

Supplementary Material

Cyclic ADP-ribose analogs without “southern” ribose inhibit ADP-ribosyl cyclase-hydrolase CD38

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Contents

Figures S1-3	S2
Crystallographic data collection and model refinement statistics	S4
HPLC of compound 7	S5
¹ H-NMR and ¹³ C-NMR of <i>N</i> 9-butyl-cIDPR compounds	S6

Figure S1: As the cyclic compound **7** peak diminished, a new peak corresponding to **7a** appeared.

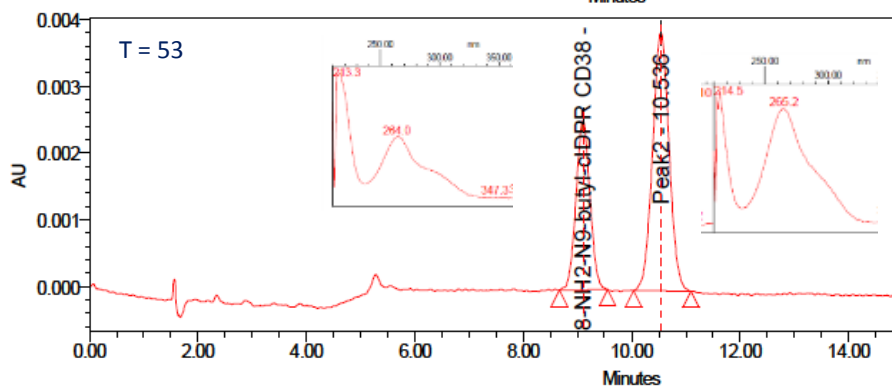
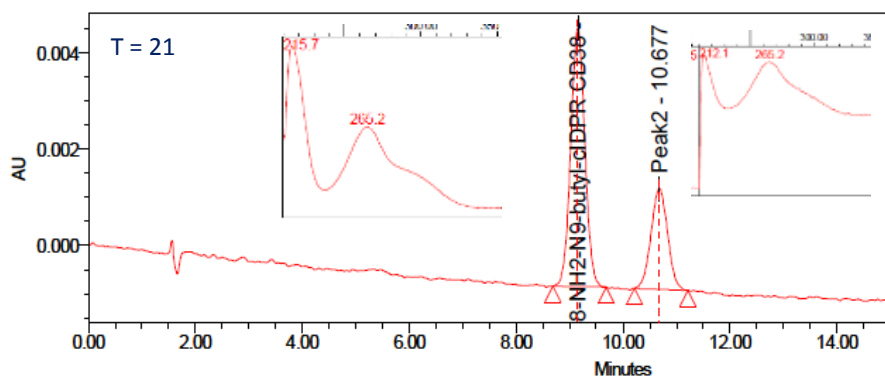
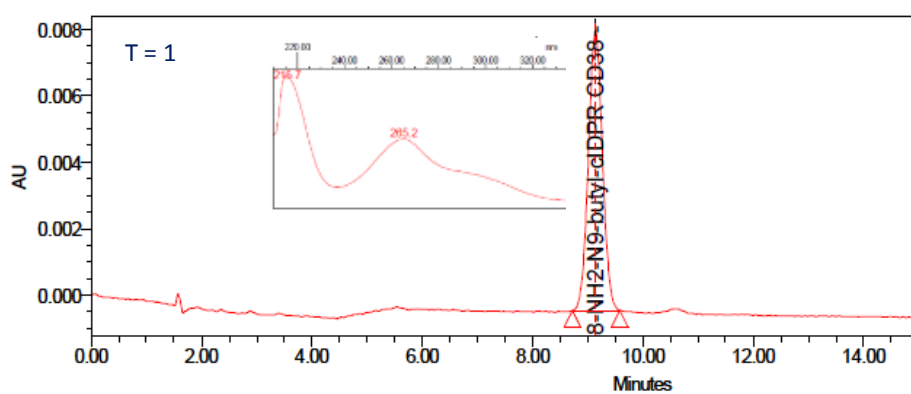
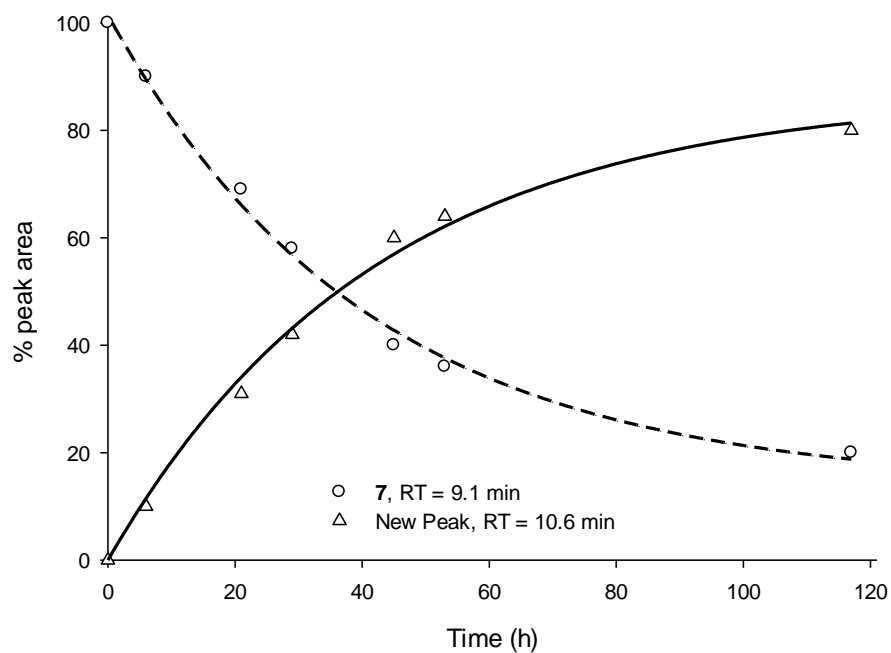


Figure S2: The rate of hydrolysis of **7** depended on the concentration of CD38 present

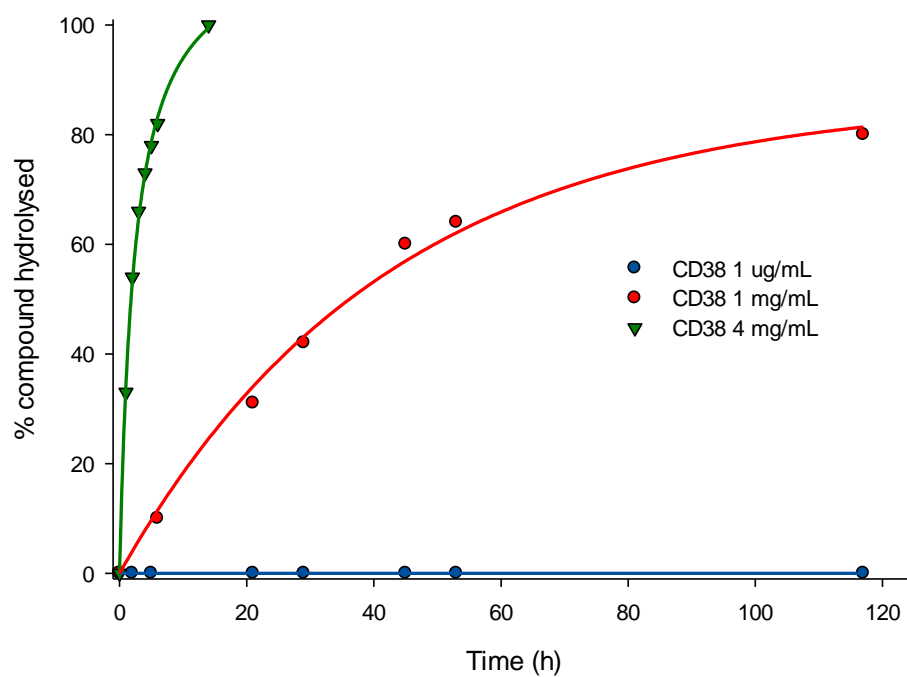


Figure S3: At concentrations of CD38 used in the enzyme assay, neither cIDPR (**2**) or 8-NH₂-N⁹-butyl-cIDPR was hydrolysed.

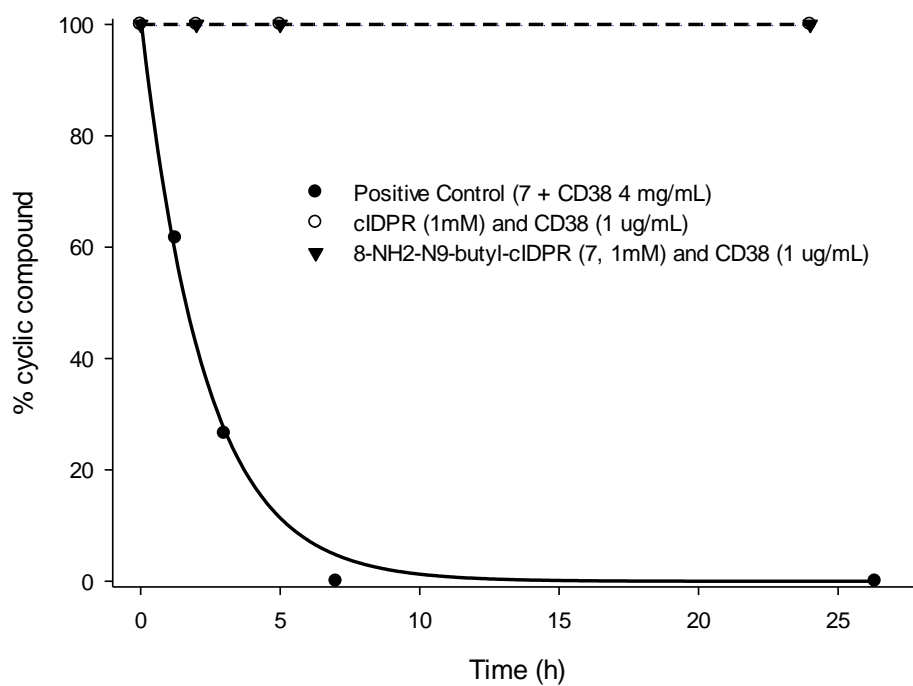


Table 1 Data collection and refinement statistics (PDB Code 4TMF)

	CD38-7a
Data collection	
Wavelength (Å)	0.9785
Space group	P1
Cell dimensions	
<i>a</i> , <i>b</i> , <i>c</i> (Å)	41.69, 54.13, 63.32
α , β , γ (°)	108.58, 90.98, 93.98
Resolution (Å)	50~2.05(2.12~2.05) *
<i>R</i> _{merge}	0.046(0.528)*
Completeness (%)	97.6(97.3)*
Redundancy	3.9(3.9)*
<i>I</i> / σI	24.6(2.6)*
Refinement	
Resolution (Å)	50~2.05
No. reflections	30312
<i>R</i> _{work} / <i>R</i> _{free}	0.1980/0.2270
No. atoms	
Protein	3946
ligand#	66
Water	80
Ramachandran plot	
Favored (%)	98
Outliers (%)	0.21
Clashscore	3.33
<i>B</i> -factors	
Protein	67.60
ligand	69.50
Water	52.00
R.m.s. deviations	
Bond lengths (Å)	0.011
Bond angles (°)	1.42

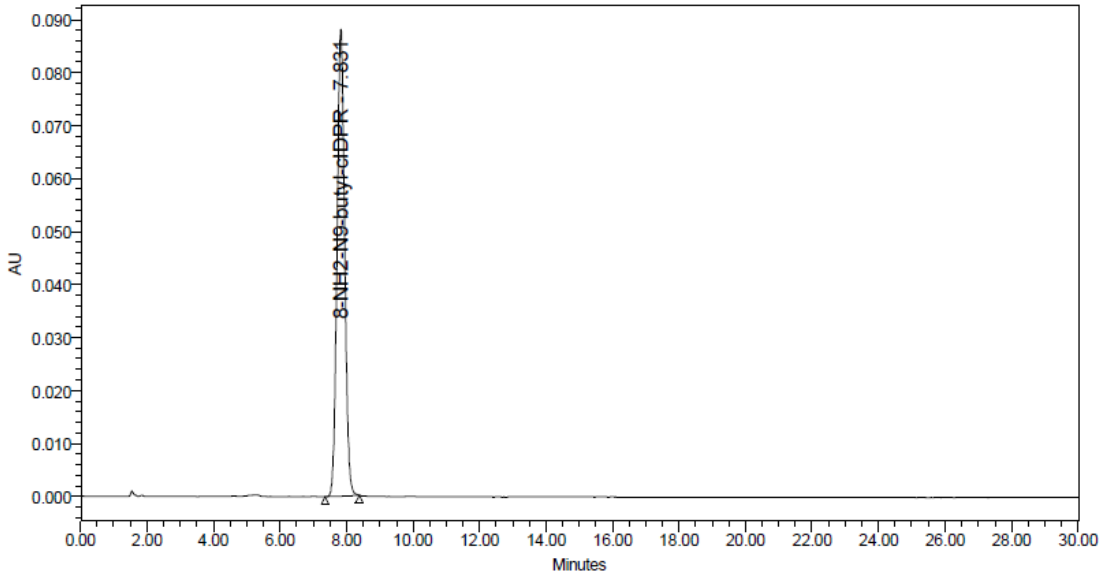
*Values in parentheses are for highest-resolution shell.

#ligand: hydrolysed compound (**7a**).

HPLC traces for Compound 7 (8-NH₂-N₉-butyl cIDPR)

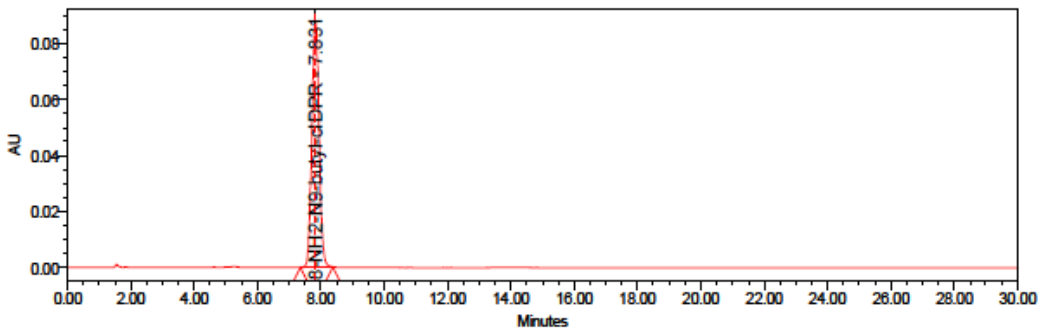
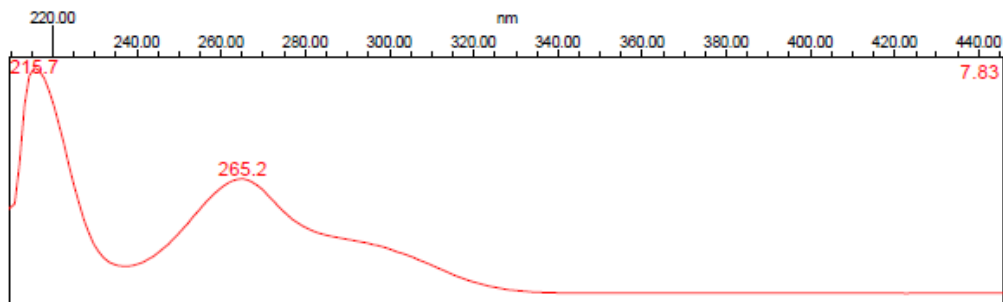
SAMPLE INFORMATION

Sample Name:	JMS 687 A5	Acquired By:	Christelle
Sample Type:	Unknown	Date Acquired:	24/04/2012 5:47:38 PM
Vial:	5	Acq. Method Set:	isocratic new PDA Jo
Injection #:	1	Date Processed:	04/05/2012 1:07:49 PM
Injection Volume:	10.00 ul	Processing Method:	8_NH2 N9 butyl cIDPR
Run Time:	30.0 Minutes	Channel Name:	Wvlm Ch1
Sample Set Name:	JMS 687 A	Proc. Chnl. Descr.:	PDA 254.0 nm



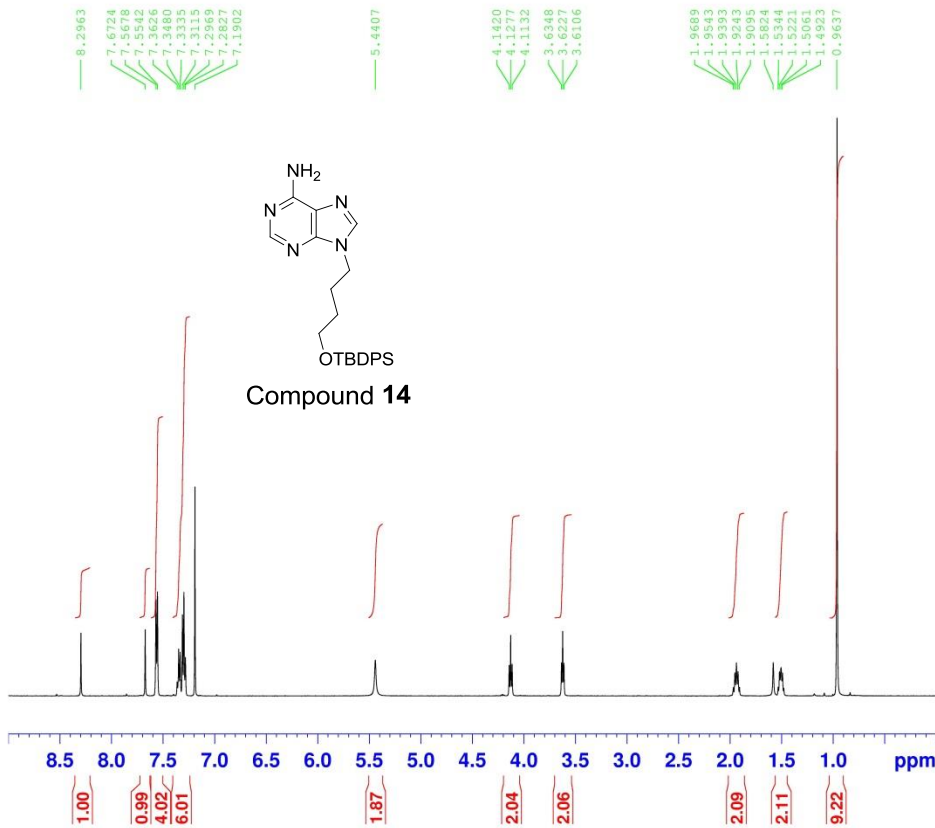
	Peak Name	RT	Area	% Area	Height
1	8-NH ₂ -N ₉ -butyl-cIDPR	7.831	1400095	100.00	88097

Spectrum Index Plot
8-NH₂-N₉-butyl-cIDPR - 7.831



PDA Result Table

	Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	8-NH ₂ -N ₉ -butyl-cIDPR	7.831	1400095			No				No

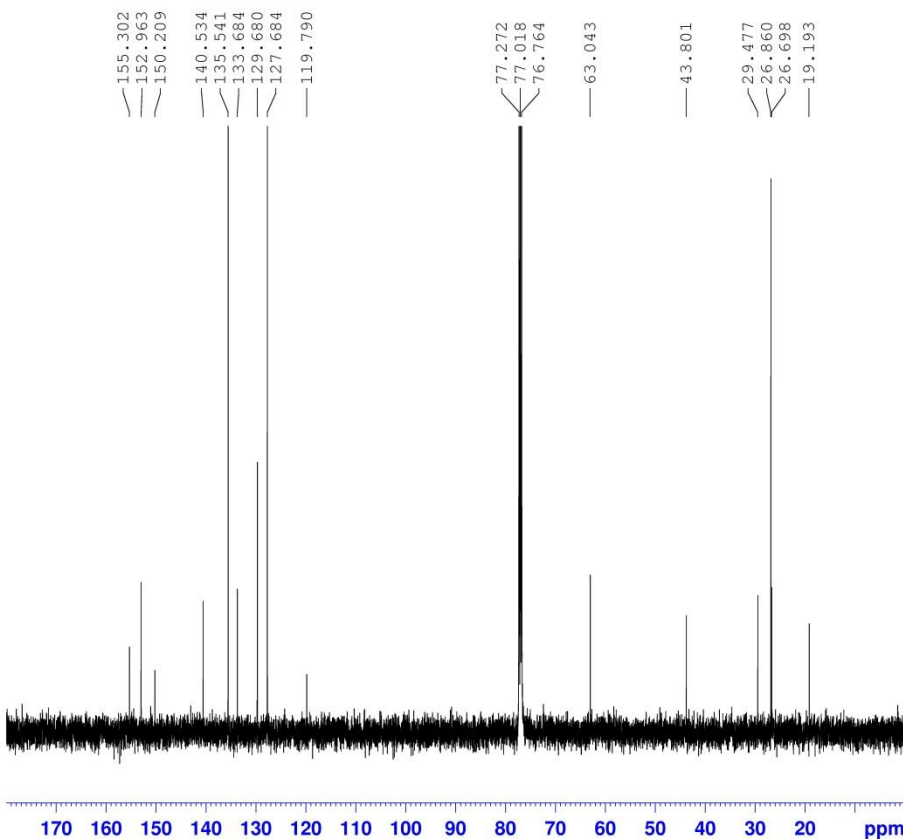


```

NAME      Nov26-2012-JMS663
EXPNO     1
PROCNO    1
Date_     20121126
Time      16.22
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1719923 sec
RG         287
DW         48.400 usec
DE         13.94 usec
TE         298.2 K
D1         1.00000000 sec
TDO        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1         10.30 usec
PL1        -0.12 dB
PL1W      19.35150909 W
SFO1      500.1330885 MHz
SI         32768
SF         500.1300482 MHz
WDW        EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00
  
```



```

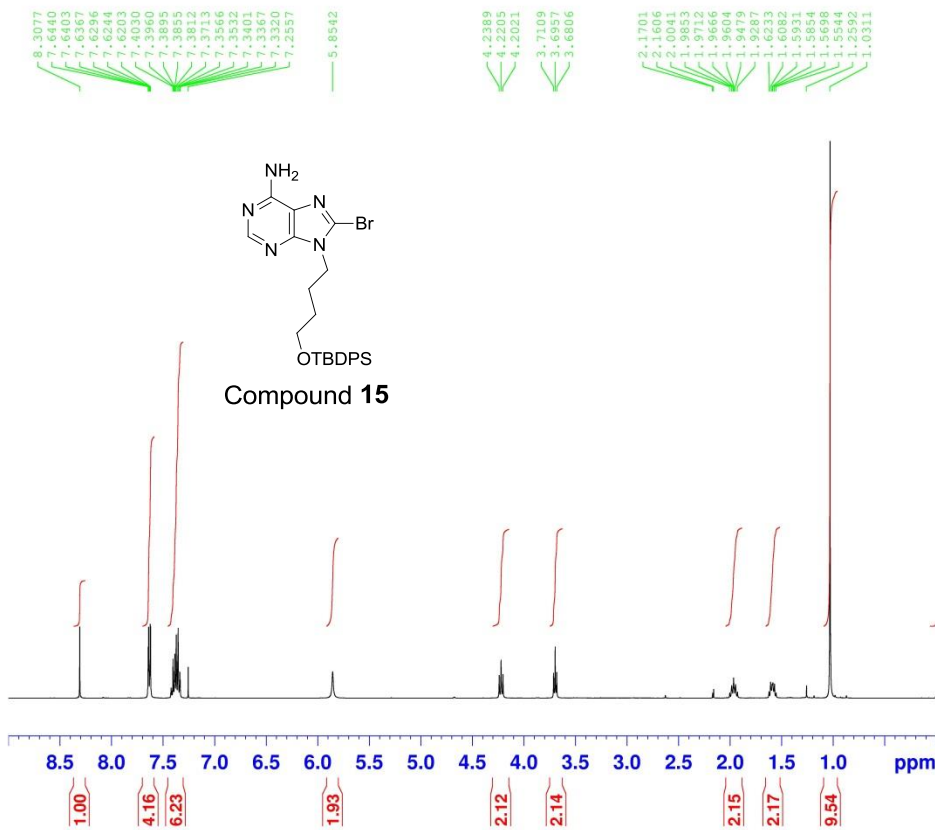
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EXPNO     11
PROCNO    1
Date_     20121127
Time      4.49
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH        29761.904 H:
FIDRES     0.454131 H:
AQ         1.1010548 se
RG         2050
DW         16.800 u:
DE         8.43 u:
TE         298.0 K
D1         2.00000000 se
D11        0.03000000 se
TDO        1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1         9.50 u:
PL1        -0.51 dl
PL1W      99.92730713 W
SFO1      125.7703643 MI
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 u:
PL2        -0.12 dl
PL12      17.94 dl
PL13      21.00 dl
PL2W      19.35150909 W
PL12W     0.30249262 W
PL13W     0.14952536 W
SFO2      500.1320005 MI
SI         32768
SF         125.7577890 MI
WDW        EM
SSB         0
LB         1.00 H:
GB         0
PC         1.40
  
```

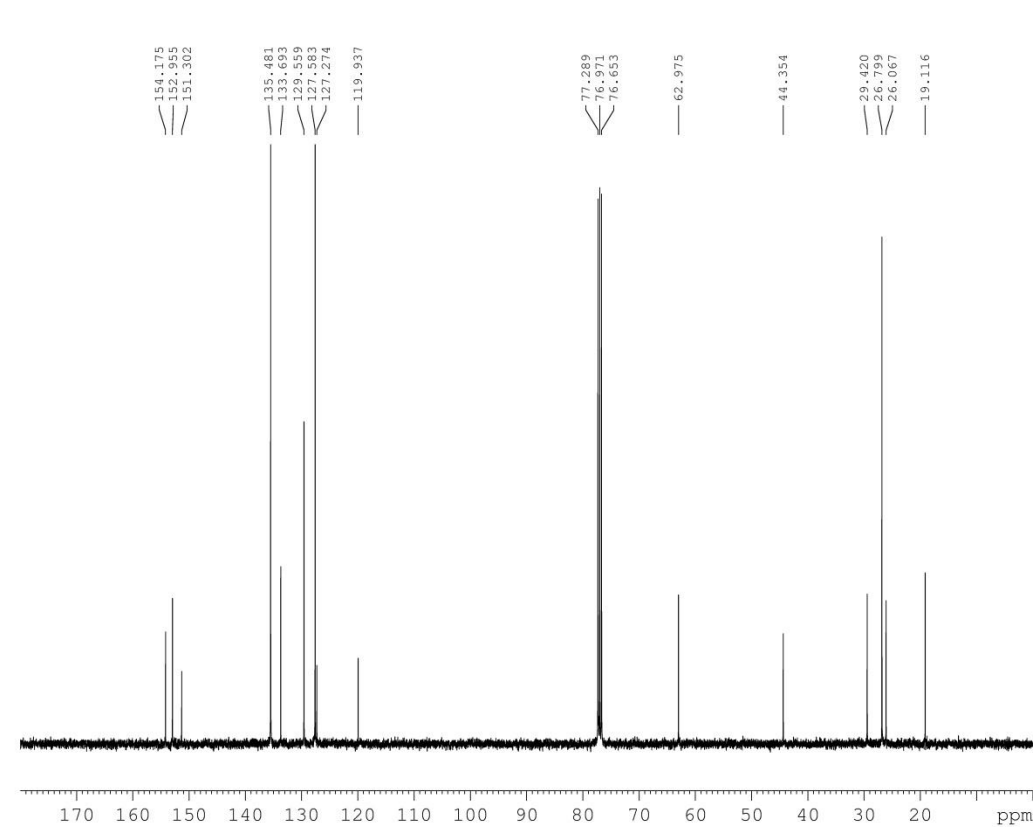


```

NAME      Aug19-2010-JMS4833
EXPNO     1
PROCNO    1
Date_     20100820
Time      7.04
INSTRUM   AVIII400
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         101
DW         60.800 usec
DE         17.24 usec
TE         298.0 K
D1         1.00000000 sec
D10        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        13.00 usec
PL1       0.00 dB
PL1W      9.74611950 W
SFO1      400.0424704 MHz
SI        65536
SF        400.0400148 MHz
WDW       EM
SSB       0
LB        0.20 Hz
GB        0
PC        1.00
  
```



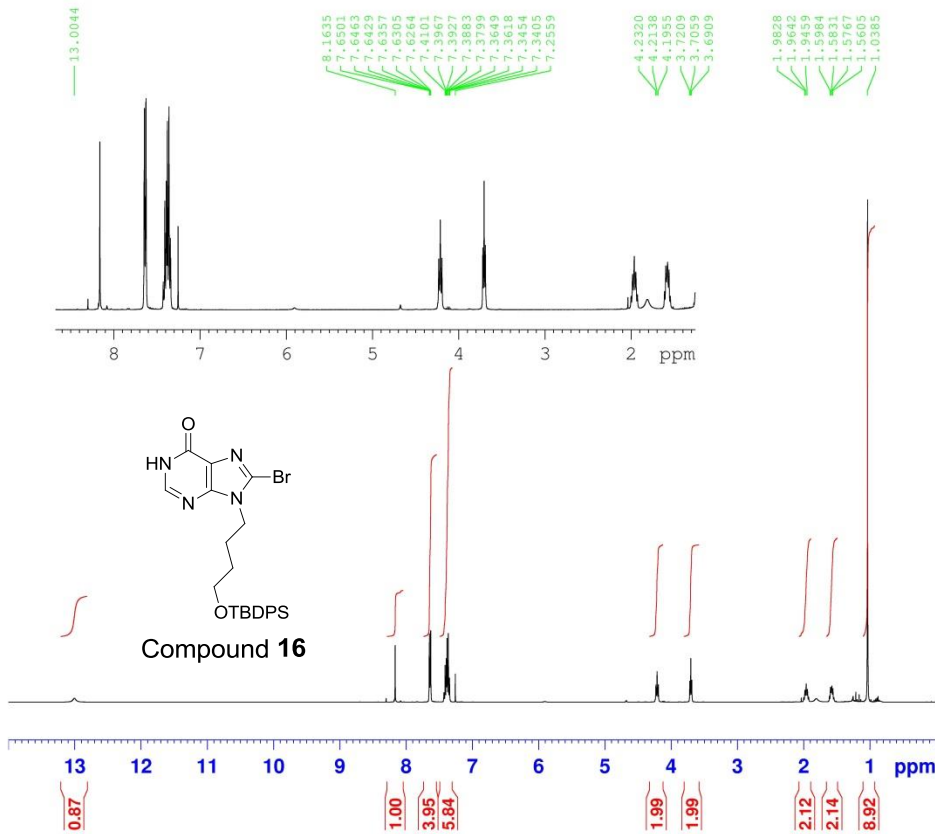
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EXPNO     11
PROCNO    11
Date_     20130128
Time      19.34
INSTRUM   AVIII400
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         512
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         1620
DW         20.800 usec
DE         6.50 usec
TE         298.0 K
D1         2.00000000 sec
D11        0.03000000 sec
D10        1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        8.75 usec
PL1       -2.00 dB
PL1W      58.91986084 W
SFO1      100.6001970 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       0.00 dB
PL2W      15.75 dB
PL3       19.00 dB
PL3W      9.74611950 W
PL12W     0.25753233 W
PL13W     0.12269837 W
SFO2      400.0416002 MHz
SI        65536
SF        100.5901380 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



```

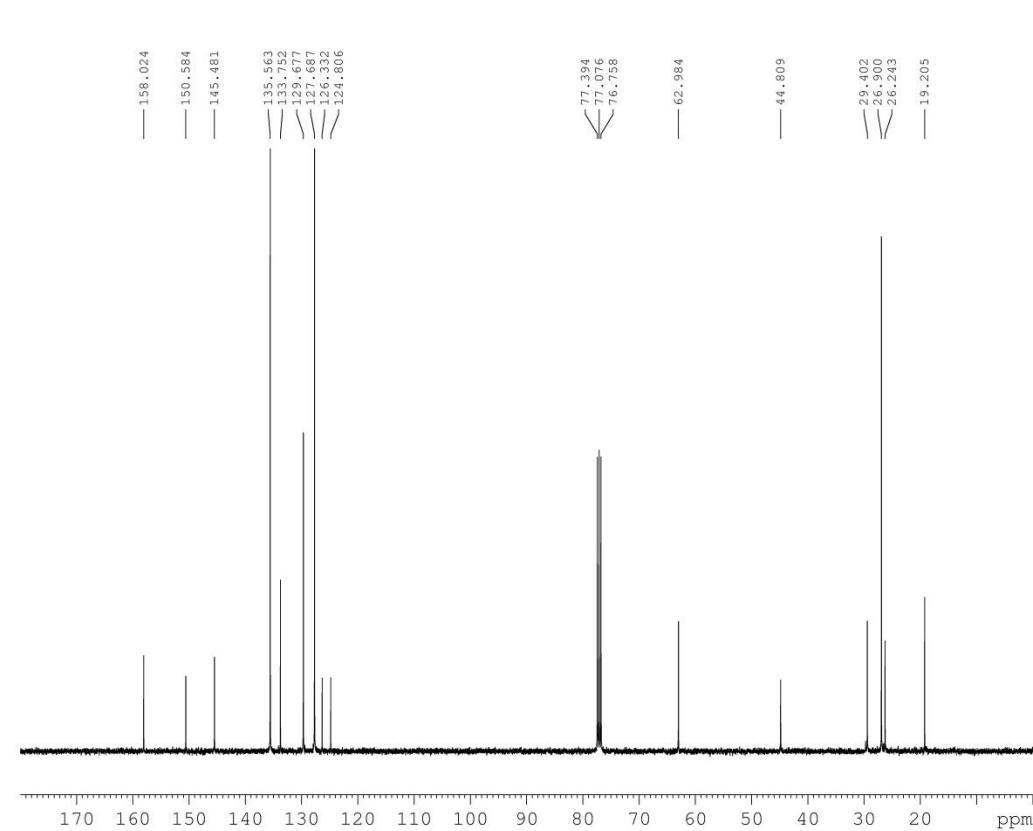
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PROCNO    1
Date_     20100603
Time      11.08
INSTRUM   AVIII400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         101
DW         60.800 usec
DE         17.24 usec
TE         297.9 K
D1         1.00000000 sec
D10        1
TD0        1

```

```

===== CHANNEL f1 =====
NUC1      1H
P1        13.00 usec
PL1       0.00 dB
PL1W      9.74611950 W
SFO1      400.0424704 MHz
SI        65536
SF        400.0400148 MHz
WDW       EM
SSB       0
LB        0.20 Hz
GB        0
PC        1.00

```



```

NAME      Jul01-2010-JMS3247
EXPNO     11
PROCNO    1
Date_     20100701
Time      23.20
INSTRUM   AVIII400
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         298.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

===== CHANNEL f1 =====
NUC1      13C
P1        8.75 usec
PL1       -2.00 dB
PL1W      58.91986084 W
SFO1      100.6001970 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       0.00 dB
PL12      15.75 dB
PL13      19.00 dB
PL2W      9.74611950 W
PL12W     0.25753233 W
PL13W     0.12269637 W
SFO2      400.0416002 MHz
SI        65536
SF        100.5901380 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

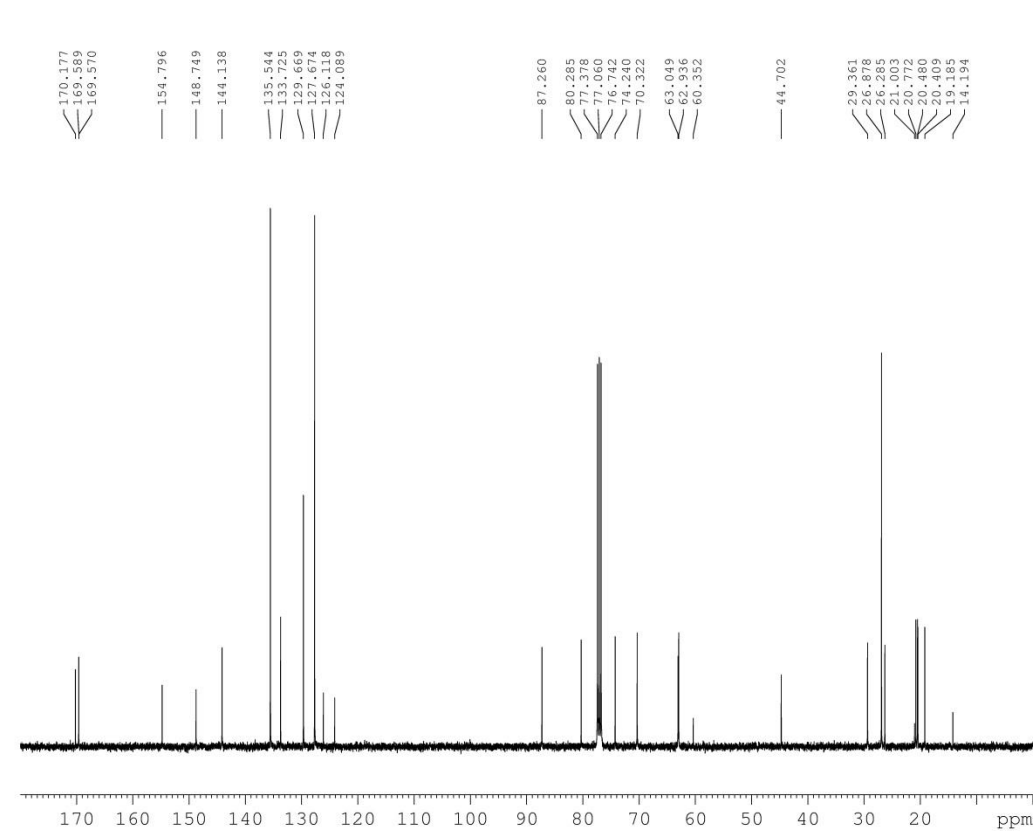
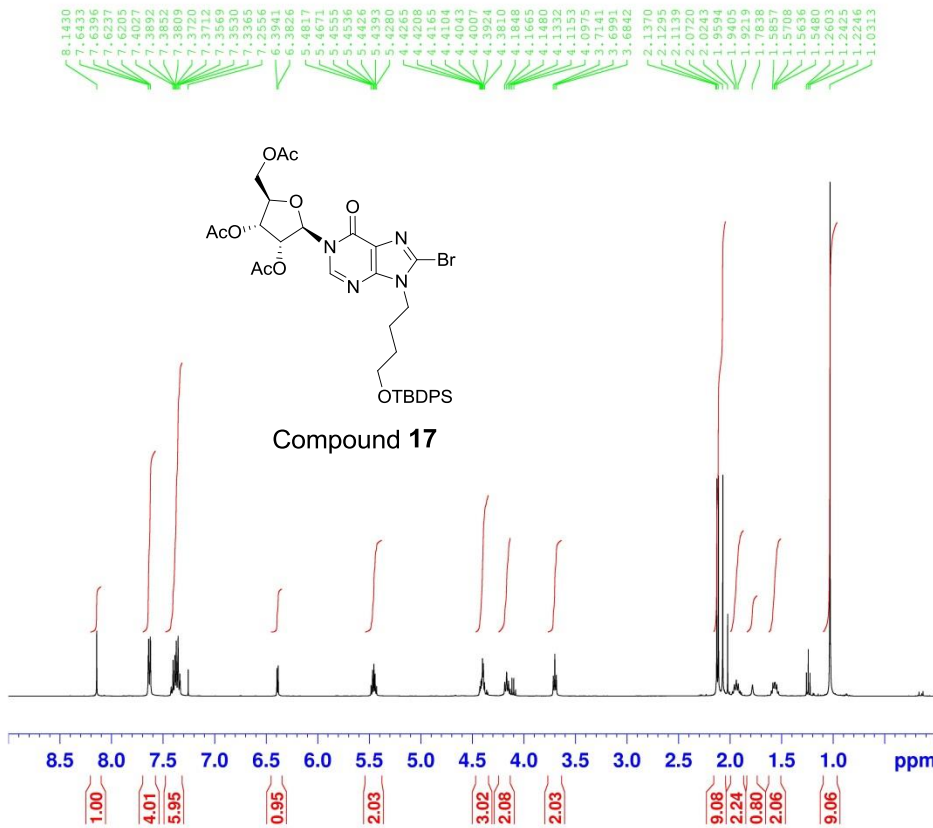



```

NAME      Jul105-2010-JMS3318
EXPNO     10
PROCNO    1
Date_     20100705
Time      18.34
INSTRUM   AVIII400
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         64
DW        60.800 usec
DE        17.24 usec
TE        298.0 K
D1        1.00000000 sec
D10       1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        13.00 usec
PL1       0.00 dB
PL1W     9.74611950 W
SFO1     400.0424704 MHz
SI        65536
SF       400.0400148 MHz
WDW       EM
SSB       0
LB        0.20 Hz
GB        0
PC        1.00
  
```



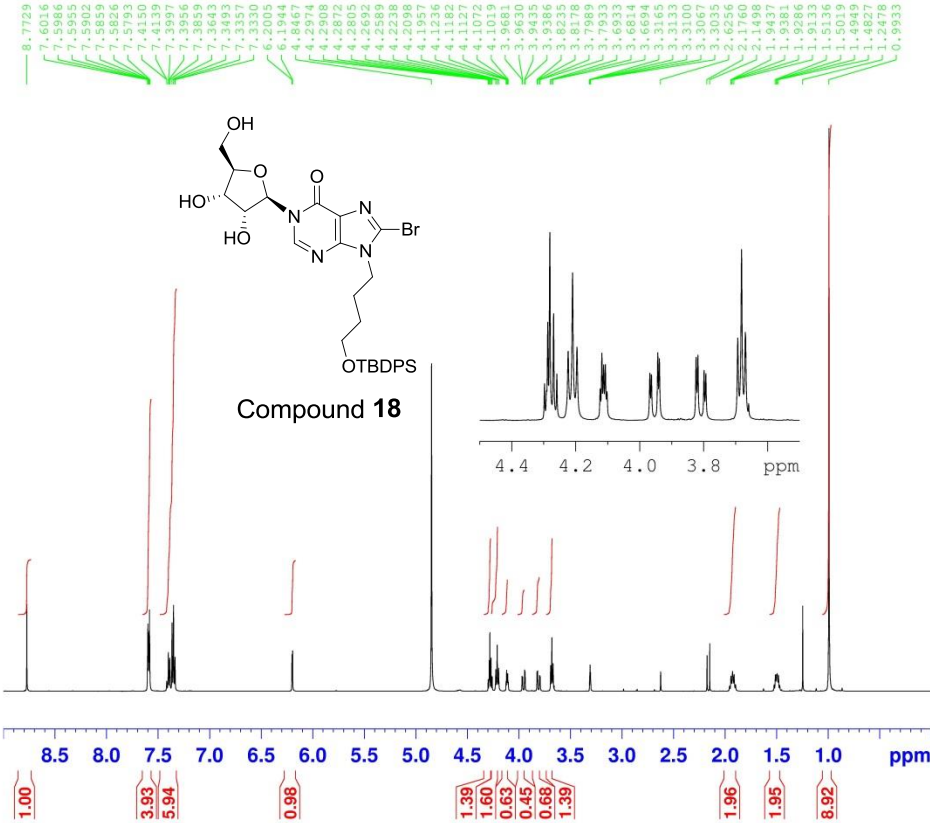
```

NAME      Jul105-2010-JMS3318
EXPNO     11
PROCNO    1
Date_     20100706
Time      4.54
INSTRUM   AVIII400
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        298.0 K
D1        2.00000000 sec
D11       0.03000000 sec
D10       1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        8.75 usec
PL1       -2.00 dB
PL1W     58.91986084 W
SFO1     100.6001970 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       0.00 dB
PL12     15.75 dB
PL13     19.00 dB
PL2W     9.74611950 W
PL12W    0.25753233 W
PL13W    0.12269637 W
SFO2     400.0416002 MHz
SI        65536
SF       100.5901380 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

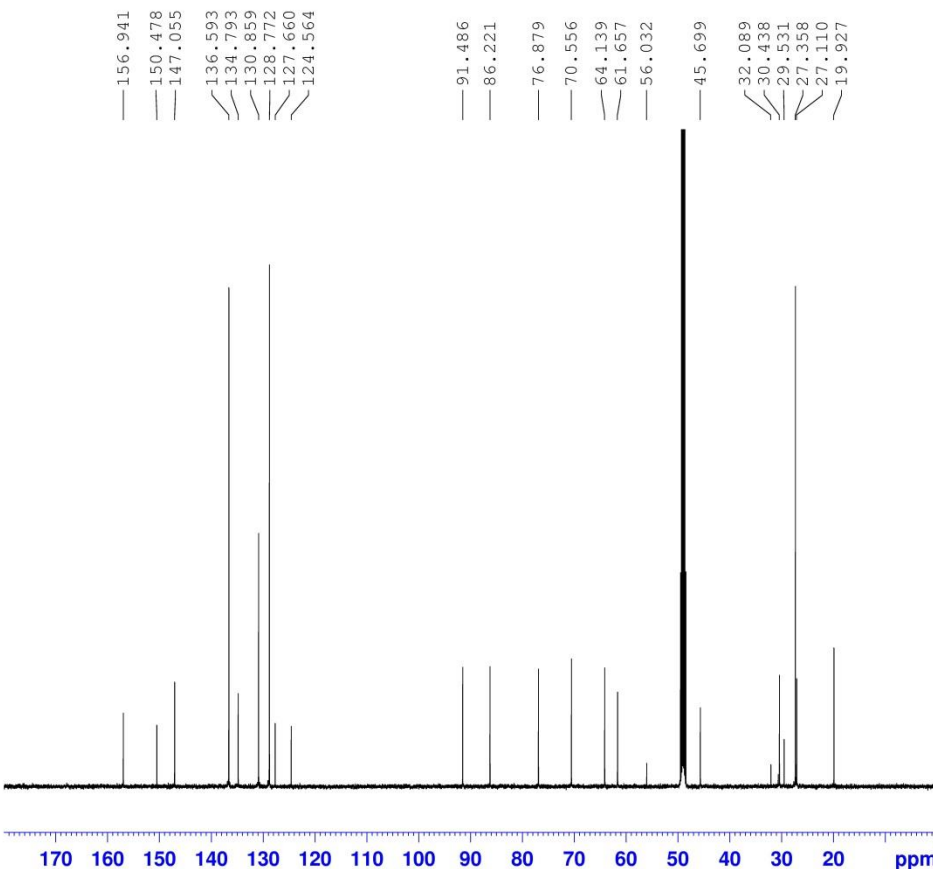


```

NAME      JMS218
EXPNO     10
PROCNO    1
Date_     20100721
Time      0.26
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   MeOD
NS         16
DS         2
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ         3.171923 sec
RG         64
DW         48.400 usec
DE         12.94 usec
TE         300.0 K
D1         1.00000000 sec
TDO        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1         10.30 usec
PL1        0.00 dB
PL1W      19.34152603 W
SFO1      500.1330885 MHz
SI         32768
SF         500.1300110 MHz
WDW        EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00
  
```



```

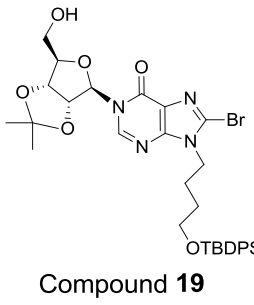
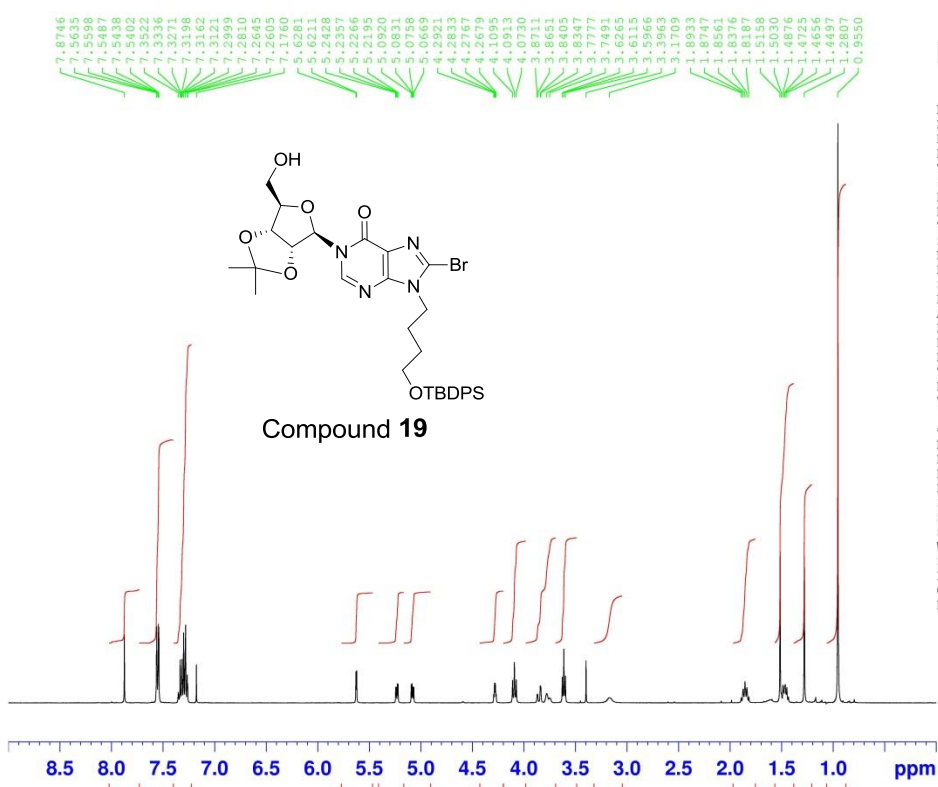
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EXPNO     11
PROCNO    1
Date_     20100721
Time      0.32
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   MeOD
NS         1024
DS         4
SWH       29761.904 H
FIDRES    0.454131 H
AQ         1.1010548 s
RG         2050
DW         16.800 u
DE         9.53 u
TE         300.3 K
D1         2.00000000 s
D11        0.03000000 s
TDO        1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1         9.50 u
PL1        0.00 dB
PL1W      114.29083252 W
SFO1      125.7703643 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 u
PL2        0.00 dB
PL12      18.06 dB
PL13      21.00 dB
PL12W     19.34152603 W
PL12W     0.30233663 W
PL13W     0.15363520 W
SFO2      500.1320005 MHz
SI         32768
SF         125.7576165 MHz
WDW        EM
SSB         0
LB         1.00 H
GB         0
PC         1.40
  
```

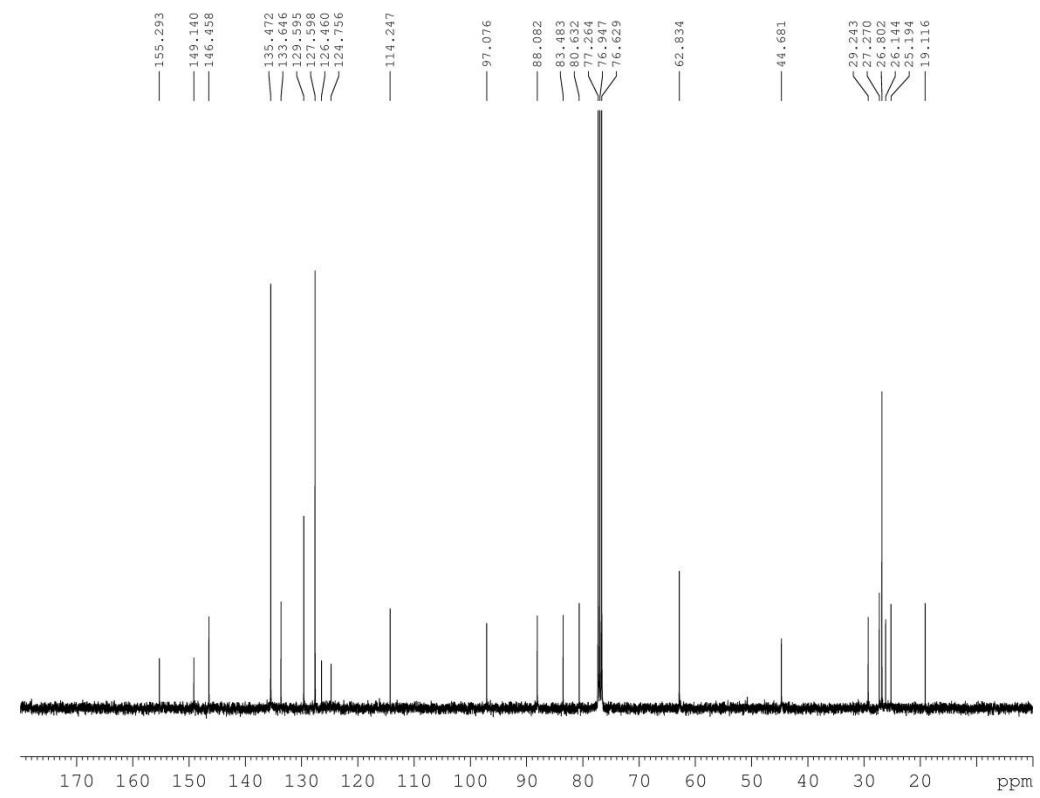


Compound 19



```

NAME      Oct04-2010-JMS4219
EXPNO    10
PROCNO   1
Date_    20101004
Time     15.50
INSTRUM  AVIII400
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        114
DW        60.800 usec
DE        17.24 usec
TE        298.0 K
D1        1.00000000 sec
D10       1
----- CHANNEL f1 -----
NUC1      1H
P1        13.00 usec
PL1       0.00 dB
PL1W      9.74611950 W
SFO1      400.0424704 MHz
SI        65536
SF        400.0400148 MHz
WDW       EM
SSB       0
LB        0.20 Hz
GB        0
PC        1.00
  
```



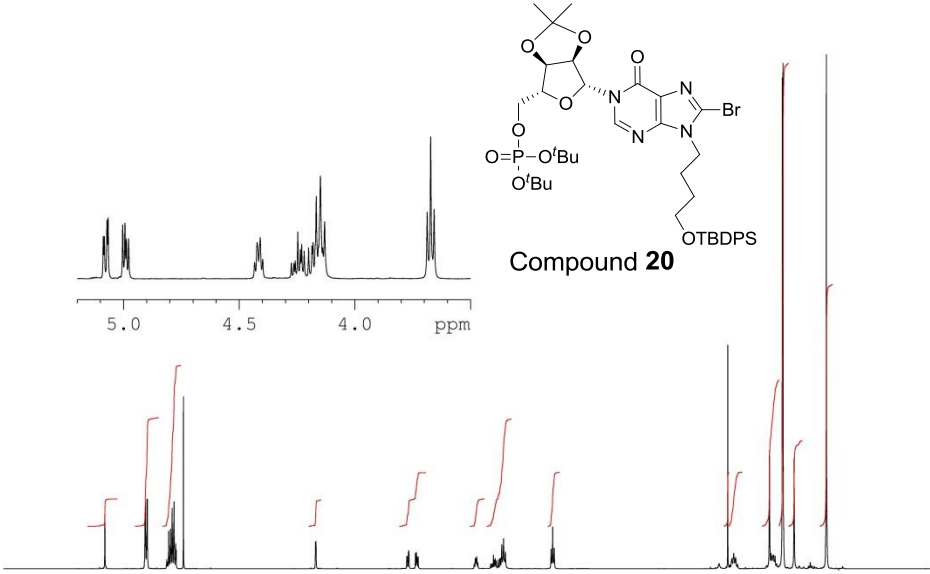
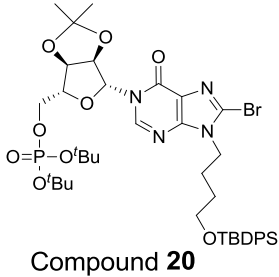
```

NAME      Oct04-2010-JMS4219
EXPNO    11
PROCNO   1
Date_    20101004
Time     20.48
INSTRUM  AVIII400
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
ID        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        298.0 K
D1        2.00000000 sec
D11       0.03000000 sec
D10       1
----- CHANNEL f1 -----
NUC1      13C
P1        8.75 usec
PL1       -2.00 dB
PL1W      58.91986084 W
SFO1      100.6001970 MHz
----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       0.00 dB
PL12     15.75 dB
PL13     19.00 dB
PL2W      9.74611950 W
PL12W    0.25753233 W
PL13W    0.12269837 W
SFO2      400.0416002 MHz
SI        65536
SF        100.5901380 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

8.0154
7.6268
7.6231
7.6196
7.6124
7.6071
7.6031
7.5966
7.5826
7.3790
7.3748
7.3631
7.3599
7.3485
7.3450
7.3284
7.3243
7.2533
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5.9673
5.0864
5.0817
5.0704
5.0657
4.9827
4.9827
4.9865
4.9767
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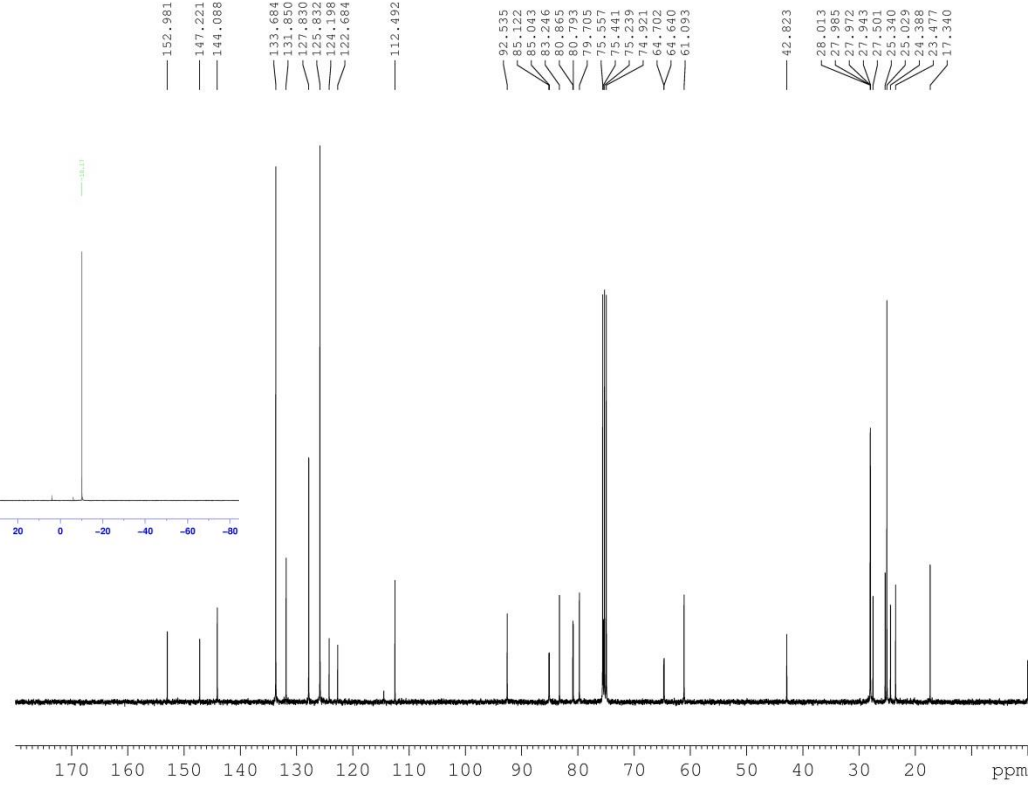
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INSTRUM AVIII400
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 32
DW 60.800 usec
DE 17.24 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1



----- CHANNEL f1 -----
NUC1 1H
P1 13.00 usec
PL1 0.00 dB
PL1W 9.74611950 W
SFO1 400.0424704 MHz
SI 65536
SF 400.0399837 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

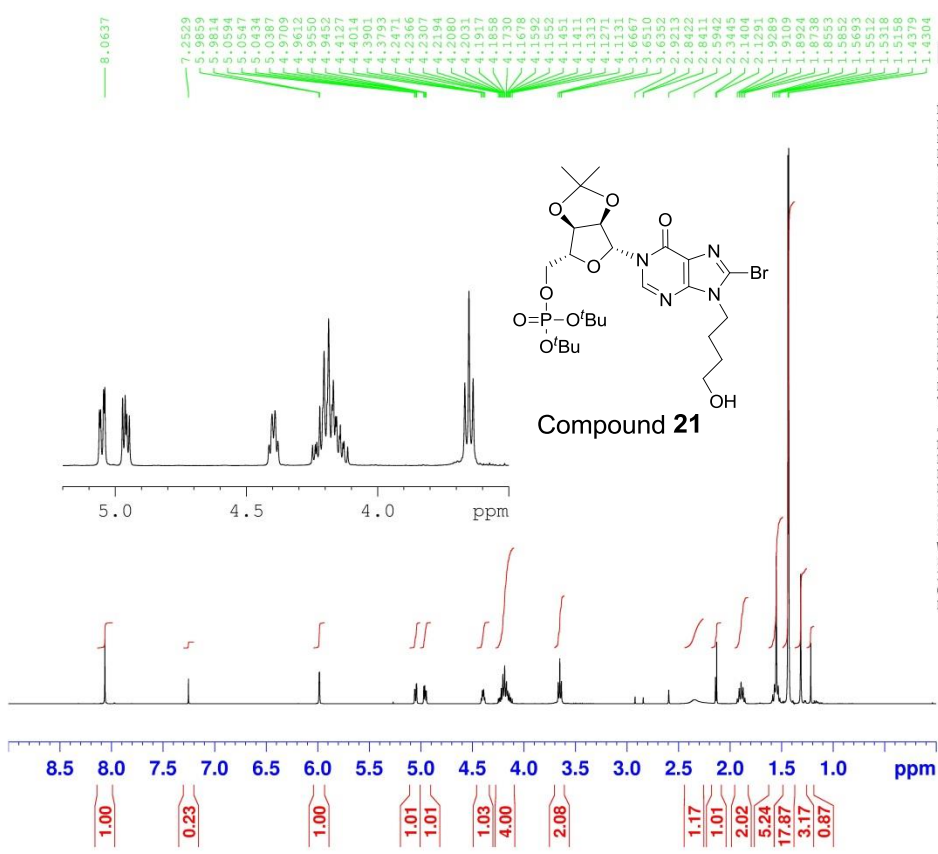
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

1.00 3.96 5.86 0.97 1.96 1.01 3.91 1.97 1.96 1.98 5.34 16.89 3.13 8.81



NAME Mar02-2011-JMS8363
EXPNO 13
PROCNO 1
Date_ 20110303
Time 2.54
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
ID 65536
SOLVENT CDCl3
NS 1000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 1820
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 8.75 usec
PL1 -2.00 dB
PL1W 58.9198608 W
SFO1 100.6001970 MHz
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL2 15.75 dB
PL13 19.00 dB
PL2W 9.74611950 W
PL12W 0.25753233 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz
SI 65536
SF 100.5903156 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

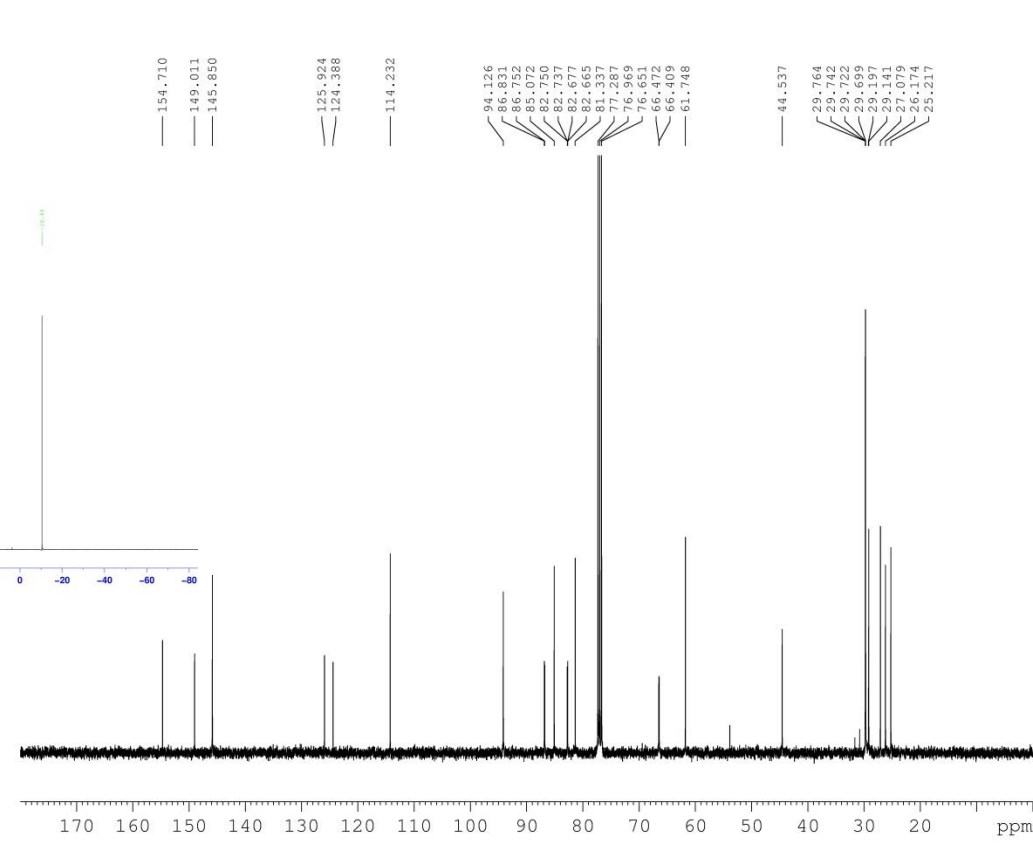


```

NAME      Dec13-2010-JMS6860
EXPNO    10
PROCNO   1
Date_    20101214
Time     2.20
INSTRUM  AVIII400
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       57
DW       60.800 usec
DE       17.24 usec
TE       298.0 K
D1       1.00000000 sec
TDO     1

----- CHANNEL f1 -----
NUC1     1H
P1       13.00 usec
PL1      0.00 dB
PL1W     9.74611950 W
SFO1     400.0424704 MHz
SI       65536
SF       400.0399837 MHz
WDW      EM
SSB      0
LB       0.20 Hz
GB       0
PC       1.00

```



```

NAME      Dec13-2010-JMS6860
EXPNO    13
PROCNO   1
Date_    20101214
Time     3.14
INSTRUM  AVIII400
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       298.0 K
D1       2.00000000 sec
D11     0.03000000 sec
TDO     1

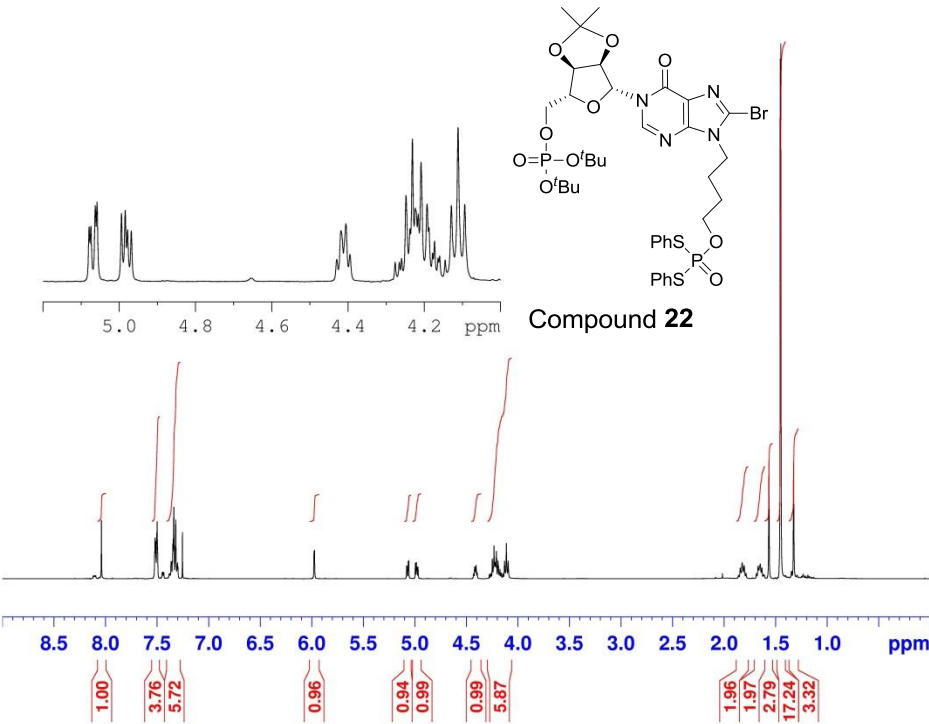
----- CHANNEL f1 -----
NUC1     13C
P1       8.75 usec
PL1      -2.00 dB
PL1W     58.91986084 W
SFO1     100.6001970 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
PCPD2   80.00 usec
PL2      0.00 dB
PL12    15.75 dB
PL13    19.00 dB
PL2W     9.74611950 W
PL12W   0.25753233 W
PL13W   0.12269837 W
SFO2     400.0416002 MHz
SI       65536
SF       100.5901380 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

```

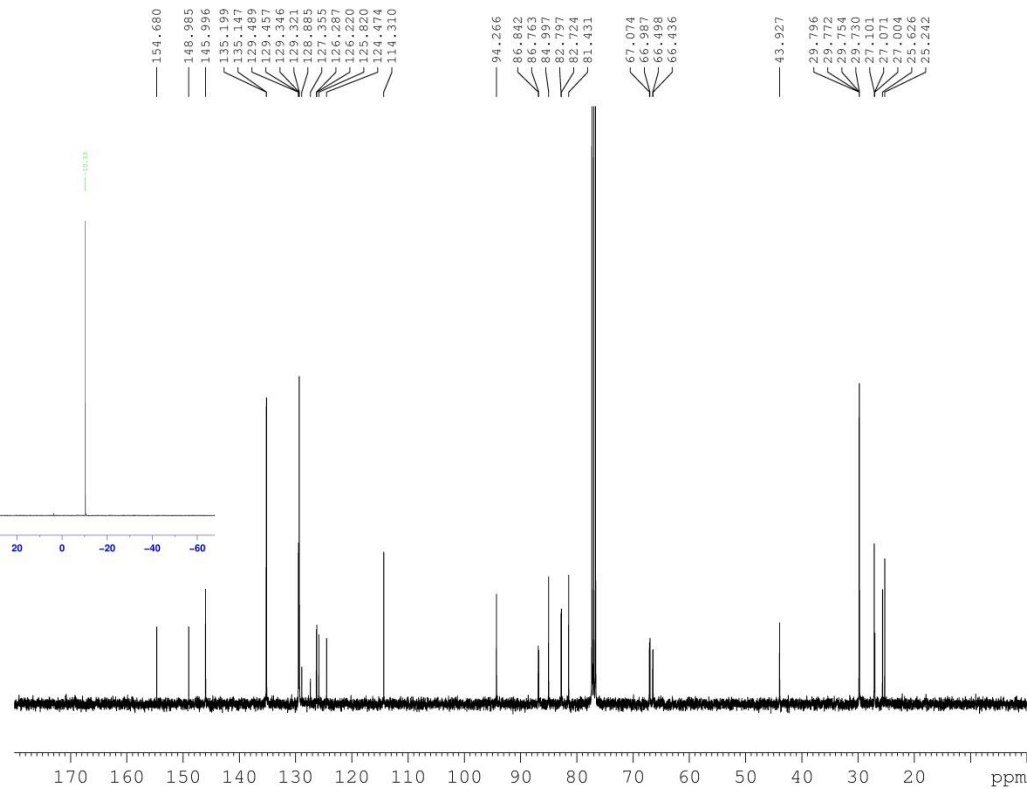


8.0391
7.5178
7.5178
7.5145
7.5095
7.5034
7.4990
7.4938
7.3639
7.3509
7.3469
7.3428
7.3373
7.3225
7.3180
7.3011
7.2830
7.2530
5.9768
5.9723
5.0785
5.0738
5.0624
5.0578
4.9839
4.9778
4.9678
4.4180
4.4051
4.3945
4.2876
4.2711
4.2331
4.2155
4.2080
4.1922
4.1874
4.1777
4.1726
4.1119
4.0934
1.8419
1.8238
1.8047
1.6698
1.6553
1.6482
1.6324
1.3640
1.3491
1.3246



```
NAME      Dec15-2010-JMS6942
EXPNO    10
PROCNO   1
Date_    20101215
Time     18.54
INSTRUM  AVIII400
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        71.8
DW        60.800 usec
DE        17.24 usec
TE        298.0 K
D1        1.00000000 sec
D10      1
TDO       1
```

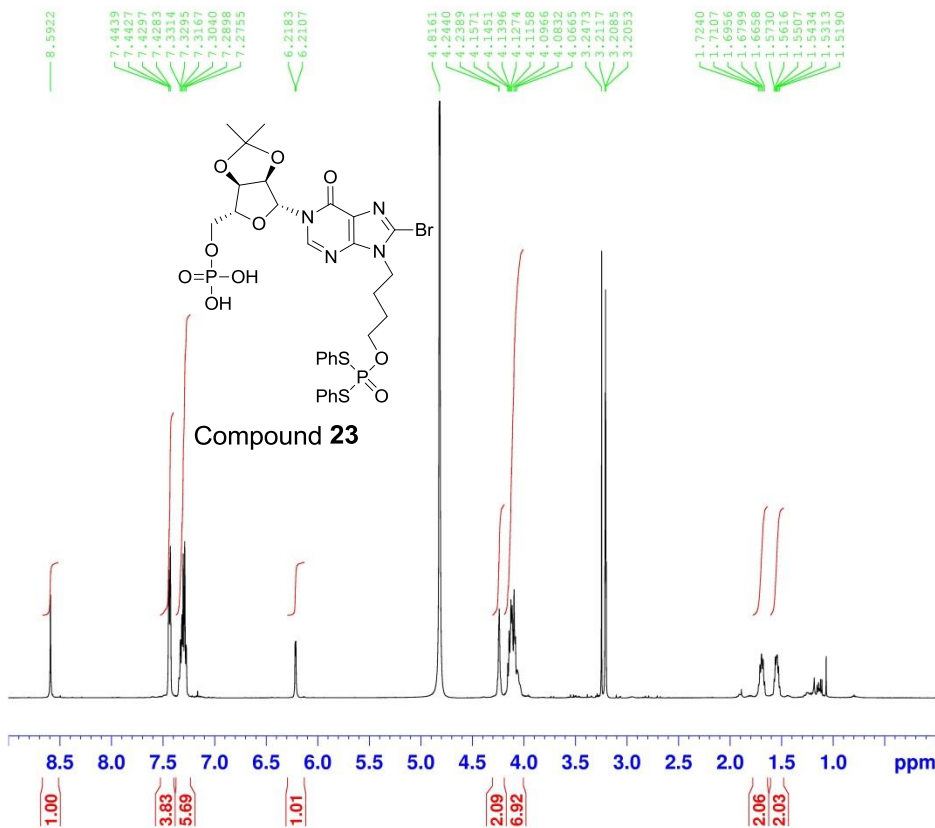
```
----- CHANNEL f1 -----
NUC1      1H
P1        13.00 usec
PL1       0.00 dB
PL1W      9.74611950 W
SFO1      400.0424704 MHz
SI        65536
SF        400.0399837 MHz
WDW       EM
SSB       0
LB        0.20 Hz
GB        0
PC        1.00
```



```
NAME      Dec15-2010-JMS6942
EXPNO    12
PROCNO   1
Date_    20101215
Time     19.31
INSTRUM  AVIII400
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
ID        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        298.0 K
D1        2.00000000 sec
D11       0.03000000 sec
TDO       1
```

```
----- CHANNEL f1 -----
NUC1      13C
P1        8.75 usec
PL1       -2.00 dB
PL1W      58.91986084 W
SFO1      100.6001970 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       0.00 dB
PL12     15.75 dB
PL13     19.00 dB
PL2W     9.74611950 W
PL12W    0.25753233 W
PL13W    0.12269837 W
SFO2     400.0416002 MHz
SI        65536
SF        100.5901380 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

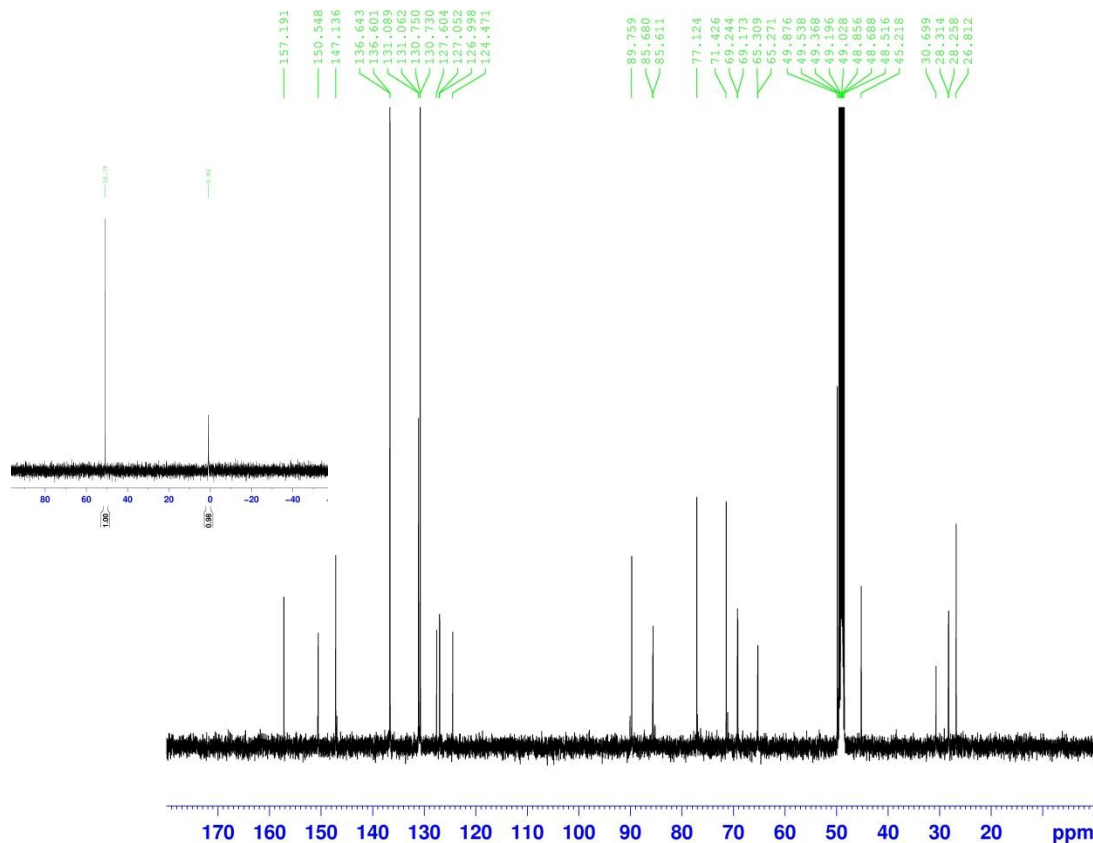


```

NAME      Mar15-2011-JMS404
EXPNO    10
PROCNO   1
Date_    20110315
Time     17.42
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  MeOD
NS       64
DS       2
SWH      10330.578 Hz
FIDRES   0.157632 Hz
AQ       3.1719923 sec
RG       114
DW       48.400 usec
DE       13.94 usec
TE       294.0 K
D1       1.00000000 sec
TDO      1
  
```

```

----- CHANNEL f1 -----
NUC1     1H
P1       10.30 usec
PL1      0.00 dB
PL1W     19.34152603 W
SFO1     500.1330885 MHz
SI       32768
SF       500.1300616 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```



```

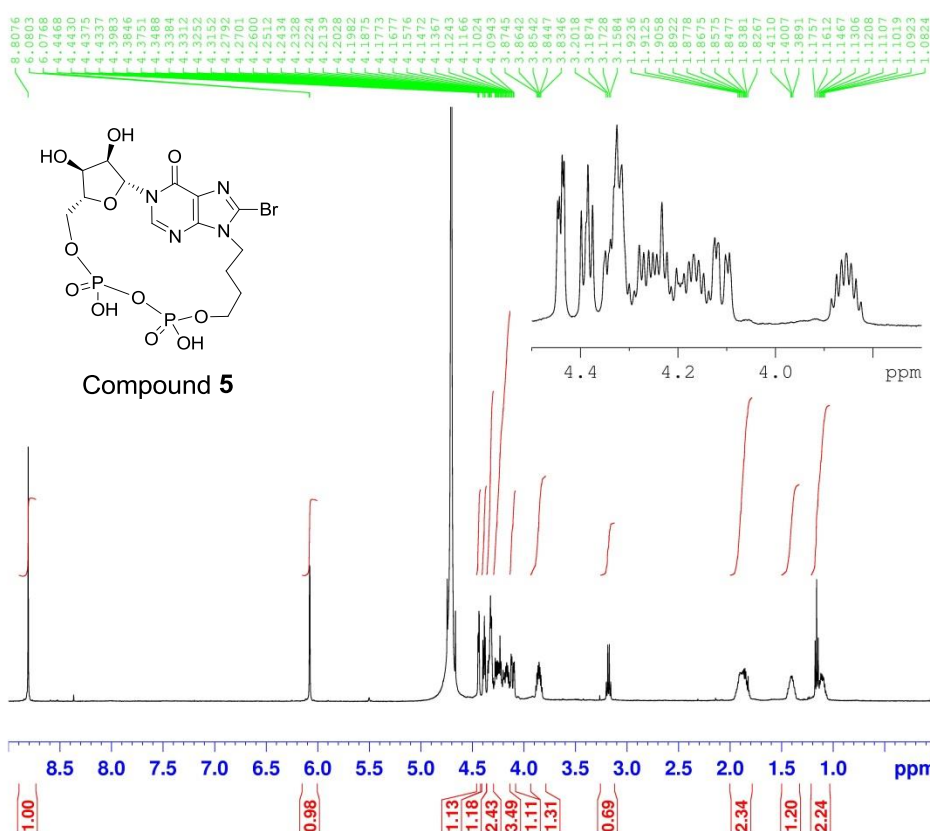
NAME      Jan07-2011-JMS362
EXPNO    12
PROCNO   1
Date_    20110107
Time     19.32
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  MeOD
NS       2048
DS       4
SWH      29761.904 Hz
FIDRES   0.454131 Hz
AQ       1.1010548 sec
RG       2050
DW       16.800 usec
DE       9.48 usec
TE       300.0 K
D1       2.00000000 sec
D11      0.03000000 sec
TDO      1
  
```

```

----- CHANNEL f1 -----
NUC1     13C
P1       14.50 usec
PL1      0.00 dB
PL1W     114.29083252 W
SFO1     125.7703643 MHz
  
```

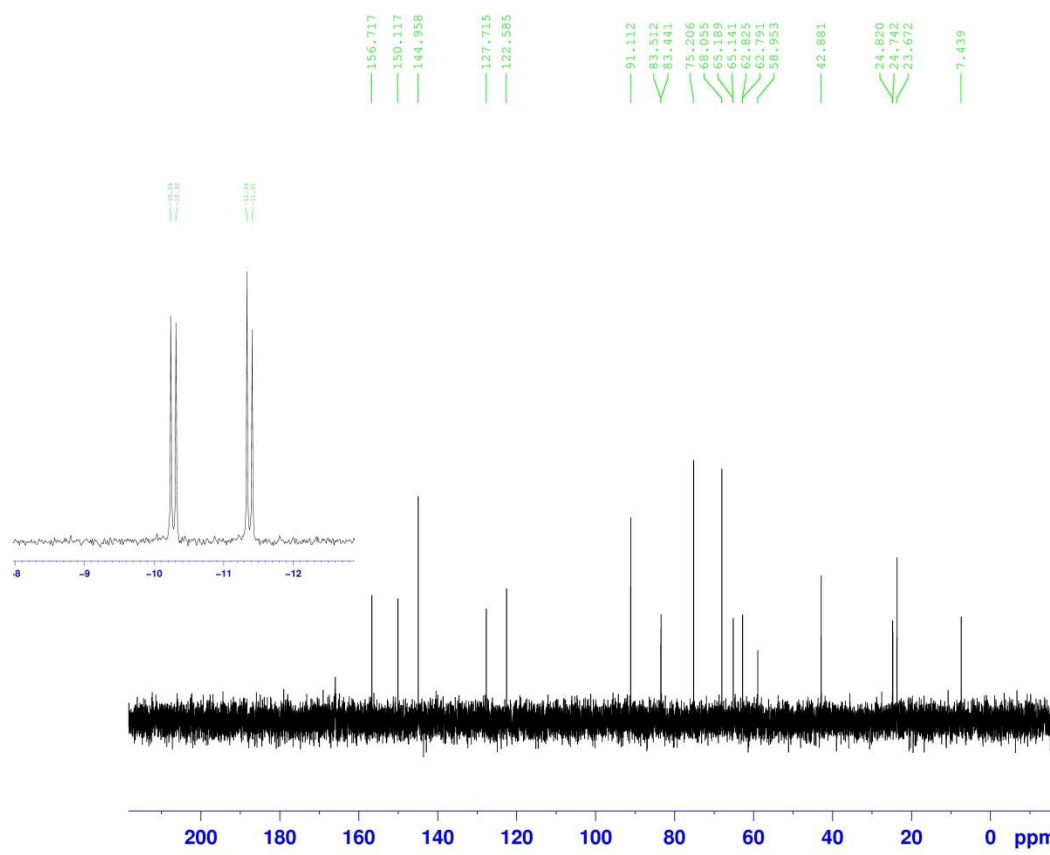
```

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      0.00 dB
PL12     18.06 dB
PL13     21.00 dB
PL2W     19.34152603 W
PL12W    0.30233663 W
PL13W    0.15363520 W
SFO2     500.1320005 MHz
SI       32768
SF       125.7576104 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```



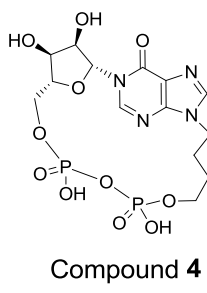
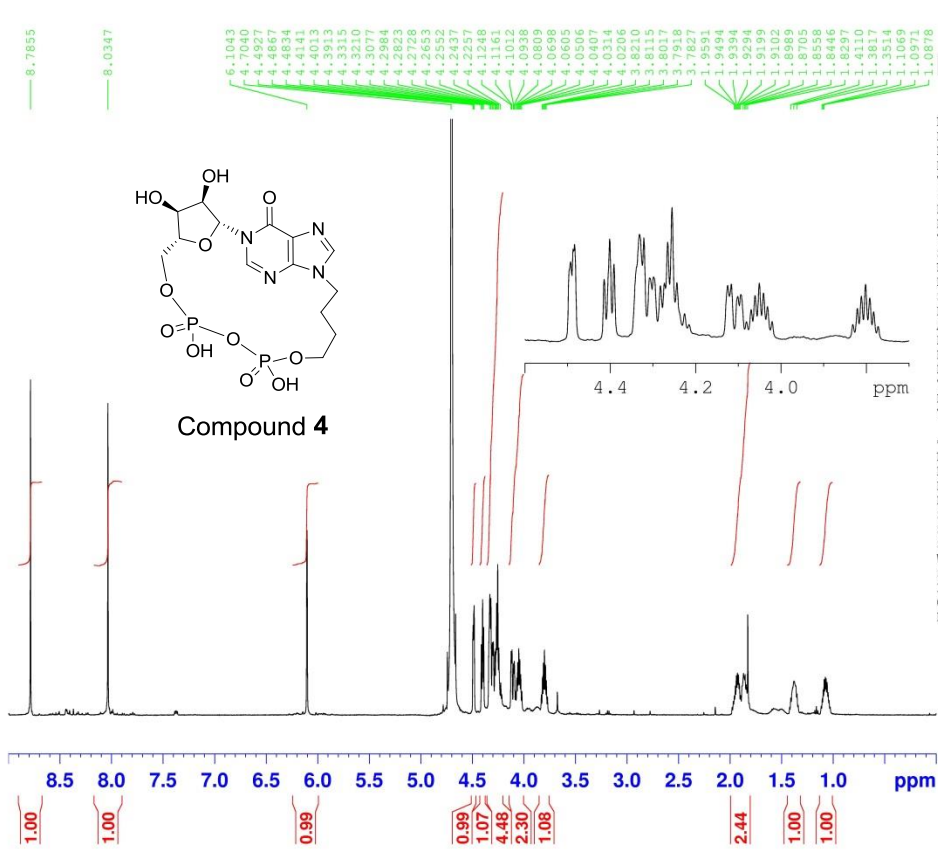
```

NAME      Jan24-2011-JMS369
EXPNO    10
PROCNO   1
Date_    20110124
Time     16.37
INSTRUM spect
PROBHD   5 mm PABBO BB-
PULPROG zg30
TD       65536
SOLVENT  D2O
NS       64
DS       2
SWH      10330.578 Hz
FIDRES   0.157632 Hz
AQ       3.1719923 sec
RG       256
DW       48.400 usec
DE       13.94 usec
TE       298.0 K
D1       1.00000000 sec
TD0      1
----- CHANNEL f1 -----
NUC1     1H
P1       10.30 usec
PL1      0.00 dB
PL1W     19.34152603 W
SFO1     500.1330885 MHz
SI       32768
SF       500.1300000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```

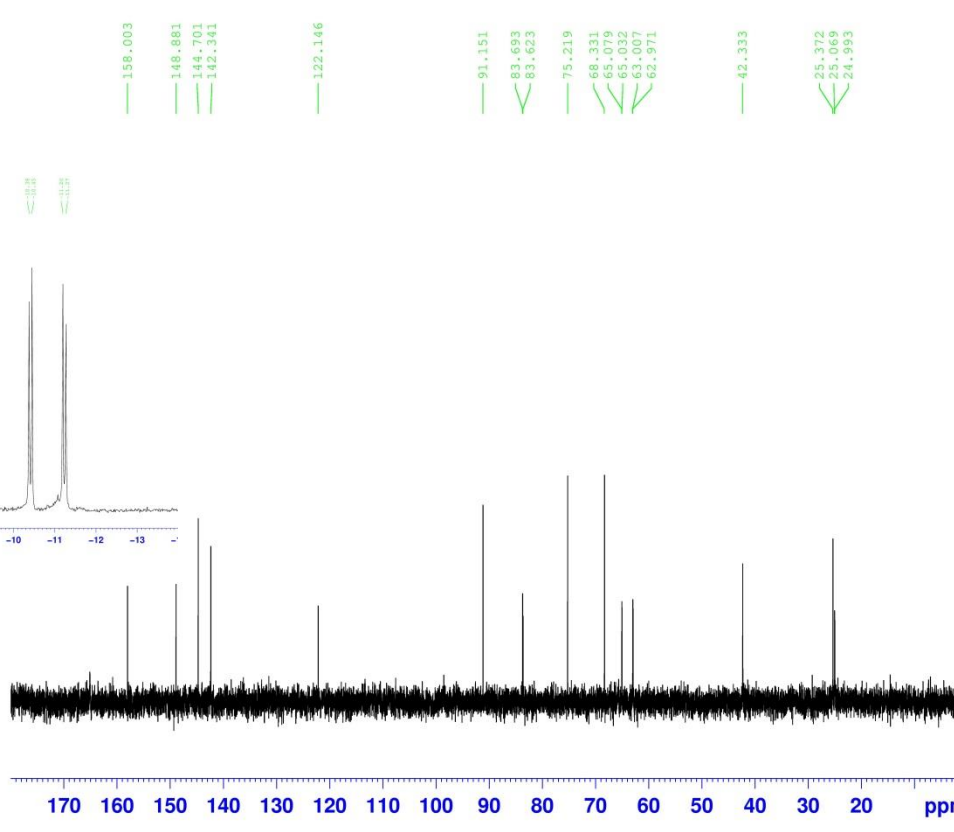


```

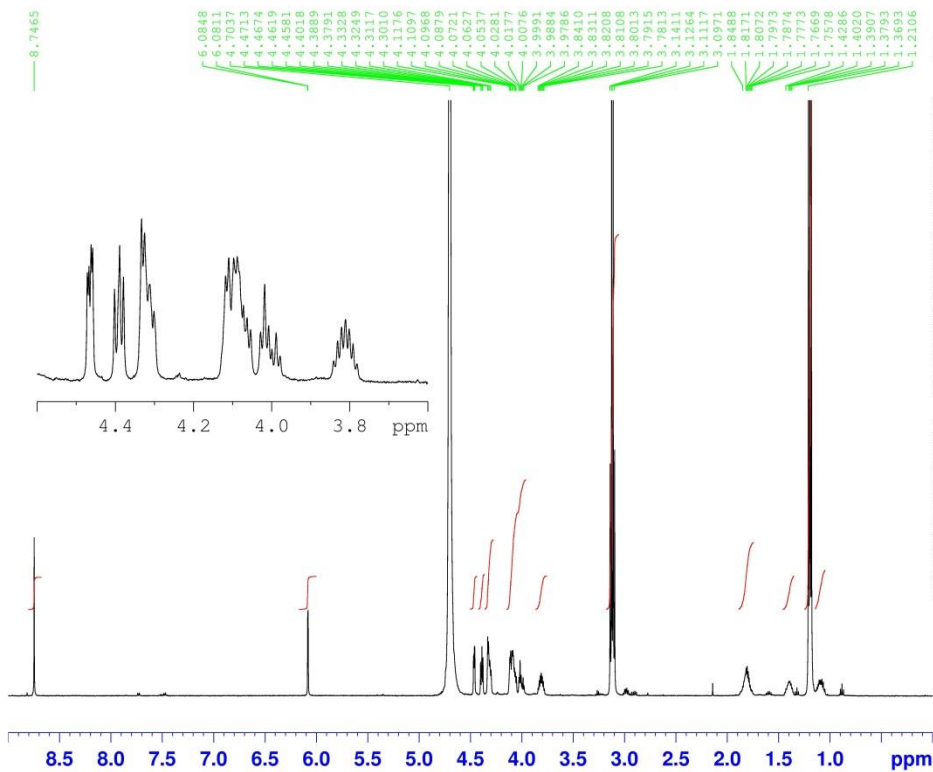
NAME      Jan24-2011-JMS369
EXPNO    13
PROCNO   1
Date_    20110125
Time     1.53
INSTRUM spect
PROBHD   5 mm PABBO BB-
PULPROG zgpg30
TD       65536
SOLVENT  D2O
NS       10240
DS       4
SWH      29761.904 Hz
FIDRES   0.454131 Hz
AQ       1.1010548 sec
RG       2050
DW       16.800 usec
DE       9.48 usec
TE       298.0 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
----- CHANNEL f1 -----
NUC1     13C
P1       14.50 usec
PL1      0.00 dB
PL1W     114.29083252 W
SFO1     125.7703643 MHz
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      0.00 dB
PL12     18.06 dB
PL13     21.00 dB
PL2W     19.34152603 W
PL12W    0.30233663 W
PL13W    0.15363520 W
SFO2     500.1320005 MHz
SI       32768
SF       125.7577890 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```

NAME May27-2011-JMS452Na
 EXPNO 11
 PROCNO 1
 Date_ 20110527
 Time 12.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 128
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 228
 DW 48.400 usec
 DE 13.94 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 10.30 usec
 PL1 -0.12 dB
 PL1W 19.35150909 W
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1330000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NAME May27-2011-JMS452Na
 EXPNO 13
 PROCNO 1
 Date_ 20110527
 Time 14.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 10240
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 2050
 DW 16.800 usec
 DE 8.43 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 ===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -0.51 dB
 PL1W 99.92730713 W
 SFO1 125.7703643 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -0.12 dB
 PL12 17.94 dB
 PL13 21.00 dB
 PL2W 19.35150909 W
 PL12W 0.30249262 W
 PL13W 0.14952536 W
 SFO2 500.1320005 MHz
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



```

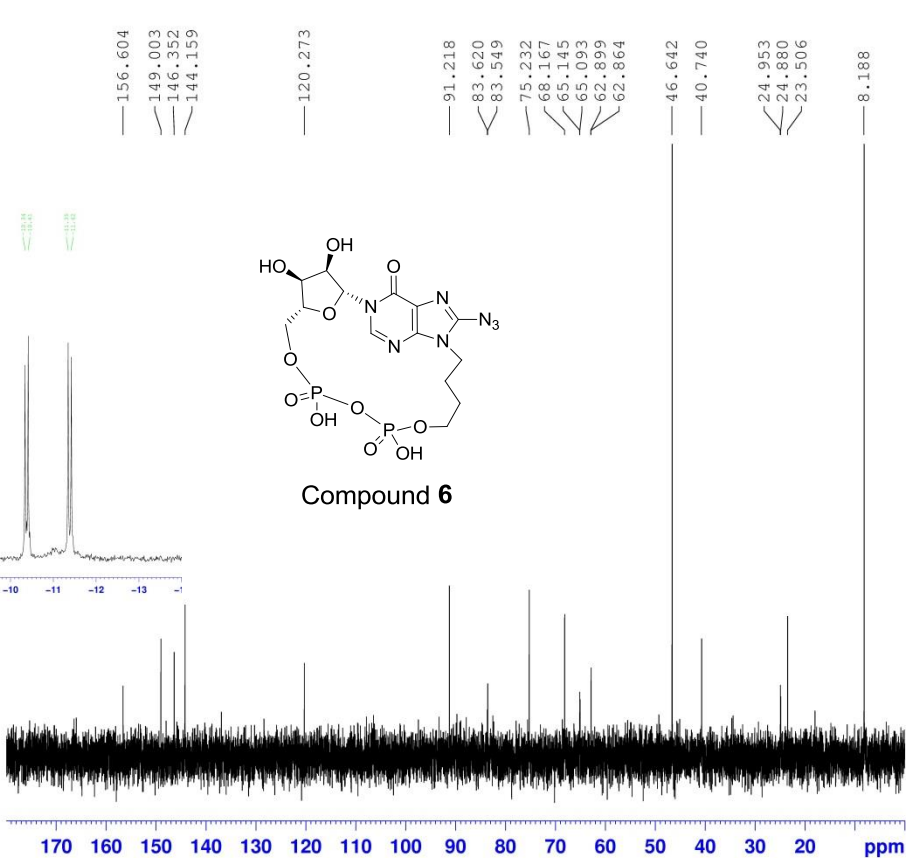
NAME      JMS AZIDE HPLC
EXPNO     10
PROCNO    1
Date_     20120601
Time      14.47
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT   D2O
NS        146
DS        2
SWH       10330.573 Hz
FIDRES    0.157632 Hz
AQ        3.1719923 sec
RG        203
DW        48.400 usec
DE        13.94 usec
TE        298.0 K
D1        1.00000000 sec
TD0       1

```

```

===== CHANNEL f1 =====
NUC1      1H
P1        10.30 usec
PL1       -0.12 dB
PL1W      19.35150909 W
SF01      500.1330885 MHz
SI        32768
SF        500.1300000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

```



```

NAME      JMS AZIDE HPLC
EXPNO     24
PROCNO    1
Date_     20120605
Time      8.55
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   D2O
NS        20480
DS        4
SWH       29761.904 H:
FIDRES    0.454131 H:
AQ        1.1010548 se
RG        2050
DW        16.800 u:
DE        8.43 u:
TE        298.0 K
D1        2.00000000 se
D11       0.03000000 se
TD0       1

```

```

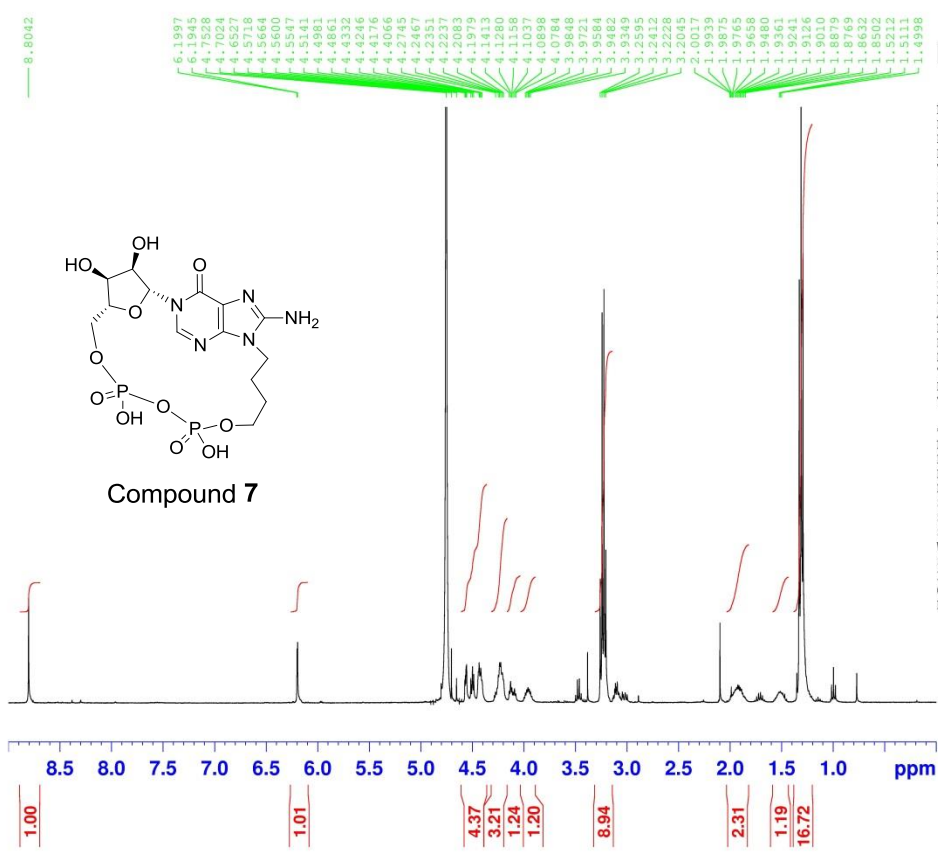
===== CHANNEL f1 =====
NUC1      13C
P1        9.50 u:
PL1       -0.51 dl
PL1W      99.92730713 W
SF01      125.7703643 MI

```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 u:
PL2       -0.12 dl
PL12      17.94 dl
PL13      21.00 dl
PL2W      19.35150909 W
PL12W     0.30249262 W
PL13W     0.14952536 W
SF02      500.1320005 MI
SI        32768
SF        125.7577890 MI
WDW       EM
SSB       0
LB        1.00 H:
GB        0
PC        1.40

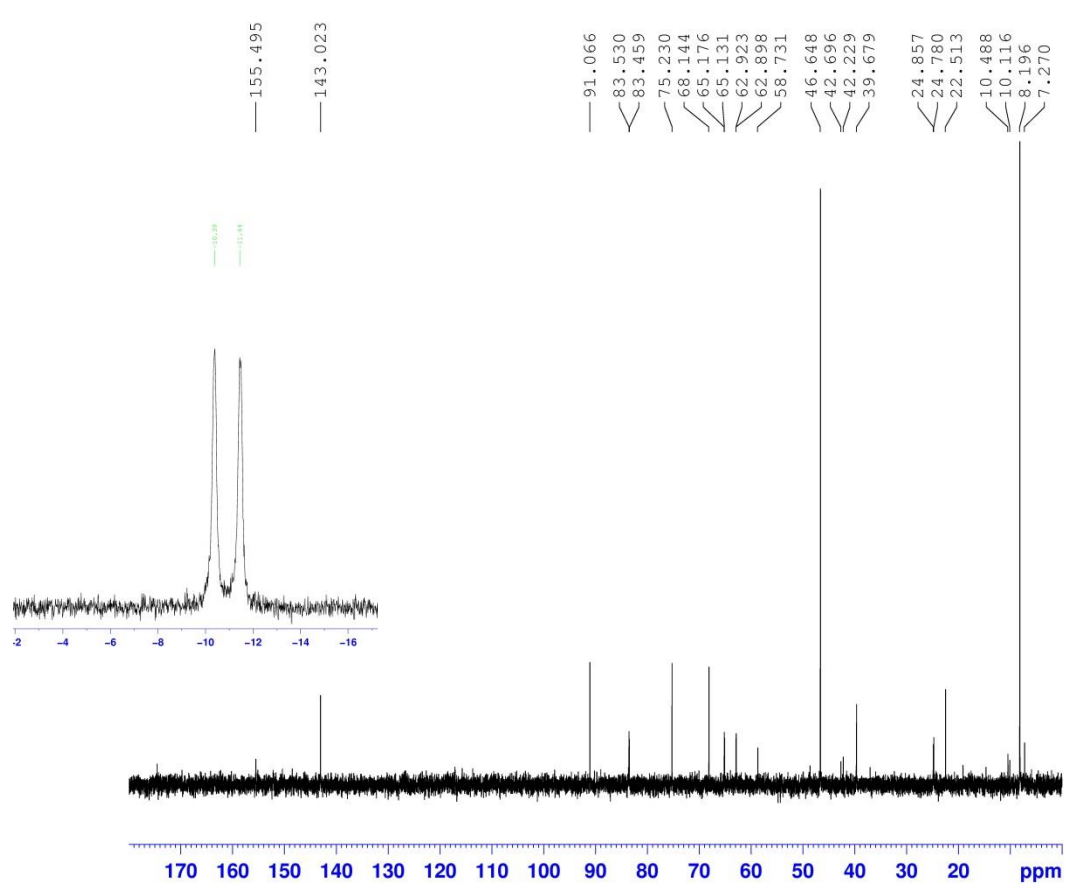
```



```

NAME      Apr26-2012-JMS17669
EXPNO     1
PROCNO    1
Date_     20120426
Time      22.29
INSTRUM   AVIII400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   D2O
NS         160
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         228
DW         60.800 usec
DE         17.24 usec
TE         298.0 K
D1         1.00000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1      1H
P1        13.00 usec
PL1       0.00 dB
PL1W      9.74611950 W
SF01      400.0424704 MHz
SI        65536
SF        400.0399837 MHz
WDW       EM
SSB       0
LB        0.20 Hz
GB        0
PC        1.00
  
```



```

NAME      JMS 687 HPLC RT :
EXPNO     18
PROCNO    1
Date_     20120427
Time      17.34
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zpgp30
TD         65536
SOLVENT   D2O
NS         10240
DS         4
SWH        29761.904 H:
FIDRES     0.454131 H:
AQ         1.1010548 s:
RG         2050
DW         16.800 u:
DE         8.43 u:
TE         298.1 K
D1         2.00000000 s:
D11        0.03000000 s:
TDO        1

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 u:
PL1       -0.51 dB
PL1W      99.92730713 W
SF01      125.7703643 M:

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 u:
PL2       -0.12 dB
PL12      17.94 dB
PL13      21.00 dB
PL2W      19.35150909 W
PL12W     0.30249262 W
PL13W     0.14952536 W
SF02      500.1320005 M:
SI        32768
SF        125.7577890 M:
WDW       EM
SSB       0
LB        1.00 H:
GB        0
PC        1.40
  
```