

Supporting Information

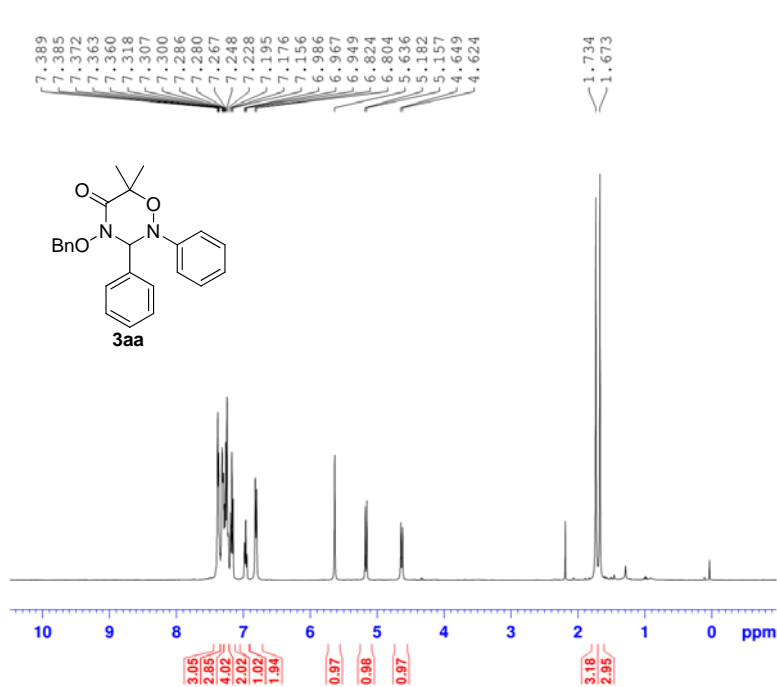
A facile access to novel 1,2,4-oxadiazinan-5-ones via [3+3]
cycloaddition of in situ generated azaoxyallyl cations with
nitrones

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Hai-Liang Pang, Xiao-Qin Chen, Xiu-Qing Song, Juan Du

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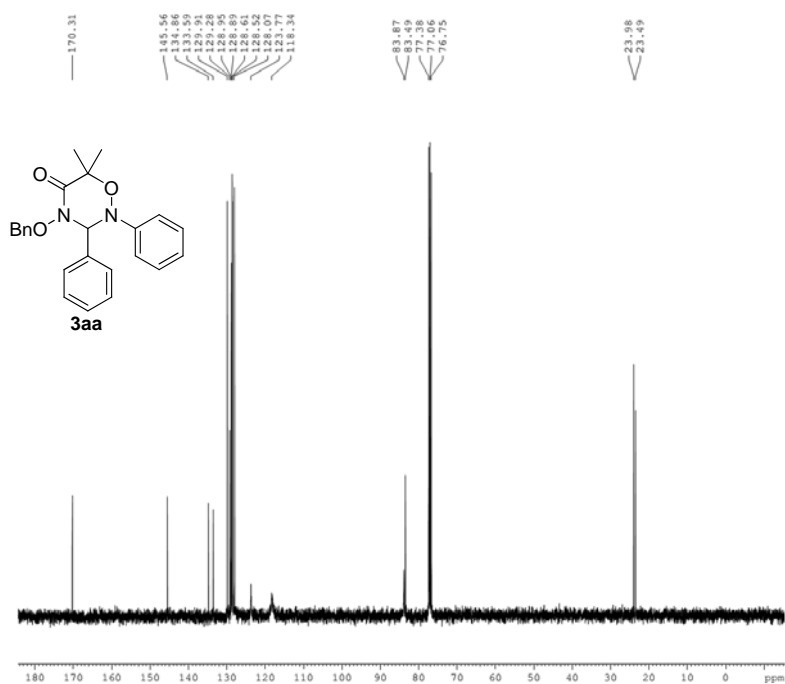
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1. ¹H and ¹³C NMR spectra



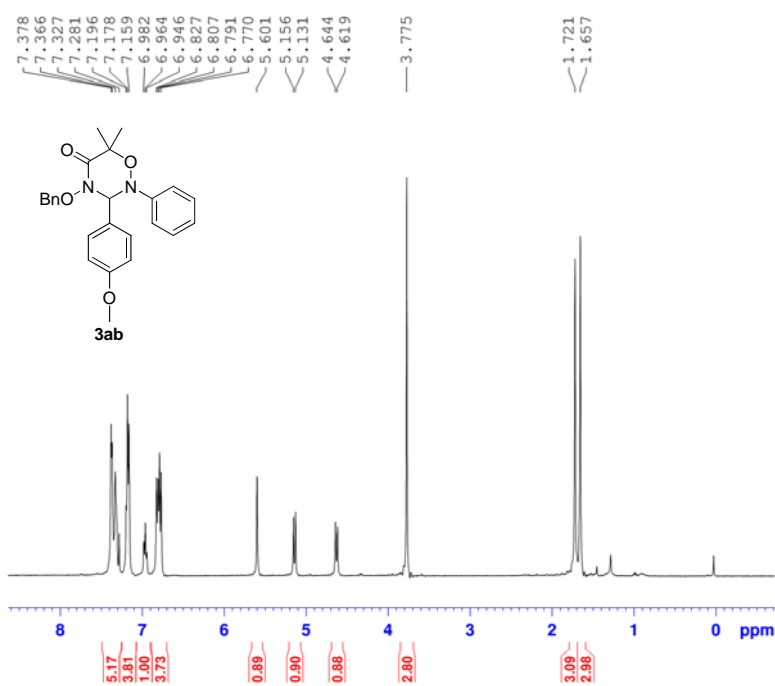
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NAME          NMR2
EXPNO         4187
PROCNO        1
Date_         20160429
Time          12.06
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD             65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8223.695 Hz
FIDRES       0.125483 Hz
AQ           3.9846387 sec
RG           128
DW           60.800 usec
DE           6.50 usec
TE           294.9 K
D1           1.00000000 sec
TDO          1
===== CHANNEL f1 =====
NUC1          1H
P1            14.50 usec
PL1          -2.83 dB
PL1W        16.91636658 W
SF01        400.1724712 MHz
SI           32768
SF          400.1700000 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
FC           1.00
    
```



```

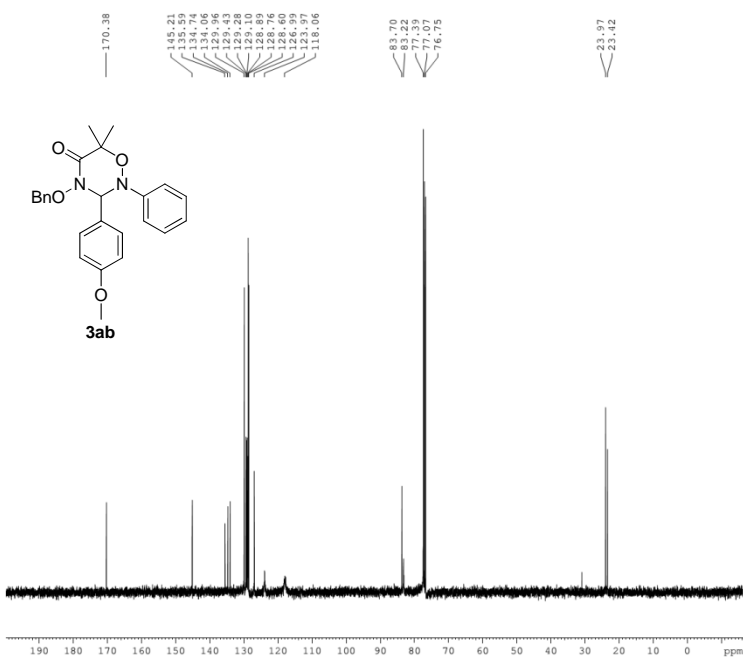
NAME          NMR2
EXPNO         4238
PROCNO        1
Date_         20160523
Time          13.36
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD             65536
SOLVENT       CDCl3
NS            128
DS            4
SWH           24038.461 Hz
FIDRES       0.366798 Hz
AQ           1.3631988 sec
RG           2050
DW           20.800 usec
DE           6.50 usec
TE           298.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TDO          1
===== CHANNEL f1 =====
NUC1          13C
P1            11.70 usec
PL1          -2.00 dB
PL1W        48.76812744 W
SF01        100.6328888 MHz
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
FCPD2        80.00 usec
PL2          -2.83 dB
PL12         12.00 dB
PL13         14.00 dB
PL2W        16.91636658 W
PL12W       0.55629748 W
PL13W       0.35100001 W
SF02        400.1716007 MHz
SI           32768
SF          100.6228270 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
FC           1.40
    
```



```

NAME          NMR2
EXPNO         4232
PROCNO        1
Date_         20160523
Time         11.25
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            2
DS            2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            128
DW            60.800 usec
DE            6.50 usec
TE            298.7 K
D1            1.00000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          1H
P1            14.50 usec
PL1           -2.83 dB
PL1W          16.91636658 W
SF01          400.1724712 MHz
SI            32768
SF            400.1700000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

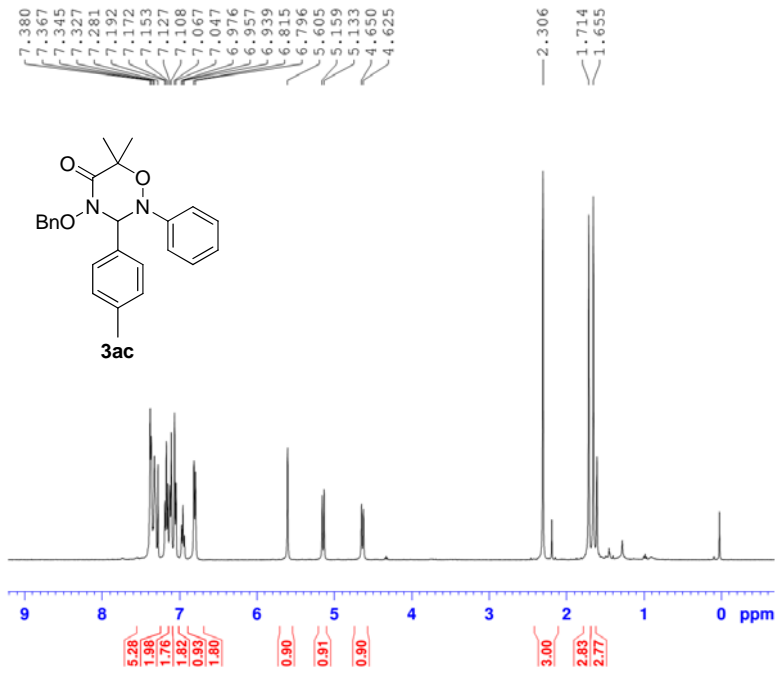


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NAME          NMR2
EXPNO         4250
PROCNO        1
Date_         20160524
Time         15.54
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            110
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            2050
DW            20.800 usec
DE            6.50 usec
TE            297.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          13C
P1            11.70 usec
PL1           -2.00 dB
PL1W          48.76812744 W
SF01          100.6328888 MHz

----- CHANNEL f2 -----
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -2.83 dB
PL12          12.00 dB
PL13          14.00 dB
PL2W          16.91636658 W
PL12W         0.55629748 W
PL13W         0.35100001 W
SF02          400.1716007 MHz
SI            32768
SF            100.6228270 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

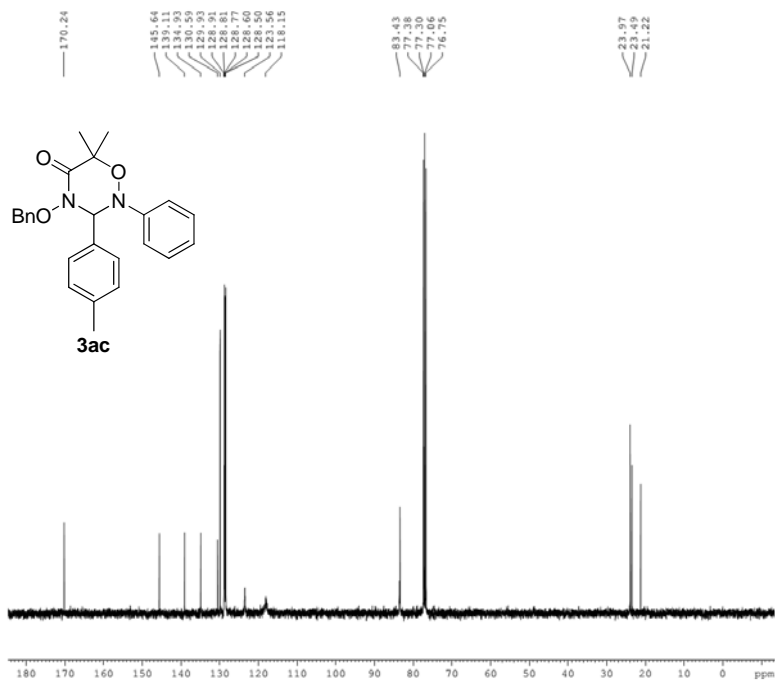


```

NAME      NMR2
EXPNO    4234
PROCNO   1
Date_    20160523
Time     11.38
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       8223.685 Hz
FIDRES   0.125483 Hz
AQ        3.9846387 sec
RG        128
DW        60.800 usec
DE        6.50 usec
TE        298.6 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1        14.50 usec
PL1       -2.83 dB
PL1W      16.91636658 W
SFO1      400.1724712 MHz
SI        32768
SF        400.1700000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

```



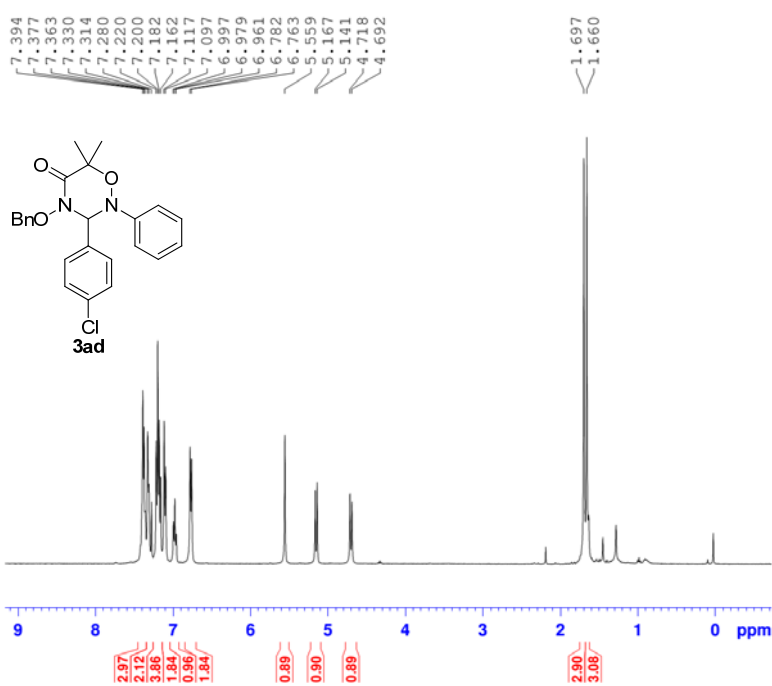
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NAME      NMR2
EXPNO    4263
PROCNO   1
Date_    20160525
Time     13.37
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        164
DS        4
SWH       24038.461 Hz
FIDRES   0.366798 Hz
AQ        1.3631988 sec
RG        2050
DW        20.800 usec
DE        6.50 usec
TE        297.9 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      13C
P1        11.70 usec
PL1       -2.00 dB
PL1W      48.76812744 W
SFO1      100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       -2.83 dB
PL12     12.00 dB
PL13     14.00 dB
PL2W     16.91636658 W
PL12W    0.55629748 W
PL13W    0.35100001 W
SFO2     400.1716007 MHz
SI        32768
SF        100.6228270 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

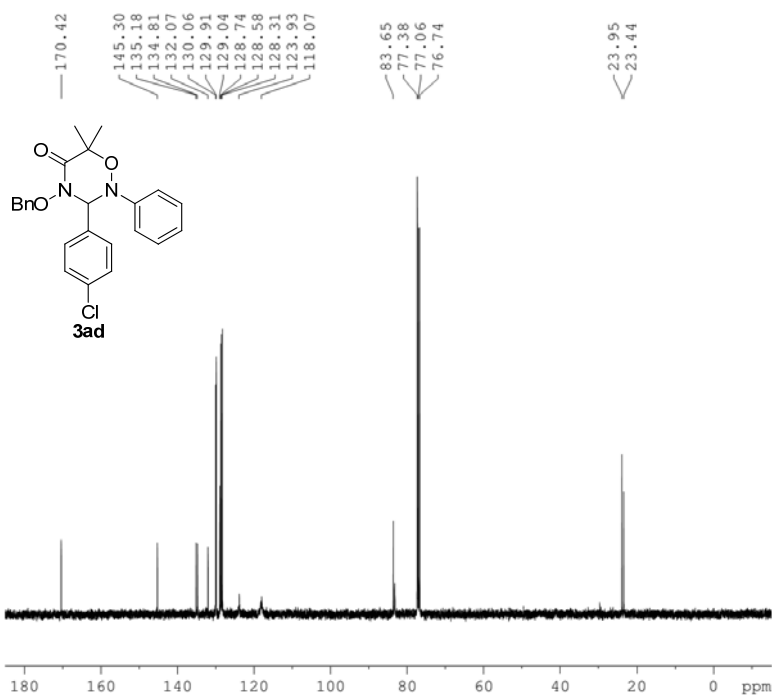


```

NAME      NMR2
EXPNO    4236
PROCNO   1
Date_    20160523
Time     11.52
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       7
DS       2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ       3.9846387 sec
RG       128
DW       60.800 usec
DE       6.50 usec
TE       298.3 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     1H
P1       14.50 usec
PL1      -2.32 dB
PL1W    16.91636658 W
SFO1    400.1724712 MHz
SI       32768
SF       400.1700000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

```



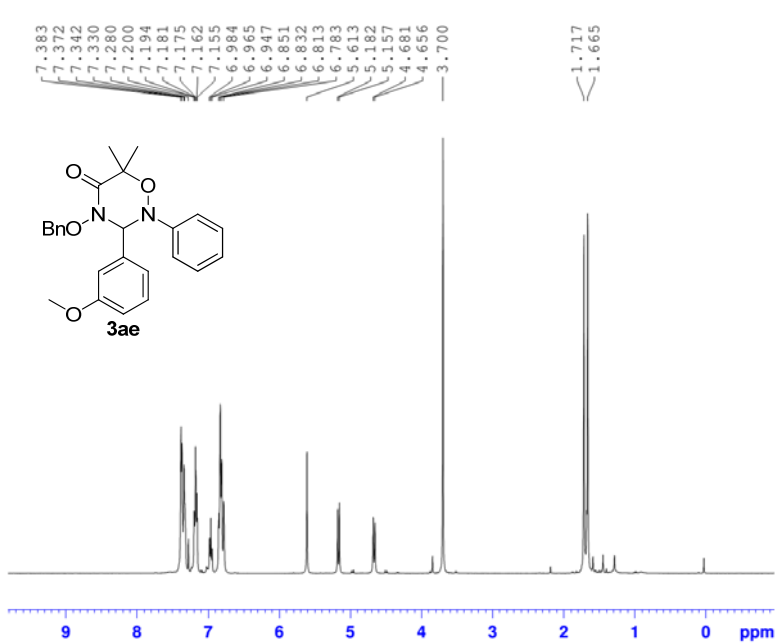
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NAME      NMR2
EXPNO    4261
PROCNO   1
Date_    20160525
Time     11.02
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       109
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631988 sec
RG       2050
DW       20.800 usec
DE       6.50 usec
TE       299.0 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     13C
P1       11.70 usec
PL1      -2.00 dB
PL1W    48.76812744 W
SFO1    100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      -2.83 dB
PL12     12.00 dB
PL13     14.00 dB
PL1W    16.91636658 W
PL12W   0.55629748 W
PL13W   0.35100001 W
SFO2    400.1716007 MHz
SI       32768
SF       100.6228270 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

```

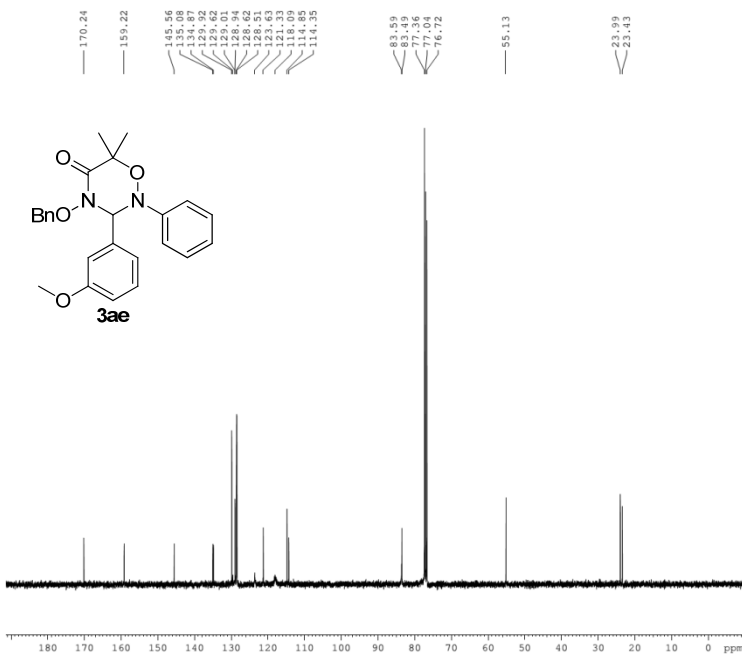


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NAME          NMR2
EXPNO         4304
PROCNO        1
Date_         20160601
Time         11.48
INSTRUM      spect
PROBHD        5 mm PABBO BB-
PULPROG      zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8223.685 Hz
FIDRES       0.125483 Hz
AQ           3.9846387 sec
RG            128
DW           60.800 usec
DE           6.50 usec
TE           298.3 K
D1           1.00000000 sec
TDO          1

===== CHANNEL f1 =====
NUC1          1H
P1            14.50 usec
PL1          -2.83 dB
PL1W         16.91636658 W
SFO1         400.1724712 MHz
SI           32768
SF           400.1700000 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00

```



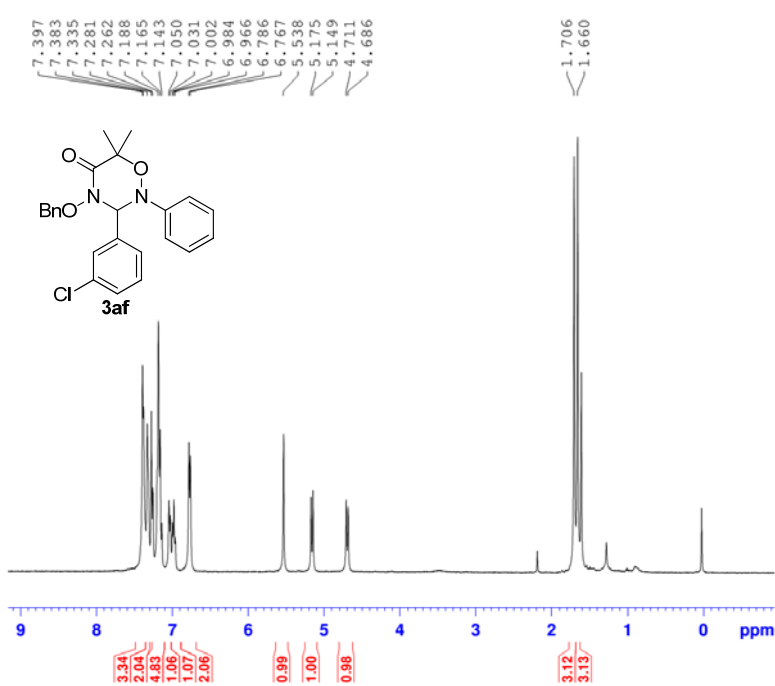
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NAME          NMR
EXPNO         4305
PROCNO        1
Date_         20160601
Time         11.44
INSTRUM      spect
PROBHD        5 mm PABBO BB-
PULPROG      zgpg30
TD            65536
SOLVENT       CDCl3
NS            183
DS            4
SWH           24038.461 Hz
FIDRES       0.366798 Hz
AQ           1.3631988 sec
RG            2050
DW           20.800 usec
DE           6.50 usec
TE           299.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TDO          1

===== CHANNEL f1 =====
NUC1          13C
P1            11.70 usec
PL1          -2.00 dB
PL1W         48.76812744 W
SFO1         100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2          -2.83 dB
PL12         12.00 dB
PL13         14.00 dB
PL2W         16.91636658 W
PL12W        0.55629748 W
PL13W        0.35100001 W
SFO2         400.1716007 MHz
SI           32768
SF           100.6228270 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40

```

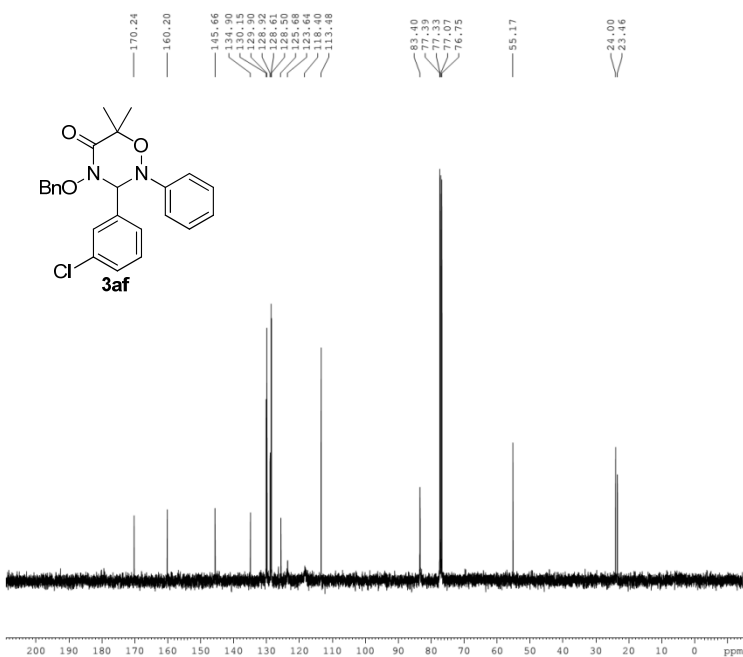


```

NAME      NMR2
EXPNO     4318
PROCNO    1
Date_     20160606
Time      15.38
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         7
DS         2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ         3.9846387 sec
RG         128
DW         60.800 usec
DE         6.50 usec
TE         673.2 K
D1         1.00000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1      1H
P1        14.50 usec
PL1       -2.83 dB
PL1W      16.91636658 W
SFO1      400.1724712 MHz
SI         32768
SF         400.1700000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```



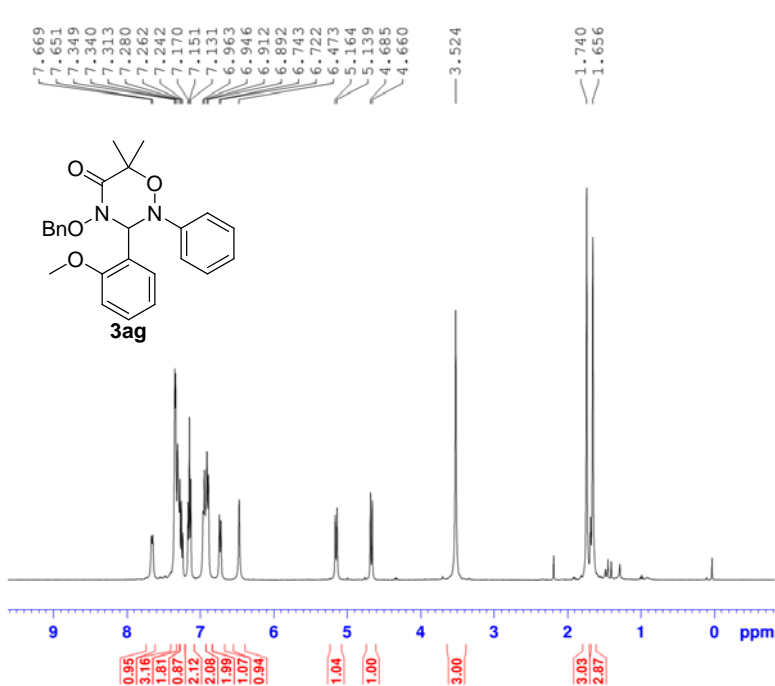
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NAME      NMR2
EXPNO     4252
PROCNO    1
Date_     20160524
Time      16.38
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         53
DS         4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ         1.3631988 sec
RG         2050
DW         20.800 usec
DE         6.50 usec
TE         297.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1      13C
P1        11.70 usec
PL1       -2.00 dB
PL1W      48.76812744 W
SFO1      100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -2.83 dB
PL12      12.00 dB
PL13      14.00 dB
PL2W      16.91636658 W
PL12W     0.55629748 W
PL13W     0.35100001 W
SFO2      400.1716007 MHz
SI         32768
SF         100.6228270 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

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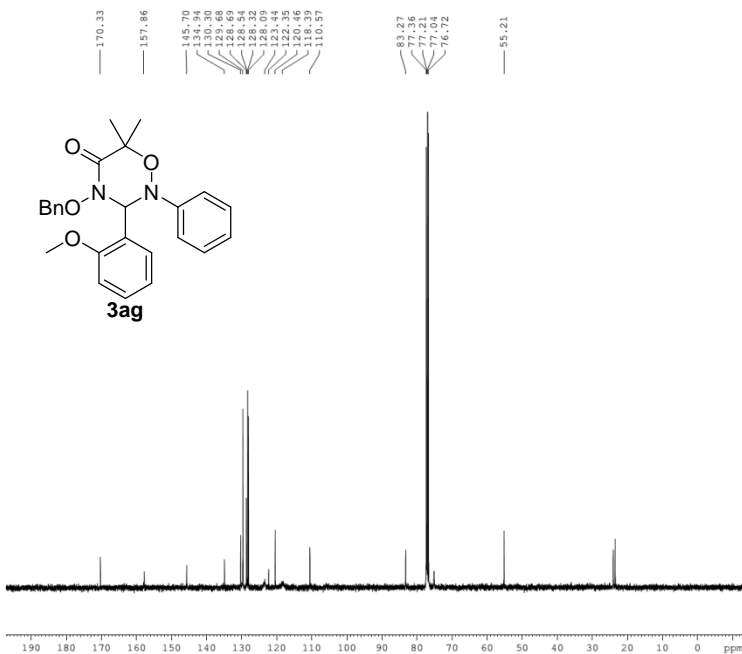


```

NAME          NMR2
EXPNO         4307
PROCNO        1
Date_         20160601
Time          12.00
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDC13
NS            4
DS            2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            128
DW            60.800 usec
DE            6.50 usec
TE            297.8 K
D1            1.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.50 usec
PL1           -2.83 dB
PL1W          16.91636658 W
SF01          400.1724712 MHz
SI            32768
SF            400.1700000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

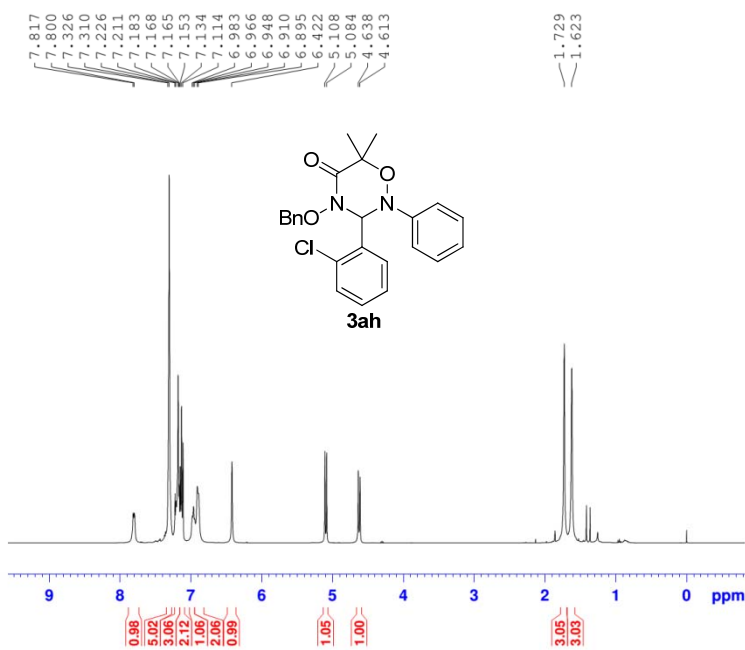
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EXPNO         4308
PROCNO        1
Date_         20160601
Time          12.04
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDC13
NS            4
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            2050
DW            20.800 usec
DE            6.50 usec
TE            298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            11.70 usec
PL1           -2.00 dB
PL1W          48.76812744 W
SF01          100.6328888 MHz
  
```

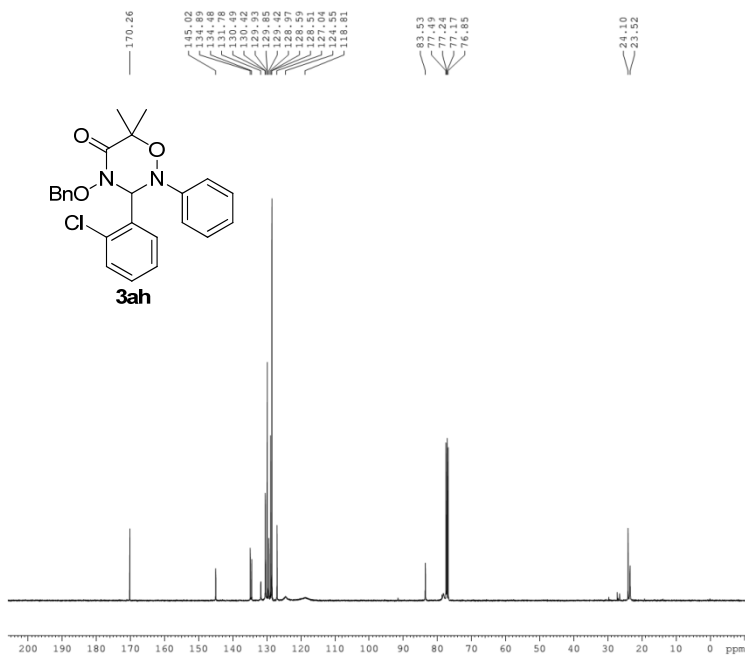
```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
FCHD2         80.00 usec
PL2           -2.83 dB
PL12          12.00 dB
PL13          14.00 dB
PL2W          16.91636658 W
PL12W         0.55629748 W
PL13W         0.35100001 W
SF02          400.1716007 MHz
SI            32768
SF            100.6228270 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

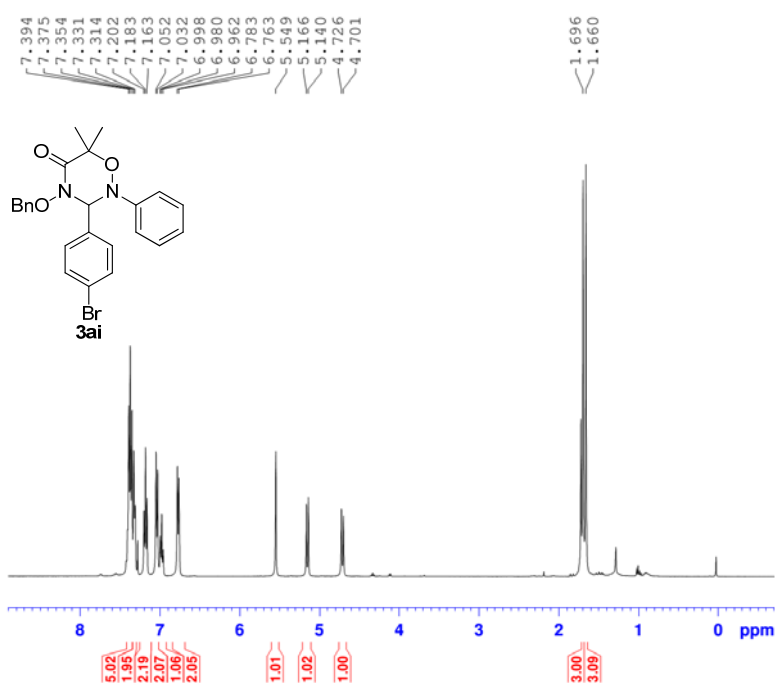
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NAME          NMR2
EXPNO         9
PROCNO        1
Date_         20170215
Time          13.48 h
INSTRUM       spect
PROBHD        z116098_0406 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            19.71
DW            62.400 usec
DE            6.50 usec
TE            291.6 K
D1            1.00000000 sec
TDO           1
SFO1          400.1324708 MHz
NUC1          1H
P1            10.00 usec
SI            65536
SF            400.1300227 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

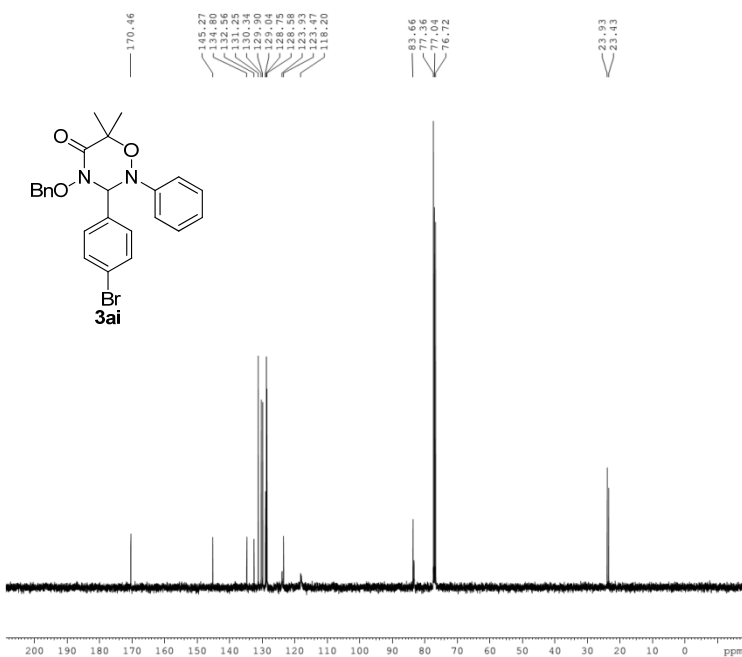
NAME          NMR2
EXPNO         10
PROCNO        1
Date_         20170215
Time          14.48 h
INSTRUM       spect
PROBHD        z116098_0406 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            1024
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            196.12
DW            20.800 usec
DE            6.50 usec
TE            292.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TDO           1
SFO1          100.6228298 MHz
NUC1          13C
P1            10.00 usec
SI            32768
SF            100.6127685 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



```

NAME          NMR
EXPNO         4348
PROCNO        1
Date_         20160907
Time         11.37
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            9
DS            2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            114
DW            60.800 usec
DE            6.50 usec
TE            673.2 K
D1            1.00000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          1H
P1            14.50 usec
PL1           -2.83 dB
PL1W          16.91636658 W
SFO1          400.1724712 MHz
SI            32768
SF            400.1700000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

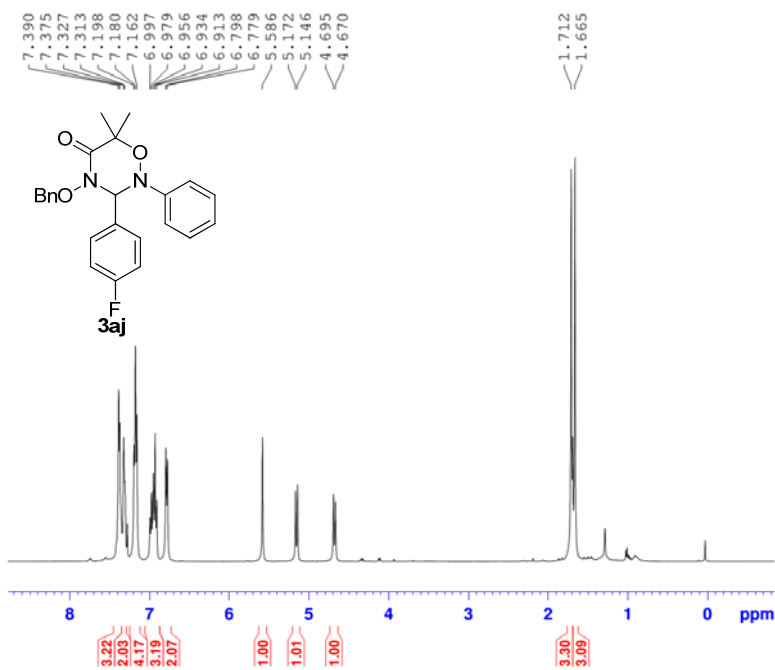


```

NAME          NMR
EXPNO         4349
PROCNO        1
Date_         20160907
Time         11.41
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            128
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            2050
DW            20.800 usec
DE            6.50 usec
TE            673.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          13C
P1            11.70 usec
PL1           -2.00 dB
PL1W          48.76812744 W
SFO1          100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -2.83 dB
PL12          12.00 dB
PL13          14.00 dB
PL2W          16.91636658 W
PL12W         0.55629748 W
PL13W         0.35100001 W
SFO2          400.1716007 MHz
SI            32768
SF            100.6228270 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

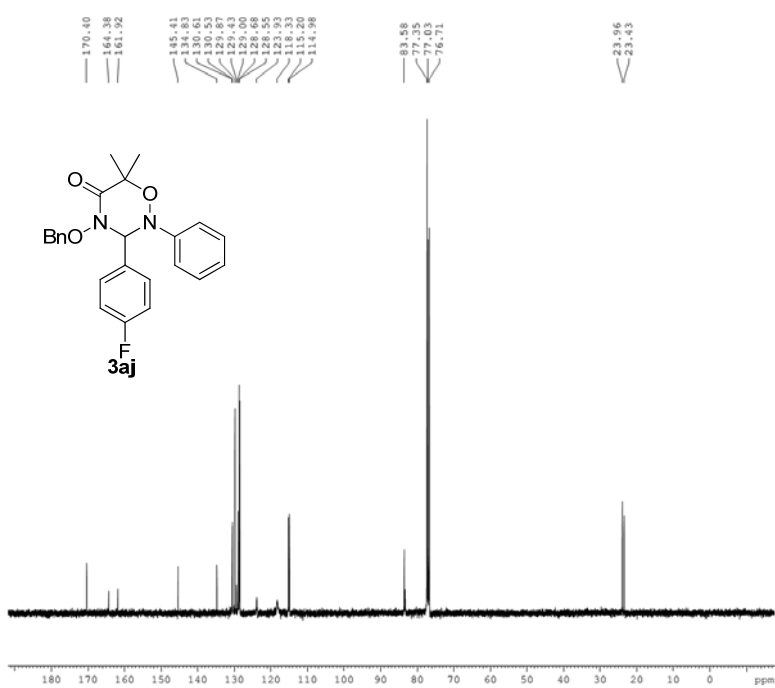


```

NAME          NMR
EXPNO         4355
PROCNO        1
Date_         20160907
Time          15.06
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            128
DW            60.800 usec
DE            6.50 usec
TE            673.2 K
D1            1.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.50 usec
PL1           -2.32 dB
PL1W          16.91636658 W
SFO1          400.1724712 MHz
SI            32768
SF            400.1700000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



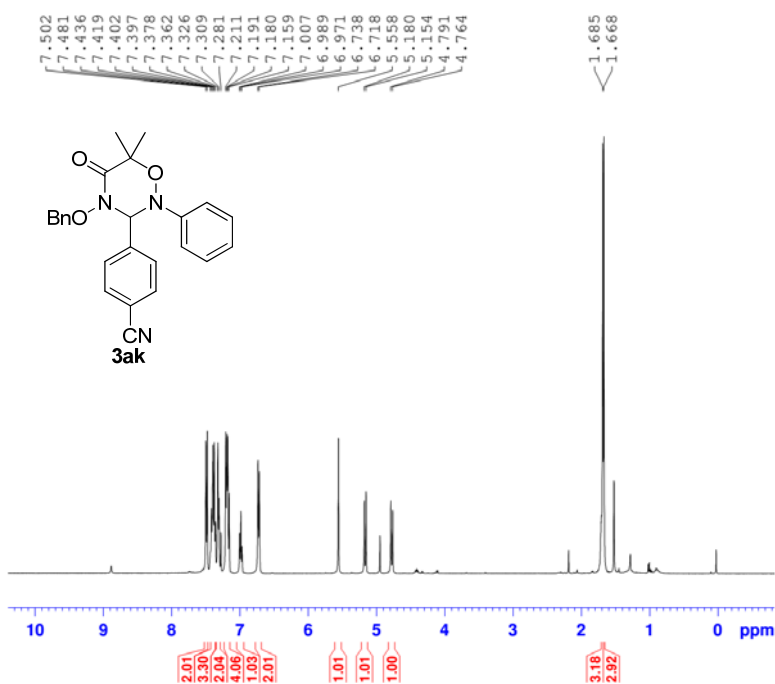
```

NAME          NMR
EXPNO         4354
PROCNO        1
Date_         20160907
Time          12.11
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            256
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            2050
DW            20.800 usec
DE            6.50 usec
TE            673.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            11.70 usec
PL1           -2.00 dB
PL1W          48.76812744 W
SFO1          100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -2.83 dB
PL12          12.00 dB
PL13          14.00 dB
PL2W          16.91636658 W
PL12W         0.55629748 W
PL13W         0.35100001 W
SFO2          400.1716007 MHz
SI            32768
SF            100.6228270 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

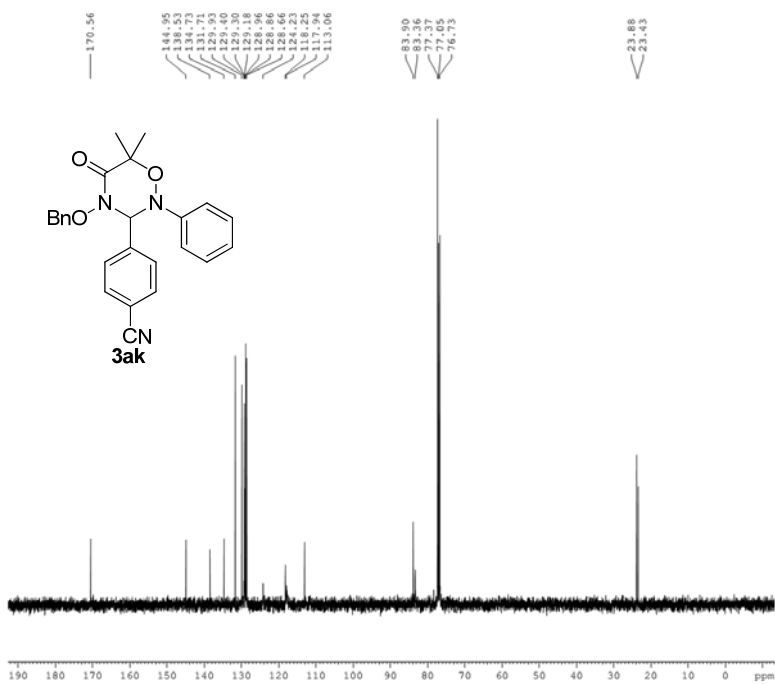


```

NAME      NMR
EXPNO     4352
PROCNO    1
Date_     20160907
Time      12.01
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         4
DS         2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ        3.9846387 sec
RG         128
DW         60.800 usec
DE         6.50 usec
TE         673.2 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      1H
P1         14.50 usec
PL1        -2.83 dB
PL1W      16.91636658 W
SFO1      400.1724712 MHz
SI         32768
SF         400.1700000 MHz
WDW        EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00

```



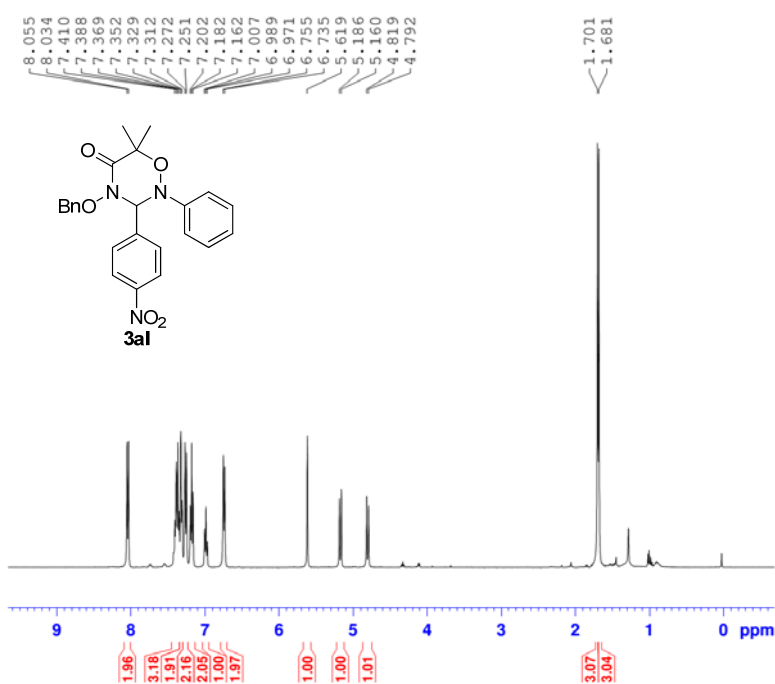
```

NAME      NMR
EXPNO     4353
PROCNO    1
Date_     20160907
Time      12.04
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         64
DS         4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG         2050
DW         20.800 usec
DE         6.50 usec
TE         673.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      13C
P1         11.70 usec
PL1        -2.00 dB
PL1W      48.76812744 W
SFO1      100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2        -2.83 dB
PL12      12.00 dB
PL13      14.00 dB
PL2W      16.91636658 W
PL12W     0.55629748 W
PL13W     0.35100001 W
SFO2      400.1716007 MHz
SI         32768
SF         100.6228270 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40

```

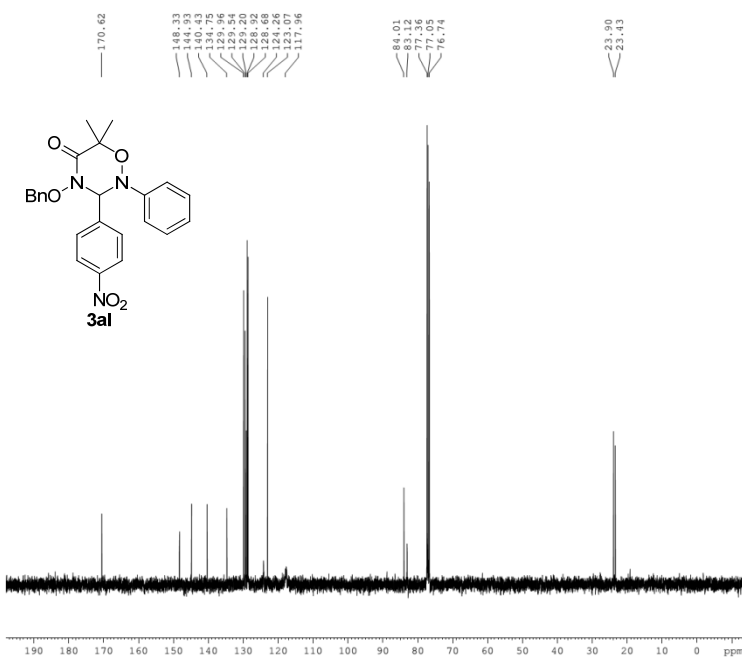


```

NAME          NMR
EXPNO         4351
PROCNO        1
Date_         20160907
Time          11.57
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            4
DS            2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            128
DW            60.800 usec
DE            6.50 usec
TE            673.2 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            14.50 usec
PL1          -2.83 dB
PL1W         16.91636658 W
SF01         400.1724712 MHz
SI           32768
SF           400.1700000 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00

```



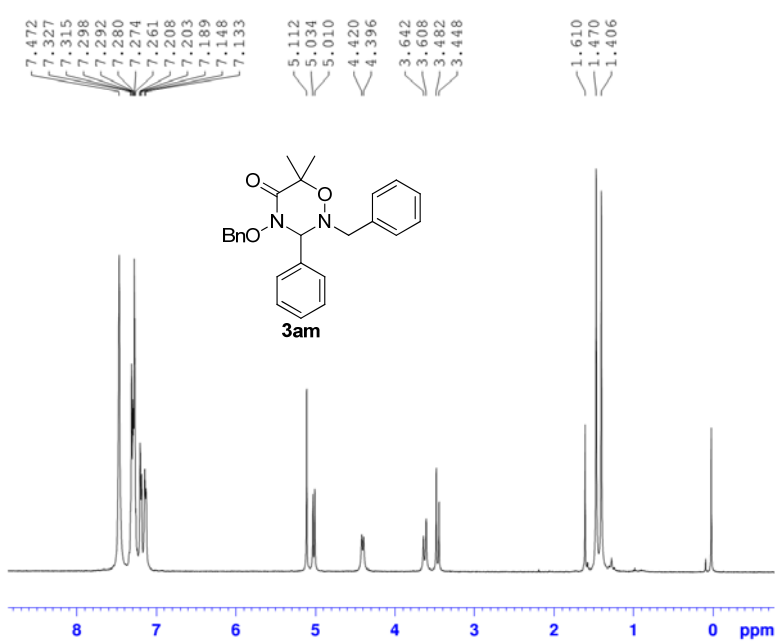
```

NAME          NMR
EXPNO         4350
PROCNO        1
Date_         20160907
Time          11.51
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            52
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            2050
DW            20.800 usec
DE            6.50 usec
TE            673.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            11.70 usec
PL1          -2.00 dB
PL1W         48.76812744 W
SF01         100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2        80.00 usec
PL2          -2.83 dB
PL12         12.00 dB
PL13         14.00 dB
PL2W         16.91636658 W
PL12W        0.55629748 W
PL13W        0.35100001 W
SF02         400.1716007 MHz
SI           32768
SF           100.6228270 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40

```

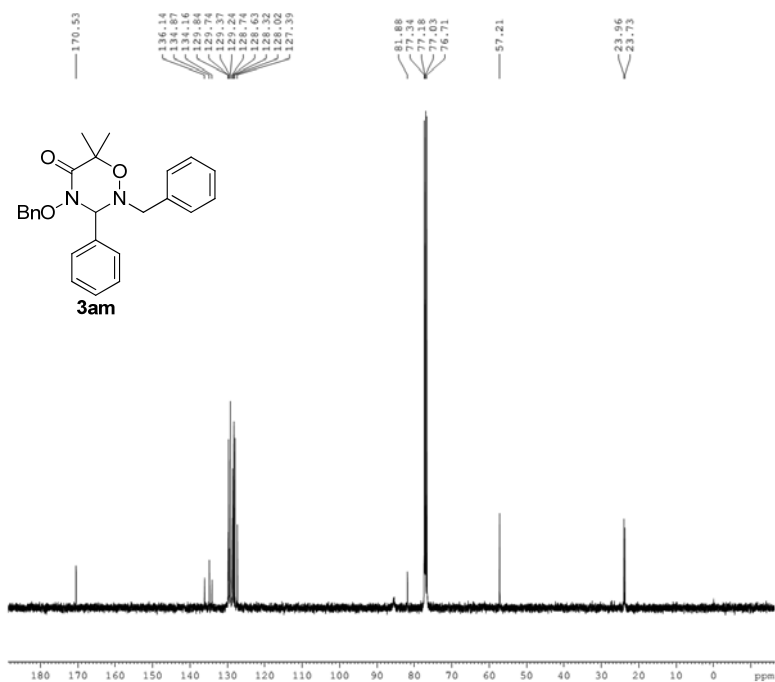


```

NAME      NMR2
EXPNO    4190
PROCNO    1
Date_    20160504
Time      8.40
INSTRUM  spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS         8
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         128
DW         60.800 usec
DE         6.50 usec
TE         294.5 K
D1         1.00000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1      1H
P1        14.50 usec
PL1       -2.33 dB
PL1W      16.91636658 W
SFO1      400.1724712 MHz
SI        32768
SF        400.1700000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

```



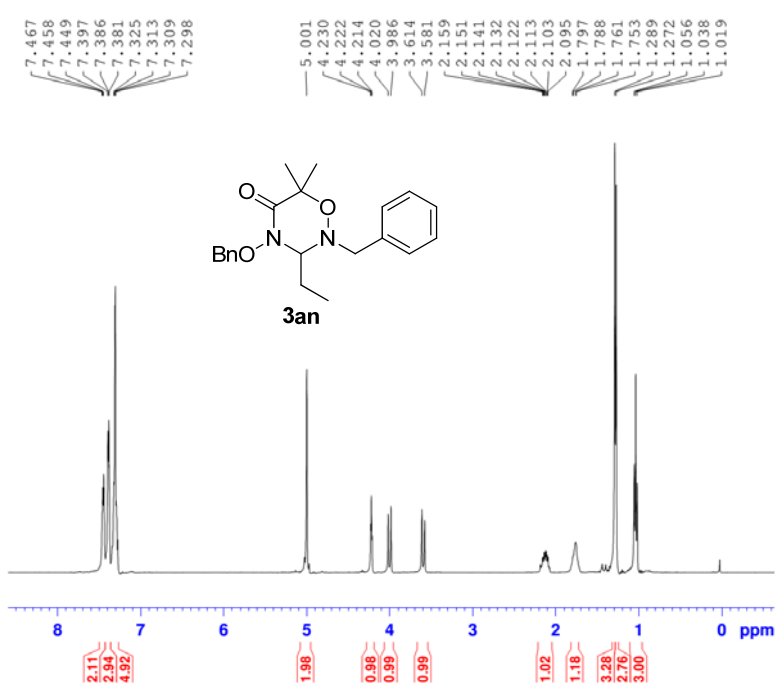
```

NAME      NMR
EXPNO    4341
PROCNO    1
Date_    20160907
Time      9.47
INSTRUM  spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS         376
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         2050
DW         20.800 usec
DE         6.50 usec
TE         673.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1      13C
P1        11.70 usec
PL1       -2.00 dB
PL1W      48.76812744 W
SFO1      100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -2.83 dB
PL12      12.00 dB
PL13      14.00 dB
PL2W      16.91636658 W
PL12W     0.55629748 W
PL13W     0.35100001 W
SFO2      400.1716007 MHz
SI        32768
SF        100.6228270 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

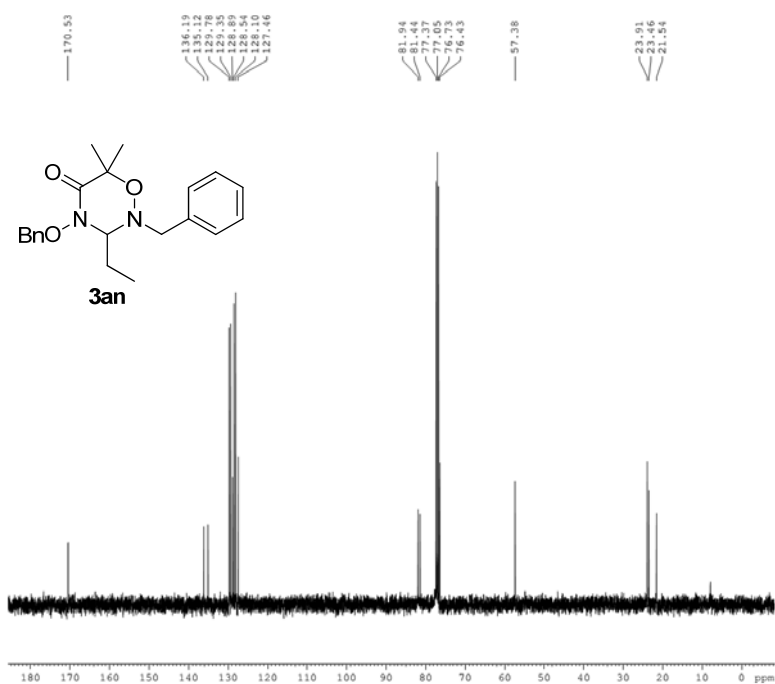
```



```

NAME      NMR2
EXPNO    4296
PROCNO    1
Date_     20160531
Time      17.12
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         4
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         128
DW         60.800 usec
DE         6.50 usec
TE         297.7 K
D1         1.0000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.50 usec
PL1        -2.83 dB
PL1W       16.91636658 W
SF01       400.1724712 MHz
SI         32768
SF         400.1700000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

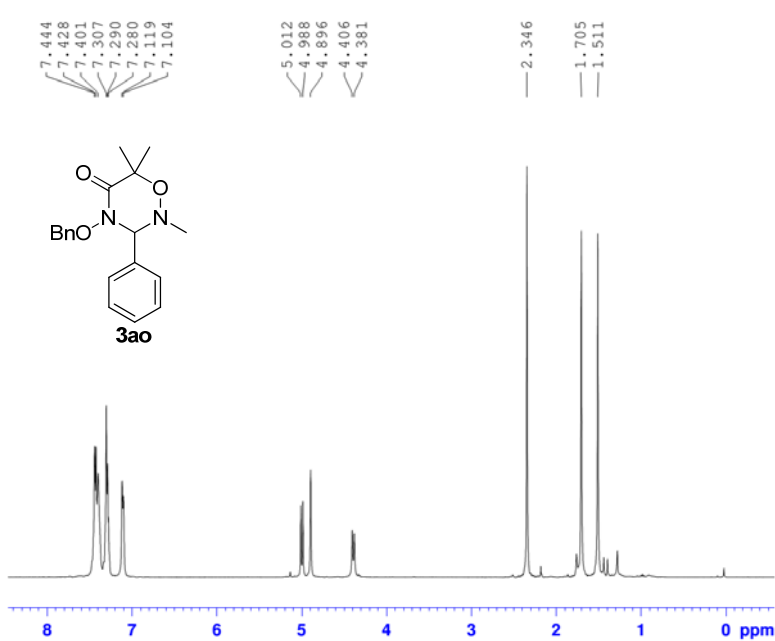


```

NAME      NMR2
EXPNO    4295
PROCNO    1
Date_     20160531
Time      16.17
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         40
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         2050
DW         20.600 usec
DE         6.50 usec
TE         298.2 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         11.70 usec
PL1        -2.00 dB
PL1W       48.76812744 W
SF01       100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -2.83 dB
PL12       12.00 dB
PL13       14.00 dB
PL2W       16.91636658 W
PL12W      0.55629748 W
PL13W      0.35100001 W
SF02       400.1716007 MHz
SI         32768
SF         100.6228270 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

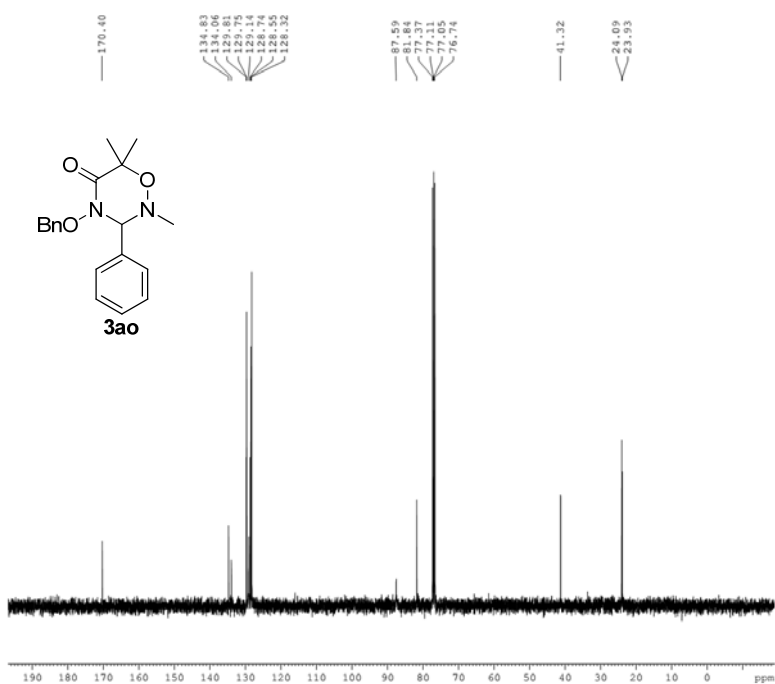


```

NAME      NMR2
EXPNO     4293
PROCNO    1
Date_     20160531
Time      16.06
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         4
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         128
DW         60.800 usec
DE         6.50 usec
TE         297.8 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      1H
P1         14.50 usec
PL1        -2.83 dB
PL1W       16.91636658 W
SFO1       400.1724712 MHz
SI         32768
SF         400.1700000 MHz
WDW        EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00

```



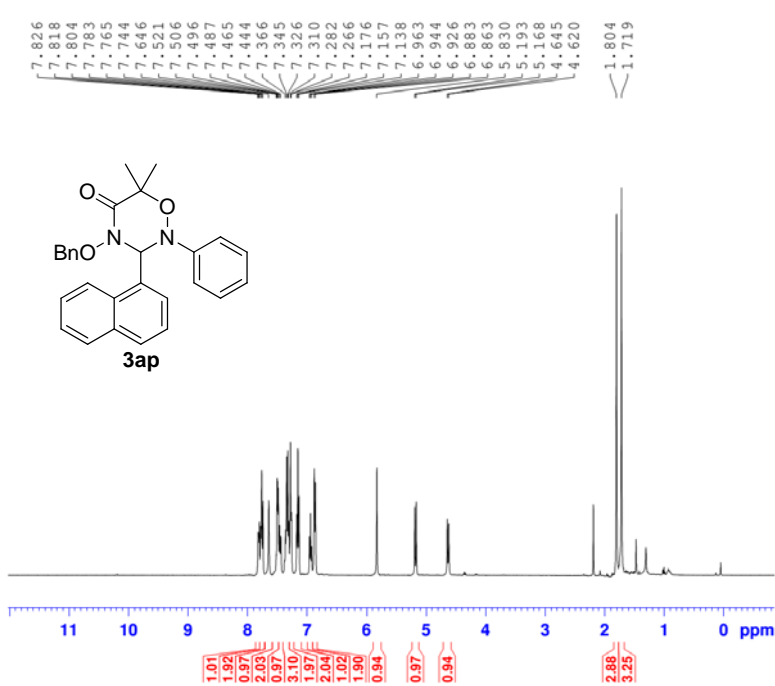
```

NAME      NMR2
EXPNO     4294
PROCNO    1
Date_     20160531
Time      16.09
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         54
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         2050
DW         20.800 usec
DE         6.50 usec
TE         297.8 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      13C
P1         11.70 usec
PL1        -2.00 dB
PL1W       48.76812744 W
SFO1       100.6228270 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2        -2.83 dB
PL12       12.00 dB
PL13       14.00 dB
PL12W     16.91636658 W
PL12W     0.55629748 W
PL13W     0.35100001 W
SFO2       400.1716007 MHz
SI         32768
SF         100.6228270 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40

```

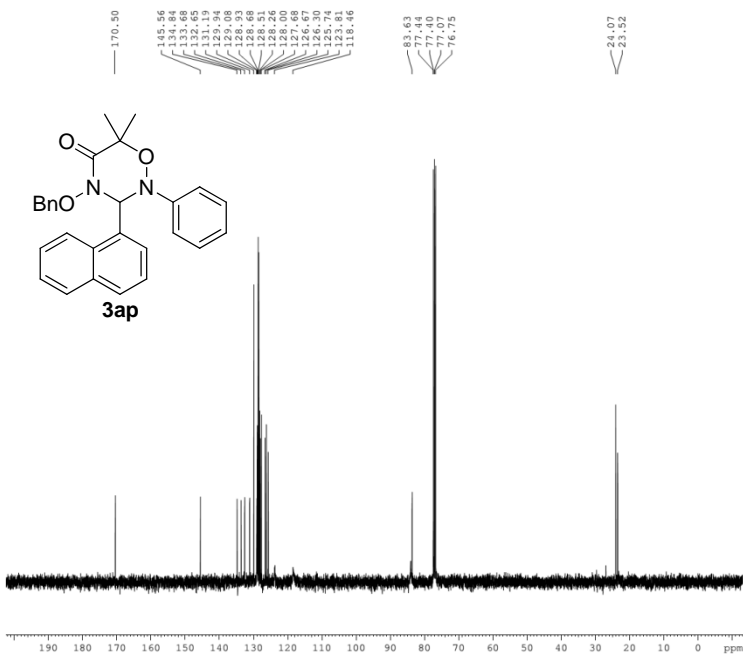



```

NAME          NMR2
EXPNO         4258
PROCNO        1
Date_         20160525
Time          10.37
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            2
DS            2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            128
DW            60.800 usec
DE            6.50 usec
TE            298.0 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            14.50 usec
PL1           -2.83 dB
PL1W          16.91636658 W
SFO1          400.1724712 MHz
SI            32768
SF            400.1700000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



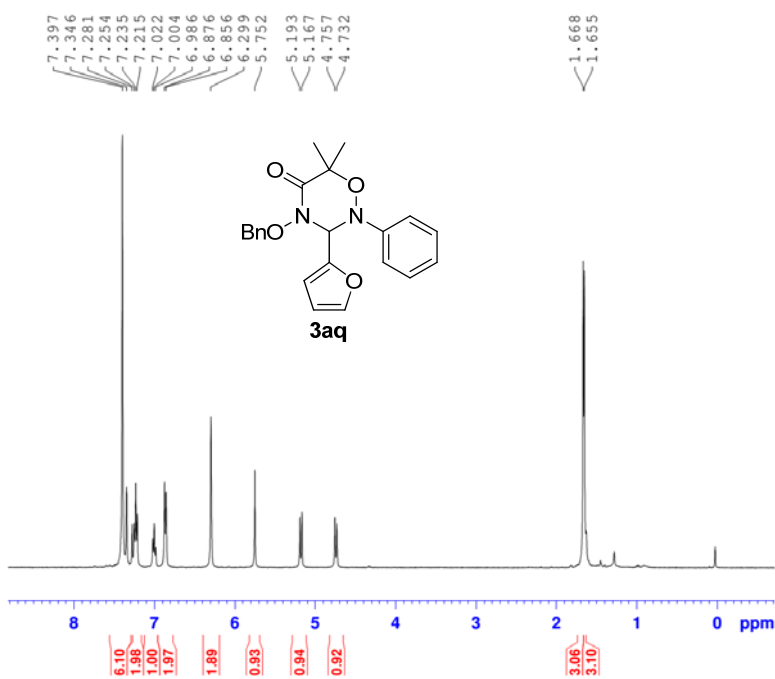
```

NAME          NMR2
EXPNO         4259
PROCNO        1
Date_         20160525
Time          10.40
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            60
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            2050
DW            20.800 usec
DE            6.50 usec
TE            298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            11.70 usec
PL1           -2.00 dB
PL1W          48.76812744 W
SFO1          100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -2.83 dB
PL12          12.00 dB
PL13          14.00 dB
PL2W          16.91636658 W
PL12W         0.55629748 W
PL13W         0.35100001 W
SFO2          400.1716007 MHz
SI            32768
SF            100.6228270 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

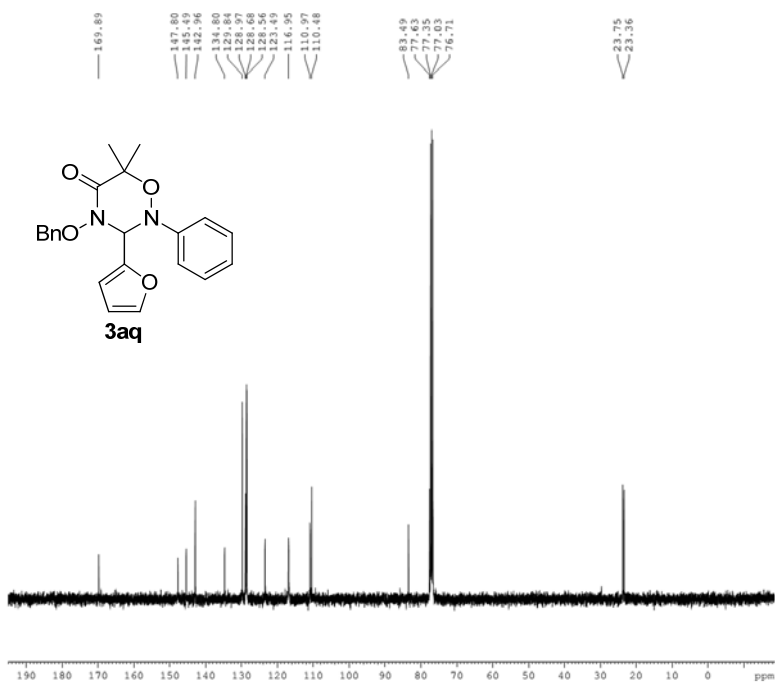
```



```

NAME          NMR2
EXPNO         4235
PROCNO        1
Date_         20160523
Time          11.43
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            2
DS            2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            128
DW            60.800 usec
DE            6.50 usec
TE            298.5 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            14.50 usec
PL1           -2.83 dB
PL1W          16.91636658 W
SFO1          400.1724712 MHz
SI            32768
SF            400.1700000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

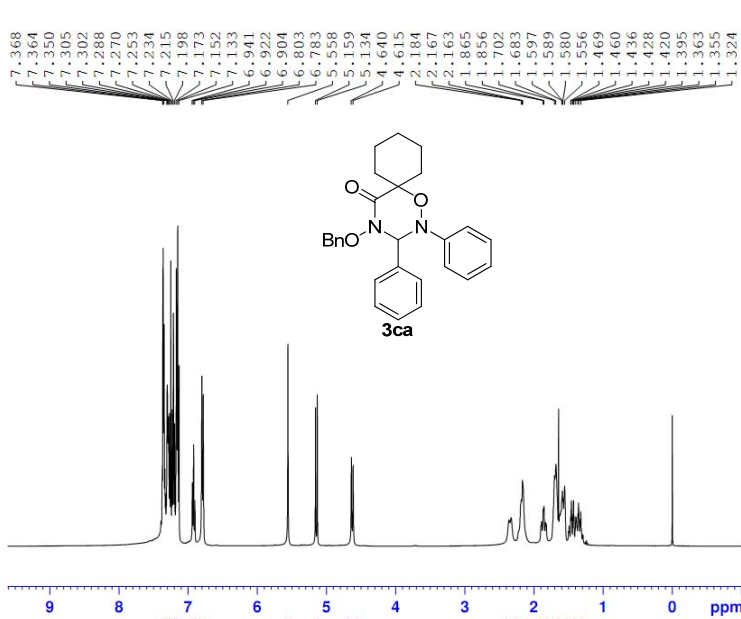


```

NAME          NMR
EXPNO         4342
PROCNO        1
Date_         20160907
Time          10.21
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            198
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            2050
DW            20.800 usec
DE            6.50 usec
TE            673.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

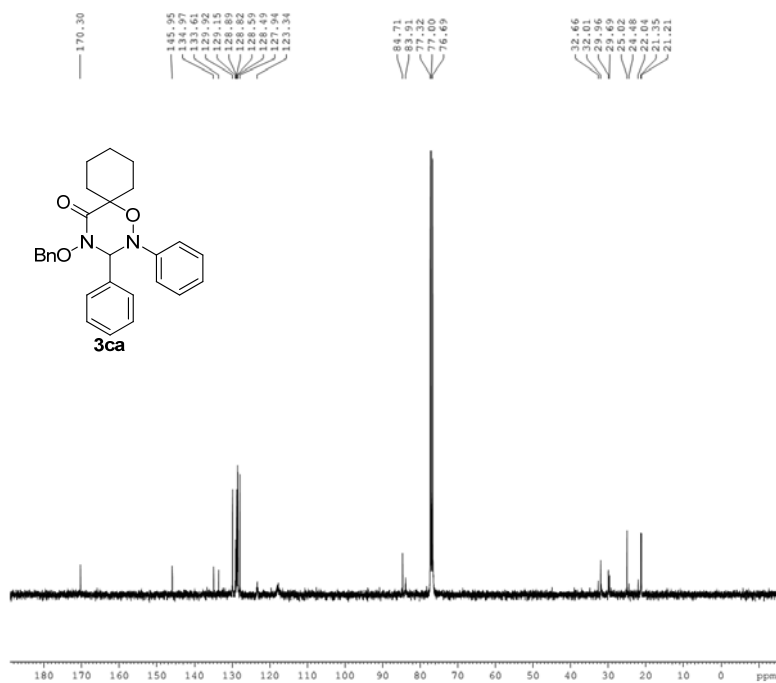
===== CHANNEL f1 =====
NUC1          13C
P1            11.70 usec
PL1           -2.00 dB
PL1W          48.76812744 W
SFO1          100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -2.83 dB
PL12          12.00 dB
PL13          14.00 dB
PL1W          16.91636658 W
PL12W         0.55629748 W
PL13W         0.35100001 W
SFO2          400.1716007 MHz
SI            32768
SF            100.6228270 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



```

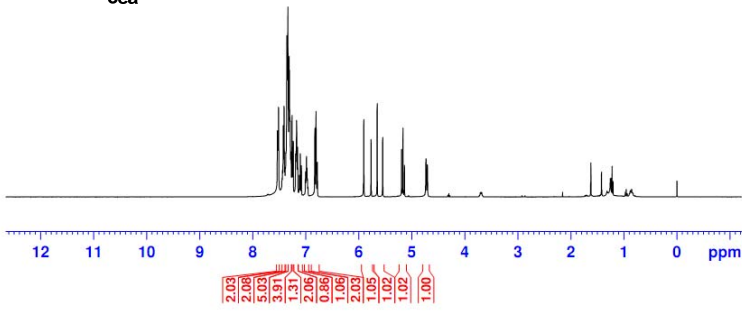
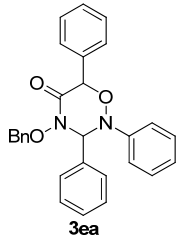
NAME          NMR
EXPNO         20
PROCNO        1
Date_         20170216
Time          12.26 h
INSTRUM       spect
PROBHD        z116098_0406 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ           4.0894966 sec
RG           63.47
DW           62.400 usec
DE           6.50 usec
TE           292.2 K
D1           1.00000000 sec
TDO          1
SFO1         400.1324708 MHz
NUC1          1H
F1           10.00 usec
SI           65536
SF           400.1300126 MHz
WDW           EM
SSB           0
LB           0.30 Hz
GB           0
PC           1.00
  
```



```

NAME          NMR
EXPNO         4359
PROCNO        1
Date_         20160907
Time          15.52
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            512
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ           1.3631988 sec
RG           2050
DW           20.800 usec
DE           6.50 usec
TE           273.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TDO          1
***** CHANNEL f1 *****
NUC1          13C
F1           11.70 usec
PL1          -2.00 dB
PL1W        48.76812744 W
SFO1         100.6228888 MHz
***** CHANNEL f2 *****
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2          -2.83 dB
PL12        12.00 dB
PL13        14.00 dB
PL1W        16.91636658 W
PL2W        0.55629748 W
PL13W       0.35100001 W
SFO2         400.1716007 MHz
SI           32768
SF           100.6228270 MHz
WDW           EM
SSB           0
LB           1.00 Hz
GB           0
PC           1.40
  
```

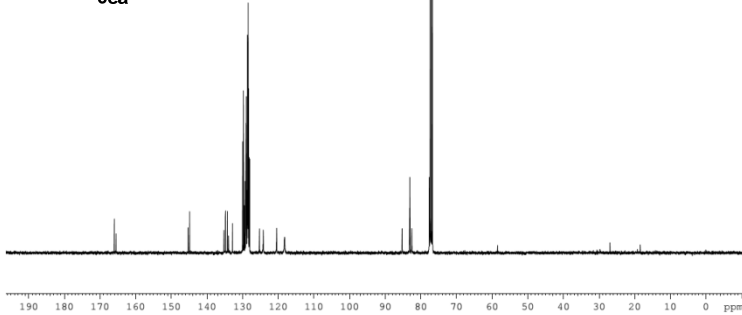
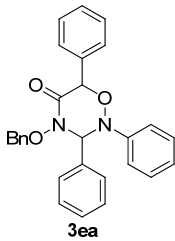
7.535
7.516
7.427
7.412
7.410
7.358
7.355
7.345
7.339
7.316
7.311
7.261
7.244
7.241
7.238
7.195
7.185
7.175
7.156
7.124
7.105
7.085
7.007
6.989
6.829
6.808
6.785
5.907
5.770
5.654
5.550
5.184
5.168
5.140
4.735
4.711



```

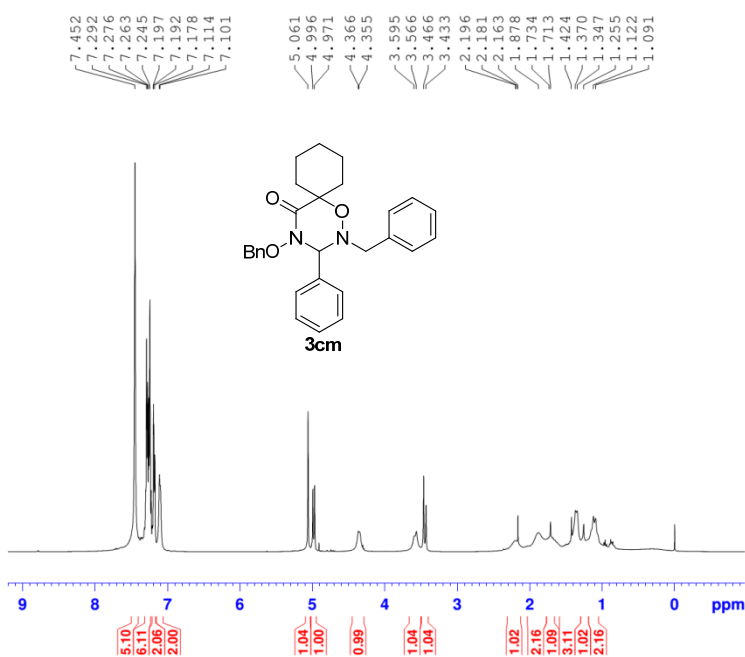
NAME          NMR2
EXPNO         15
PROCNO        1
Date_         20170215
Time          17.02 h
INSTRUM       spect
PROBHD        Z116098_0406 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            50.56
DW            62.400 usec
DE            6.50 usec
TE            292.2 K
D1            1.00000000 sec
TD0           1
SF01          400.1324708 MHz
NUC1          1H
P1            10.00 usec
SI            65536
SF            400.1300189 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

166.05
157.32
155.32
144.32
135.29
134.88
134.85
134.28
132.87
130.04
129.85
129.85
129.37
129.16
129.01
129.01
128.97
128.67
128.67
128.61
128.35
128.35
128.35
128.17
124.26
123.32
123.32
118.26
85.24
83.09
82.09
82.59
77.68
77.10
76.78



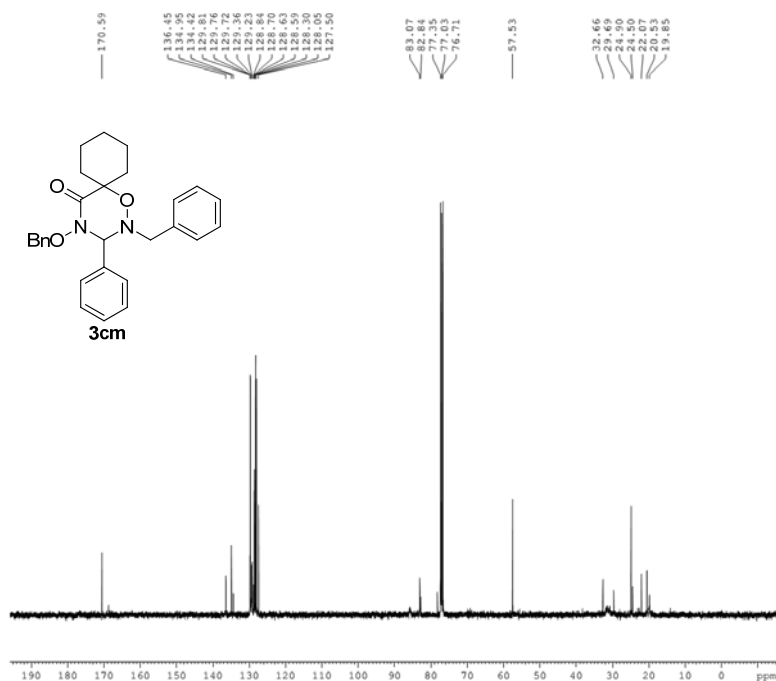
```

NAME          NMR2
EXPNO         16
PROCNO        1
Date_         20170215
Time          18.02 h
INSTRUM       spect
PROBHD        Z116098_0406 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            1024
DS            4
SWH           24033.461 Hz
FIDRES        0.368798 Hz
AQ            1.3631988 sec
RG            196.12
DW            20.800 usec
DE            6.50 usec
TE            292.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
SF01          100.6228298 MHz
NUC1          13C
P1            10.00 usec
SI            32768
SF            100.6127685 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



```

NAME          NMR2
EXPNO         3
PROCNO        1
Date_         20170215
Time          10.32 h
INSTRUM       spect
PROBHD        z116098_0406 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            30.91
DW            62.400 usec
DE            6.50 usec
TE            292.0 K
D1            1.00000000 sec
TDO           1
SFO1          400.1324708 MHz
NUC1          1H
P1            10.00 usec
SI            65536
SF            400.1300142 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

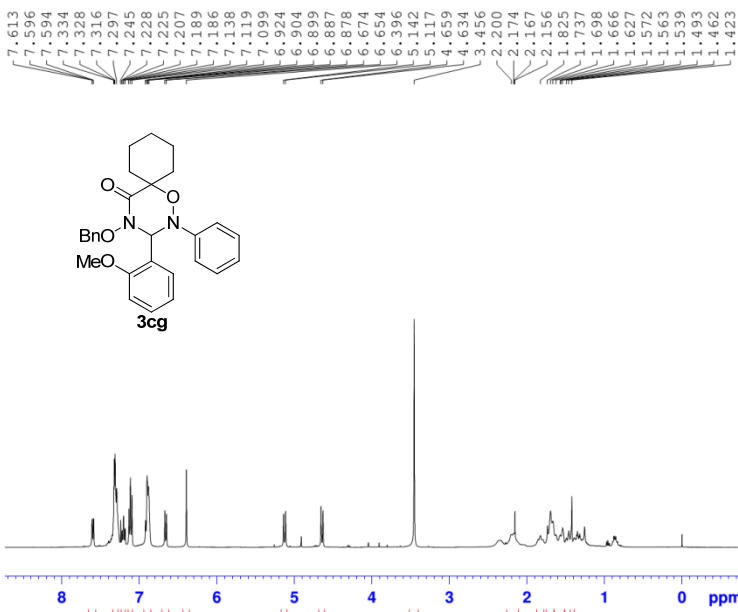


```

NAME          NMR
EXPNO         4364
PROCNO        1
Date_         20160907
Time          16.55
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            304
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            2050
DW            20.800 usec
DE            6.50 usec
TE            673.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TDO           1

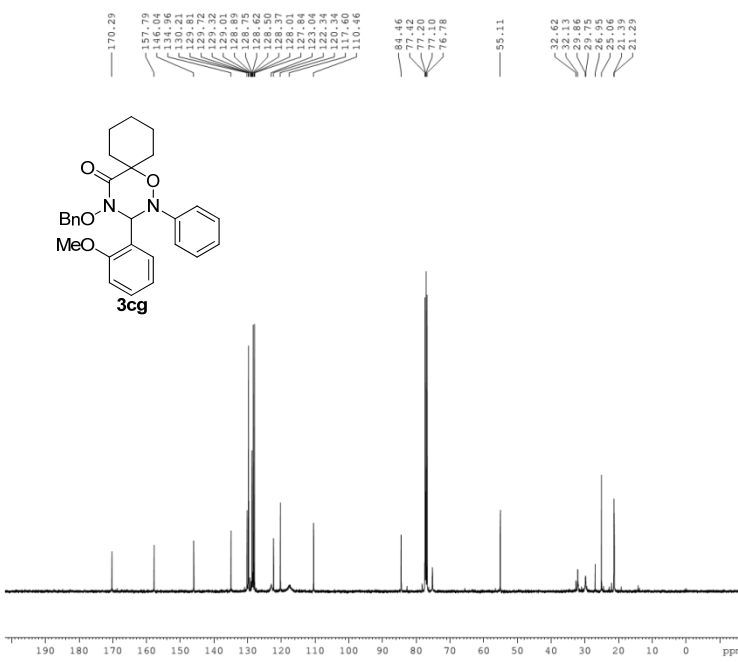
===== CHANNEL f1 =====
NUC1          13C
P1            11.70 usec
PL1           -2.00 dB
PL1W          48.76812744 W
SFO1          100.6328888 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -2.83 dB
PL12          12.00 dB
PL13          14.00 dB
PL2W          16.91636658 W
PL12W         0.55629748 W
PL13W         0.35100001 W
SFO2          400.1716007 MHz
SI            32768
SF            100.6228270 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



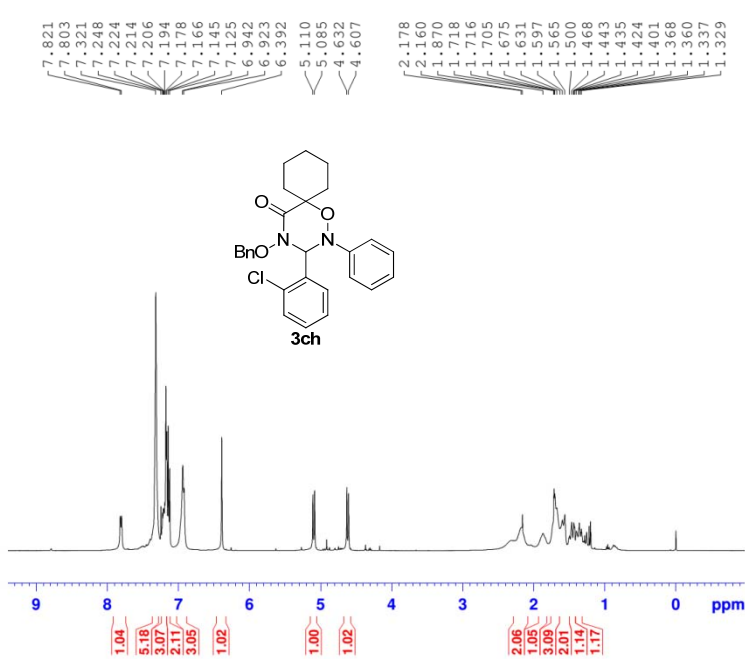
```

NAME          NMR2
EXPNO         13
PROCNO        1
Date_         20170211
Time          15.58 h
INSTRUM       spect
PROBHD        z116098_0406 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            30.91
DW            62.400 usec
DE            6.50 usec
TE            292.1 K
D1            1.00000000 sec
TD0           1
SF01          400.1324708 MHz
NUC1          1H
P1            10.00 usec
SI            65536
SF            400.1300159 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



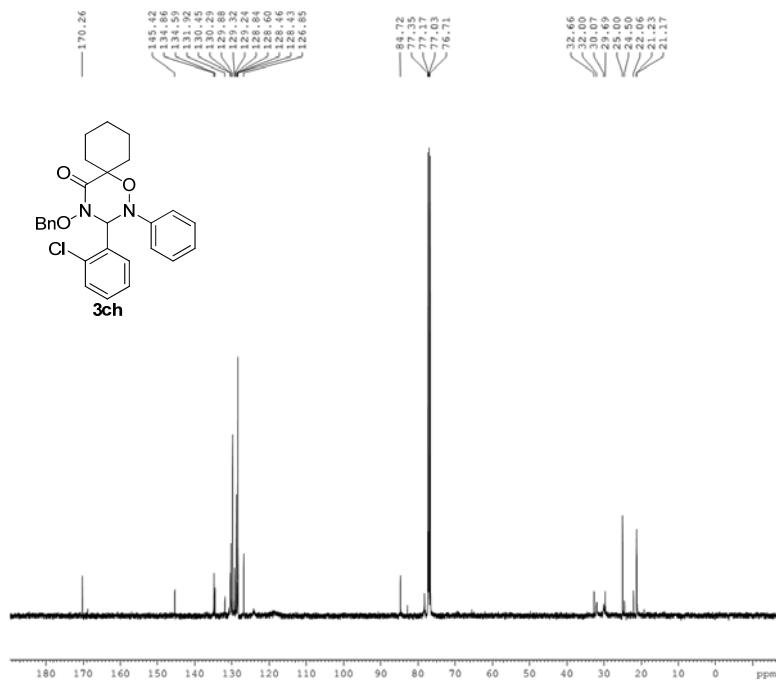
```

NAME          NMR2
EXPNO         14
PROCNO        1
Date_         20170211
Time          16.57 h
INSTRUM       spect
PROBHD        z116098_0406 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            1024
DS            4
SWH           24033.461 Hz
FIDRES        0.368798 Hz
AQ            1.3631988 sec
RG            196.12
DW            20.800 usec
DE            6.50 usec
TE            292.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
SF01          100.6228298 MHz
NUC1          13C
P1            10.00 usec
SI            32768
SF            100.6127685 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



```

NAME          NMR2
EXPNO         5
PROCNO       1
Date_        20170215
Time         11.36 h
INSTRUM      spect
PROBHD       Z116098_0406 (
PULPROG      zg30
TD           65536
SOLVENT      CDCl3
NS           16
DS           2
SWH          8012.820 Hz
FIDRES       0.122266 Hz
AQ           4.0894966 sec
RG           30.91
DW           62.400 usec
DE           6.50 usec
TE           292.2 K
D1           1.00000000 sec
TD0          1
SFO1         400.1324708 MHz
NUC1         1H
P1           10.00 usec
SI           65536
SF           400.1300144 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```



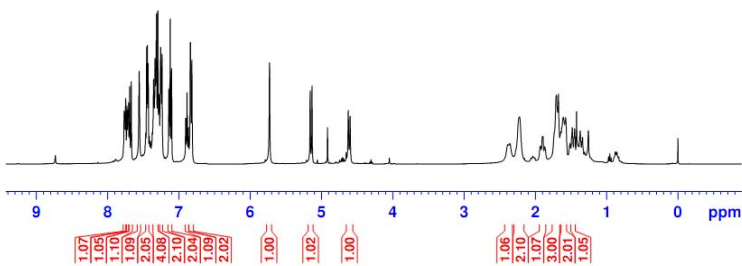
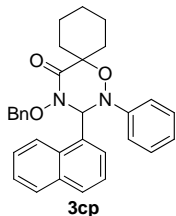
```

NAME          NMR
EXPNO         4343
PROCNO       1
Date_        20160907
Time         10.38
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           637
DS           4
SWH          24038.461 Hz
FIDRES       0.366798 Hz
AQ           1.3631988 sec
RG           2050
DW           20.800 usec
DE           6.50 usec
TE           673.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0          1

***** CHANNEL f1 *****
NUC1         13C
P1           11.70 usec
PL1         -2.00 dB
PL1W        48.76812744 W
SFO1         100.6328888 MHz

***** CHANNEL f2 *****
CPDPRG2      waltz16
NUC2         1H
PCPD2       80.00 usec
PL2         -2.83 dB
PL12        12.00 dB
PL13        14.00 dB
PL2W        16.91636658 W
PL12W       0.55629748 W
PL13W       0.35100001 W
SFO2         400.1716007 MHz
SI           32768
SF           100.6228270 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

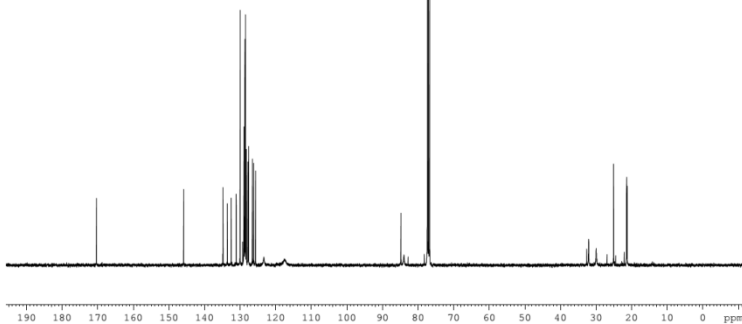
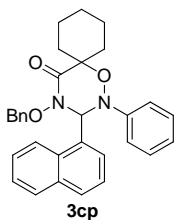
7.772
7.762
7.749
7.732
7.718
7.709
7.693
7.671
7.559
7.454
7.444
7.434
7.356
7.337
7.330
7.316
7.298
7.282
7.258
7.239
7.144
7.124
7.104
6.906
6.888
6.870
6.840
6.820
5.731
5.160
5.134
4.625
4.599
2.222
1.902
1.894
1.706
1.676
1.609
1.574
1.490
1.483
1.458
1.450



```

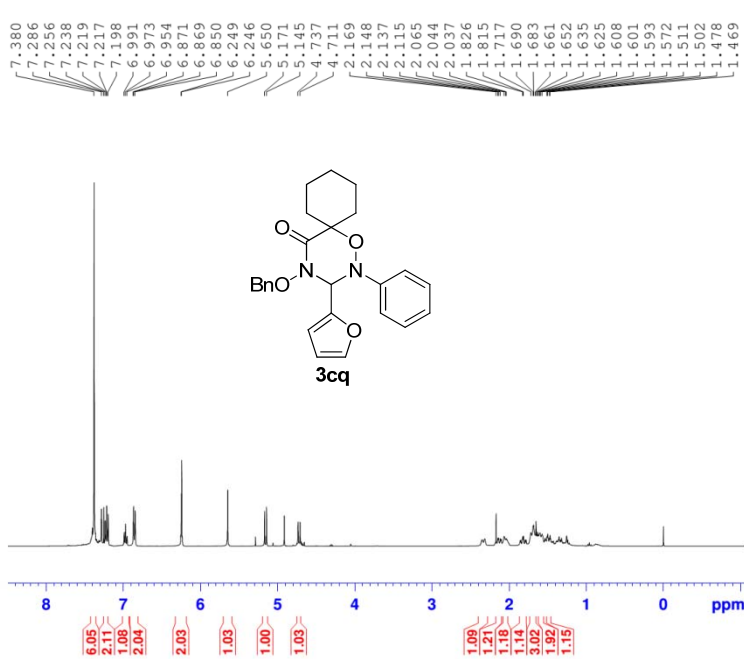
NAME          NMR2
EXPNO         7
PROCNO        1
Date_         20170215
Time          12.40 h
INSTRUM       spect
PROBHD        z116098_0406 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            30.91
DW            62.400 usec
DE            6.50 usec
TE            292.2 K
D1            1.00000000 sec
TD0           1
SFO1          400.1324708 MHz
NUC1          1H
P1            10.00 usec
SI            65536
SF            400.1300180 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

170.44
165.81
154.92
154.86
153.61
153.61
151.15
151.02
150.02
148.98
148.94
148.94
148.95
148.53
148.39
148.39
147.66
147.66
146.23
146.23
145.72
145.72
142.97
142.97
84.84
77.30
77.30
77.09
76.77
32.62
32.09
32.09
26.98
26.98
23.05
23.05
23.50
23.50
21.41
21.41
21.26



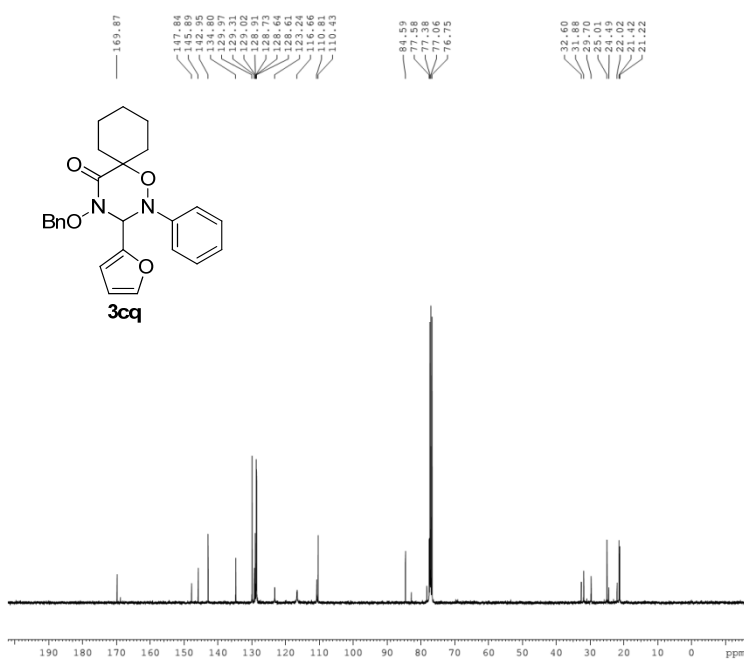
```

NAME          NMR2
EXPNO         8
PROCNO        1
Date_         20170215
Time          13.39 h
INSTRUM       spect
PROBHD        z116098_0406 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            1024
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            196.12
DW            20.800 usec
DE            6.50 usec
TE            292.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
SFO1          100.6228298 MHz
NUC1          13C
P1            10.00 usec
SI            32768
SF            100.6127685 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

```

NAME          NMR2
EXPNO         1
PROCNO       1
Date_        20170215
Time         9.27 h
INSTRUM      spect
PROBHD       z116098_0406 (
PULPROG      zg30
TD           65536
SOLVENT      CDCl3
NS           16
DS           2
SWH          8012.820 Hz
FIDRES       0.122266 Hz
AQ           4.0894966 sec
RG           63.47
DW           62.400 usec
DE           6.50 usec
TE           291.8 K
D1           1.00000000 sec
TDO          1
SFO1         400.1324708 MHz
NUC1         1H
P1           10.00 usec
SI           65536
SF           400.1300112 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```



```

NAME          NMR2
EXPNO         2
PROCNO       1
Date_        20170215
Time        10.27 h
INSTRUM      spect
PROBHD       z116098_0406 (
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           1024
DS           4
SWH          24038.461 Hz
FIDRES       0.366798 Hz
AQ           1.3631988 sec
RG           196.12
DW           20.800 usec
DE           6.50 usec
TE           292.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TDO          1
SFO1         100.6228298 MHz
NUC1         13C
P1           10.00 usec
SI           32768
SF           100.6127685 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

2. X-Ray crystal data of compound 3ad

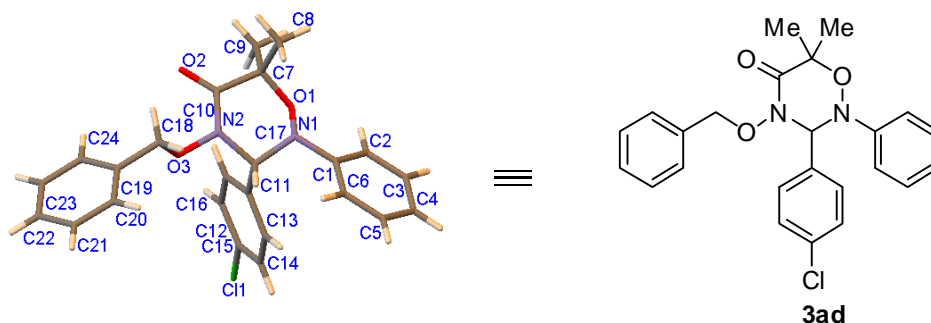


Figure 1. X-ray single crystal structure of 3ad (with thermal ellipsoids shown at the 50% probability level)

| | |
|---------------------------------|--|
| Identification code | 3ad |
| Empirical formula | $C_{24}H_{23}ClN_2O_3$ |
| Formula weight | 422.89 |
| Temperature | 113(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Orthorhombic, $Pca2(1)$ |
| Unit cell dimensions | a = 22.150(4) Å alpha = 90 deg. b = 5.9700(10) Å beta = 90 deg. c = 15.611(3) Å gamma = 90 deg. |
| Volume | 2064.2(6) Å ³ |
| Z, Calculated density | 4, 1.361 Mg/m ³ |
| Absorption coefficient | 0.214 mm ⁻¹ |
| F(000) | 888 |
| Crystal size | 0.2 x 0.18 x 0.12 mm |
| Theta range for data collection | 3.193 to 27.501 deg. |
| Limiting indices | -27 ≤ h ≤ 28, -7 ≤ k ≤ 7, -20 ≤ l ≤ 19 |

| | |
|-----------------------------------|---|
| Reflections collected / unique | 19944 / 4605 [R(int) = 0.0245] |
| Completeness to theta = 27.55 | 99.8 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 1.000 and 0.941 |
| Refinement method | Full-matrix least-squares on F ² |
| Data / restraints / parameters | 4605 / 1 / 273 |
| Goodness-of-fit on F ² | 1.041 |
| Final R indices [I > 2σ(I)] | R1 = 0.0221, wR2 = 0.0583 |
| R indices (all data) | R1 = 0.0231, wR2 = 0.0588 |
| Absolute structure parameter | -0.009(14) |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.204 and -0.150 e.Å ⁻³ |