)	51(3)	-6(2)	2(2)	4(2)
C(16)	38(3)	31(3)	61(3)	17(2)	-10(2)	-1(2)
C(17)	47(3)	41(3)	29(2)	12(2)	-1(2)	-4(2)
C(18)	32(3)	28(2)	32(2)	6(2)	3(2)	3(2)
O(1)	64(3)	38(2)	79(3)	-9(2)	-19(2)	5(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for RHNCR.

	x	y	z	U(eq)
H(6A)	-924	8072	4747	65
H(6B)	1061	8294	5157	65
H(6C)	646	7359	4760	65
H(7A)	1524	10304	4336	75
H(7B)	3578	9988	4356	75
H(7C)	2285	9568	4957	75
H(8A)	2905	9823	2020	88
H(8B)	3850	10138	2871	88
H(8C)	1850	10459	2566	88
H(9A)	-120	8484	1433	77
H(9B)	1079	7628	1610	77
H(9C)	2034	8538	1460	77
H(10A)	-470	6725	3510	69
H(10B)	-8	6738	2600	69
H(10C)	-1790	7212	2840	69
H(12A)	4730	8480	5144	53
H(12B)	6615	8185	5612	53
H(12C)	4757	7938	5959	53
H(14)	6927	5882	4351	39
H(15)	8173	4606	4925	46
H(16)	8152	4367	6300	53
H(17)	6858	5374	7078	47
H(18)	5648	6662	6526	37
H(1N)	4550(60)	6730(20)	4120(20)	25(13)
H(1O)	2380(70)	6020(30)	1780(30)	61(18)
H(2O)	2100(70)	5200(30)	1530(30)	70(20)

b) Crystal structures of Rhodacycle complexes 15:

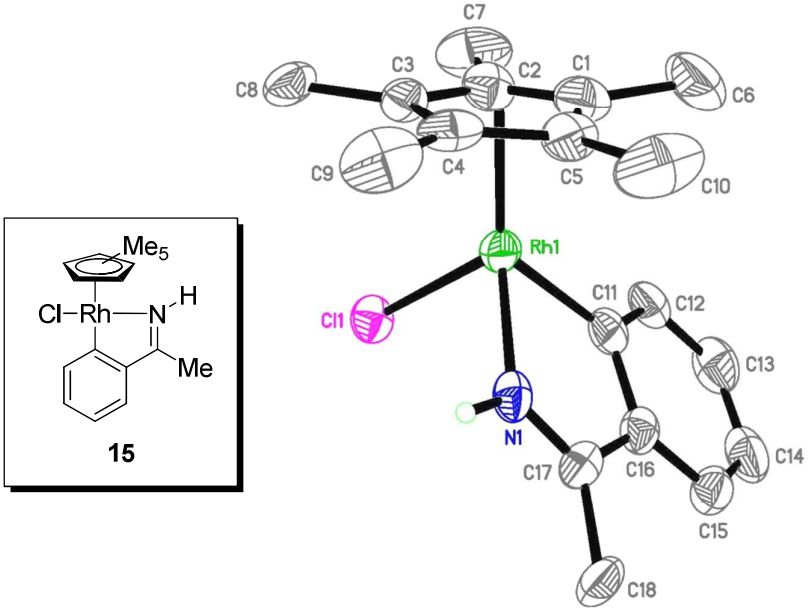


Figure 2. ORTEP drawing of one molecule of complex **15** with 30% atomic displacement parameters.

An orange crystal of Rhodacycle complex **15**, shaped as a needle of approximate dimensions 0.18 × 0.02 × 0.01 mm, was used for crystal- and intensity-data collection. The structure was solved by direct methods. All non-hydrogen atoms were refined anisotropically. The N–H hydrogen atoms were located and refined freely, and the remaining hydrogen atoms were generated in idealized positions and refined in a riding model. Details on crystal data, intensity collection, and refinement details are given in Table 1. Selected bond lengths and bond angles are presented in Table 2.

Table 1. Crystal data and structure refinement for **RhNR2**.

Identification code	rhnr2	
Empirical formula	$C_{18}H_{23}ClNRh$	
Formula weight	391.73	
Temperature	243(2) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 27.150(9) Å	α = 90°
	b = 15.576(5) Å	β = 90°
	c = 8.563(3) Å	γ = 90°
Volume	3621(2) Å^3	
Z	8	
Density (calculated)	1.437 Mg/m^3	
Absorption coefficient	1.084 mm^{-1}	
F(000)	1600	
Crystal size	0.18 × 0.02 × 0.01 mm^3	
θ range for data collection	1.50–26.21°	
Index ranges	$-31 \le h \le 33$, $-14 \le k \le 19$, $-10 \le l \le 10$	
Reflections collected	22087	
Independent reflections	7014 [R(int) = 0.1110]	
Completeness to θ = 26.21°	98.7%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9892 and 0.8287	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	7014/1/397	
Goodness-of-fit on F^2	0.785	
Final R indices [$I > 2\sigma(I)$]	$R1$ = 0.0495, $wR2$ = 0.0639	
R indices (all data)	$R1$ = 0.1282, $wR2$ = 0.0861	
Absolute structure parameter	−0.04(4)	
Largest diff. peak and hole	0.573 and −0.387 e·Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rhnr2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	-1954(1)	-927(1)	-3988(1)	54(1)
Rh(2)	284(1)	3057(1)	931(1)	48(1)
Cl(1)	-1295(1)	-586(2)	-5757(3)	59(1)
Cl(2)	828(1)	3318(2)	3126(3)	69(1)
N(1)	-1471(3)	-1418(5)	-2345(10)	53(2)
N(2)	410(3)	1750(4)	1009(15)	51(2)
C(1)	-2743(3)	-747(8)	-4060(30)	96(3)
C(2)	-2579(4)	-743(7)	-5561(14)	71(3)
C(3)	-2392(3)	-1591(7)	-5865(12)	57(3)
C(4)	-2419(4)	-2069(7)	-4473(14)	73(4)
C(5)	-2617(4)	-1539(11)	-3260(15)	98(5)
C(6)	-3037(4)	-30(8)	-3146(17)	175(8)
C(7)	-2643(4)	-61(6)	-6740(15)	117(5)
C(8)	-2213(3)	-1879(6)	-7418(11)	72(3)
C(9)	-2246(3)	-3003(6)	-4270(20)	104(4)
C(10)	-2721(5)	-1863(10)	-1591(14)	172(7)
C(11)	-1778(3)	121(6)	-2672(12)	59(3)
C(12)	-1907(3)	976(7)	-2908(11)	65(3)
C(13)	-1752(4)	1615(7)	-1863(16)	84(4)
C(14)	-1467(4)	1410(7)	-564(16)	89(4)
C(15)	-1325(3)	576(7)	-290(12)	69(3)
C(16)	-1471(3)	-62(6)	-1344(11)	55(3)
C(17)	-1309(3)	-957(6)	-1273(11)	51(2)
C(18)	-954(3)	-1242(5)	0(10)	68(3)
C(19)	111(4)	3135(5)	-1507(10)	57(3)
C(20)	616(4)	3462(6)	-1372(11)	49(3)
C(21)	589(4)	4174(5)	-406(10)	53(3)
C(22)	85(4)	4306(5)	82(10)	58(3)
C(23)	-210(4)	3683(6)	-701(11)	54(2)
C(24)	-32(3)	2375(5)	-2526(11)	75(3)
C(25)	1049(3)	3118(6)	-2193(12)	75(3)
C(26)	1033(3)	4705(5)	125(11)	82(4)

C(27)	-100(3)	5077(4)	951(15)	84(3)
C(28)	-764(4)	3645(6)	-709(13)	82(3)
C(29)	-240(3)	2651(5)	2394(10)	53(3)
C(30)	-576(4)	3139(6)	3285(12)	66(3)
C(31)	-929(4)	2757(7)	4200(13)	83(3)
C(32)	-964(4)	1859(7)	4340(13)	80(3)
C(33)	-632(4)	1364(6)	3534(12)	63(3)
C(34)	-279(3)	1753(5)	2639(10)	49(2)
C(35)	117(3)	1272(6)	1777(10)	50(2)
C(36)	159(3)	309(5)	1810(10)	66(3)

Table 3. Bond lengths [Å] and angles [°] for rhnr2.

Rh1–C11	2.040(10)
Rh1–N1	2.070(8)
Rh(1)-C(5)	2.130(11)
Rh(1)-C(1)	2.161(9)
Rh(1)-C(2)	2.185(11)
Rh(1)-C(4)	2.221(10)
Rh(1)-C(3)	2.250(10)
Rh1–Cl1	2.405(3)
Rh2–C29	1.999(10)
Rh2–N2	2.066(6)
Rh(2)-C(19)	2.144(8)
Rh(2)-C(22)	2.145(8)
Rh(2)-C(23)	2.169(9)
Rh(2)-C(21)	2.240(8)
Rh(2)-C(20)	2.258(9)
Rh2–Cl2	2.424(3)
N1–C17	1.246(10)
N1–HN1	0.77(5)
N2–C35	1.273(10)
N2–HN2	0.87(5)
C(1)-C(2)	1.36(2)
C(1)-C(5)	1.452(17)
C(1)-C(6)	1.580(16)
C(2)-C(3)	1.440(13)
C(2)-C(7)	1.475(12)
C(3)-C(4)	1.407(13)
C(3)-C(8)	1.485(12)
C(4)-C(5)	1.431(15)
C(4)-C(9)	1.539(12)
C(5)-C(10)	1.542(15)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(6)-H(6C)	0.9700
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(7)-H(7C)	0.9700

C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(8)-H(8C)	0.9700
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(9)-H(9C)	0.9700
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(10)-H(10C)	0.9700
C(11)-C(12)	1.392(11)
C(11)-C(16)	1.439(11)
C(12)-C(13)	1.402(13)
C(12)-H(12)	0.9400
C(13)-C(14)	1.392(14)
C(13)-H(13)	0.9400
C(14)-C(15)	1.376(12)
C(14)-H(14)	0.9400
C(15)-C(16)	1.401(11)
C(15)-H(15)	0.9400
C(16)-C(17)	1.463(11)
C(17)-C(18)	1.521(11)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(18)-H(18C)	0.9700
C(19)-C(23)	1.400(11)
C(19)-C(20)	1.469(13)
C(19)-C(24)	1.521(10)
C(20)-C(21)	1.385(11)
C(20)-C(25)	1.470(12)
C(21)-C(22)	1.445(11)
C(21)-C(26)	1.532(11)
C(22)-C(23)	1.425(11)
C(22)-C(27)	1.500(11)
C(23)-C(28)	1.505(11)
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(24)-H(24C)	0.9700
C(25)-H(25A)	0.9700

C(25)-H(25B)	0.9700
C(25)-H(25C)	0.9700
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(26)-H(26C)	0.9700
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(27)-H(27C)	0.9700
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(28)-H(28C)	0.9700
C(29)-C(30)	1.411(12)
C(29)-C(34)	1.419(10)
C(30)-C(31)	1.374(12)
C(30)-H(30)	0.9400
C(31)-C(32)	1.407(11)
C(31)-H(31)	0.9400
C(32)-C(33)	1.373(12)
C(32)-H(32)	0.9400
C(33)-C(34)	1.368(11)
C(33)-H(33)	0.9400
C(34)-C(35)	1.503(11)
C(35)-C(36)	1.505(10)
C(36)-H(36A)	0.9700
C(36)-H(36B)	0.9700
C(36)-H(36C)	0.9700

C11–Rh1–N1	76.8(4)
C(11)-Rh(1)-C(5)	113.3(5)
N(1)-Rh(1)-C(5)	99.8(5)
C(11)-Rh(1)-C(1)	98.4(4)
N(1)-Rh(1)-C(1)	134.1(6)
C(5)-Rh(1)-C(1)	39.5(5)
C(11)-Rh(1)-C(2)	114.7(4)
N(1)-Rh(1)-C(2)	163.6(3)
C(5)-Rh(1)-C(2)	65.4(5)
C(1)-Rh(1)-C(2)	36.5(6)
C(11)-Rh(1)-C(4)	151.3(4)

N(1)-Rh(1)-C(4)	101.0(4)
C(5)-Rh(1)-C(4)	38.3(4)
C(1)-Rh(1)-C(4)	62.3(4)
C(2)-Rh(1)-C(4)	63.2(4)
C(11)-Rh(1)-C(3)	152.4(4)
N(1)-Rh(1)-C(3)	130.5(3)
C(5)-Rh(1)-C(3)	63.7(5)
C(1)-Rh(1)-C(3)	61.0(5)
C(2)-Rh(1)-C(3)	37.9(3)
C(4)-Rh(1)-C(3)	36.7(3)
C11–Rh1–Cl1	89.8(2)
N1–Rh1–Cl1	92.2(2)
C(5)-Rh(1)-Cl(1)	155.8(4)
C(1)-Rh(1)-Cl(1)	133.7(6)
C(2)-Rh(1)-Cl(1)	99.3(3)
C(4)-Rh(1)-Cl(1)	118.9(3)
C(3)-Rh(1)-Cl(1)	92.6(3)
C29–Rh2–N2	77.6(4)
C(29)-Rh(2)-C(19)	118.2(4)
N(2)-Rh(2)-C(19)	97.1(4)
C(29)-Rh(2)-C(22)	108.7(4)
N(2)-Rh(2)-C(22)	161.1(4)
C(19)-Rh(2)-C(22)	64.1(3)
C(29)-Rh(2)-C(23)	96.1(3)
N(2)-Rh(2)-C(23)	124.4(4)
C(19)-Rh(2)-C(23)	37.9(3)
C(22)-Rh(2)-C(23)	38.6(3)
C(29)-Rh(2)-C(21)	146.0(3)
N(2)-Rh(2)-C(21)	136.1(4)
C(19)-Rh(2)-C(21)	62.6(3)
C(22)-Rh(2)-C(21)	38.4(3)
C(23)-Rh(2)-C(21)	63.3(3)
C(29)-Rh(2)-C(20)	156.9(4)
N(2)-Rh(2)-C(20)	103.7(4)
C(19)-Rh(2)-C(20)	38.9(3)
C(22)-Rh(2)-C(20)	63.4(4)
C(23)-Rh(2)-C(20)	63.8(4)
C(21)-Rh(2)-C(20)	35.9(3)

C29–Rh2–Cl2	90.0(3)
N2–Rh2–Cl2	92.3(3)
C(19)-Rh(2)-Cl(2)	151.6(3)
C(22)-Rh(2)-Cl(2)	105.4(3)
C(23)-Rh(2)-Cl(2)	143.3(3)
C(21)-Rh(2)-Cl(2)	92.4(3)
C(20)-Rh(2)-Cl(2)	112.8(3)
C(17)-N(1)-Rh(1)	120.8(7)
C(17)-N(1)-HN1	119(5)
Rh(1)-N(1)-HN1	120(5)
C(35)-N(2)-Rh(2)	119.4(7)
C(35)-N(2)-HN2	122(4)
Rh(2)-N(2)-HN2	117(4)
C(2)-C(1)-C(5)	111.9(12)
C(2)-C(1)-C(6)	129.1(15)
C(5)-C(1)-C(6)	119.0(18)
C(2)-C(1)-Rh(1)	72.8(7)
C(5)-C(1)-Rh(1)	69.1(6)
C(6)-C(1)-Rh(1)	125.3(9)
C(1)-C(2)-C(3)	106.3(10)
C(1)-C(2)-C(7)	127.7(12)
C(3)-C(2)-C(7)	125.4(11)
C(1)-C(2)-Rh(1)	70.8(7)
C(3)-C(2)-Rh(1)	73.5(6)
C(7)-C(2)-Rh(1)	127.4(7)
C(4)-C(3)-C(2)	108.3(10)
C(4)-C(3)-C(8)	128.1(10)
C(2)-C(3)-C(8)	123.6(9)
C(4)-C(3)-Rh(1)	70.5(6)
C(2)-C(3)-Rh(1)	68.6(6)
C(8)-C(3)-Rh(1)	127.3(7)
C(3)-C(4)-C(5)	109.2(11)
C(3)-C(4)-C(9)	125.5(12)
C(5)-C(4)-C(9)	125.3(12)
C(3)-C(4)-Rh(1)	72.8(6)
C(5)-C(4)-Rh(1)	67.4(7)
C(9)-C(4)-Rh(1)	124.2(7)
C(4)-C(5)-C(1)	103.7(12)

C(4)-C(5)-C(10)	123.5(14)
C(1)-C(5)-C(10)	132.3(16)
C(4)-C(5)-Rh(1)	74.3(6)
C(1)-C(5)-Rh(1)	71.4(6)
C(10)-C(5)-Rh(1)	124.9(9)
C(1)-C(6)-H(6A)	109.5
C(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(3)-C(8)-H(8A)	109.5
C(3)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(3)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(4)-C(9)-H(9A)	109.5
C(4)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(4)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(16)	116.7(9)
C(12)-C(11)-Rh(1)	128.8(8)
C(16)-C(11)-Rh(1)	114.5(7)

C(11)-C(12)-C(13)	120.7(10)
C(11)-C(12)-H(12)	119.6
C(13)-C(12)-H(12)	119.6
C(14)-C(13)-C(12)	121.0(10)
C(14)-C(13)-H(13)	119.5
C(12)-C(13)-H(13)	119.5
C(15)-C(14)-C(13)	120.6(11)
C(15)-C(14)-H(14)	119.7
C(13)-C(14)-H(14)	119.7
C(14)-C(15)-C(16)	118.8(10)
C(14)-C(15)-H(15)	120.6
C(16)-C(15)-H(15)	120.6
C(15)-C(16)-C(11)	122.2(9)
C(15)-C(16)-C(17)	124.4(10)
C(11)-C(16)-C(17)	113.3(9)
N(1)-C(17)-C(16)	114.3(10)
N(1)-C(17)-C(18)	125.8(9)
C(16)-C(17)-C(18)	119.9(8)
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(23)-C(19)-C(20)	109.3(8)
C(23)-C(19)-C(24)	126.8(9)
C(20)-C(19)-C(24)	123.6(9)
C(23)-C(19)-Rh(2)	72.0(5)
C(20)-C(19)-Rh(2)	74.7(5)
C(24)-C(19)-Rh(2)	124.7(6)
C(21)-C(20)-C(19)	105.9(9)
C(21)-C(20)-C(25)	128.4(10)
C(19)-C(20)-C(25)	125.6(9)
C(21)-C(20)-Rh(2)	71.4(5)
C(19)-C(20)-Rh(2)	66.4(5)
C(25)-C(20)-Rh(2)	129.4(7)
C(20)-C(21)-C(22)	109.7(9)
C(20)-C(21)-C(26)	124.6(10)

C(22)-C(21)-C(26)	125.6(8)
C(20)-C(21)-Rh(2)	72.8(5)
C(22)-C(21)-Rh(2)	67.2(5)
C(26)-C(21)-Rh(2)	124.0(6)
C(23)-C(22)-C(21)	107.4(8)
C(23)-C(22)-C(27)	126.2(9)
C(21)-C(22)-C(27)	125.0(8)
C(23)-C(22)-Rh(2)	71.6(5)
C(21)-C(22)-Rh(2)	74.3(5)
C(27)-C(22)-Rh(2)	130.0(7)
C(19)-C(23)-C(22)	107.3(9)
C(19)-C(23)-C(28)	126.5(9)
C(22)-C(23)-C(28)	126.2(9)
C(19)-C(23)-Rh(2)	70.1(5)
C(22)-C(23)-Rh(2)	69.8(5)
C(28)-C(23)-Rh(2)	127.1(6)
C(19)-C(24)-H(24A)	109.5
C(19)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(19)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(20)-C(25)-H(25A)	109.5
C(20)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(20)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(21)-C(26)-H(26A)	109.5
C(21)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(21)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(22)-C(27)-H(27A)	109.5
C(22)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(22)-C(27)-H(27C)	109.5

H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30)-C(29)-C(34)	113.7(9)
C(30)-C(29)-Rh(2)	129.0(7)
C(34)-C(29)-Rh(2)	117.3(7)
C(31)-C(30)-C(29)	121.8(10)
C(31)-C(30)-H(30)	119.1
C(29)-C(30)-H(30)	119.1
C(30)-C(31)-C(32)	121.8(11)
C(30)-C(31)-H(31)	119.1
C(32)-C(31)-H(31)	119.1
C(33)-C(32)-C(31)	118.1(10)
C(33)-C(32)-H(32)	121.0
C(31)-C(32)-H(32)	121.0
C(34)-C(33)-C(32)	119.6(9)
C(34)-C(33)-H(33)	120.2
C(32)-C(33)-H(33)	120.2
C(33)-C(34)-C(29)	124.9(9)
C(33)-C(34)-C(35)	123.7(9)
C(29)-C(34)-C(35)	111.5(8)
N(2)-C(35)-C(34)	114.1(8)
N(2)-C(35)-C(36)	123.0(9)
C(34)-C(35)-C(36)	122.9(8)
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for rhnr2. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	51(1)	68(1)	42(1)	-1(1)	4(1)	-4(1)
Rh(2)	62(1)	43(1)	40(1)	3(1)	1(1)	-3(1)
Cl(1)	63(2)	59(2)	55(2)	3(1)	11(2)	-7(1)
Cl(2)	85(2)	71(2)	52(2)	2(2)	-15(2)	-10(2)
N(1)	59(6)	45(6)	56(6)	-11(5)	12(4)	-2(5)
N(2)	48(5)	55(4)	49(4)	-5(7)	-2(7)	0(4)
C(1)	58(7)	110(9)	121(11)	-32(14)	-10(13)	-3(6)
C(2)	64(8)	78(9)	70(9)	14(7)	6(7)	-8(6)
C(3)	57(7)	71(7)	43(7)	10(5)	-5(6)	2(5)
C(4)	56(7)	85(8)	77(12)	18(7)	-19(6)	-24(6)
C(5)	54(8)	189(17)	50(9)	-1(10)	18(7)	-46(10)
C(6)	68(9)	228(14)	230(20)	-124(13)	0(10)	41(10)
C(7)	115(11)	100(9)	136(13)	35(9)	-59(9)	12(8)
C(8)	67(7)	111(8)	39(6)	-3(6)	-7(5)	-19(6)
C(9)	117(9)	93(7)	101(12)	30(9)	-17(12)	-39(7)
C(10)	118(12)	340(20)	61(10)	46(11)	5(8)	-126(12)
C(11)	45(6)	76(7)	57(7)	2(6)	22(5)	-9(5)
C(12)	54(6)	71(7)	68(7)	12(6)	12(6)	20(6)
C(13)	86(9)	54(7)	112(12)	-13(7)	17(8)	11(6)
C(14)	70(9)	83(9)	115(12)	-39(8)	23(8)	-1(7)
C(15)	73(8)	72(7)	62(8)	-17(6)	3(6)	-4(6)
C(16)	56(7)	60(7)	47(7)	-1(5)	12(5)	-6(5)
C(17)	57(7)	54(6)	42(6)	0(5)	5(5)	-19(5)
C(18)	78(7)	90(7)	36(6)	-8(5)	-8(5)	-5(6)
C(19)	98(9)	37(5)	36(6)	-1(4)	-10(6)	8(6)
C(20)	78(8)	38(6)	30(6)	1(4)	21(6)	-9(6)
C(21)	85(8)	37(6)	37(6)	8(4)	-3(6)	-2(6)
C(22)	89(8)	40(6)	45(6)	2(4)	2(6)	3(6)
C(23)	65(7)	47(6)	51(7)	9(5)	-2(6)	-3(5)
C(24)	99(8)	69(7)	58(7)	-6(5)	-15(6)	-13(6)
C(25)	81(8)	87(8)	57(8)	17(6)	-1(7)	-1(6)
C(26)	113(9)	64(7)	71(8)	3(5)	-2(6)	-34(6)

C(27)	134(8)	54(5)	63(6)	3(9)	19(13)	17(5)
C(28)	74(9)	98(9)	73(9)	23(6)	-12(7)	-2(7)
C(29)	68(7)	38(5)	52(6)	-3(4)	-21(5)	14(5)
C(30)	71(8)	64(7)	63(8)	7(6)	-2(6)	1(6)
C(31)	59(8)	106(10)	83(9)	13(7)	3(7)	-2(7)
C(32)	59(8)	110(10)	71(8)	17(7)	3(6)	-29(7)
C(33)	52(7)	76(7)	61(8)	21(6)	-4(6)	-21(6)
C(34)	42(6)	65(7)	41(6)	5(5)	-7(5)	2(5)
C(35)	52(6)	59(6)	38(6)	10(4)	-9(5)	-23(5)
C(36)	90(8)	49(6)	58(7)	6(5)	-12(6)	-13(5)

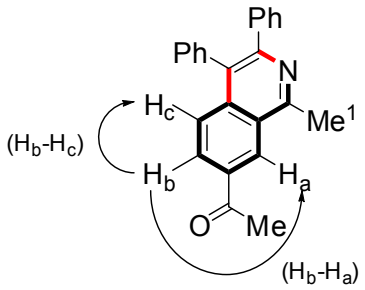
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rhnr2.

	x	y	z	U(eq)
H(6A)	-2959	528	-3582	262
H(6B)	-2945	-43	-2052	262
H(6C)	-3388	-136	-3243	262
H(7A)	-2678	489	-6220	176
H(7B)	-2936	-178	-7354	176
H(7C)	-2358	-47	-7420	176
H(8A)	-2478	-1834	-8173	109
H(8B)	-2105	-2471	-7351	109
H(8C)	-1940	-1520	-7744	109
H(9A)	-2140	-3092	-3197	156
H(9B)	-1973	-3115	-4968	156
H(9C)	-2515	-3391	-4506	156
H(10A)	-3004	-2243	-1604	258
H(10B)	-2788	-1378	-914	258
H(10C)	-2436	-2173	-1205	258
H(12)	-2100	1127	-3777	77
H(13)	-1842	2189	-2042	101
H(14)	-1371	1846	131	107
H(15)	-1133	438	588	83
H(18A)	-887	-1850	-113	102
H(18B)	-1100	-1135	1015	102
H(18C)	-649	-922	-92	102
H(24A)	-364	2193	-2268	113
H(24B)	195	1905	-2342	113
H(24C)	-18	2541	-3616	113
H(25A)	1345	3380	-1777	112
H(25B)	1022	3246	-3298	112
H(25C)	1064	2501	-2045	112
H(26A)	1331	4366	17	124
H(26B)	991	4869	1209	124
H(26C)	1059	5217	-515	124
H(27A)	130	5222	1776	126

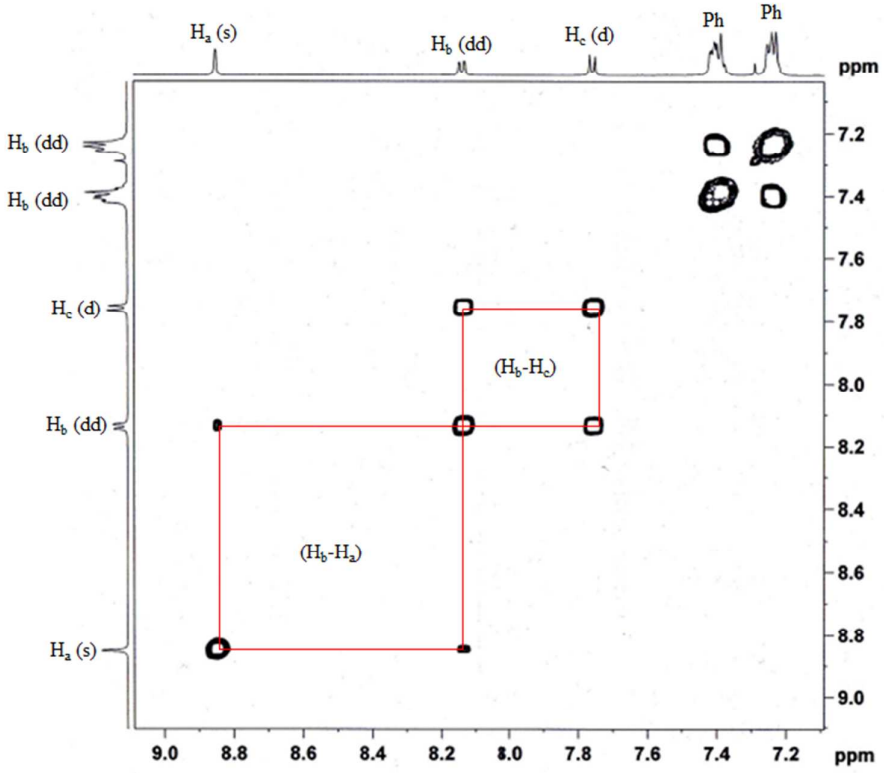
H(27B)	-419	4950	1402	126
H(27C)	-130	5557	237	126
H(28A)	-891	4048	-1473	123
H(28B)	-888	3794	318	123
H(28C)	-870	3069	-977	123
H(30)	-557	3741	3252	79
H(31)	-1154	3105	4746	99
H(32)	-1208	1605	4968	96
H(33)	-646	762	3596	76
H(36A)	440	132	1187	98
H(36B)	-138	56	1384	98
H(36C)	204	117	2878	98
HN2	690(20)	1570(30)	670(90)	30(20)
HN1	-1410(20)	-1900(30)	-2340(80)	10(20)

6. Determination of the regiochemistry of 10b and 13f by 2D NMR analysis:

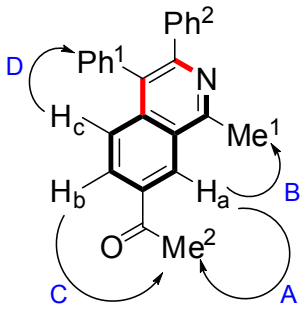
a) 2D COSY NMR on 10b in the aromatic region ($CDCl_3$, 600 MHz):



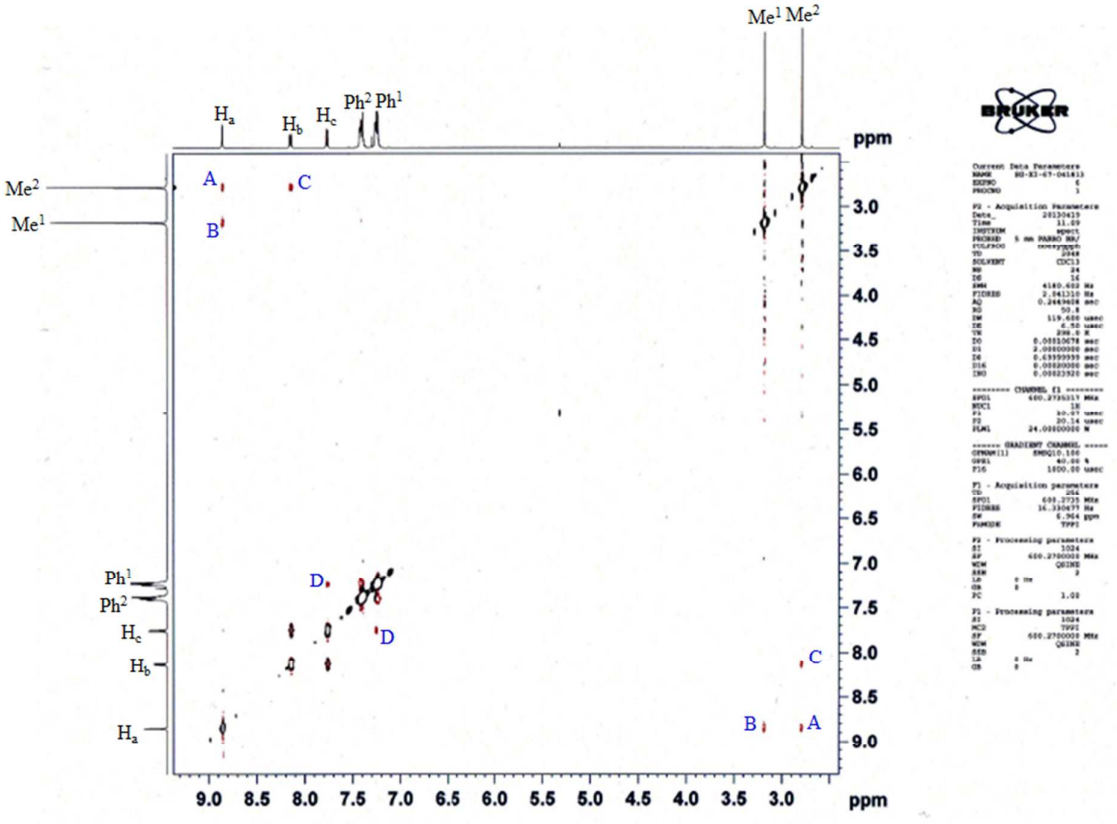
10b



b) 2D NOESY of 10b ($CDCl_3$, 600 MHz):



10b



c) 2D NOESY of 13f ($CDCl_3$, 600 MHz):