

Supporting Information

Implications of dynamic imine chemistry to the sustainable synthesis of nitrogen heterocycles via transimination followed by intramolecular cyclisation

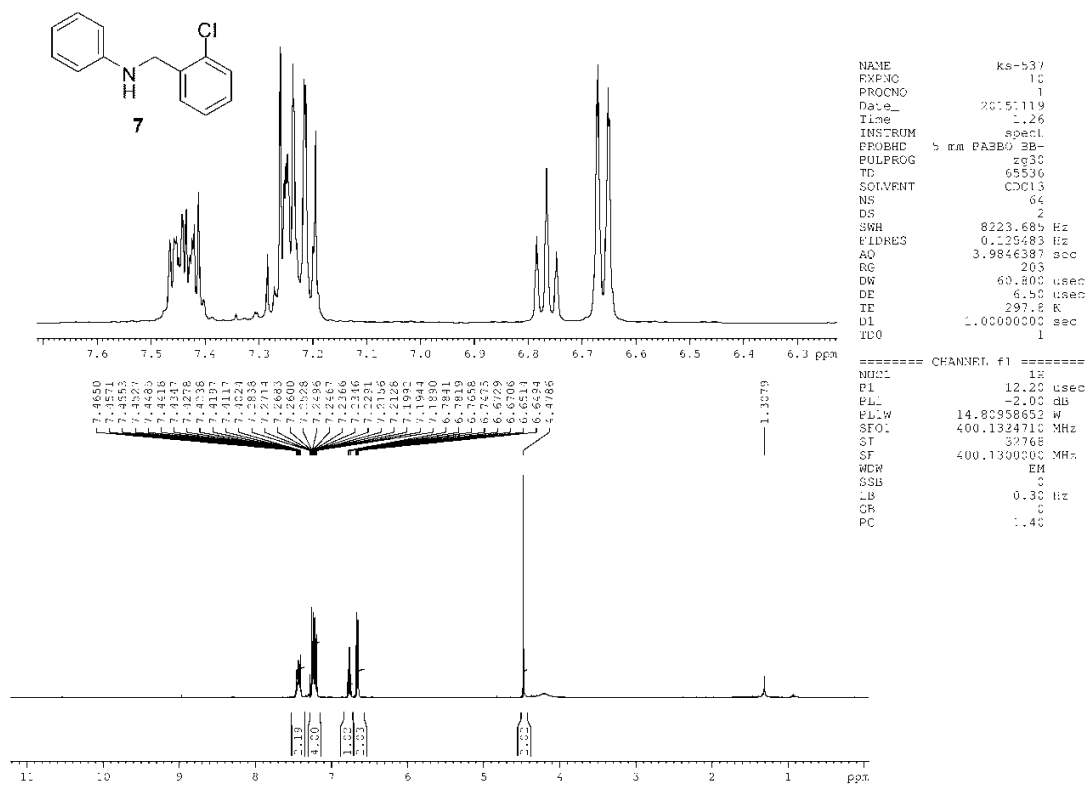
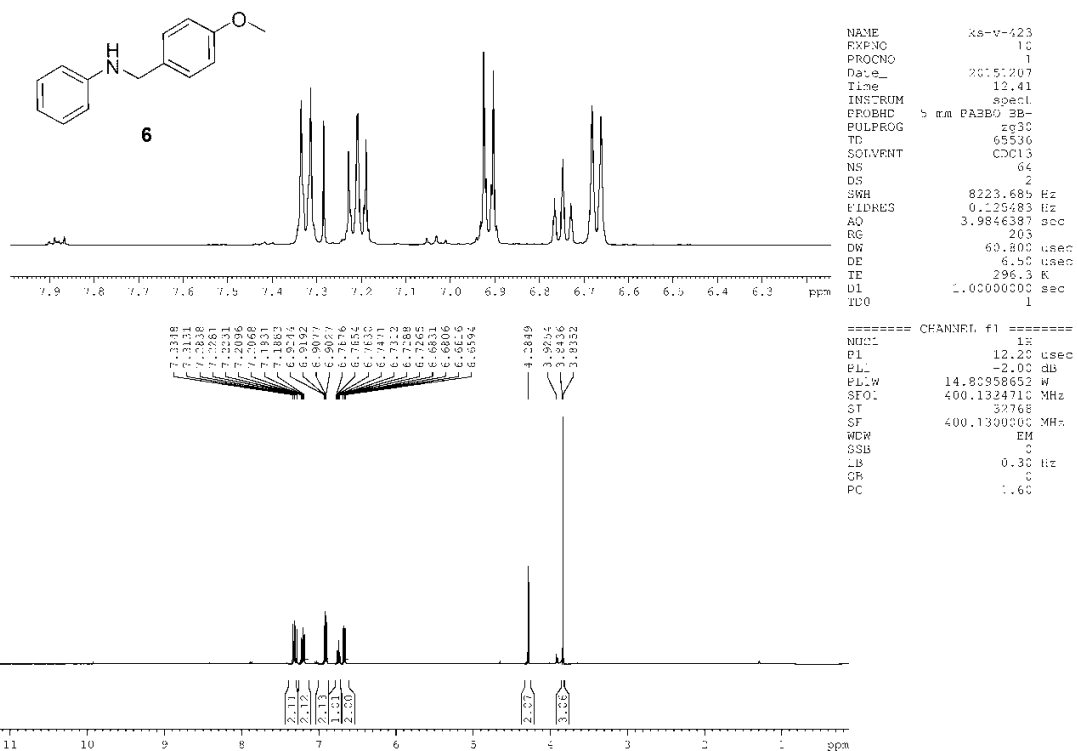
Joydev K. Laha, K. S. Satyanarayana Tummalapalli, and Krupal P. Jethava*

Department of Pharmaceutical Technology (Process Chemistry)

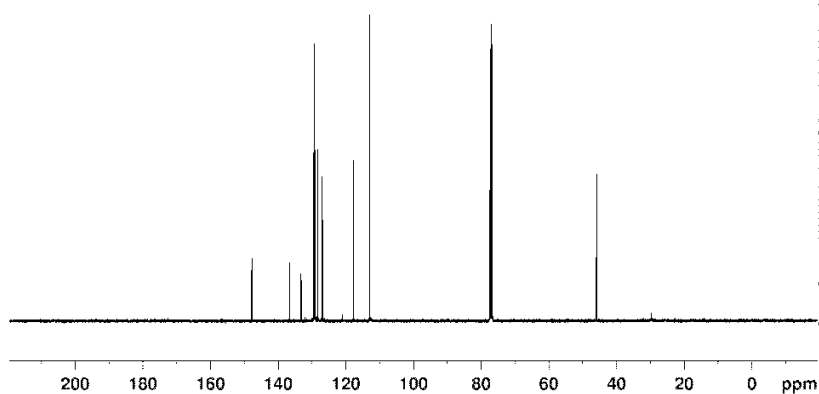
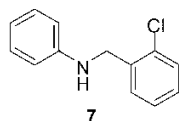
National Institute of Pharmaceutical Education and Research

S. A. S. Nagar, Punjab 160062

INDIA



ks-537
 C13CPD CDCl3 (D:\CIL\JKLara_108\NMR\2015\Nov) Administrator 20



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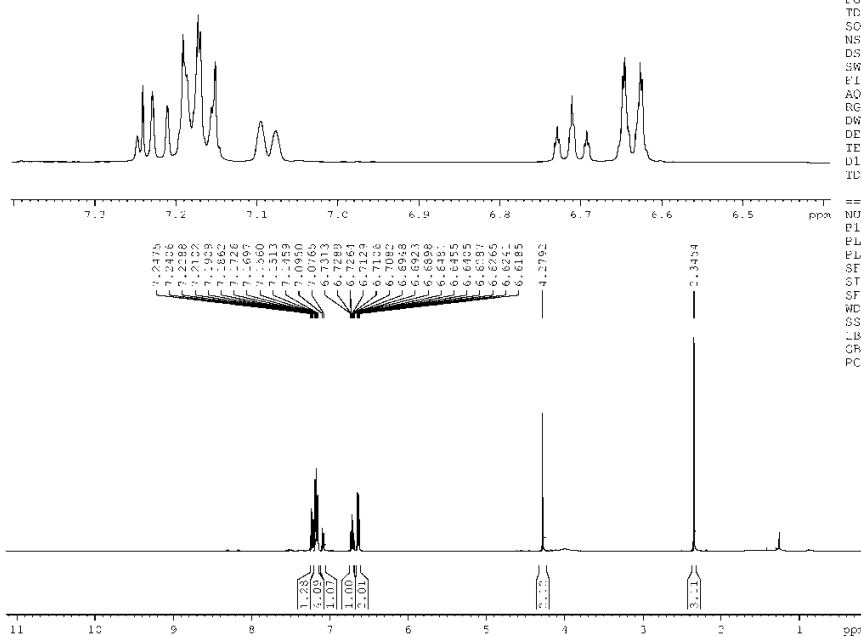
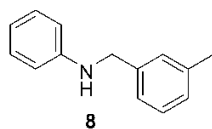
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PROCNO   1
Date_    20151119
Time     2.25
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       1024
DS       4
SWH      24038.46 Hz
FIDRES   0.366738 Hz
AQ       1.363198 sec
RG       203
DW       20.300 usec
DE       6.50 usec
TE       293.5 K
D1       2.0000000 sec
D11      0.3300000 sec
TD0      .
  
```

```

----- CHANNEL f1 -----
NUC1     13C
P1       9.50 usec
PL1     -1.00 dB
PL1W    44.90434265 W
SFO1    100.6228938 MHz
  
```

```

===== CHANNEL f2 =====
CFDPRG2  waitz15
NUC2     1H
PCPD2    89.00 usec
PL2     -2.00 dB
PL12    14.33 dB
PL13    18.33 dB
PL2W    14.30958652 W
PL12W   0.34478072 W
PL13W   0.13725965 W
SFO2    400.1316005 MHz
SI       32768
SF       100.6127630 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
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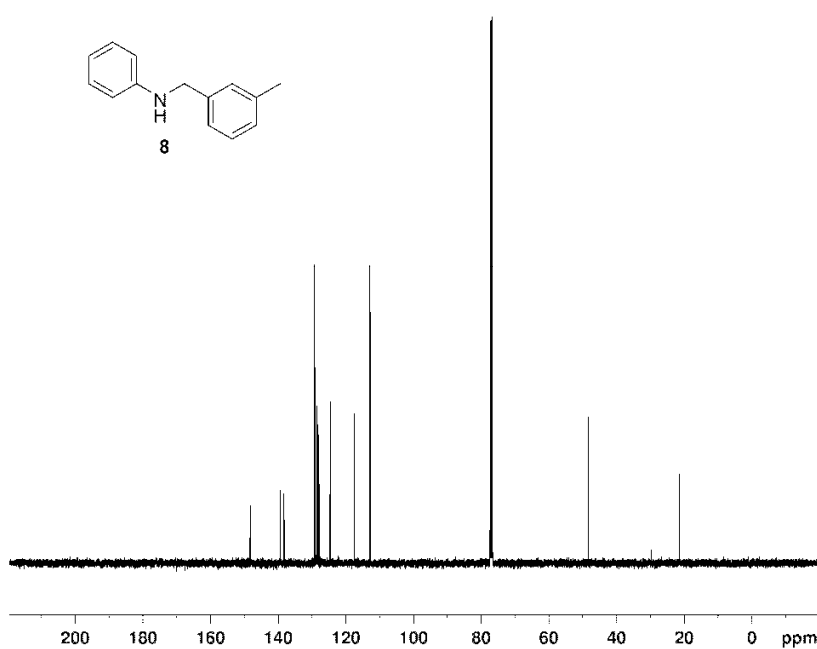
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PROCNO   1
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Time     11.52
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       64
DS       2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ       3.9846387 sec
RG       203
DW       60.800 usec
DE       6.50 usec
TE       297.8 K
D1       1.0000000 sec
TD0      1
  
```

```

===== CHANNEL f1 =====
NUC1     1H
P1       12.20 usec
PL1     -2.00 dB
PL1W    14.80398652 W
SFO1    400.1324111 MHz
SI       32768
SF       400.1300174 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.40
  
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ks-v-424
 C13CPD CDCl3 {D:\CIL\JKLabz_108\NMR\2015\July} Administrator 17

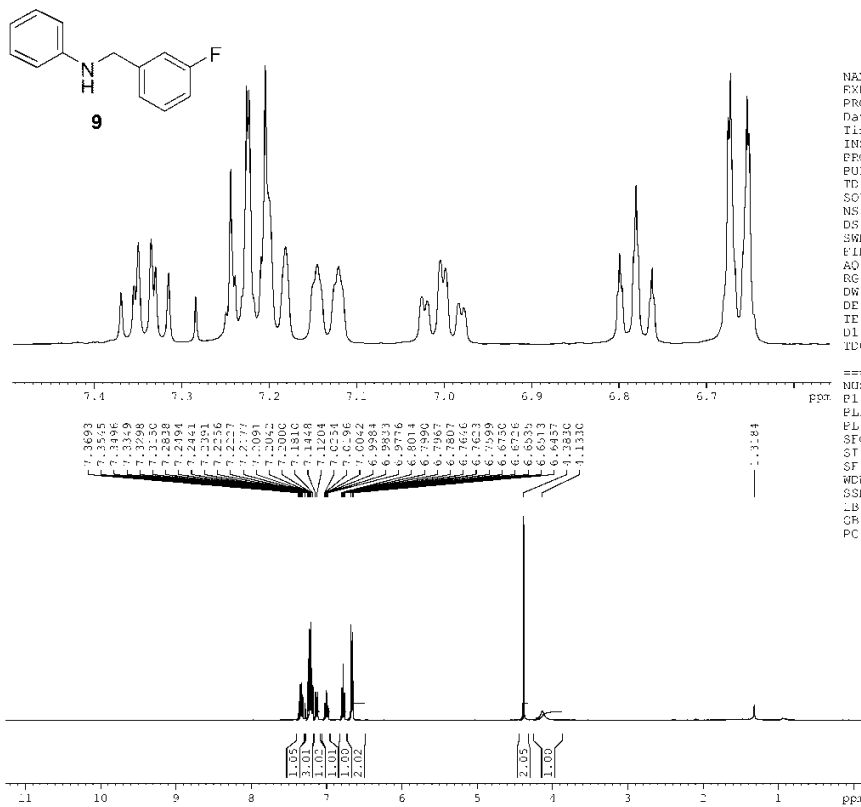


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NAME      ks v 424
EXPNO    1
PROCNO   1
Date_    20150722
Time     17.30
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        2
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG         203
DW        20.500 usec
DE        6.50 usec
TE        298.5 K
D1        2.3600000 sec
D11       0.3300000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       1.00 dB
PL1W      44.96434265 W
SFO1      100.6228298 MHz

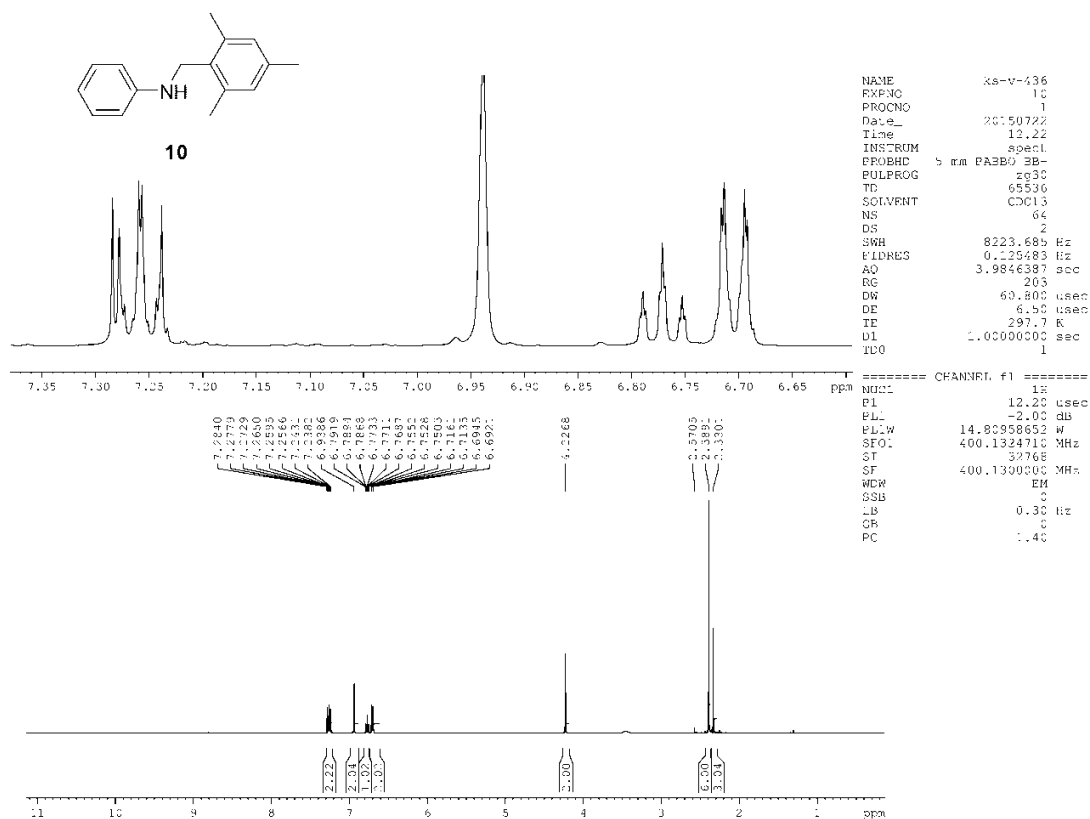
===== CHANNEL f2 =====
CPDPRG2   waitz15
NUC2       1H
PCPD2     80.00 usec
PF2       -2.00 dB
PL12      14.33 dB
PL13      18.33 dB
PL1W      14.80958652 W
PL12W     0.34478072 W
PL13W     0.13725966 W
SFO2      400.1316005 MHz
SI         32768
SF        100.6127690 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB         0
PC        1.40
  
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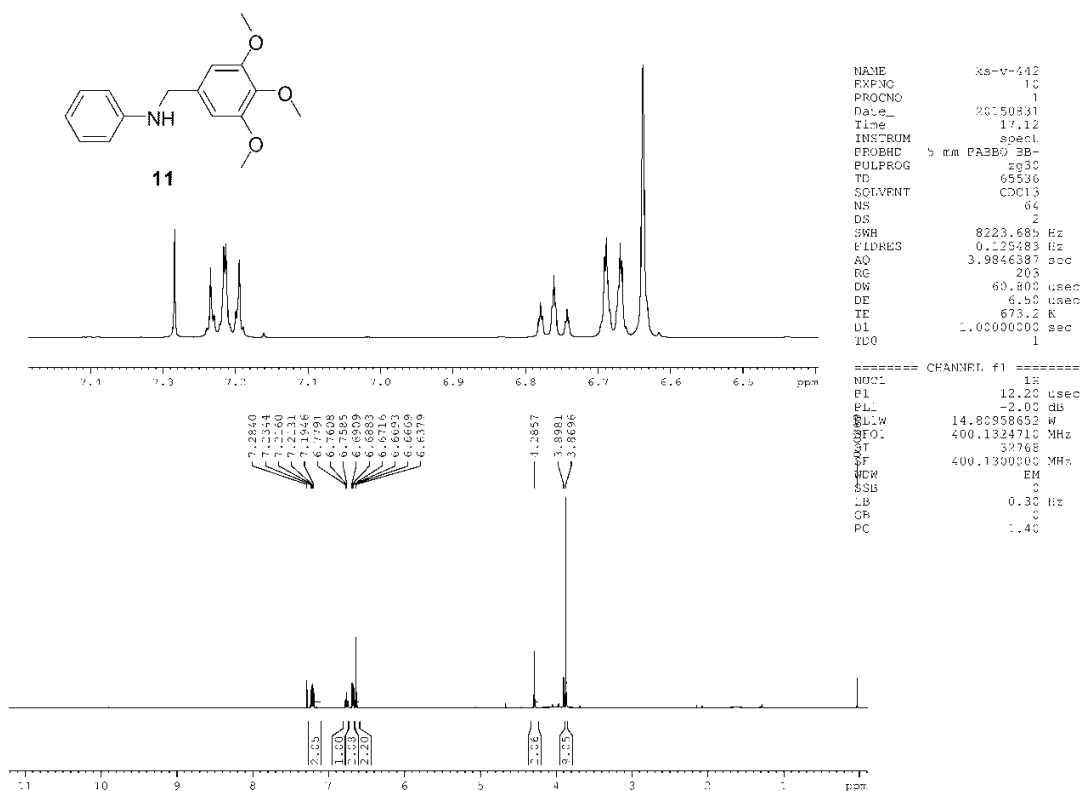


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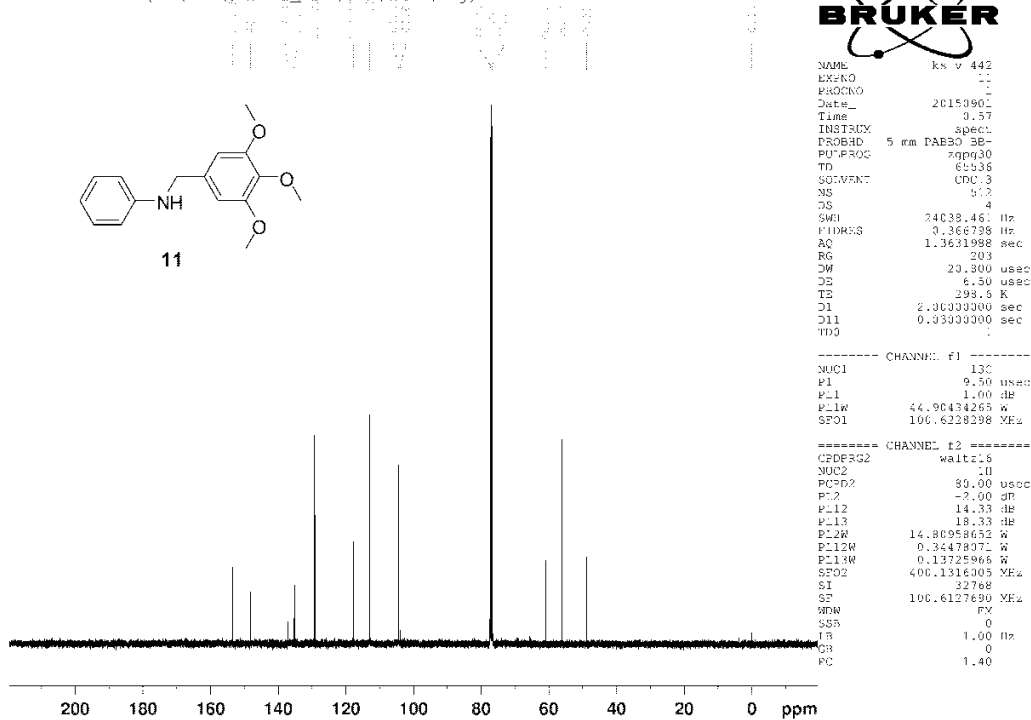
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PROCNO   1
Date_    20151119
Time     0.16
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        64
DS        2
SWH       8223.685 Hz
FIDRES    0.129483 Hz
AQ        3.9846387 sec
RG         161
DW        60.800 usec
DE        6.50 usec
TE        297.9 K
D1        1.0000000 sec
TD0       1

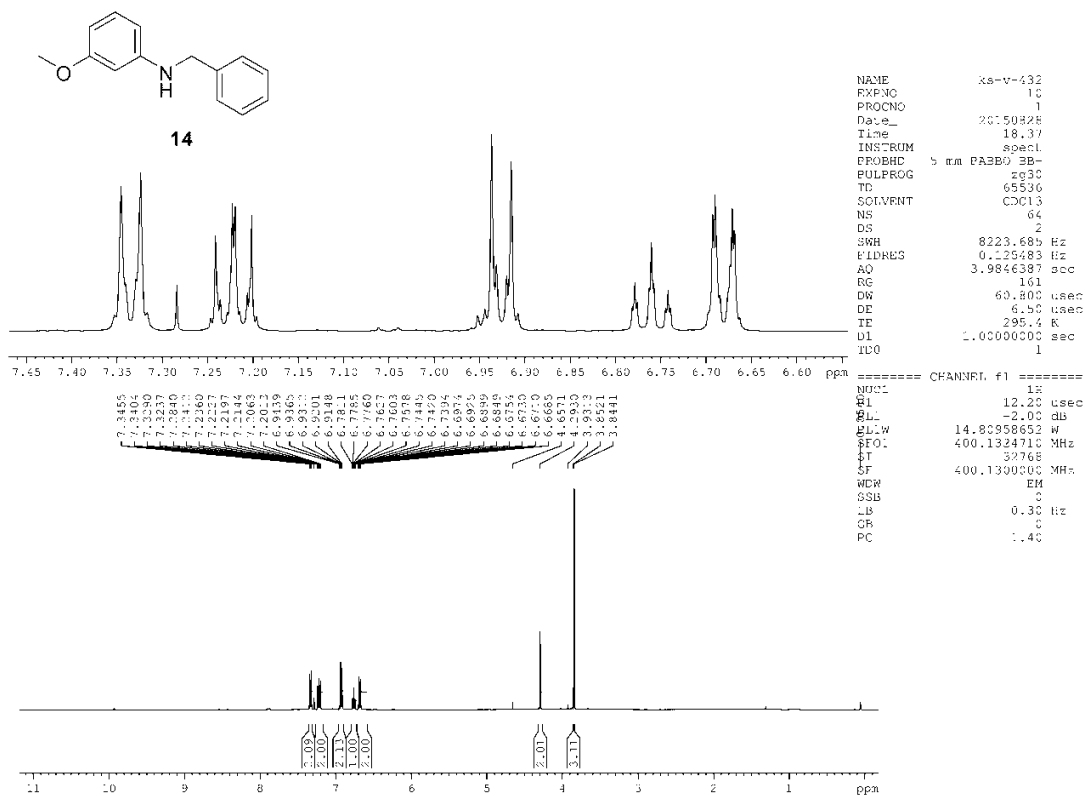
===== CHANNEL f1 =====
NUC1      1H
P1        12.00 usec
PL1       -2.00 dB
PL1W      14.80958652 W
SFO1      400.1324710 MHz
SI         32768
SF        400.1300000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB         0
PC        1.40
  
```



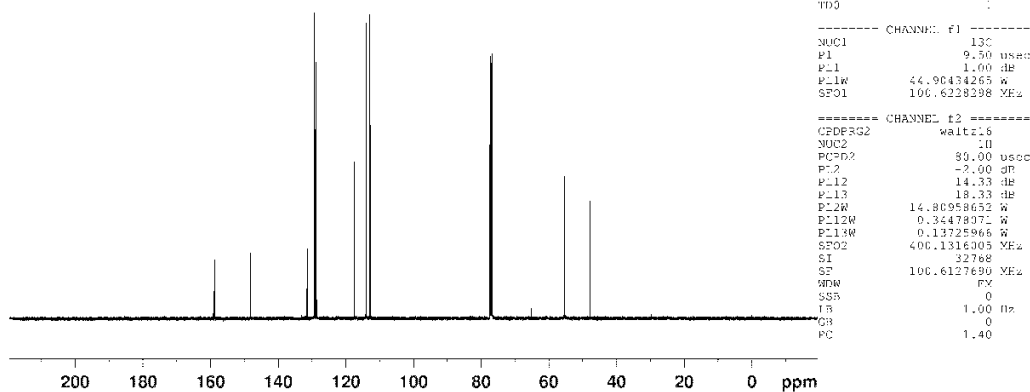
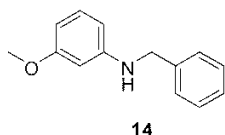


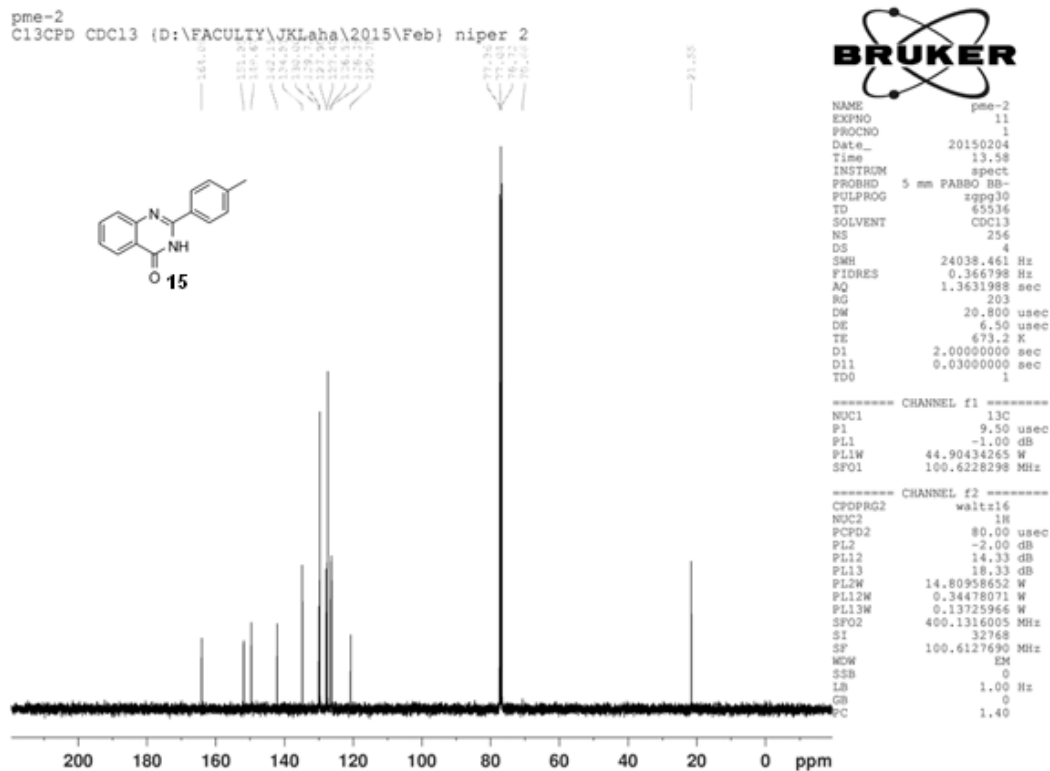
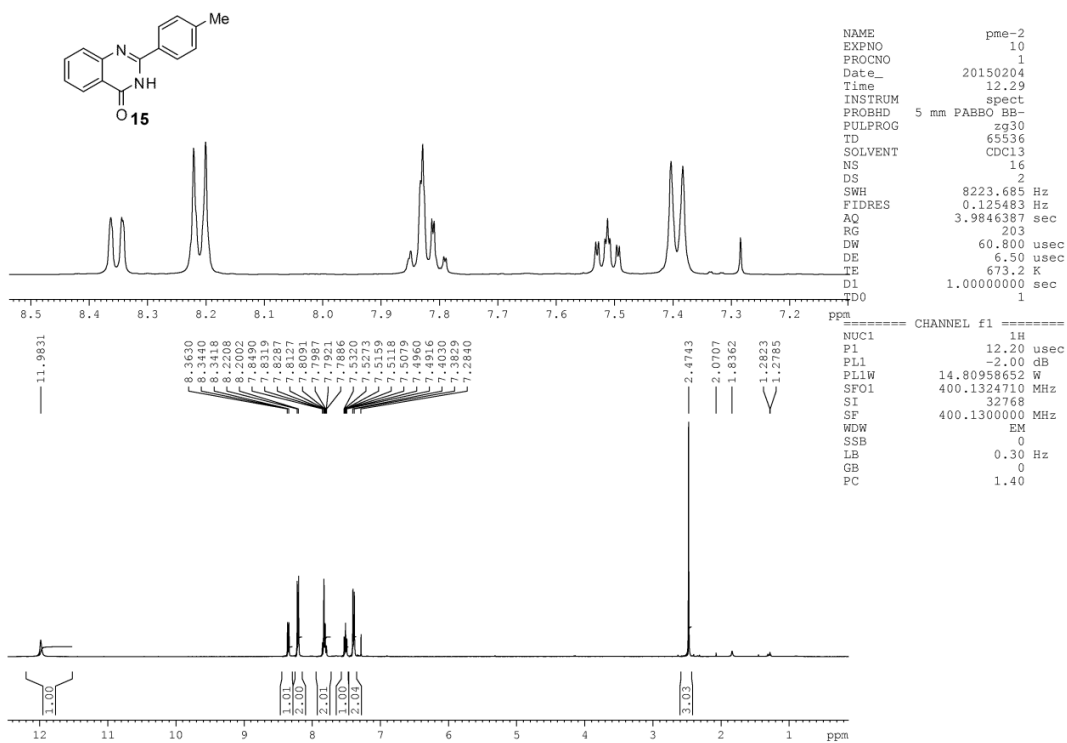
ks-v-442
C13CPD CDCl3 (D:\NCIL\JKLaha_108\NMR\2015\Aug) Administrator 24

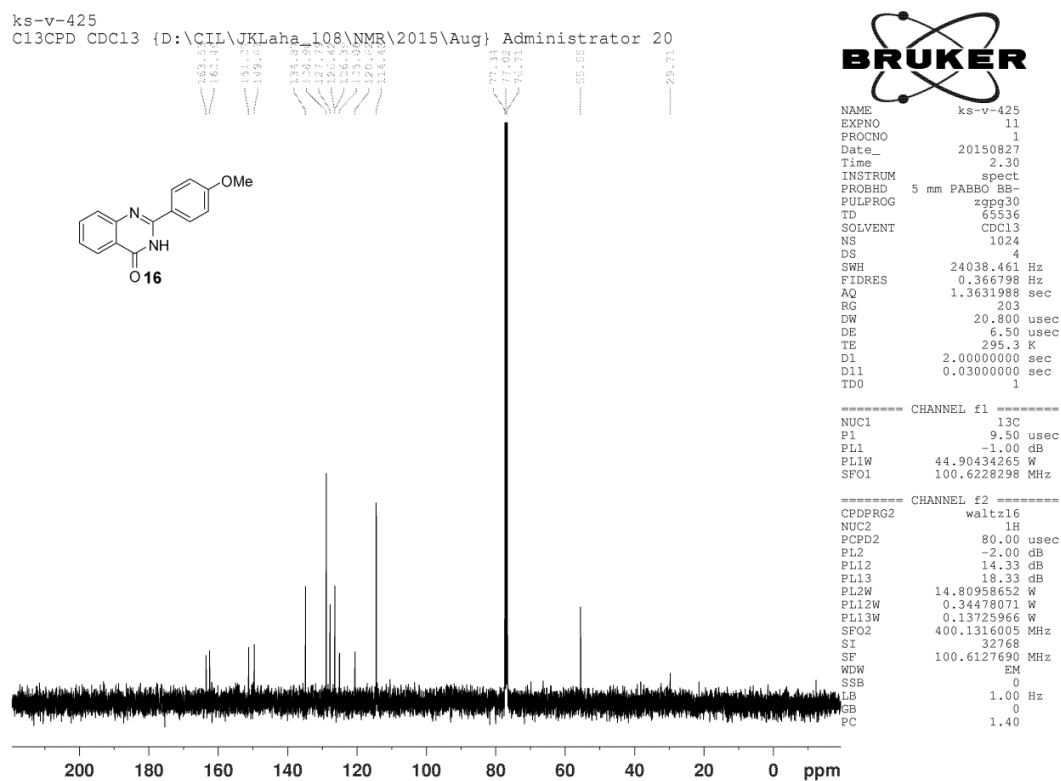
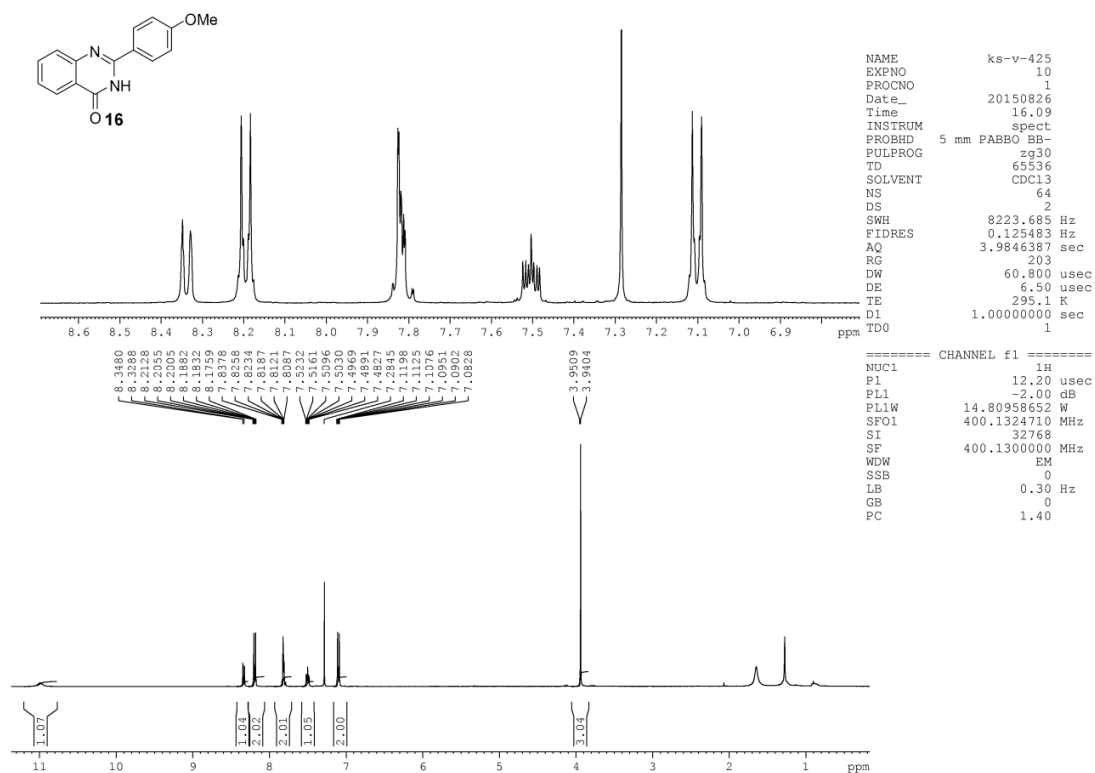


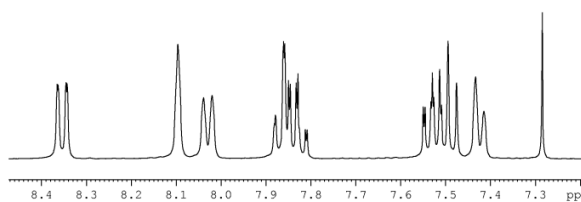
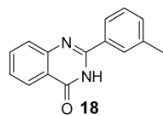


ks-v-432
 C13CPD5.L2 CDCl3 (D:\C1L\JKLaha_108\NMR\2015\Aug; Administrator 23



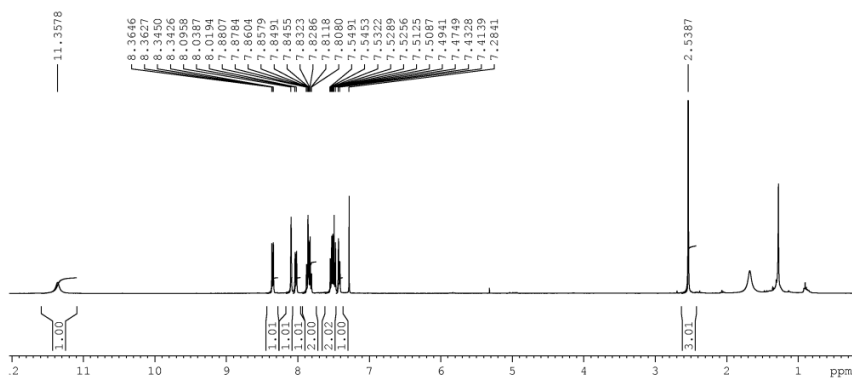






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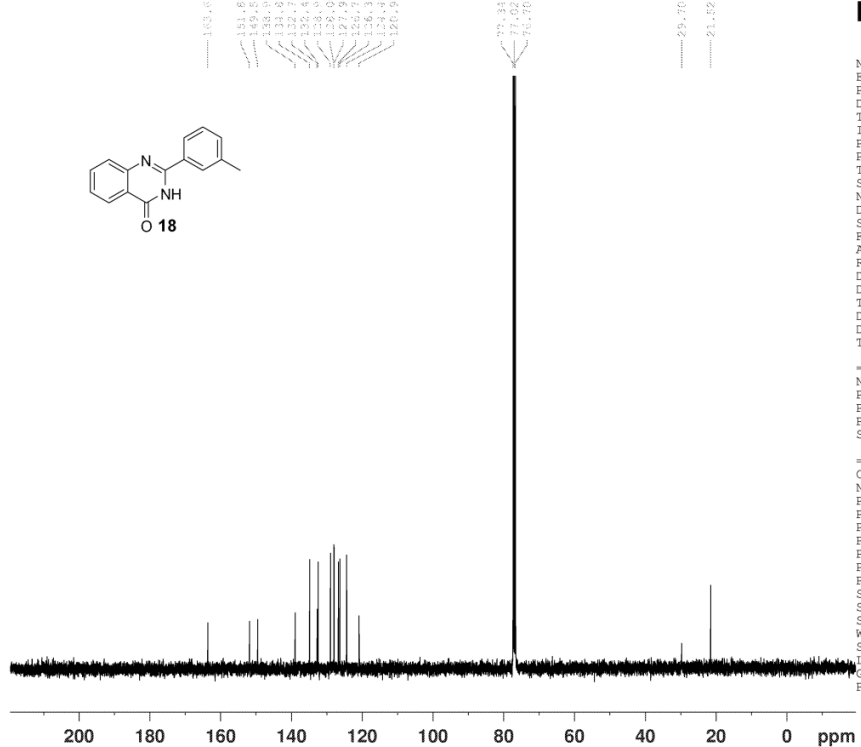
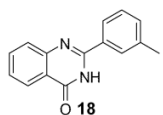
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PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       64
DS       2
SWH      8223.685 Hz
AQ       0.125483 Hz
FIDRES   3.9846387 sec
RG       203
DW       60.800 usec
DE       6.50 usec
TE       297.8 K
D1       1.00000000 sec
TD0     1
    
```



```

===== CHANNEL f1 =====
NUC1    1H
P1      12.20 usec
PL1     -2.00 dB
PL1W    14.80958652 W
SFO1    400.1324710 MHz
SI      32768
SF      400.1300000 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.40
    
```

ks-v-429-f
C13CPD512 CDCl3 (D:\CII\JKLaha_108\NMR\2015\Sep) Administrator 27



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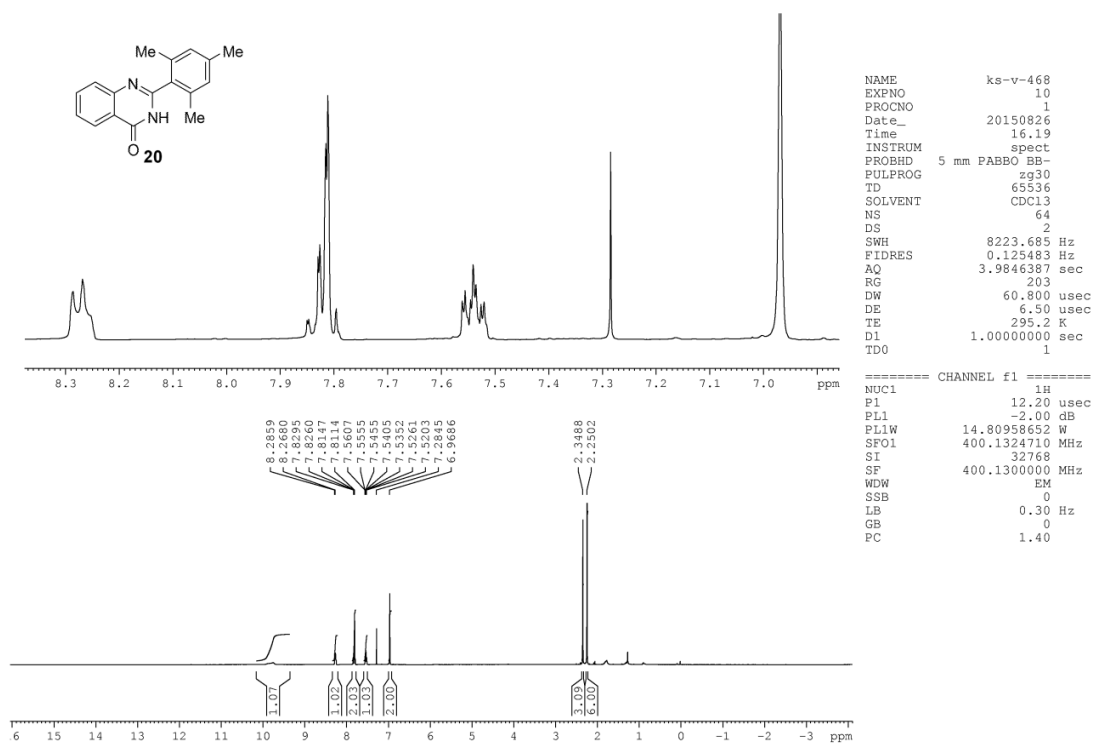
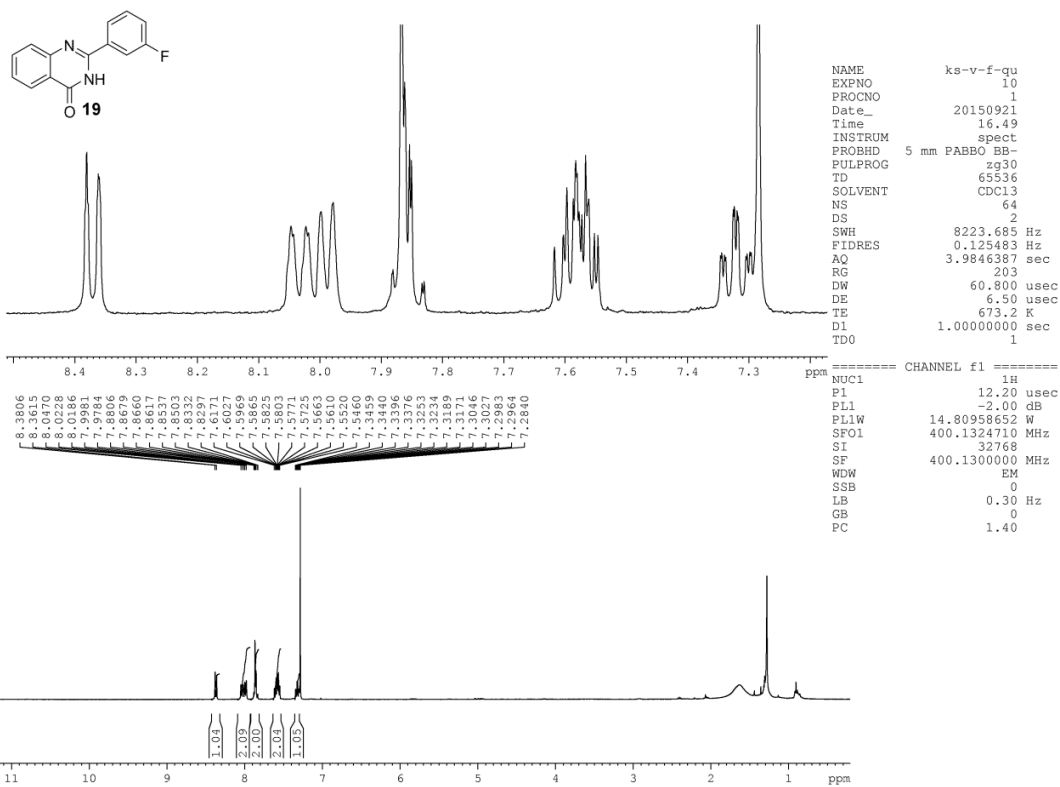
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EXPNO    11
PROCNO   1
Date_    20150918
Time     4.17
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       512
DS       4
SWH      24038.461 Hz
AQ       0.366798 Hz
FIDRES   1.3631988 sec
RG       203
DW       20.800 usec
DE       6.50 usec
TE       673.2 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0     1
    
```

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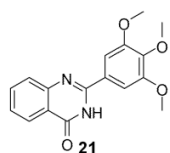
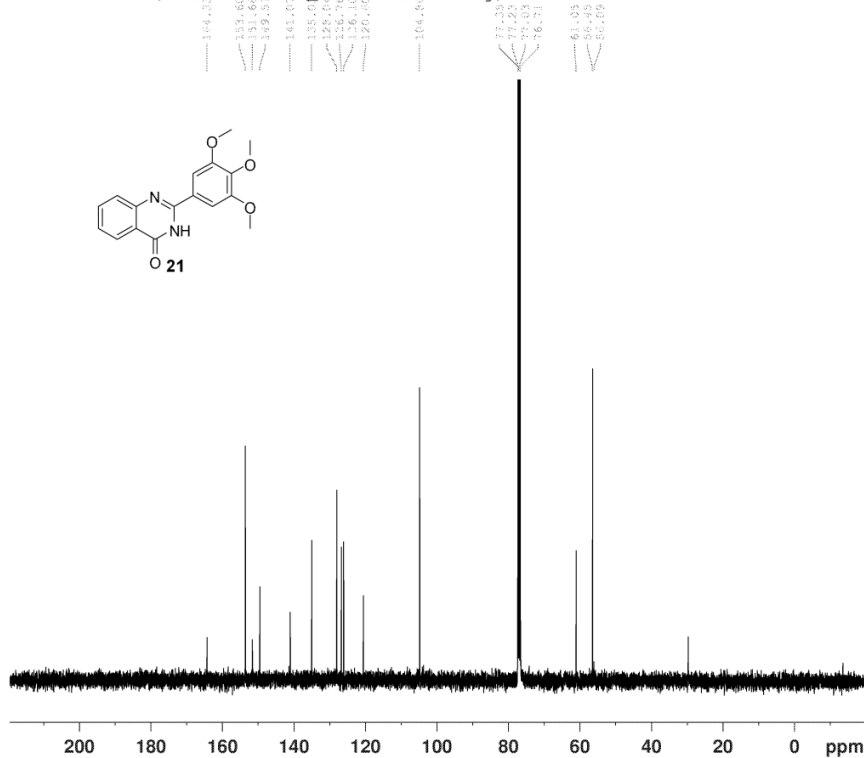
===== CHANNEL f1 =====
NUC1    13C
P1      9.50 usec
PL1     -1.00 dB
PL1W    44.90434265 W
SFO1    100.6228298 MHz
    
```

```

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2     -2.00 dB
PL12    14.33 dB
PL13    18.33 dB
PL2W    14.80958652 W
PL12W   0.34478071 W
PL13W   0.13725966 W
SFO2    400.1316005 MHz
SI      32768
SF      100.6127690 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
    
```



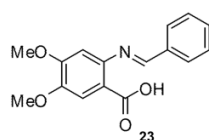
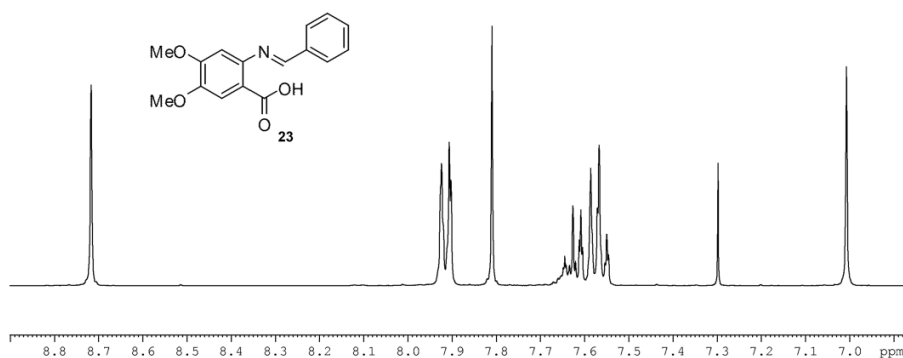
ks-v-469
 C13CPD CDC13 (D:\CIL\JKLaha_108\NMR\2015\Aug) Administrator 22



NAME ks-v-469
 EXPNO 11
 PROCNO 1
 Date_ 20150827
 Time 4.35
 INSTRUM spect
 PROBHD 5 mm PABBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 295.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

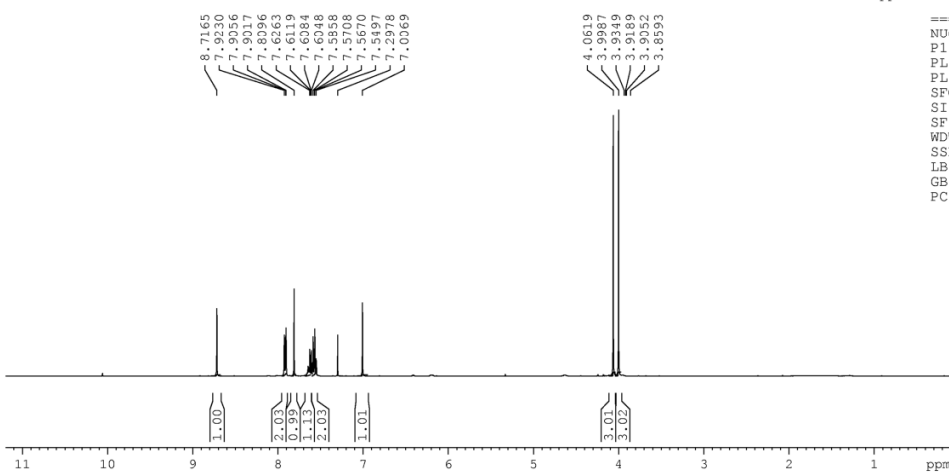
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -1.00 dB
 PL1W 44.90434265 W
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CDPBRG2 waitz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.33 dB
 PL13 18.33 dB
 PL2W 14.80958652 W
 PL12W 0.34478071 W
 PL13W 0.13725966 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

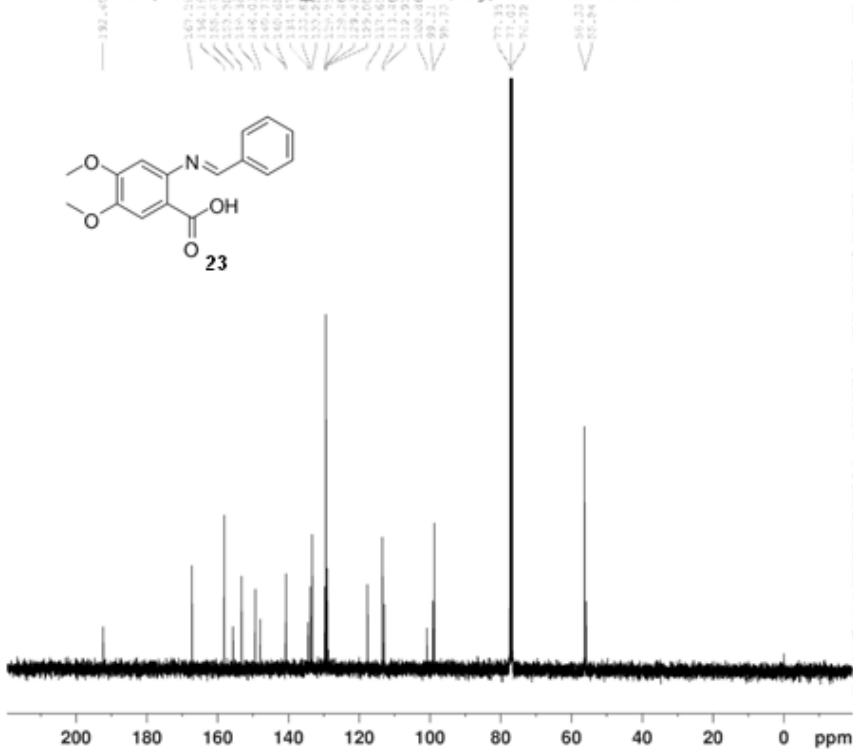


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 PROCNO 1
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 Time 18.35
 INSTRUM spect
 PROBHD 5 mm PABBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 64
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 203
 DW 60.800 usec
 DE 6.50 usec
 TE 673.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.20 usec
 PL1 -2.00 dB
 PL1W 14.80958652 W
 SFO1 400.1324710 MHz
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40



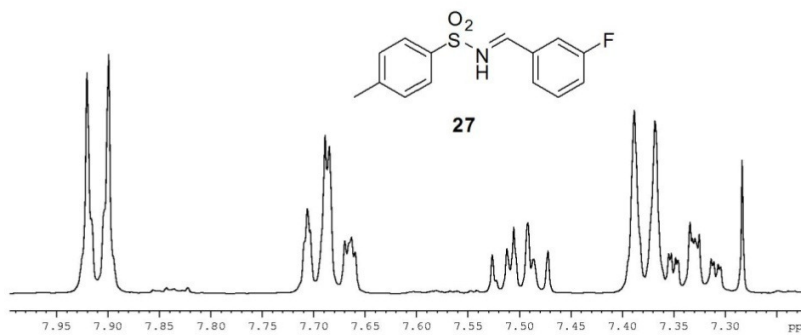
ks-im-ay
 C13CPD CDC13 (D:\CIL\JKLaha_108\NMR\2015\Aug) Administrator 25



NAME ks-im-ay
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 PROCNO 1
 Date_ 20150819
 Time 22.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DM 20.800 usec
 DE 6.50 usec
 TE 673.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

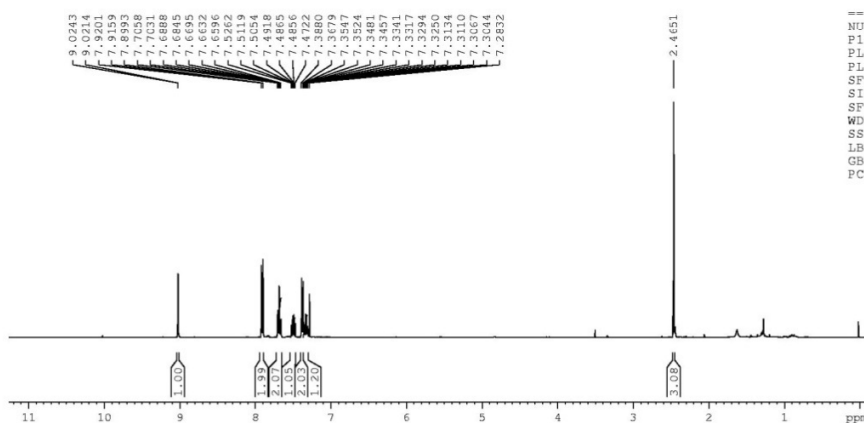
==== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -1.00 dB
 PL1W 44.90434265 W
 SFO1 100.6228298 MHz

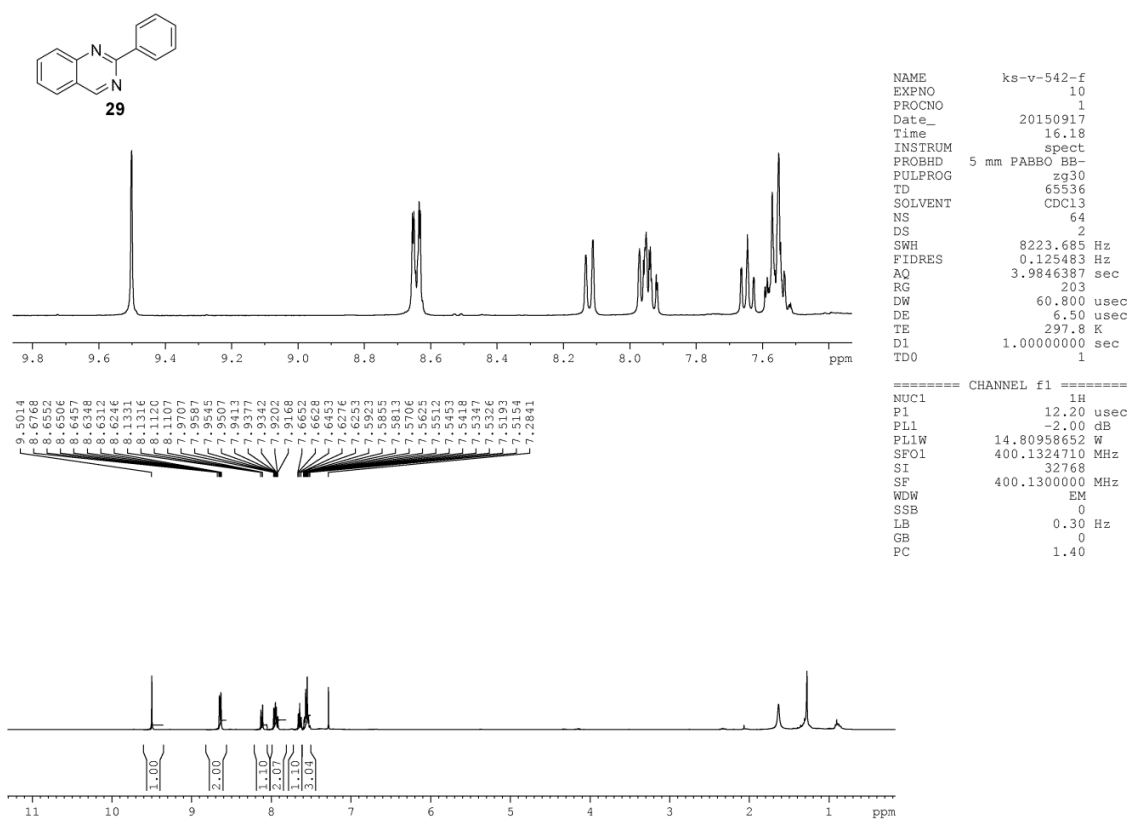
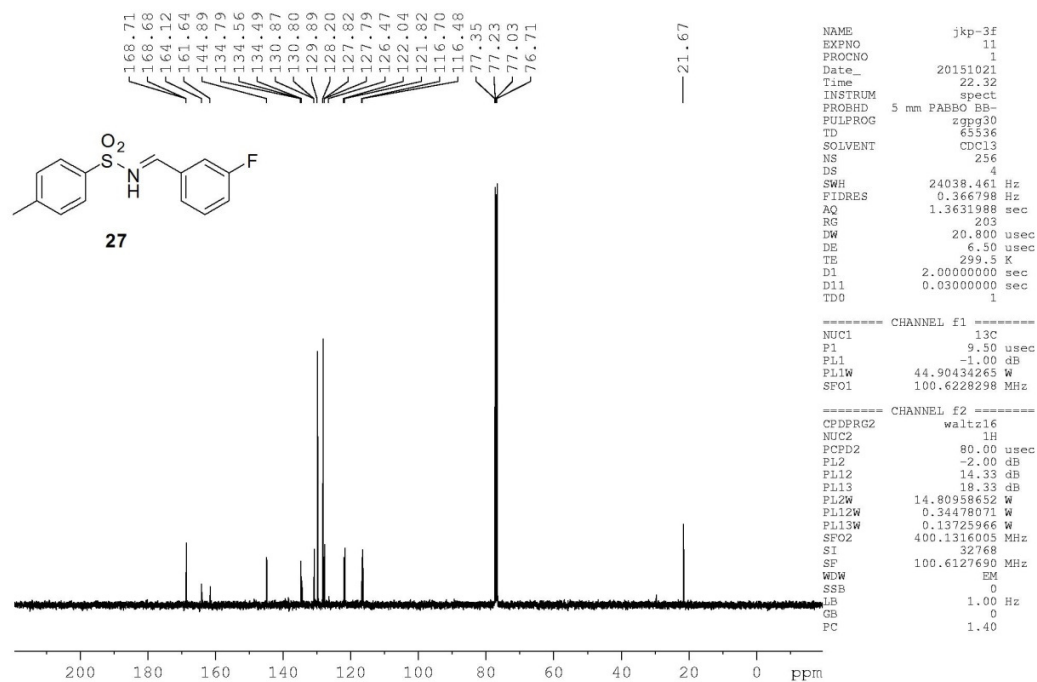
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.33 dB
 PL13 18.33 dB
 PL2W 14.80958652 W
 PL12W 0.34478071 W
 PL13W 0.13725966 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127690 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



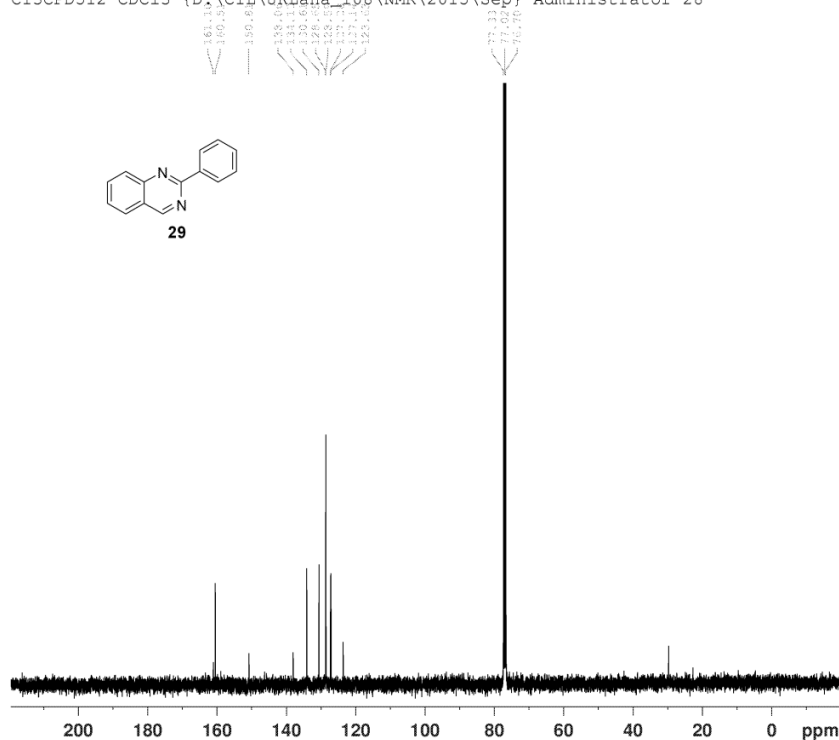
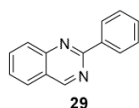
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 PROCNO 1
 Date_ 20151021
 Time 15.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 203
 DM 60.800 usec
 DE 6.50 usec
 TE 299.3 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 12.20 usec
 PL1 -2.00 dB
 PL1W 14.80958652 W
 SFO1 400.1324710 MHz
 SI 32768
 SF 400.1300000 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40





ks-v-542-f
C13CPD512 CDC13 (D:\CIL\JKLaha_108\NMR\2015\Sep) Administrator 28



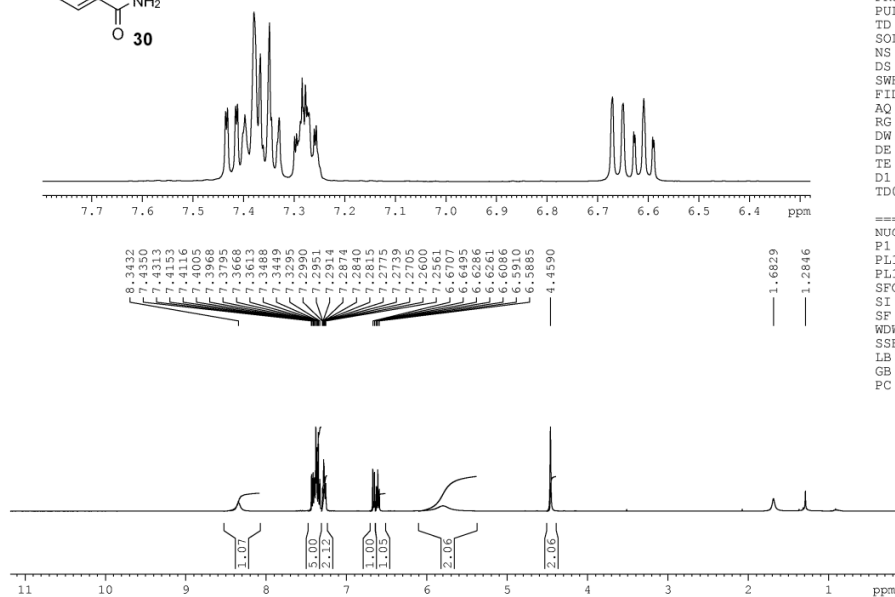
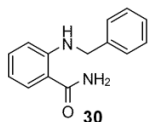
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NAME      ks-v-542-f
EXPNO     11
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Date_     20150918
Time      4.50
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   CDC13
NS        512
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        203
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        9.50 usec
PL1       -1.00 dB
PL1W     44.90434265 W
SFO1     100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -2.00 dB
PL12     14.33 dB
PL13     19.33 dB
PL2W     14.80958652 W
PL12W    0.34478071 W
PL13W    0.13725966 W
SFO2     400.1316005 MHz
SI        32768
SF        100.6127690 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

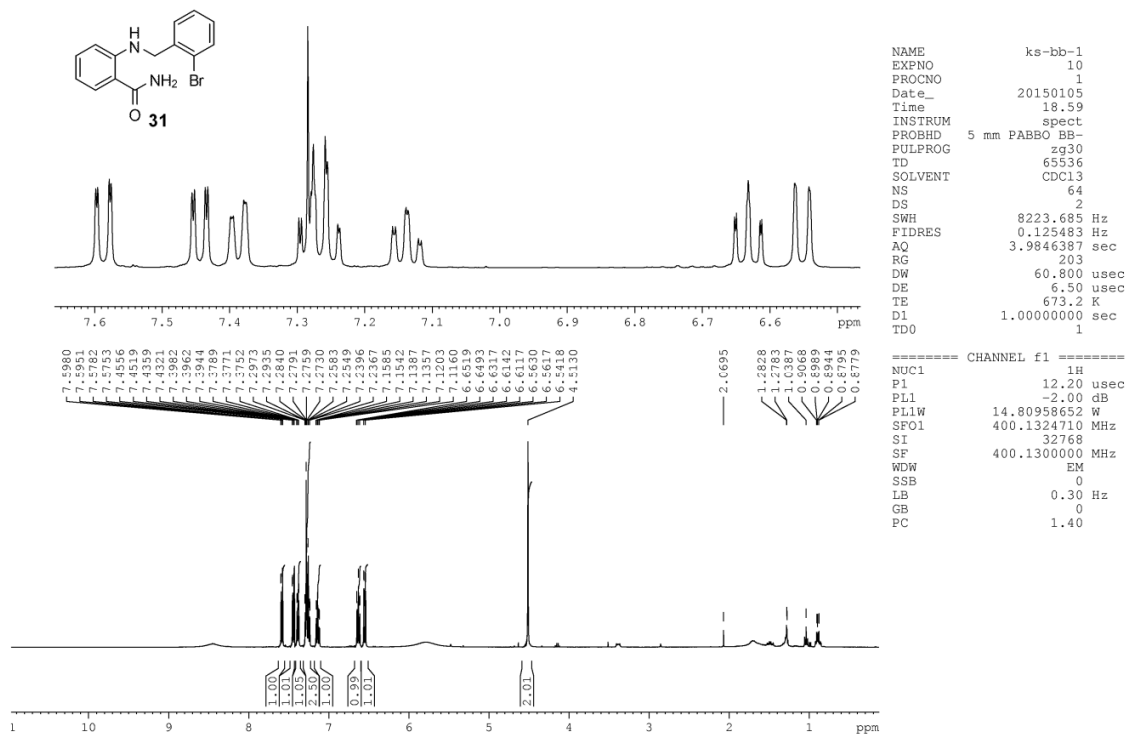


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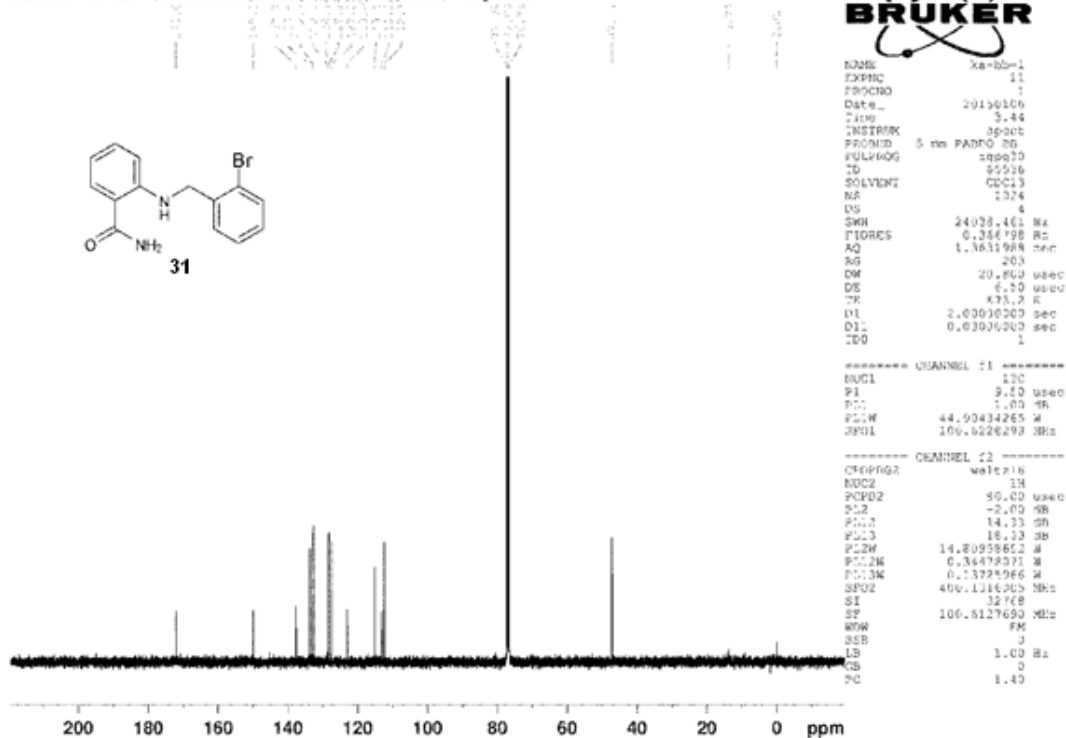
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INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT   CDC13
NS        64
DS        2
SWH       8223.695 Hz
FIDRES    0.125483 Hz
AQ        3.9846387 sec
RG        203
DW        60.800 usec
DE        6.50 usec
TE        673.2 K
D1        1.00000000 sec
TD0       1

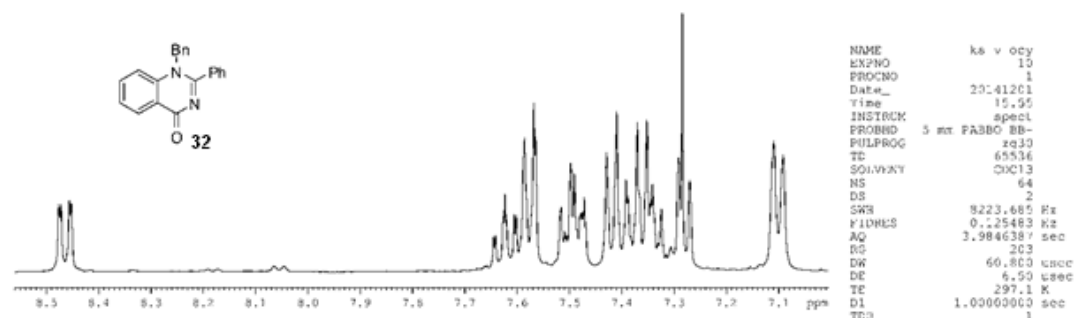
===== CHANNEL f1 =====
NUC1      1H
P1        12.20 usec
PL1       -2.00 dB
PL1W     14.80958652 W
SFO1     400.1324710 MHz
SI        32768
SF        400.1300000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.40

```



ks-bb-1
 C13CPD CDCl3 (D:\FACULTY\JKL\lab\2015\Jan) niper 34



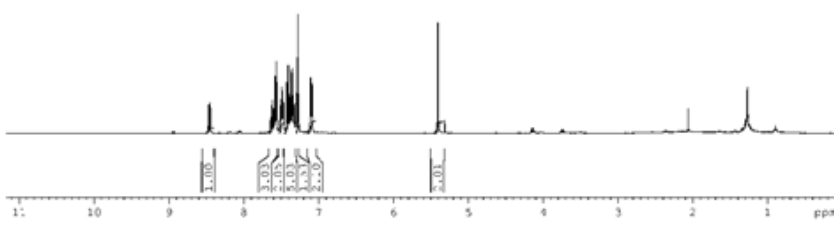


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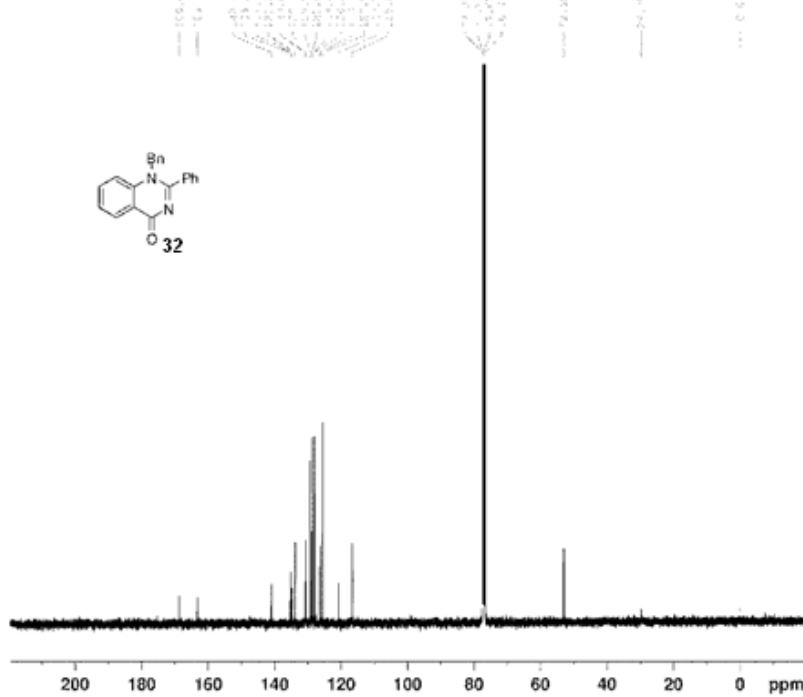
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EXPNO     15
PROCNO    1
Date_     20141201
Time      15.55
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         64
DS         2
SWH        8223.685 Hz
FIDRES     0.25483 Hz
AQ         3.9846387 sec
RG         203
DW         60.800 usec
DE         6.50 usec
TE         297.1 K
D1         1.0000000 sec
D11        1
D12        1
D13        1
D14        1
D15        1
D16        1
D17        1
D18        1
D19        1
D20        1
D21        1
D22        1
D23        1
D24        1
D25        1
D26        1
D27        1
D28        1
D29        1
D30        1
D31        1
D32        1
D33        1
D34        1
D35        1
D36        1
D37        1
D38        1
D39        1
D40        1
D41        1
D42        1
D43        1
D44        1
D45        1
D46        1
D47        1
D48        1
D49        1
D50        1
D51        1
D52        1
D53        1
D54        1
D55        1
D56        1
D57        1
D58        1
D59        1
D60        1
D61        1
D62        1
D63        1
D64        1
D65        1
D66        1
D67        1
D68        1
D69        1
D70        1
D71        1
D72        1
D73        1
D74        1
D75        1
D76        1
D77        1
D78        1
D79        1
D80        1
D81        1
D82        1
D83        1
D84        1
D85        1
D86        1
D87        1
D88        1
D89        1
D90        1
D91        1
D92        1
D93        1
D94        1
D95        1
D96        1
D97        1
D98        1
D99        1
D100       1
    
```

```

===== CHANNEL f1 =====
NUC1      13C
P1         12.20 usec
PL1        -2.00 dB
PL12W     14.80958652 W
SFO1      400.1324710 MHz
SI         32768
SF         400.1300000 MHz
MCH        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.40
    
```



ks-v-ocy
C13CPD CDCl3 (D:\FACULTY\JRLaha\2014\Dec) niper 24



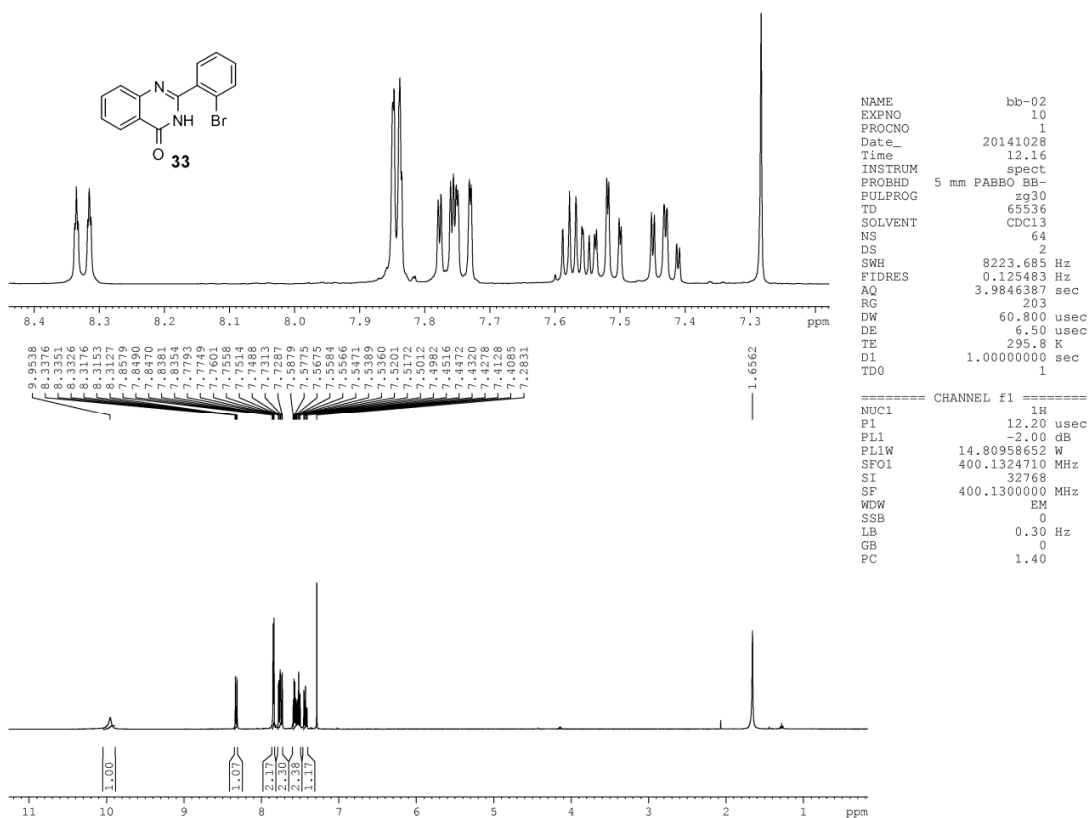
```

NAME      ks v ocy
EXPNO     11
PROCNO    1
Date_     20141202
Time      1.52
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         1500
DS         4
SWH        24038.461 Hz
FIDRES     0.364798 Hz
AQ         1.3823168 sec
RG         26.3
DW         20.800 usec
DE         6.50 usec
TE         298.2 K
D1         2.0000000 sec
D11        1.0000000 sec
D12        1
D13        1
D14        1
D15        1
D16        1
D17        1
D18        1
D19        1
D20        1
D21        1
D22        1
D23        1
D24        1
D25        1
D26        1
D27        1
D28        1
D29        1
D30        1
D31        1
D32        1
D33        1
D34        1
D35        1
D36        1
D37        1
D38        1
D39        1
D40        1
D41        1
D42        1
D43        1
D44        1
D45        1
D46        1
D47        1
D48        1
D49        1
D50        1
D51        1
D52        1
D53        1
D54        1
D55        1
D56        1
D57        1
D58        1
D59        1
D60        1
D61        1
D62        1
D63        1
D64        1
D65        1
D66        1
D67        1
D68        1
D69        1
D70        1
D71        1
D72        1
D73        1
D74        1
D75        1
D76        1
D77        1
D78        1
D79        1
D80        1
D81        1
D82        1
D83        1
D84        1
D85        1
D86        1
D87        1
D88        1
D89        1
D90        1
D91        1
D92        1
D93        1
D94        1
D95        1
D96        1
D97        1
D98        1
D99        1
D100       1
    
```

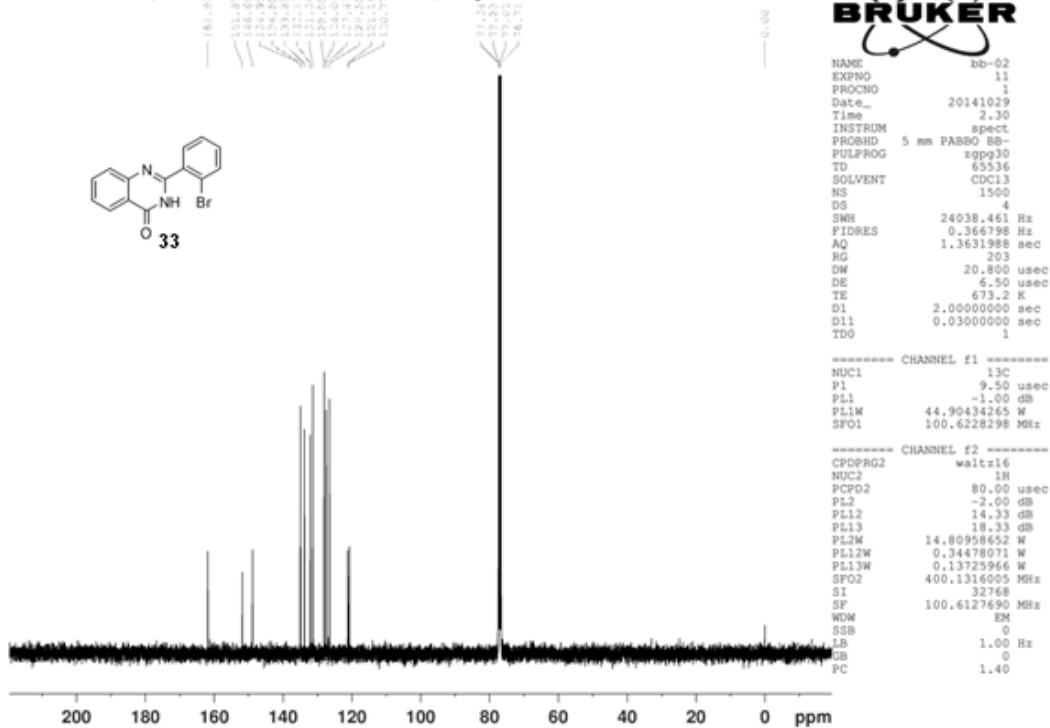
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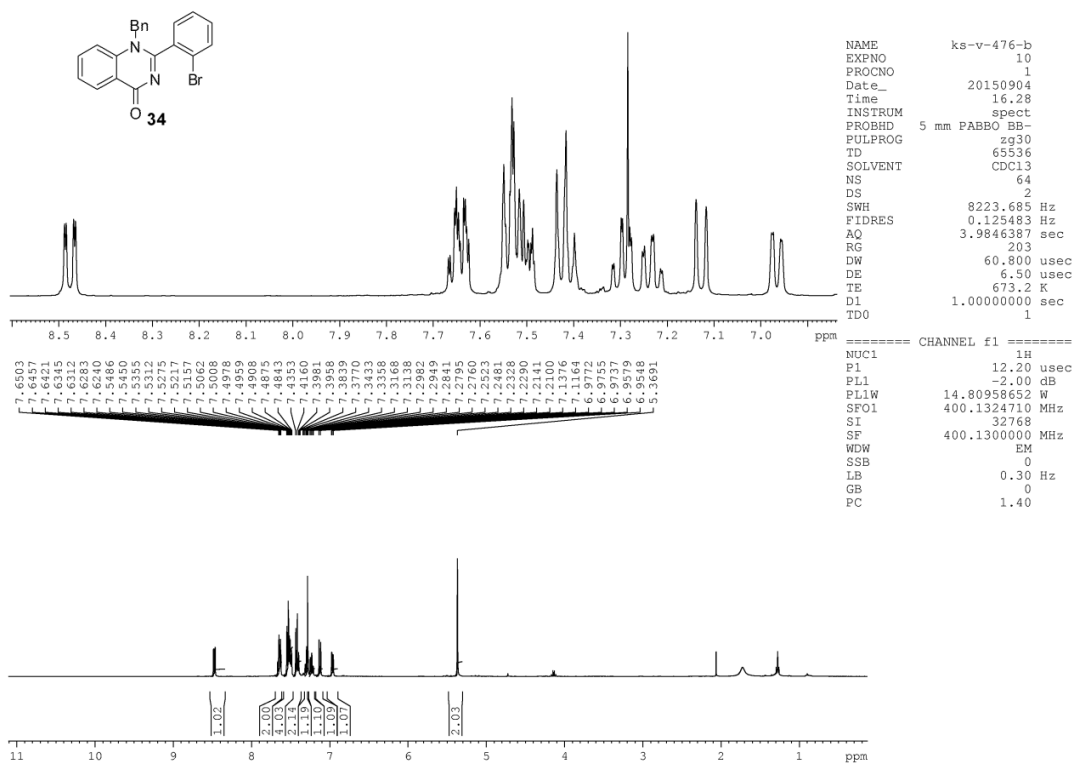
===== CHANNEL f1 =====
NUC1      13C
P1         9.50 usec
PL1        1.00 dB
PL12W     11.90434265 W
SFO1      100.6228258 MHz

===== CHANNEL f2 =====
CH01f02   wait:15
NUC2      1H
P2         50.00 usec
PL2        -2.00 dB
PL12      14.35 dB
PL13      18.33 dB
PL12W     14.80958652 W
PL13W     0.34478071 W
PL13W     1.17255665 W
SFO2      400.1114625 MHz
SI         32768
SF         100.6127650 MHz
MCH        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```



bb-02
C13CPD CDC13 {D:\FACULTY\JKLaha\2014\Oct} niper 11

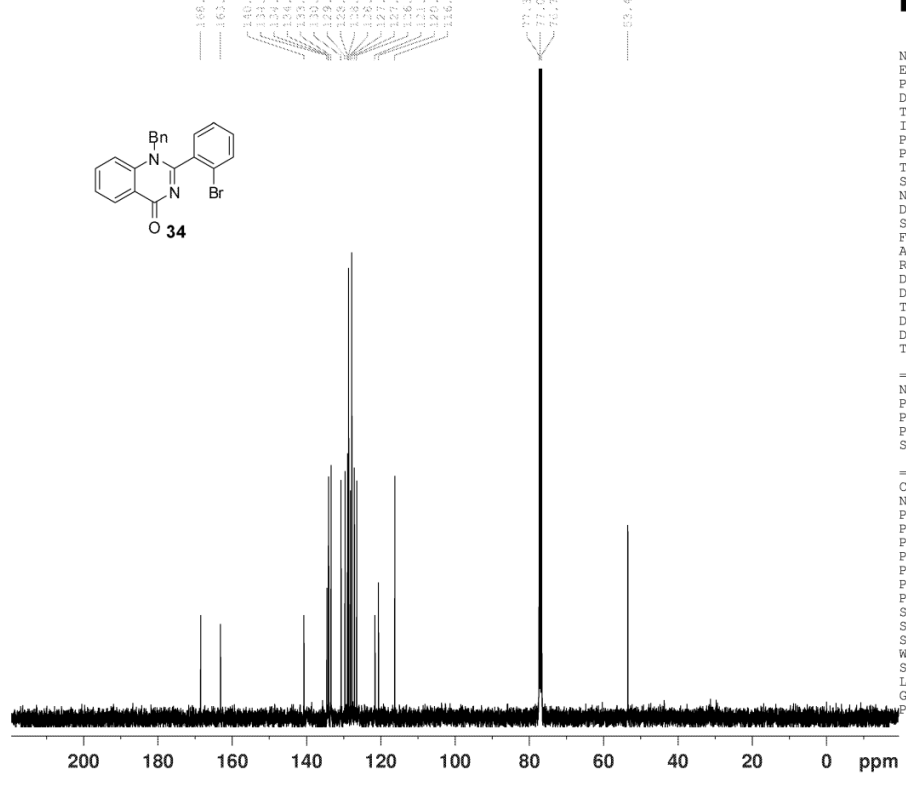




NAME ks-v-476-b
EXPNO 10
PROCNO 1
Date_ 20150904
Time 16.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

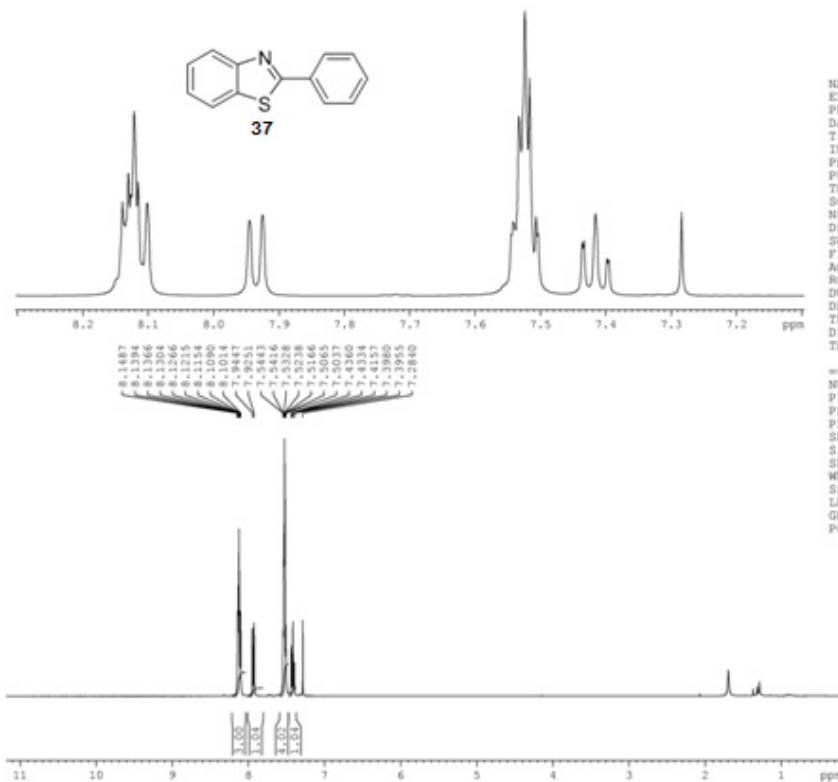
ks-v-476-b
C13CPD CDC13 {D:\CIL\JKLaha_108\NMR\2015\Sep} Administrator 20



NAME ks-v-476-b
EXPNO 11
PROCNO 1
Date_ 20150905
Time 7.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
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 9.50 usec
PL1 -1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz

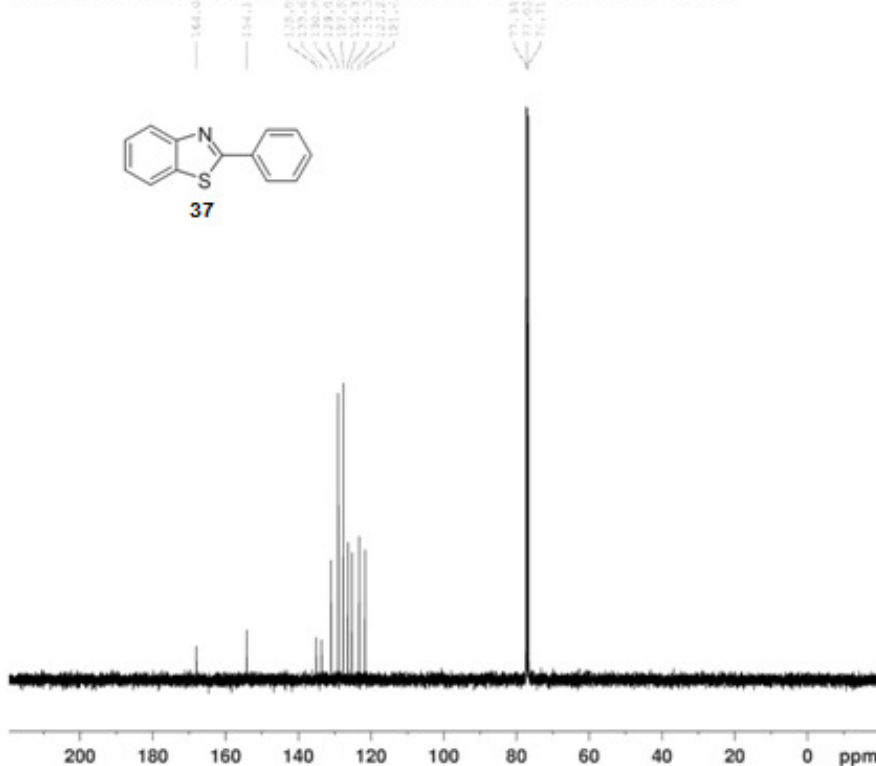
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



NAME ks-v-572
EXPNO 10
PROCNO 1
Date_ 20151020
Time 16.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
MDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

ks-v-572
C13CPD512 CDCl3 {D:\C11\JKLaha_108\NMR\2015\Oct} Administrator 28



NAME ks-v-572
EXPNO 11
PROCNO 1
Date_ 20151021
Time 1.49
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 203
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 -1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
MDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40