

Multicomponent Synthesis of 4-Aminophthalazin-1(2H)-ones by Palladium-Catalyzed Isocyanide Insertion

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2020 Antwerp, Belgium*

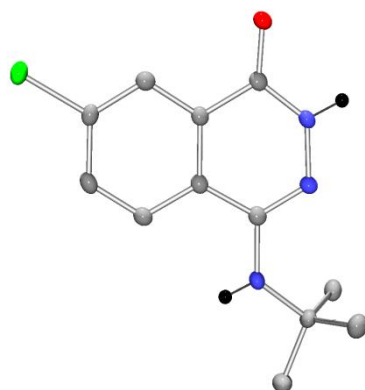
bert.maes@ua.ac.be

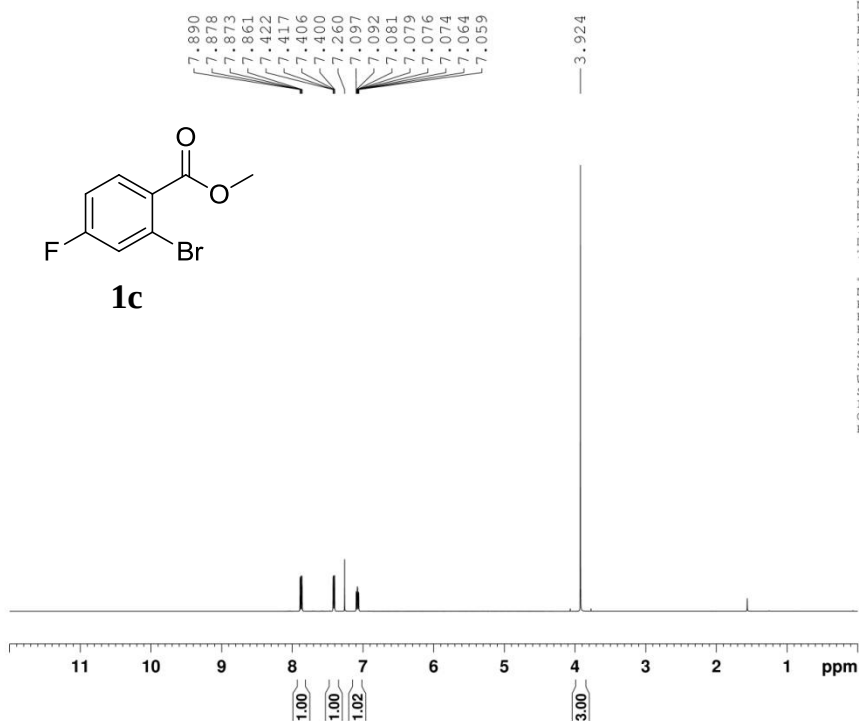
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Kingdom*

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Figure S1 - X-Ray crystal structure of compound 4b	S2
Copies of ¹ H and ¹³ C NMR spectra of new compounds	S3

Figure S1. X-ray structure of compound **4b**. Displacement ellipsoids are drawn at 50% probability level.



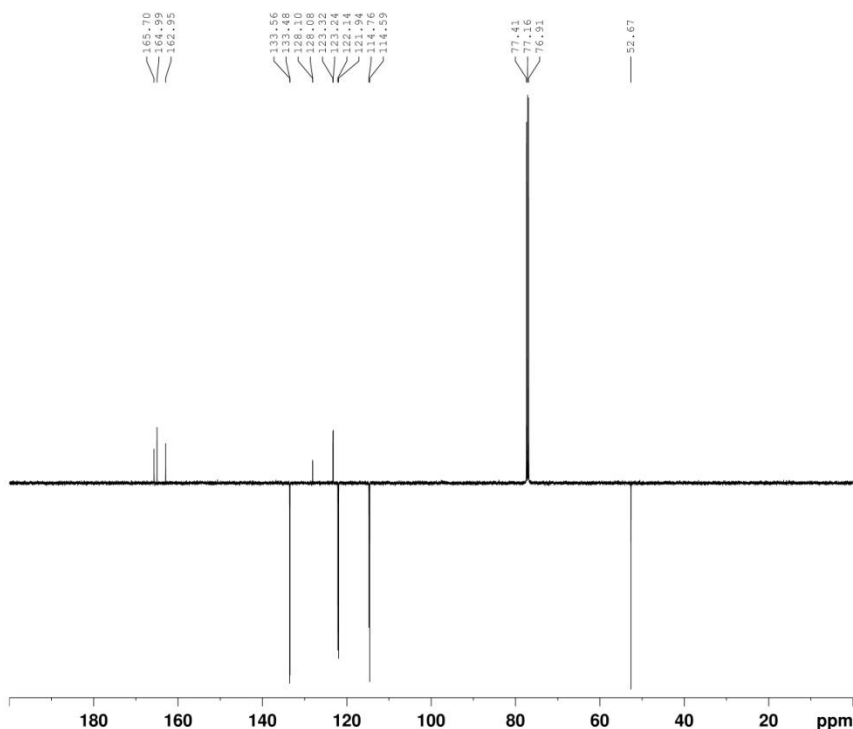


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PROCNO        1
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INSTRUM       spect
PROBHD        5 mm CPTCI 1H-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1719923 sec
RG            11.3
DW            48.400 usec
DE            6.50 usec
TE            296.1 K
D1            1.00000000 sec
D10           1
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            6.70 usec
PL1           4.00 dB
PL1W          8.72000027 W
SFO1          500.2330891 MHz
SI            32768
SF            500.2300100 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

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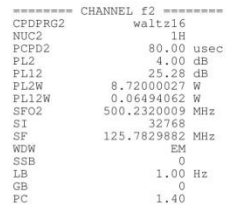
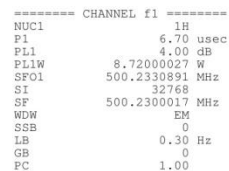
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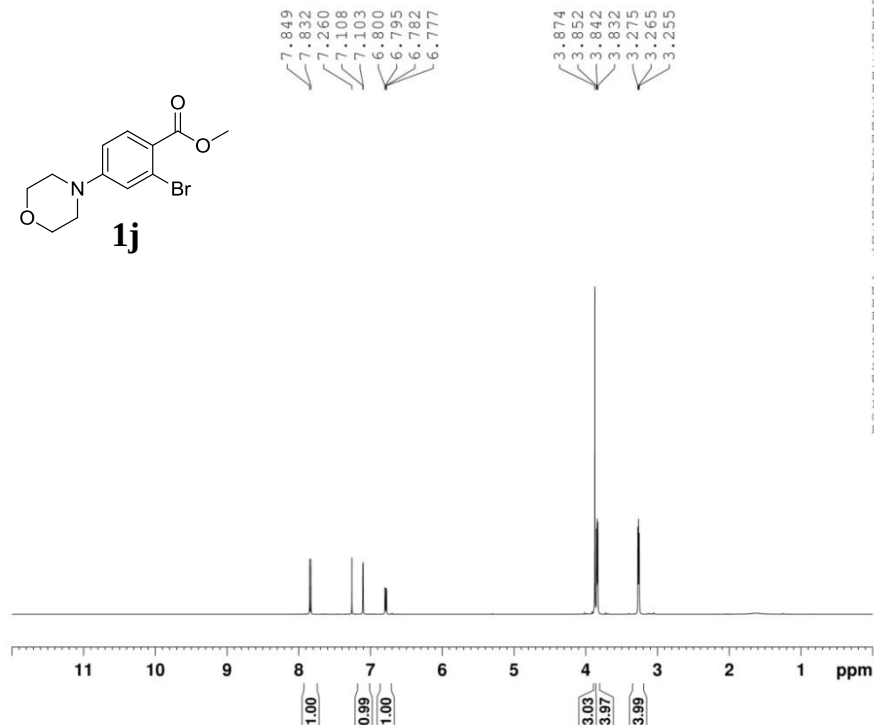
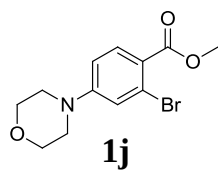
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PULPROG       3mod
TD            65536
SOLVENT       CDCl3
NS            768
DS            4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG            2050
DW            16.800 usec
DE            6.50 usec
TE            296.0 K
CNST2         145.0000000
CNST11        1.0000000
D1            2.00000000 sec
D20           0.00689655 sec
D10           1
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            11.20 usec
P2            22.40 usec
PL1           -2.00 dB
PL1W          88.77790070 W
SFO1          125.7955118 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           4.00 dB
PL12          25.28 dB
PL2W          8.72000027 W
PL12W         0.06494062 W
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WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

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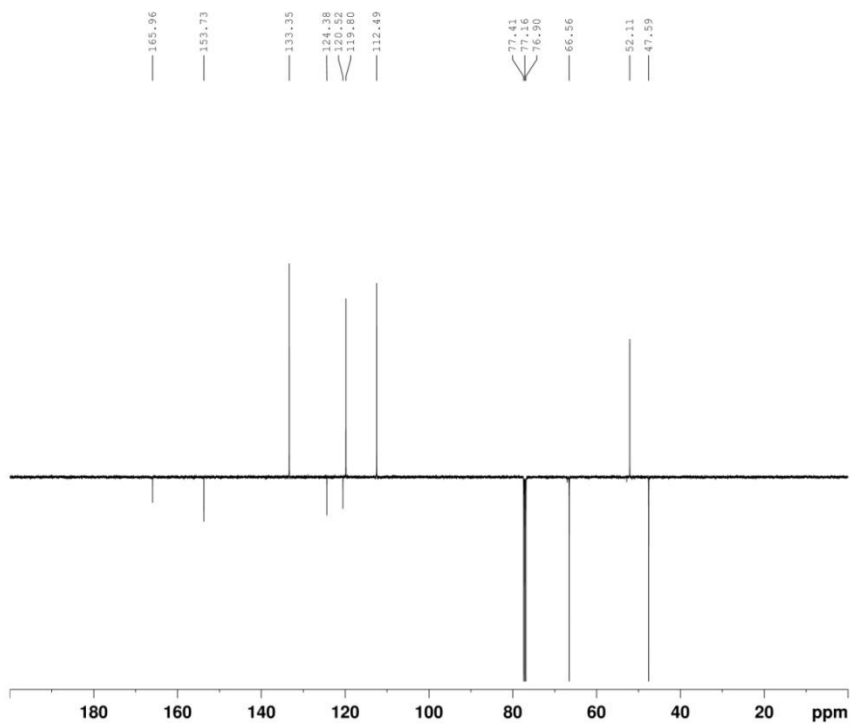


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PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1719923 sec
RG         20.2
DW         48.400 usec
DE         6.50 usec
TE         296.1 K
D1         1.00000000 sec
D10        1
  
```

```

===== CHANNEL f1 =====
NUC1       1H
P1         6.70 usec
PL1        4.00 dB
PL1W       8.72000027 W
SF01       500.2330891 MHz
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SSB        0
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GB         0
PC         1.00
  
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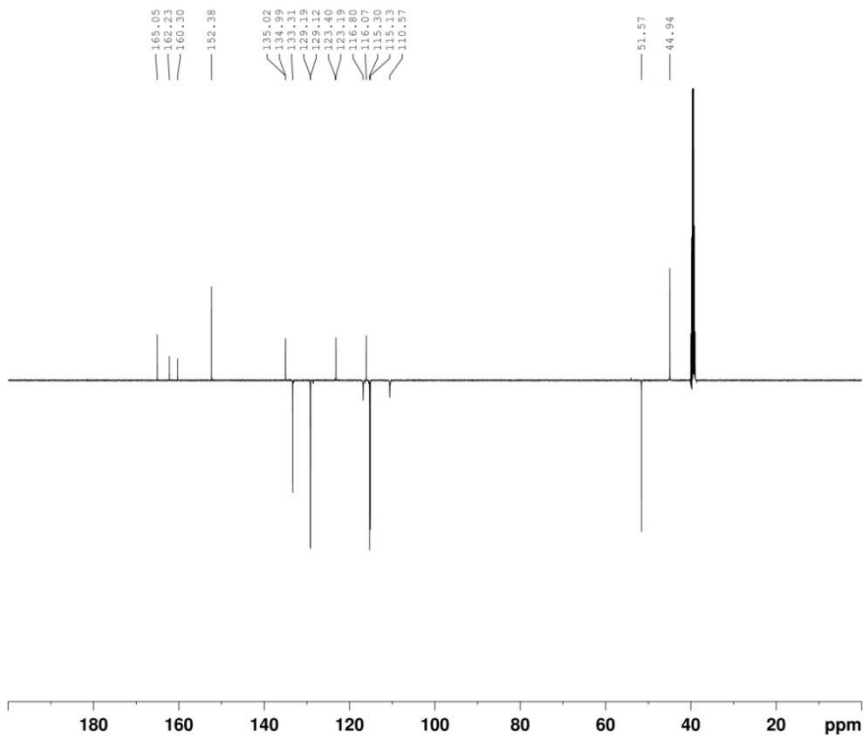
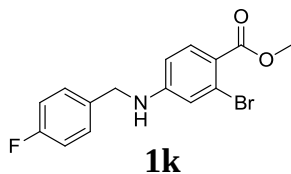
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PULPROG   jmod
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SOLVENT   CDCl3
NS         512
DS         4
SWH        29761.904 Hz
FIDRES     0.454131 Hz
AQ         1.1010548 sec
RG         2050
DW         16.800 usec
DE         6.50 usec
TE         296.1 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
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D10        1
  
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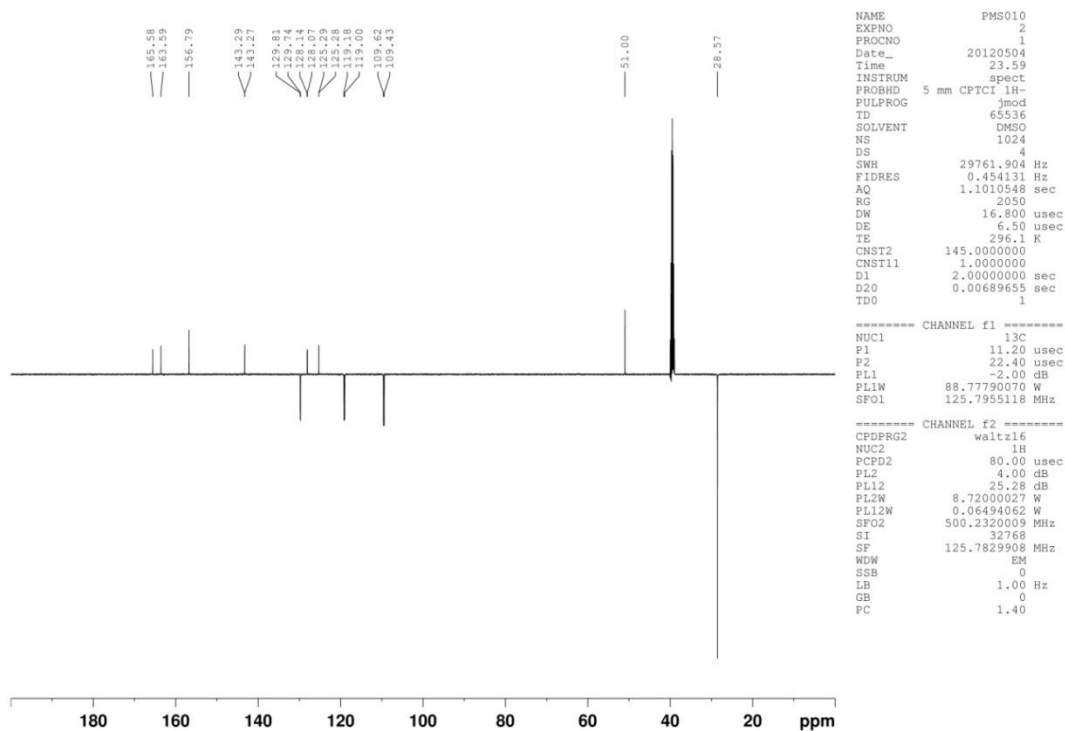
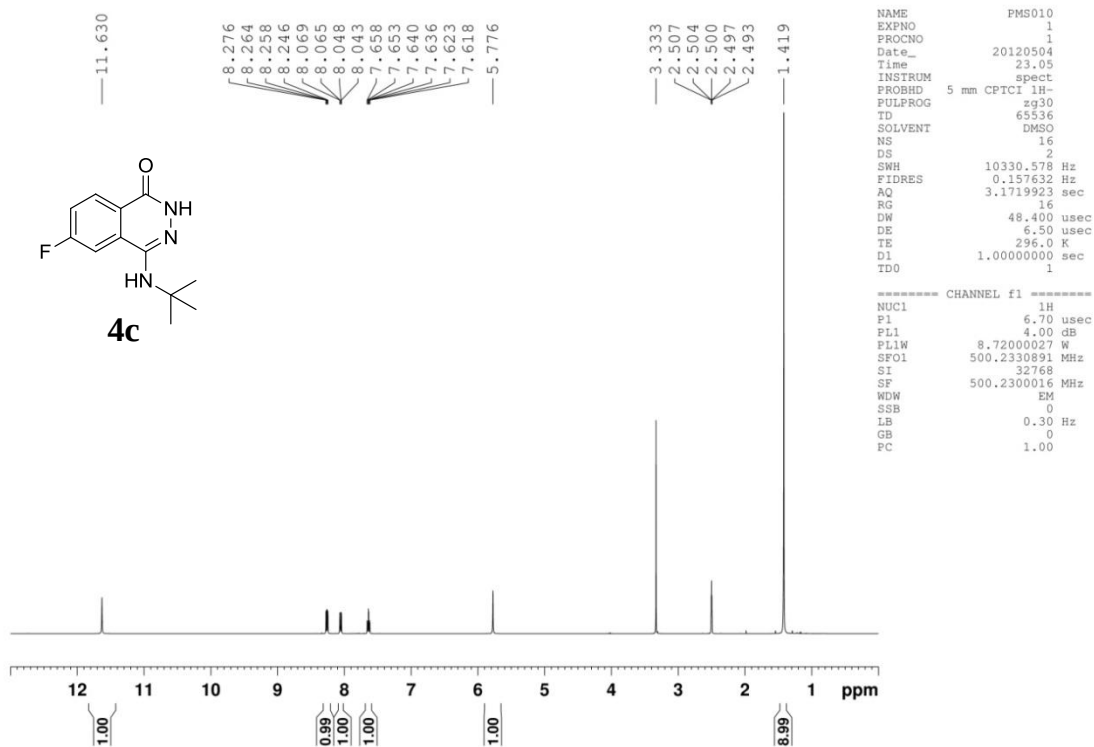
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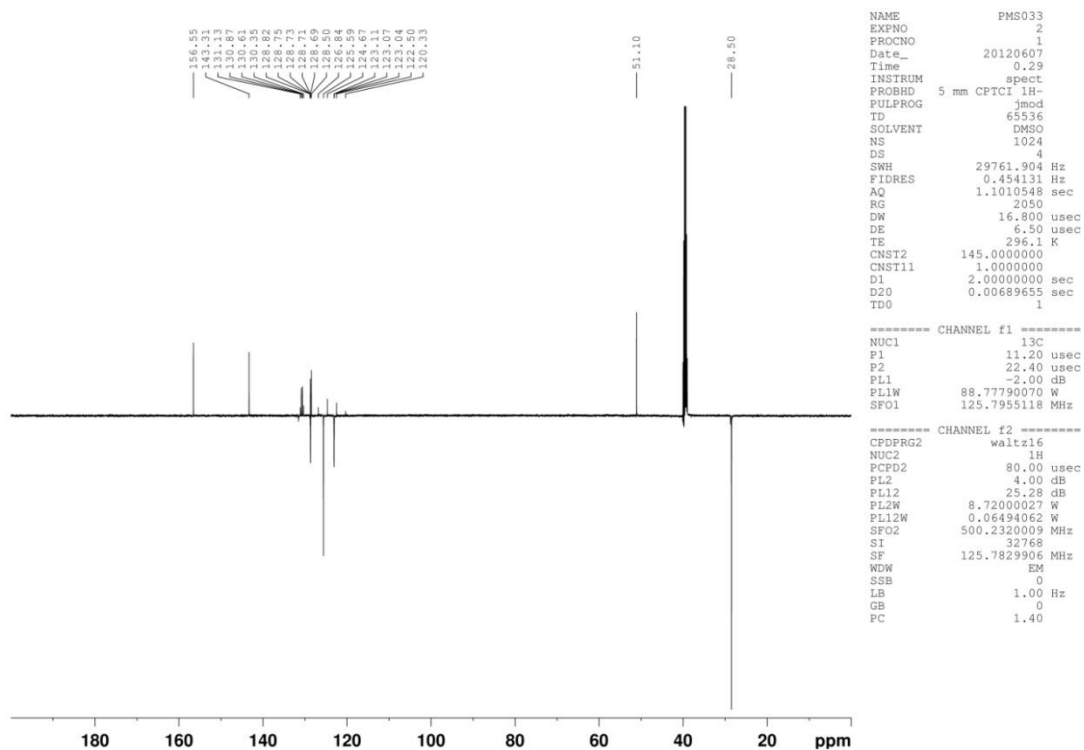
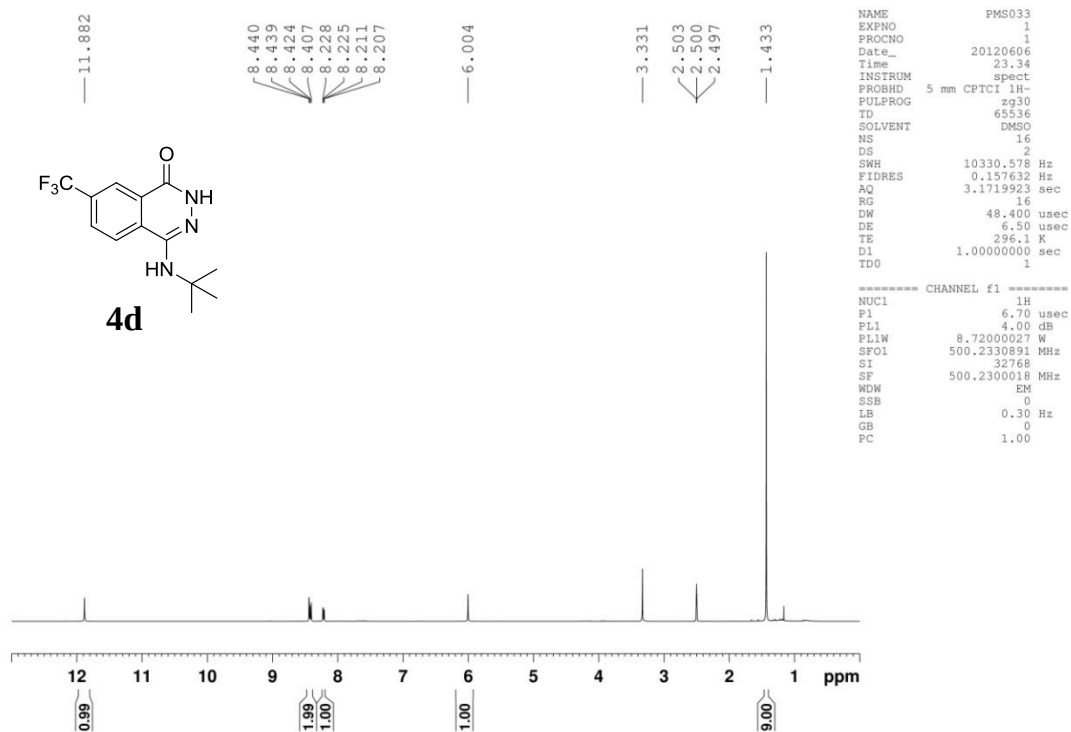
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NUC1       13C
P1         11.20 usec
P2         22.40 usec
PL1        -2.00 dB
PL1W       88.77790070 W
SF01       125.7955118 MHz
  
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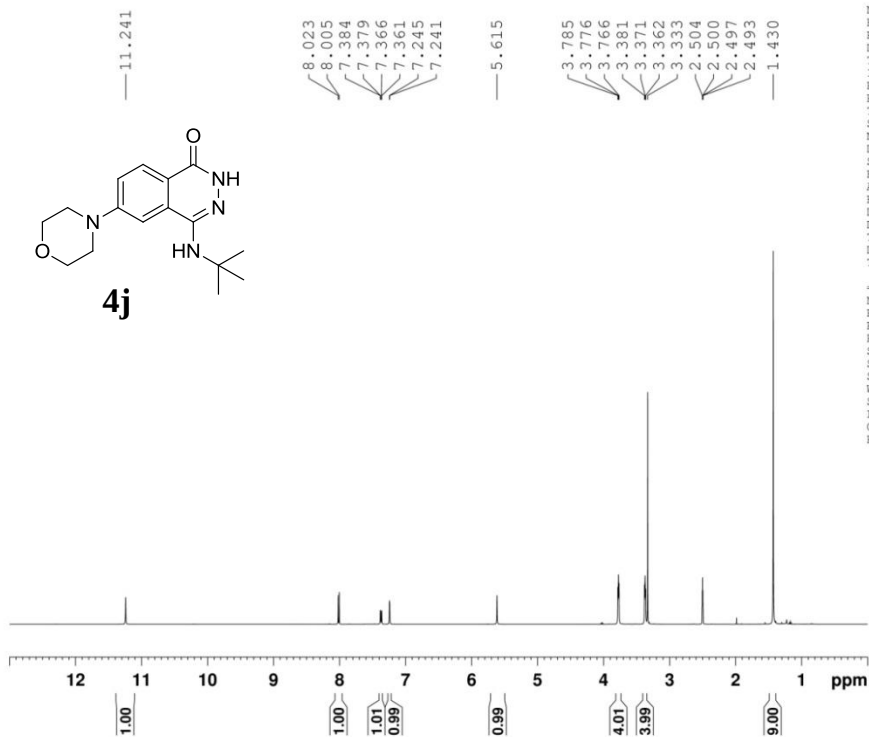
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===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        4.00 dB
PL12       25.28 dB
PL2W       8.72000027 W
PL12W      0.06494062 W
SF02       500.2320009 MHz
SI         32768
SF         125.7829176 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```









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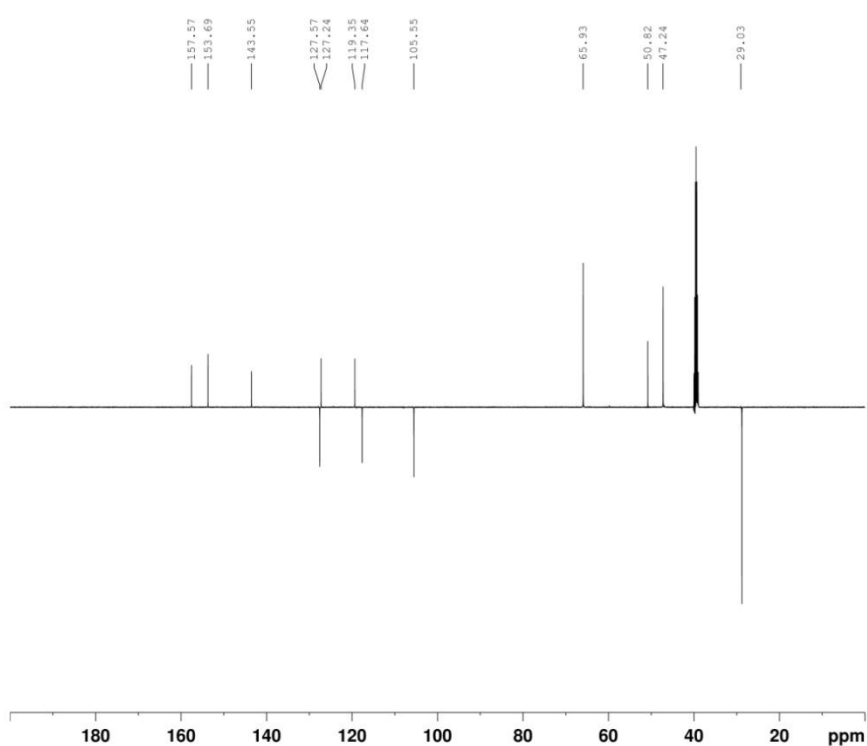
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PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1719923 sec
RG         16
DW         48.400 usec
DE         6.50 usec
TE         296.1 K
D1         1.00000000 sec
TD0        1

```

```

===== CHANNEL f1 =====
NUC1      1H
P1        6.70 usec
PL1       4.00 dB
PL1W      8.72000027 W
SFO1      500.2330891 MHz
SI        32768
SF        500.2300016 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

```



```

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EXPNO     6
PROCNO    1
Date_     20120512
Time      0.48
INSTRUM   spect
PROBHD    5 mm CPTCI 1H-
PULPROG   jmod
TD         65536
SOLVENT   DMSO
NS         2048
DS         4
SWH        29761.904 Hz
FIDRES     0.454131 Hz
AQ         1.1010548 sec
RG         2050
DW         16.800 usec
DE         6.50 usec
TE         296.1 K
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CNST11    1.0000000
D1         2.00000000 sec
D20       0.00689655 sec
TD0        1

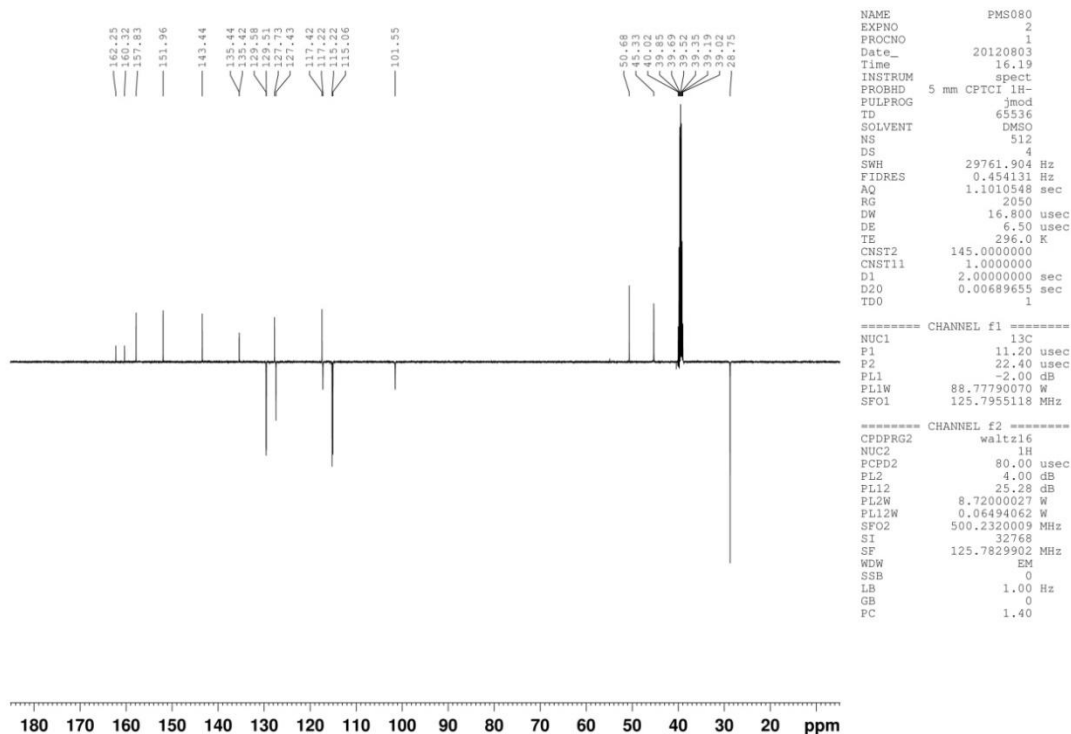
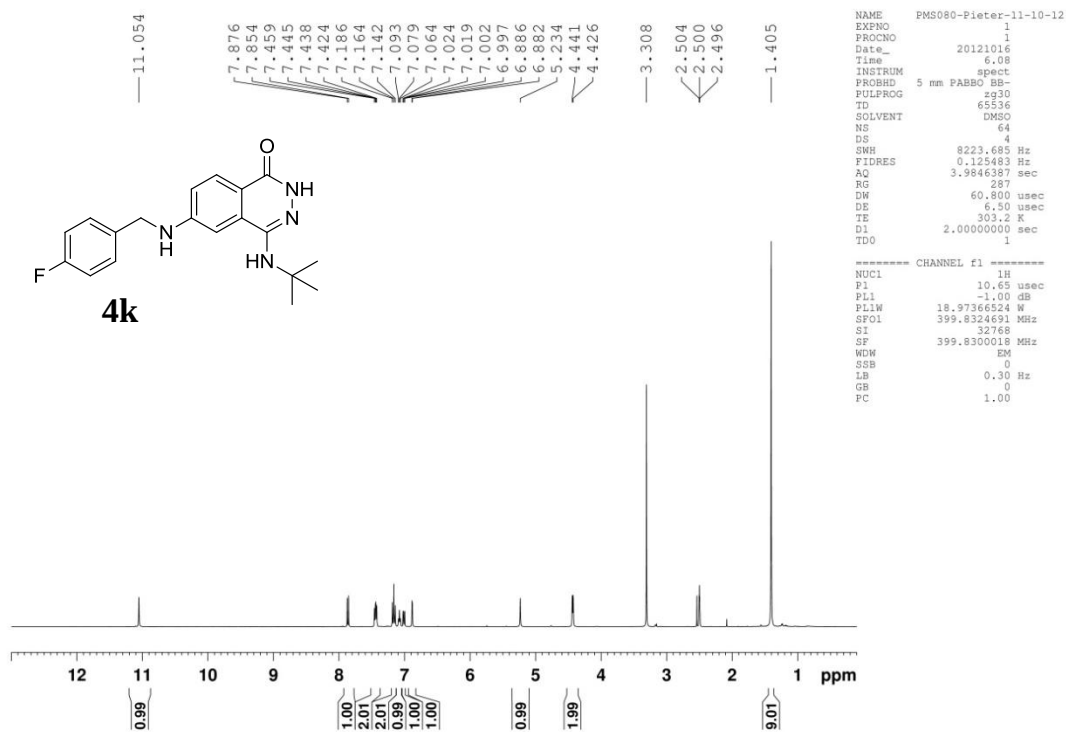
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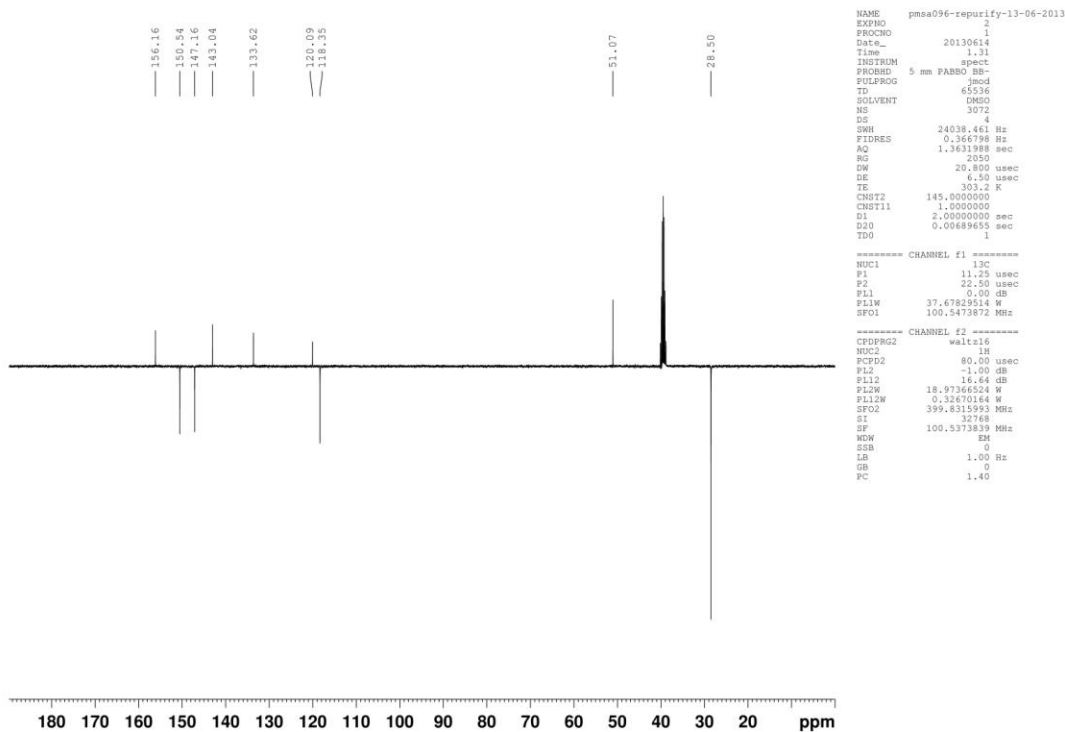
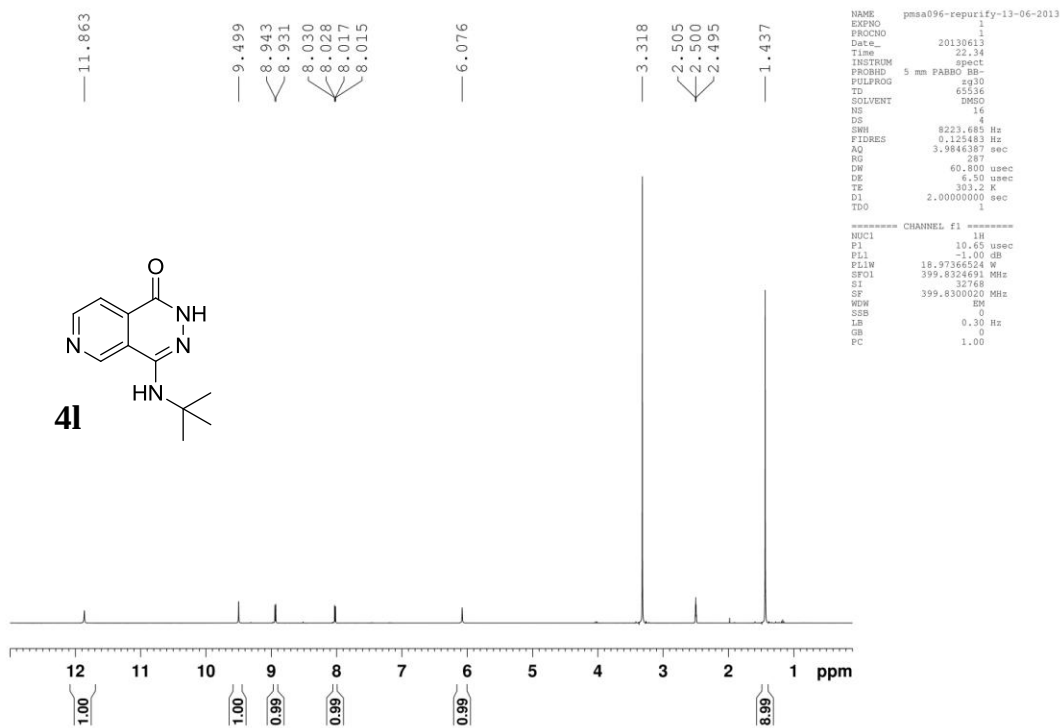
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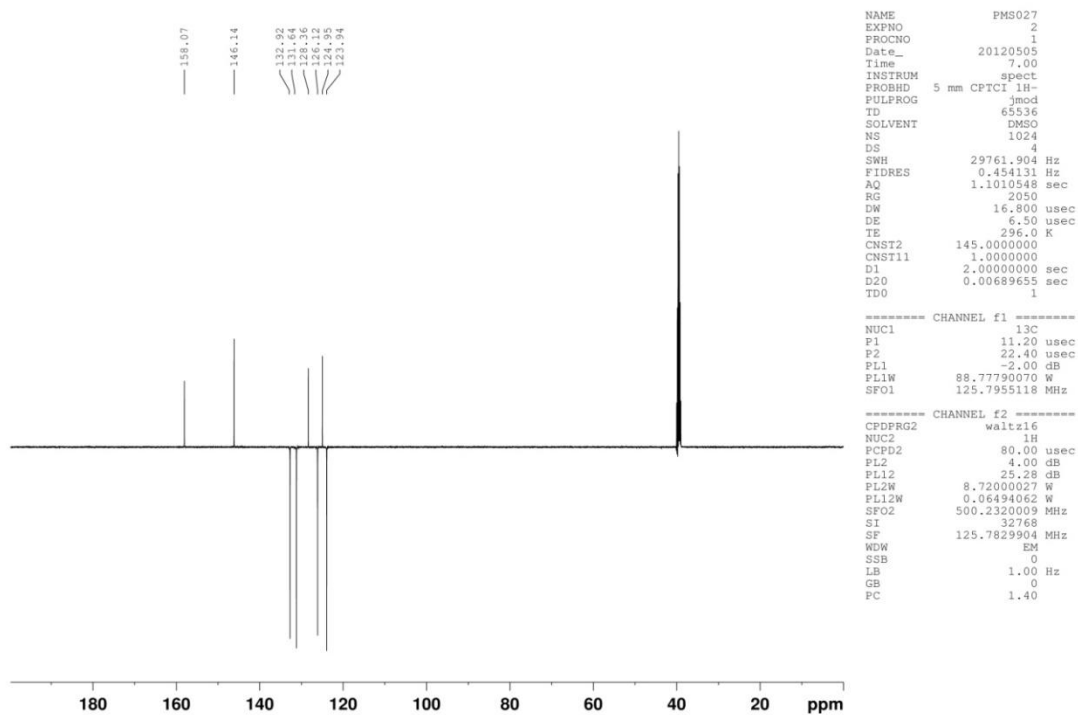
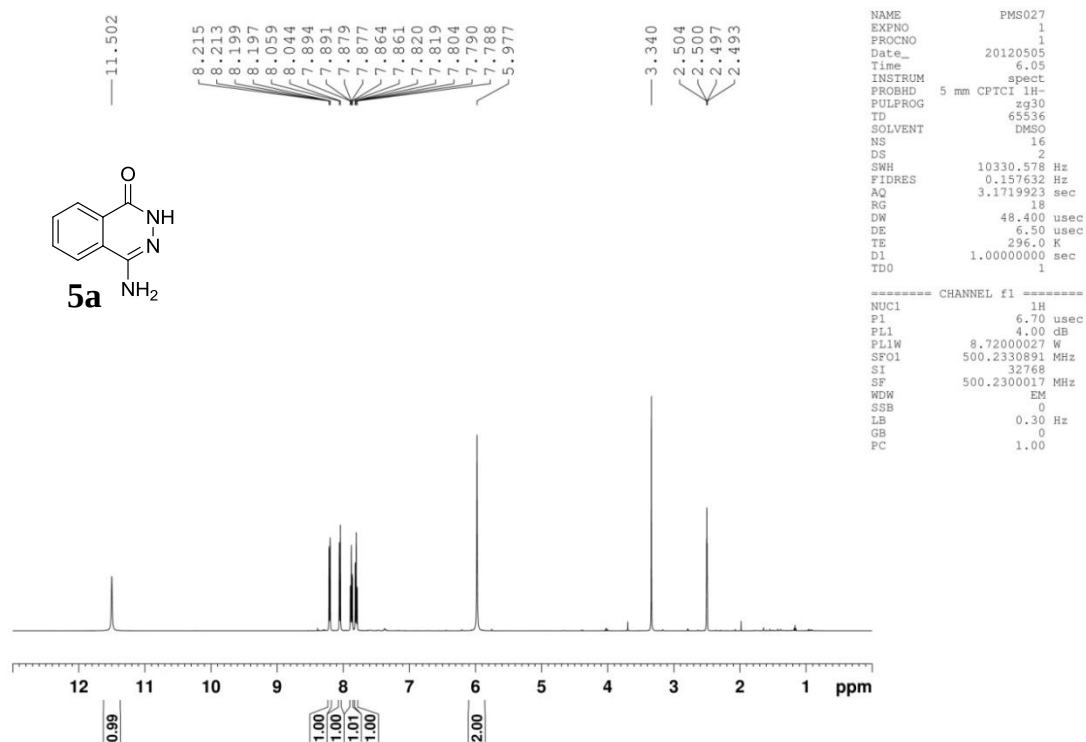
===== CHANNEL f1 =====
NUC1      13C
P1        11.20 usec
P2        22.40 usec
PL1       -2.00 dB
PL1W      88.77790070 W
SFO1      125.7955118 MHz

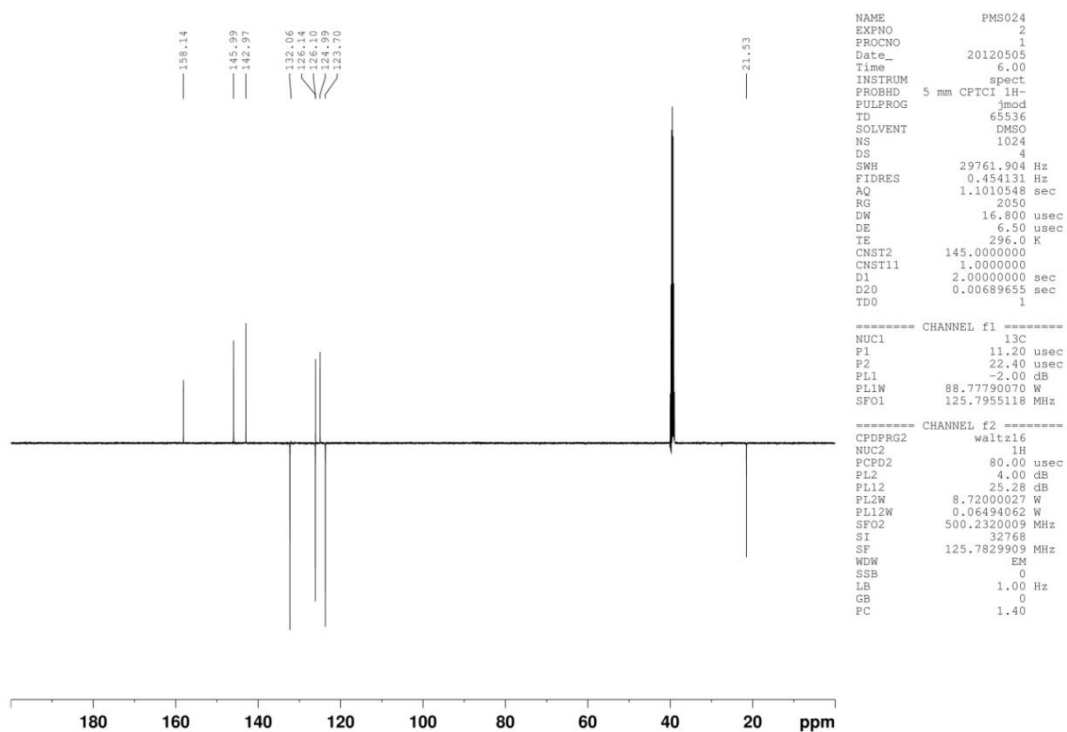
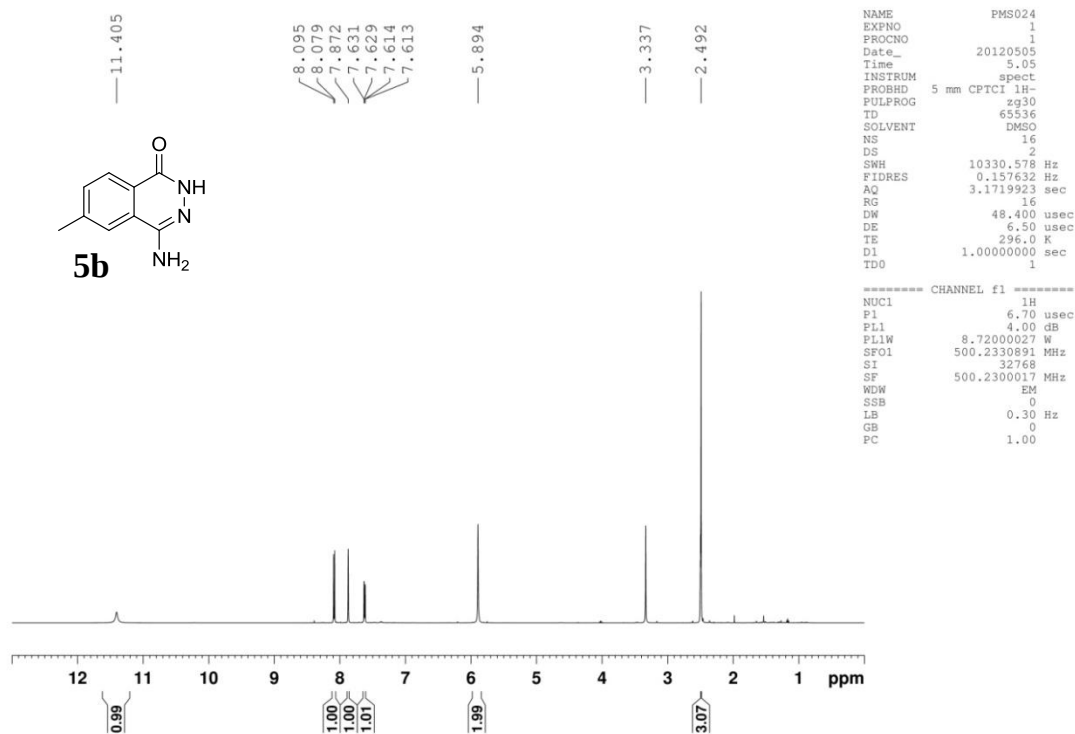
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       4.00 dB
PL12      25.28 dB
PL2W      8.72000027 W
PL12W     0.06494062 W
SFO2      500.2320009 MHz
SI        32768
SF        125.7829911 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

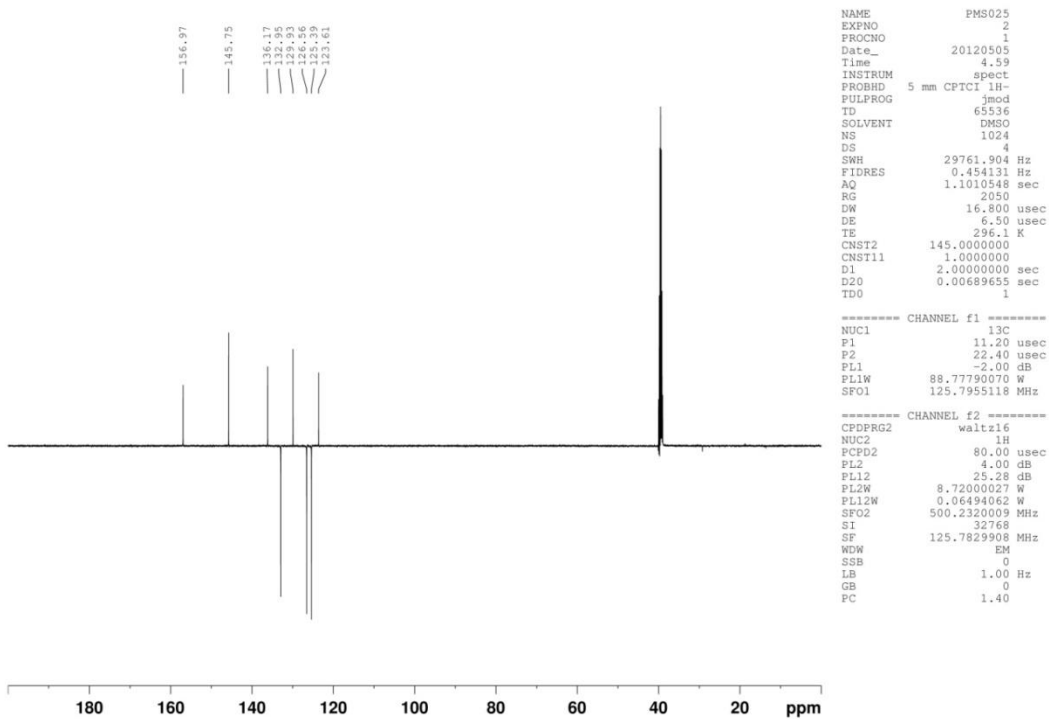
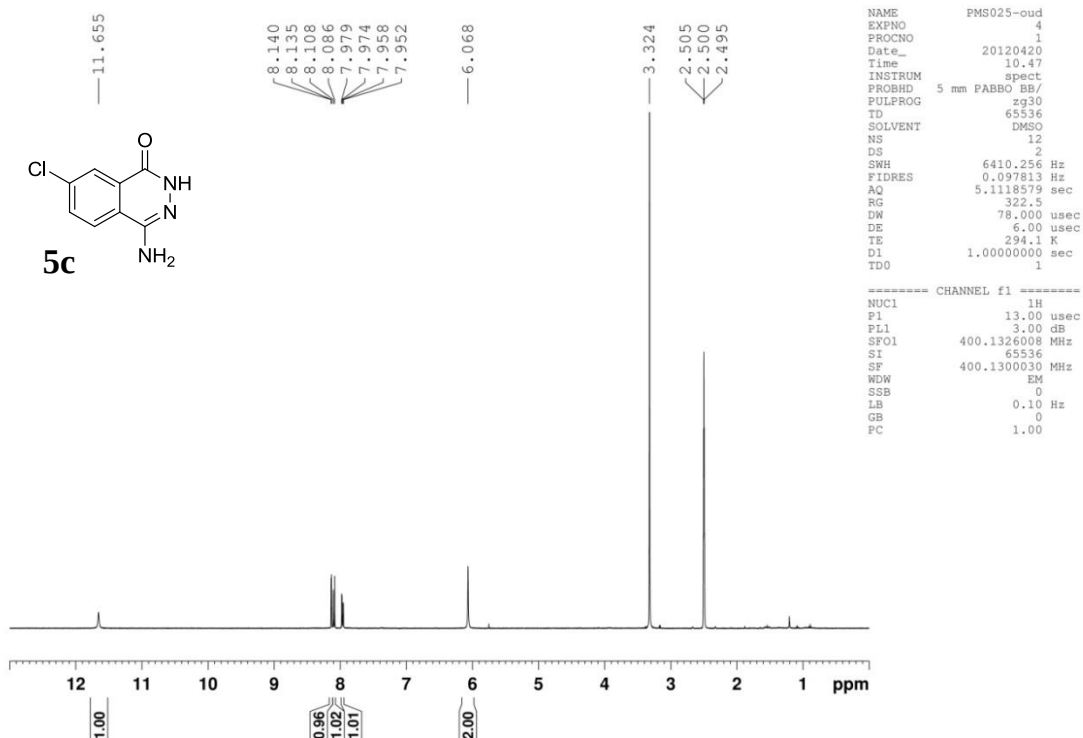
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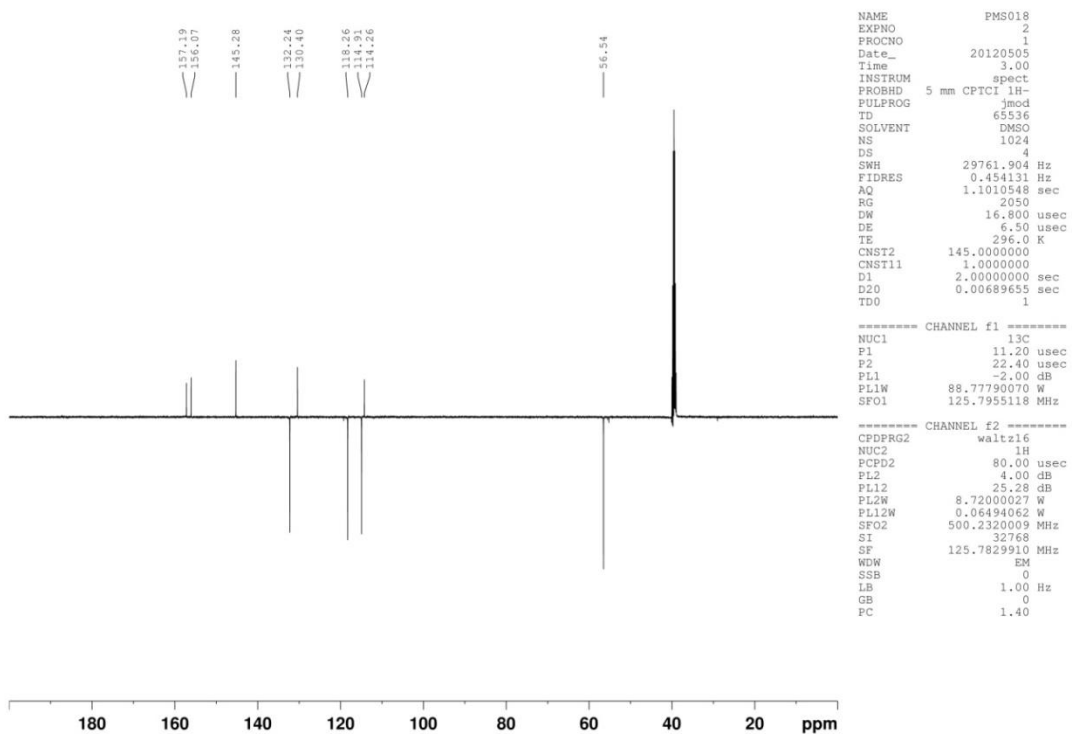
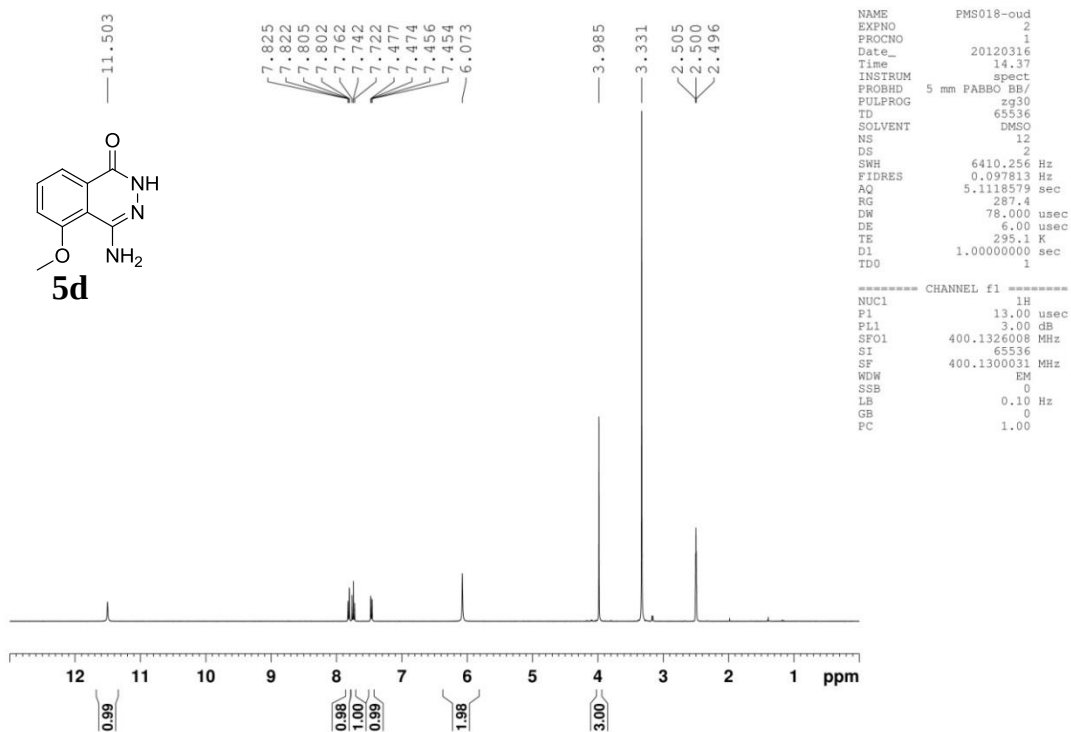


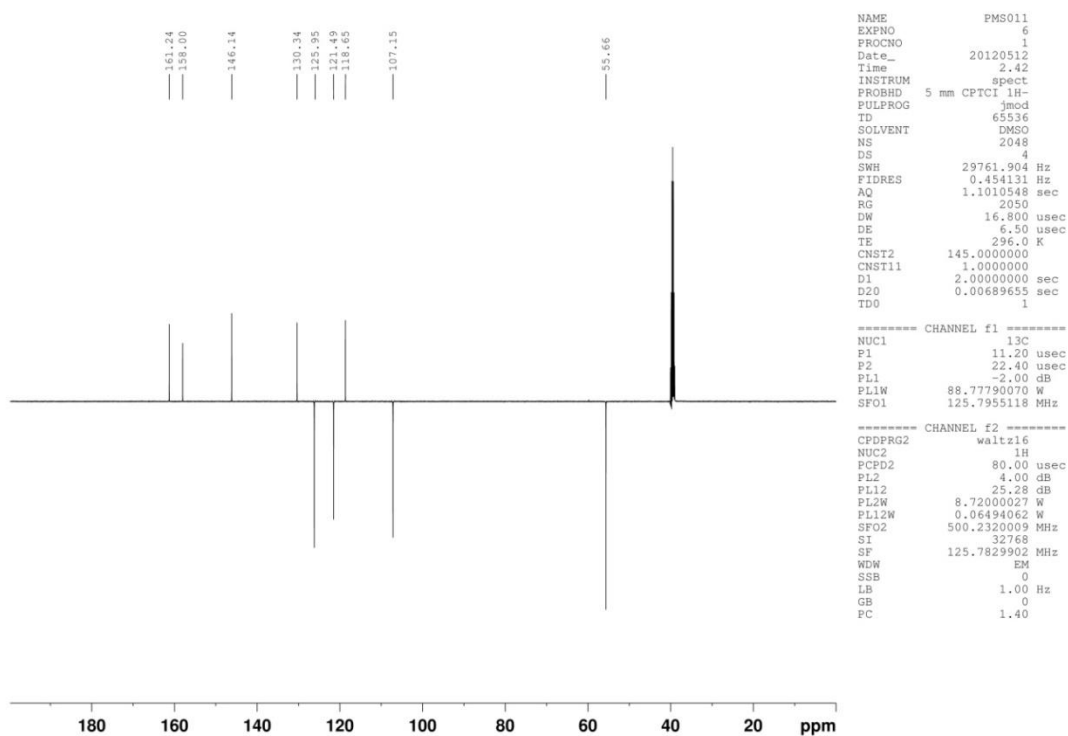
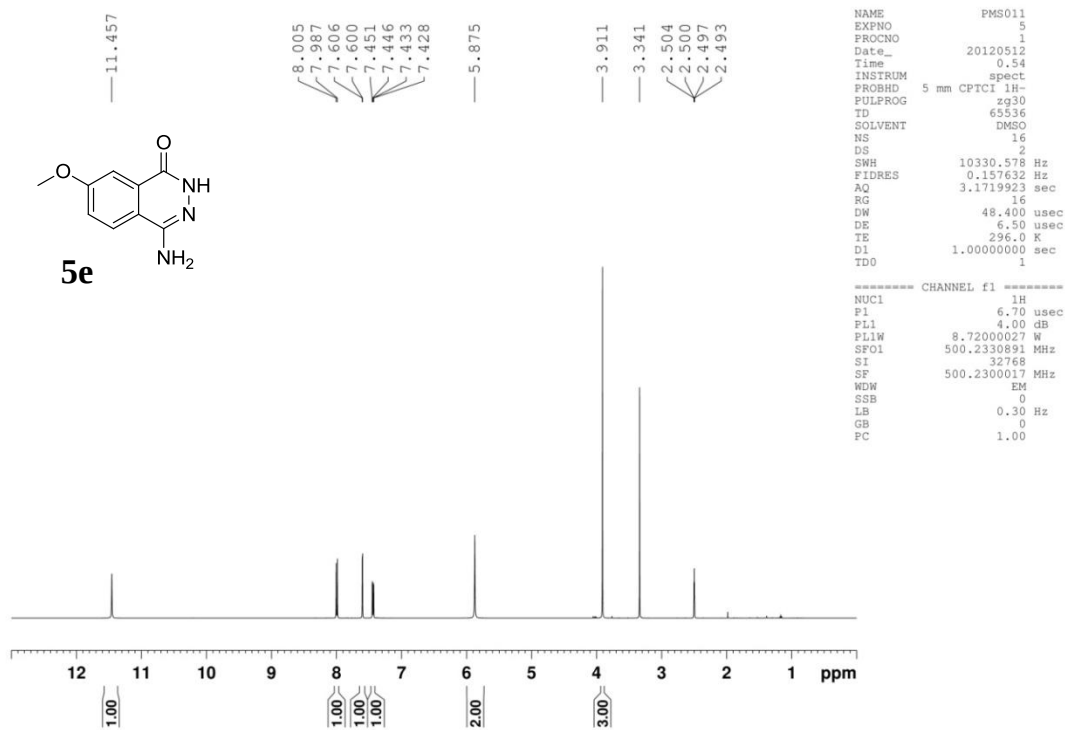


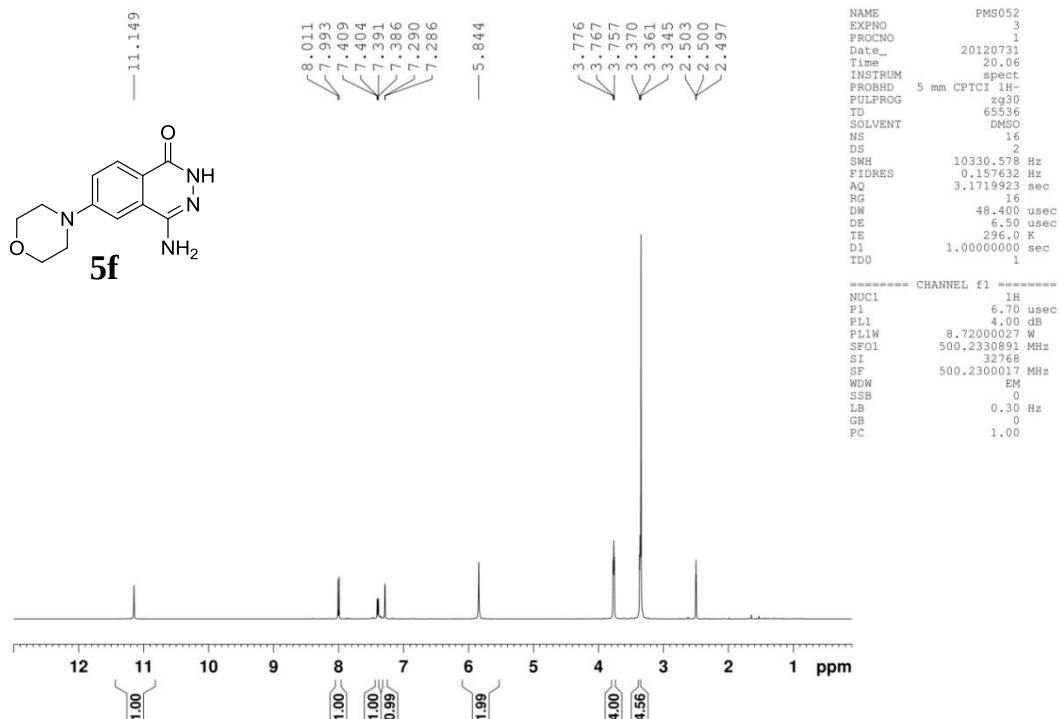
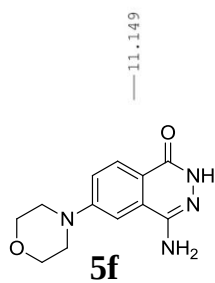










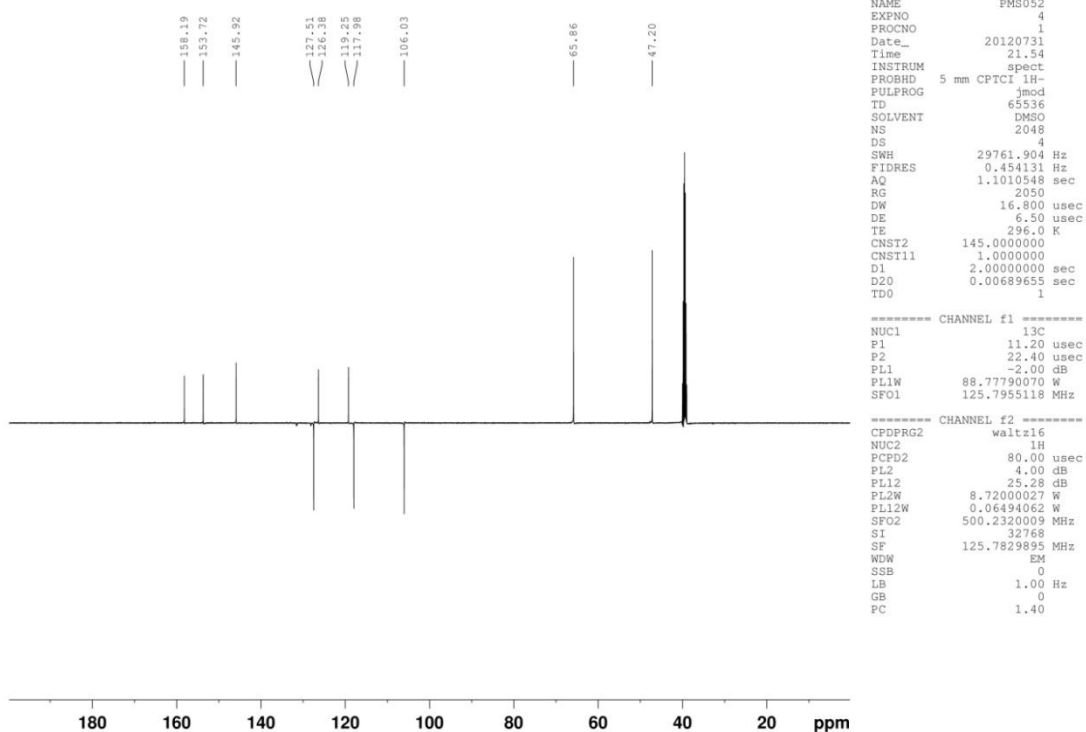


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PROCNO    1
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PROBHD    5 mm CPTCI 1H-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1719923 sec
RG         16
DW         48.400 usec
DE         6.50 usec
TE         296.0 K
D1         1.00000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1         6.70 usec
PL1        4.00 dB
PL1W       8.72000027 W
SFO1      500.2330891 MHz
SI         32768
SF         500.2300017 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



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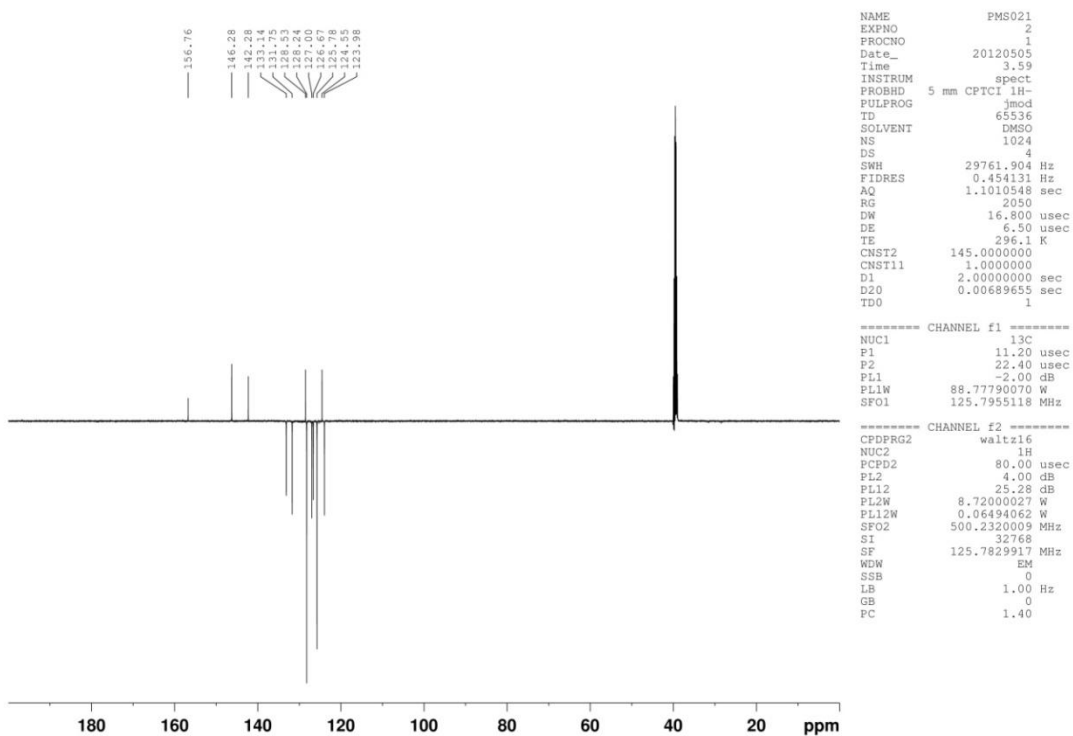
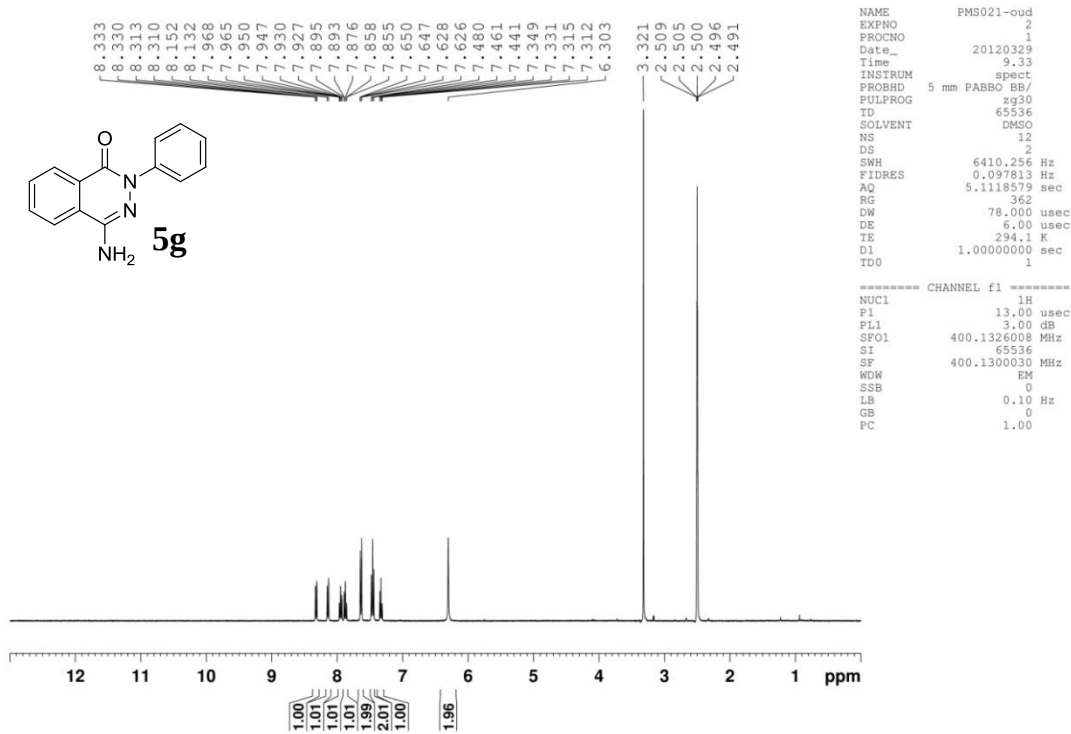
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TD         65536
SOLVENT   DMSO
NS         2048
DS         4
SWH        29761.904 Hz
FIDRES     0.454131 Hz
AQ         1.1010548 sec
RG         2050
DW         16.800 usec
DE         6.50 usec
TE         296.0 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20        0.00689655 sec
TD0        1
  
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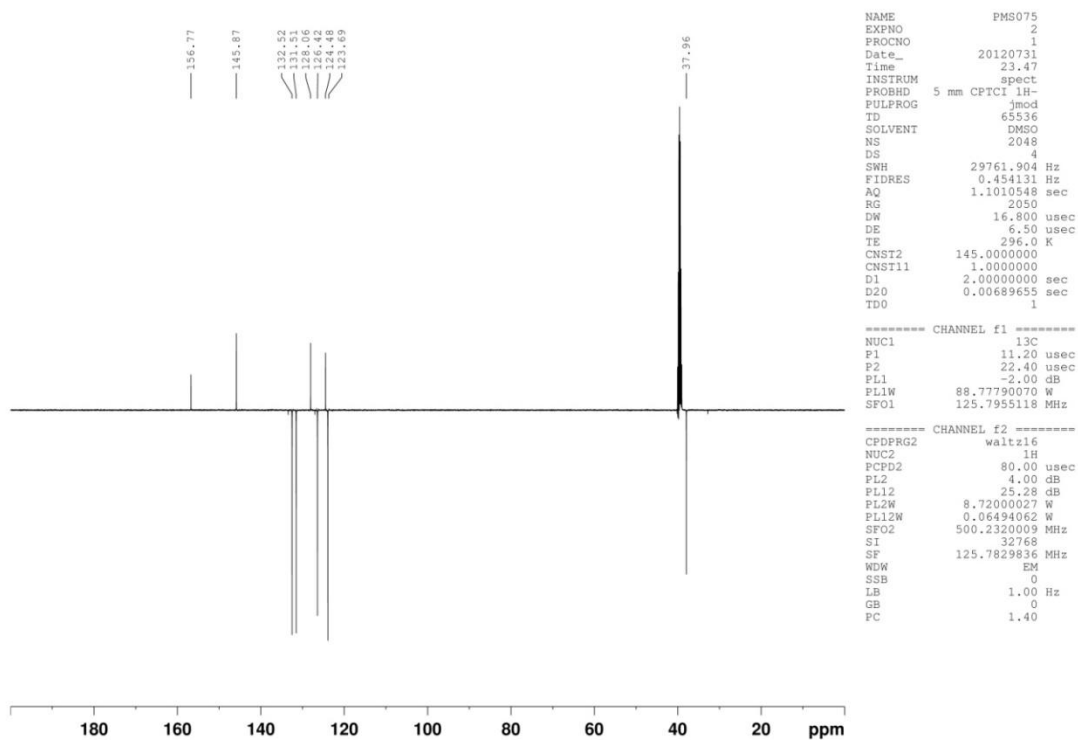
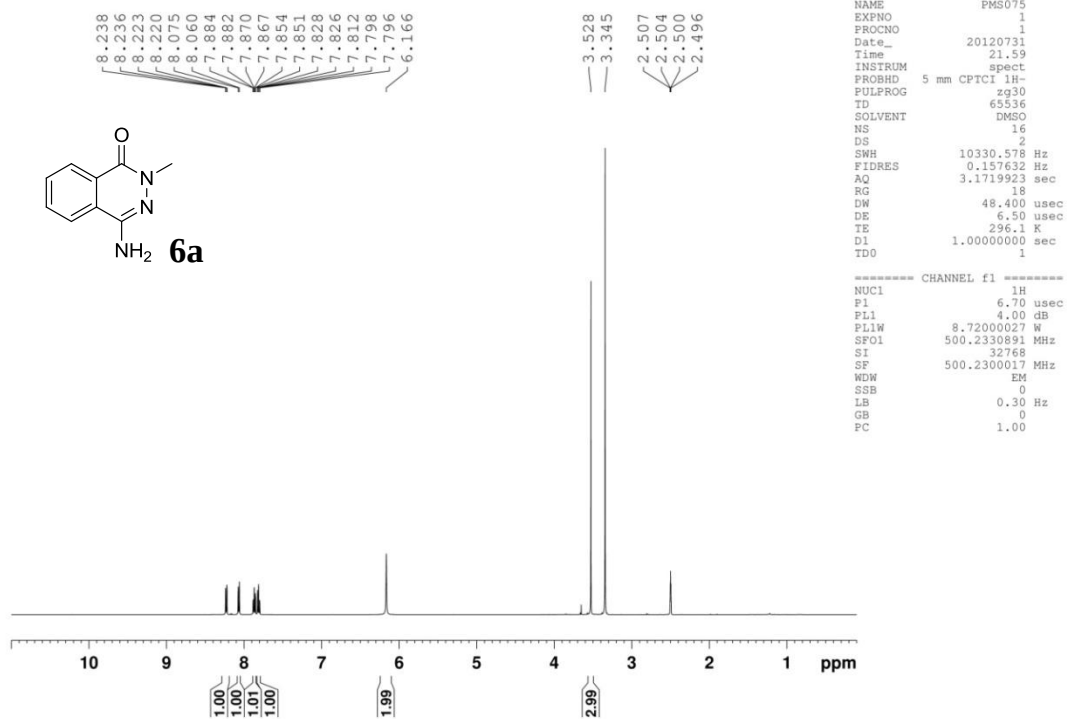
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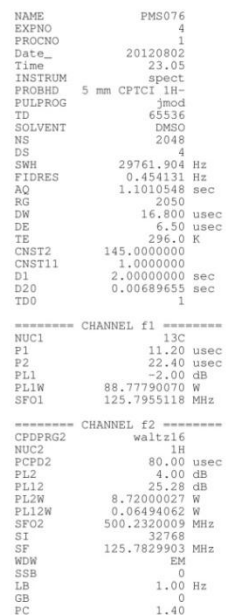
===== CHANNEL f1 =====
NUC1      13C
P1         11.20 usec
P2         22.40 usec
PL1        -2.00 dB
PL1W       88.77790070 W
SFO1      125.7955118 MHz
  
```

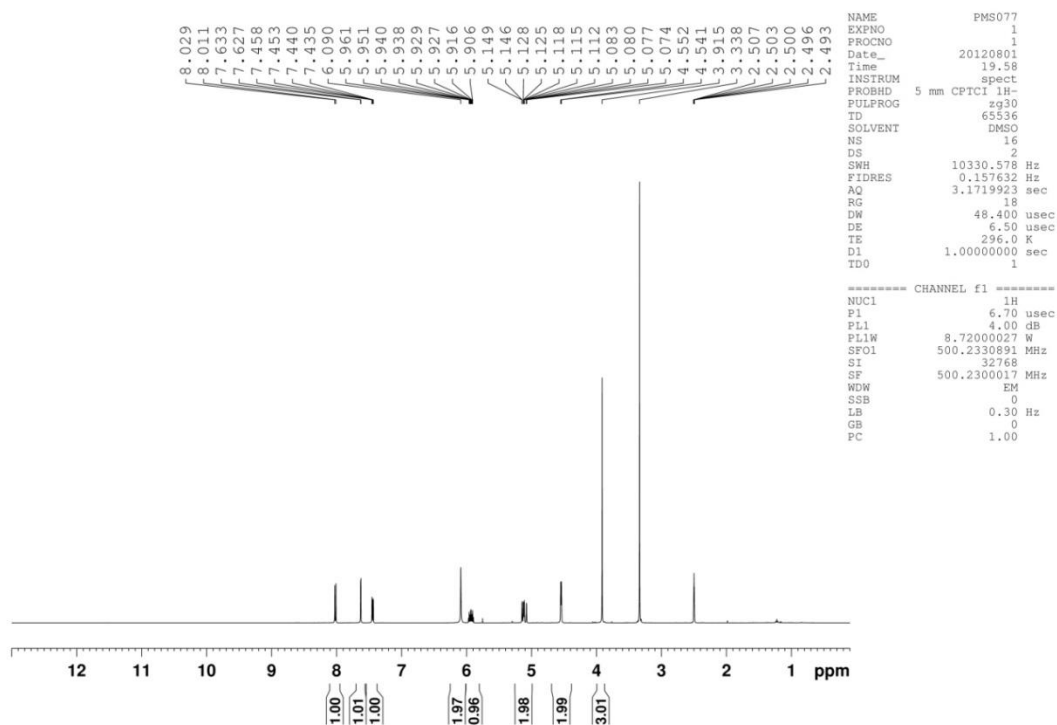
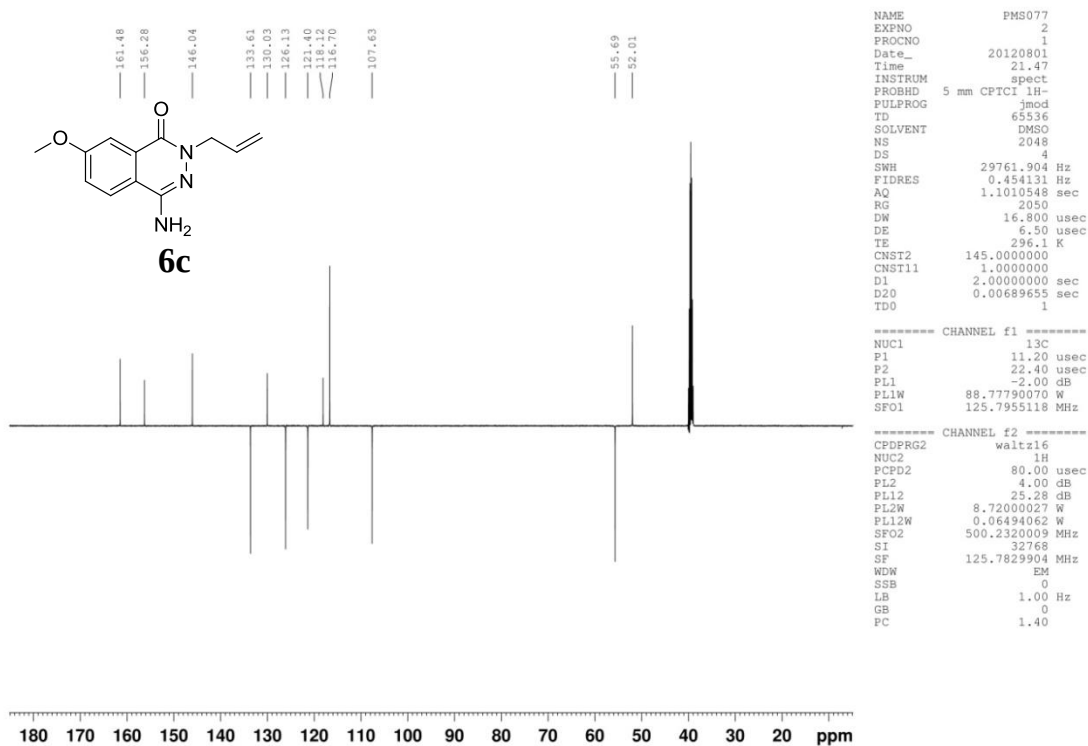
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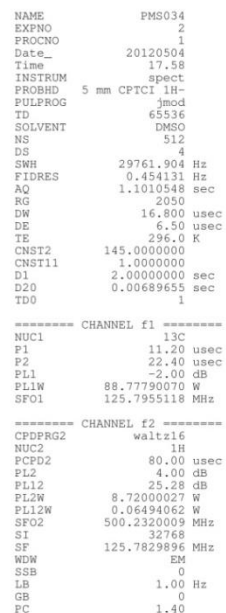
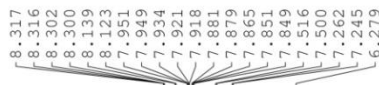
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      80.00 usec
PL2         4.00 dB
PL12       25.28 dB
PL2W       8.72000027 W
PL12W      0.06494062 W
SFO2      500.2320009 MHz
SI         32768
SF         125.7829895 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
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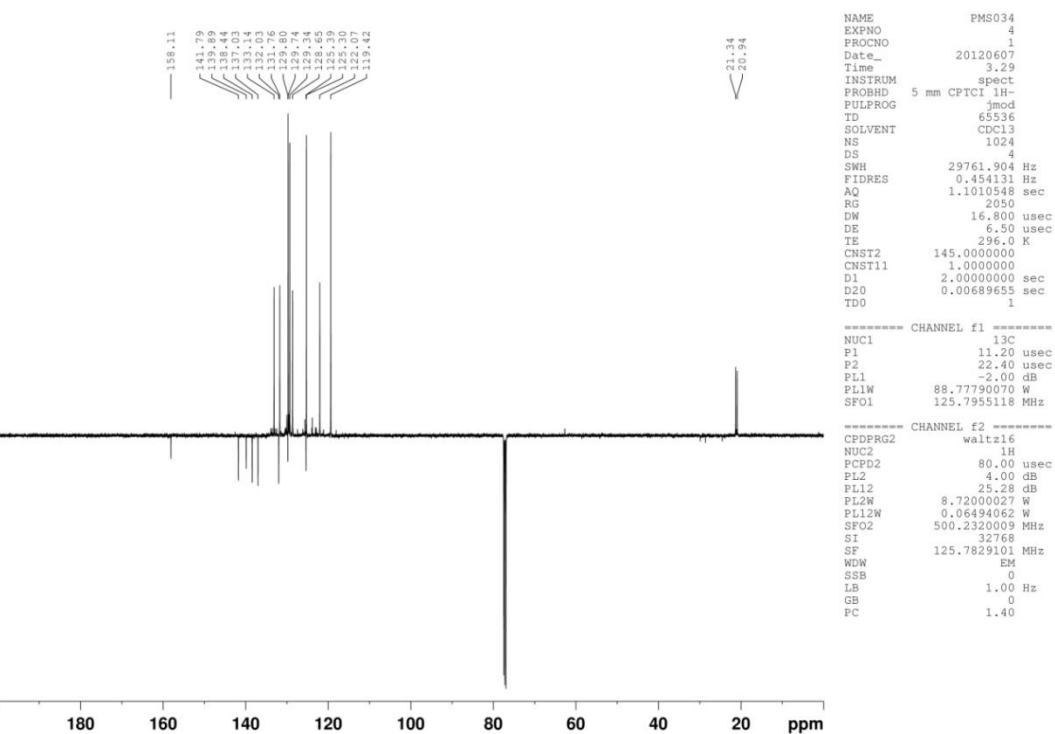


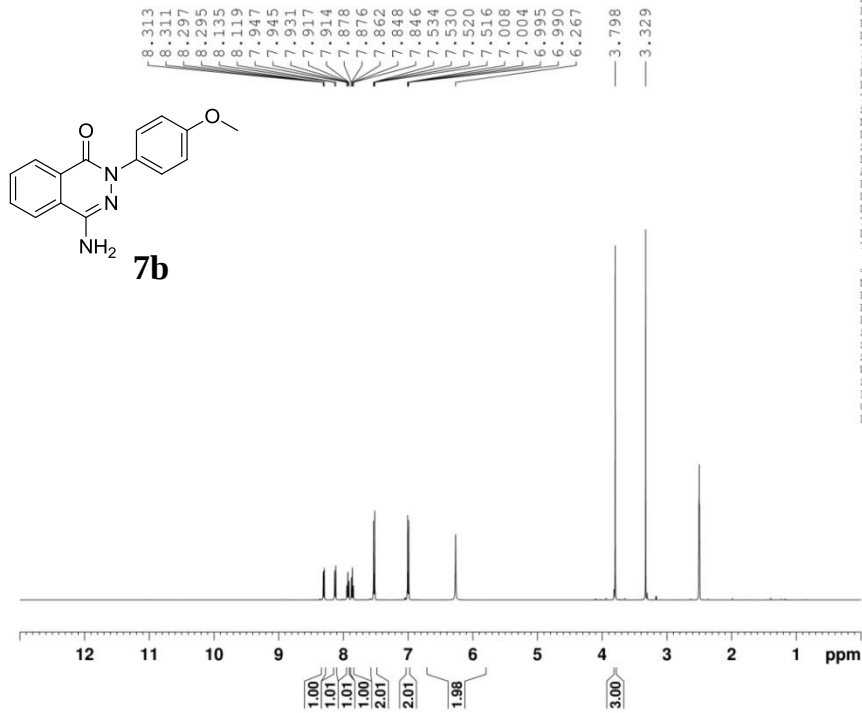






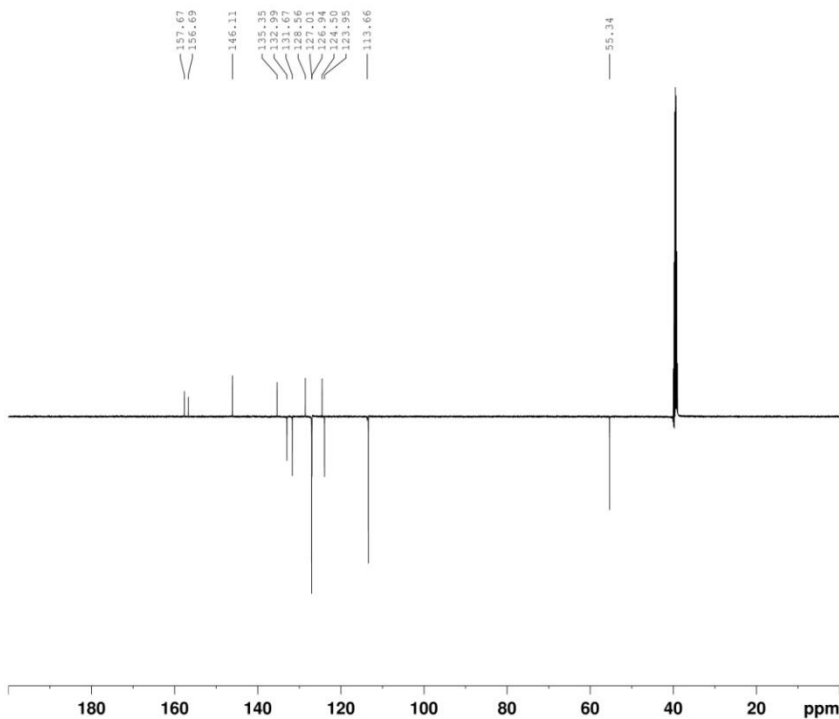






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PROCNO 1
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Time 7.06
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 18
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

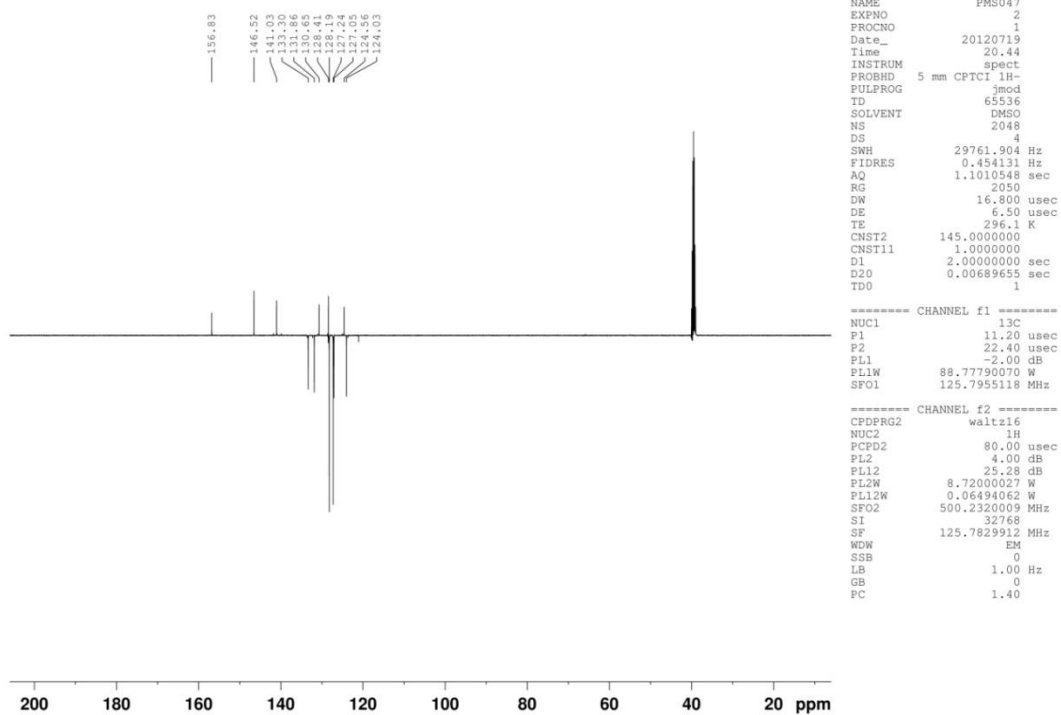
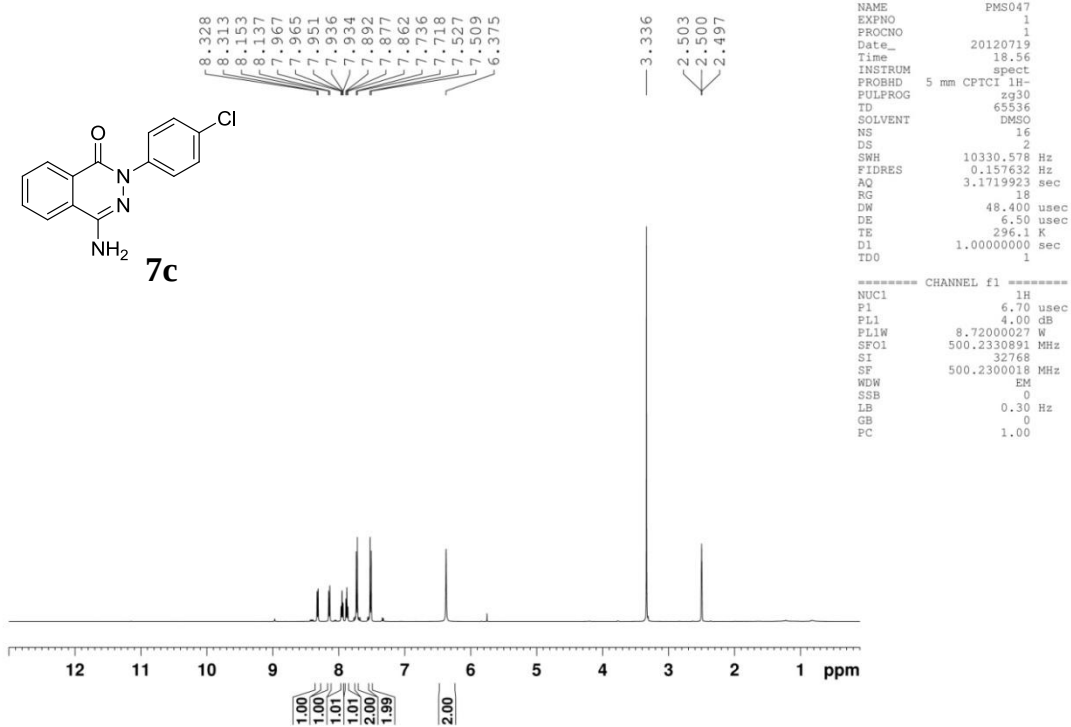
===== CHANNEL f1 =====
NUC1 1H
P1 6.70 usec
PL1 4.00 dB
PL1W 8.72000027 W
SFO1 500.2330891 MHz
SI 32768
SF 500.2300017 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

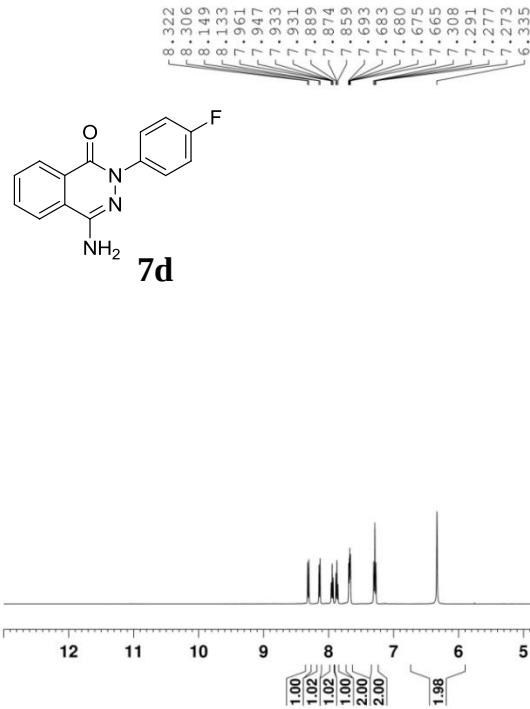


NAME PMS035
EXPNO 2
PROCNO 1
Date_ 20120505
Time 8.00
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG jmod
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.0 K
CNST2 145.0000000
CNST11 1.00000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.20 usec
P2 22.40 usec
PL1 -2.00 dB
PL1W 88.77790070 W
SFO1 125.7955118 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.28 dB
PL2W 8.72000027 W
PL12W 0.06494062 W
SFO2 500.2320009 MHz
SI 32768
SF 125.7829911 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



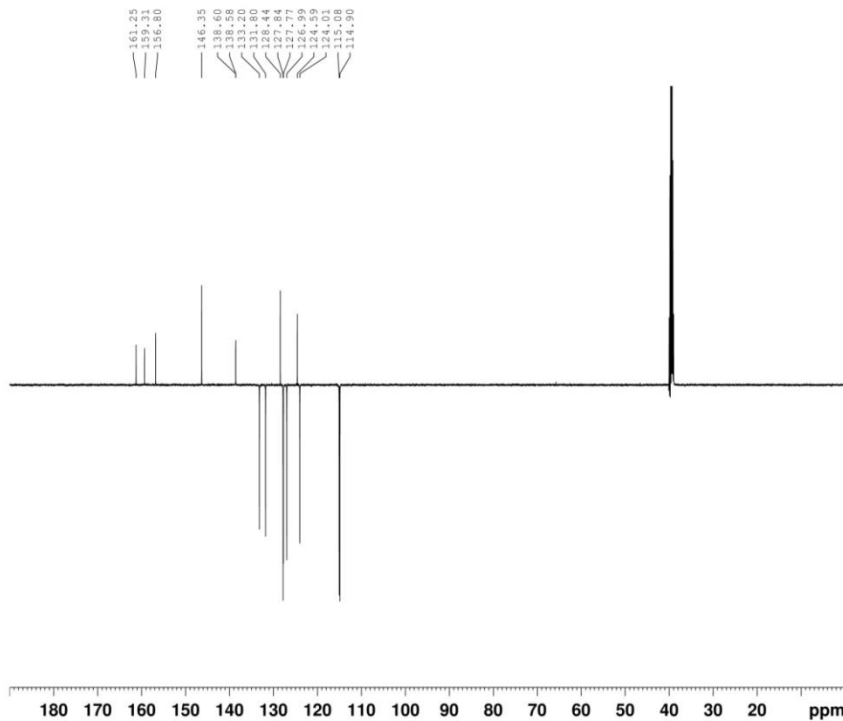


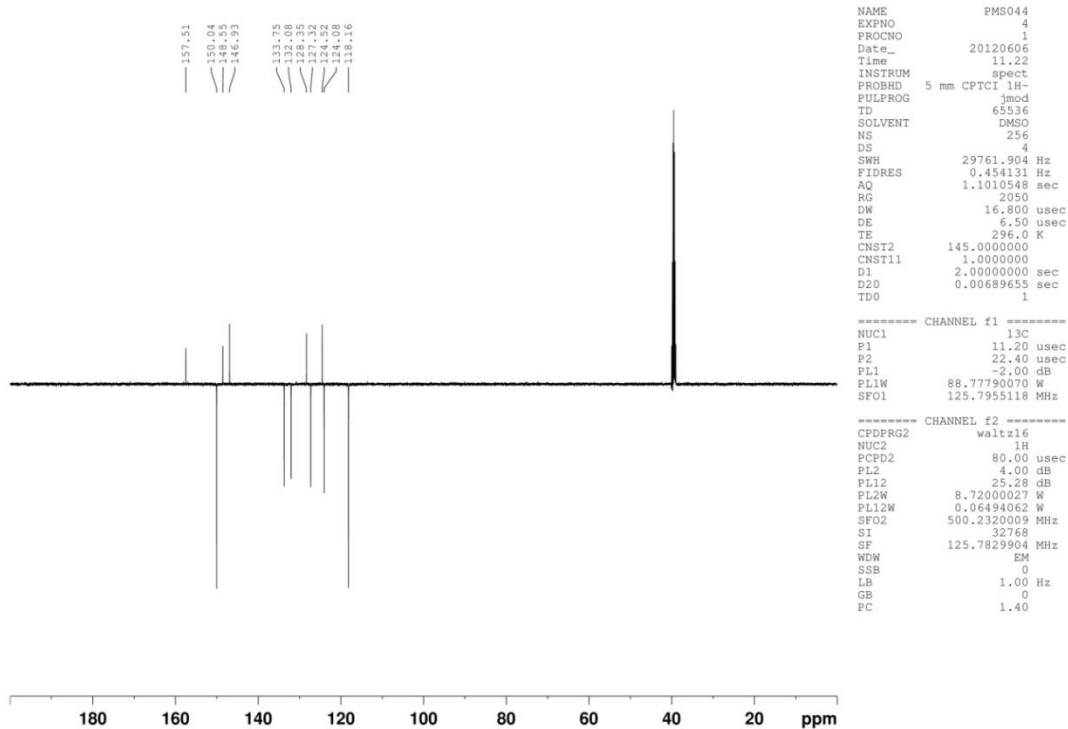
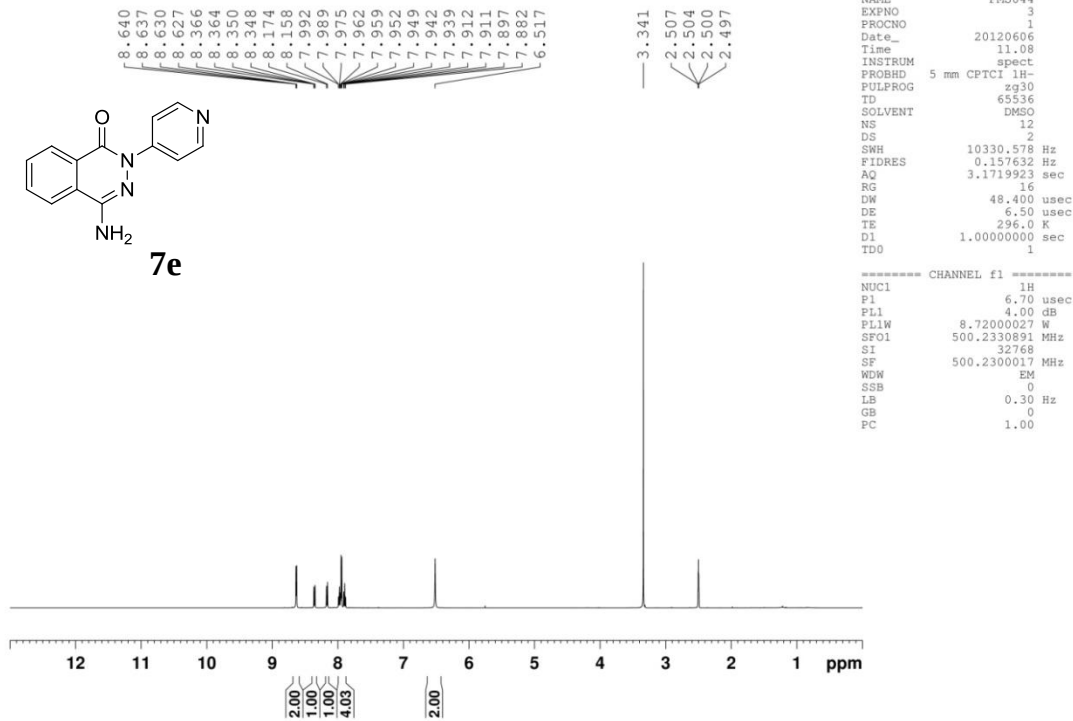
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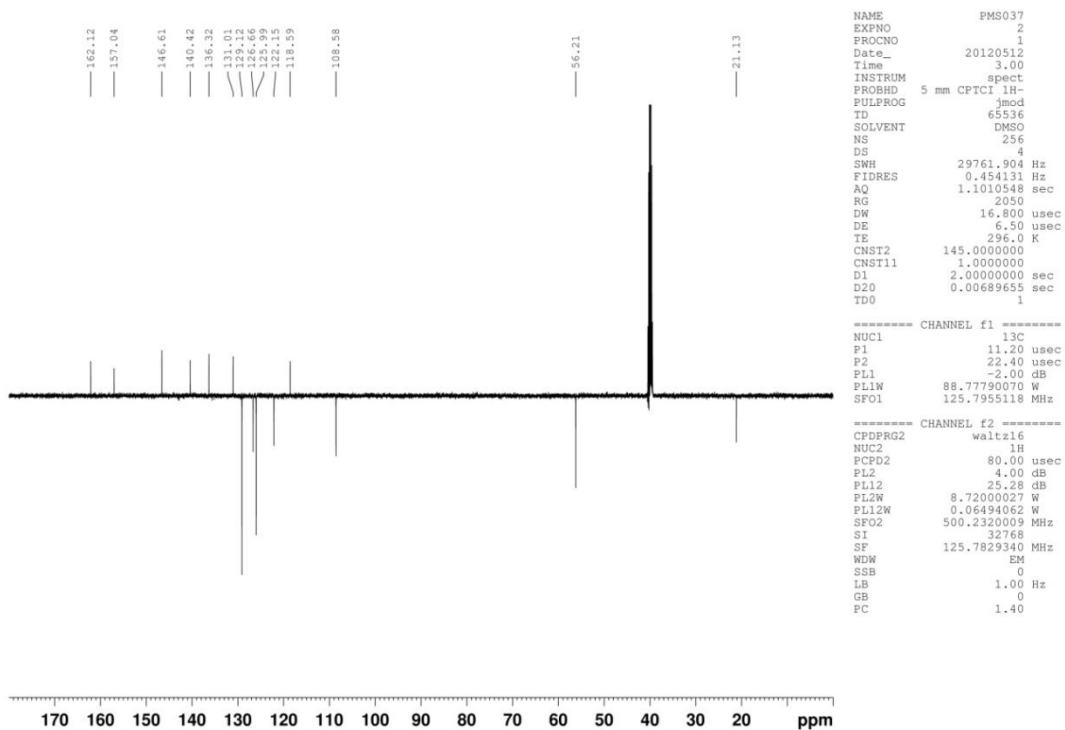
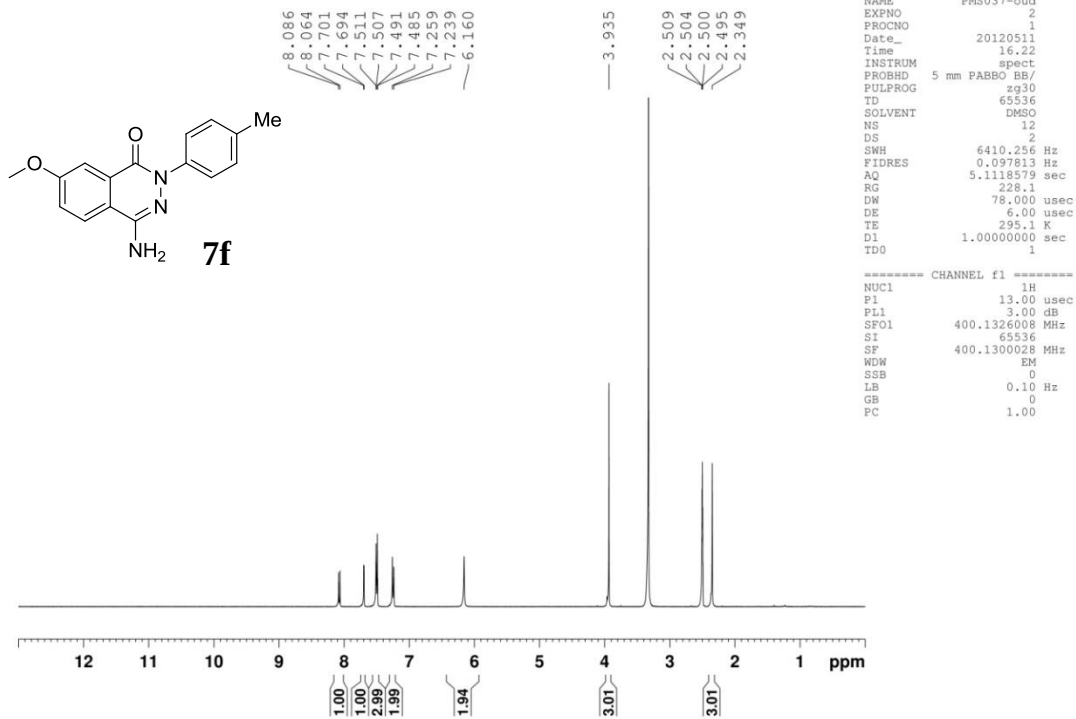
NAME      PMS048
EXPNO     1
PROCNO    1
Date_     20120719
Time      20.49
INSTRUM   spect
PROBHD    5 mm CPTCI 1H-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1719923 sec
RG         18
DW         48.400 usec
DE         6.50 usec
TE         296.0 K
D1         1.00000000 sec
TD0        1
  
```

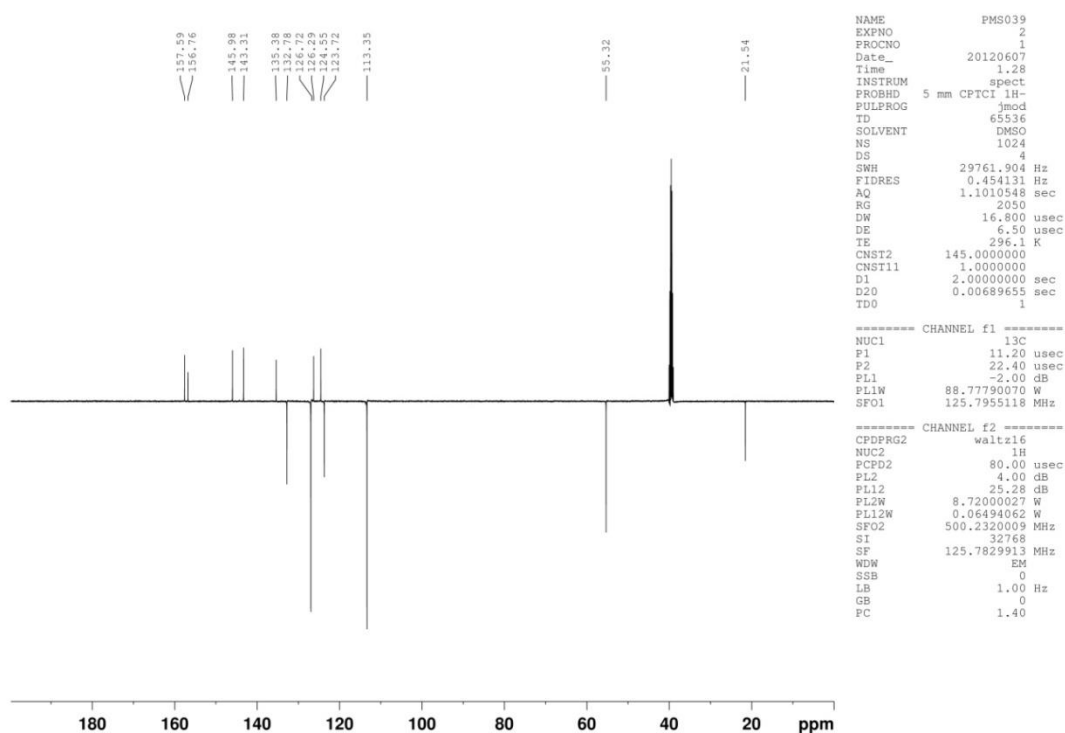
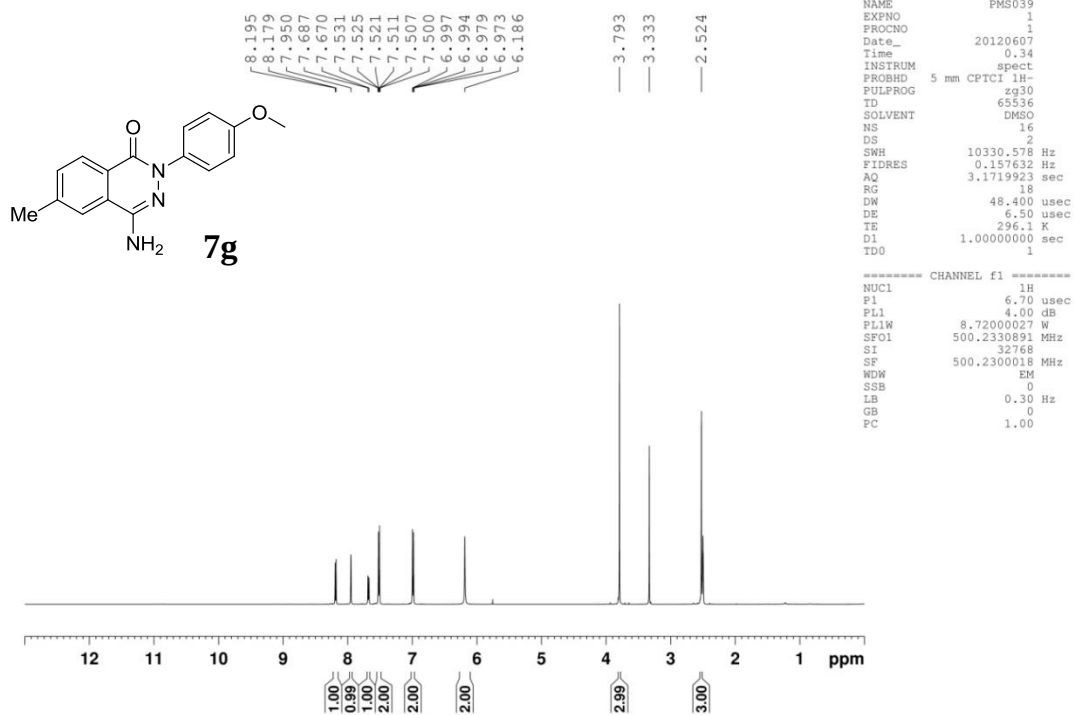
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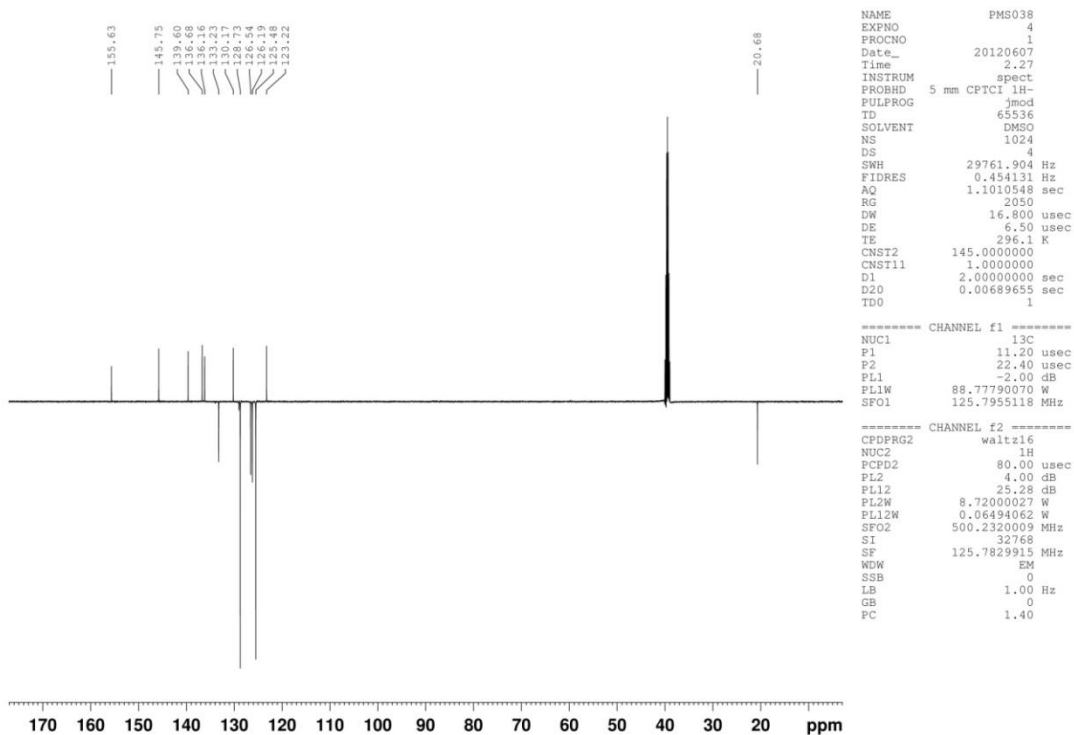
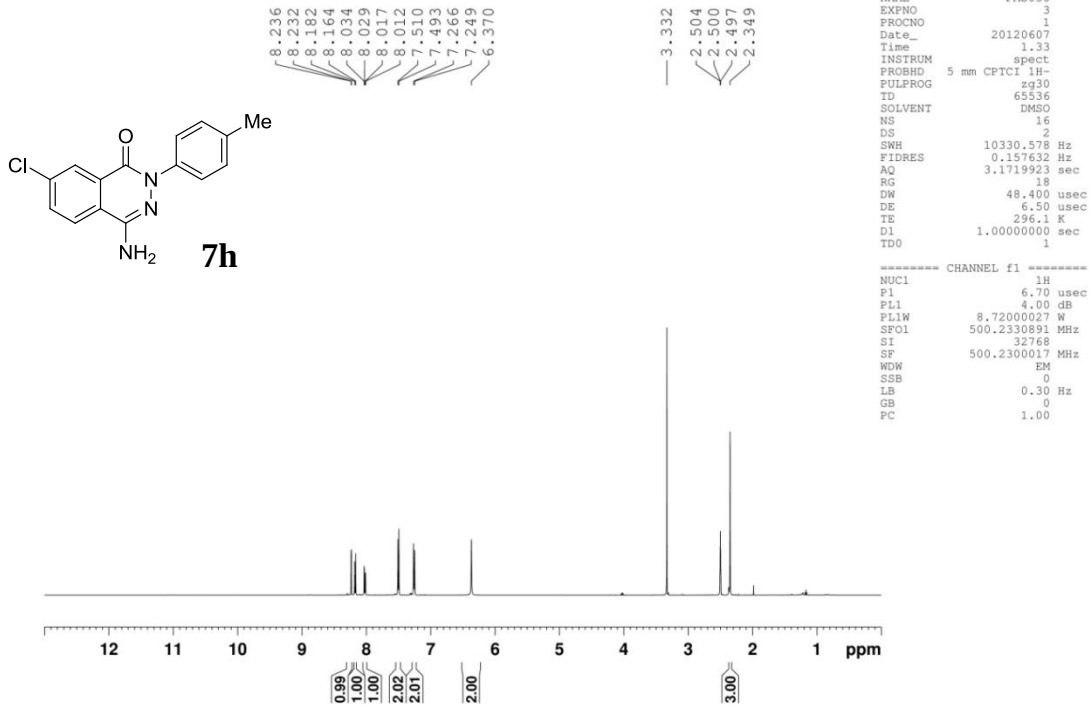
===== CHANNEL f1 =====
NUC1      1H
P1         6.70 usec
PL1        4.00 dB
PL1W       8.72000027 W
SFO1       500.2330891 MHz
SI         32768
SF         500.2300023 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

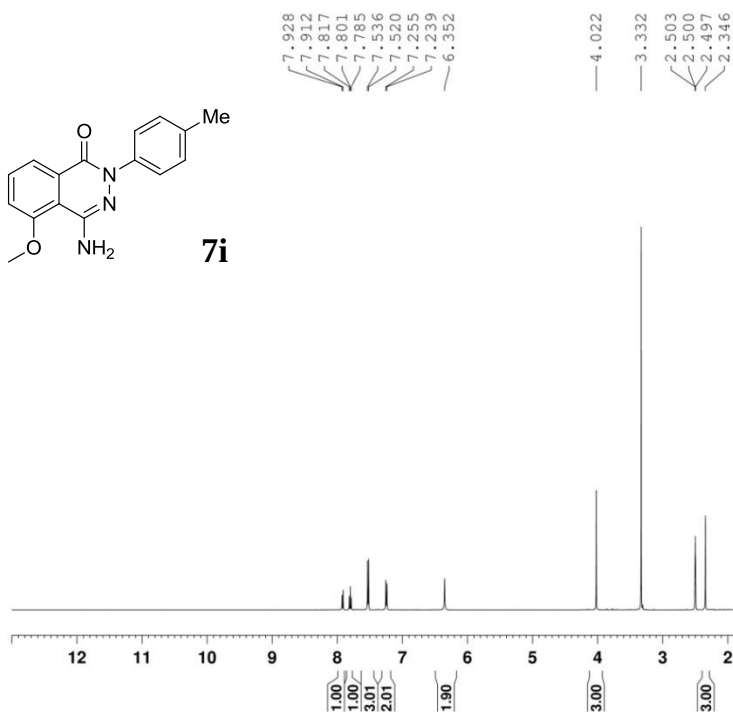
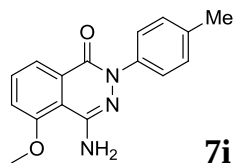










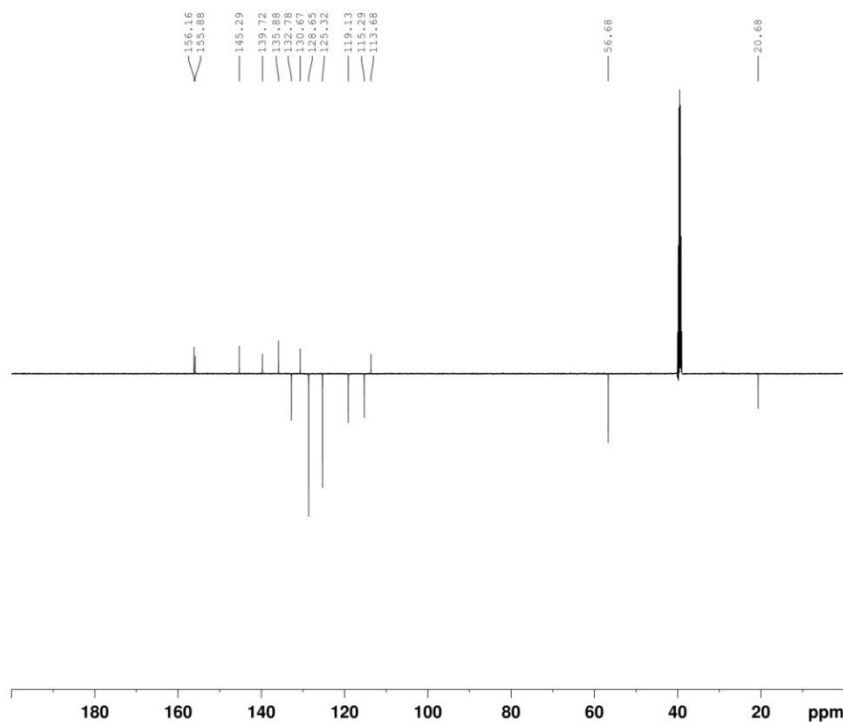


```

NAME      PMS046
EXPNO     1
PROCNO    1
Date_     20120719
Time      17.03
INSTRUM   spect
PROBHD    5 mm CPTCI 1H-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1719923 sec
RG         18
DW         48.400 usec
DE         6.50 usec
TE         296.1 K
D1         1.00000000 sec
D10        1
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1         6.70 usec
PL1        4.00 dB
PL1W       8.72000027 W
SFO1       500.2330891 MHz
SI         32768
SF         500.2300017 MHz
WDW        EM
SSB         0
LB         0.30 Hz
GB          0
PC          1.00
  
```



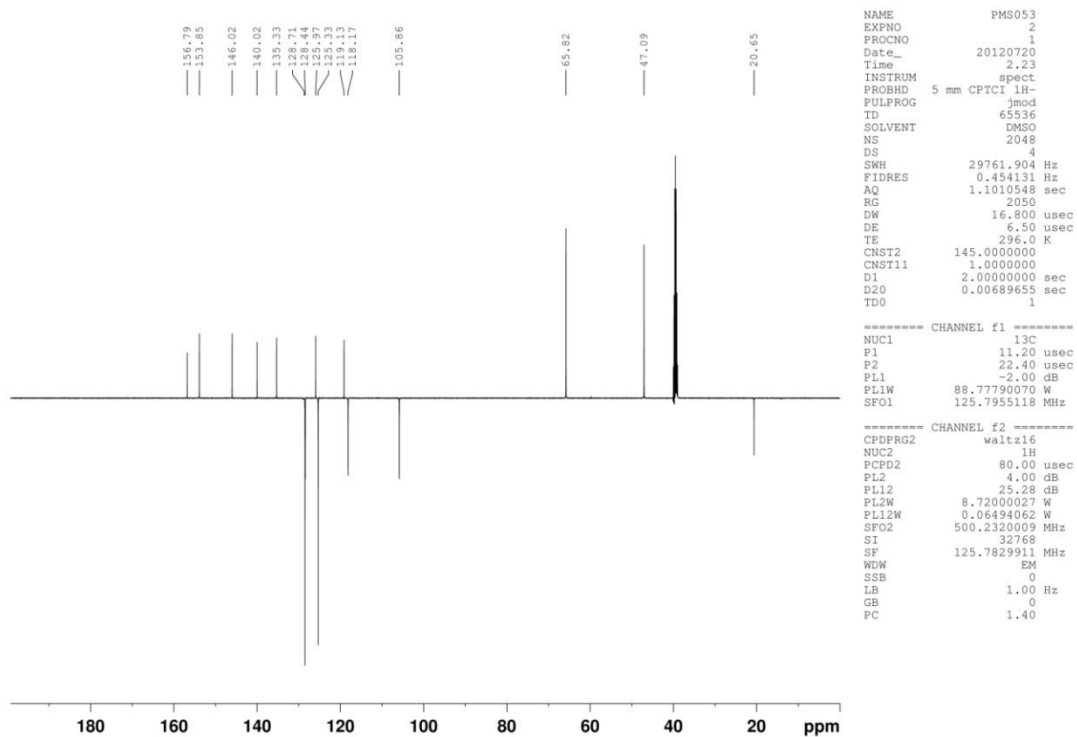
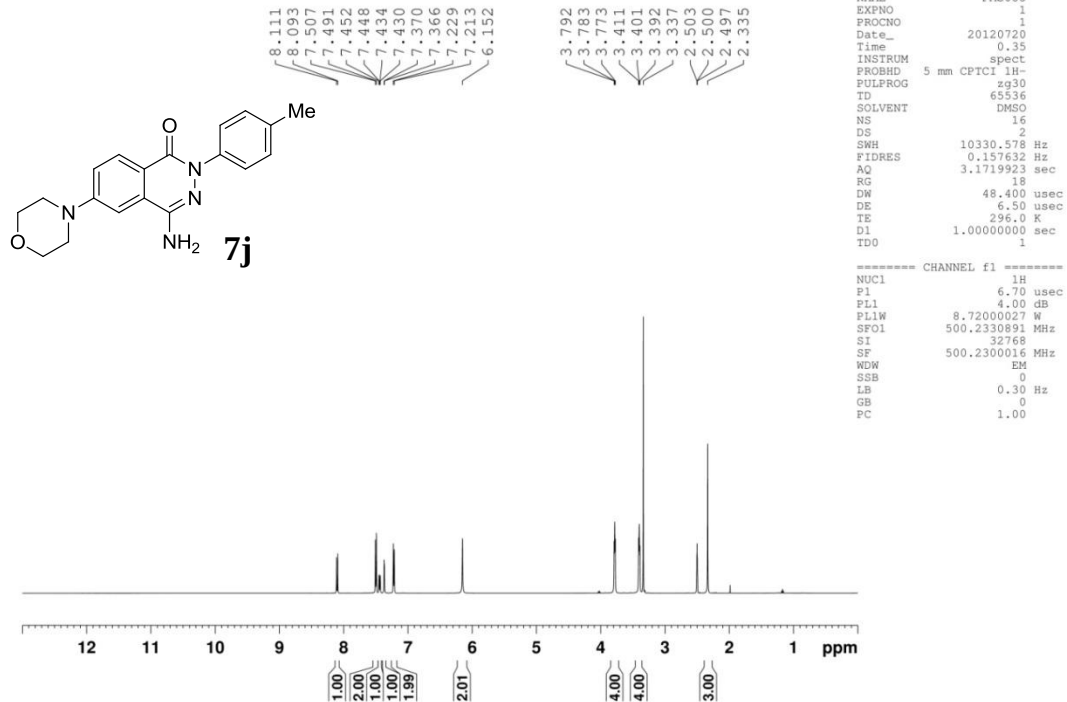
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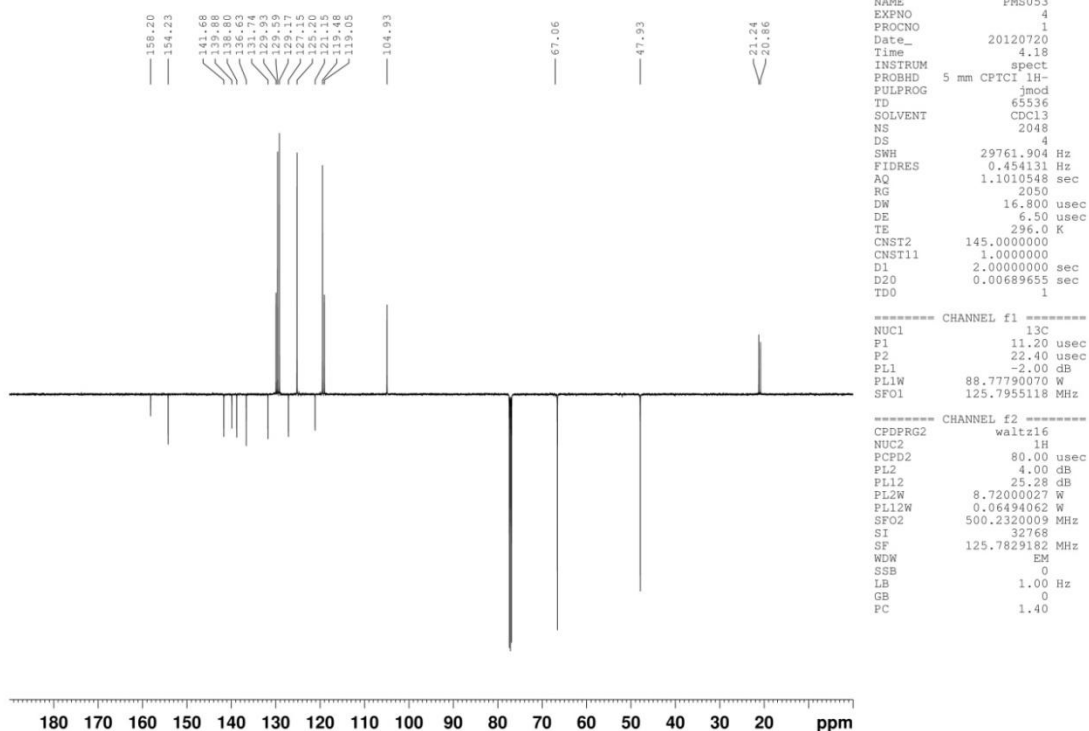
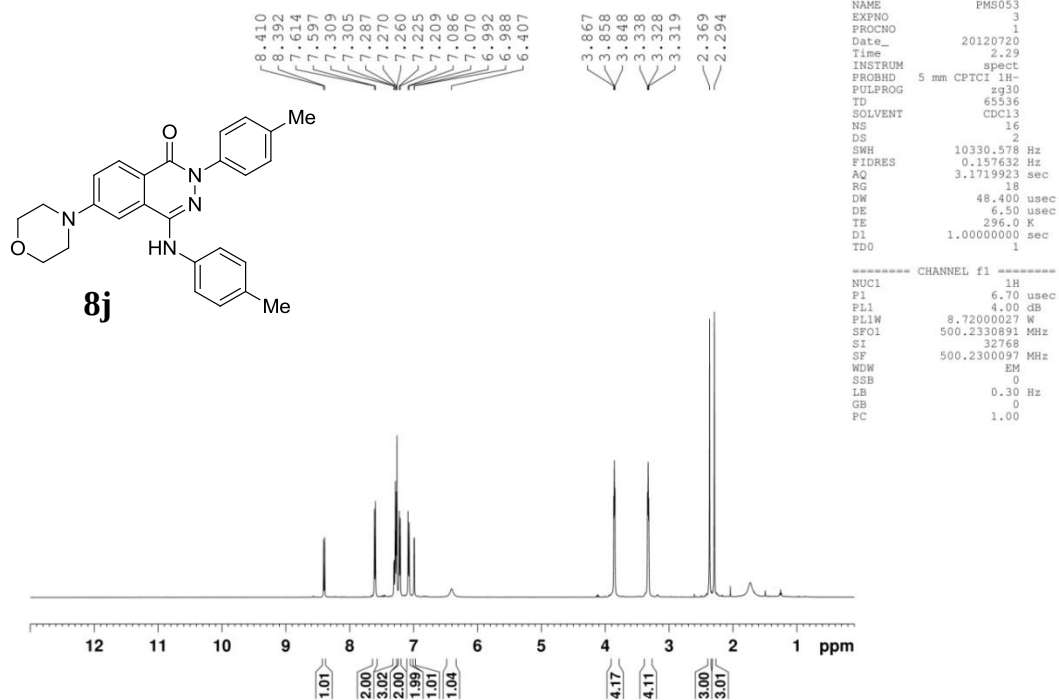
NAME      PMS046
EXPNO     2
PROCNO    1
Date_     20120719
Time      18.52
INSTRUM   spect
PROBHD    5 mm CPTCI 1H-
PULPROG   jmod
TD         65536
SOLVENT   DMSO
NS         2048
DS         4
SWH        29761.904 Hz
FIDRES     0.454131 Hz
AQ         1.1010548 sec
RG         2050
DW         16.800 usec
DE         6.50 usec
TE         296.0 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20        0.00689655 sec
D10        1
TD0        1
  
```

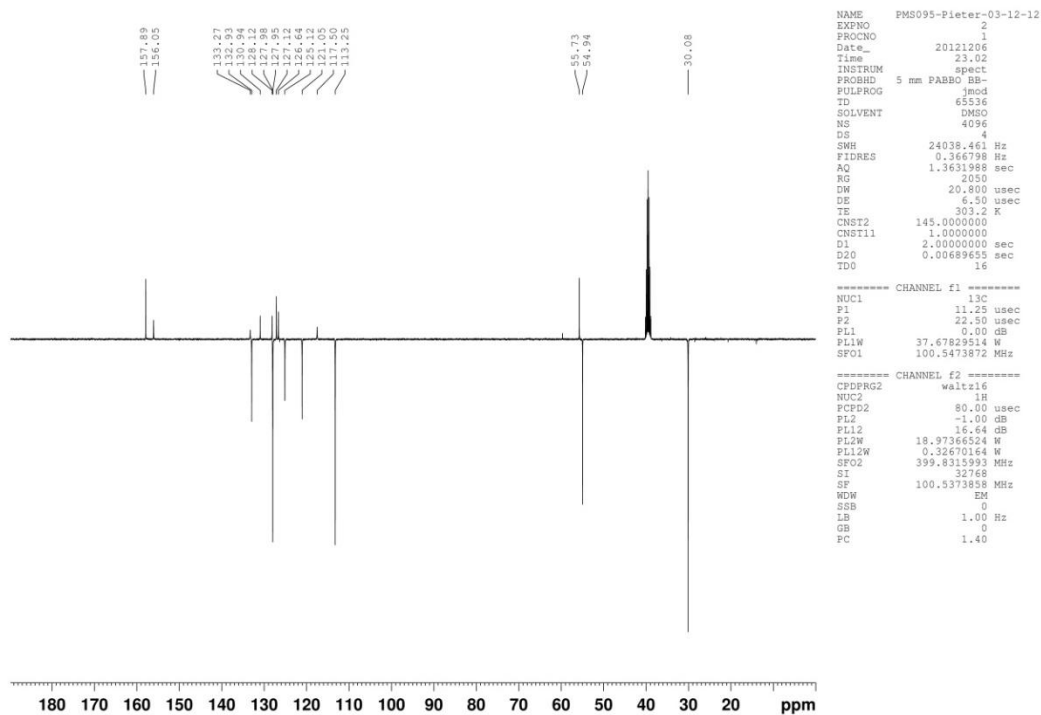
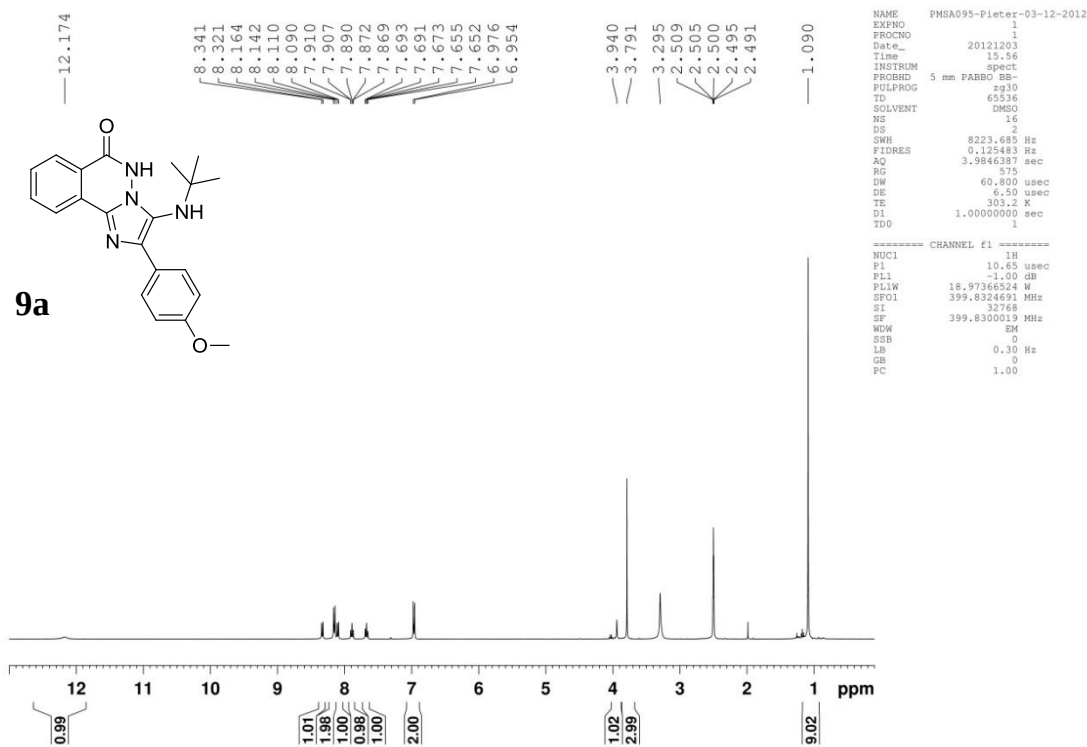
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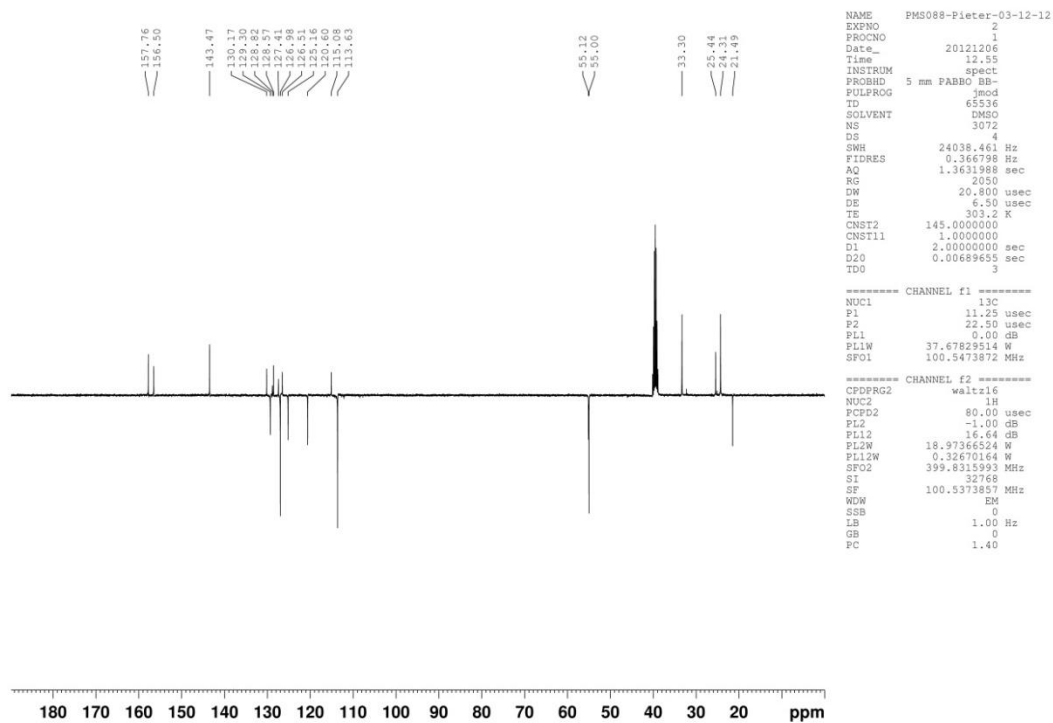
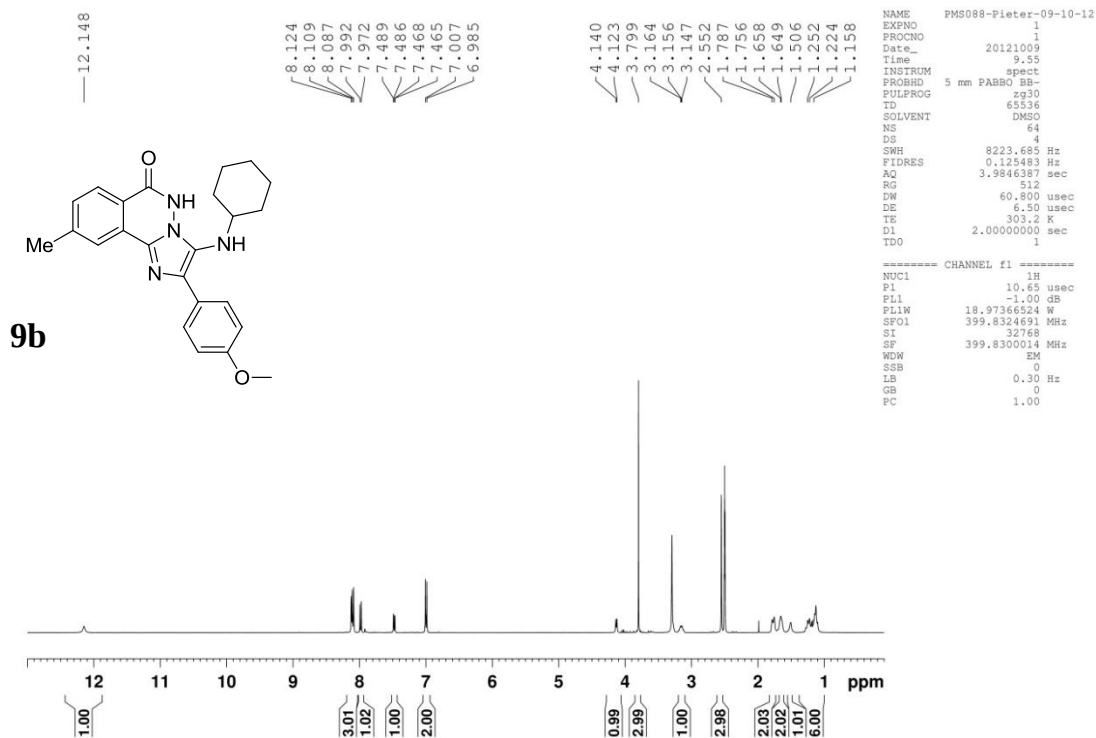
===== CHANNEL f1 =====
NUC1      13C
P1         11.20 usec
P2         22.40 usec
PL1        -2.00 dB
PL1W       88.77790070 W
SFO1       125.7955118 MHz

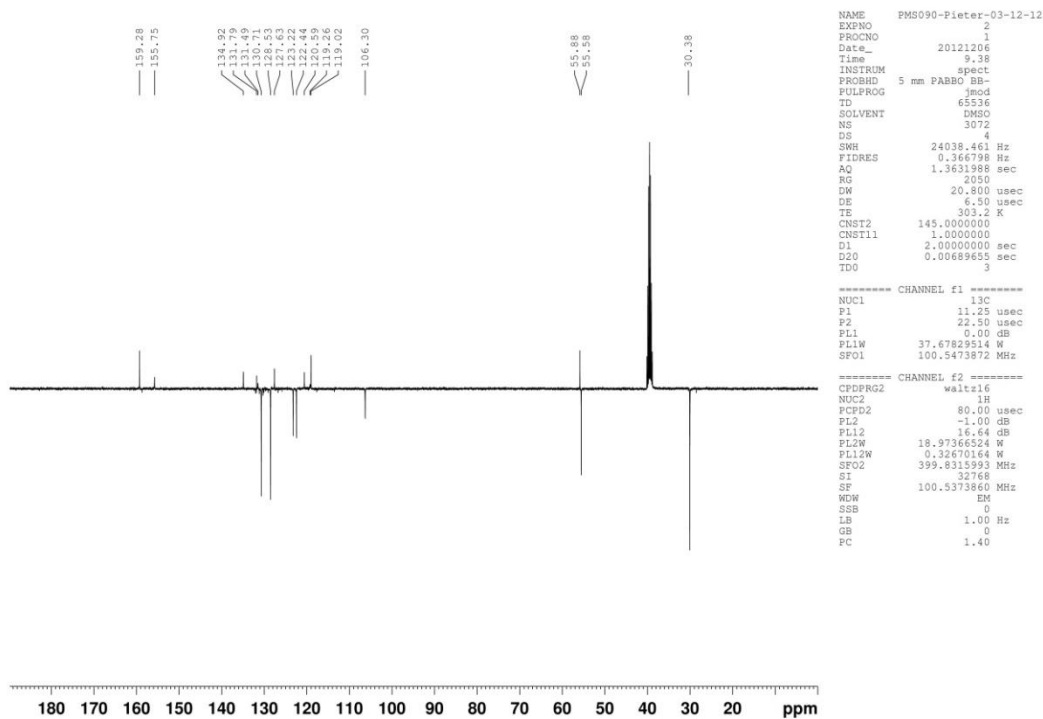
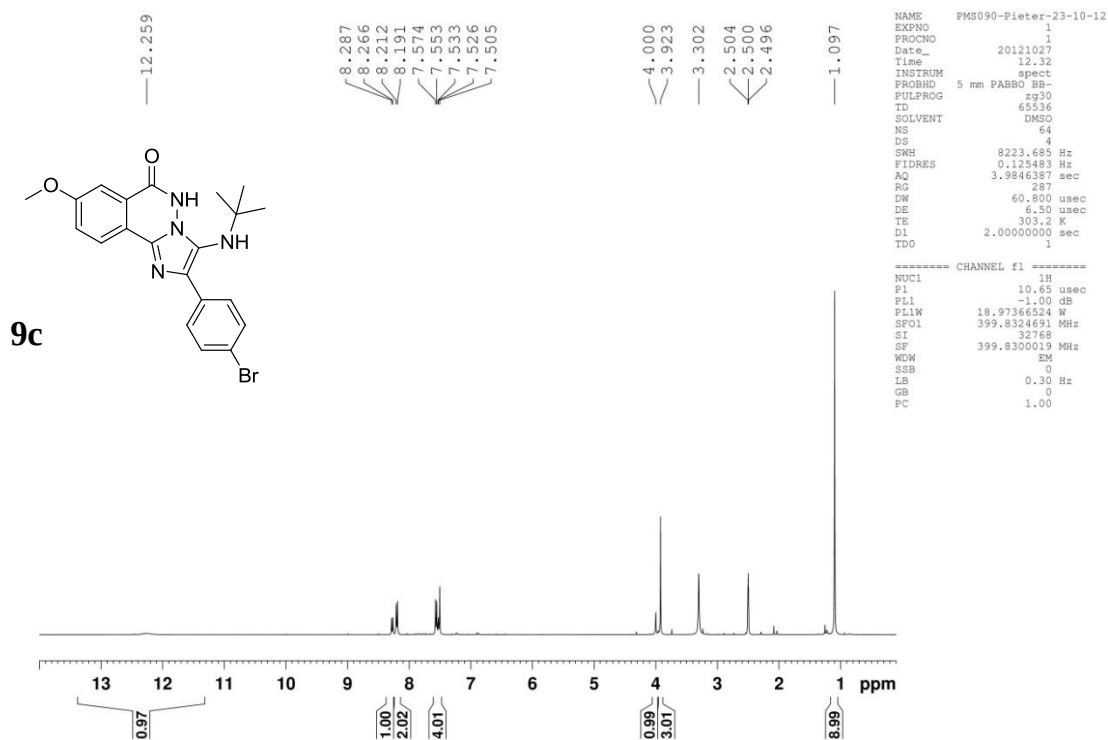
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2        4.00 dB
PL12       25.28 dB
PL2W       8.72000027 W
PL12W      0.06494062 W
SFO2       500.2320009 MHz
SI         32768
SF         125.7829907 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB          0
PC          1.40
  
```













```

===== CHANNEL f1 =====
NUC1                1H
P1                  13.00 usec
PL1                 3.00 dB
SFO1                400.1326008 MHz
SI                  65536
SF                  400.1300027 MHz
WDW                  EM
SSB                  0
LB                  0.10 Hz
GB                  0
PC                  1.00

```



```

===== CHANNEL f1 =====
NUC1                13C
P1                   8.80 usec
p2                   17.60 usec
PL1                  -1.00 dB
SFO1                100.6228298 MHz

```

```
===== CHANNEL f2 =====
CPDPRG2          waltz16
NUC2              1H
PCPD2            80.00 usec
PL2              3.00 dB
PL12             18.00 dB
SF02             400.1316005 MHz
SI               32768
SF               100.6128162 MHz
WDW              EM
SSB              0
LB               1.00 Hz
GB              0
PC               1.40
```