

Supplementary Information

Small Molecule CD38 Inhibitors: Synthesis of 8-Amino-*N*1-Inosine 5'-Monophosphate, Analogues and Early Structure-Activity Relationship

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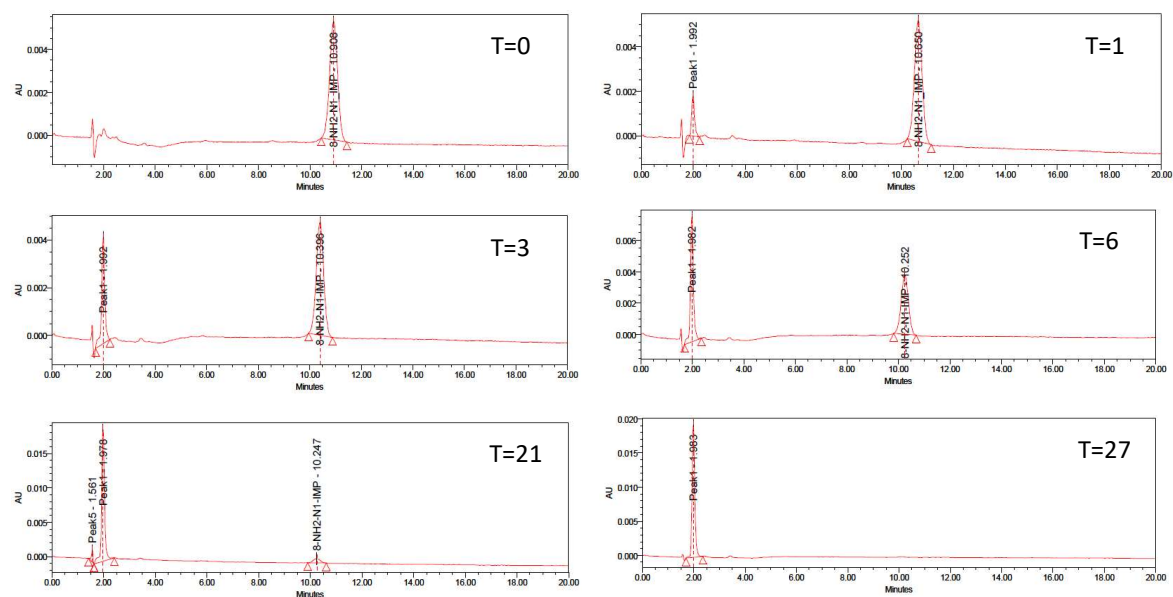
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Figure S1: Hydrolysis of 8-NH ₂ - <i>N</i> 1-IMP by high concentration of CD38 - HPLC data	p2
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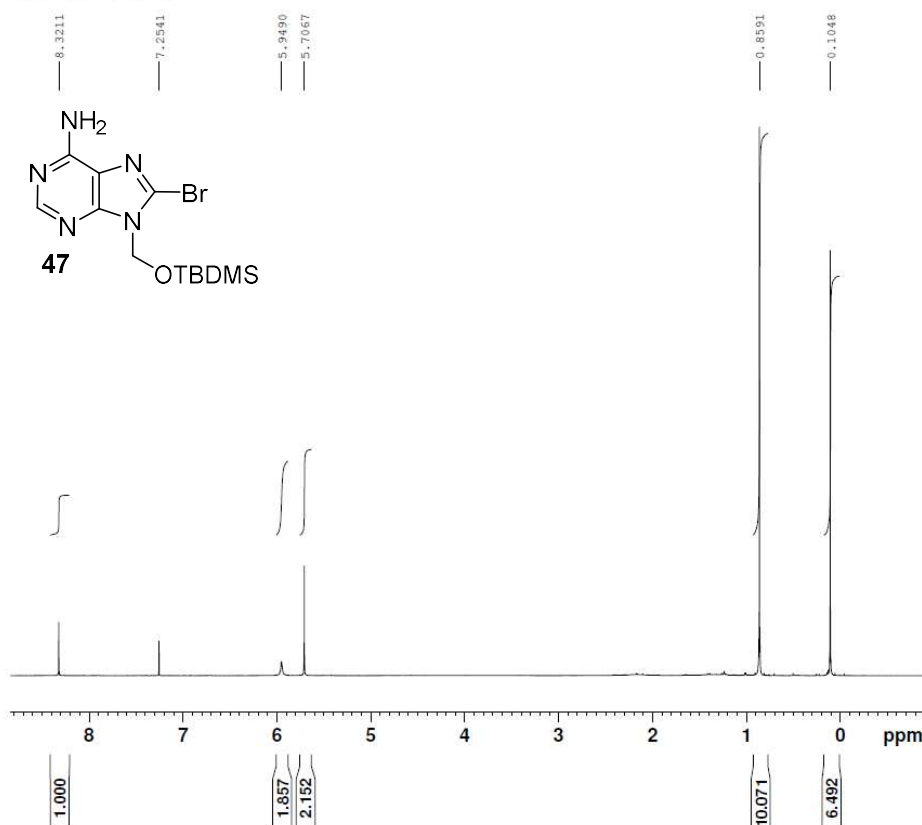
Figure S1: Hydrolysis of 8-NH₂-N1-IMP by high concentration of CD38 - HPLC data



HPLC traces showing 8-NH₂-N1-IMP (**11**) is turned over by high concentrations of CD38. HPLC conditions: eluting at 1 mL/min with an isocratic ion-pair buffer: 0.17% (m/v) cetrимide and 45% (v/v) phosphate buffer (pH 6.4) in MeOH. Time (T) in hours from addition of CD38.

Synthesis of 8-NH₂-N1-IMP (11)

JMS 834 T 13-15



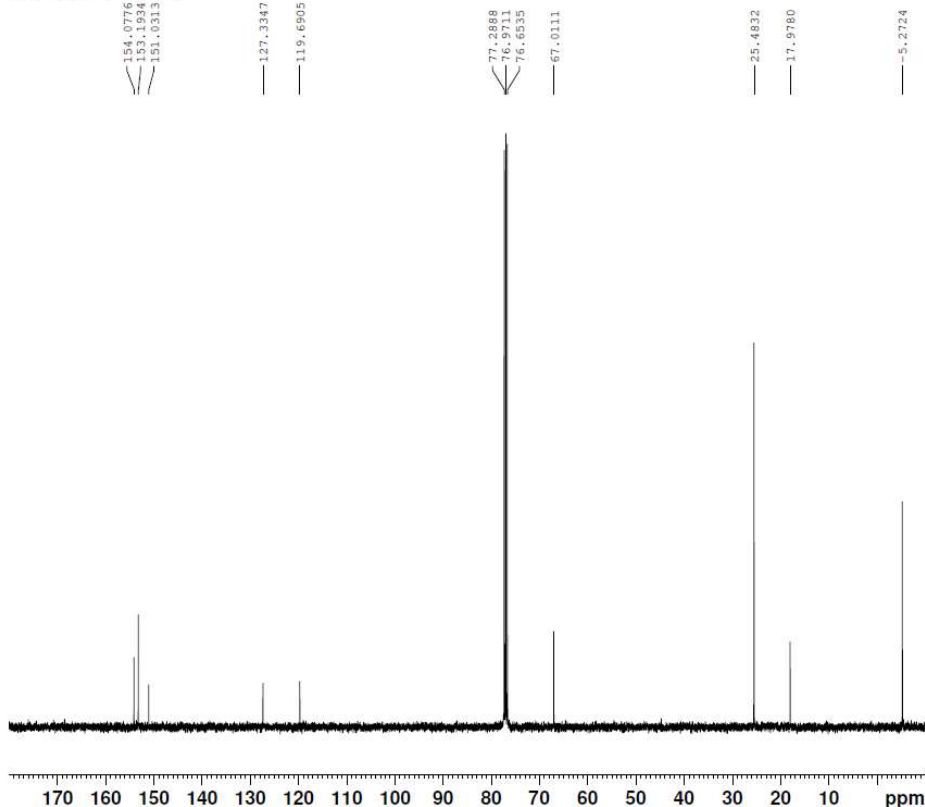
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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 114
DW 60.800 usec
DE 17.48 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 -1.00 dB
PL1W 12.26963711 W
SFO1 400.0424704 MHz

F2 - Processing parameters
SI 65536
SF 400.0399837 MHz
WDW EM
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GB 0
PC 1.00

JMS 834 T 13-15



Current Data Parameters
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EXPNO 11
PROCNO 1

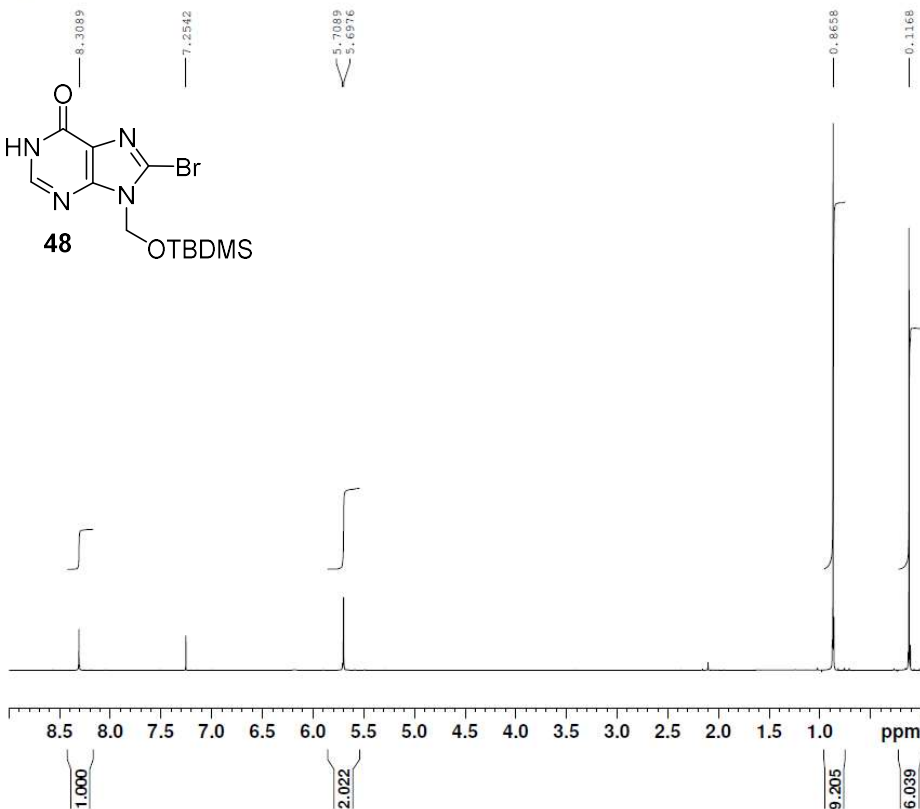
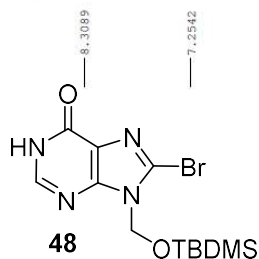
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NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 1820
DW 20.800 usec
DE 6.50 usec
TE 293.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== 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 -1.00 dB
PL12 15.55 dB
PL13 19.00 dB
PL2W 12.26963711 W
PL12W 0.27153867 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz

F2 - Processing parameters
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SF 100.5901380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

JMS 835 T 9-11



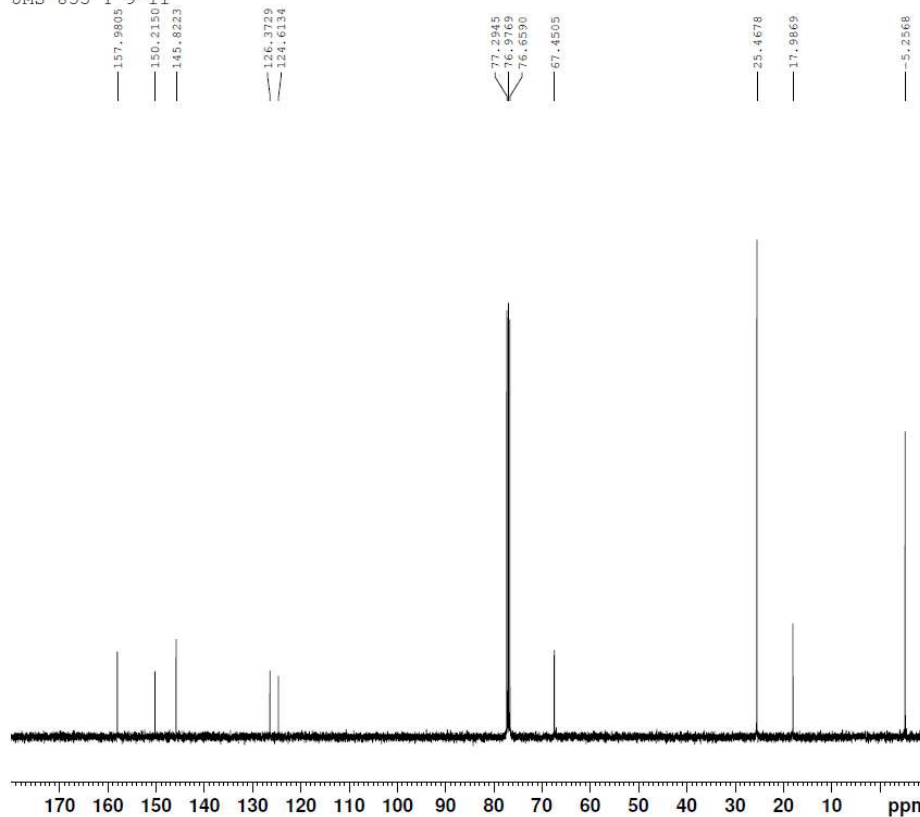
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TD 65536
SOLVENT CDC13
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SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 90.5
DW 60.800 usec
DE 17.48 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 -1.00 dB
PL1W 12.26963711 W
SFO1 400.0424704 MHz

F2 - Processing parameters
SI 65536
SF 400.0399837 MHz
WDW EM
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LB 0.20 Hz
GB 0
PC 1.00

JMS 835 T 9-11



Current Data Parameters
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PROCNO 1

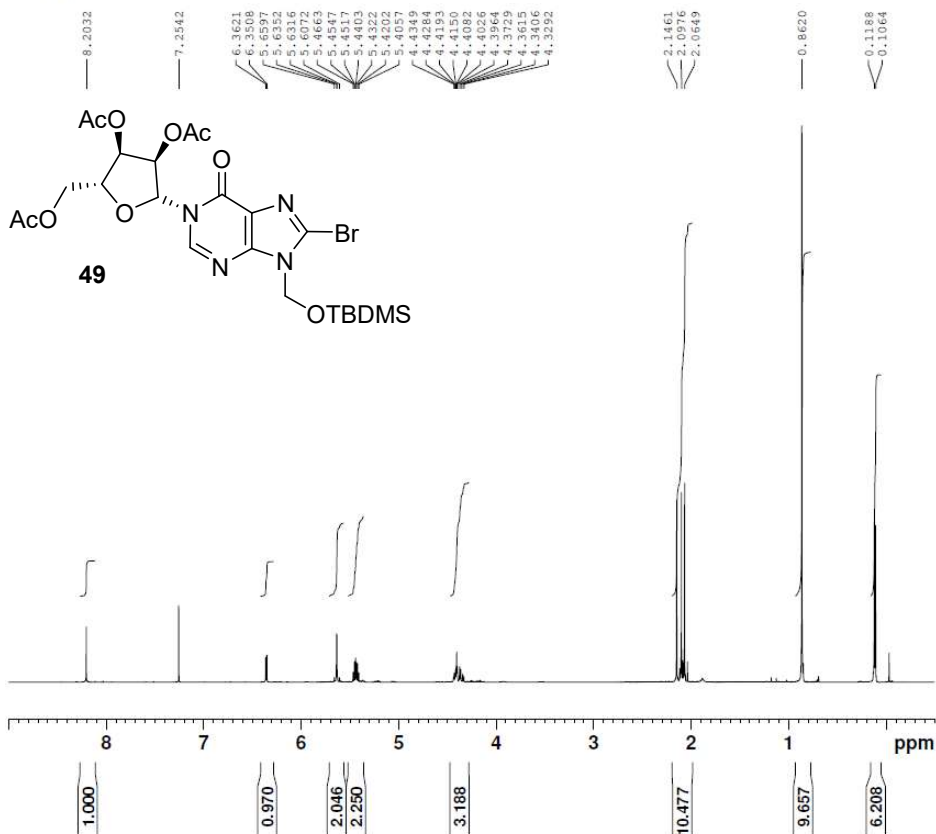
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AQ 1.3631488 sec
RG 1820
DW 20.800 usec
DE 6.50 usec
TE 293.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== 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 -1.00 dB
PL12 15.55 dB
PL13 19.00 dB
PL2W 12.26963711 W
PL12W 0.27153867 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz

F2 - Processing parameters
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SF 100.5901380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

JMS 853 T 31, 33-34

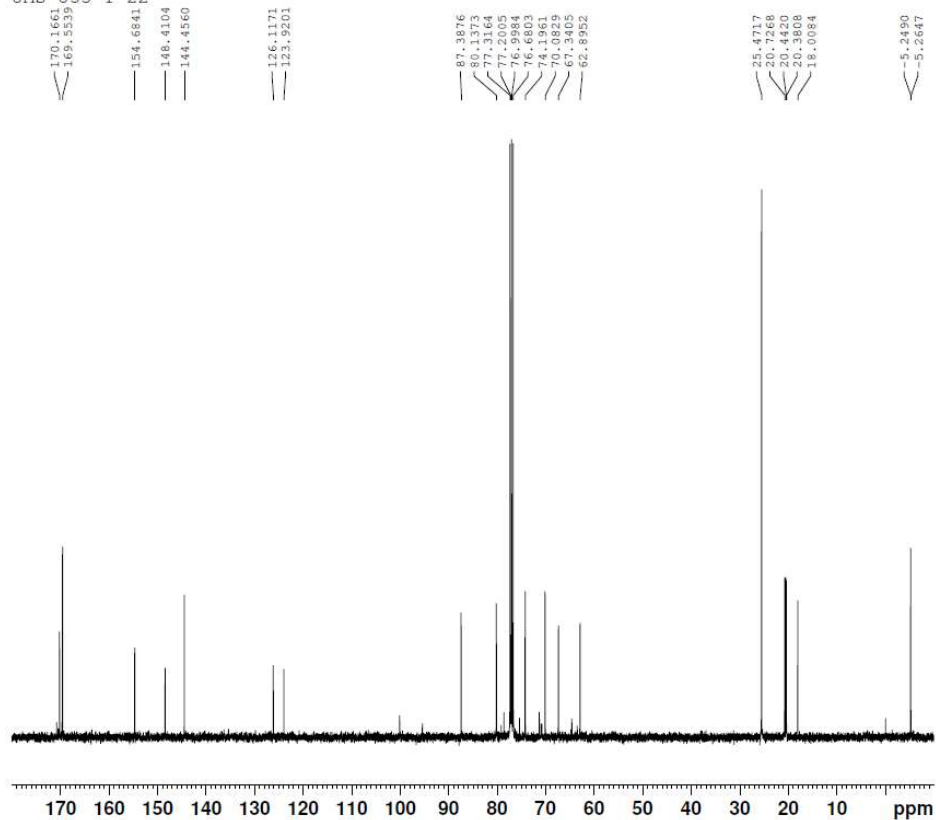


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 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 64
 DW 60.800 usec
 DE 17.48 usec
 TE 293.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.90 usec
 PL1 -1.00 dB
 PL1W 12.26963711 W
 SFO1 400.0424704 MHz

F2 - Processing parameters
 SI 65536
 SF 400.0399837 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

JMS 853 T 22



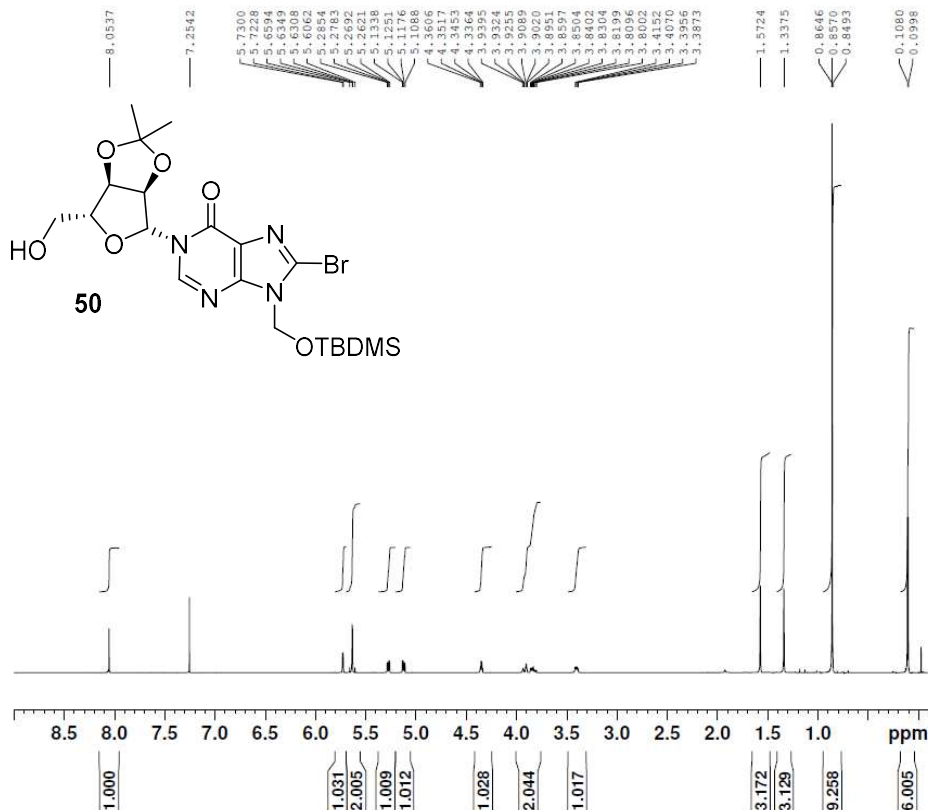
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 1820
 DW 20.800 usec
 DE 6.50 usec
 TE 293.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

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

===== CHANNEL f2 =====
 CPDPRG12 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 15.55 dB
 PL13 19.00 dB
 PL2W 12.26963711 W
 PL12W 0.27153867 W
 PL13W 0.12269637 W
 SFO2 400.0416002 MHz

F2 - Processing parameters
 SI 65536
 SF 100.5901380 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



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EXPNO      10
PROCNO     1
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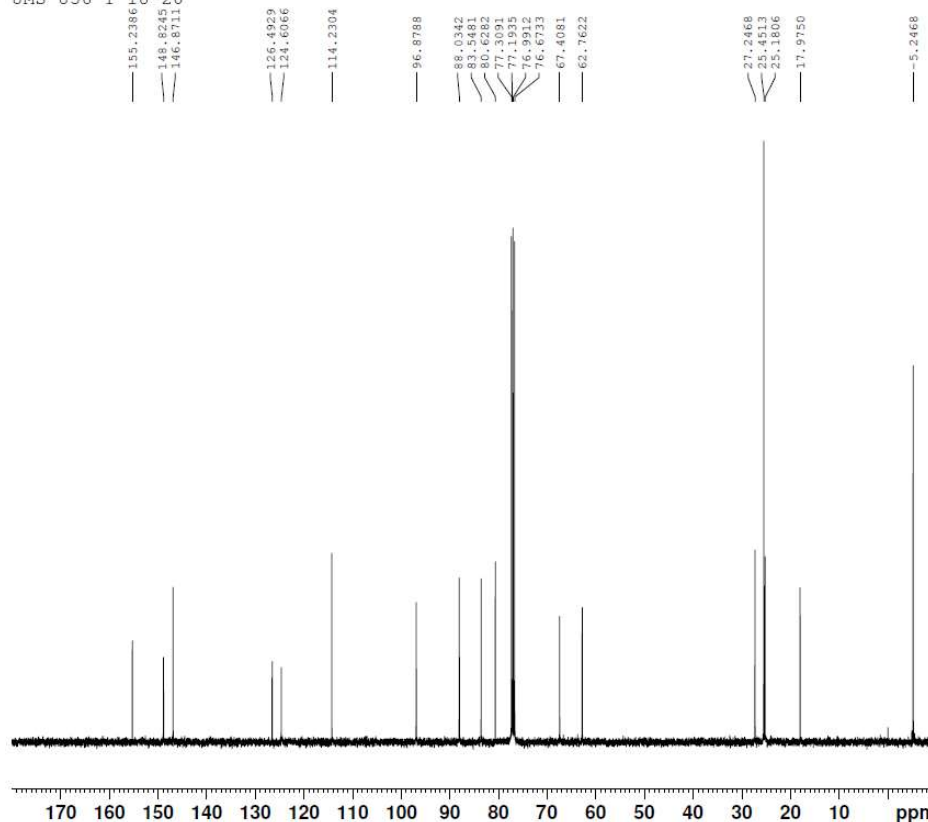
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Time       17:00
INSTRUM    AVI11407
PROBHWD    5 mm PABBO BB-
PULPROG     zg30
TD          65536
SOLVENT     CDCl3
NS          16
DS          2
SWH         8223.685 Hz
FIDRES      0.125483 Hz
AQ          3.9845889 sec
RG          64
DC          68.000 usec
DE          17.48 usec
TE          293.2 K
D1          1.00000000 sec
TDO         1
```

```

===== CHANNEL f1 =====
NUC1              1H
P1                 11.90 usec
PL1                -1.00 dB
PL1W               12.26963711 W
SFO1               400.0424704 MHz

```

```
F2 - Processing parameters
SI                65536
SF                400.0399837 MHz
WDW               EM
SSB               0
LB               0.20 Hz
GB               0
PC               1.00
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```
Current Data Parameters
NAME      Aug02-2013-JMS29398
EXPNO      11
PROCNO     1
```

```

F2 - Acquisition Parameters
Date_      20130803
Time       6.30
INSTRUM    AVII1400
PROBHD     5 mm PABBO 5B-
PULPROG    zgpg30
TD          65536
SOLVENT    CDCl3
NS          4
DS          2
SWH         24038.461 Hz
FIDRES     0.366798 Hz
AQ          1.3631488 sec
RG          1820
DE          20.800 usec
DW          6.50 usec
TE          293.2 K
D1          2.00000000 sec
D11         0.03000000 sec
TDO         1

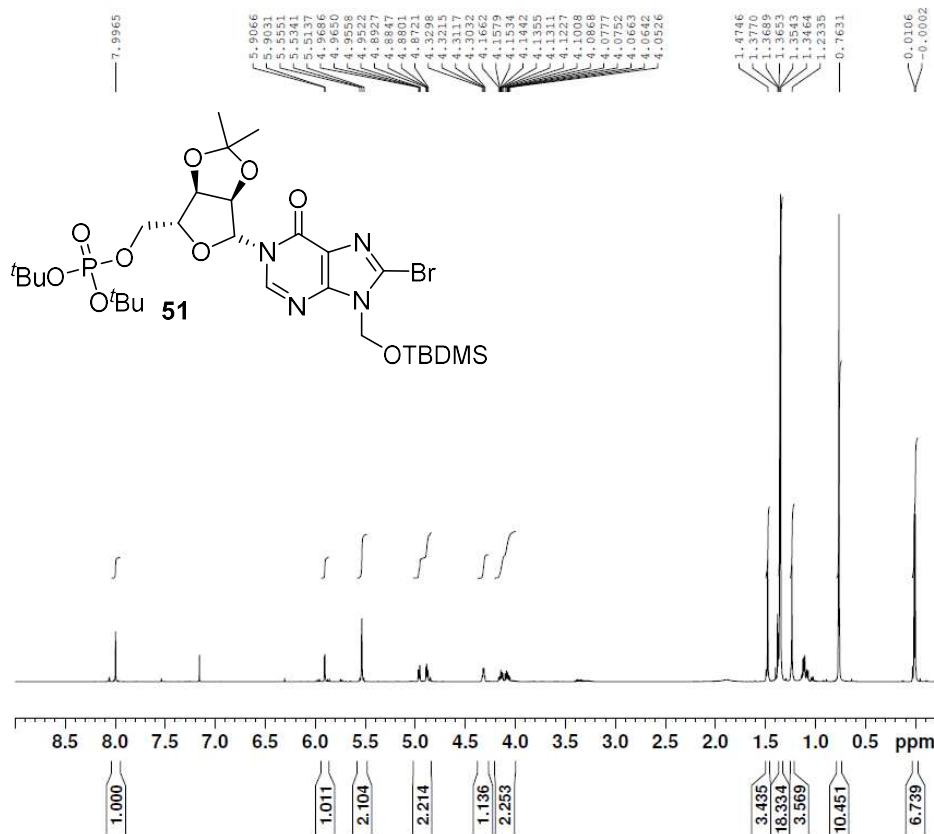
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```
===== CHANNEL f1 =====
NUC1                13C
P1                   8.75 usec
PL1                  -2.00 dB
PL1W                 58.91986084 W
SFO1                 100.6001970 MHz
```

```
===== CHANNEL f2 =====
CPDPRG[2]      waltz16
NUC2            1H
PCPD2           80.00 usec
PL2             -1.00 dB
PL12            15.55 dB
PL13            19.00 dB
PL2W            12.26963711 W
PL12W           0.27153867 W
PL13W           0.12269637 W
SF02            400.0416002 MHz
```

```
F2 - Processing parameters
SI                65536
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GB              0
PC              1.40
```

JMS 736 T 11-14



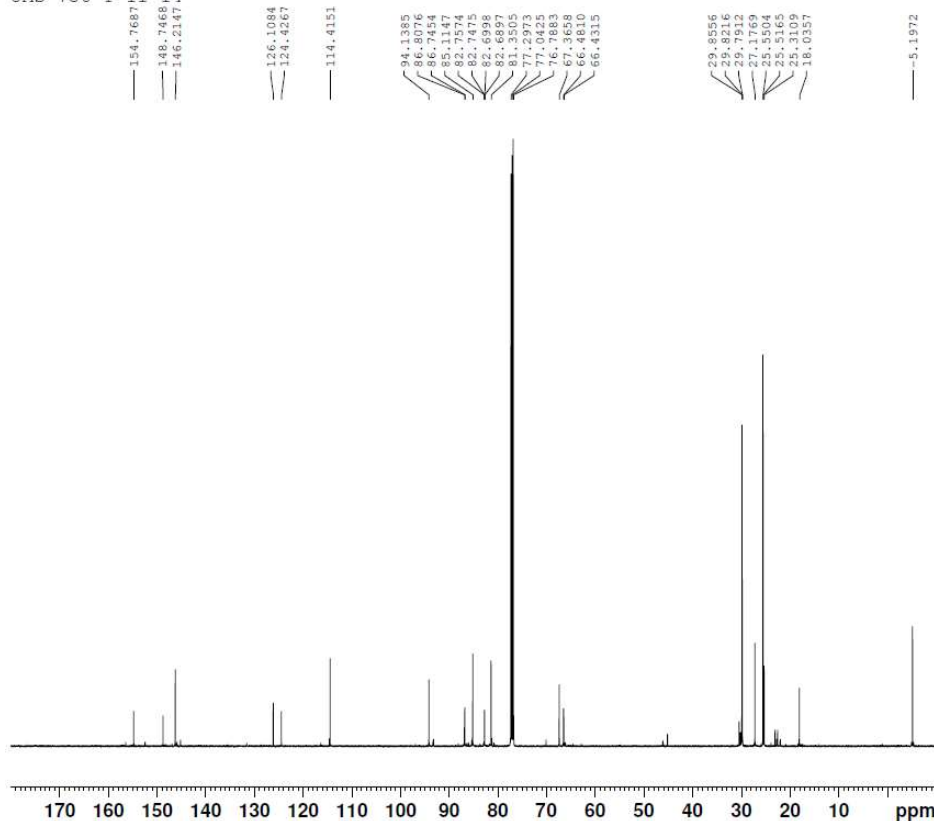
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 EXPNO 10
 PROCNO 1

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 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 3.1719425 sec
 RG 64
 DW 48.400 usec
 DE 13.94 usec
 TE 298.0 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

F2 - Processing parameters
 SI 32768
 SF 500.1300644 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

JMS 736 T 11-14



Current Data Parameters
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 EXPNO 12
 PROCNO 1

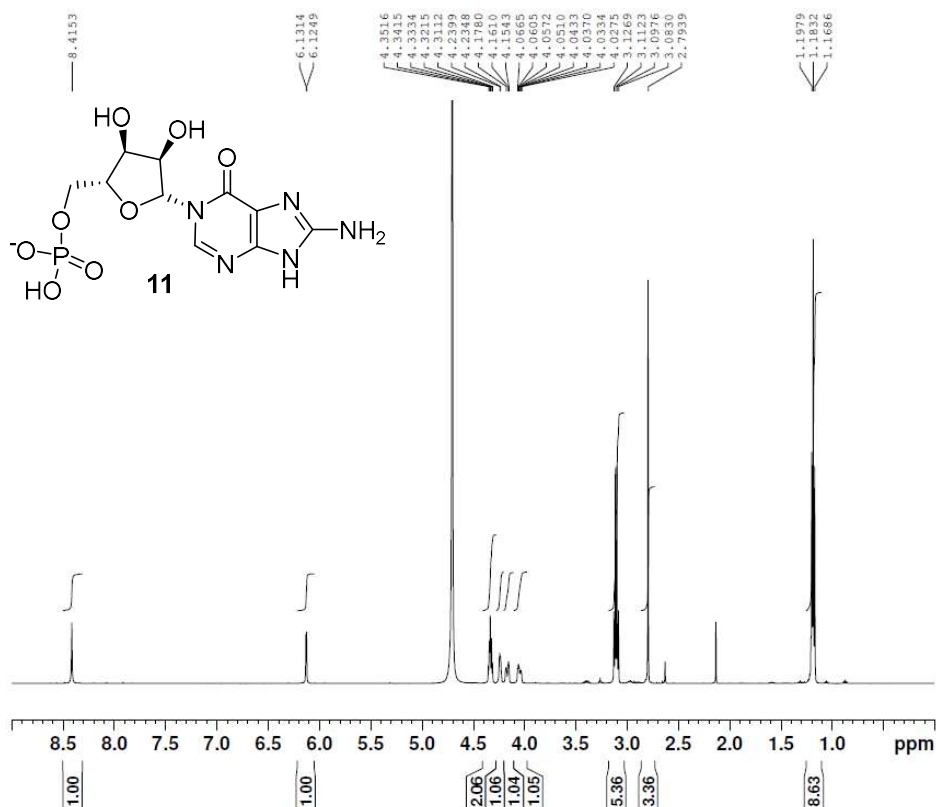
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 Time 17.53
 INSTRUM spect
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 5000
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 2050
 DW 16.800 usec
 DE 8.43 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -0.51 dB
 PL1W 99.92730713 W
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====
 CPDPRG[2] 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

F2 - Processing parameters
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 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

JMS 746 HPLC again



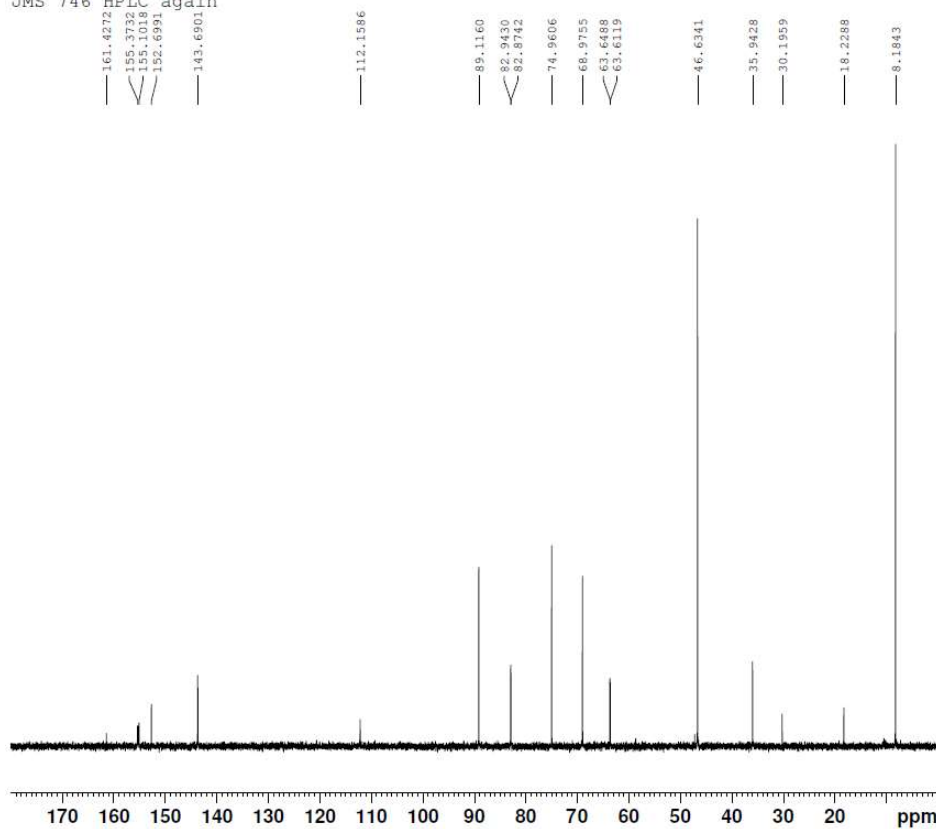
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NAME Oct24-2012-JMS 746
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INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT D2O
NS 128
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 80.6
DW 48.400 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -0.12 dB
PL1W 19.35150909 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

JMS 746 HPLC again



Current Data Parameters
NAME Oct24-2012-JMS 746
EXPNO 12
PROCNO 1

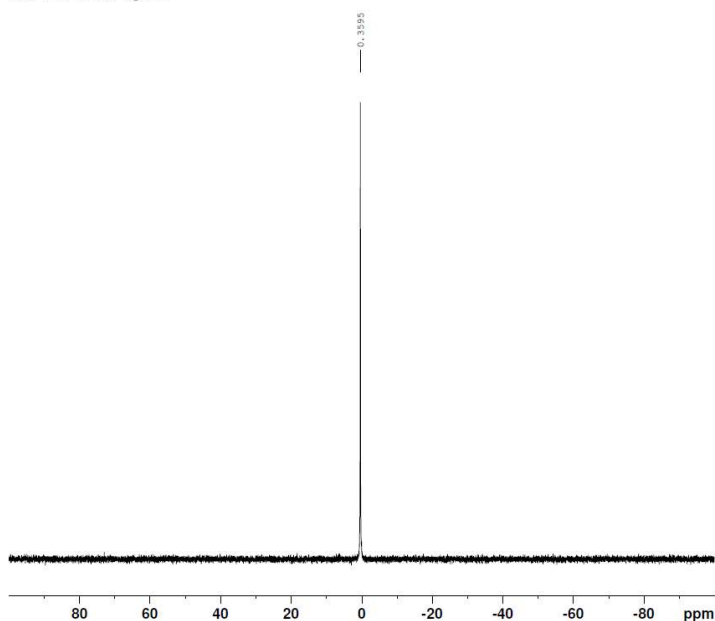
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PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 5000
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 8.43 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== 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

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

JMS 746 HPLC again



```

Current Data Parameters
NAME      Oct24-2012-JMS 746
EXPNO     11
PROCNO    1

F2 - Acquisition Parameters
Date_     20121024
Time      18.43
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   D2O
NS         256
DS         4
SWH        81821.742 Hz
FIDRES     1.243823 Hz
AQ         0.4019541 sec
RG         2050
DW         6.133 usec
DE         6.50 usec
TE         297.9 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       31P
P1         12.00 usec
PL1        -0.46 dB
PL1W       90.28126526 W
SFO1       202.4462121 MHz

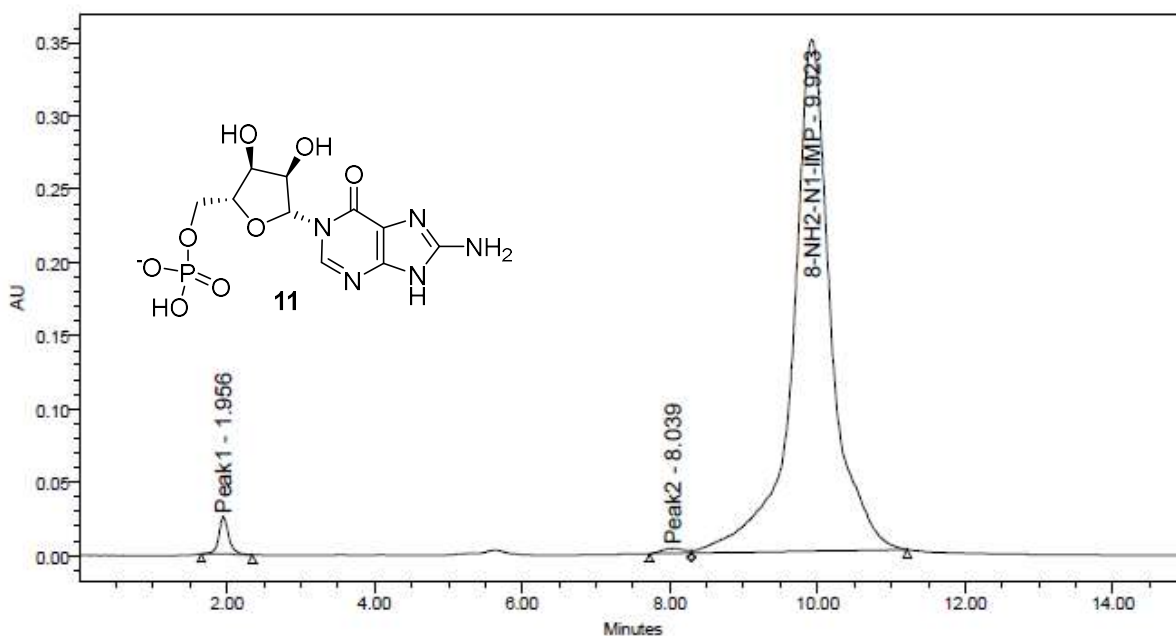
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -0.12 dB
PL12       17.94 dB
PL13       21.00 dB
PL1W       19.35150909 W
PL12W      0.30249262 W
PL13W      0.14952536 W
SFO2       500.1320005 MHz

F2 - Processing parameters
SI         32768
SF         202.4563350 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40
  
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SAMPLE INFORMATION

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 Vial: 2
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 15.0 Minutes
 Sample Set Name: JMS 3 deoxy and 746

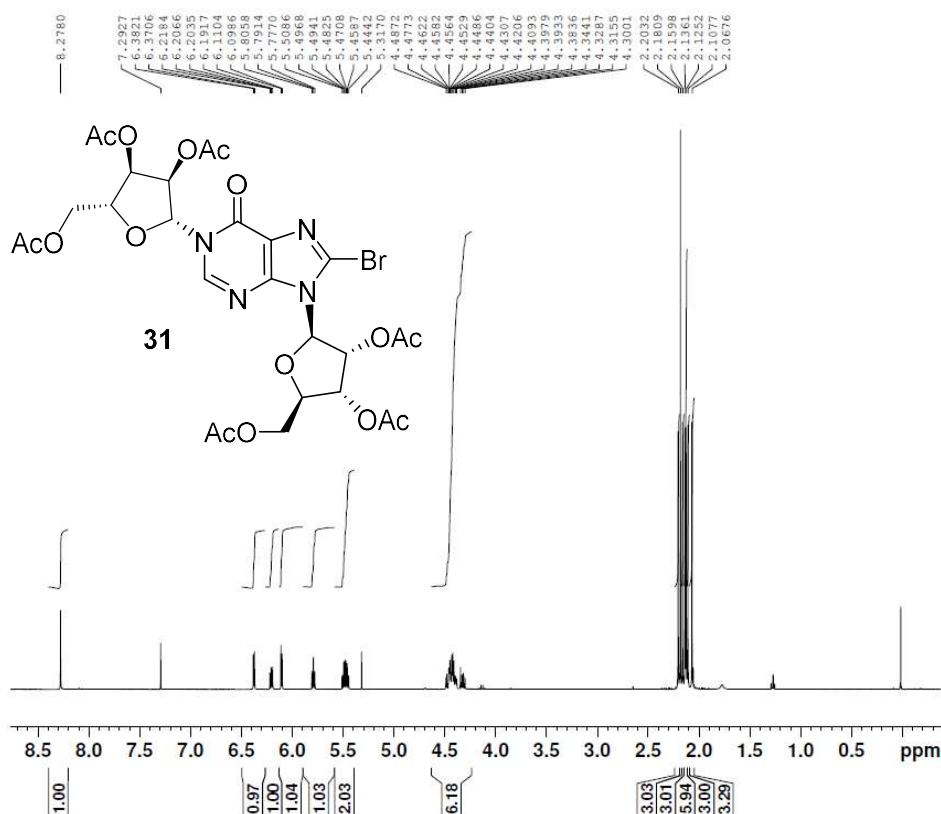
Acquired By: Joanna
 Date Acquired: 25/10/2012 2:59:32 PM
 Acq. Method Set: isocratic new PDA Jo
 Date Processed: 09/04/2021 3:09:01 PM
 Processing Method: 8_NH2_N1_IMP
 Channel Name: Wwin Ch1
 Proc. Chnl. Descr.: PDA 254.0 nm



	Peak Name	RT	Area	% Area	Height
1	Peak1	1.956	237655	1.84	25525
2	Peak2	8.039	74802	0.58	3473
3	8-NH2-N1-IMP	9.923	12615673	97.58	348912

N1-Ribosyl-inosine analogues (14-17):

JMS 112 T 43-44



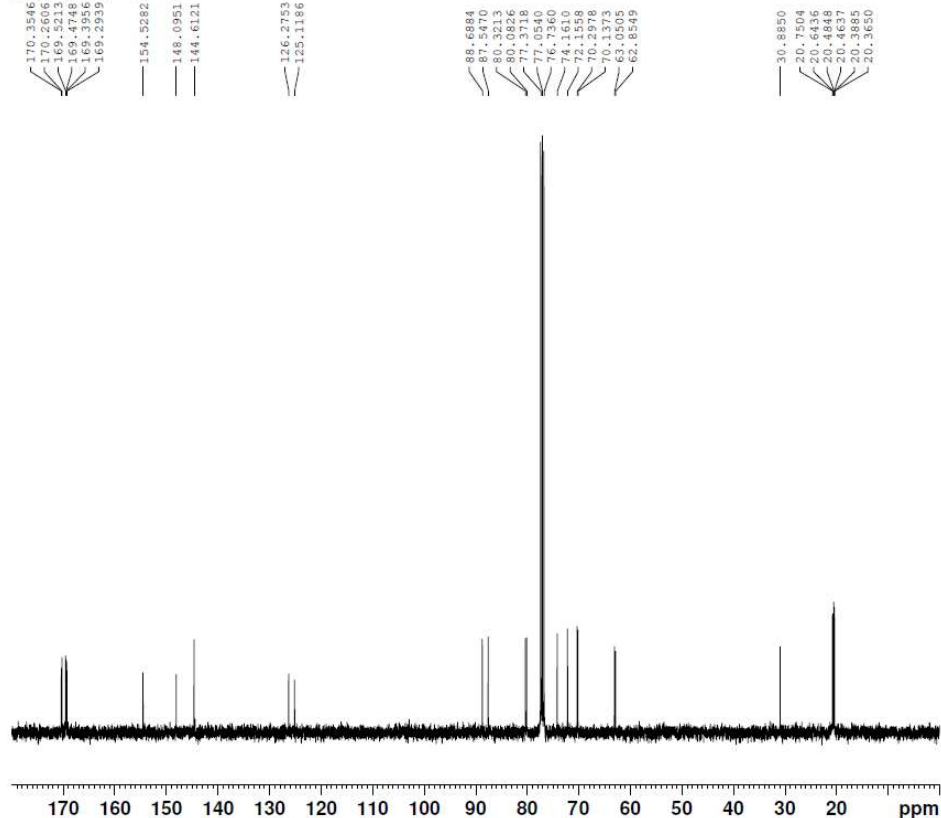
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EXPNO 10
PROCNO 1

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PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 114
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 dB
PL1W 9.74611950 W
SFO1 400.0424704 MHz

F2 - Processing parameters
SI 65536
SF 400.0400000 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

JMS 112 T 43-44



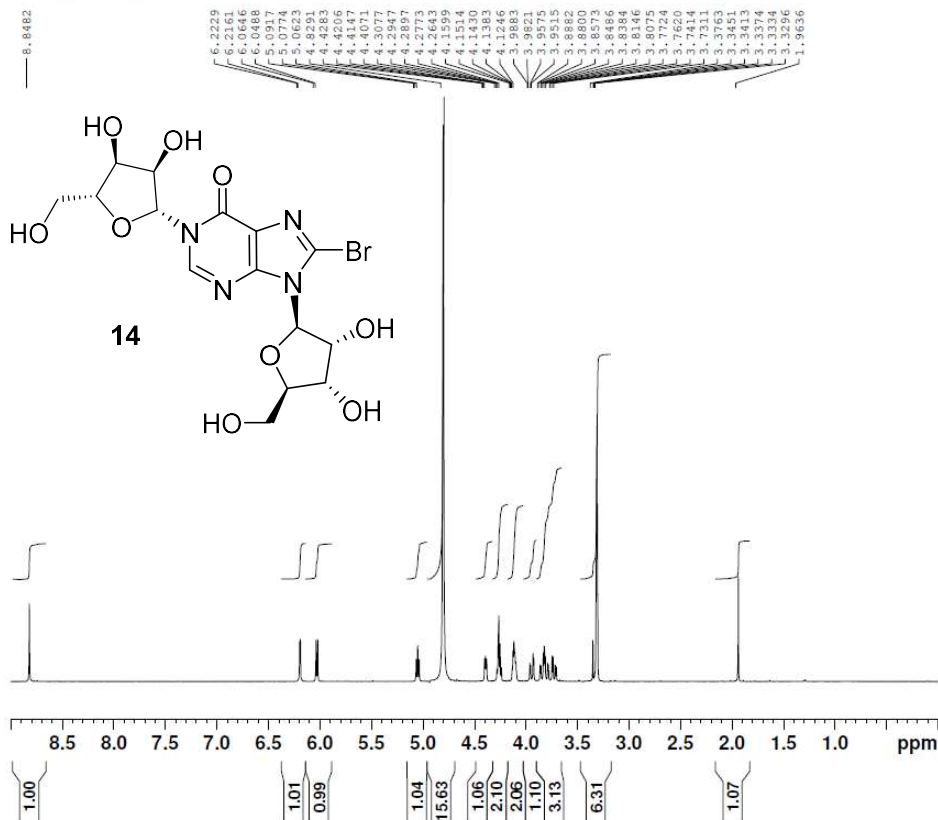
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EXPNO 17
PROCNO 1

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Time 9.54
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 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 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.78 dB
PL13 19.00 dB
PL2W 9.74611950 W
PL12W 0.25753233 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz

F2 - Processing parameters
SI 65536
SF 100.5901380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



```
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EXPNO      10
PROCNO     1
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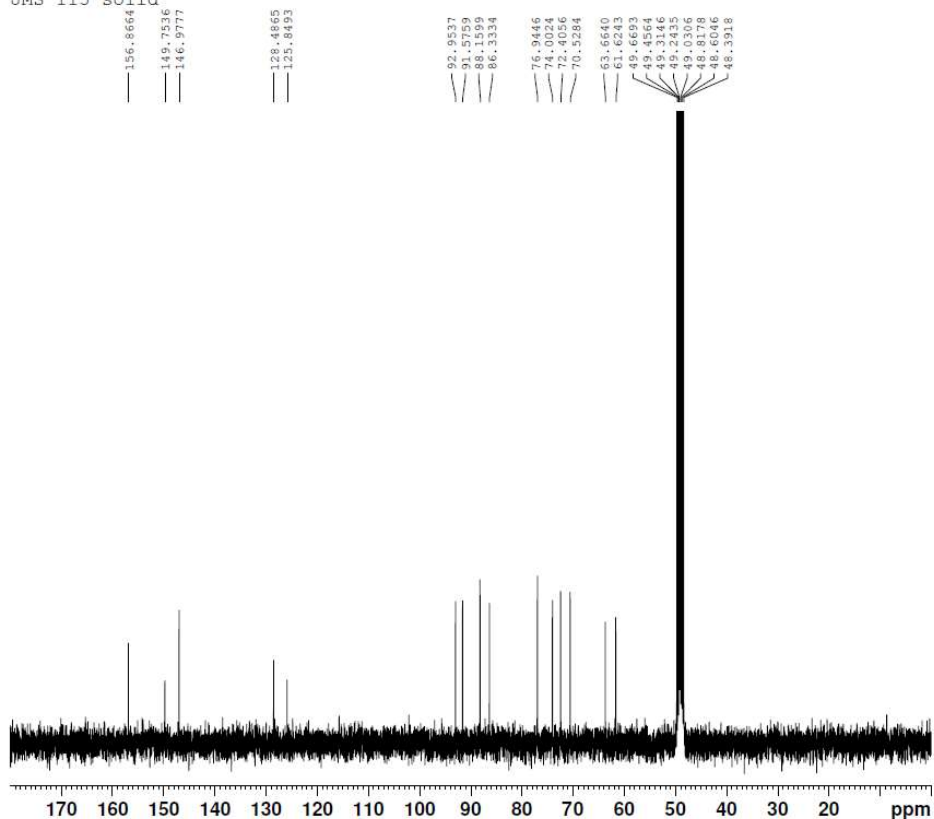
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Time_         11.33
INSTRUM       AVIII400
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       MeOD
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9845889 sec
RG            144
DEW           60.800 usec
DE            6.50 usec
TE            298.0 K
D1            1.00000000 sec
TDO           1

```

```
===== CHANNEL f1 =====
NUC1                1H
P1                  13.00 usec
PL1                 0 dB
PL1W                9.74611950 W
SFO1                400.0424704 MHz
```

F2 - Processing parameters	
SI	32768
SF	400.0400110 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



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Current Data Parameters
NAME      Mar31-2010-JMS0372
EXPNO      11
PROCNO     1
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F2 - Acquisition Parameters
Date_          20100331
Time_          14.59
INSTRUM        AVII1400
PROBHD         5 mm PABBO BB-
PULPROG        zgpg30
TD             65536
SOLVENT        MeOD
NS             512
DS             4
SWH            24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG            2050
DW            20.800 usec
DE            6.50 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

```

```

===== CHANNEL f1 =====
NUC1                13C
P1                   8.75 usec
PL1                  -2.00 dB
PL1W                 58.91986084 W
SF01                 100.6001970 MHz

```

```

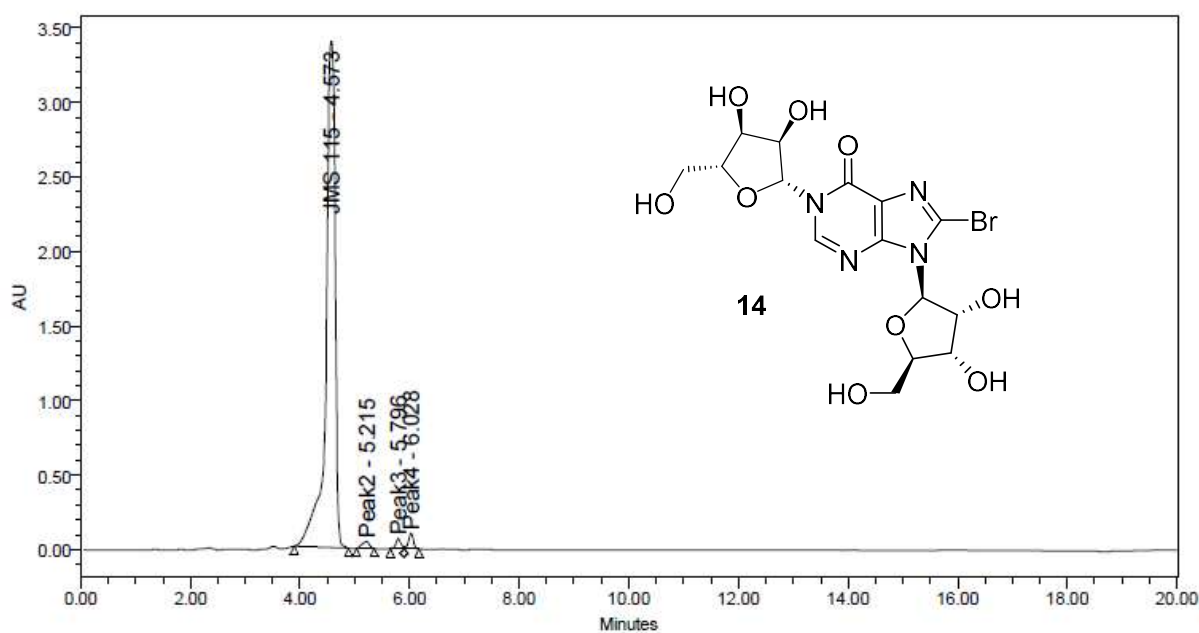
===== CHANNEL f2 =====
CPDPRG[2]          waltz16
NUC2                1H
PCPD2              80.00 usec
PL2                 0 dB
PL12               15.78 dB
PL13               19.00 dB
PL2W               9.74611950 W
PL12W              0.25753233 W
PL13W              0.12269637 W
SFO2               400.0416002 MHz

```

```
F2 - Processing parameters.
SI          65536
SF          100.5899952 MHz
WDW          EM
SSB          0
LB          1.00 Hz
GB          0
PC          1.40
```

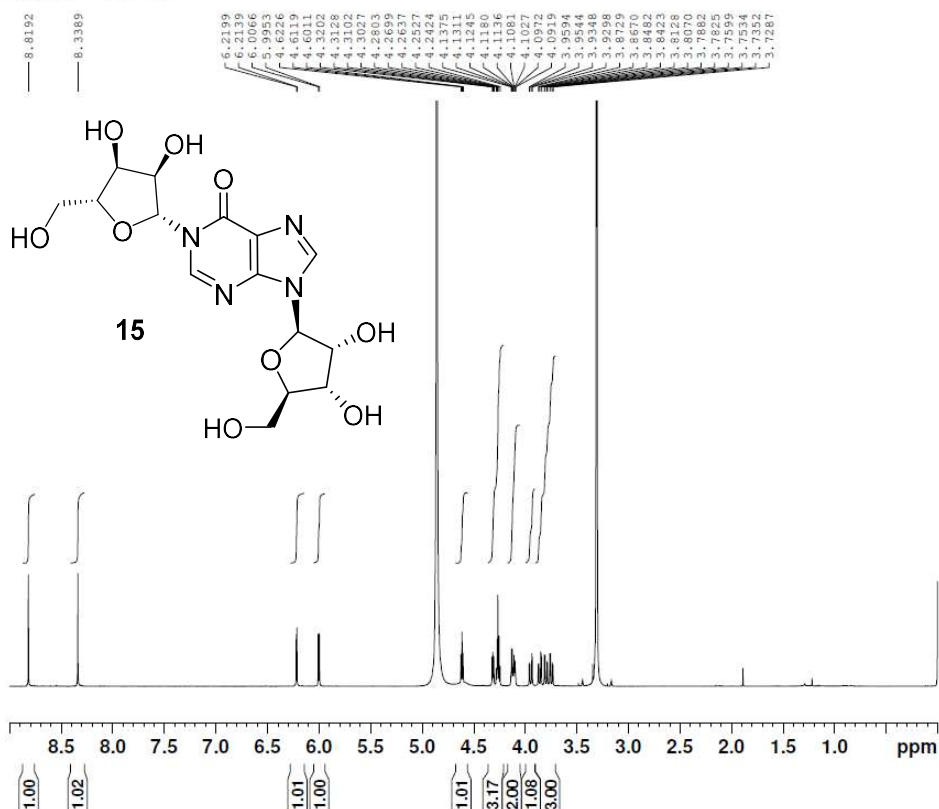
SAMPLE INFORMATION

Sample Name: JMS 115 solid	Acquired By: Christelle	Date Acquired: 04/10/2011 3:37:32 PM
Sample Type: Unknown	Date Acquired: 04/10/2011 3:37:32 PM	Acq. Method Set: RP18 LC
Vial: 6	Acq. Method Set: RP18 LC	Date Processed: 05/10/2011 10:12:15 AM
Injection #: 1	Date Processed: 05/10/2011 10:12:15 AM	Processing Method: JMS 115
Injection Volume: 10.00 ul	Processing Method: JMS 115	Channel Name: WvlnCh1
Run Time: 20.0 Minutes	Channel Name: WvlnCh1	Proc. Chnl. Descr.: PDA 262.1 nm
Sample Set Name: JMS 545 JMS 137 JMS 115	Proc. Chnl. Descr.: PDA 262.1 nm	



	Peak Name	RT	Area	% Area	Height
1	JMS 115	4.573	39715120	96.29	3391937
2	Peak2	5.215	419731	1.02	46549
3	Peak3	5.796	442067	1.07	65376
4	Peak4	6.028	668389	1.62	108342

JMS137 T15-16



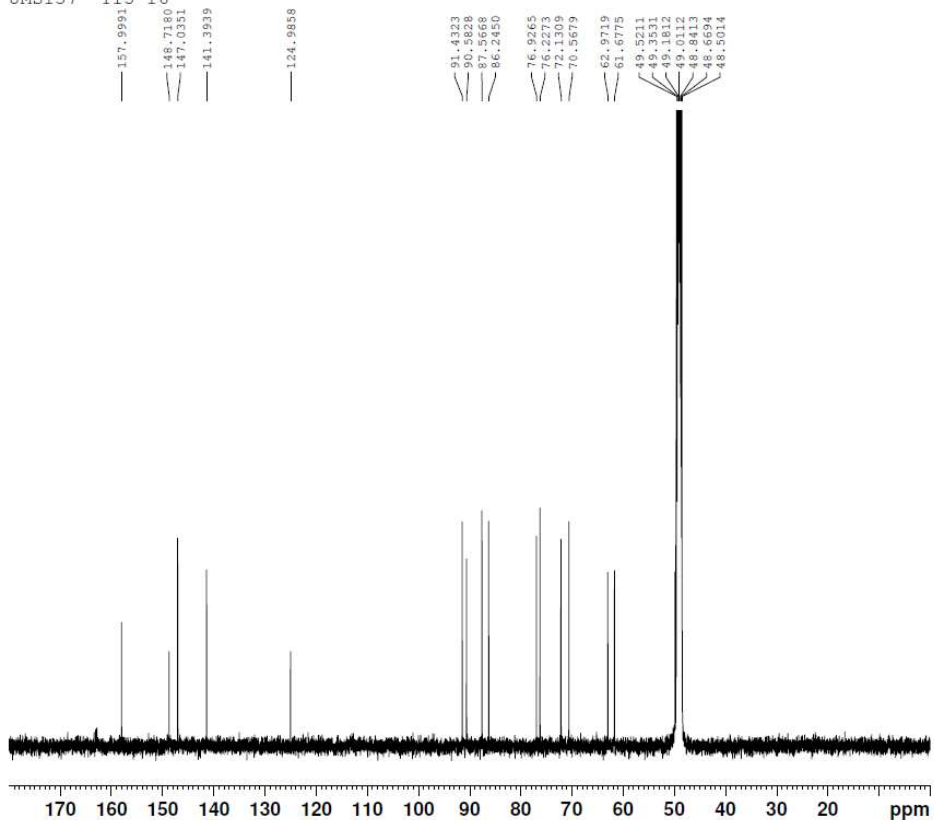
Current Data Parameters
NAME JMS137 T15-16
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111007
Time 22.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 256
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 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

F2 - Processing parameters
SI 32768
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

JMS137 T15-16



Current Data Parameters
NAME JMS137 T15-16
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111010
Time 4.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 61440
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 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

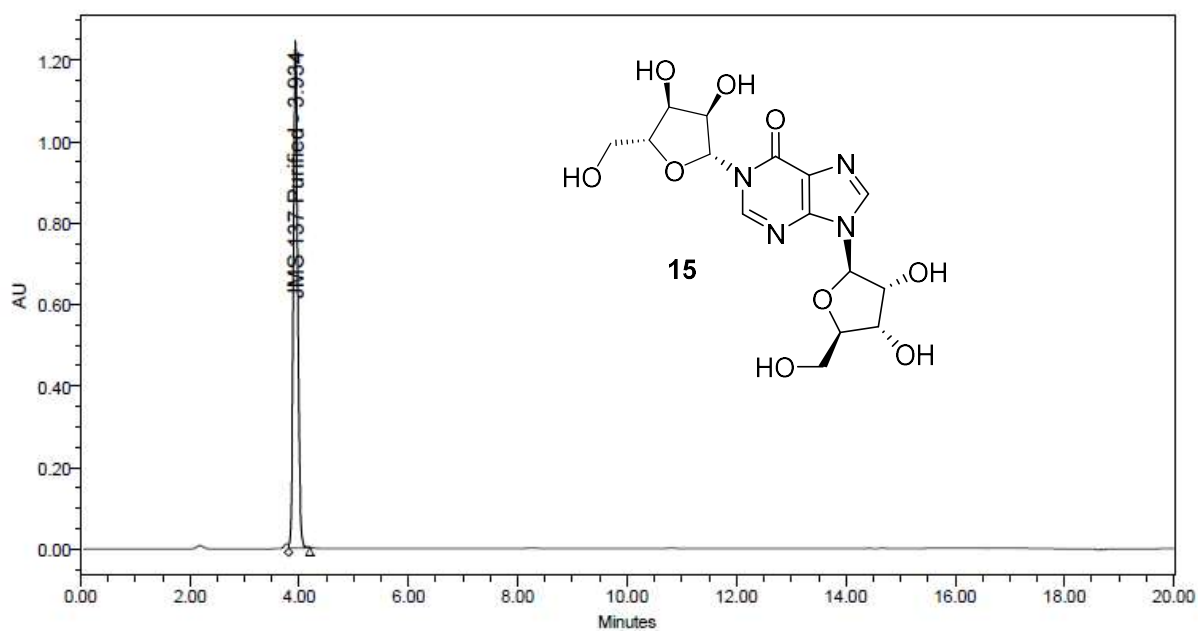
===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.12 dB
PL12 17.94 dB
PL13 21.00 dB
PL12W 19.35150909 W
PL12W 0.30249262 W
PL13W 0.14952536 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7576104 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

SAMPLE INFORMATION

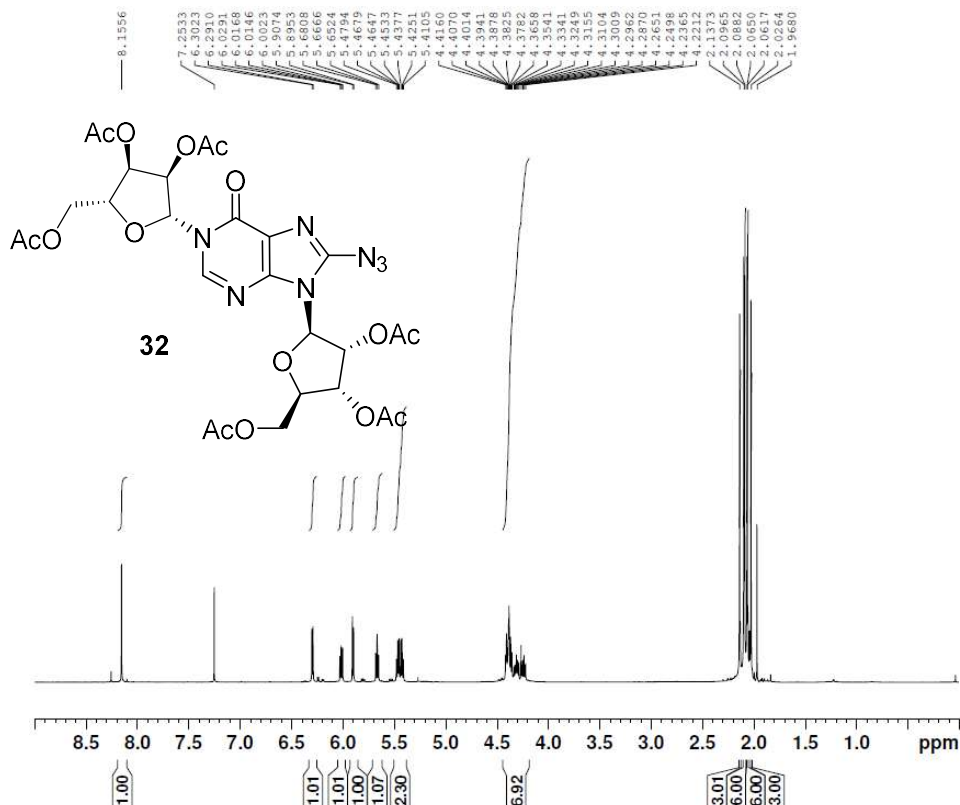
Sample Name: JMS 137 HPLC
 Sample Type: Unknown
 Vial: 26
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 20.0 Minutes
 Sample Set Name: JMS 137 HPLC 2

Acquired By: Joanna
 Date Acquired: 17/10/2011 3:27:24 PM
 Acq. Method Set: RP18 LC
 Date Processed: 17/10/2011 3:49:45 PM
 Processing Method: JMS 137 Purified
 Channel Name: WvlnCh1
 Proc. Chnl. Descr.: PDA 262.1 nm



	Peak Name	RT	Area	% Area	Height
1	JMS 137 Purified	3.934	7025028	100.00	1244149

JMS 492 PRODUCT



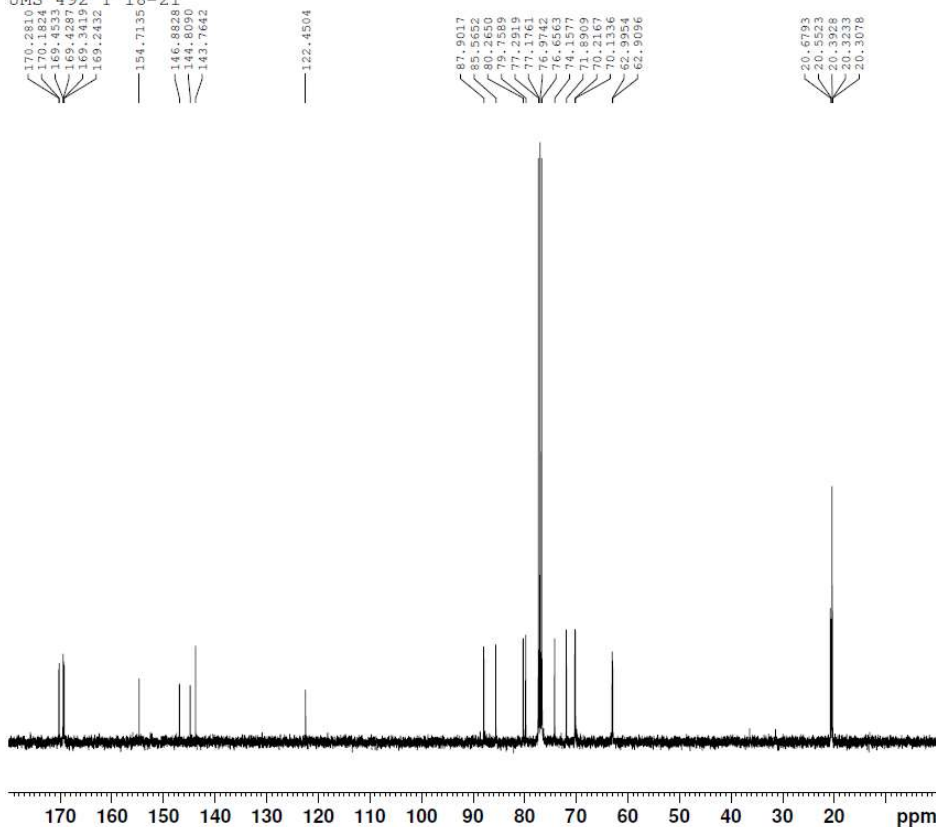
Current Data Parameters
NAME Jul26-2011-JMS11649
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110726
Time 17.25
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 3.9845889 sec
RG 71.8
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 dB
PL1W 9.74611950 W
SFO1 400.0424704 MHz

F2 - Processing parameters
SI 65536
SF 400.0399837 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

JMS 492 T 18-21



Current Data Parameters
NAME Jul18-2011-JMS11462
EXPNO 11
PROCNO 1

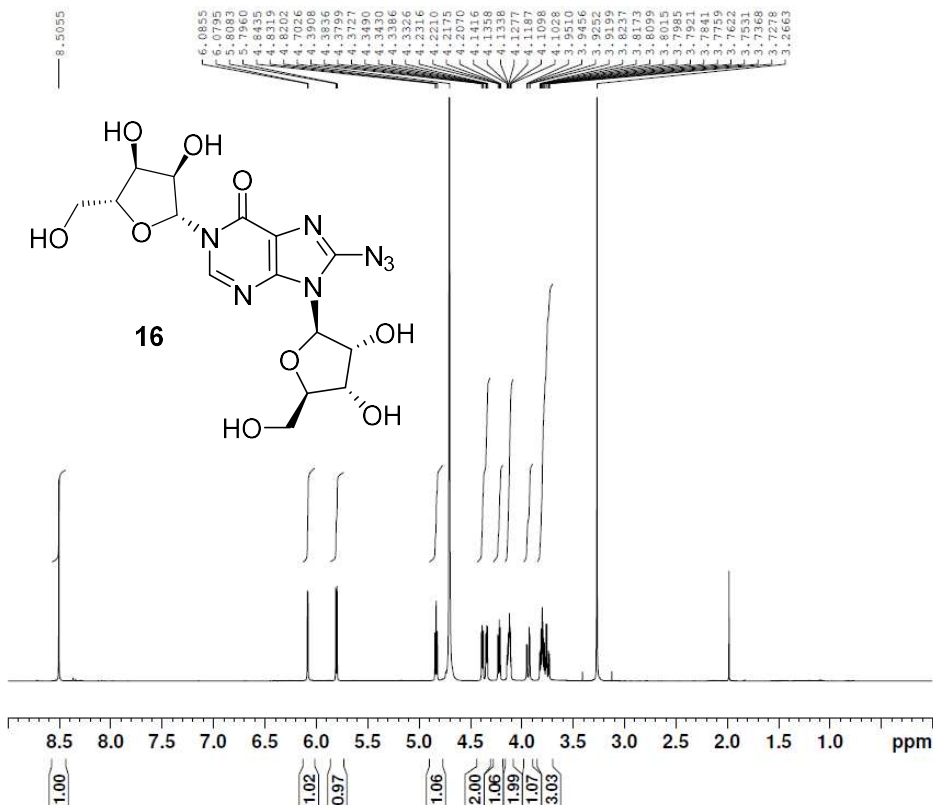
F2 - Acquisition Parameters
Date_ 20110719
Time 0.59
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.78 dB
PL13 19.00 dB
PL2W 9.74611950 W
PL12W 0.25753233 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz

F2 - Processing parameters
SI 65536
SF 100.5901380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

JMS 510 HPLC



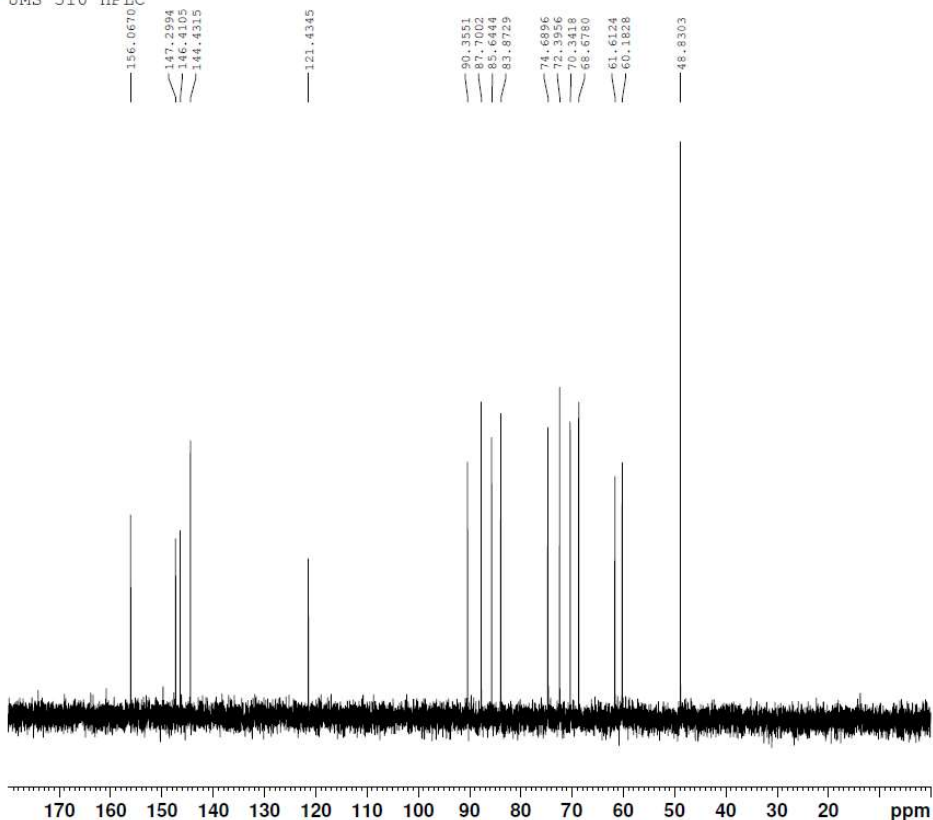
Current Data Parameters
NAME JMS510HPLC
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111019
Time 9.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 732
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 128
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

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

JMS 510 HPLC



Current Data Parameters
NAME JMS510HPLC
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111019
Time 10.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 827
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 8.43 usec
TE 298.2 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

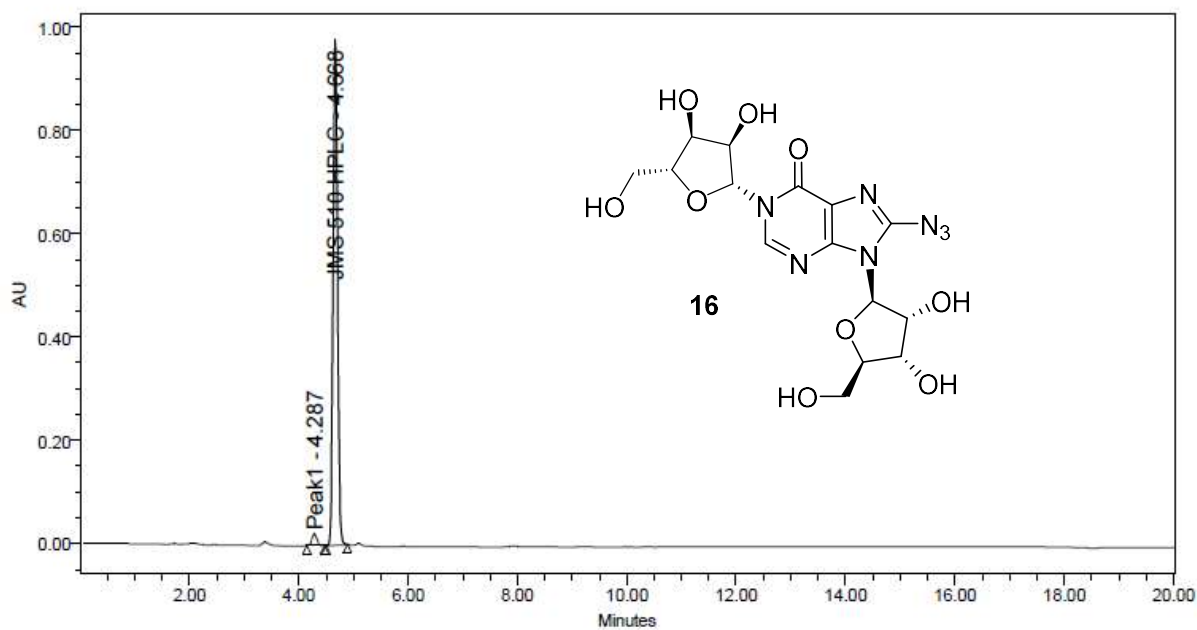
===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.12 dB
PL12 17.94 dB
PL13 21.00 dB
PL2W 19.35150909 W
PL12W 0.30249262 W
PL13W 0.14952536 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

SAMPLE INFORMATION

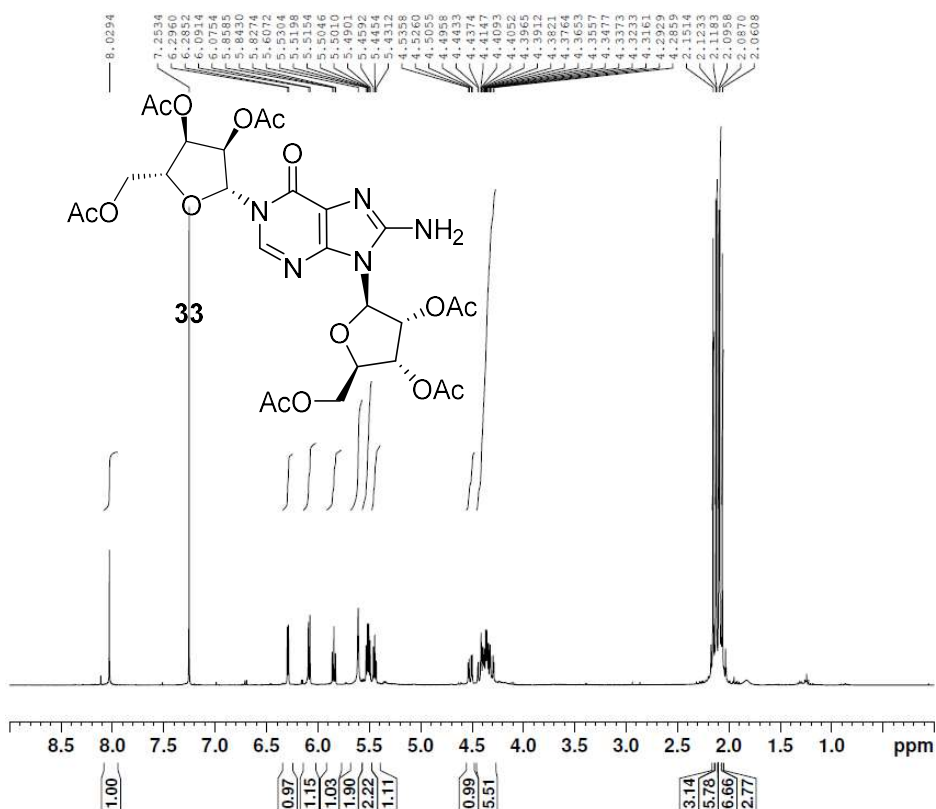
Sample Name: JMS 510 HPLC
 Sample Type: Unknown
 Vial: 1
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 20.0 Minutes
 Sample Set Name: JMS 510 HPLC

Acquired By: Christelle
 Date Acquired: 25/10/2011 5:14:47 PM
 Acq. Method Set: RP18 LC
 Date Processed: 28/10/2011 12:20:44 PM
 Processing Method: JMS 510 HPLC
 Channel Name: WvlnCh1
 Proc. Chnl. Descr.: PDA 262.1 nm



	Peak Name	RT	Area	% Area	Height
1	Peak1	4.287	143472	2.55	23047
2	JMS 510 HPLC	4.668	5486409	97.45	979291

JMS 503 T 4

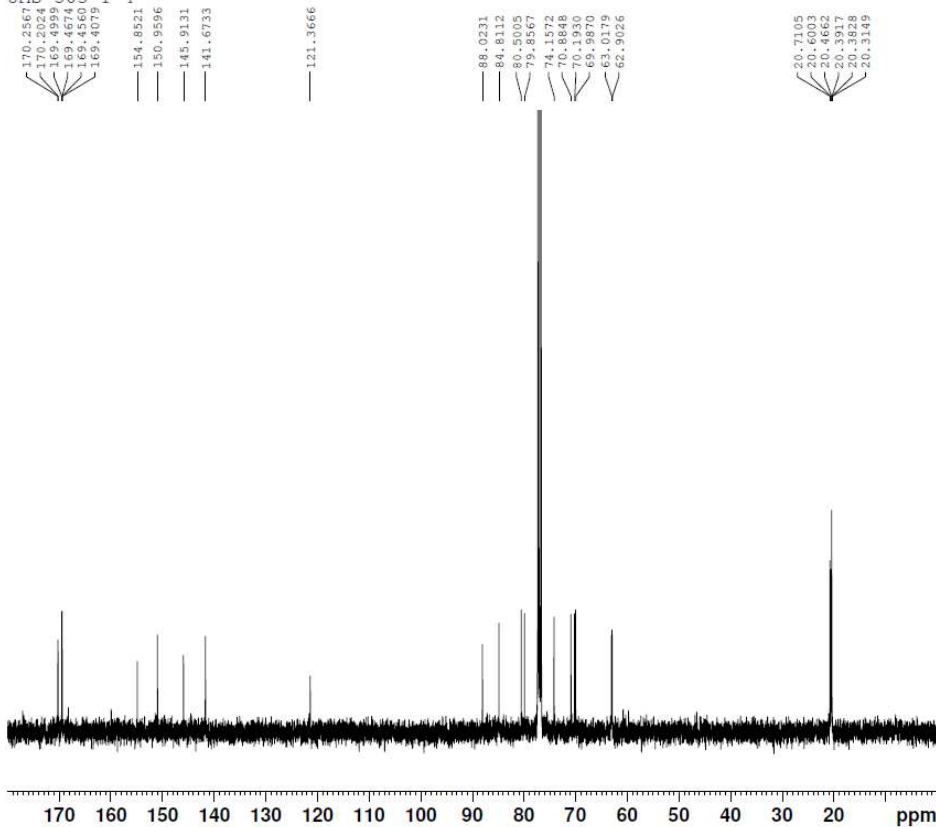


Current Data Parameters
 NAME Jul26-2011-JMS11651
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110726
 Time 17.15
 INSTRUM AVII1400
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 144
 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 dB
 PL1W 9.74611950 W
 SFO1 400.0424704 MHz
 F2 - Processing parameters
 SI 65536
 SF 400.0399837 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

JMS 503 T 4



Current Data Parameters
 NAME Jul26-2011-JMS11651
 EXPNO 14
 PROCNO 1

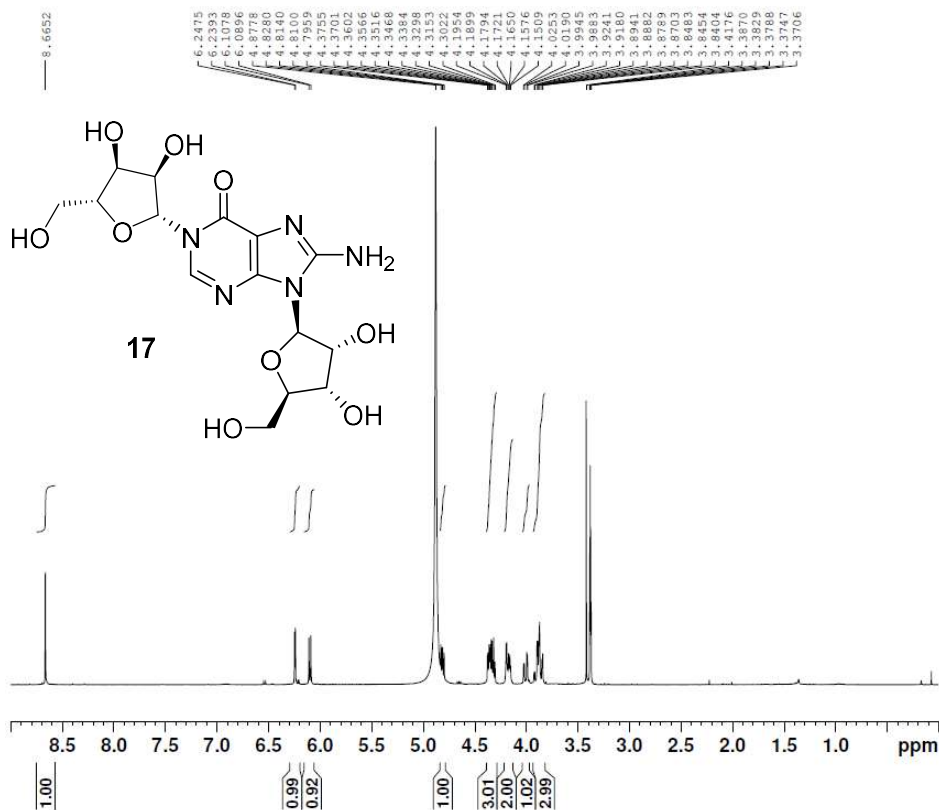
F2 - Acquisition Parameters
 Date_ 20110726
 Time 19.43
 INSTRUM AVII1400
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 2050
 DW 20.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 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 dB
 PL12 15.78 dB
 PL13 19.00 dB
 PL2W 9.74611950 W
 PL12W 0.25753233 W
 PL13W 0.12269637 W
 SFO2 400.0416002 MHz

F2 - Processing parameters
 SI 65536
 SF 100.5901380 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

JMS 509 T 9-11



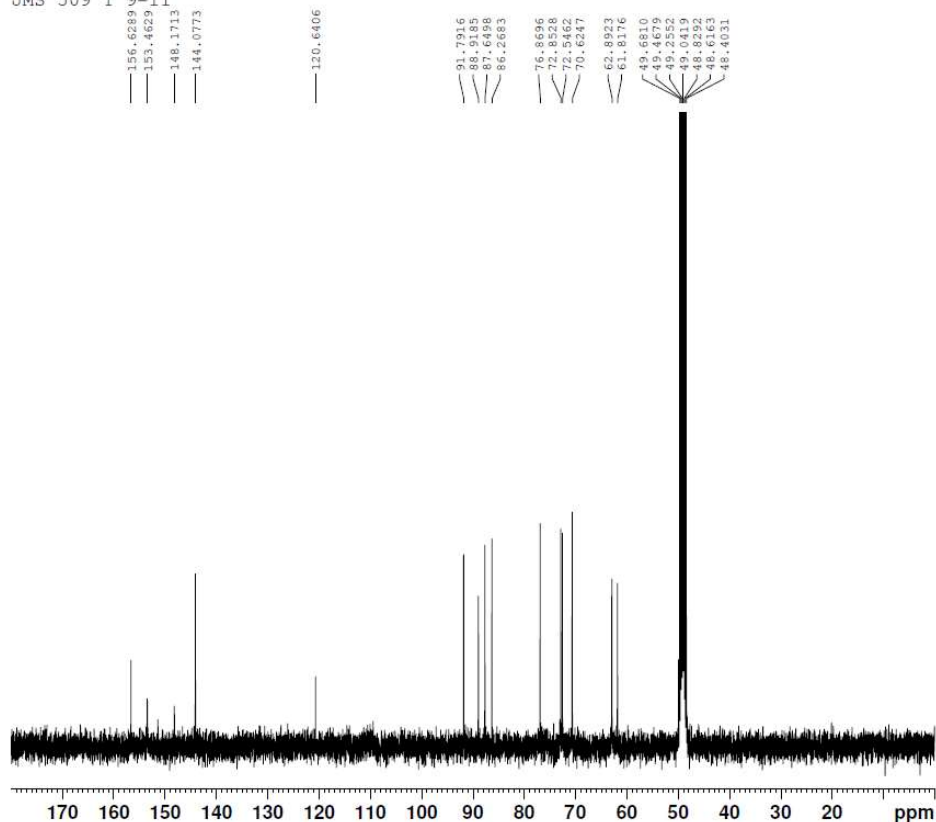
Current Data Parameters
 NAME Aug08-2011-JMS11943
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110808
 Time 16.58
 INSTRUM AVIII400
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 161
 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 dB
 PL1W 9.74611950 W
 SFO1 400.0424704 MHz

F2 - Processing parameters
 SI 65536
 SF 400.0399837 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

JMS 509 T 9-11



Current Data Parameters
 NAME Aug08-2011-JMS11943
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110809
 Time 5.47
 INSTRUM AVIII400
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 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

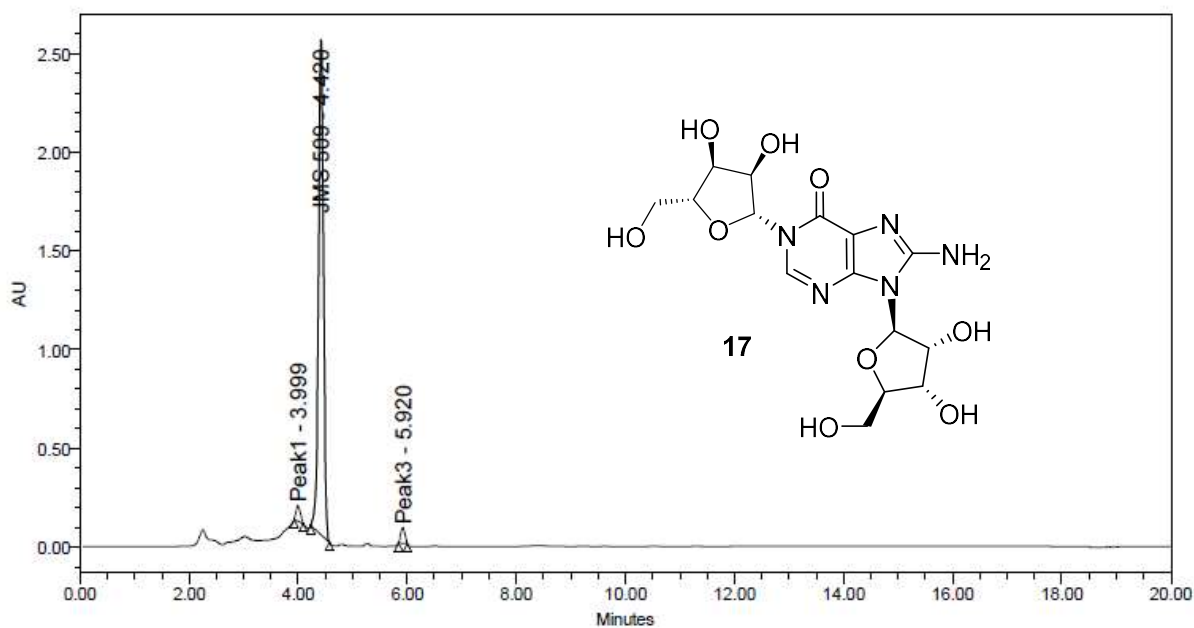
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0 dB
 PL12 15.78 dB
 PL13 19.00 dB
 PL2W 9.74611950 W
 PL12W 0.25753233 W
 PL13W 0.12269637 W
 SFO2 400.0416002 MHz

F2 - Processing parameters
 SI 65536
 SF 100.5899952 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

SAMPLE INFORMATION

Sample Name: JMS 509
 Sample Type: Unknown
 Vial: 31
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 20.0 Minutes
 Sample Set Name: JMS 509 510 519 533

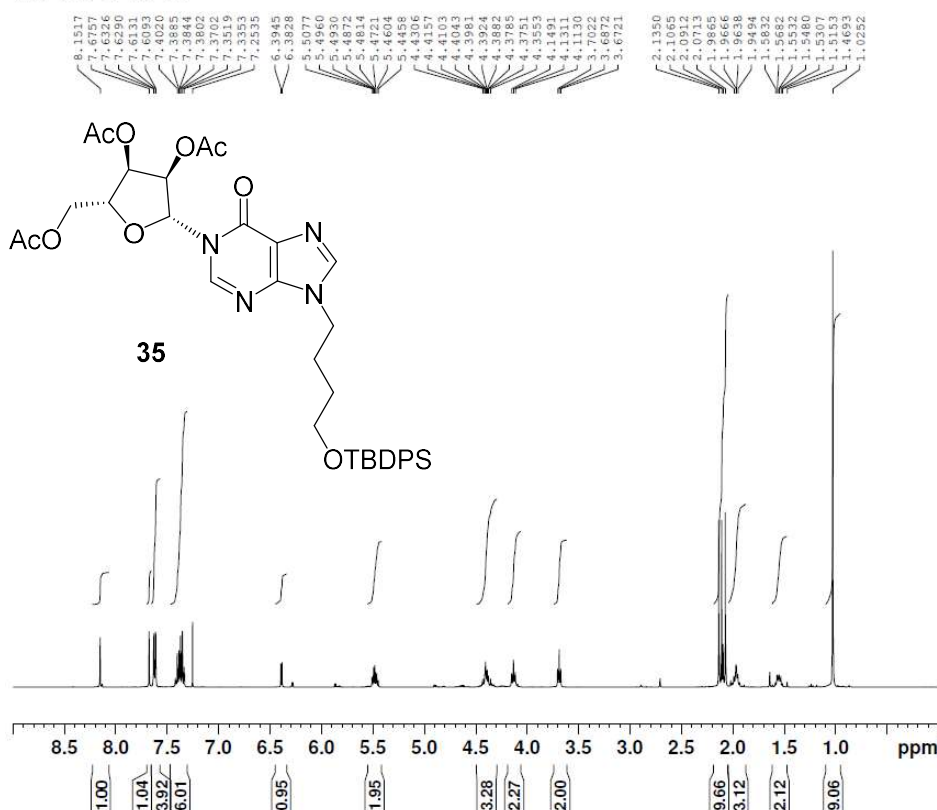
Acquired By: Joanna
 Date Acquired: 17/08/2011 3:48:55 PM
 Acq. Method Set: RP18 LC
 Date Processed: 18/08/2011 5:45:27 PM
 Processing Method: JMS 509
 Channel Name: WvInCh1
 Proc. Chnl. Descr.: PDA 262.1 nm



	Peak Name	RT	Area	% Area	Height
1	Peak1	3.999	428563	2.53	77203
2	JMS 509	4.420	16065701	95.02	2513493
3	Peak3	5.920	413227	2.44	80736

Total synthesis of N9-(4-hydroxybutyl)-N1-Inosine analogues (18-21)

JMS 523 T 10-12



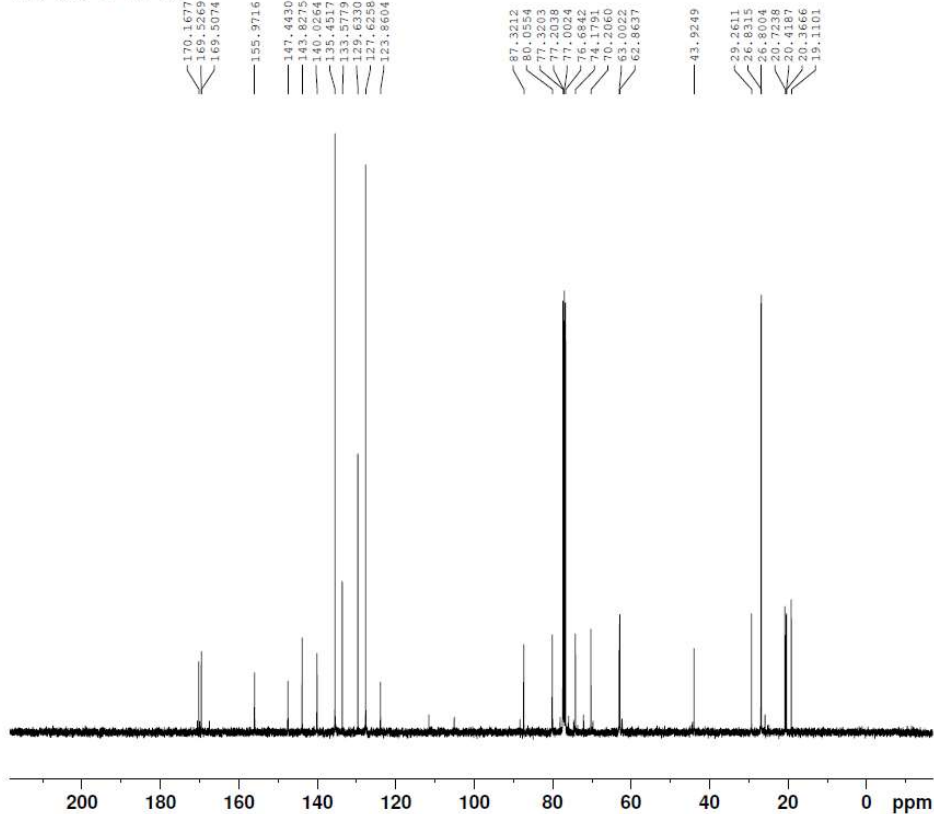
Current Data Parameters
NAME Aug08-2011-JMS11944
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110808
Time 17.04
INSTRUM AVI1400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 57
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 dB
PL1W 9.74611950 W
SFO1 400.0424704 MHz

F2 - Processing parameters
SI 65536
SF 400.0399837 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

JMS 523 T 10-12



Current Data Parameters
NAME Aug08-2011-JMS11944
EXPNO 14
PROCNO 1

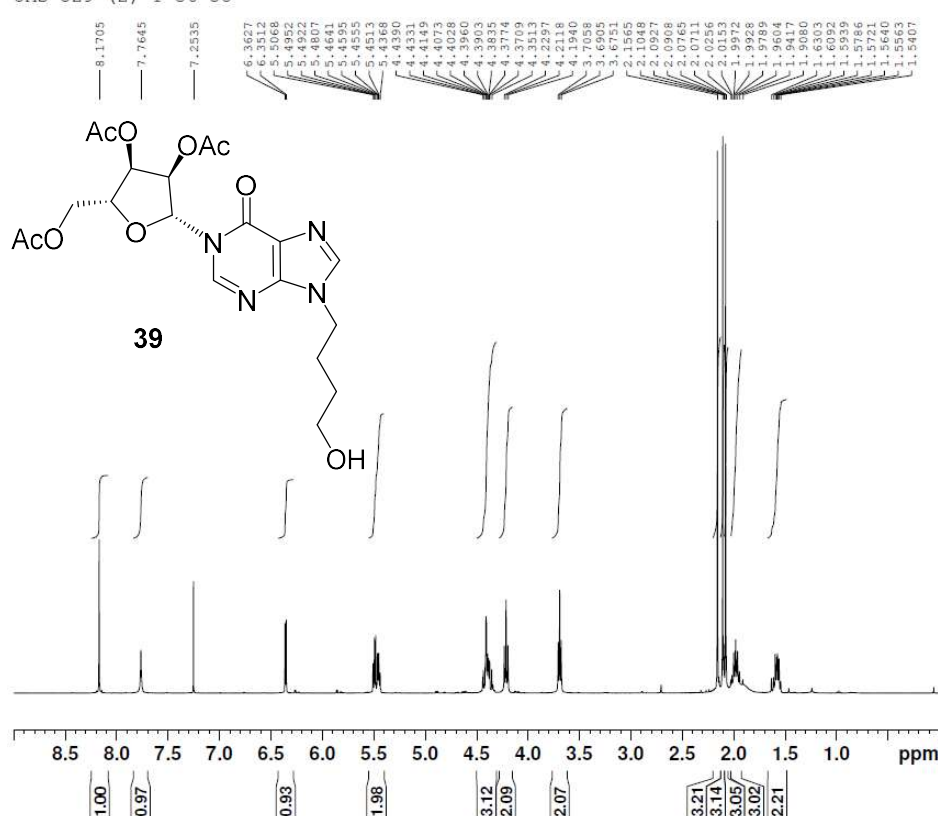
F2 - Acquisition Parameters
Date_ 20110809
Time 6.21
INSTRUM AVI1400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== 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 dB
PL12 15.78 dB
PL13 19.00 dB
PL2W 9.74611950 W
PL12W 0.25753233 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz

F2 - Processing parameters
SI 65536
SF 100.5901380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

JMS 529 (2) T 36-38



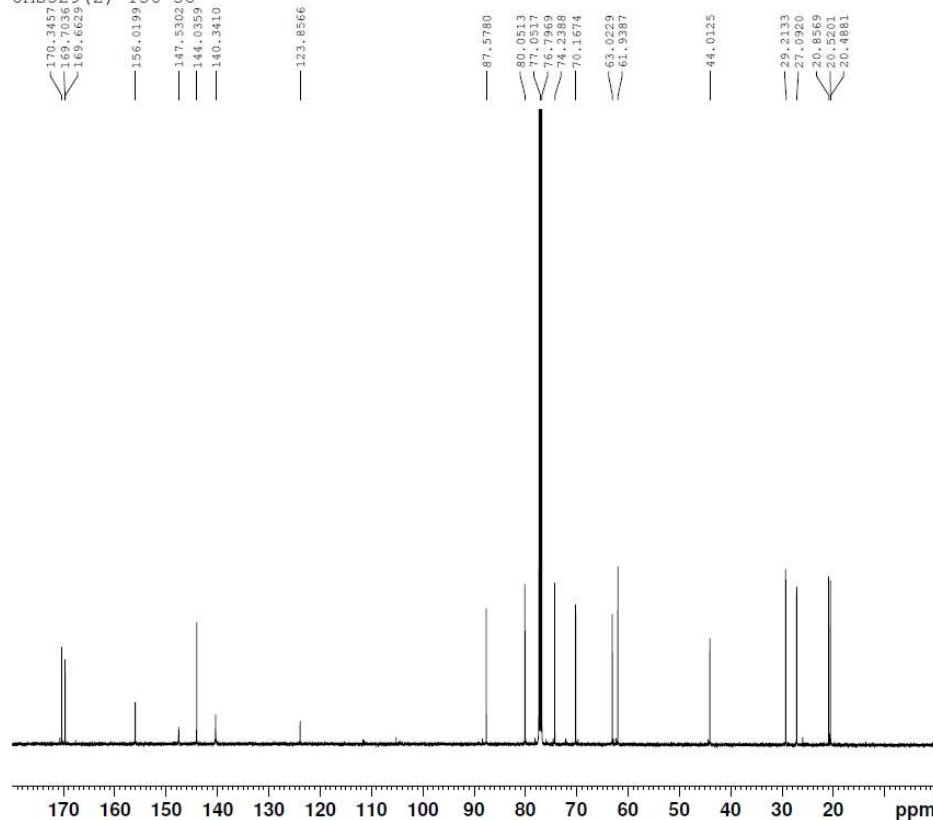
Current Data Parameters
 NAME Sep28-2011-JMS12570
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110928
 Time 18.29
 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 3.9845889 sec
 RG 161
 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 dB
 PL1W 9.74611950 W
 SFO1 400.0424704 MHz

F2 - Processing parameters
 SI 65536
 SF 400.0399837 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

JMS529 (2) T36-38



Current Data Parameters
 NAME JMS529-2 T36-38
 EXPNO 10
 PROCNO 1

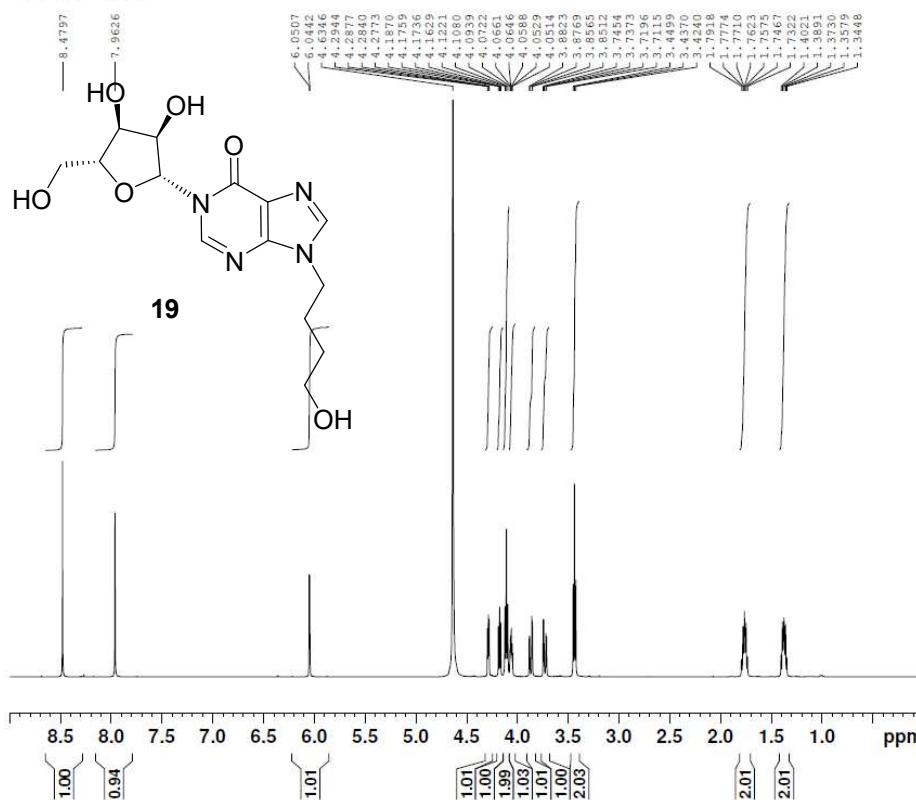
F2 - Acquisition Parameters
 Date_ 20110929
 Time 12.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 3850
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 2050
 DW 16.800 usec
 DE 8.43 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 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
 PL12W 19.35150909 W
 PL12W 0.30249262 W
 PL13W 0.14952536 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

JMS 545 HPLC



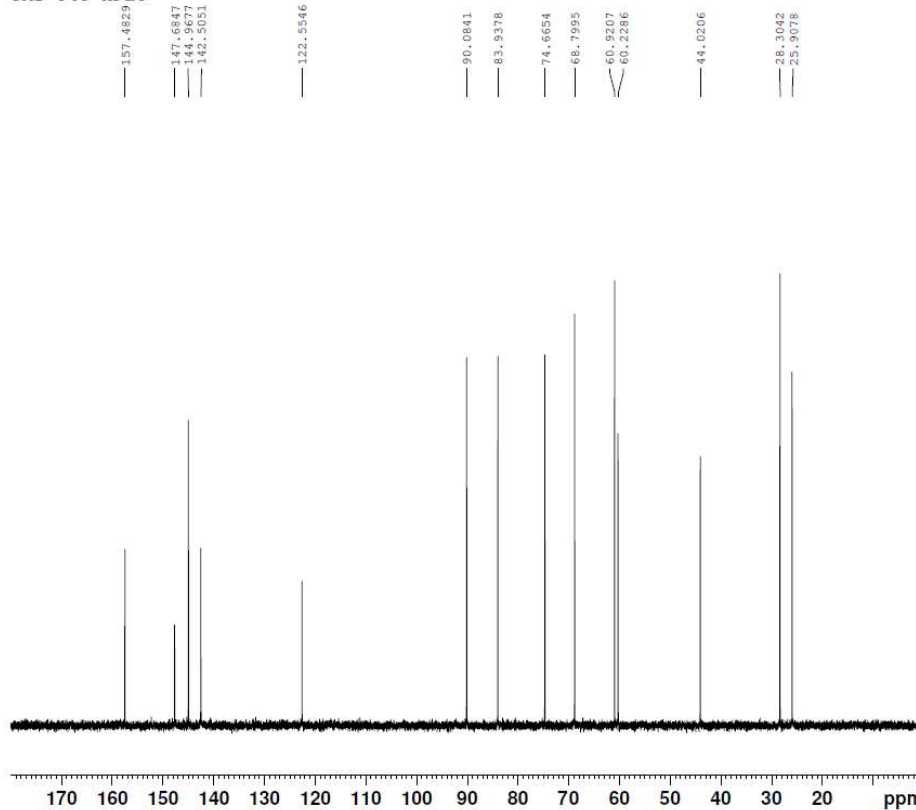
Current Data Parameters
 NAME Oct24-2011-JMS545HPLC
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111024
 Time 19.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 1600
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 128
 DW 48.400 usec
 DE 13.94 usec
 TE 297.9 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

F2 - Processing parameters
 SI 32768
 SF 500.1300345 MHz
 WDW EM
 SSB 0
 LB 0.3 Hz
 GB 0
 PC 1.00

JMS 545 HPLC



Current Data Parameters
 NAME Oct24-2011-JMS545HPLC
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111025
 Time 6.10
 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 1.1010048 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

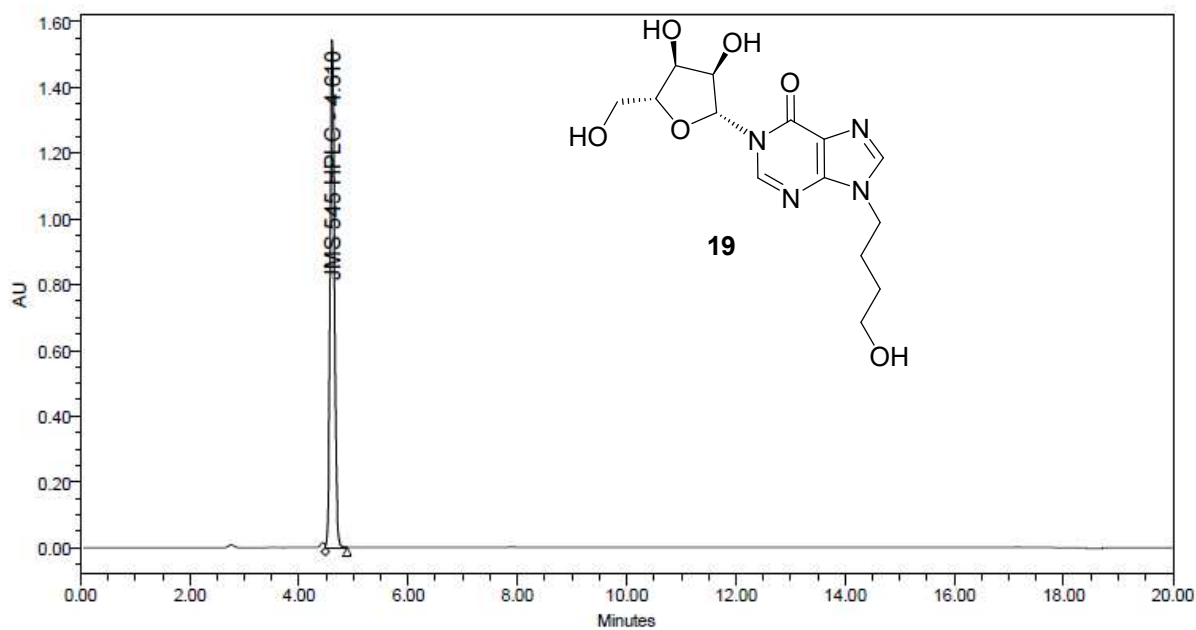
===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -0.12 dB
 PL12 17.94 dB
 PL13 21.00 dB
 PL2W 19.35150909 W
 PL12W 0.30249262 W
 PL13W 0.14952536 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

SAMPLE INFORMATION

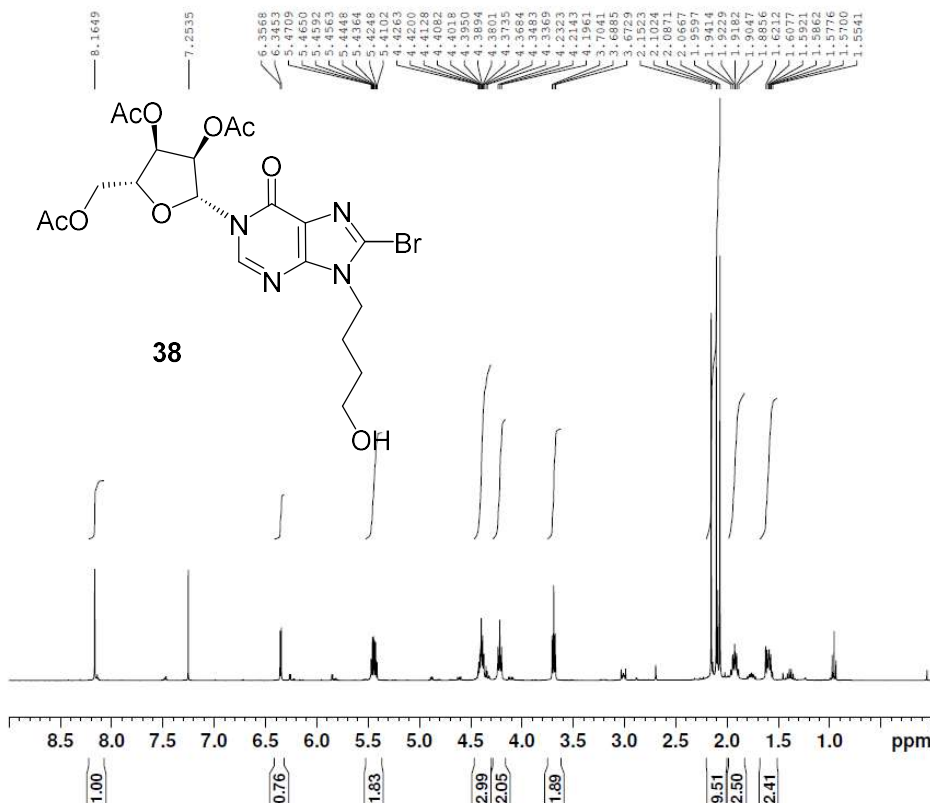
Sample Name: JMS 545 HPLC
 Sample Type: Unknown
 Vial: 3
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 20.0 Minutes
 Sample Set Name: JMS 510 533 545 HPLC

Acquired By: Christelle
 Date Acquired: 25/10/2011 4:45:44 PM
 Acq. Method Set: RP18 LC
 Date Processed: 28/10/2011 12:25:15 PM
 Processing Method: JMS 545 HPLC
 Channel Name: WvInCh1
 Proc. Chnl. Descr.: PDA 262.1 nm



	Peak Name	RT	Area	% Area	Height
1	JMS 545 HPLC	4.610	8540932	100.00	1541489

JMS 522 T 8-10



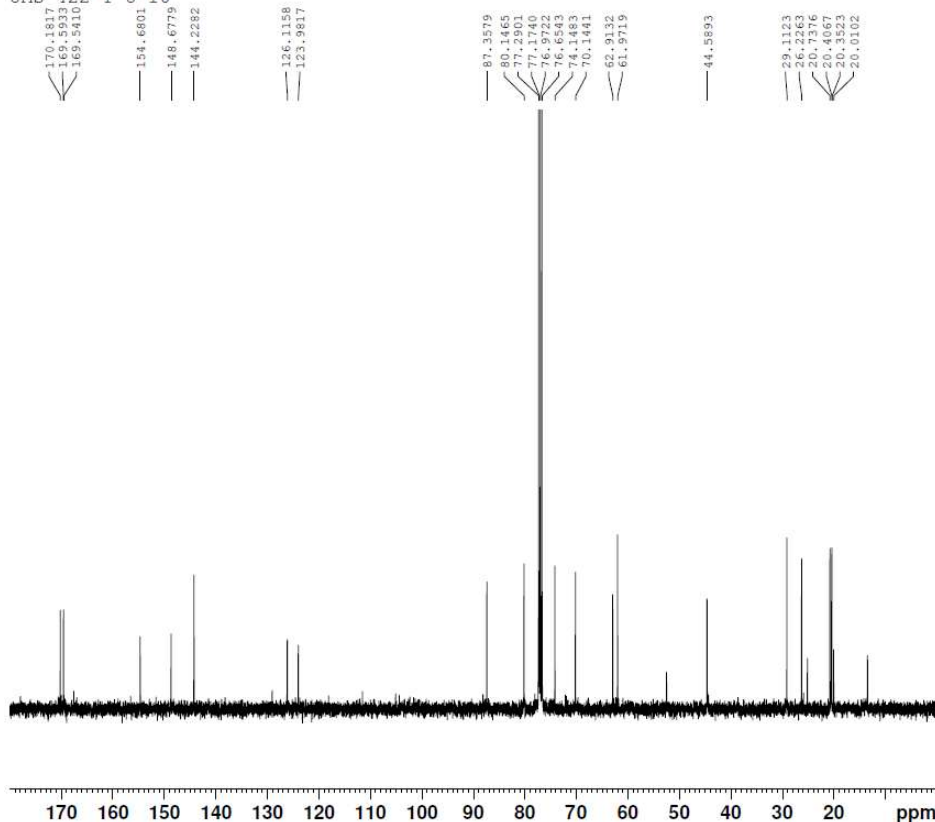
Current Data Parameters
 NAME Aug08-2011-JMS11949
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110809
 Time 7.03
 INSTRUM AVII400
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 128
 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 dB
 PL1W 9.74611950 W
 SFO1 400.0424704 MHz

F2 - Processing parameters
 SI 65536
 SF 400.0399837 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

JMS 422 T 8-10



Current Data Parameters
 NAME Aug08-2011-JMS11949
 EXPNO 14
 PROCNO 1

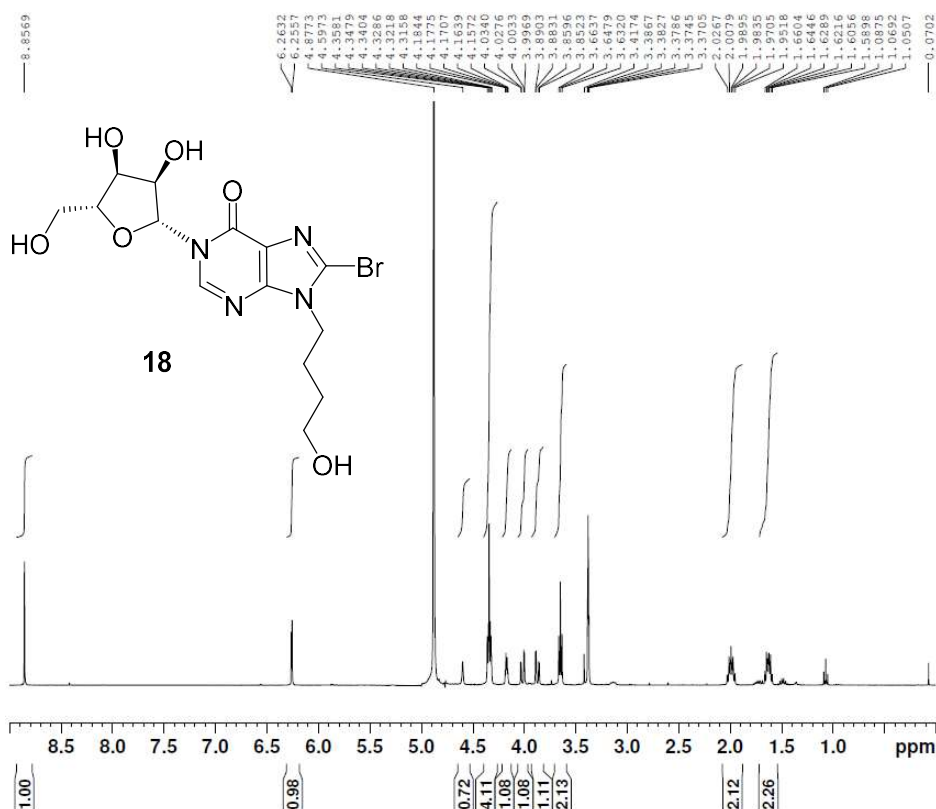
F2 - Acquisition Parameters
 Date_ 20110809
 Time 19.35
 INSTRUM AVII400
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 2050
 DW 20.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 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 dB
 PL12 15.78 dB
 PL13 19.00 dB
 PL2W 9.74611950 W
 PL12W 0.25753233 W
 PL13W 0.12269637 W
 SFO2 400.0416002 MHz

F2 - Processing parameters
 SI 65536
 SF 100.5901380 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

JMS 532 T 7-9



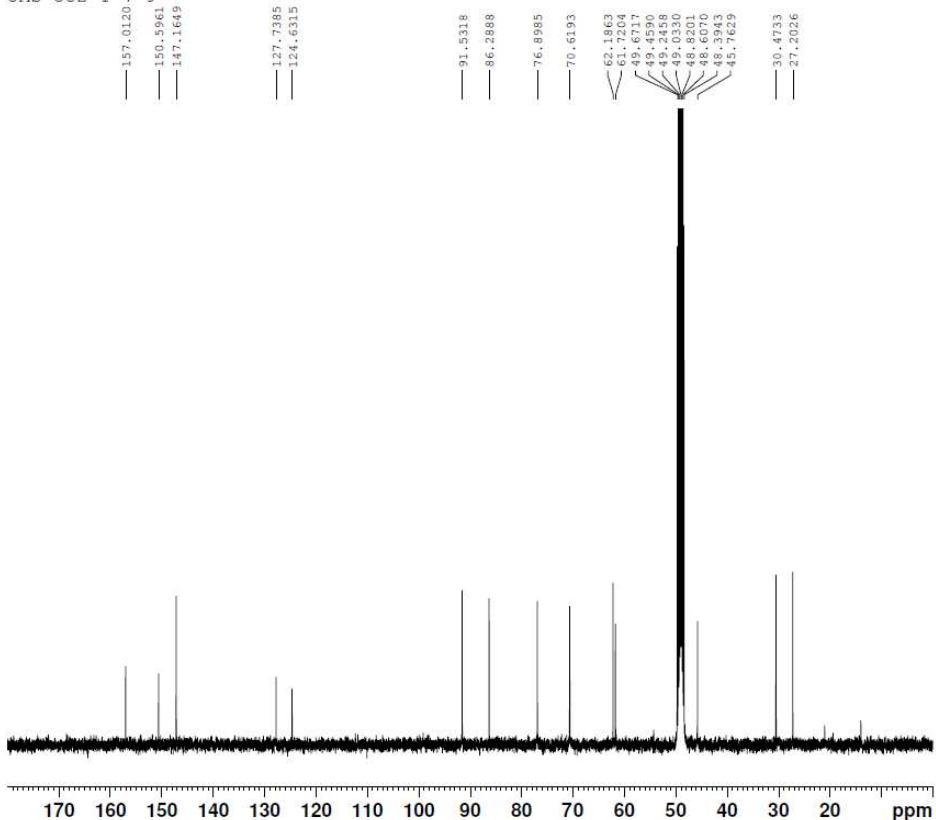
Current Data Parameters
 NAME Aug12-2011-JMS10255
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110812
 Time 16.55
 INSTRUM AVII1400
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 161
 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 dB
 PL1W 9.74611950 W
 SFO1 400.0424704 MHz

F2 - Processing parameters
 SI 65536
 SF 400.0399837 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

JMS 532 T 7-9



Current Data Parameters
 NAME Aug12-2011-JMS10255
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110813
 Time 2.24
 INSTRUM AVII1400
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 2048
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 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 58.91986084 W
 SFO1 100.6001970 MHz

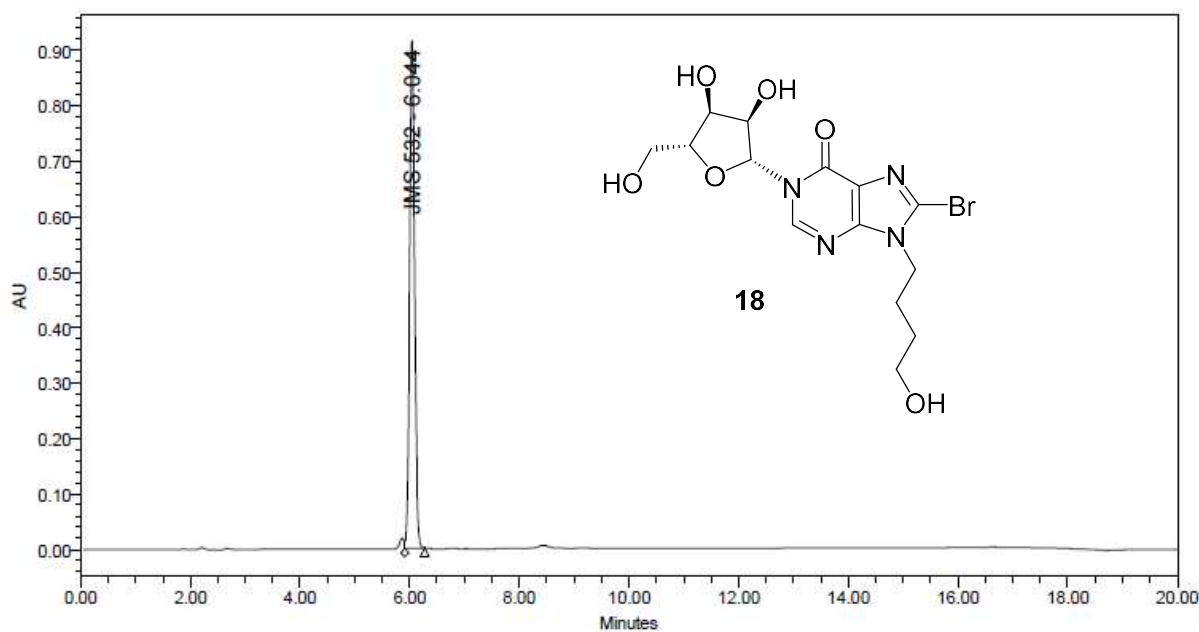
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0 dB
 PL12 15.78 dB
 PL13 19.00 dB
 PL1W 9.74611950 W
 PL12W 0.25753233 W
 PL13W 0.12269637 W
 SFO2 400.0416002 MHz

F2 - Processing parameters
 SI 65536
 SF 100.5899952 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

SAMPLE INFORMATION

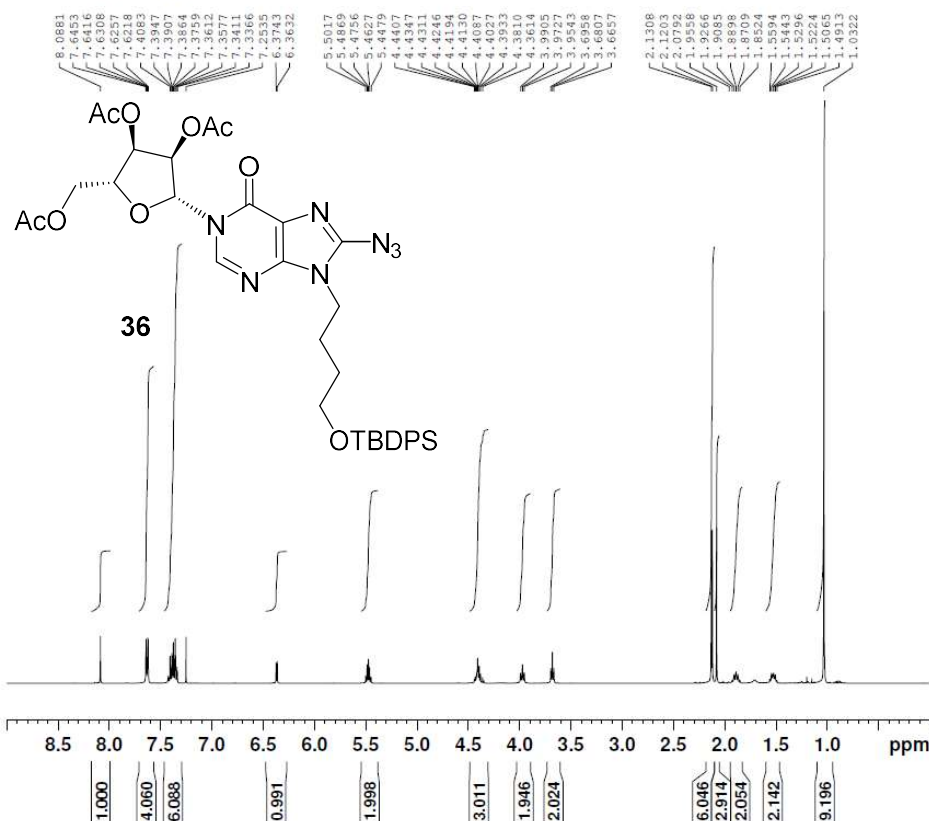
Sample Name: JMS 532
 Sample Type: Unknown
 Vial: 34
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 20.0 Minutes
 Sample Set Name: JMS 509 510 519 532 533

Acquired By: Joanna
 Date Acquired: 18/08/2011 1:33:24 PM
 Acq. Method Set: RP18 LC
 Date Processed: 18/08/2011 5:00:47 PM
 Processing Method: JMS 532
 Channel Name: WvlnCh1
 Proc. Chnl. Descr.: PDA 262.1 nm



	Peak Name	RT	Area	% Area	Height
1	JMS 532	6.044	5950121	100.00	917702

JMS 496 T 13-14



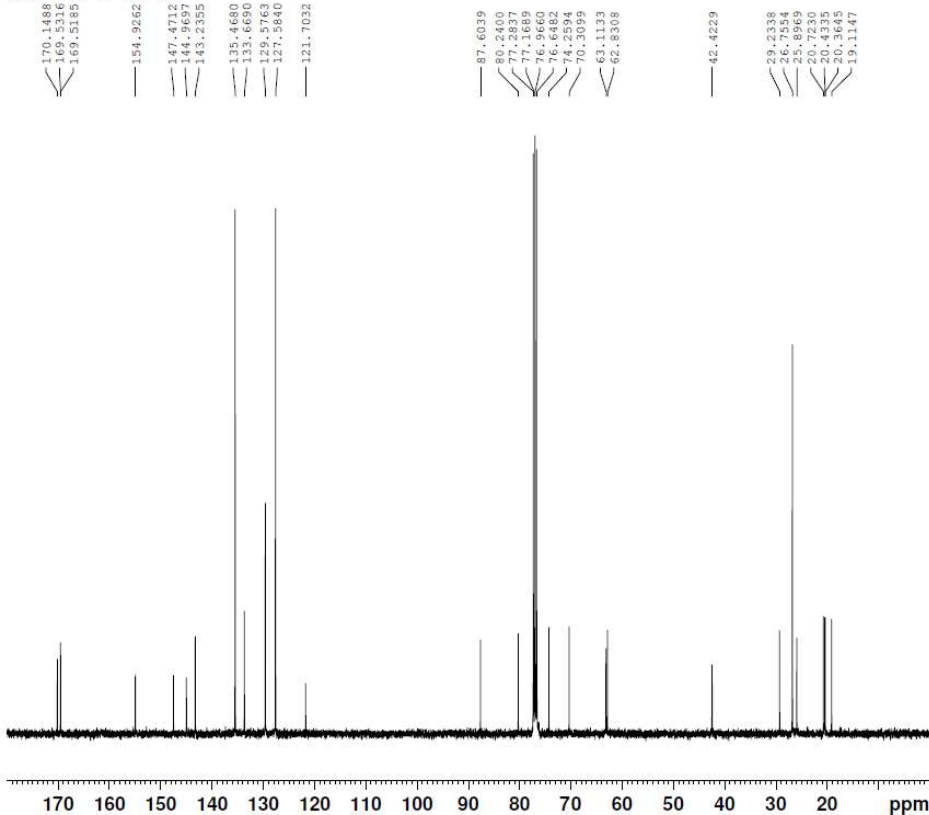
Current Data Parameters
 NAME Aug03-2011-JMS11846
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110803
 Time 15.08
 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 3.9845889 sec
 RG 101
 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 dB
 PL1W 9.74611950 W
 SFO1 400.0424704 MHz

F2 - Processing parameters
 SI 65536
 SF 400.0399837 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

JMS 496 T 13-14



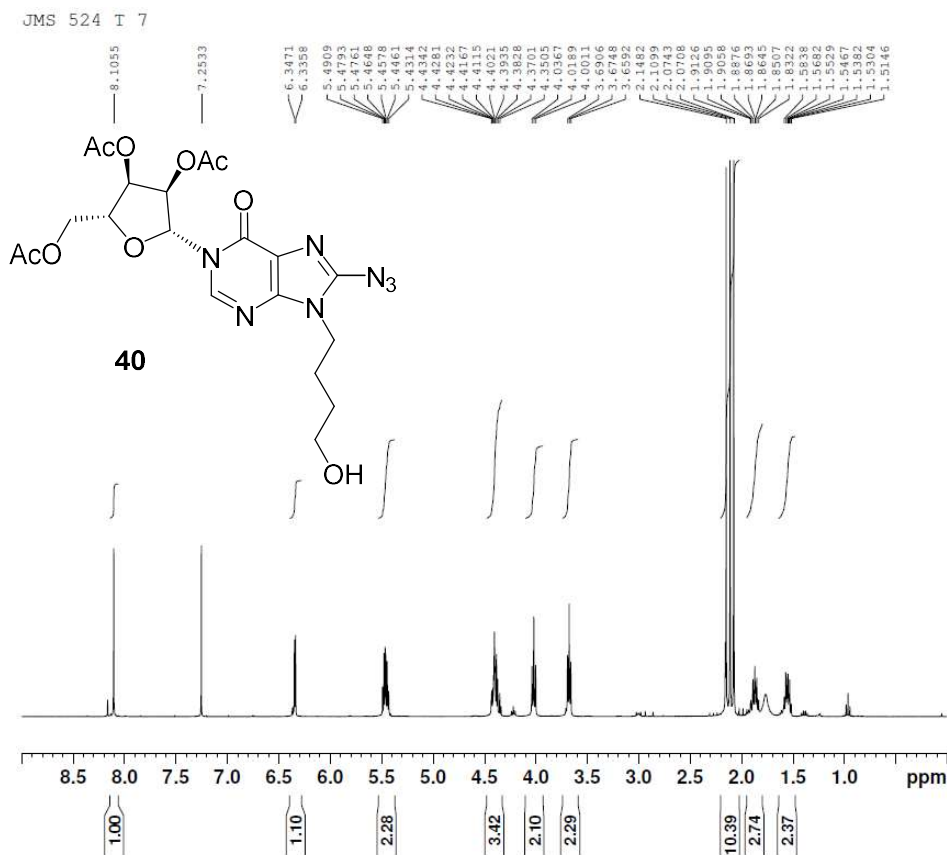
Current Data Parameters
 NAME Aug03-2011-JMS11846
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110803
 Time 22.35
 INSTRUM AVIII400
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 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 dB
 PL12 15.78 dB
 PL13 19.00 dB
 PL2W 9.74611950 W
 PL12W 0.25753233 W
 PL13W 0.12269637 W
 SFO2 400.0416002 MHz

F2 - Processing parameters
 SI 65536
 SF 100.5901380 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

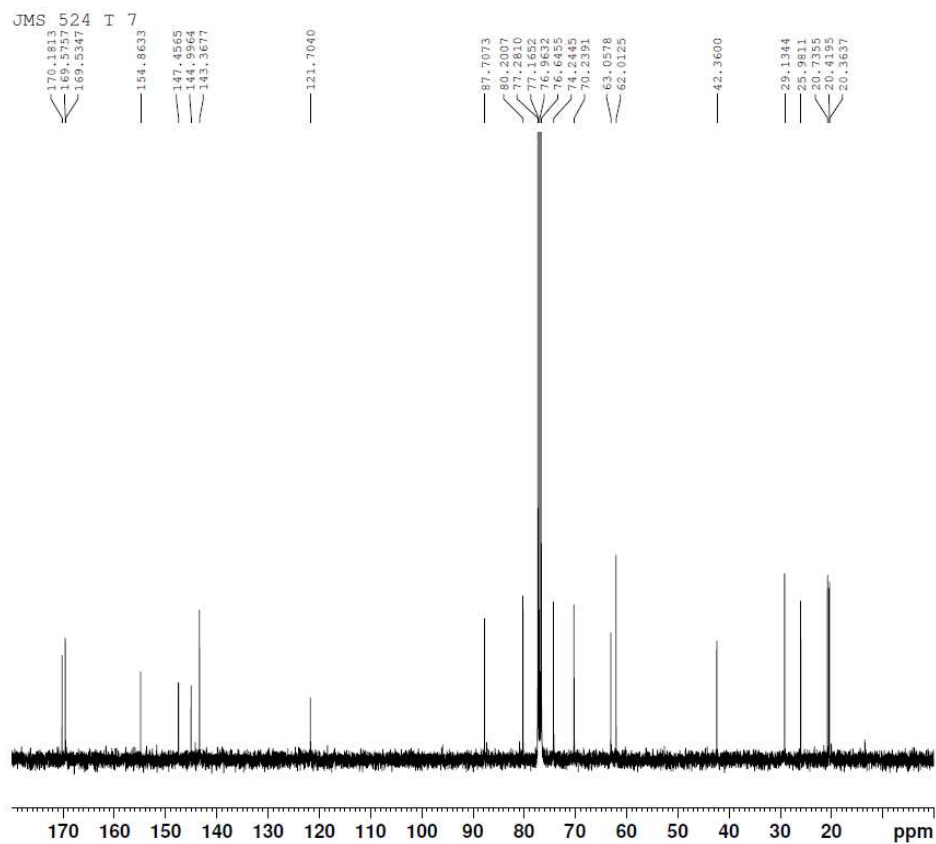


Current Data Parameters
NAME Aug08-2011-JMS11950
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110809
Time 7.46
INSTRUM AVII1400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 161
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 dB
PL1W 9.74611950 W
SFO1 400.0424704 MHz

F2 - Processing parameters
SI 65536
SF 400.0399837 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00



Current Data Parameters
NAME Aug08-2011-JMS11950
EXPNO 14
PROCNO 1

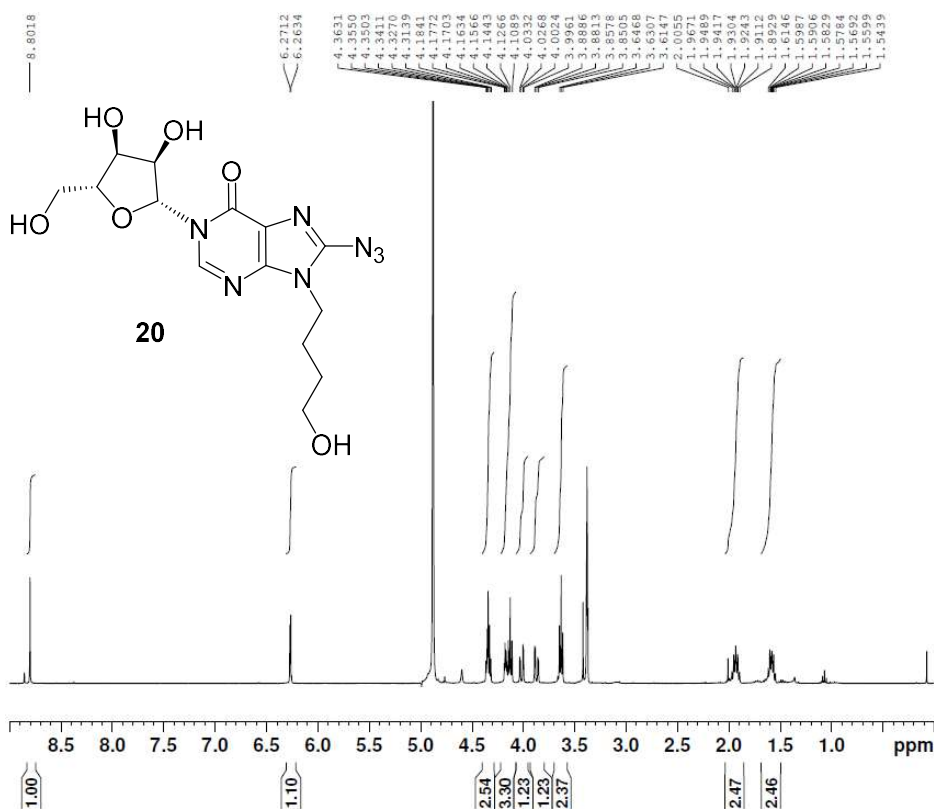
F2 - Acquisition Parameters
Date_ 20110809
Time 20.44
INSTRUM AVII1400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.75 usec
PL1 -2.00 dB
PL1W 58.91986084 W
SFO1 100.6001970 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.78 dB
PL13 19.00 dB
PL2W 9.74611950 W
PL12W 0.25753233 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz

F2 - Processing parameters
SI 65536
SF 100.5901380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

JMS 533 T 6-8



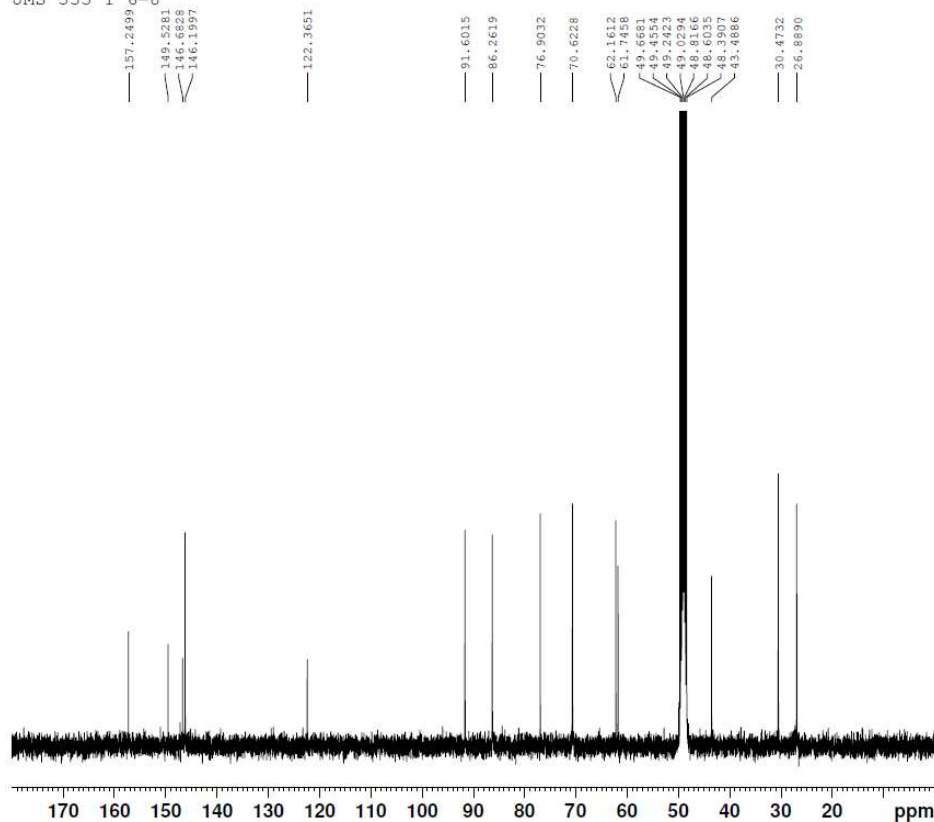
Current Data Parameters
 NAME Aug12-2011-JMS10256
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110812
 Time 17.06
 INSTRUM AVII400
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 181
 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 dB
 PL1W 9.74611950 W
 SFO1 400.0424704 MHz

F2 - Processing parameters
 SI 65536
 SF 400.0399837 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

JMS 533 T 6-8



Current Data Parameters
 NAME Aug12-2011-JMS10256
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110813
 Time 5.33
 INSTRUM AVII400
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 2048
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 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

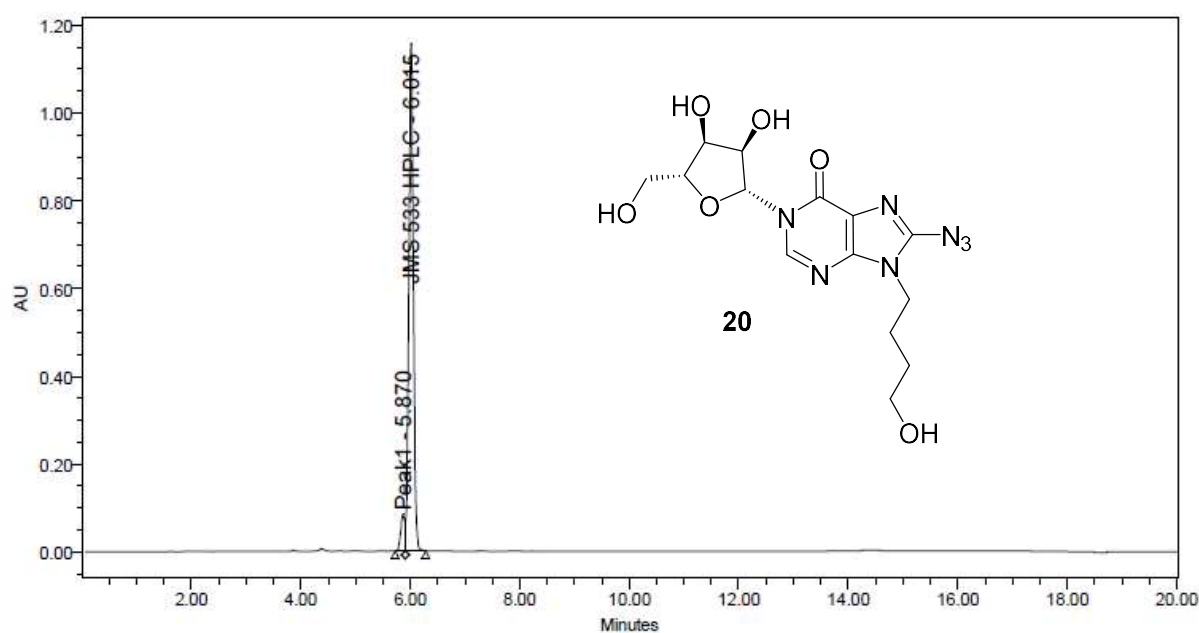
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0 dB
 PL12 15.78 dB
 PL13 19.00 dB
 PL2W 9.74611950 W
 PL12W 0.25753233 W
 PL13W 0.12269637 W
 SFO2 400.0416002 MHz

F2 - Processing parameters
 SI 65536
 SF 100.5899952 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

SAMPLE INFORMATION

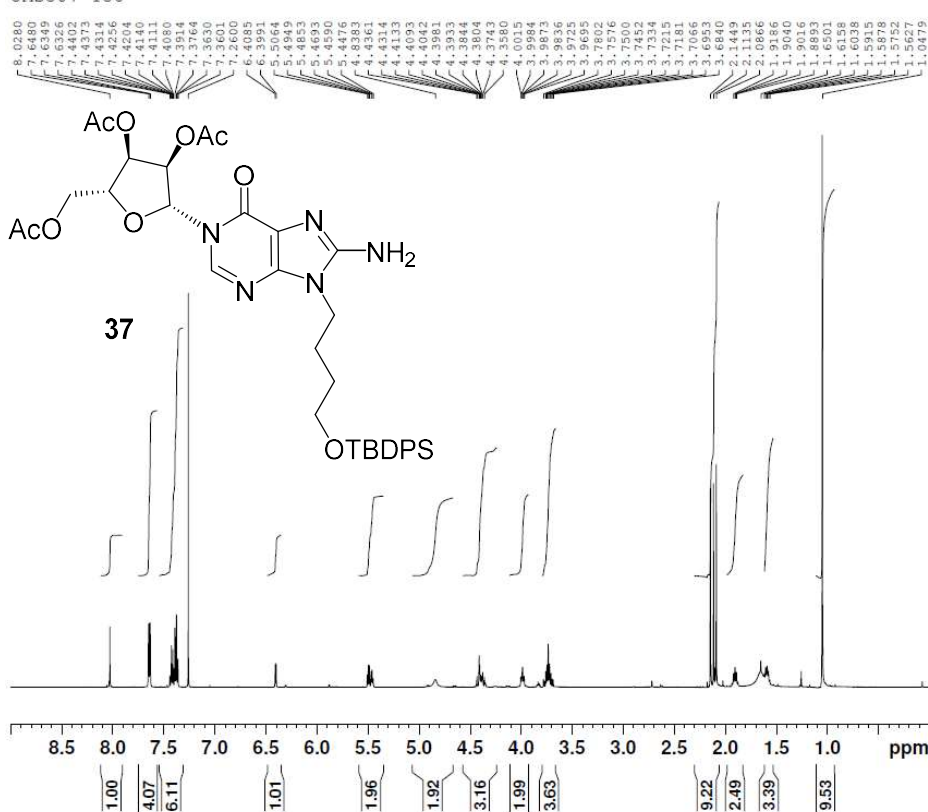
Sample Name: JMS 533 HPLC
 Sample Type: Unknown
 Vial: 2
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 20.0 Minutes
 Sample Set Name: JMS 510 533 545 HPLC

Acquired By: Christelle
 Date Acquired: 25/10/2011 4:24:49 PM
 Acq. Method Set: RP18 LC
 Date Processed: 28/10/2011 12:23:30 PM
 Processing Method: JMS 533 HPLC
 Channel Name: WvlnCh1
 Proc. Chnl. Descr.: PDA 262.1 nm



	Peak Name	RT	Area	% Area	Height
1	Peak1	5.870	424215	5.84	83250
2	JMS 533 HPLC	6.015	6835625	94.16	1157681

JMS507 T30

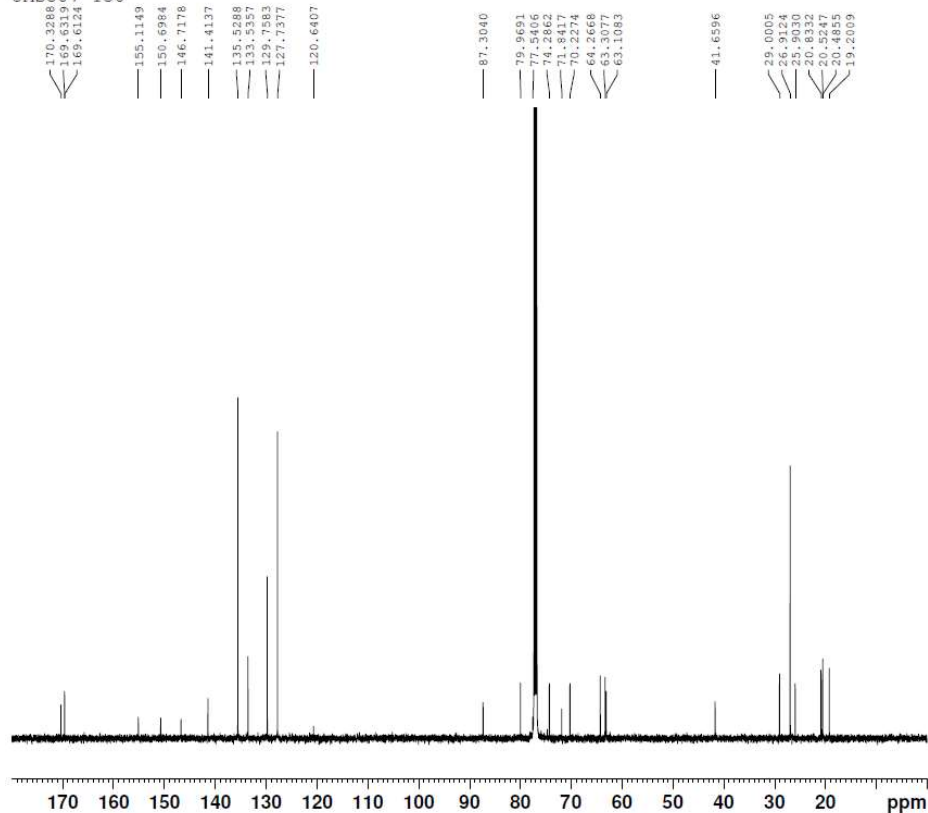


Current Data Parameters
 NAME JMS507 T30
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110802
 Time 19.47
 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 3.1719425 sec
 RG 256
 DW 48.400 usec
 DE 13.94 usec
 TE 297.9 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
 F2 - Processing parameters
 SI 32768
 SF 500.1300132 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

JMS507 T30



Current Data Parameters
 NAME JMS507 T30
 EXPNO 11
 PROCNO 1

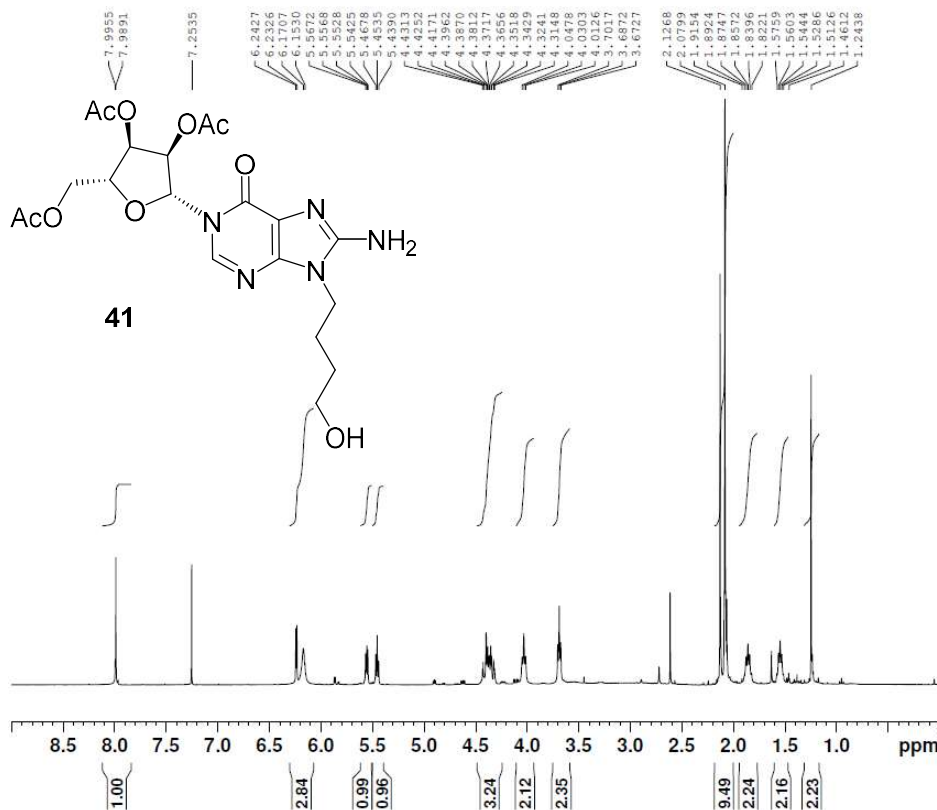
F2 - Acquisition Parameters
 Date_ 20110803
 Time 4.50
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10240
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 2050
 DW 16.800 usec
 DE 8.43 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 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
 P2 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

F2 - Processing parameters
 SI 32768
 SF 125.7577905 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

JMS 514 T 10-18



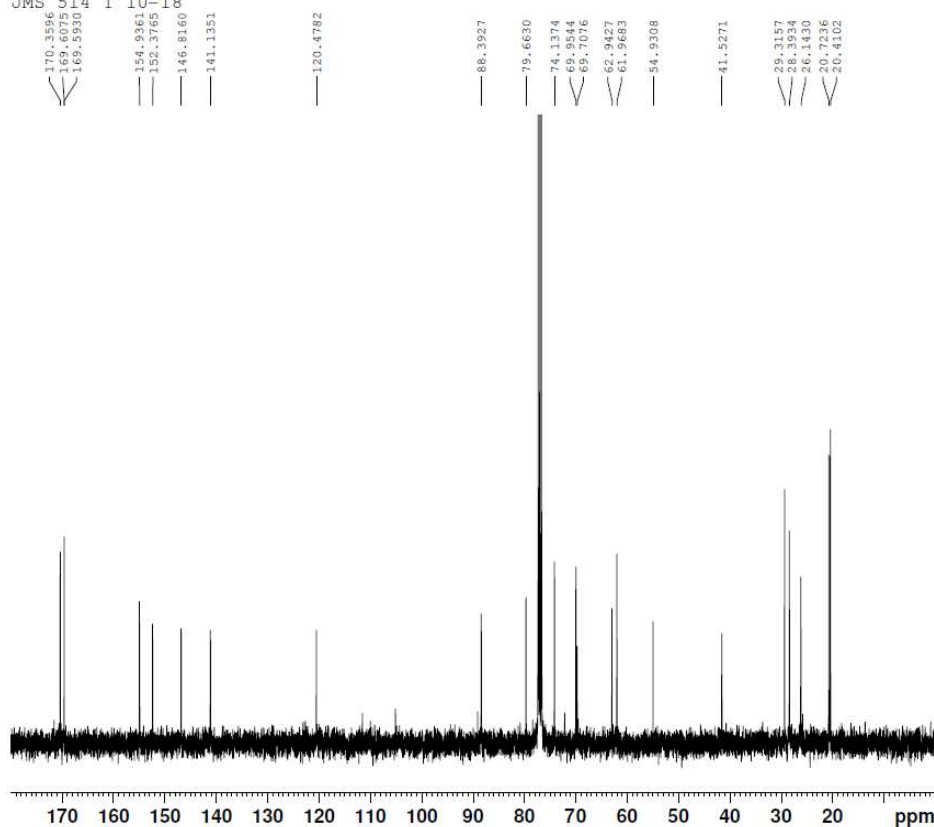
Current Data Parameters
NAME Aug02-2011-JMS11809
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110802
Time 17.38
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 3.9845889 sec
RG 101
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 dB
PL1W 9.74611950 W
SFO1 400.0424704 MHz

F2 - Processing parameters
SI 65536
SF 400.0399837 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

JMS 514 T 10-18



Current Data Parameters
NAME Aug02-2011-JMS11809
EXPNO 14
PROCNO 1

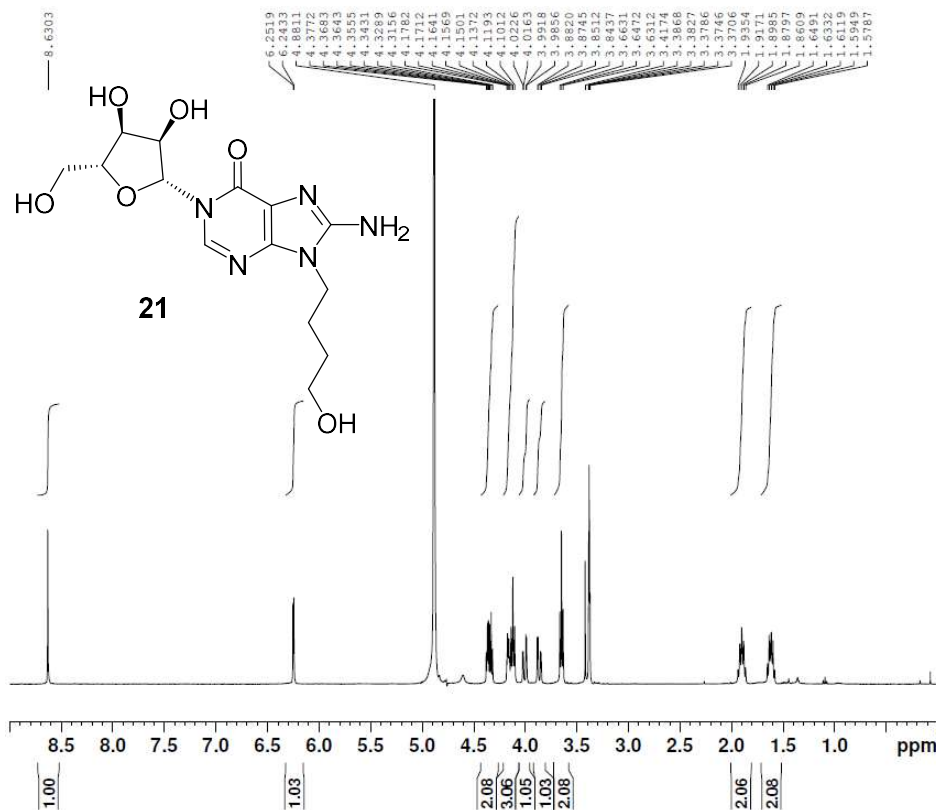
F2 - Acquisition Parameters
Date_ 20110803
Time 7.45
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== 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 dB
PL12 15.78 dB
PL13 19.00 dB
PL2W 9.74611950 W
PL12W 0.25753233 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz

F2 - Processing parameters
SI 65536
SF 100.5901380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

JMS 519 T 10-11



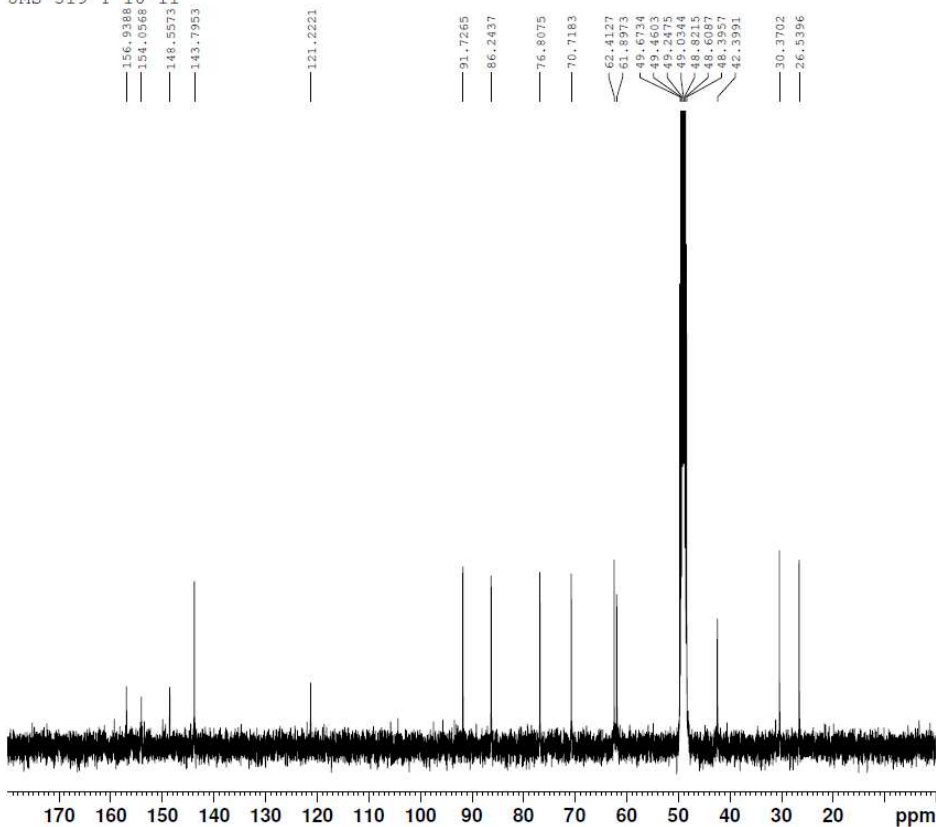
Current Data Parameters
 NAME Aug08-2011-JMS11948
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110809
 Time 8.02
 INSTRUM AVIII400
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 144
 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 dB
 PL1W 9.74611950 W
 SFO1 400.0424704 MHz

F2 - Processing parameters
 SI 65536
 SF 400.0399837 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

JMS 519 T 10-11



Current Data Parameters
 NAME Aug08-2011-JMS11948
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110809
 Time 22.22
 INSTRUM AVIII400
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 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 58.91986084 W
 SFO1 100.6001970 MHz

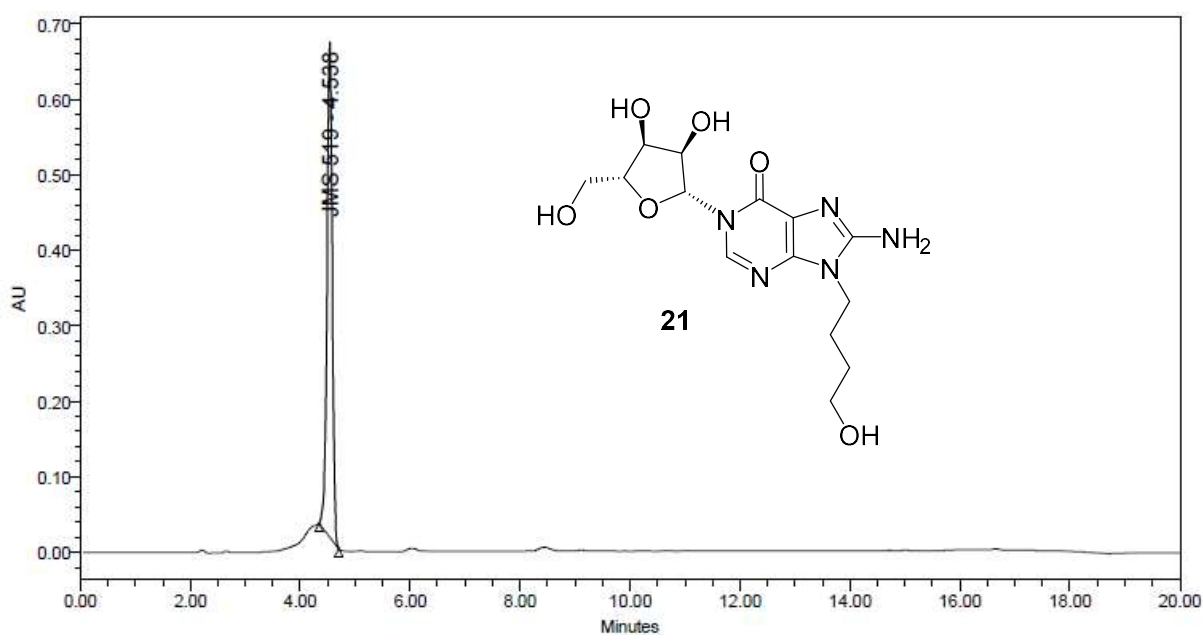
===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0 dB
 PL12 15.78 dB
 PL13 19.00 dB
 PL2W 9.74611950 W
 PL12W 0.25753233 W
 PL13W 0.12269637 W
 SFO2 400.0416002 MHz

F2 - Processing parameters
 SI 65536
 SF 100.5899952 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

SAMPLE INFORMATION

Sample Name: JMS 519
 Sample Type: Unknown
 Vial: 33
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 20.0 Minutes
 Sample Set Name: JMS 509 510 519 532 533

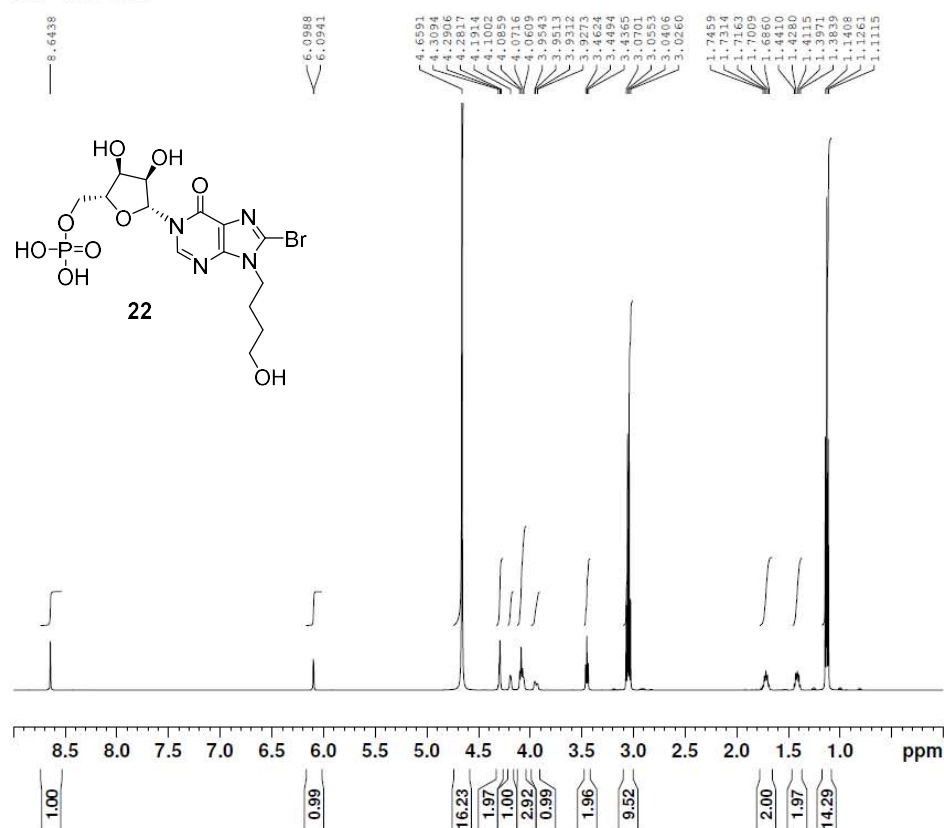
Acquired By: Joanna
 Date Acquired: 18/08/2011 1:12:30 PM
 Acq. Method Set: RP18 LC
 Date Processed: 18/08/2011 4:35:57 PM
 Processing Method: JMS 519
 Channel Name: WvlnCh1
 Proc. Chnl. Descr.: PDA 262.1 nm



	Peak Name	RT	Area	% Area	Height
1	JMS 519	4.538	4357041	100.00	656981

Total synthesis of *N*9-(4-hydroxybutyl)-*N*1-IMP analogues (22-25)

JMS 728 HPLC



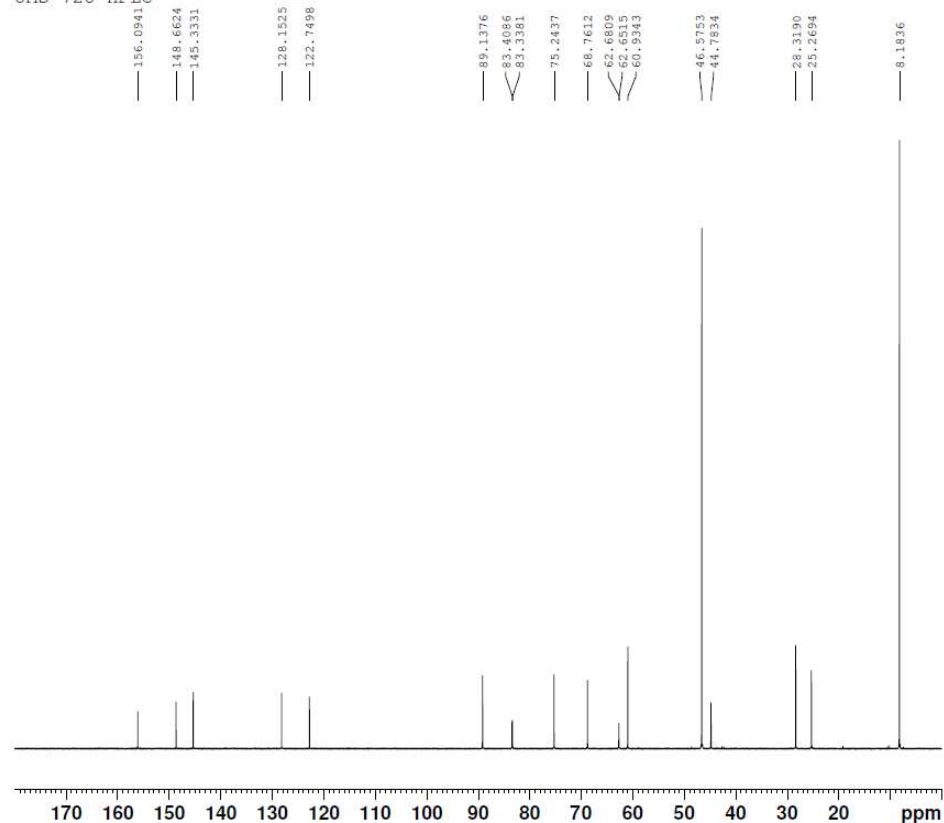
Current Data Parameters
NAME Aug14-2012-JMS728
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120814
Time 22.58
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 3.1719425 sec
RG 32
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

F2 - Processing parameters
SI 32768
SF 500.1300222 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

JMS 728 HPLC



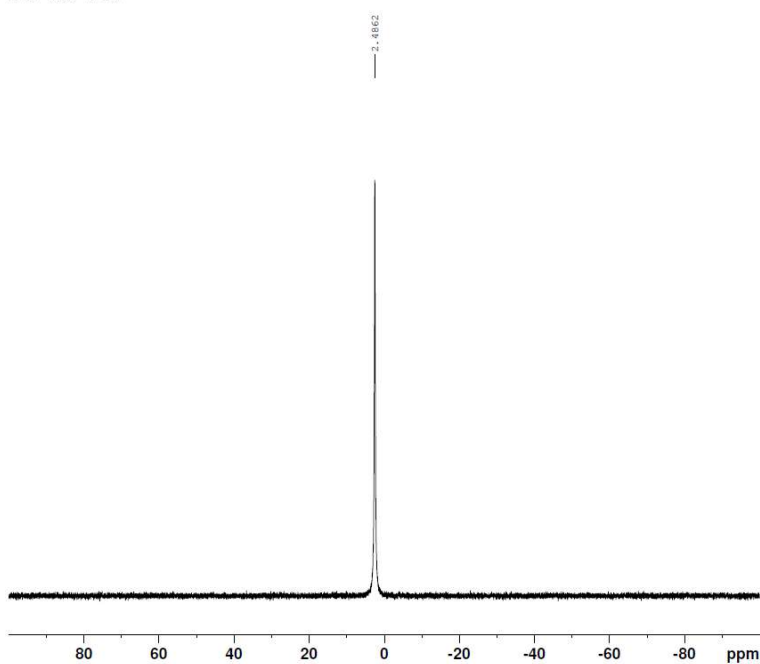
Current Data Parameters
NAME Aug14-2012-JMS728
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120815
Time 3.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 5000
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 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 =====
CPDPRG[2] 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

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME Aug14-2012-JMS728
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120815
Time 4.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 256
DS 4
SWH 81521.742 Hz
FIDRES 1.243923 Hz
AQ 0.4019541 sec
RG 2050
DW 6.133 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 12.00 usec
PL1 -0.46 dB
PL1W 90.28126526 W
SFO1 202.4462121 MHz

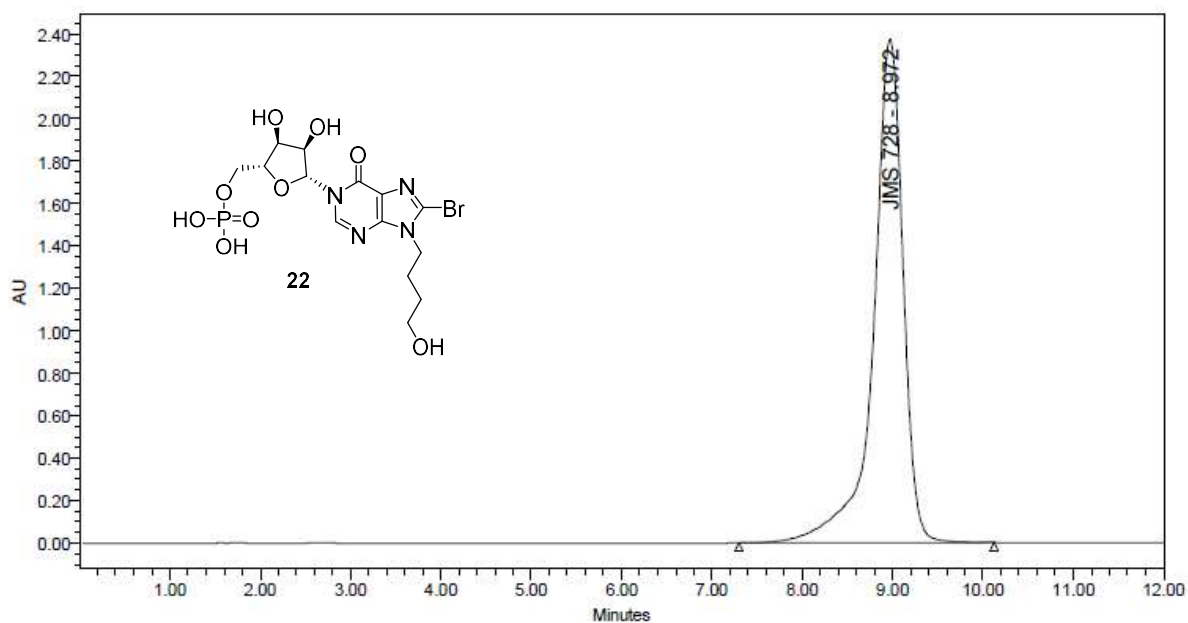
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.12 dB
PL12 17.94 dB
PL13 21.00 dB
PL2W 19.35150909 W
PL12W 0.30249262 W
PL13W 0.14952536 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 202.4563350 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

SAMPLE INFORMATION

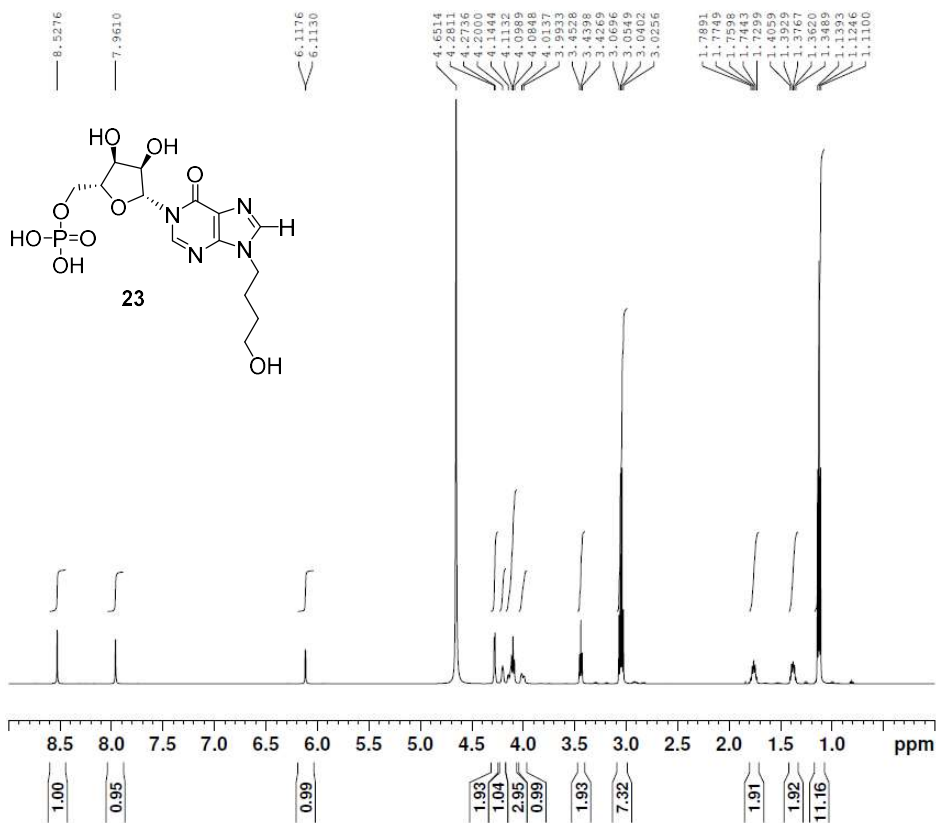
Sample Name: JMS 728 B4
Sample Type: Unknown
Vial: 4
Injection #: 1
Injection Volume: 10.00 ul
Run Time: 12.0 Minutes
Sample Set Name: JMS 728 HPLC B

Acquired By: Joanna
Date Acquired: 02/08/2012 2:03:42 PM
Acq. Method Set: isocratic new PDA Jo
Date Processed: 11/09/2012 10:40:43 AM
Processing Method: JMS 728
Channel Name: WvIn Ch1
Proc. Chnl. Descr.: PDA 254.0 nm



	Peak Name	RT	Area	% Area	Height
1	JMS 728	8.972	54319768	100.00	2372340

JMS 729 HPLC



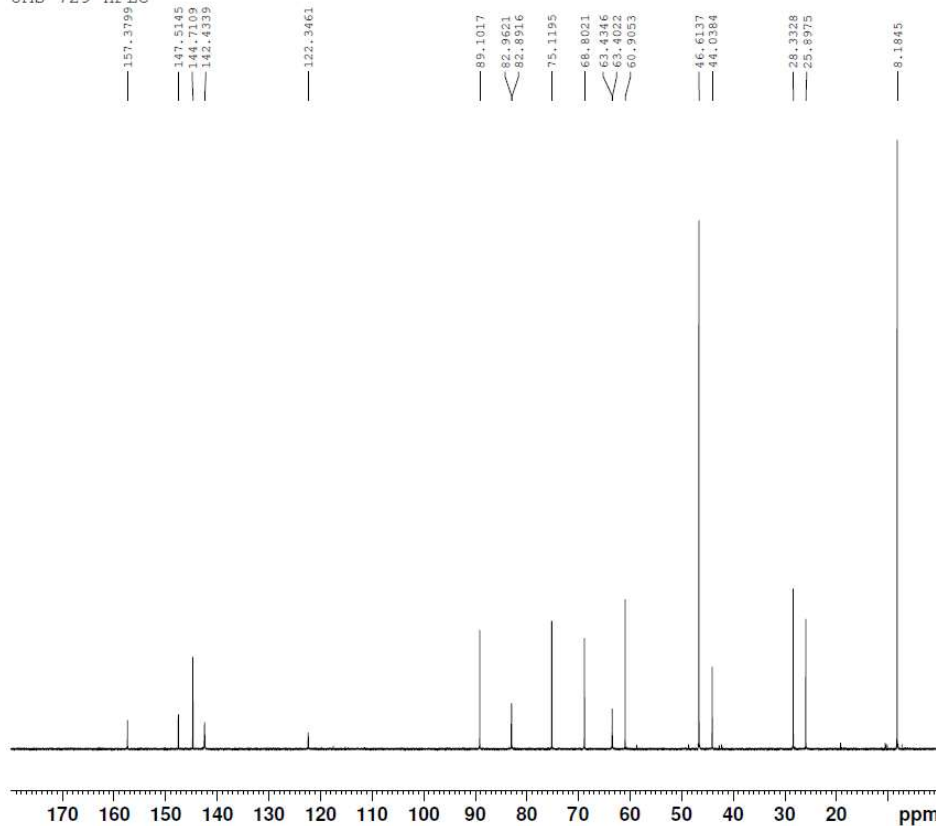
Current Data Parameters
 NAME Aug14-2012-JMS729
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120814
 Time 16.30
 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 3.1719425 sec
 RG 50.8
 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

F2 - Processing parameters
 SI 32768
 SF 500.1300262 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

JMS 729 HPLC



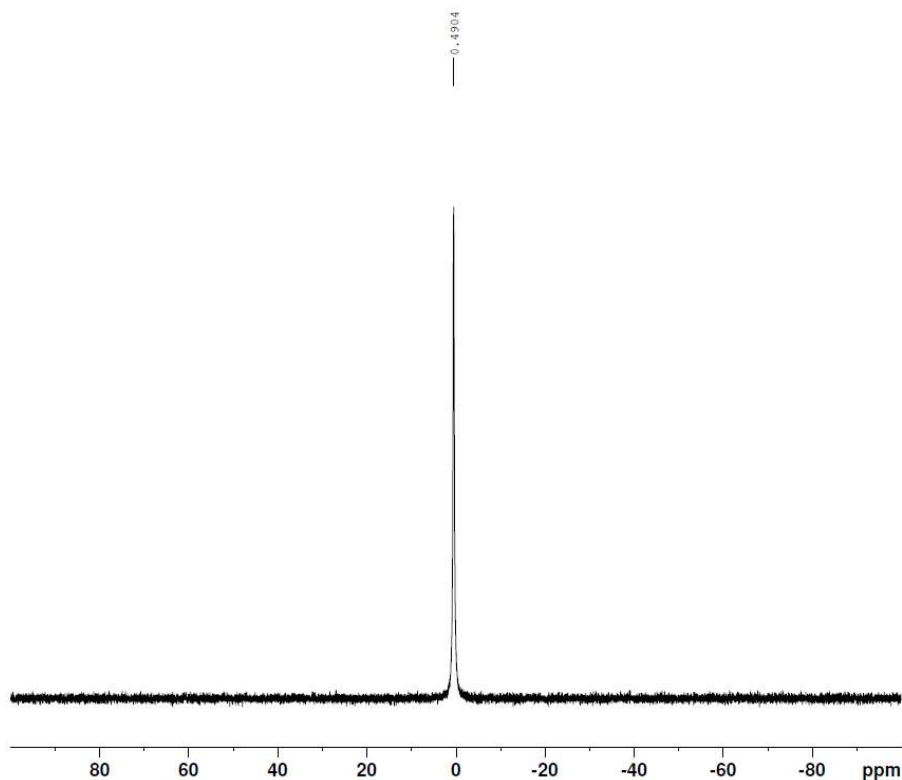
Current Data Parameters
 NAME Aug14-2012-JMS729
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120814
 Time 18.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 5000
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 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

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME Aug14-2012-JMS729
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120814
 Time 21.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 256
 DS 4
 SWH 81521.742 Hz
 FIDRES 1.243923 Hz
 AQ 0.4019541 sec
 RG 2050
 DW 6.133 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 31P
 P1 12.00 usec
 PL1 -0.46 dB
 PL1W 90.28126526 W
 SFO1 202.4462121 MHz

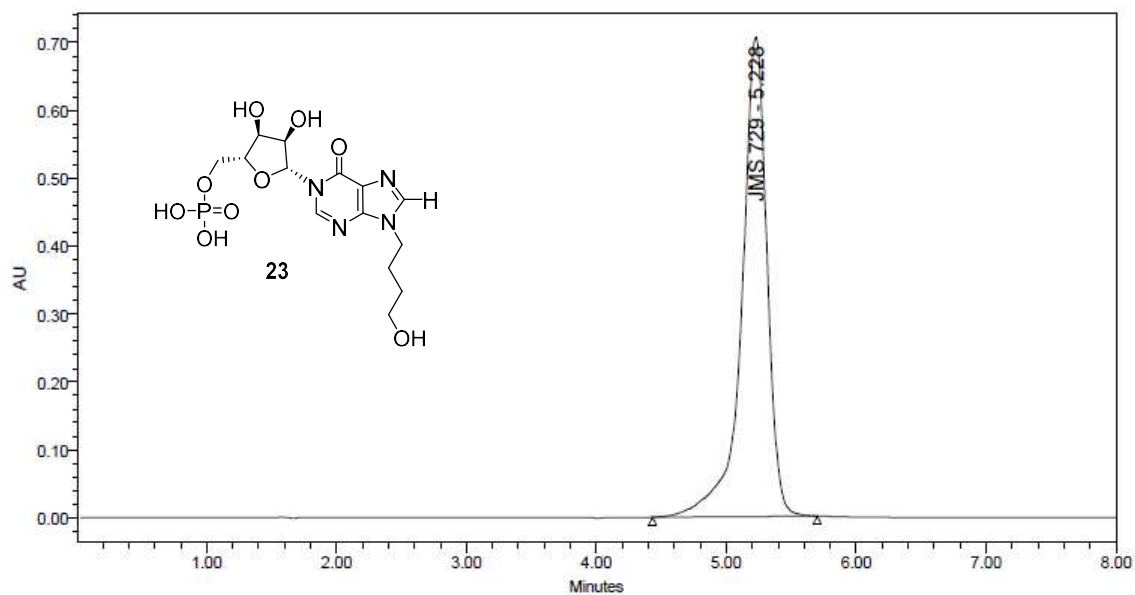
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -0.12 dB
 PL12 17.94 dB
 PL13 21.00 dB
 PL2W 19.35150909 W
 PL12W 0.30249262 W
 PL13W 0.14952536 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 202.4563350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

SAMPLE INFORMATION

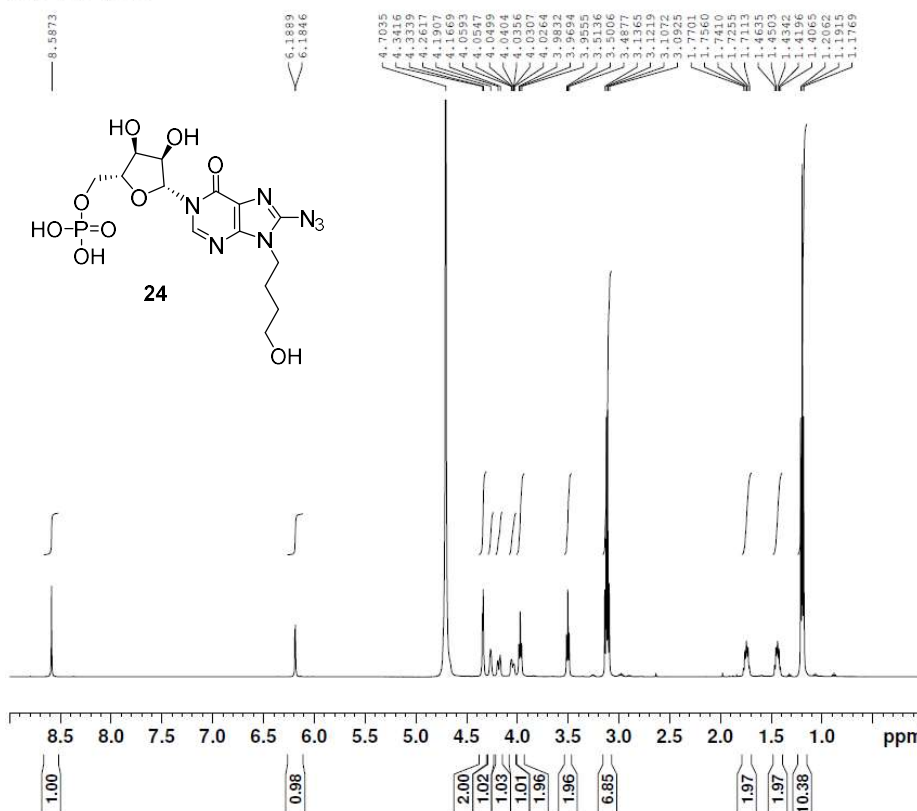
Sample Name: JMS 729 D5
 Sample Type: Unknown
 Vial: 54
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 8.0 Minutes
 Sample Set Name: JMS 729 HPLC D

Acquired By: Joanna
 Date Acquired: 01/08/2012 6:46:31 PM
 Acq. Method Set: isocratic new PDA Jo
 Date Processed: 11/09/2012 10:41:43 AM
 Processing Method: JMS 729
 Channel Name: WvIn Ch1
 Proc. Chnl. Descr.: PDA 254.0 nm



	Peak Name	RT	Area	% Area	Height
1	JMS 729	5.228	9565167	100.00	706064

JMS 742 HPLC



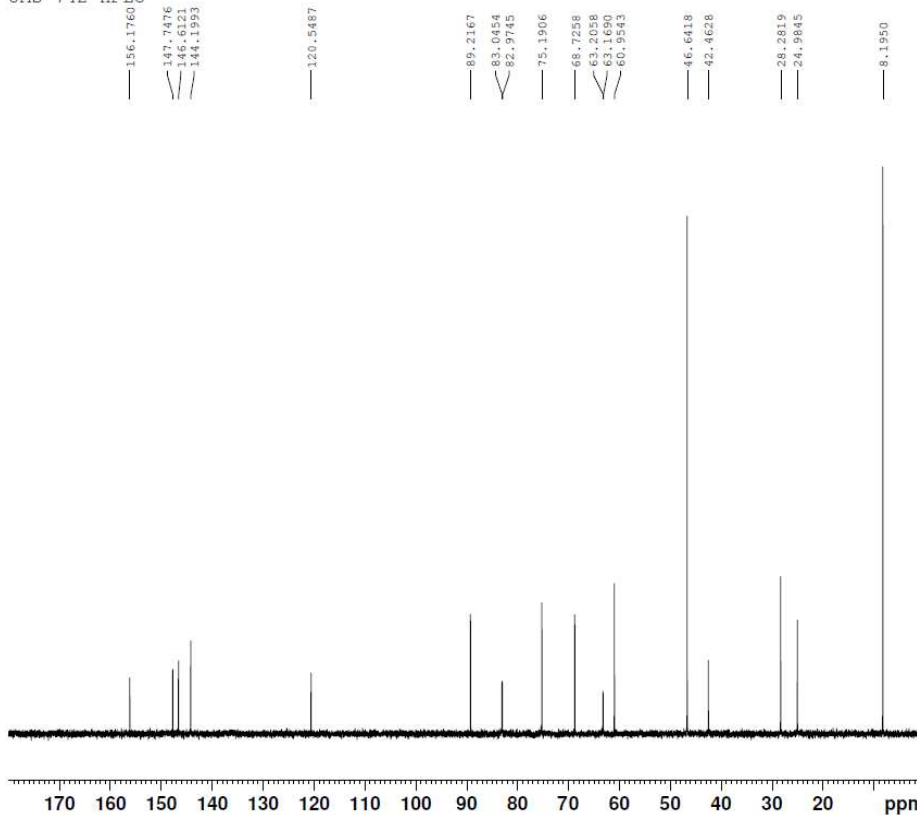
Current Data Parameters
 NAME Oct10-2012-JMS742HPLC
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121010
 Time 17.17
 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 3.1719425 sec
 RG 114
 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

F2 - Processing parameters
 SI 32768
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.3 Hz
 GB 0
 PC 1.00

JMS 742 HPLC



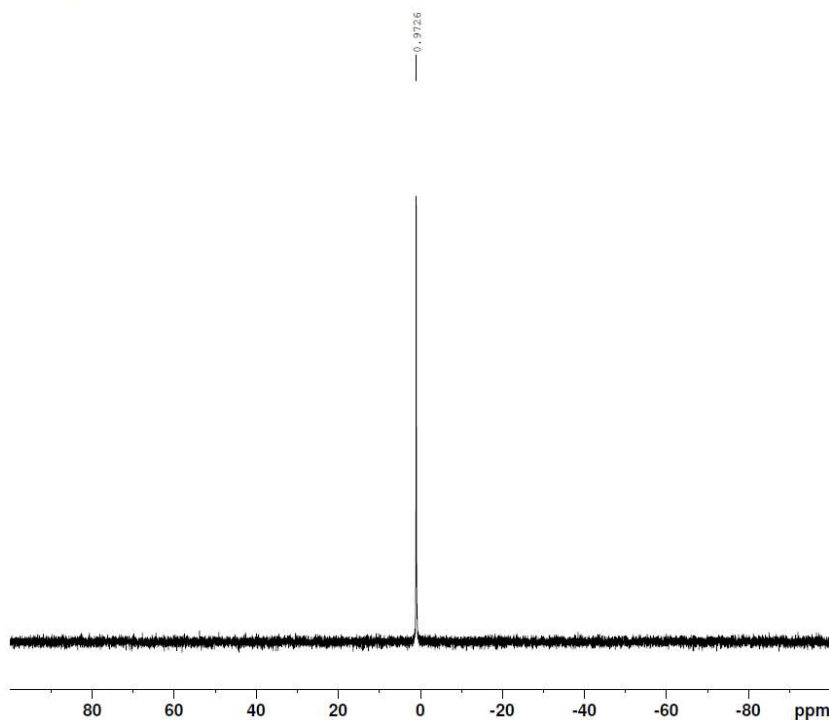
Current Data Parameters
 NAME Oct10-2012-JMS742HPLC
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121010
 Time 21.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 5000
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 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 =====
 CPDPRG[2] 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

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME Oct10-2012-JMS742HPLC
 EXPNO 18
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121011
 Time 11.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 127
 DS 4
 SWH 81521.742 Hz
 FIDRES 1.243923 Hz
 AQ 0.4019541 sec
 RG 2050
 DW 6.133 usec
 DE 6.50 usec
 TE 297.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 31P
 P1 12.00 usec
 PL1 -0.46 dB
 PL1W 90.28126526 W
 SFO1 202.4462121 MHz

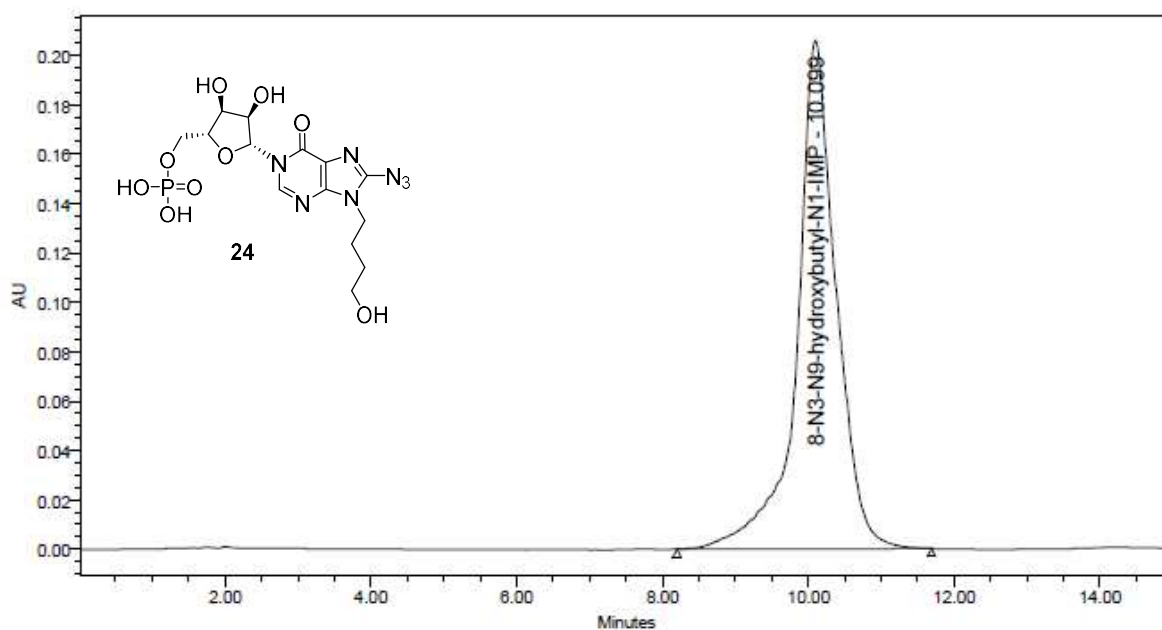
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -0.12 dB
 PL12 17.94 dB
 PL13 21.00 dB
 PL2W 19.35150909 W
 PL12W 0.30249262 W
 PL13W 0.14952536 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 202.4563350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

SAMPLE INFORMATION

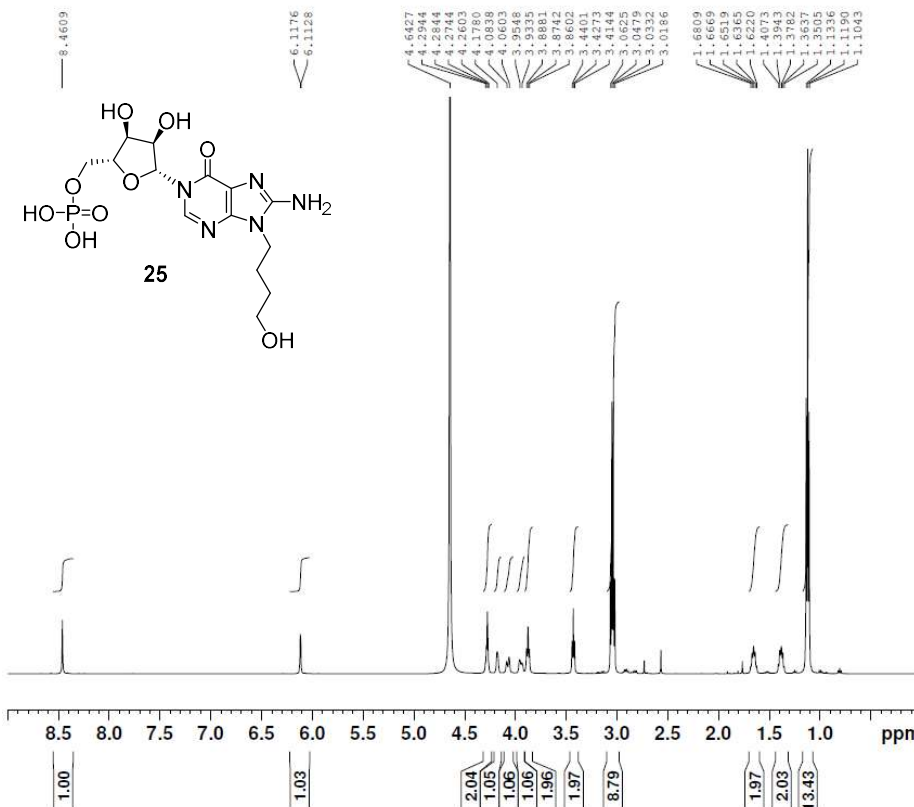
Sample Name: JMS 742 C4
 Sample Type: Unknown
 Vial: 28
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 15.0 Minutes
 Sample Set Name: JMS 742 C

Acquired By: Joanna
 Date Acquired: 09/10/2012 7:32:55 PM
 Acq. Method Set: isocratic new PDA Jo
 Date Processed: 09/04/2021 3:04:01 PM
 Processing Method: 8_N3_butyl_IMP
 Channel Name: Wvln Ch1
 Proc. Chnl. Descr.: PDA 254.0 nm



	Peak Name	RT	Area	% Area	Height
1	8-N3-N9-hydroxybutyl-N1-IMP	10.099	7699465	100.00	205493

JMS 741 HPLC



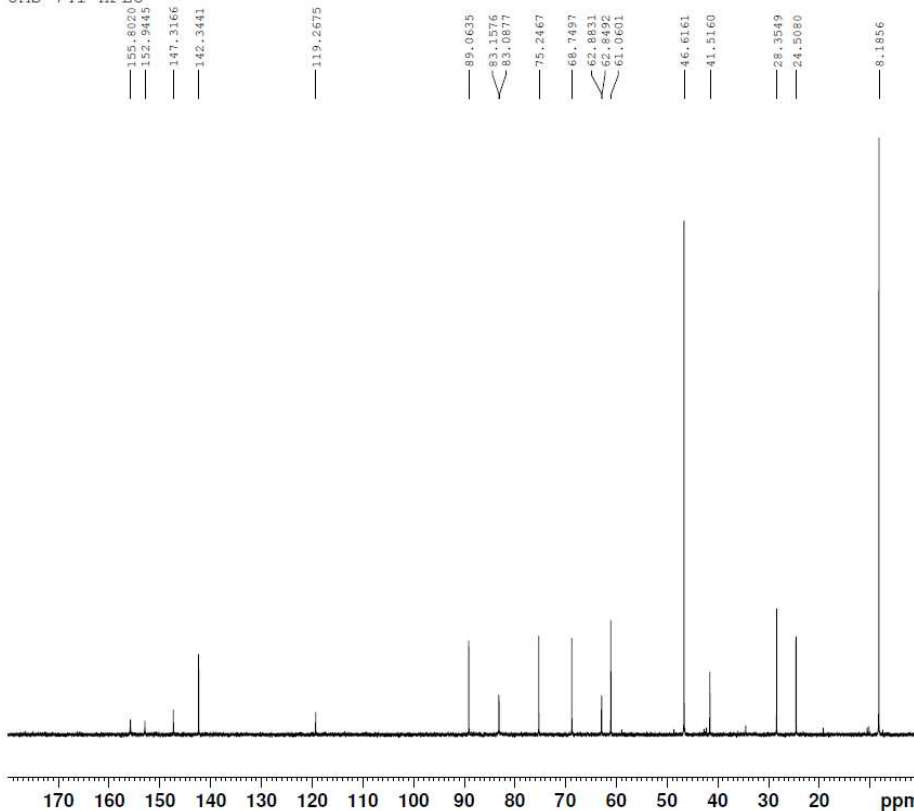
Current Data Parameters
 NAME Oct08-2012-JMS741HPLC
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121008
 Time 12.11
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 100
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 71.8
 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

F2 - Processing parameters
 SI 32768
 SF 500.1300305 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

JMS 741 HPLC



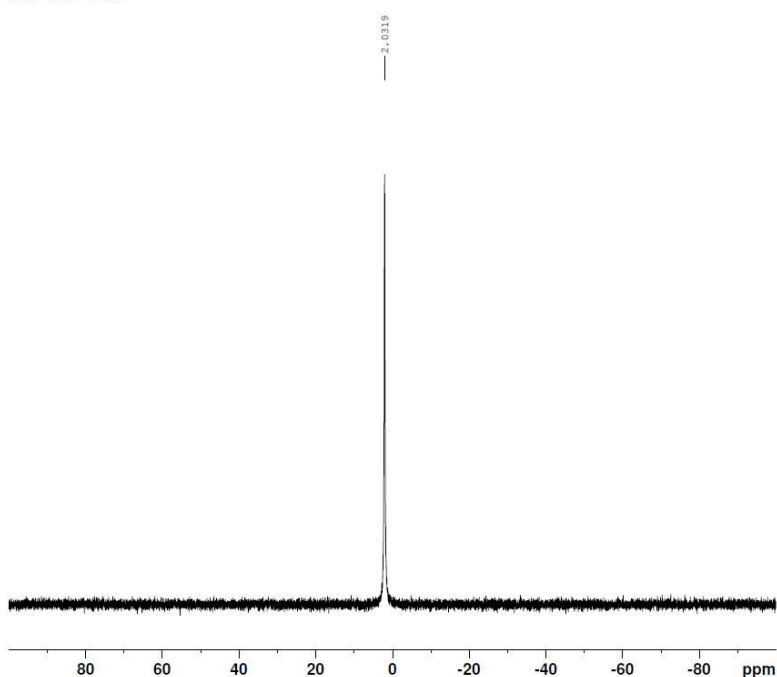
Current Data Parameters
 NAME Oct08-2012-JMS741HPLC
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121008
 Time 16.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 5000
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 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 =====
 CPDPRG[2] 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

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME Oct08-2012-JMS741HPLC
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121008
 Time 12.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 256
 DS 4
 SWH 81521.742 Hz
 FIDRES 1.243923 Hz
 AQ 0.4019541 sec
 RG 2050
 DW 6.133 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 31P
 P1 12.00 usec
 PL1 -0.46 dB
 PL1W 90.28126526 W
 SFO1 202.4462121 MHz

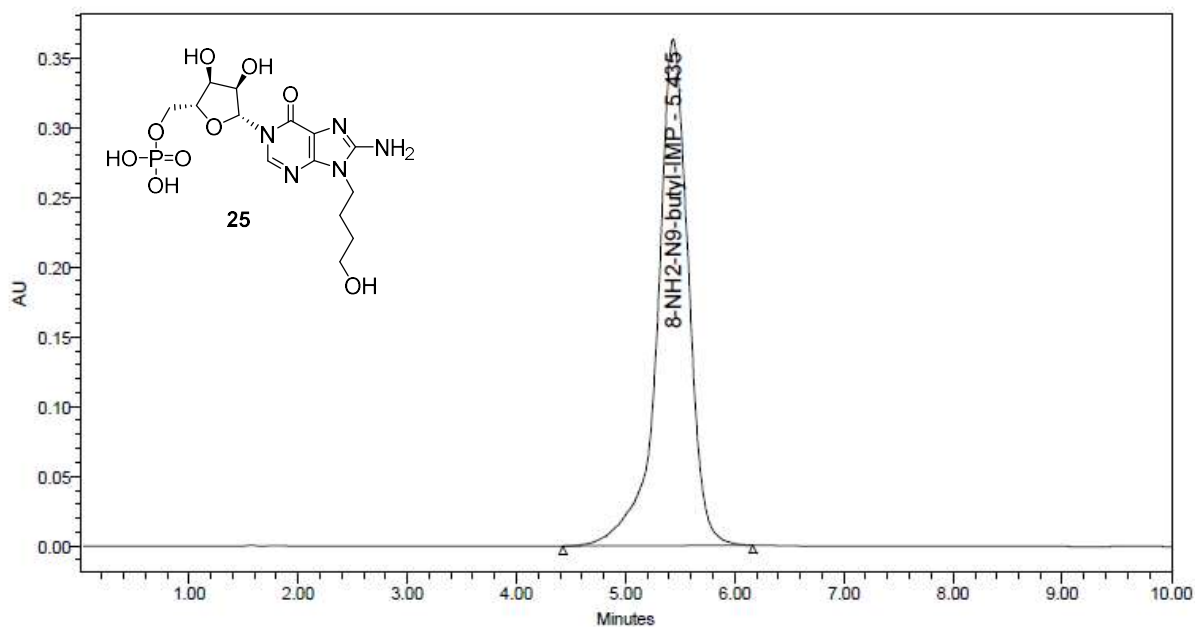
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -0.12 dB
 PL12 17.94 dB
 PL13 21.00 dB
 PL2W 19.35150909 W
 PL12W 0.30249262 W
 PL13W 0.14952536 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 202.4563350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

SAMPLE INFORMATION

Sample Name: JMS 743 E4
 Sample Type: Unknown
 Vial: 39
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 10.0 Minutes
 Sample Set Name: JMS 743 E

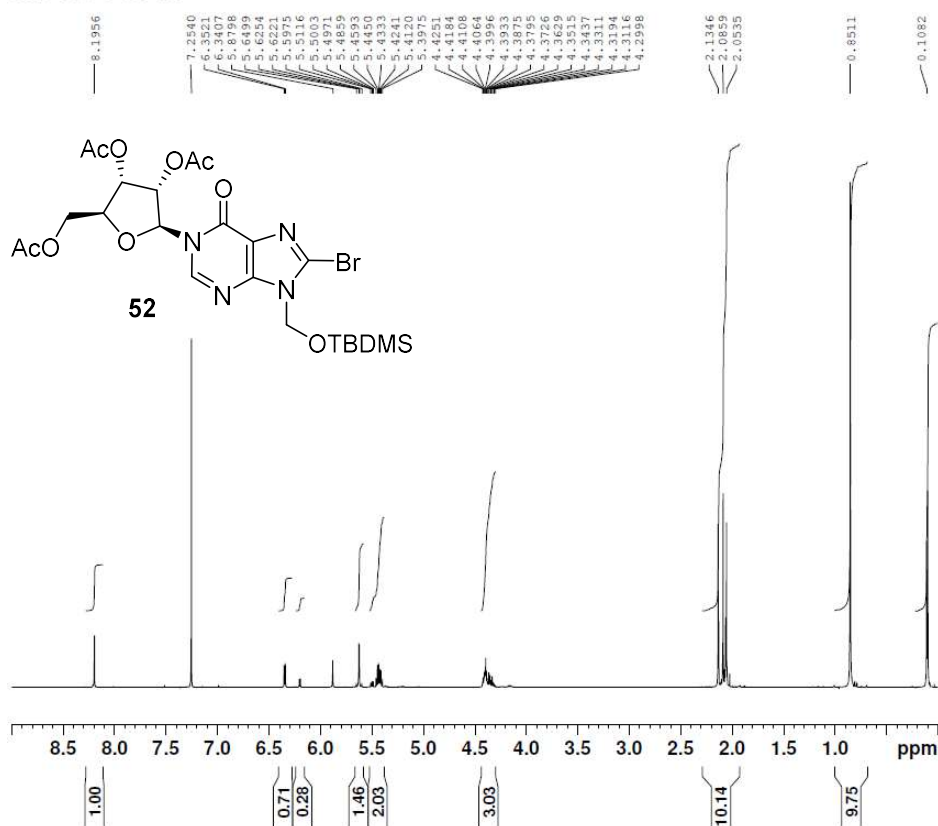
Acquired By: Joanna
 Date Acquired: 05/10/2012 10:41:28 AM
 Acq. Method Set: isocratic new PDA Jo
 Date Processed: 05/10/2012 12:33:23 PM
 Processing Method: 8NH2 N9butyl IMP
 Channel Name: WvIn Ch1
 Proc. Chnl. Descr.: PDA 254.0 nm



	Peak Name	RT	Area	% Area	Height
1	8-NH2-N9-butyl-IMP	5.435	7152416	100.00	362896

Total synthesis of L-N1-IMP analogues (26-27)

JMS 837 T 18-20



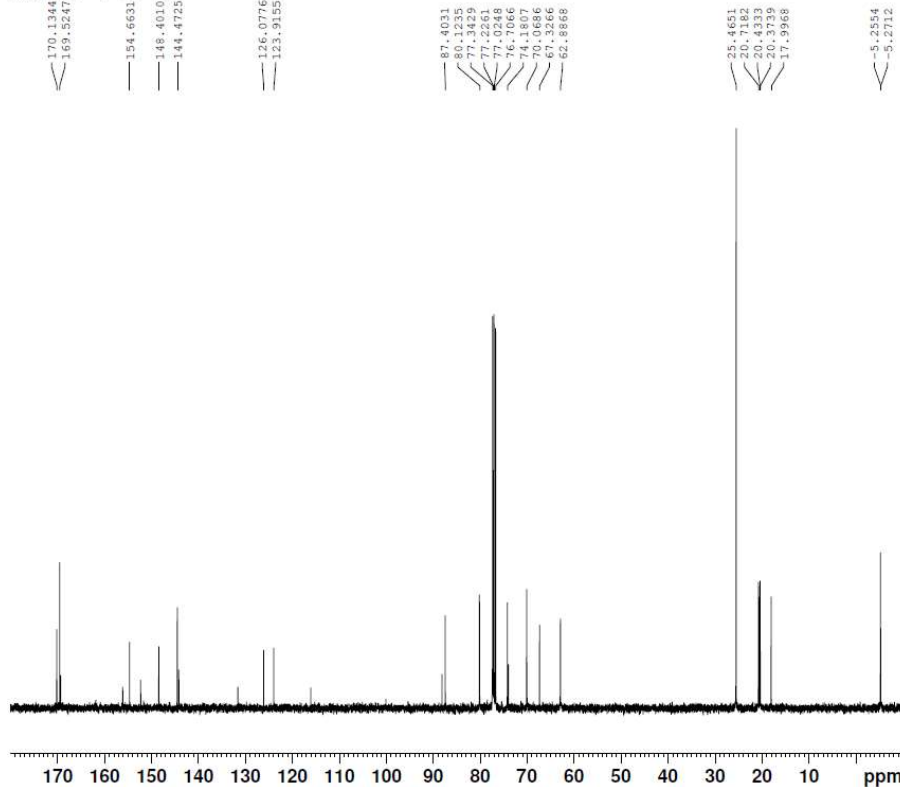
Current Data Parameters
 NAME Jun27-2013-JMS29010
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130627
 Time 12.28
 INSTRUM AVII400
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 64
 DW 60.800 usec
 DE 17.48 usec
 TE 293.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.90 usec
 PL1 -1.00 dB
 PL1W 12.26963711 W
 SFO1 400.0424704 MHz

F2 - Processing parameters
 SI 65536
 SF 400.0399837 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

JMS 837 T 18-20



Current Data Parameters
 NAME Jun27-2013-JMS29010
 EXPNO 11
 PROCNO 1

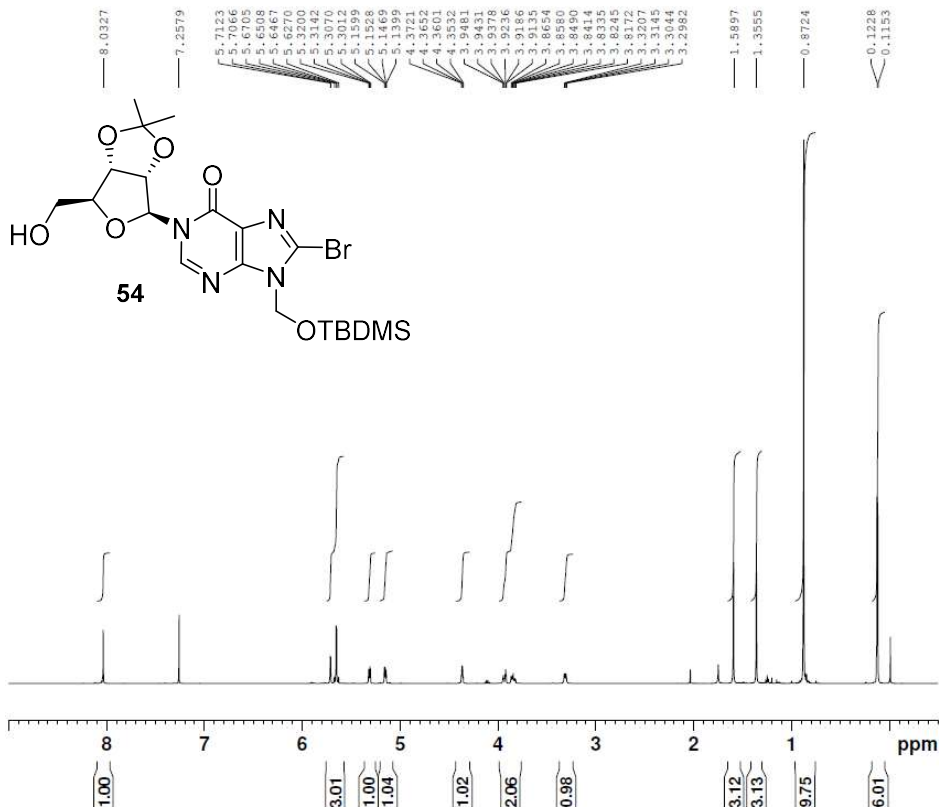
F2 - Acquisition Parameters
 Date_ 20130627
 Time 12.46
 INSTRUM AVII400
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 1820
 DW 20.800 usec
 DE 6.50 usec
 TE 293.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 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 -1.00 dB
 PL12 15.55 dB
 PL13 19.00 dB
 PL2W 12.26963711 W
 PL12W 0.27153867 W
 PL13W 0.12269637 W
 SFO2 400.0416002 MHz

F2 - Processing parameters
 SI 65536
 SF 100.5901380 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

JMS841 T18-20



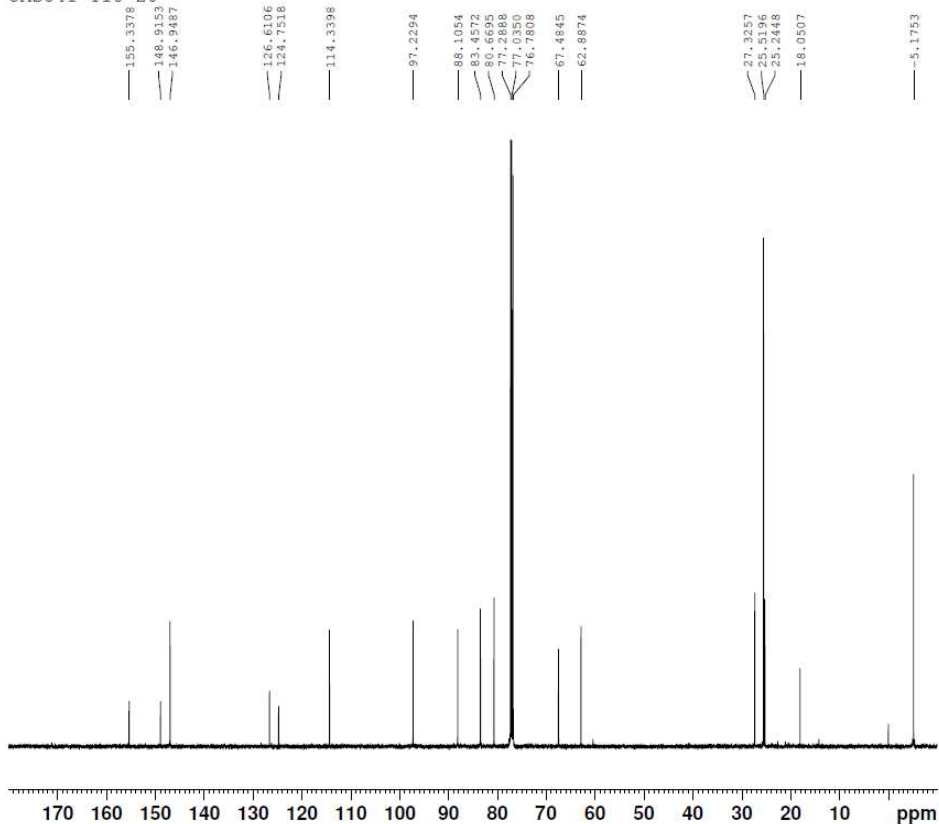
Current Data Parameters
NAME JMS841 T18-20
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130704
Time 15.52
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 3.1719425 sec
RG 101
DW 48.400 usec
DE 14.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -0.12 dB
PL1W 19.35150909 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

JMS841 T18-20



Current Data Parameters
NAME JMS841 T18-20
EXPNO 12
PROCNO 1

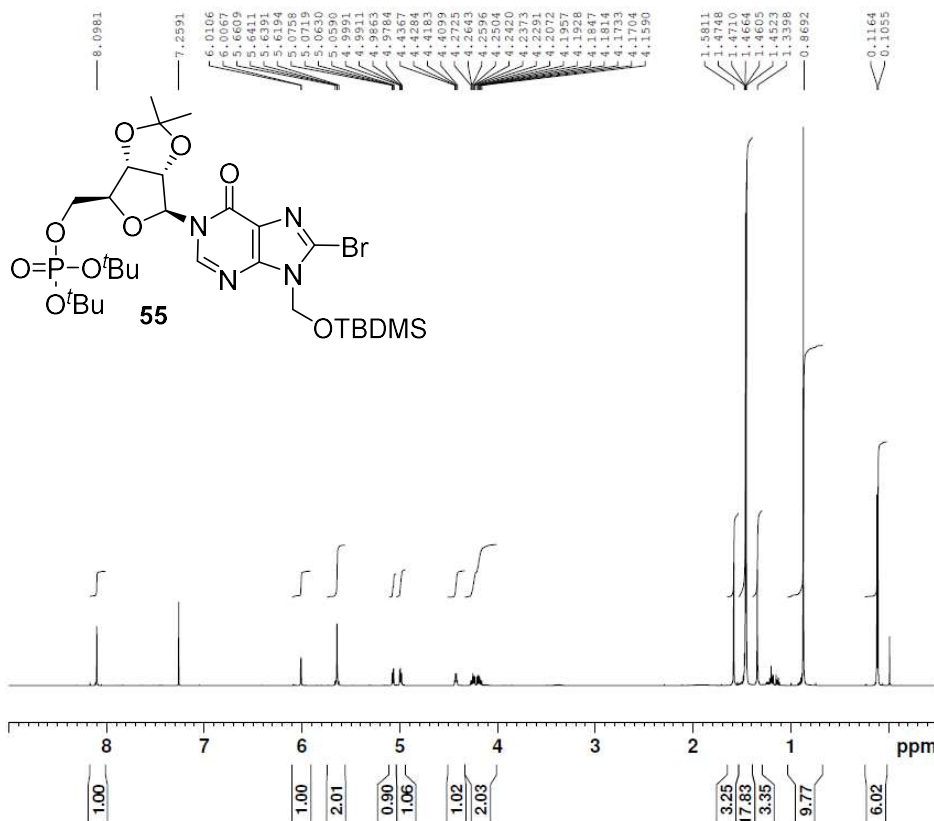
F2 - Acquisition Parameters
Date_ 20130704
Time 16.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 8.45 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -0.51 dB
PL1W 99.92730713 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG[2] 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

F2 - Processing parameters
SI 32768
SF 125.7577895 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

JMS 843 T 22-25



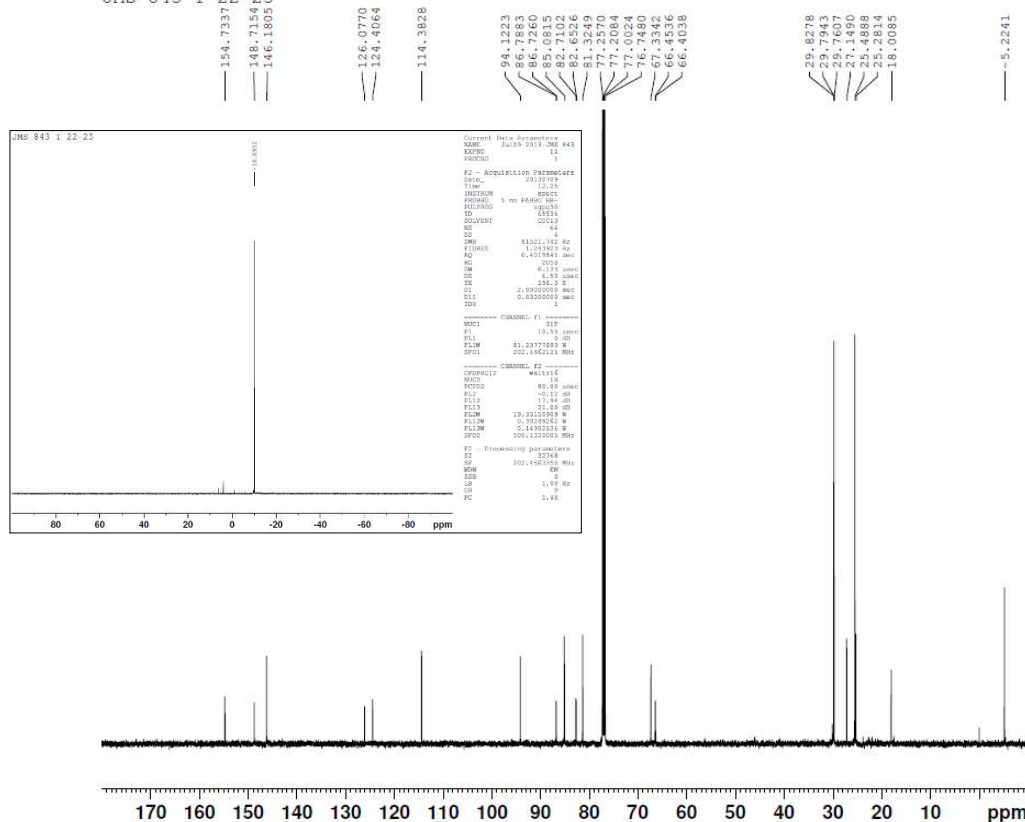
Current Data Parameters
NAME Jul09-2013-JMS 843
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130709
Time 12.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 90.5
DW 48.400 usec
DE 14.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -0.12 dB
PL1W 19.35150909 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

JMS 843 T 22-25



Current Data Parameters
NAME Jul09-2013-JMS 843
EXPNO 12
PROCNO 1

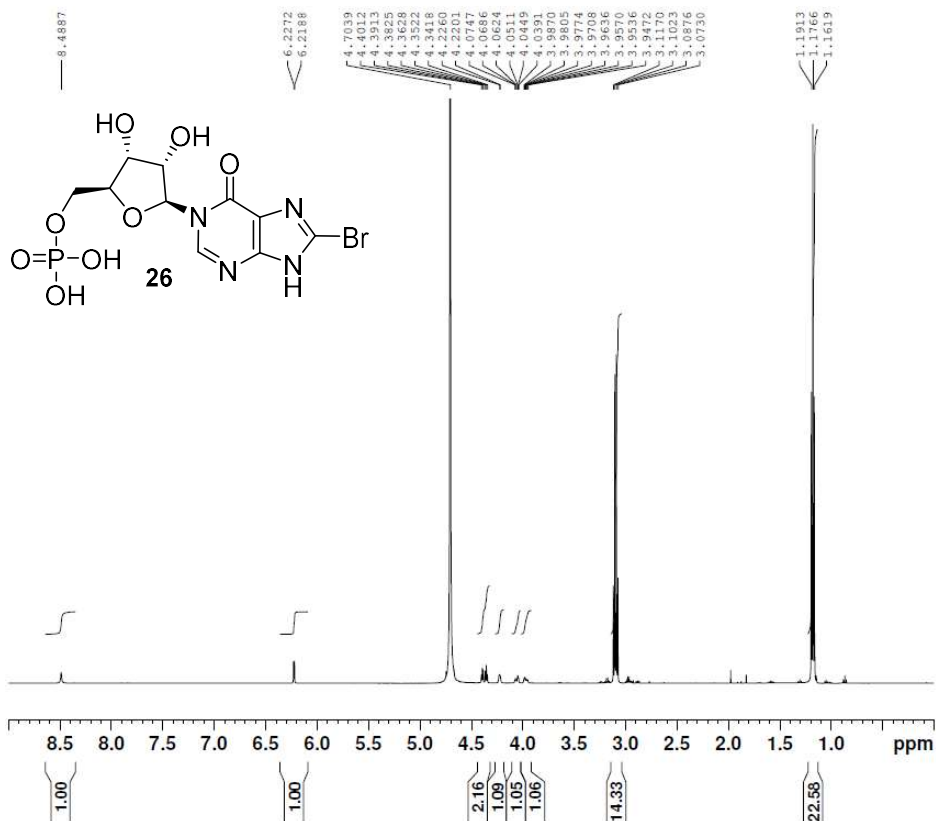
F2 - Acquisition Parameters
Date_ 20130709
Time 13.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 676
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 8.45 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 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

F2 - Processing parameters
SI 32768
SF 125.7577932 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

JMS 845 HPLC



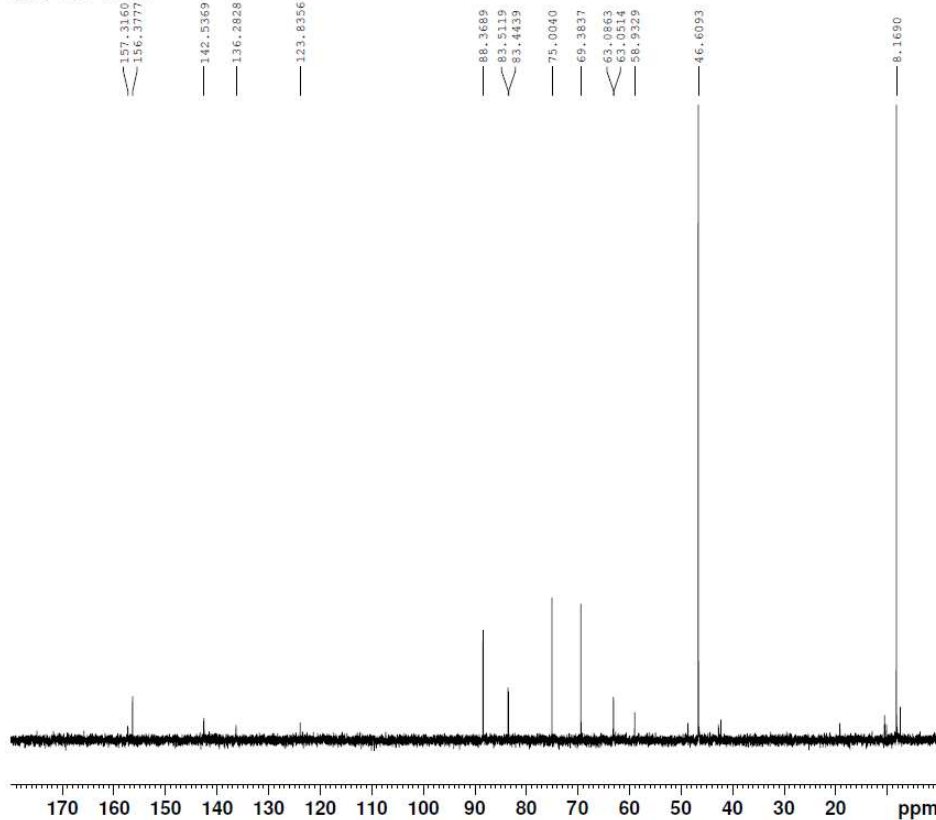
Current Data Parameters
NAME JMS 845 HPLC
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130718
Time 15.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT D2O
NS 128
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 80.6
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -0.12 dB
PL1W 19.35150909 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

JMS 845 HPLC



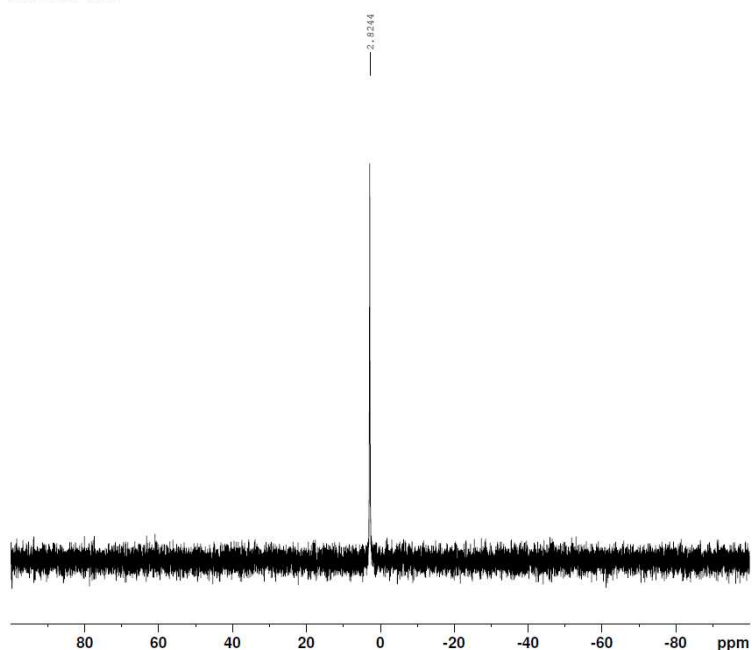
Current Data Parameters
NAME JMS 845 HPLC
EXPNO 19
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130719
Time 9.36
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 1.1010048 sec
RG 2050
DW 16.800 usec
DE 8.45 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -0.51 dB
PL1W 99.92730713 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG[2] 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

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME JMS 845 HPLC
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130718
Time 15.59
INSTRUM spect
PROBHD 5 mm PARBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 256
DS 4
SWH 81521.742 Hz
FIDRES 1.243923 Hz
AQ 0.4019541 sec
RG 2050
DW 6.133 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 10.50 usec
PL1 0 dB
PL1W 81.20777893 W
SFO1 202.4462121 MHz

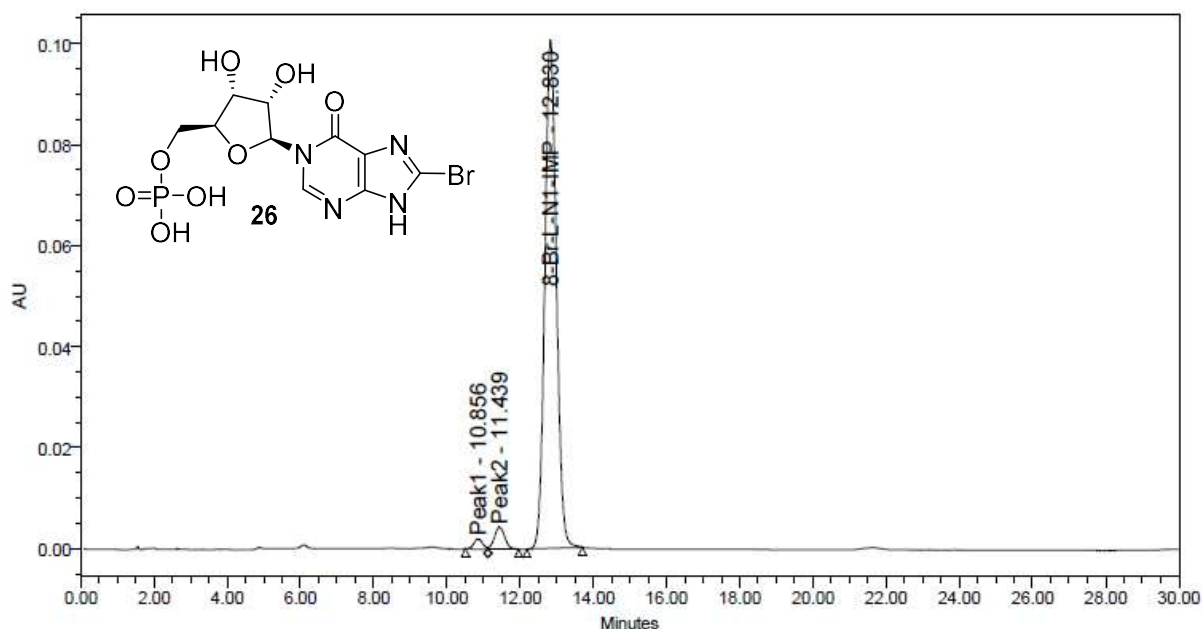
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.12 dB
PL12 17.94 dB
PL13 21.00 dB
PL2W 19.35150909 W
PL12W 0.30249262 W
PL13W 0.14952536 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 202.4563350 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

SAMPLE INFORMATION

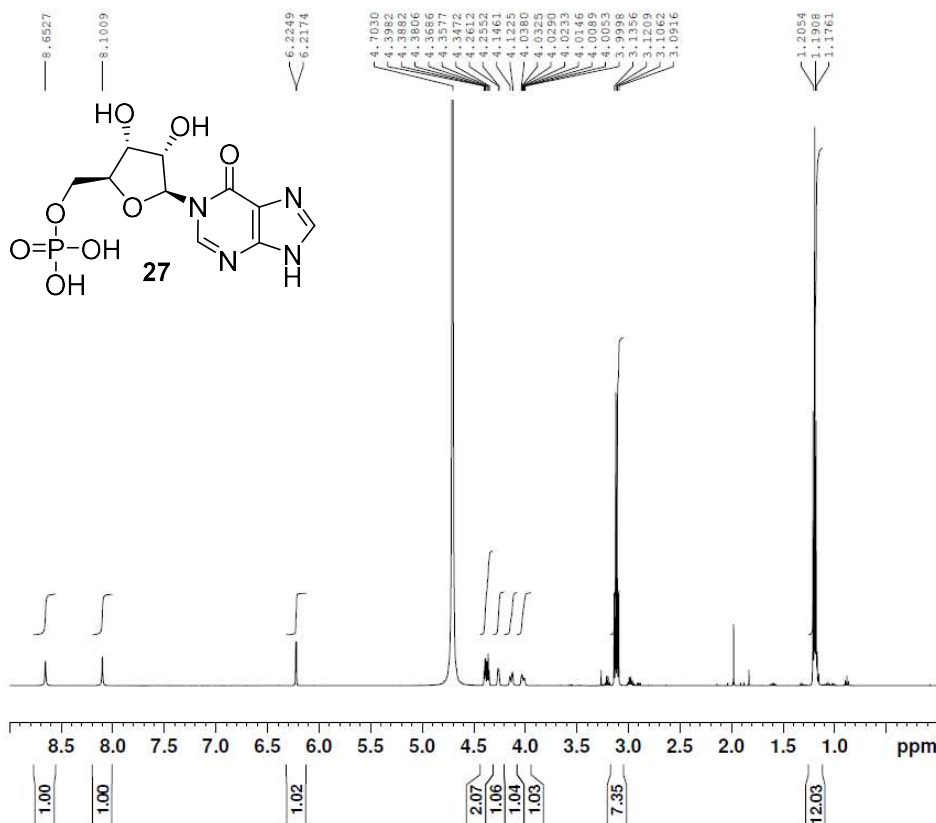
Sample Name: JMS 845 Batch 1 from UV
Sample Type: Unknown
Vial: 56
Injection #: 1
Injection Volume: 10.00 ul
Run Time: 30.0 Minutes
Sample Set Name: JMS 845 Batch 1

Acquired By: Joanna
Date Acquired: 26/09/2013 3:32:14 PM
Acq. Method Set: isocratic new PDA Jo
Date Processed: 27/09/2013 3:44:26 PM
Processing Method: 8 Br L N1 IMP
Channel Name: WvIn Ch1
Proc. Chnl. Descr.: PDA 254.0 nm



	Peak Name	RT	Area	% Area	Height
1	Peak1	10.856	32649	1.41	2001
2	Peak2	11.439	84320	3.64	4337
3	8-Br-L-N1-IMP	12.830	2197357	94.95	100598

JMS 847 HPLC



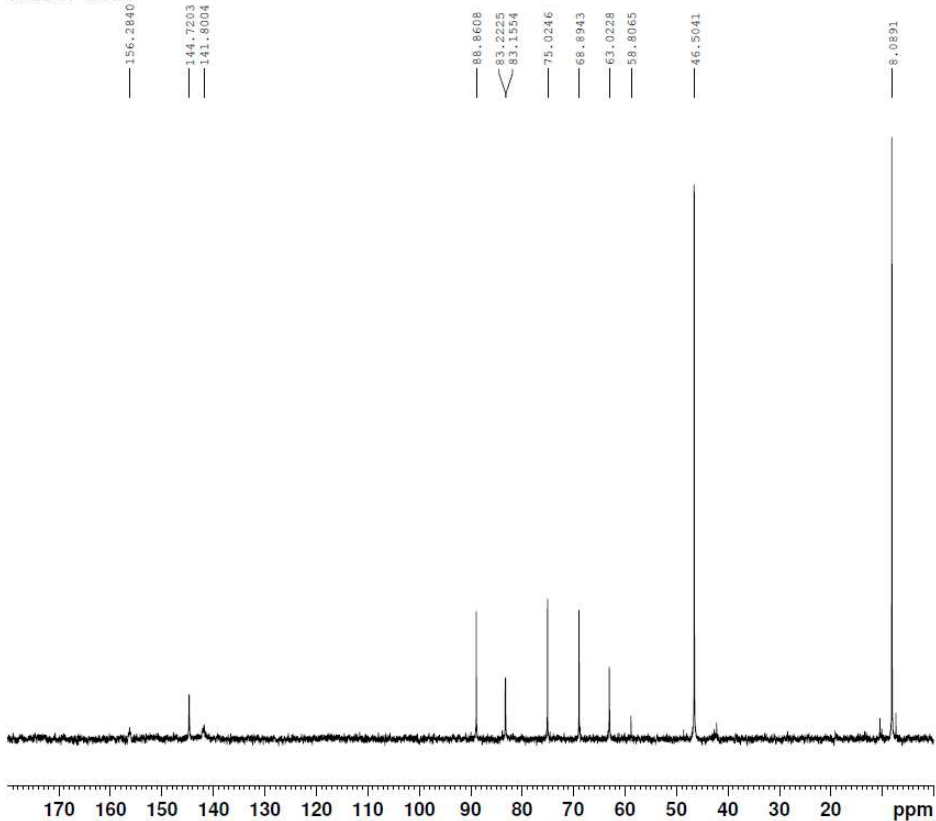
Current Data Parameters
NAME JMS 847 HPLC
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130716
Time 15.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT D2O
NS 128
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 80.6
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -0.12 dB
PL1W 19.35150909 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

JMS847 conc



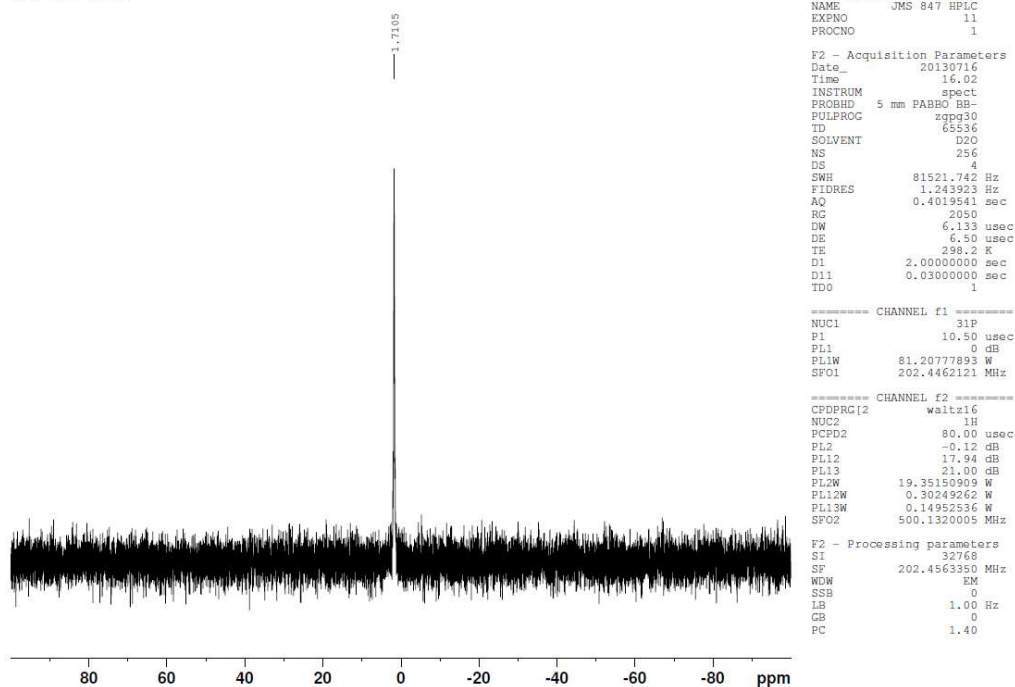
Current Data Parameters
NAME JMS847 conc
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130725
Time 17.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 16384
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 8.45 usec
TE 293.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -0.51 dB
PL1W 99.92730713 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG[2] 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

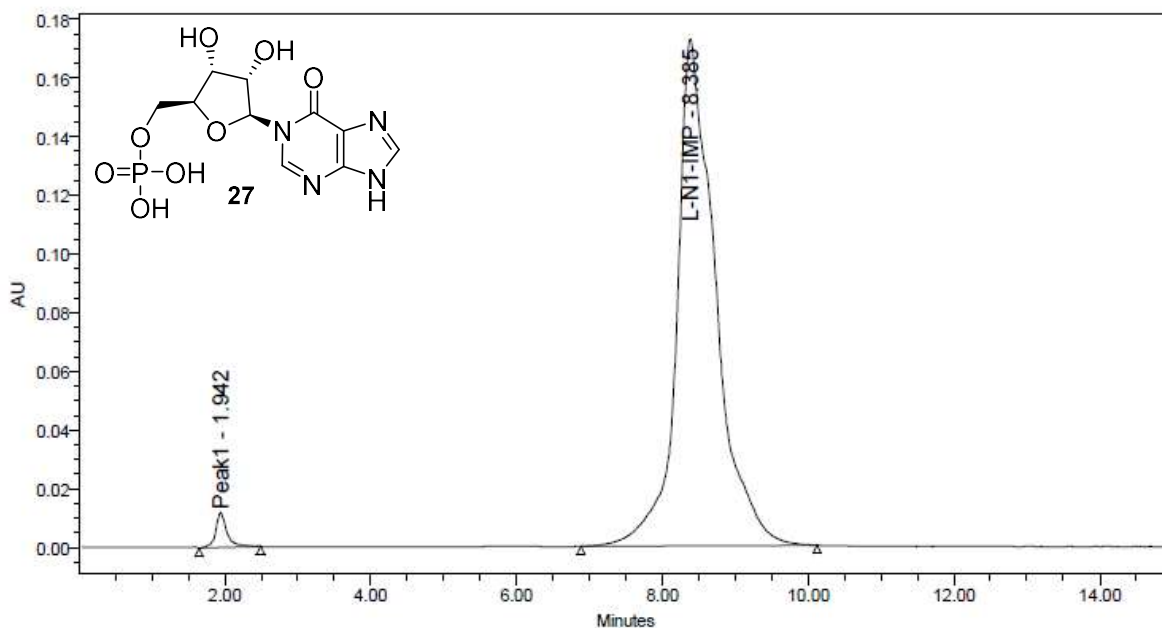
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



SAMPLE INFORMATION

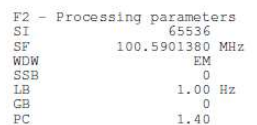
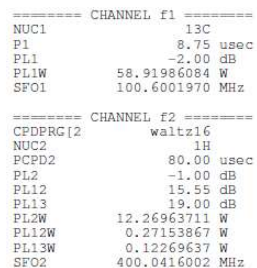
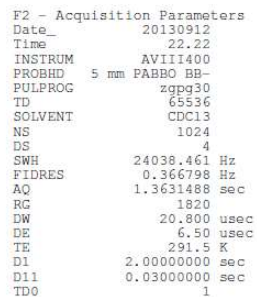
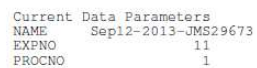
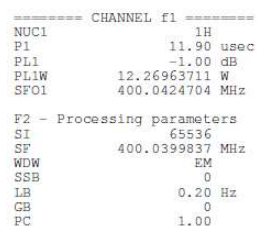
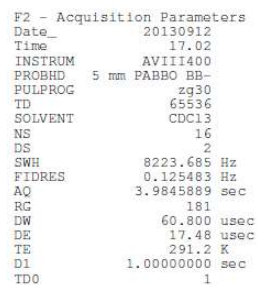
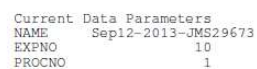
Sample Name: JMS 847 uv
Sample Type: Unknown
Vial: 2
Injection #: 1
Injection Volume: 10.00 ul
Run Time: 15.0 Minutes
Sample Set Name: JMS 847 and 845 uv

Acquired By: Joanna
Date Acquired: 24/07/2013 3:10:17 PM
Acq. Method Set: isocratic new PDA Jo
Date Processed: 27/09/2013 3:48:56 PM
Processing Method: L N1 IMP
Channel Name: Wvin Ch1
Proc. Chnl. Descr.: PDA 254.0 nm

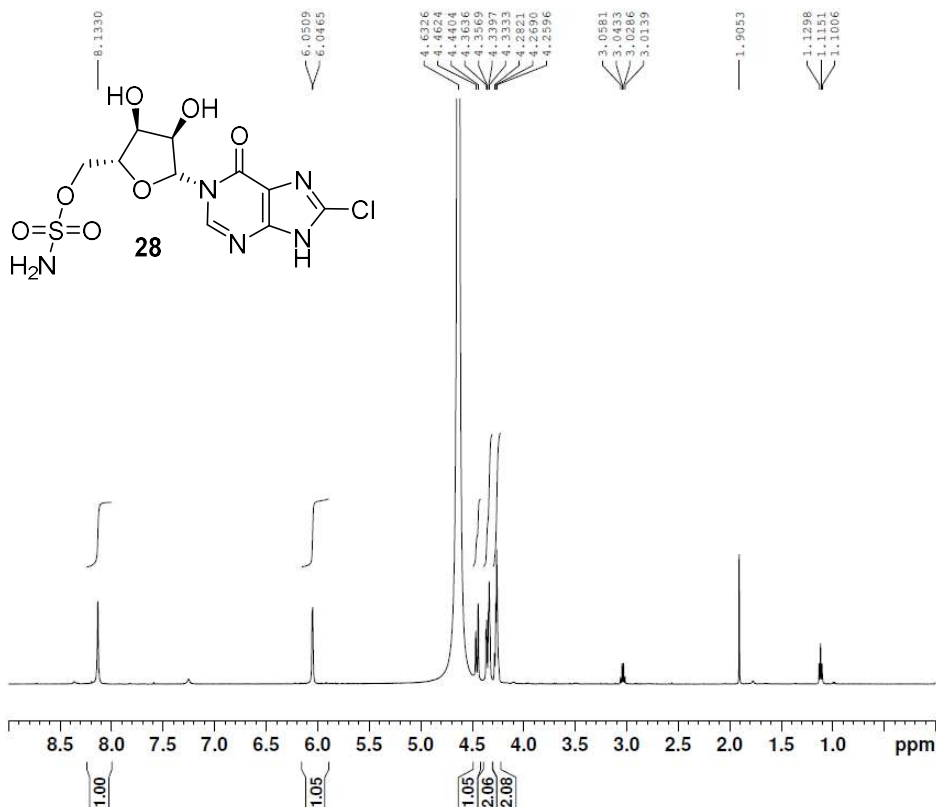


	Peak Name	RT	Area	% Area	Height
1	Peak1	1.942	129676	2.00	11947
2	L-N1-IMP	8.385	6365515	98.00	172494

JMS 870 T 6



JMS879 HPLC



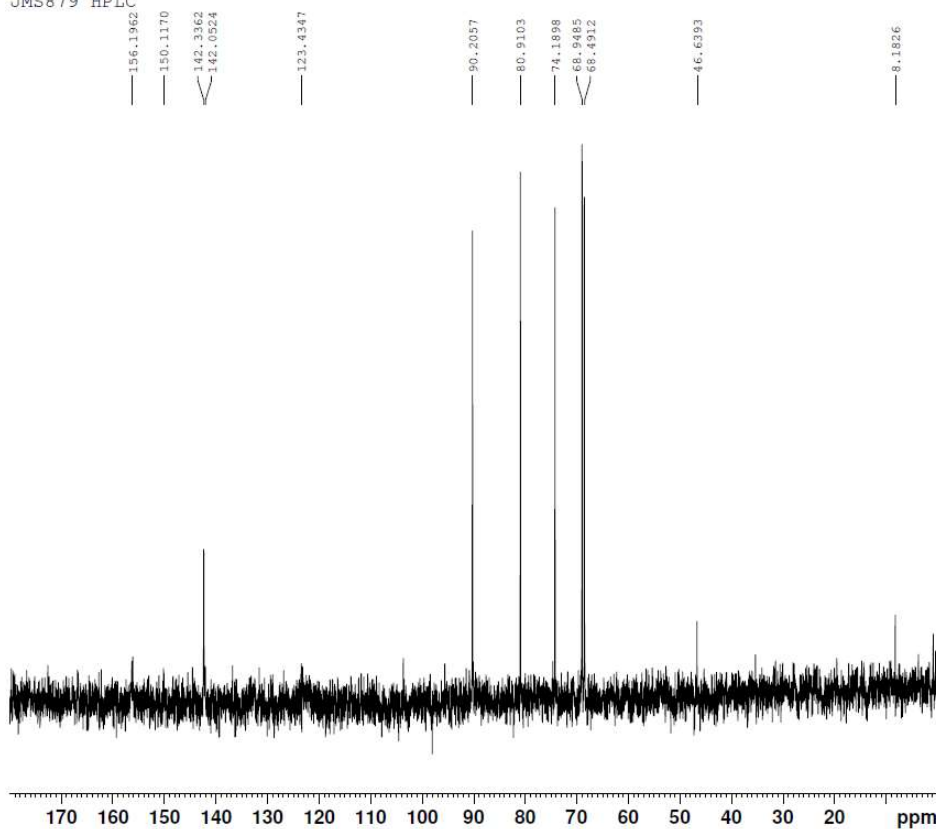
Current Data Parameters
NAME JMS879 HPLC
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131129
Time 5.53
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 3.1719425 sec
RG 228
DW 48.400 usec
DE 14.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -0.12 dB
PL1W 19.35150909 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300350 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

JMS879 HPLC



Current Data Parameters
NAME JMS879 HPLC
EXPNO 17
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131201
Time 23.06
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 1.1010048 sec
RG 2050
DW 16.800 usec
DE 8.45 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -0.51 dB
PL1W 99.92730713 W
SFO1 125.7703643 MHz

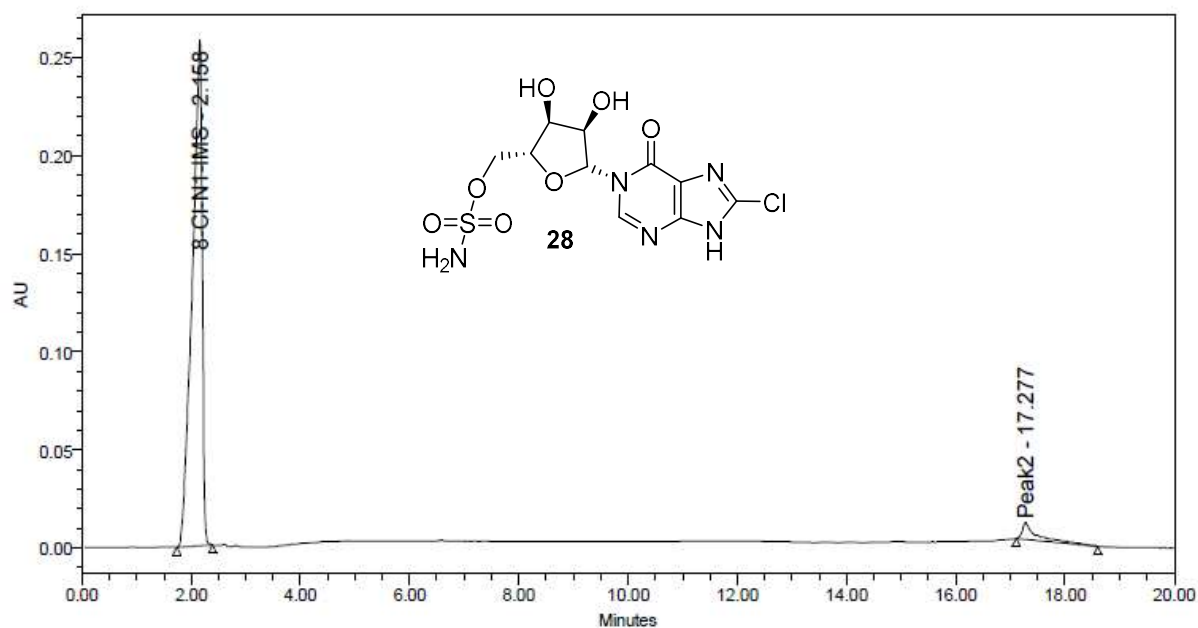
===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.12 dB
PL12 17.94 dB
PL13 21.00 dB
PL2W 19.35150909 W
PL12W 0.30249262 W
PL13W 0.14952536 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

SAMPLE INFORMATION

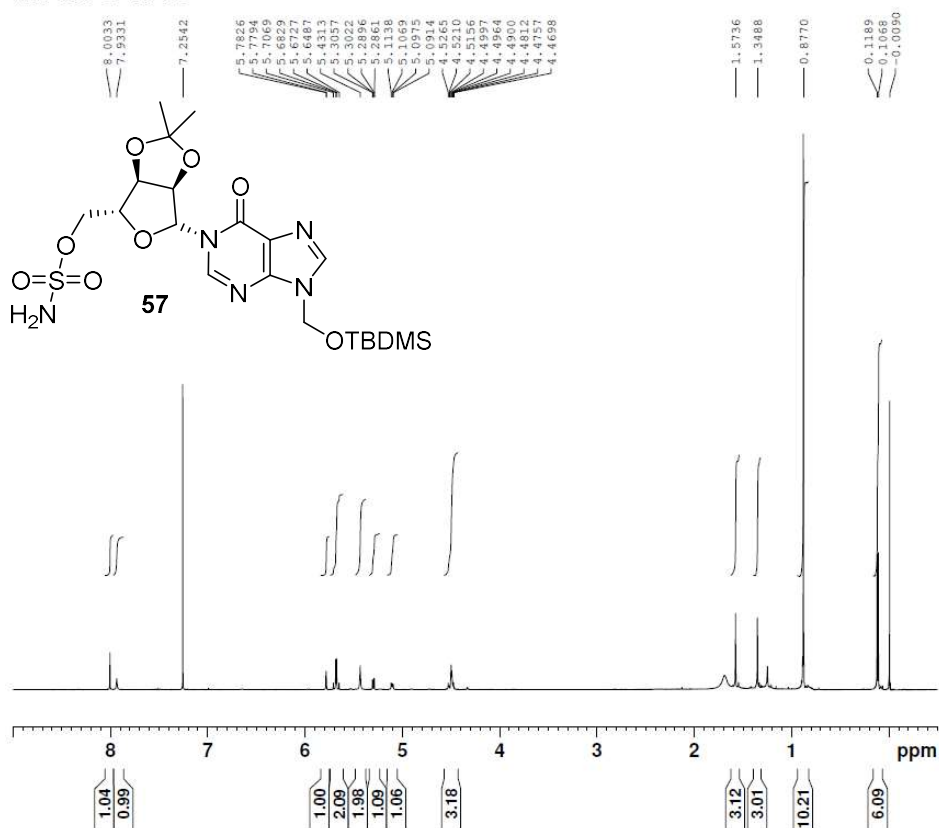
Sample Name: JMS 879 B9
 Sample Type: Unknown
 Vial: 94
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 20.0 Minutes
 Sample Set Name: JMS 879 HPLC B

Acquired By: Joanna
 Date Acquired: 27/11/2013 3:35:18 AM
 Acq. Method Set: RP18 LC
 Date Processed: 18/12/2013 11:48:24 AM
 Processing Method: 8Cl_N1_IMS in MeCN_H2O
 Channel Name: WvInCh1
 Proc. Chnl. Descr.: PDA 262.1 nm



	Peak Name	RT	Area	% Area	Height
1	8-Cl-N1-IMS	2.158	3256505	95.31	257699
2	Peak2	17.277	160233	4.69	8449

JMS 899 T 10-11



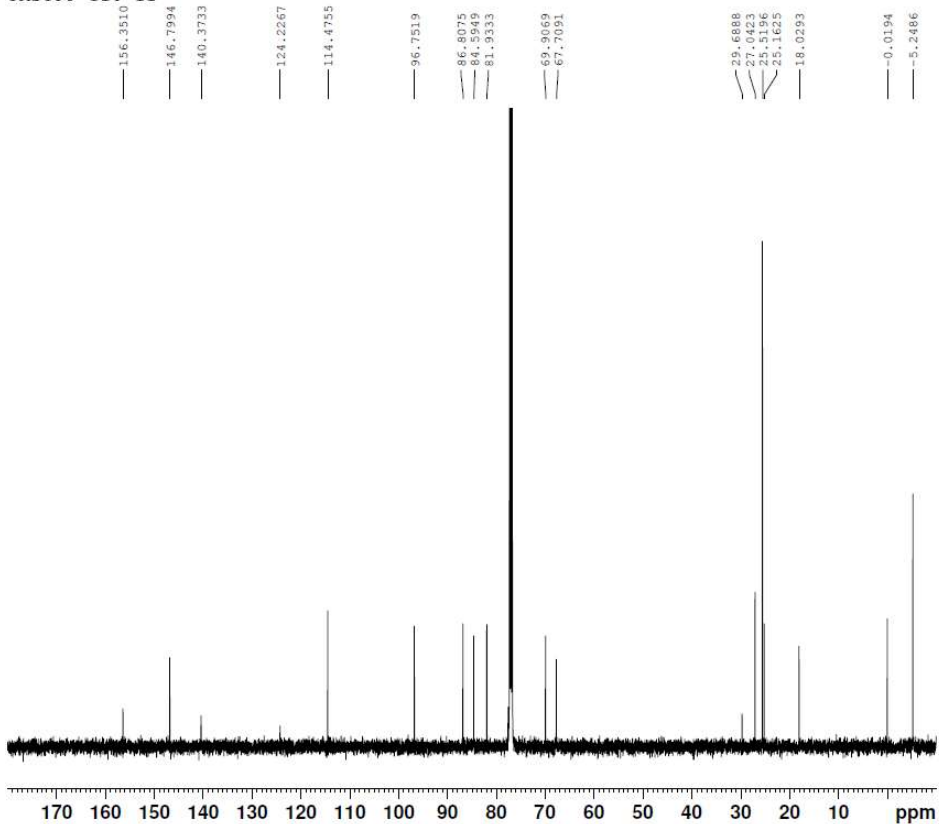
Current Data Parameters
NAME Oct21-2013-JMS30022
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131021
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 3.9845889 sec
RG 228
DW 60.800 usec
DE 17.48 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 -1.00 dB
PL1W 12.26963711 W
SFO1 400.0424704 MHz

F2 - Processing parameters
SI 65536
SF 400.0399837 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

JMS899 T10-11



Current Data Parameters
NAME JMS899 T10-11
EXPNO 16
PROCNO 1

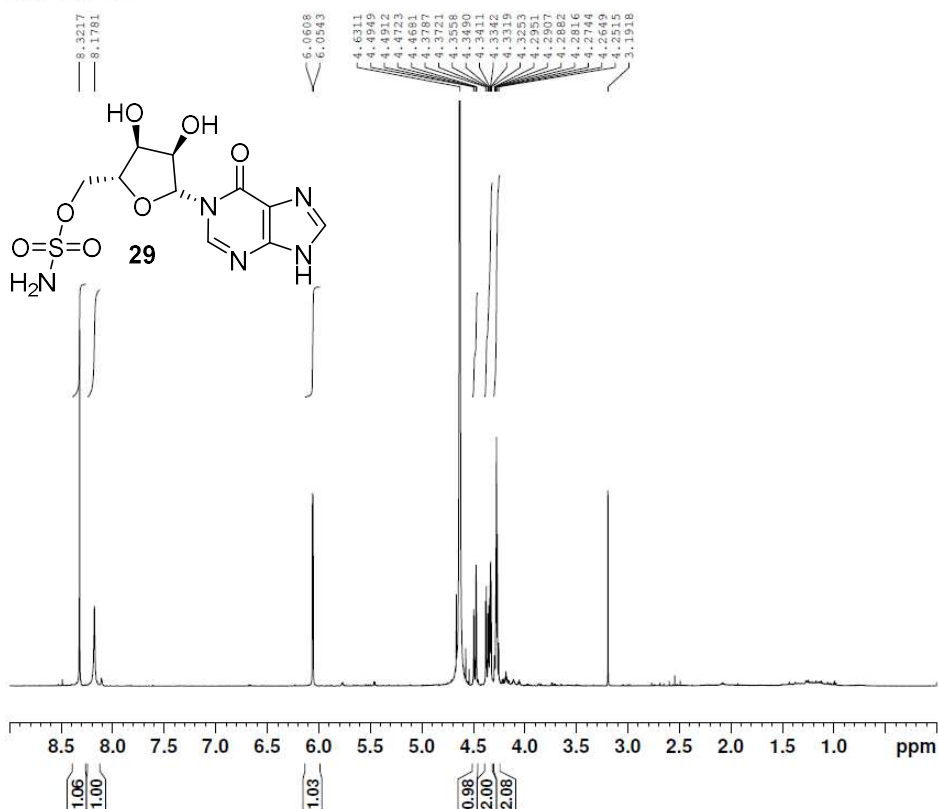
F2 - Acquisition Parameters
Date_ 20131022
Time 14.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 8.45 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -0.51 dB
PL1W 99.92730713 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG[2] 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

F2 - Processing parameters
SI 32768
SF 125.7577914 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

JMS 908 D2O



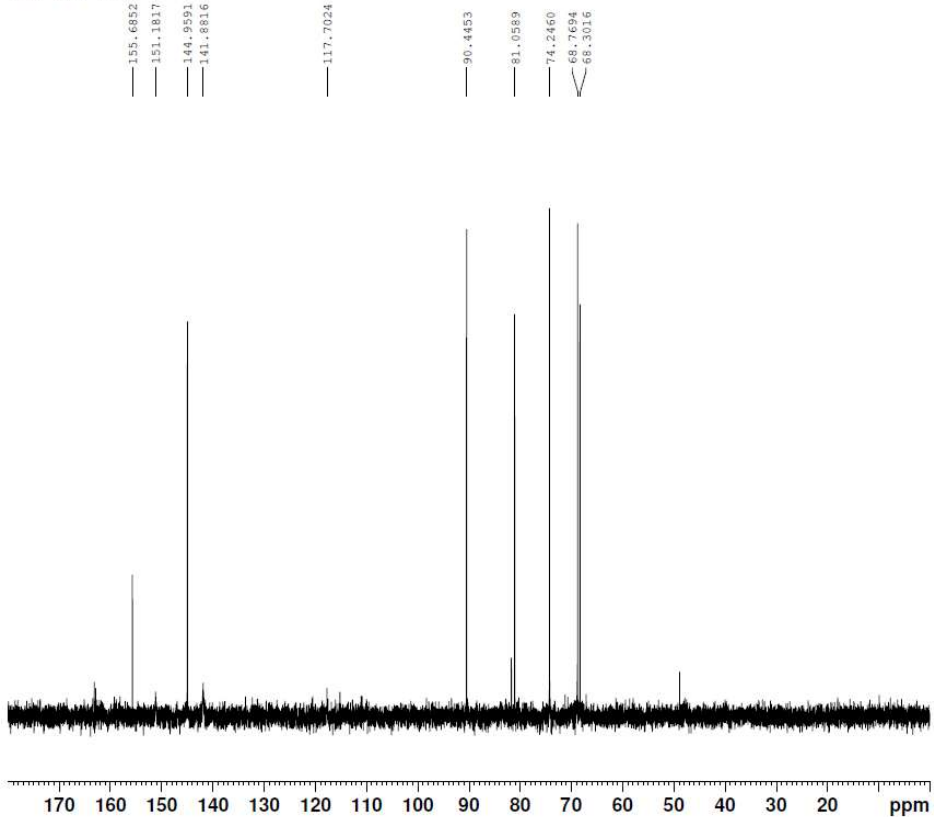
Current Data Parameters
NAME JMS 908-2
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131101
Time 16.42
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 3.1719425 sec
RG 228
DW 48.400 usec
DE 14.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -0.12 dB
PL1W 19.35150909 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300364 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

JMS 908 D2O



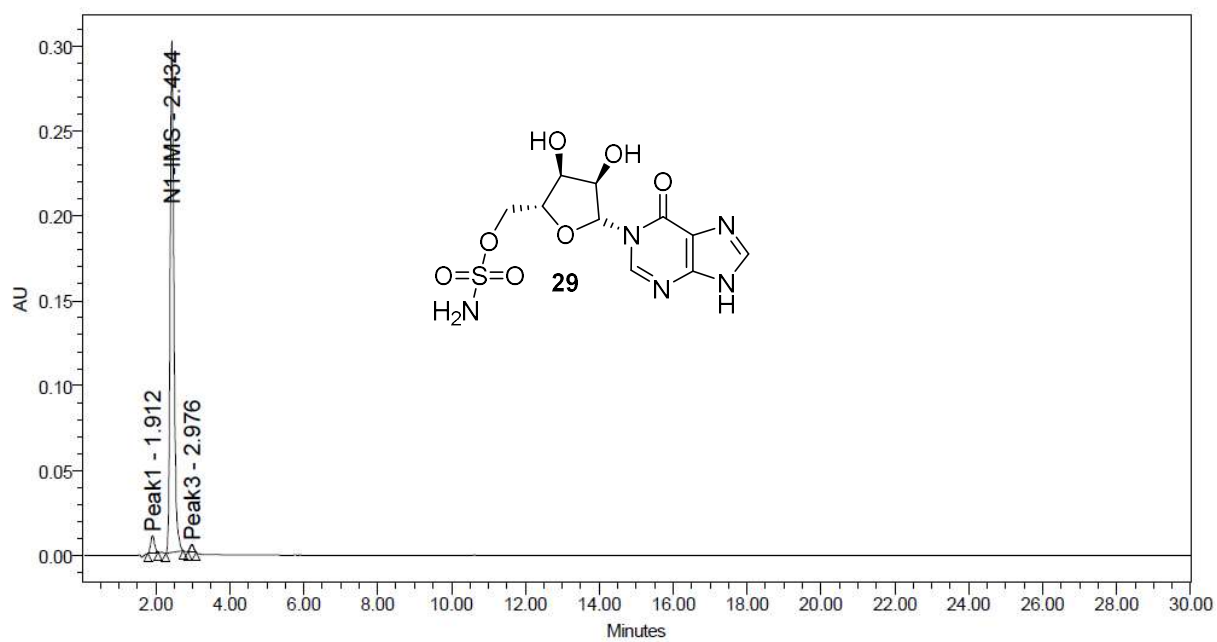
Current Data Parameters
NAME JMS 908-2
EXPNO 17
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131102
Time 22.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 20480
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 8.45 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -0.51 dB
PL1W 99.92730713 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG12 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

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



	Peak Name	RT	Area	% Area	Height
1	Peak1	1.912	73083	3.25	10284
2	N1-IMS	2.434	2148227	95.41	301144
3	Peak3	2.976	30303	1.35	4335