

Supporting Information

Synthesis of 2'-deoxy-9-deaza-nucleosides using Heck methodology

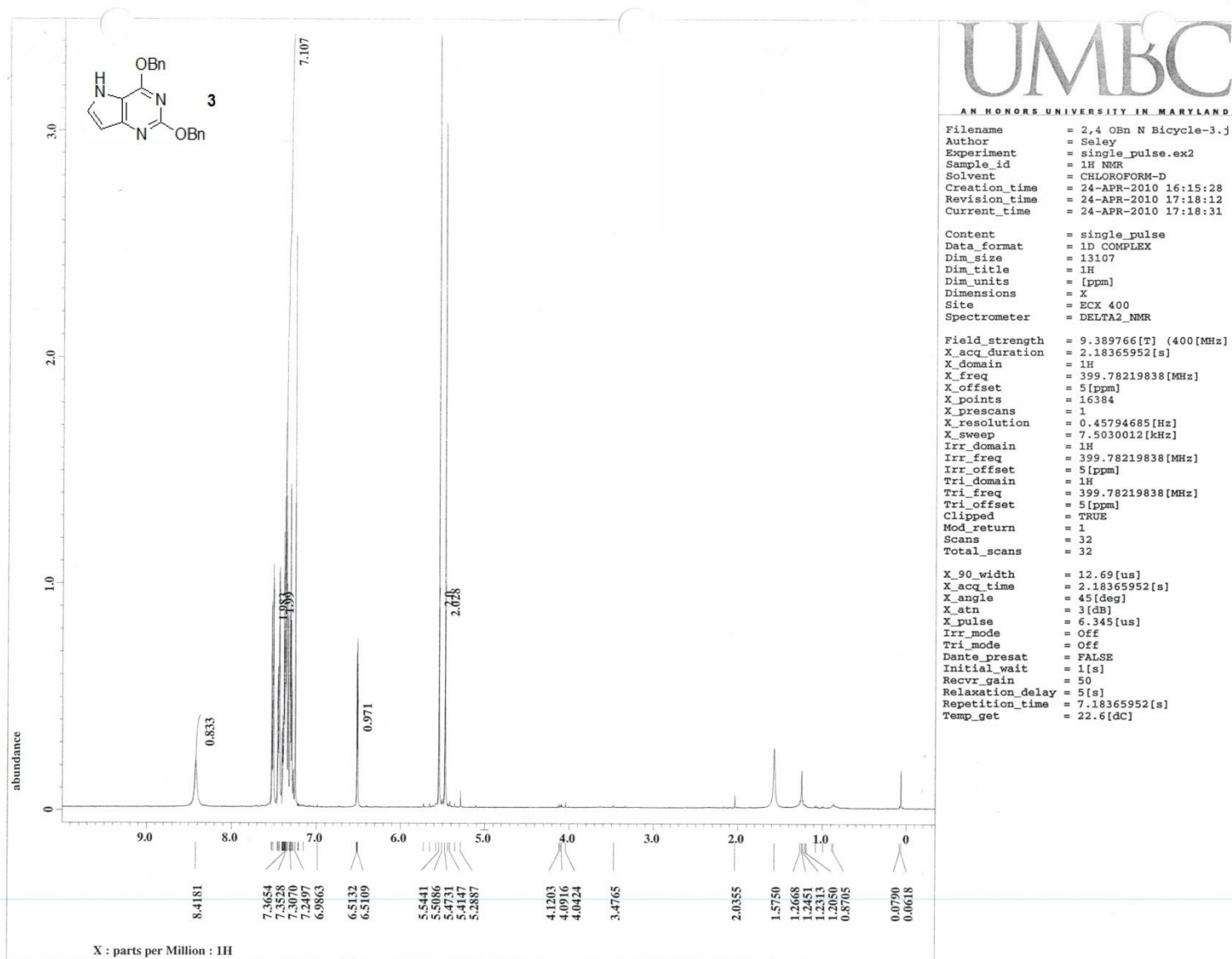
Kartik Temburnikar, Kelin Brace and Katherine L. Seley-Radtke*

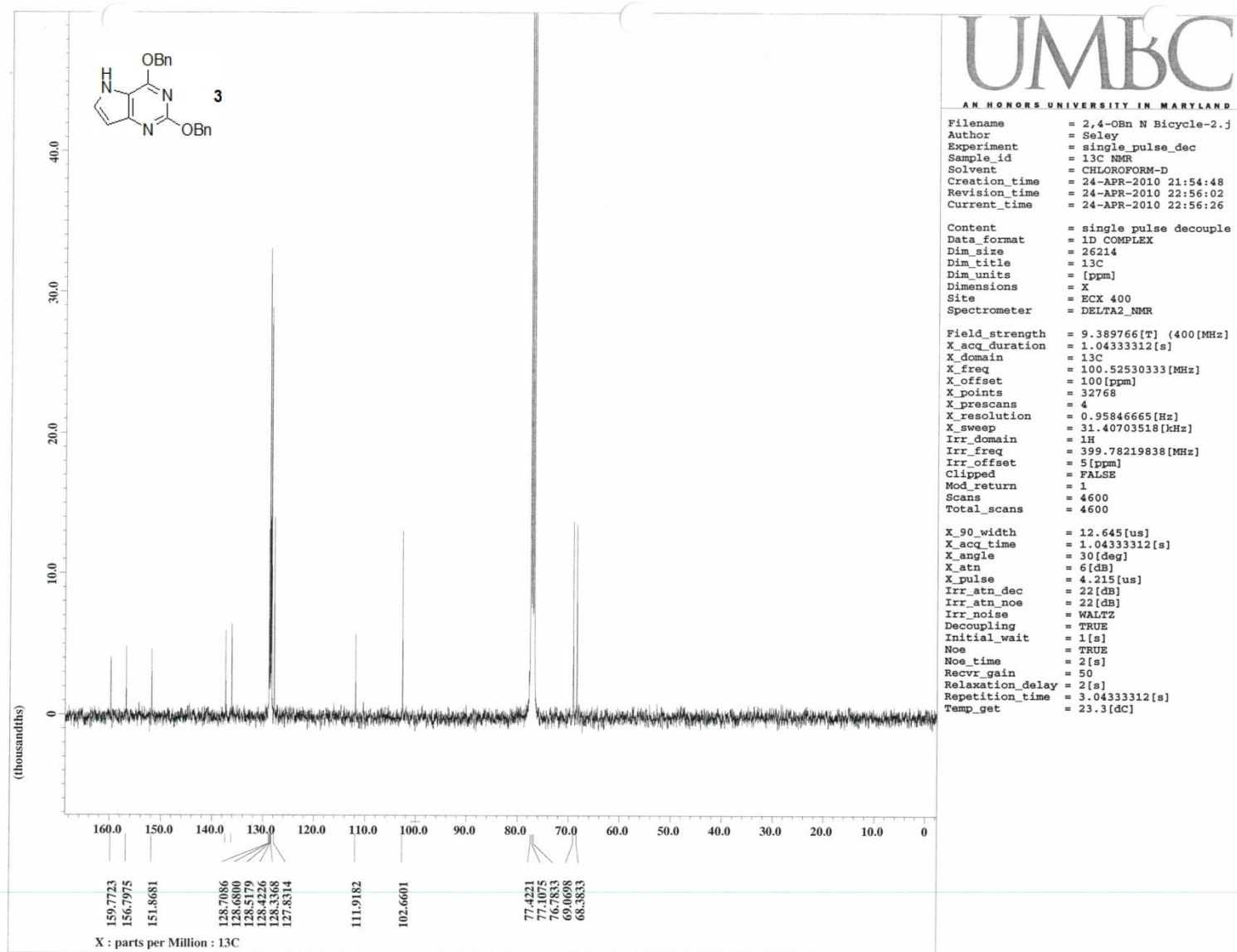
University of Maryland Baltimore County, 1000 Hilltop Circle, Baltimore, MD 21250, USA

*kseley@umbc.edu

Table of contents

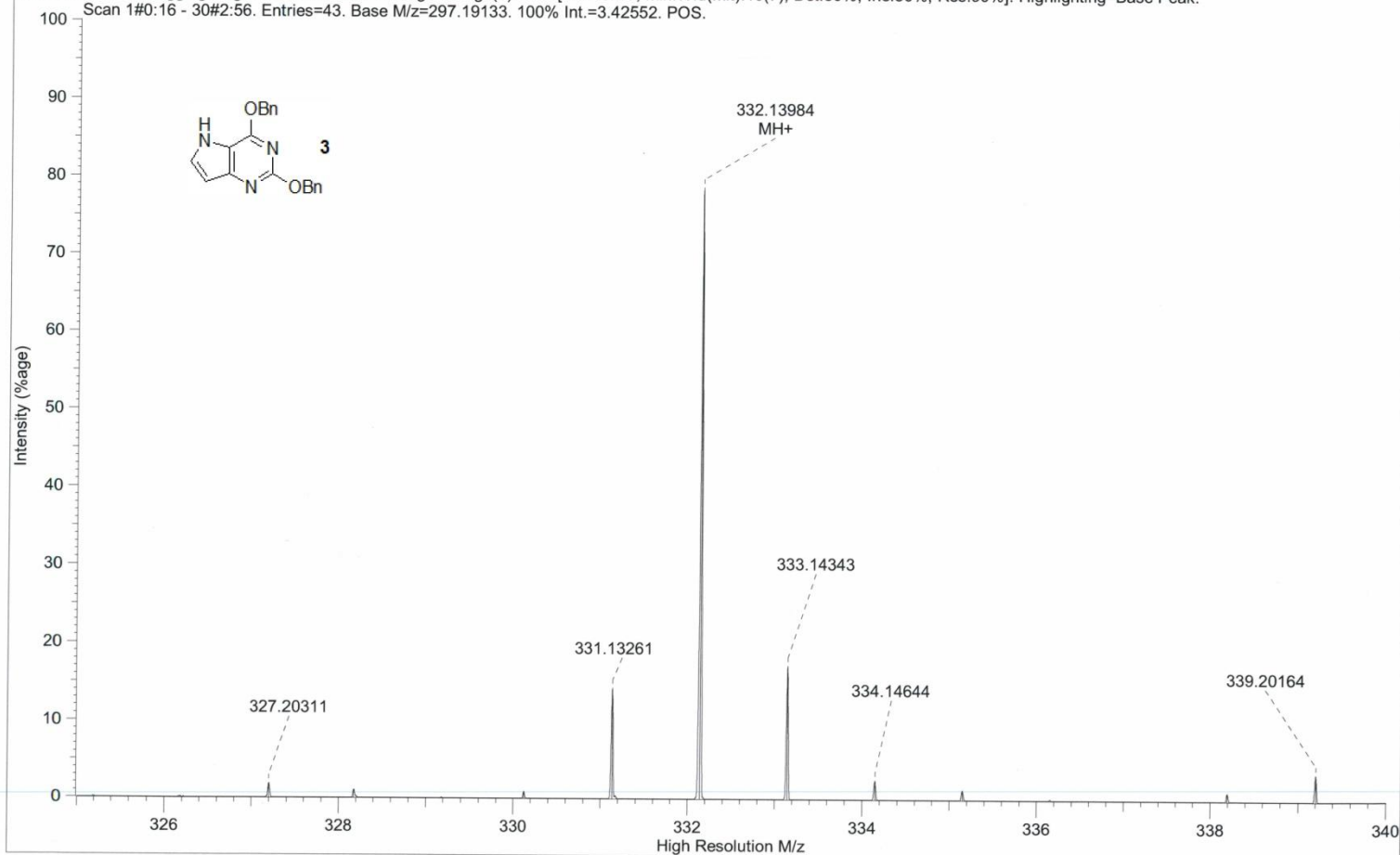
^1H NMR, ^{13}C NMR and Mass spectrometry spectra S2-S73

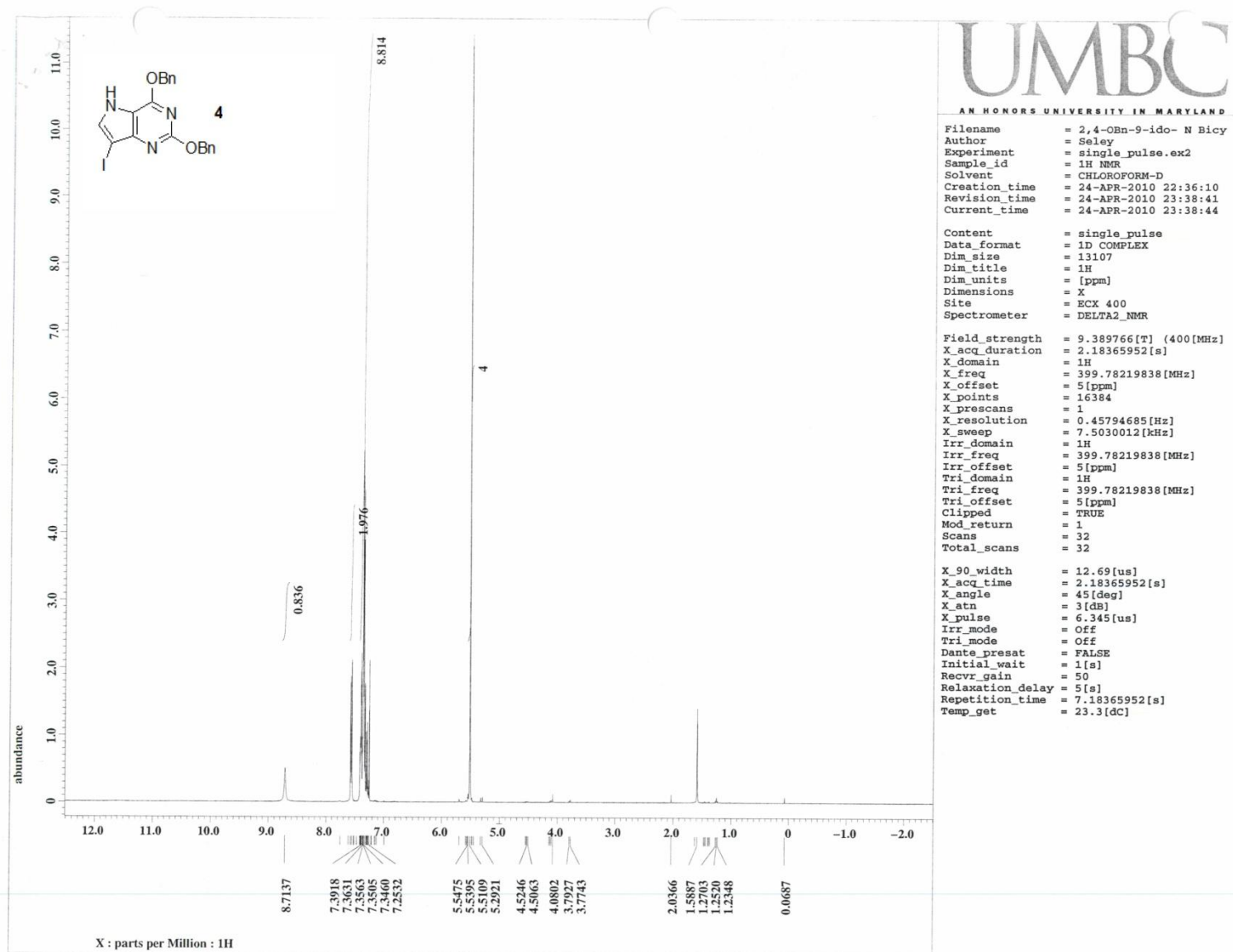


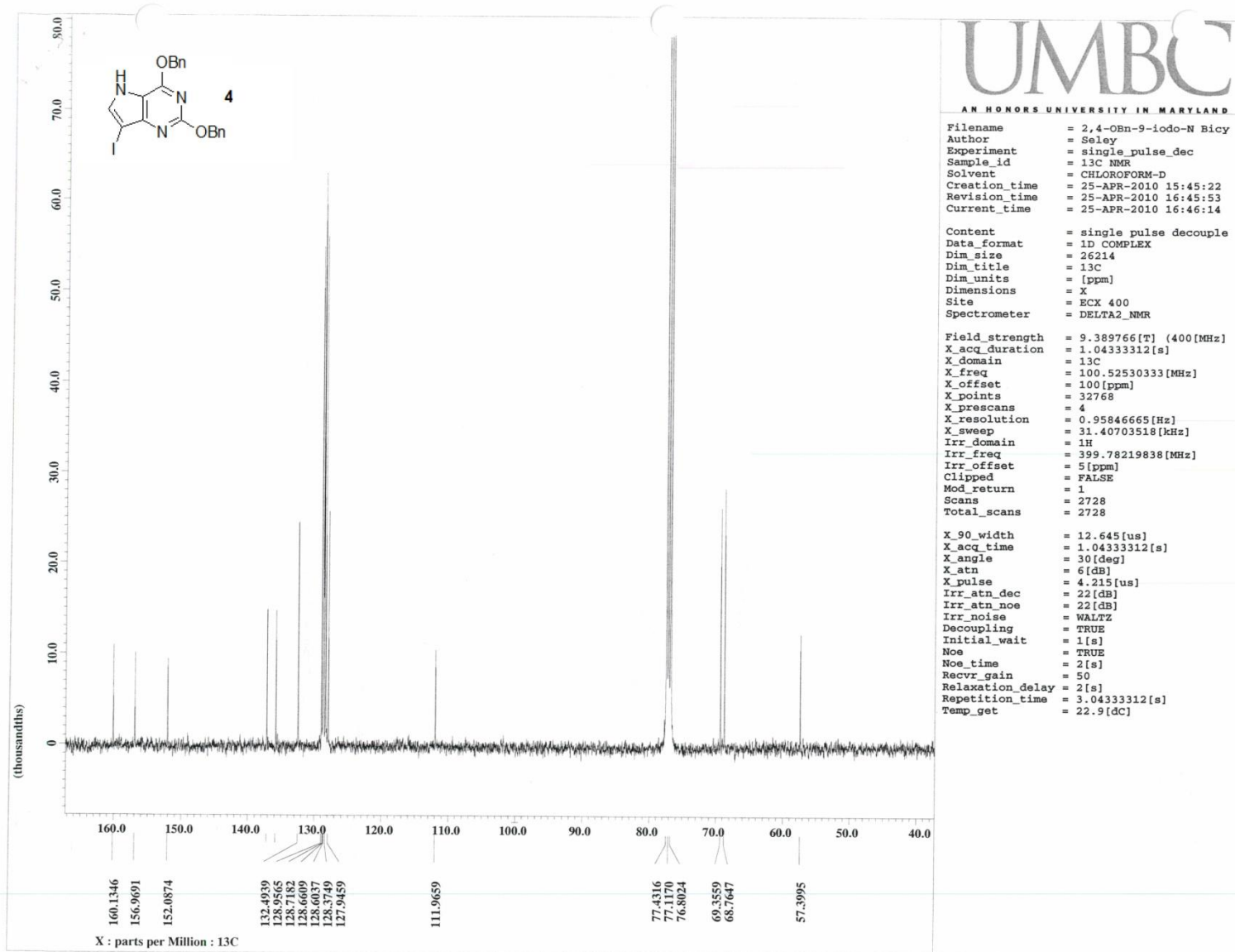


File Name : D:\VG70S Data\20130125\Zimmermann\KT_021_123\AccMass20PC_KT_021_123_20130128_1.ms2
Creation Date/Time : 1/28/2013 at 13:00:11
File Type : V/E raw data
File Source : Acquired on MASPEC II system [II32/1240]
File Title : FAB Accurate Mass Scan KT-02-123
Instrument : VG70SE
Notes : R = 10000, 20% Sweepwidth m/z = 291-350 amu, S = 25sec/dec
Sample in mNBA matrix on slated probe tip, PEGMME 350 mass ref
Gun = 28kV @ 2uA

SCAN GRAPH. Flagging=High Resolution M/z. Rolling Average(5). Ctd=[Thr:10mV, Min.Wid(Mlt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
Scan 1#0:16 - 30#2:56. Entries=43. Base M/z=297.19133. 100% Int.=3.42552. POS.

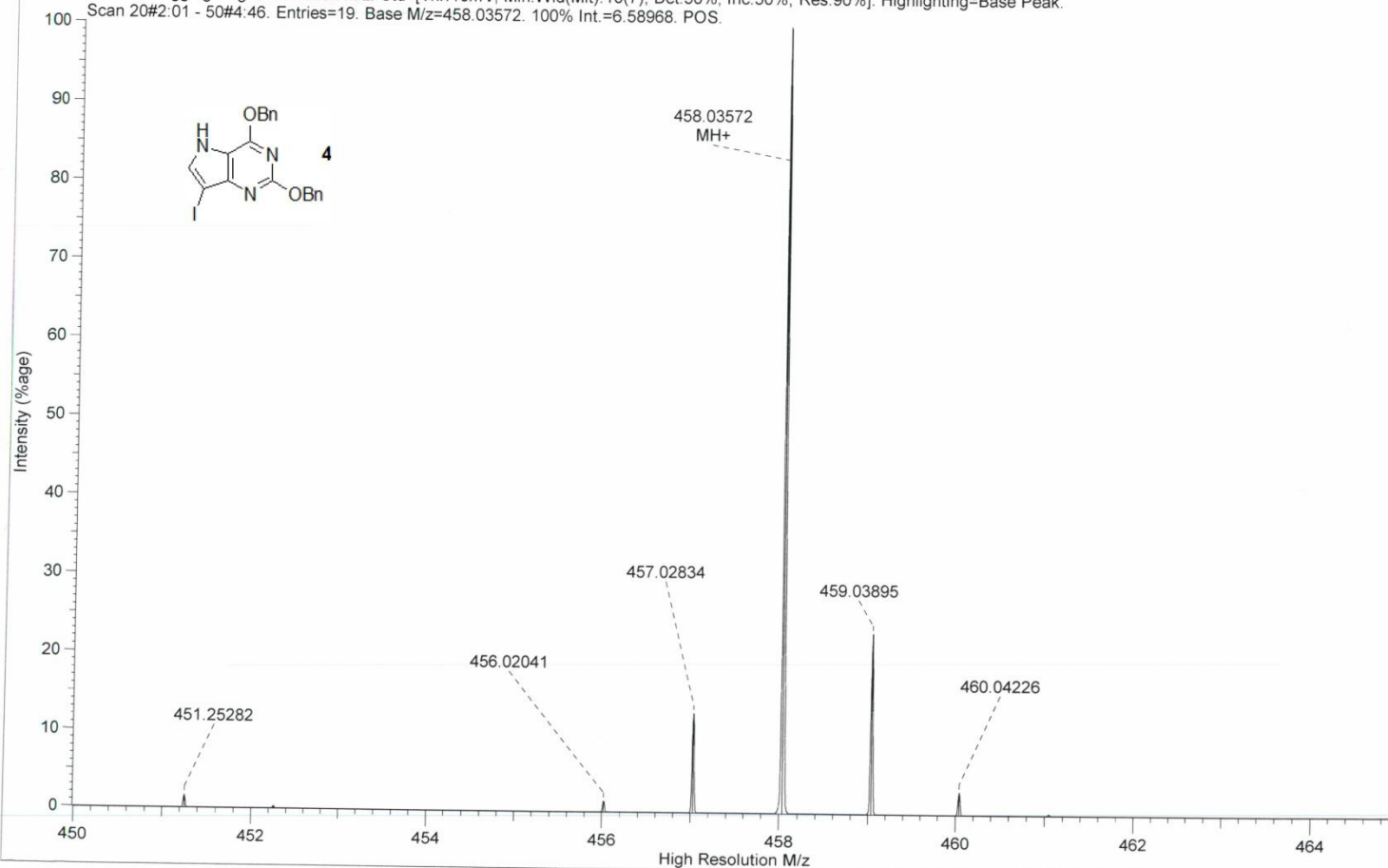


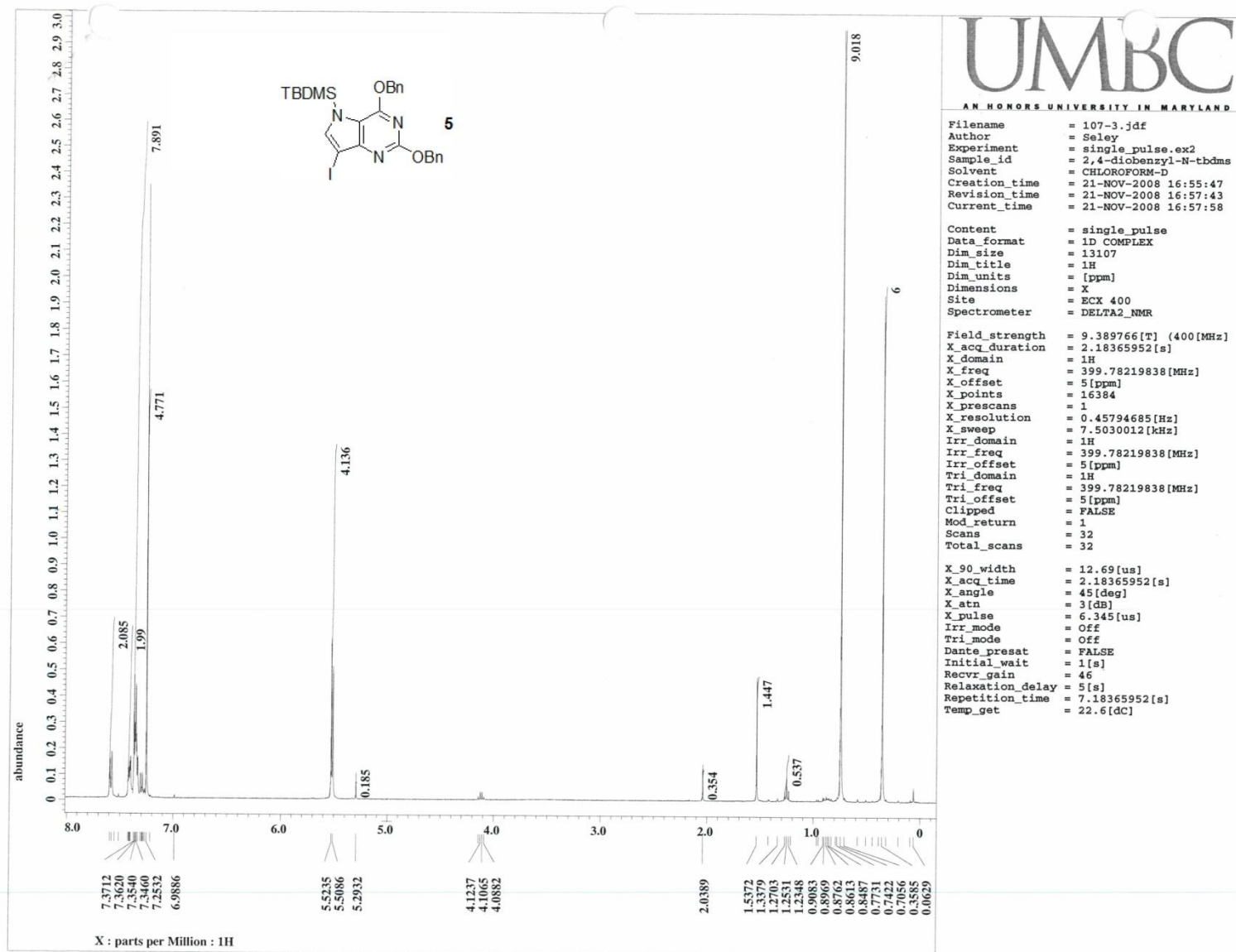


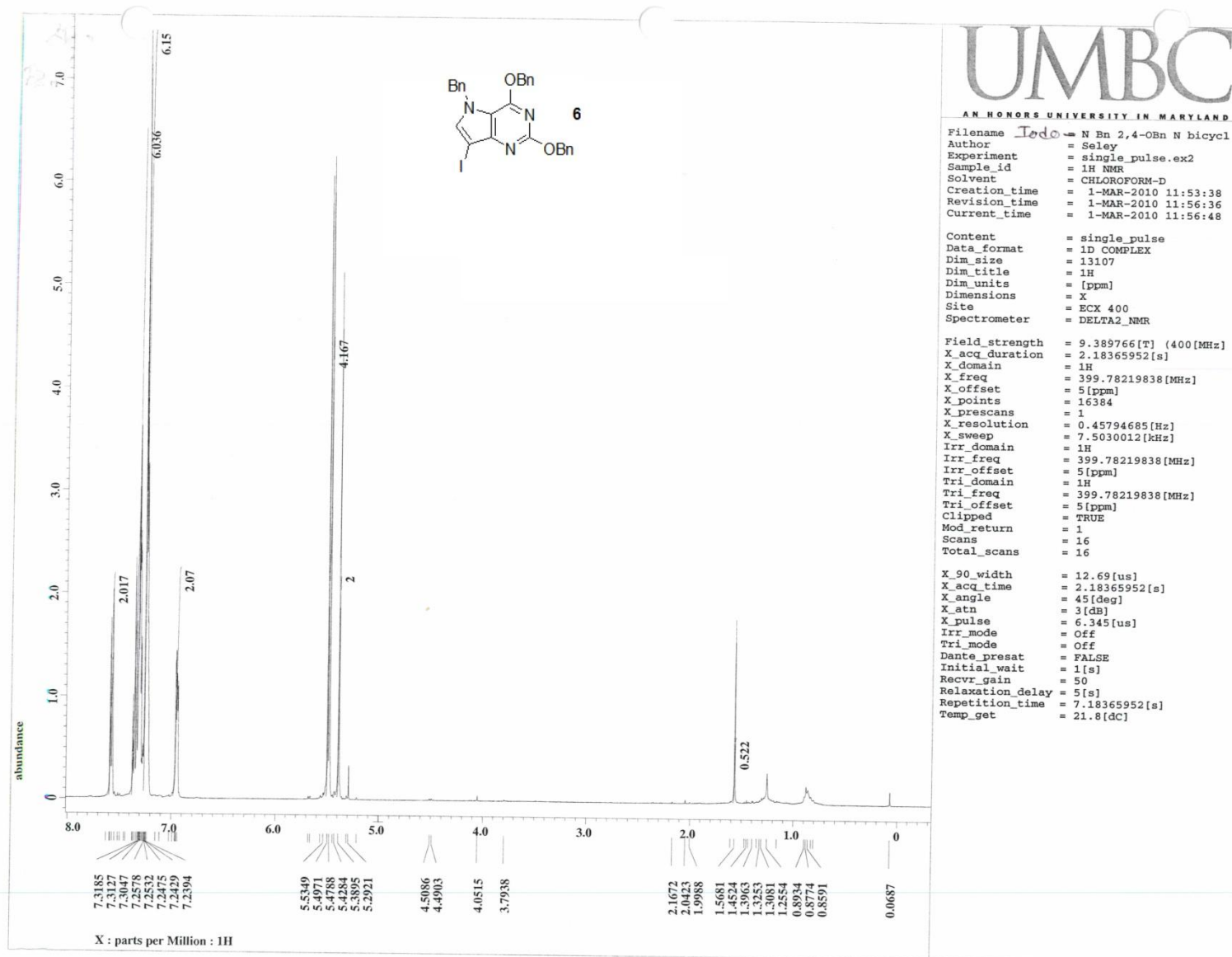


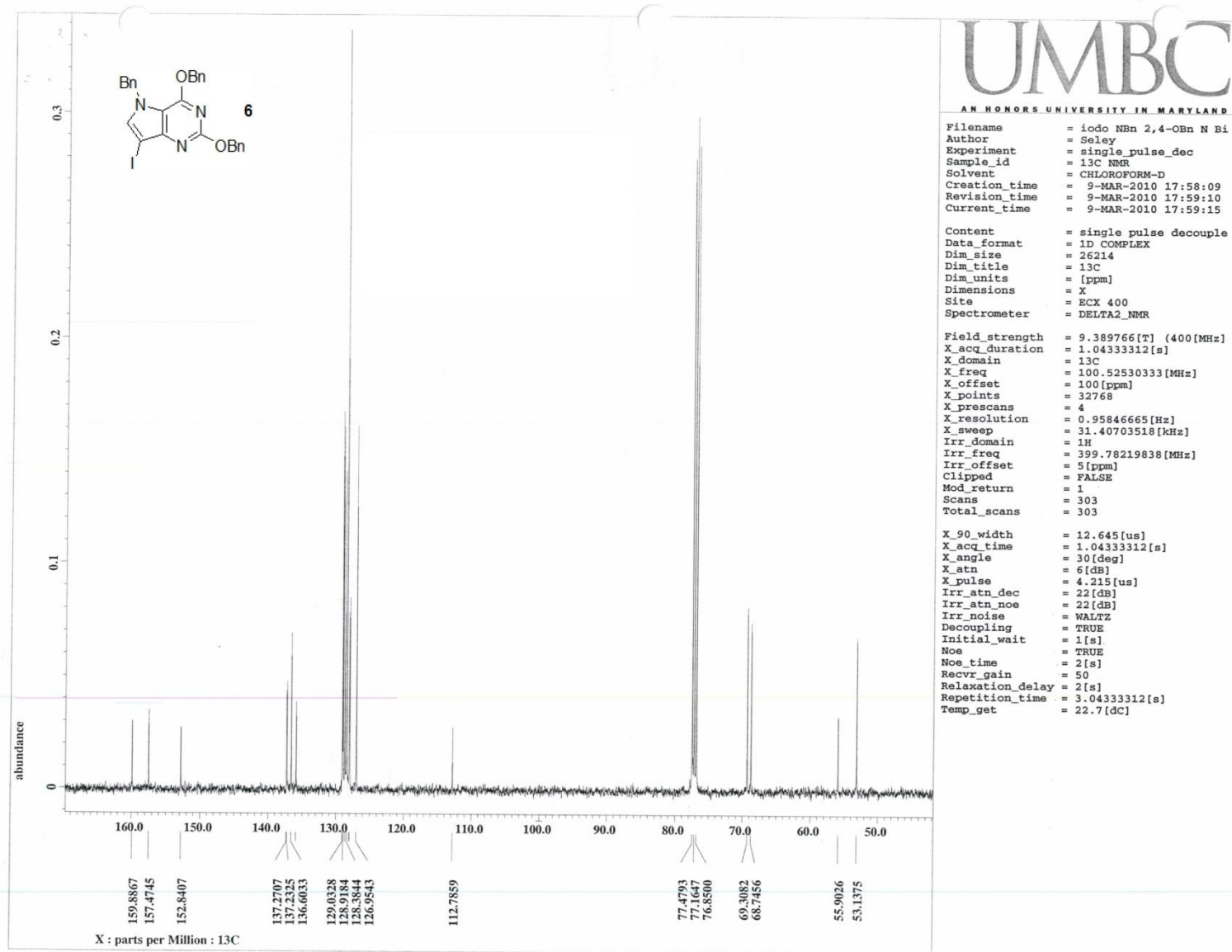
File Name : D:\VG70S Data\20100707\Kartik\KT_03_126\AccMass20PC_KT_03_126_20100708_1.ms2
Creation Date/Time : 7/8/2010 at 18:40:18
File Type : V/E raw data
File Source : Acquired on MASPEC II system [II32/1240]
File Title : FAB Accurate Mass Scan KT-3-126
Instrument : VG70S
Notes : R = 10000, 20% Sweepwidth m/z = 426-480 amu, S = 25sec/dec
Sample in mNBA matrix on slated probe tip, PEGME 550 mass ref
Gun = 28kV @ 2uA

SCAN GRAPH. Flagging=High Resolution M/z. Ctd=[Thr:10mV, Min.Wid(Mlt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
Scan 20#2:01 - 50#4:46. Entries=19. Base M/z=458.03572. 100% Int.=6.58968. POS.



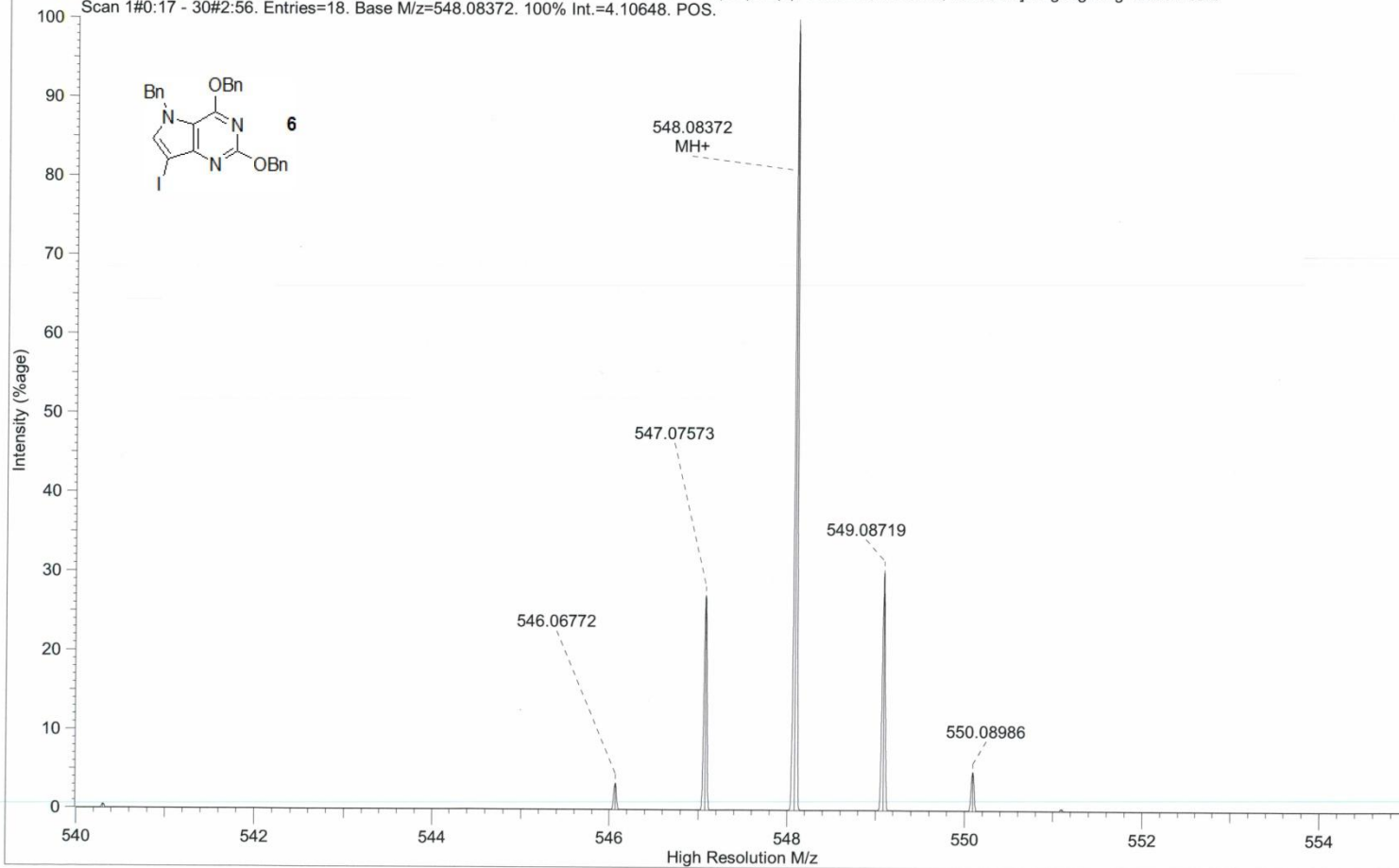


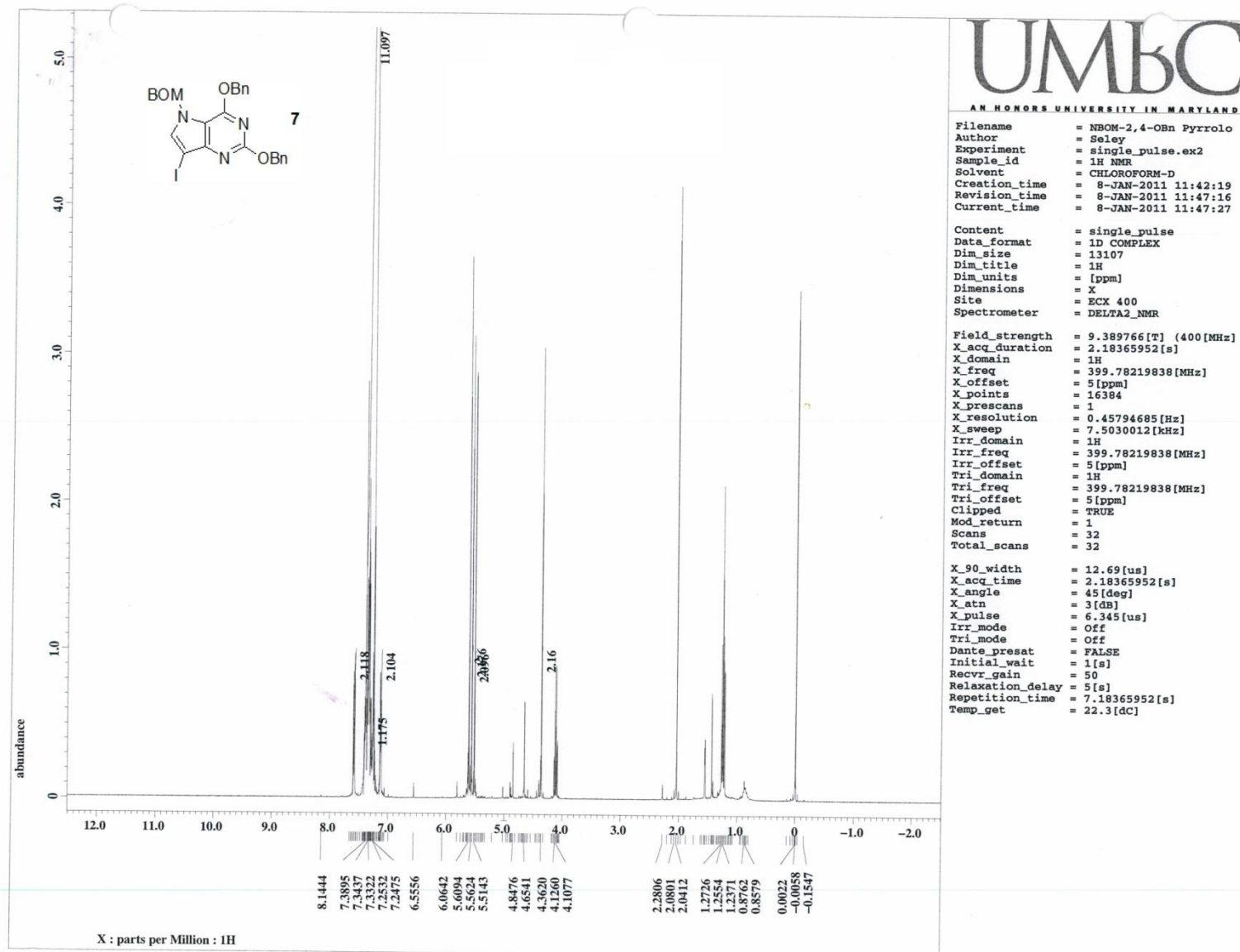


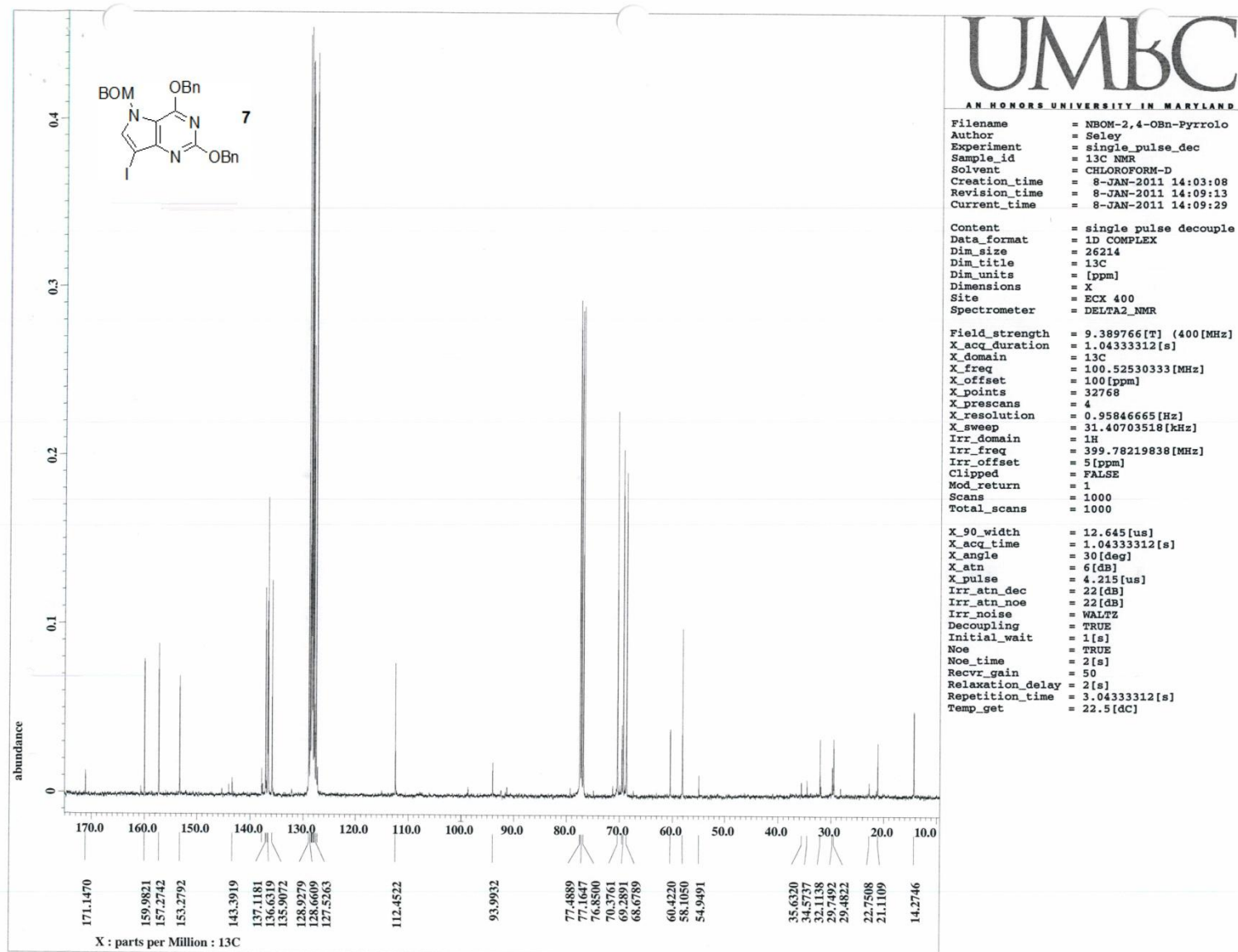


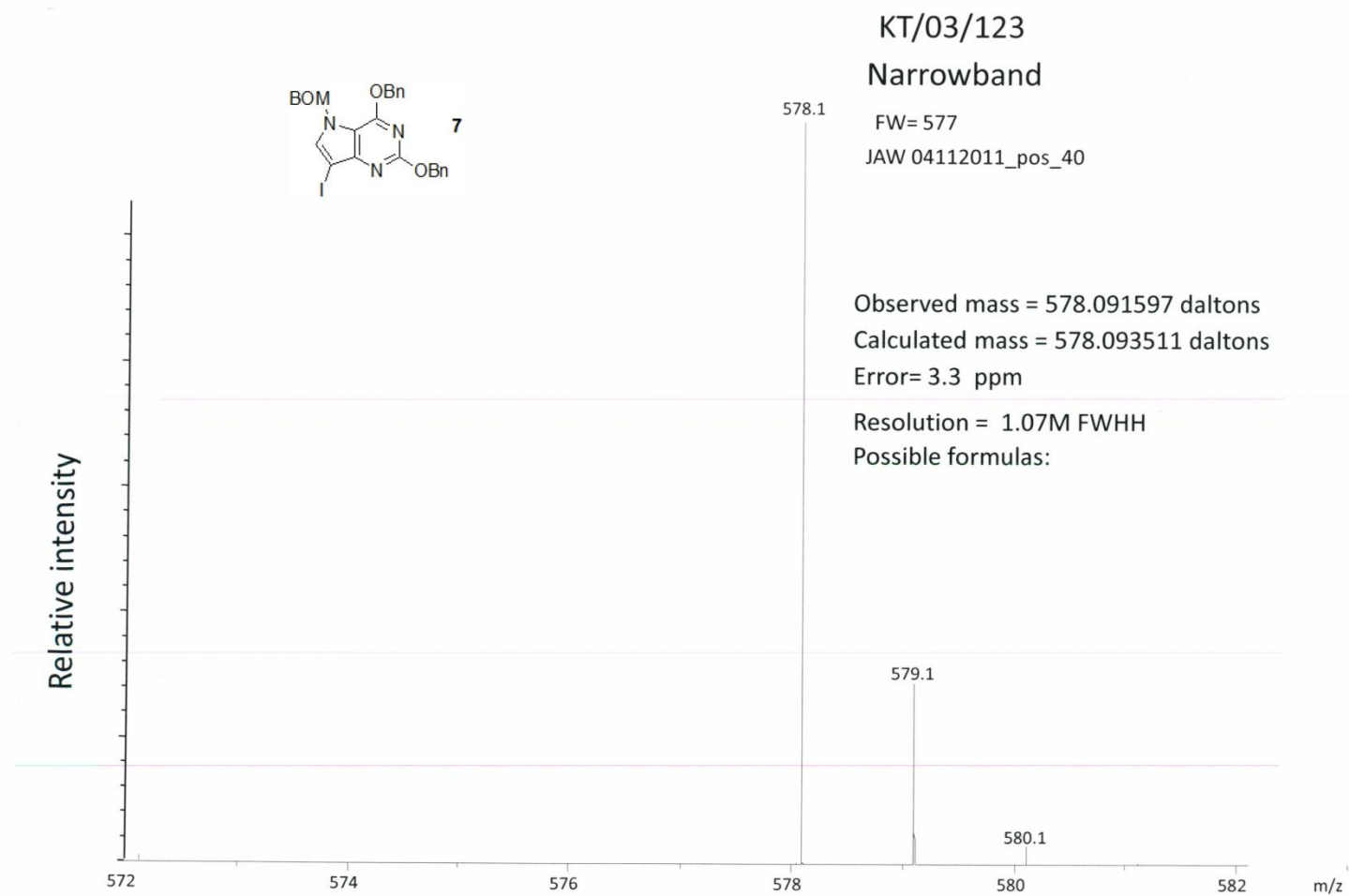
File Name : D:\VG70S Data\20130313\Kartik\KT_03_36\AccMass20PC_KT_03_36_20130314_2.ms2
Creation Date/Time : 3/14/2013 at 19:08:31
File Type : V/E raw data
File Source : Acquired on MASPEC II system [II32/1240]
File Title : FAB Accurate Mass Scan KT-03-36
Instrument : VG70SE
Notes : R = 10000, 20% Sweepwidth m/z = 511-565 amu, S = 25sec/dec
Sample in mNBA matrix on slated probe tip, PEGMME 550 mass ref
Gun = 28kV @ 2uA

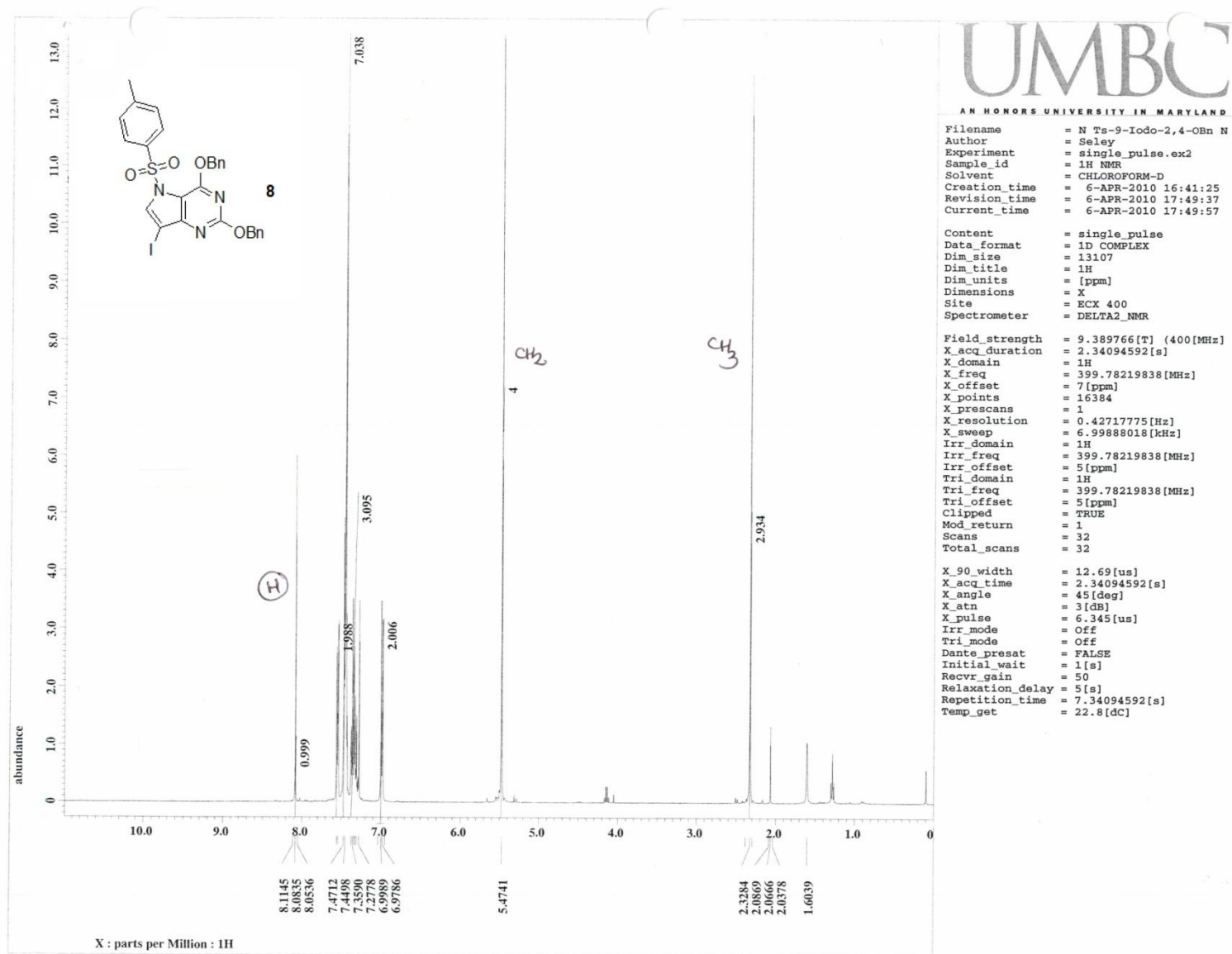
SCAN GRAPH. Flagging=High Resolution M/z. Rolling Average(5). Ctd=[Thr:10mV, Min.Wid(MIt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
Scan 1#0:17 - 30#2:56. Entries=18. Base M/z=548.08372. 100% Int.=4.10648. POS.

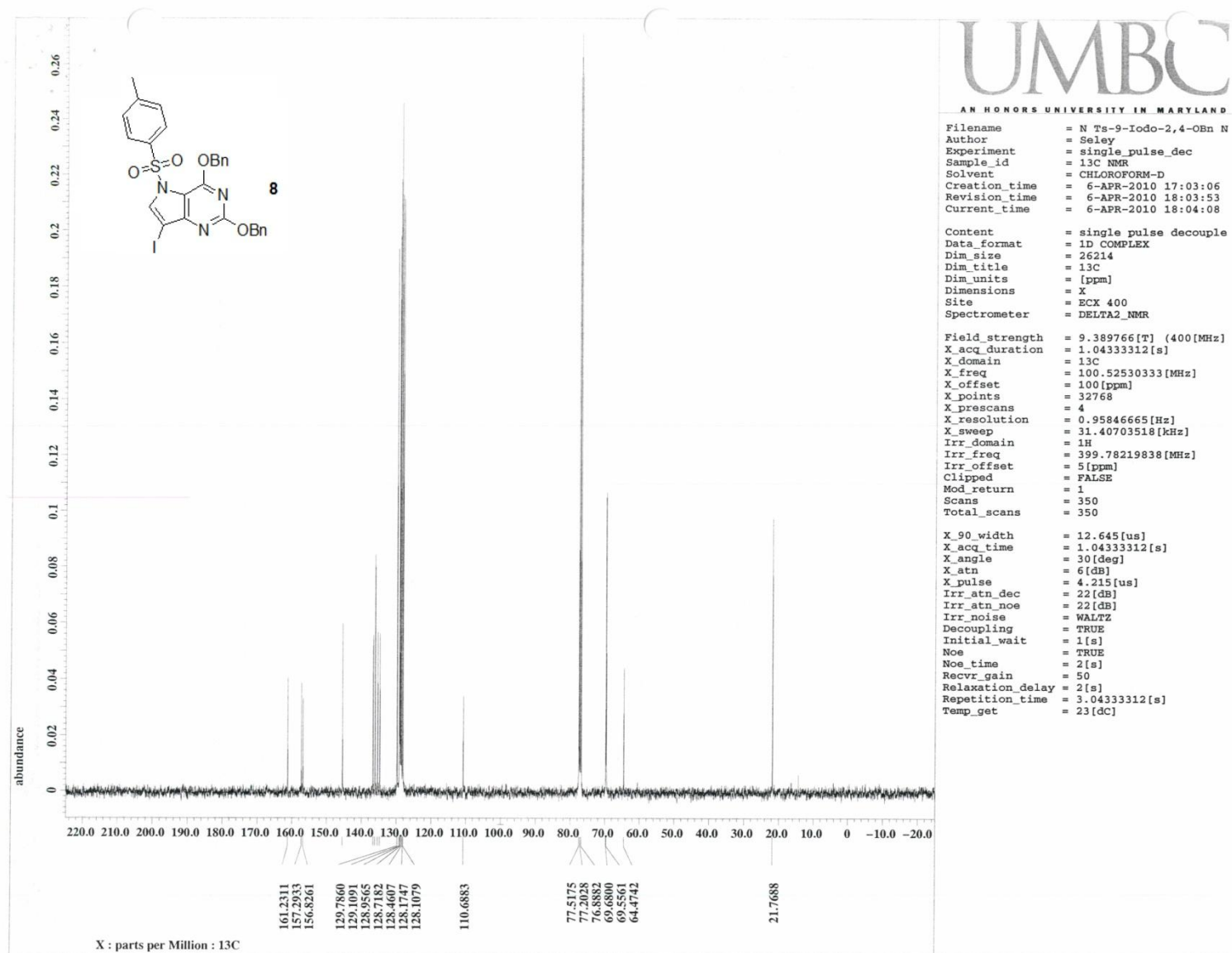






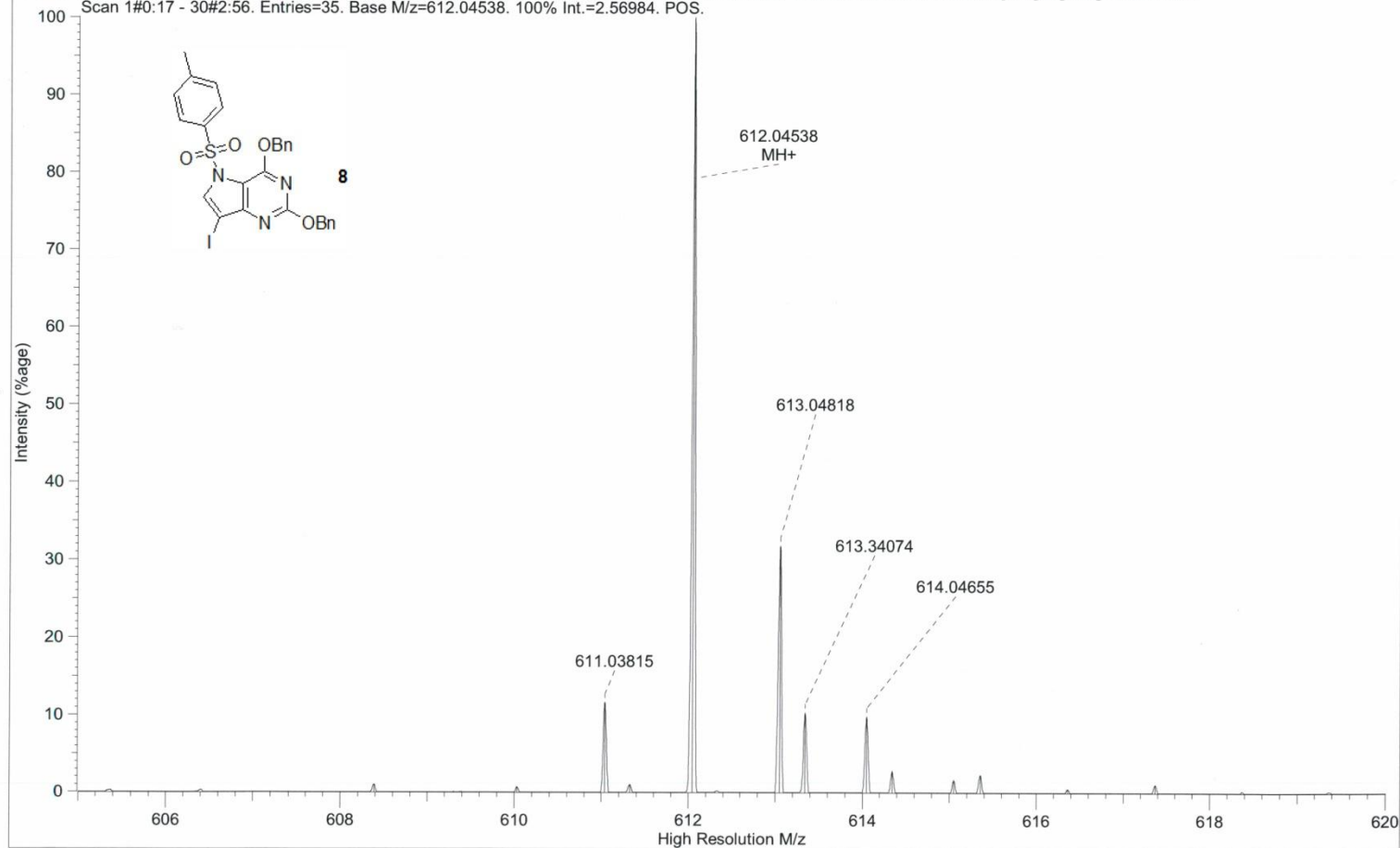


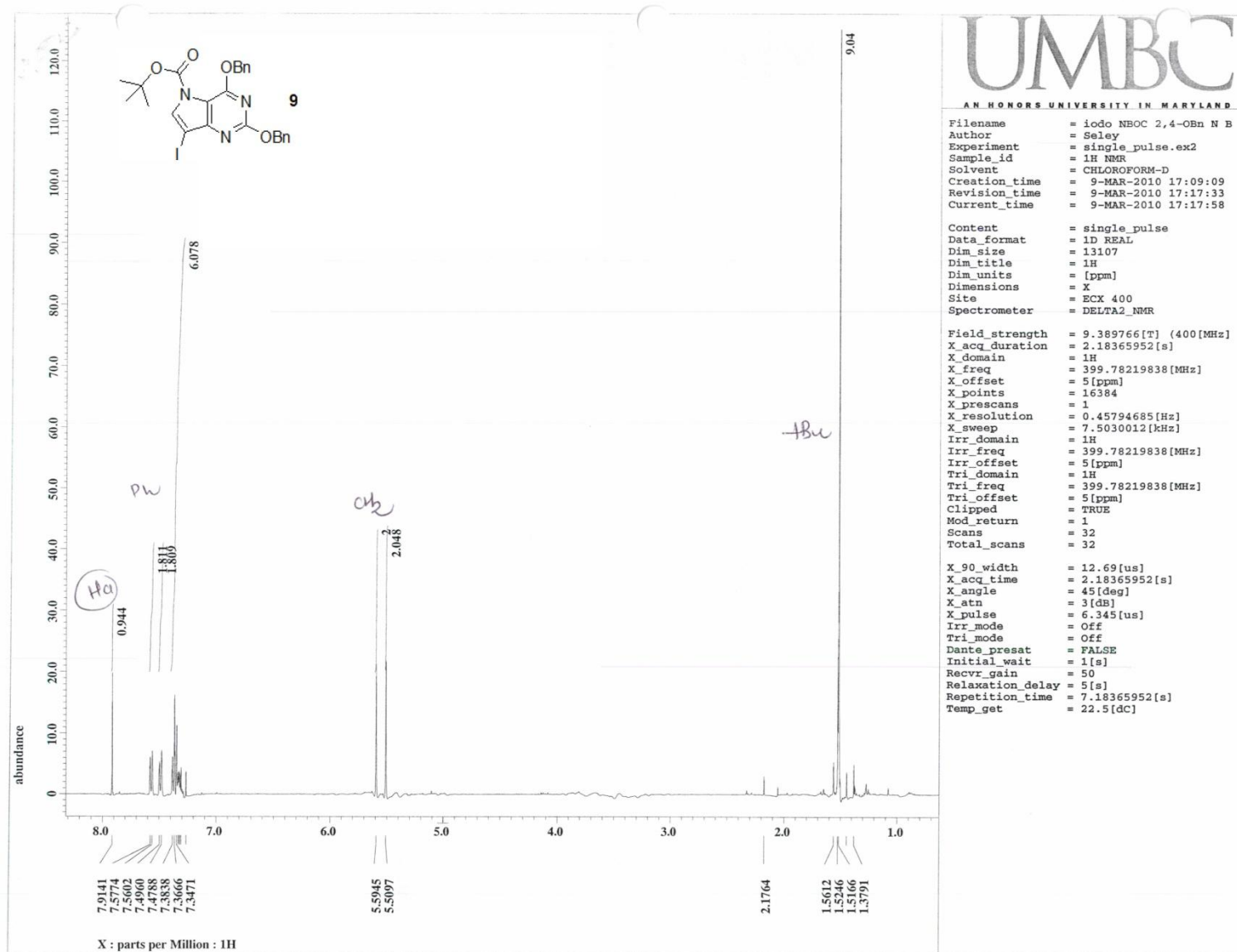


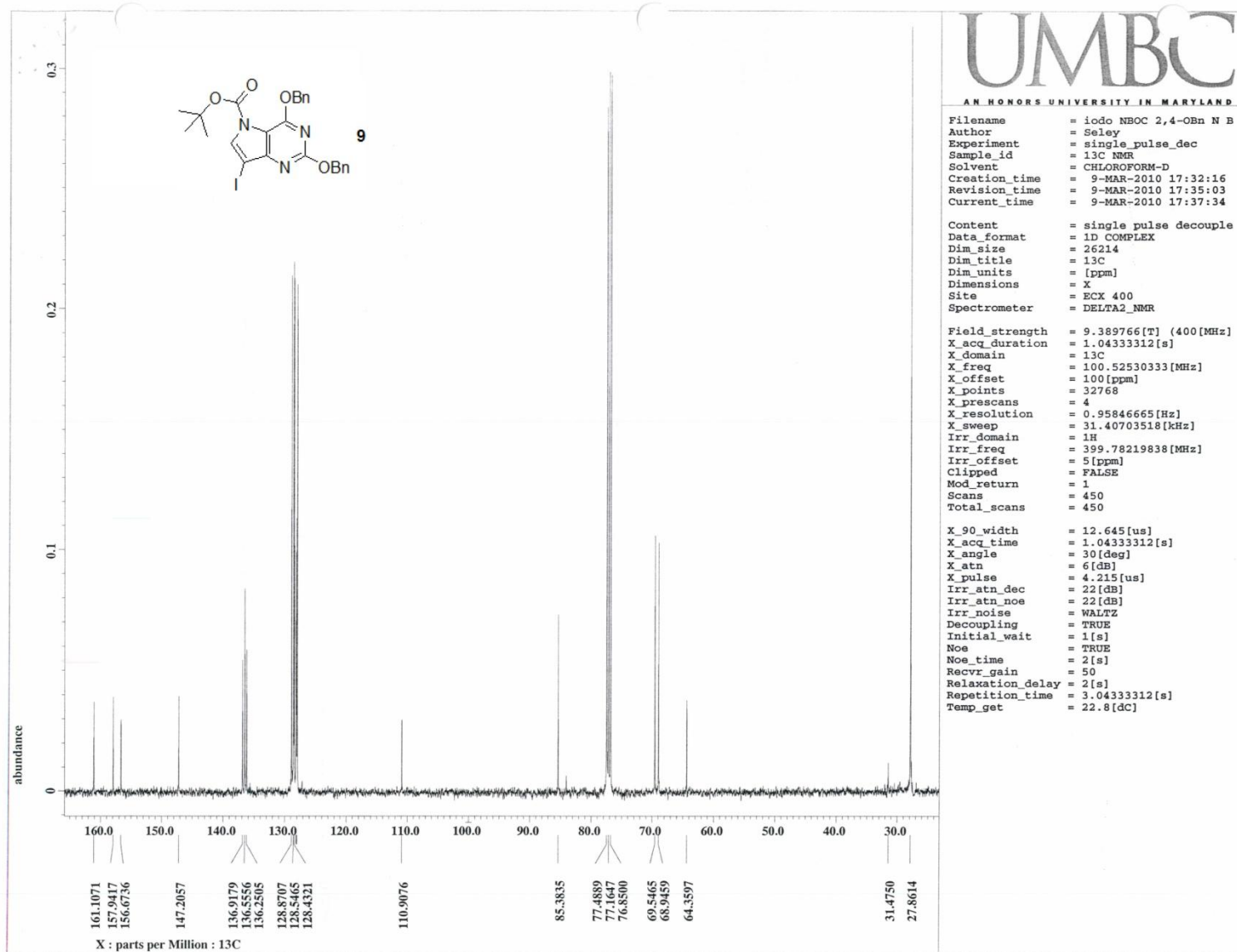


File Name : D:\VG70S Data\20130313\Kartik\KT_03_51\AccMass20PC_KT_03_51_20130314_1.ms2
Creation Date/Time : 3/14/2013 at 18:08:37
File Type : V/E raw data
File Source : Acquired on MASPEC II system [I132/1240]
File Title : FAB Accurate Mass Scan KT-03-51
Instrument : VG70SE
Notes : R = 10000, 20% Sweepwidth m/z = 586-640 amu, S = 25sec/dec
Sample in mNBA matrix on slated probe tip, PEG 600 mass ref
Gun = 28kV @ 2uA

SCAN GRAPH. Flagging=High Resolution M/z. Rolling Average(5). Ctd=[Thr:10mV, Min.Wid(Mlt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
Scan 1#0:17 - 30#2:56. Entries=35. Base M/z=612.04538. 100% Int.=2.56984. POS.

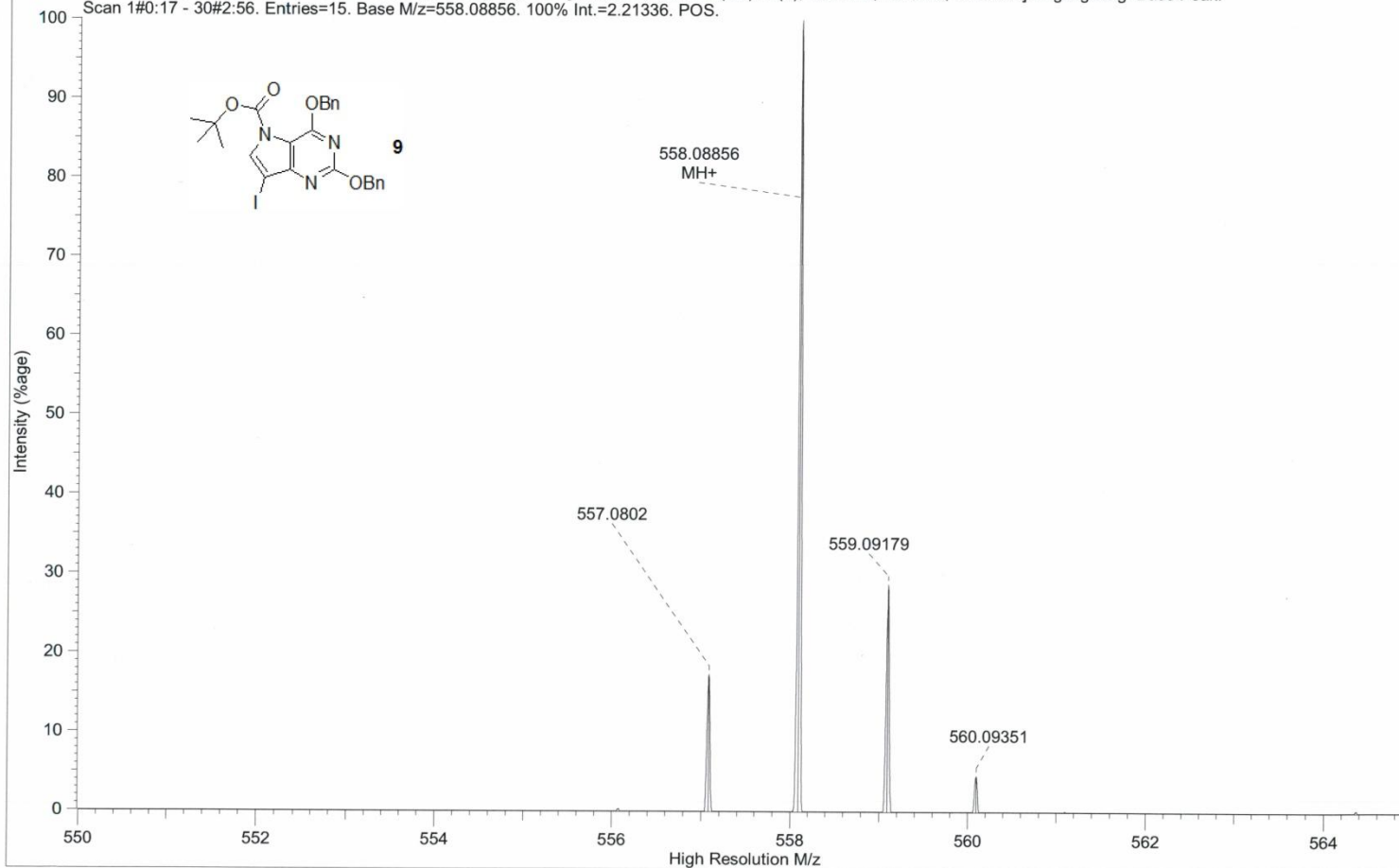


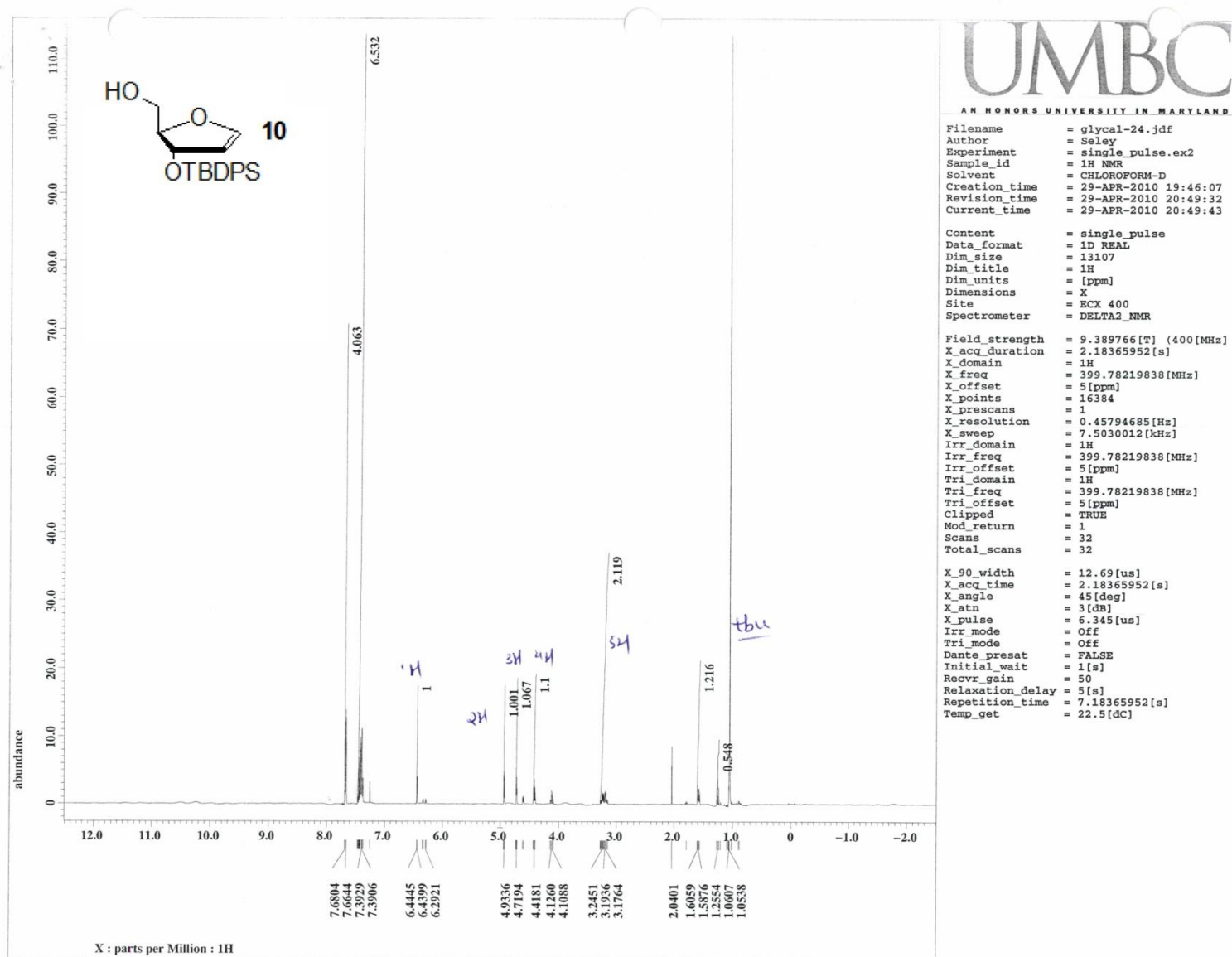


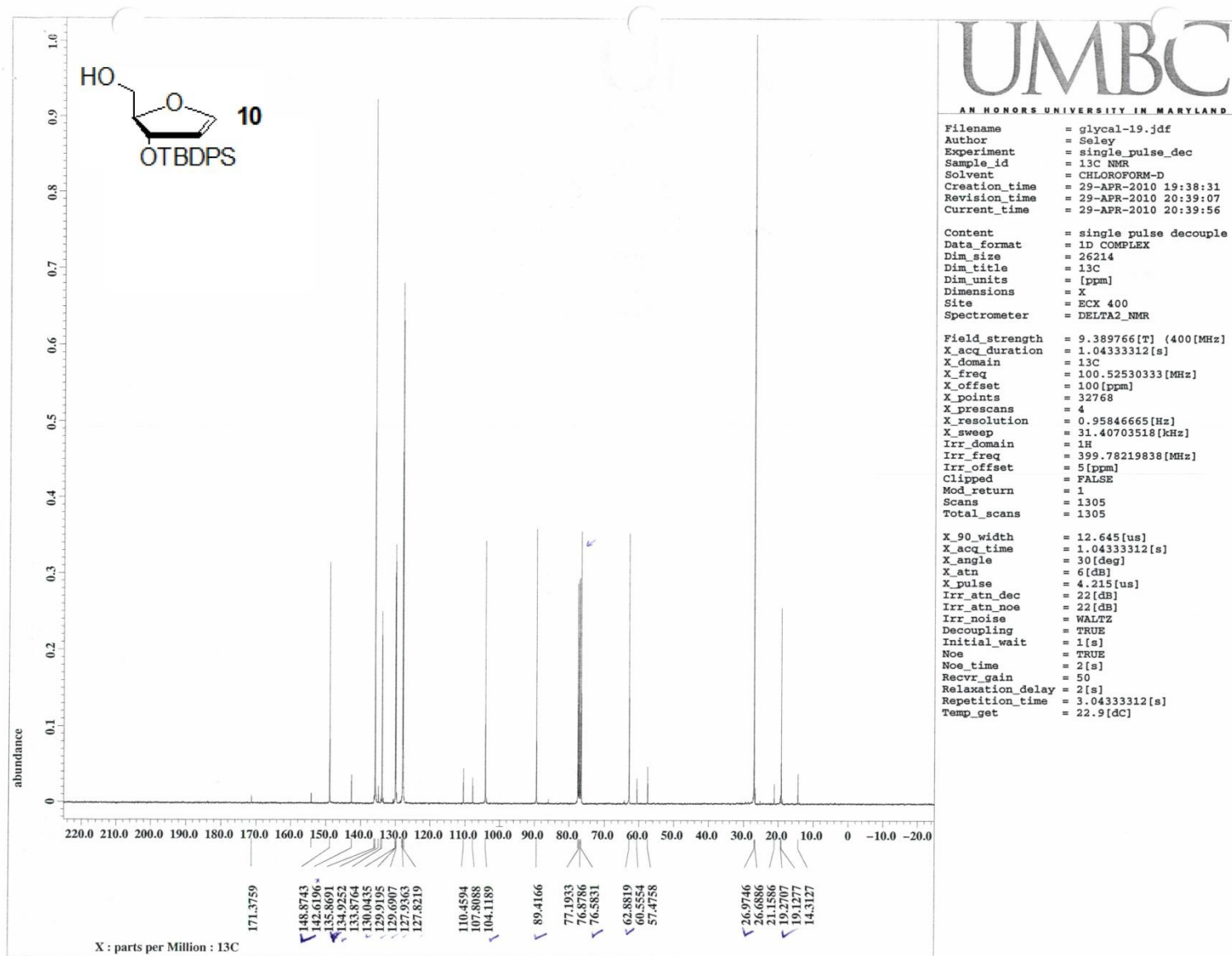


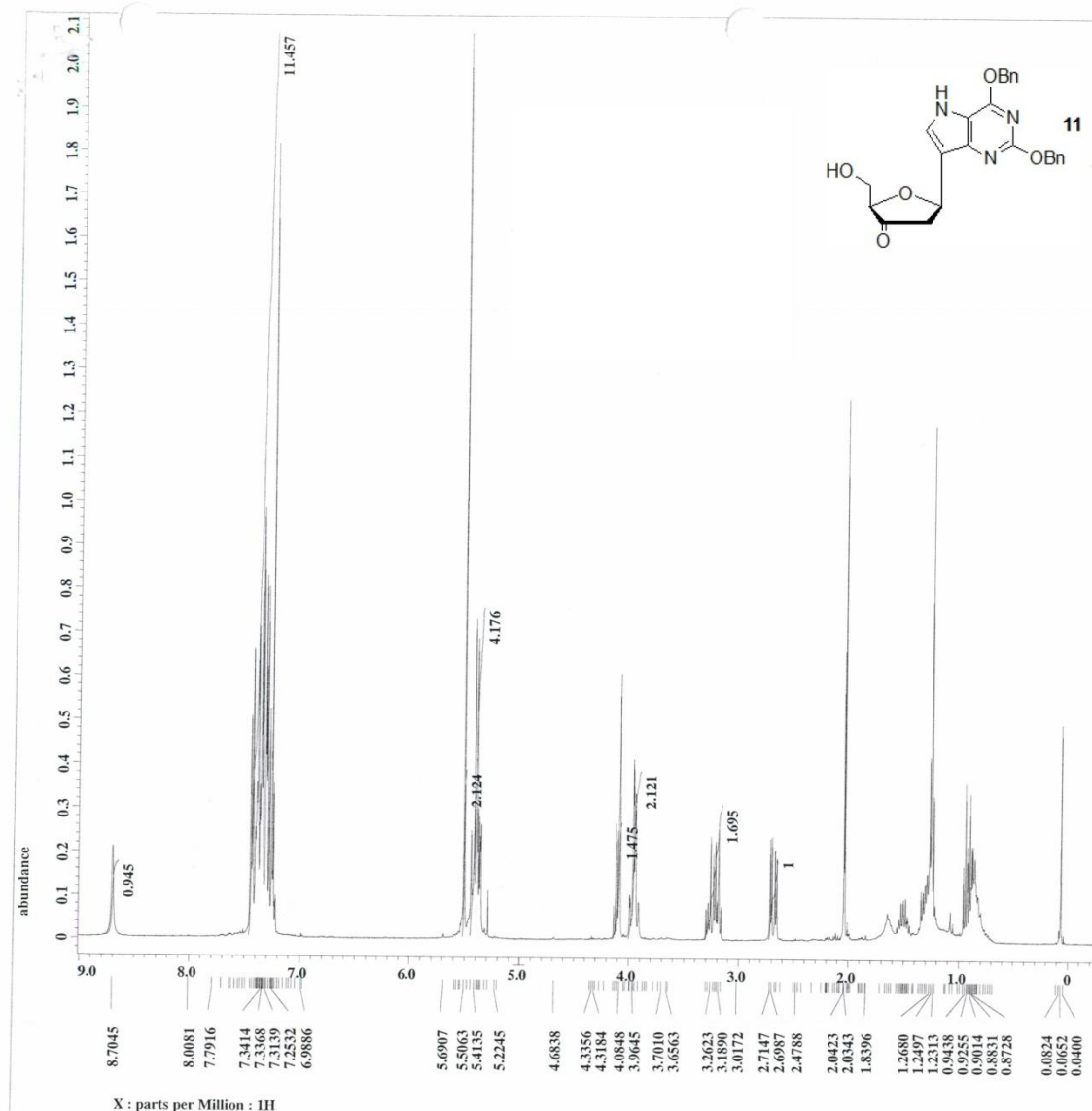
File Name : D:\VG70S Data\20130313\Kartik\VG197\AccMass20PC_VGF197_20130314_2.ms2
Creation Date/Time : 3/14/2013 at 19:20:41
File Type : V/E raw data
File Source : Acquired on MASPEC II system [I132/1240]
File Title : FAB Accurate Mass Scan VGF197
Instrument : VG70SE
Notes : R = 10000, 20% Sweepwidth m/z = 541-600 amu, S = 25sec/dec
Sample in mNBA matrix on slated probe tip, PEG 600 mass ref
Gun = 28kV @ 2uA

SCAN GRAPH. Flagging=High Resolution M/z. Rolling Average(5). Ctd=[Thr:10mV, Min.Wid(Mlt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
Scan 1#0:17 - 30#2:56. Entries=15. Base M/z=558.08856. 100% Int.=2.21336. POS.









UMBC

AN HONORS UNIVERSITY IN MARYLAND

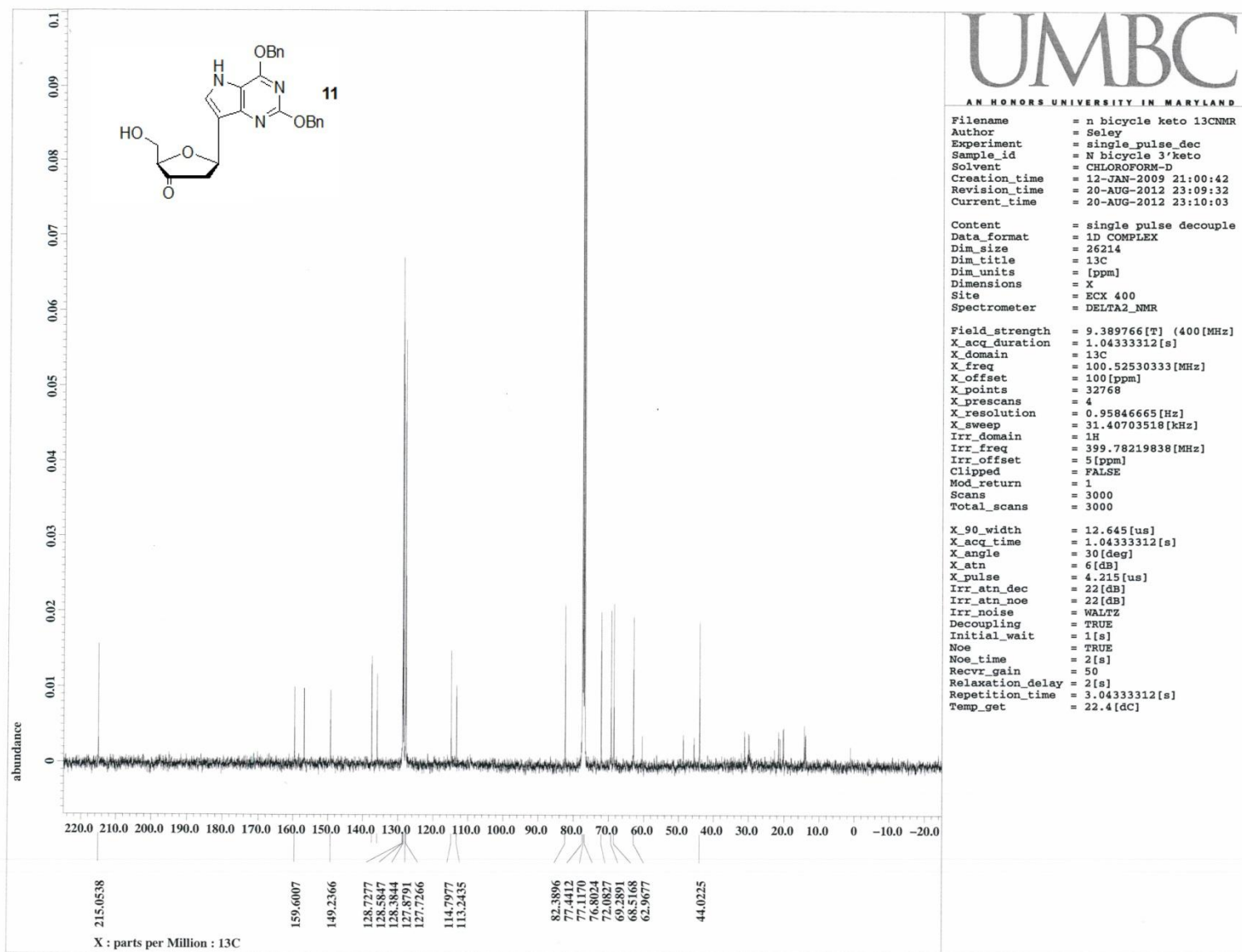
Filename = n bicycle keto-3.jdf
 Author = Seley
 Experiment = single_pulse.ex2
 Sample_id = n bicycle 3' keto
 Solvent = CHLOROFORM-D
 Creation_time = 12-JAN-2009 18:17:05
 Revision_time = 12-JAN-2009 18:19:09
 Current_time = 12-JAN-2009 18:19:22

Content = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 2.18365952[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.45794685[Hz]
 X_sweep = 7.5030012[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 32
 Total_scans = 32

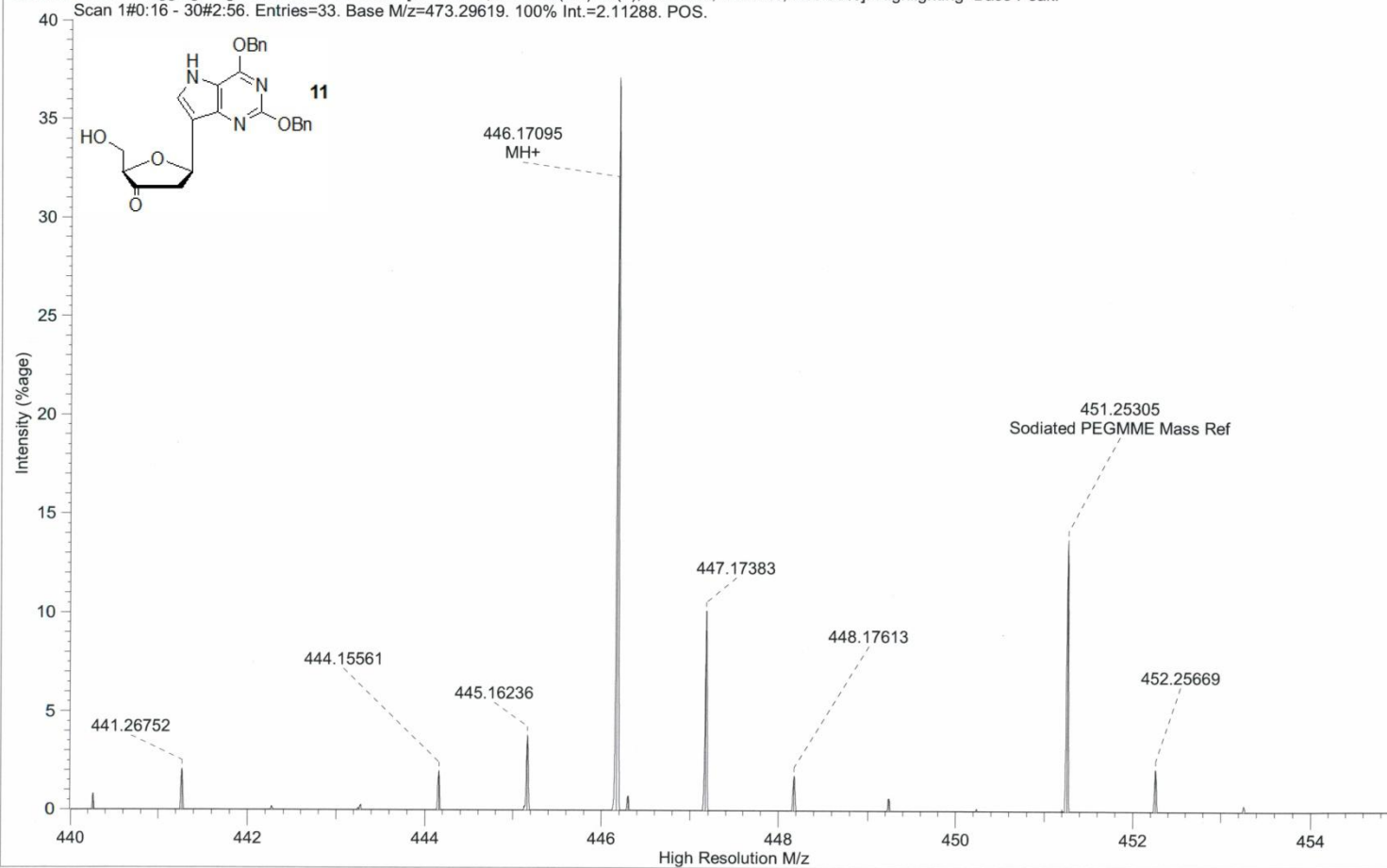
X_90_width = 12.69[us]
 X_acq_time = 2.18365952[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 6.345[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 40
 Relaxation_delay = 5[s]
 Repetition_time = 7.18365952[s]
 Temp_get = 22.1[dC]

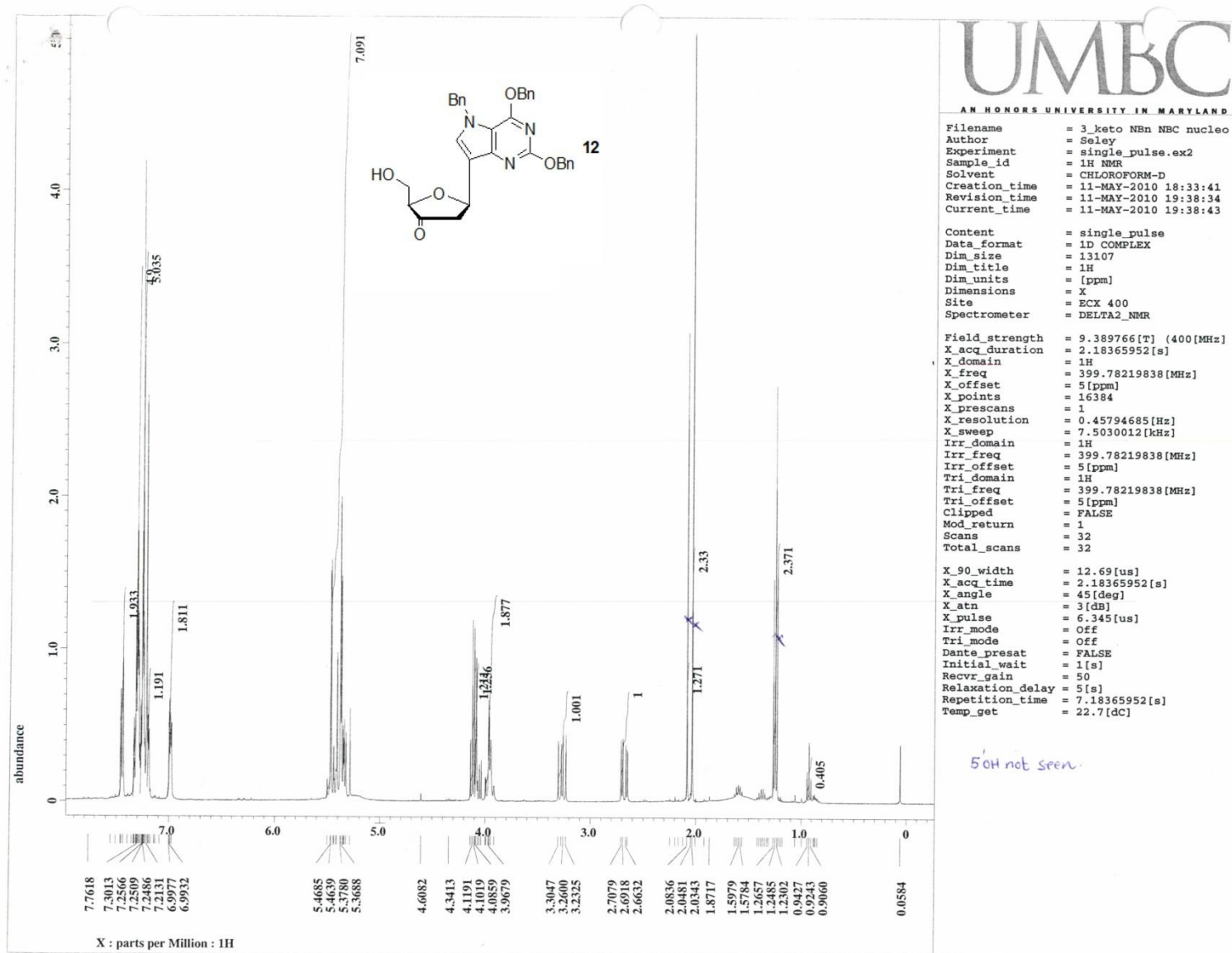
5' OH not seen.

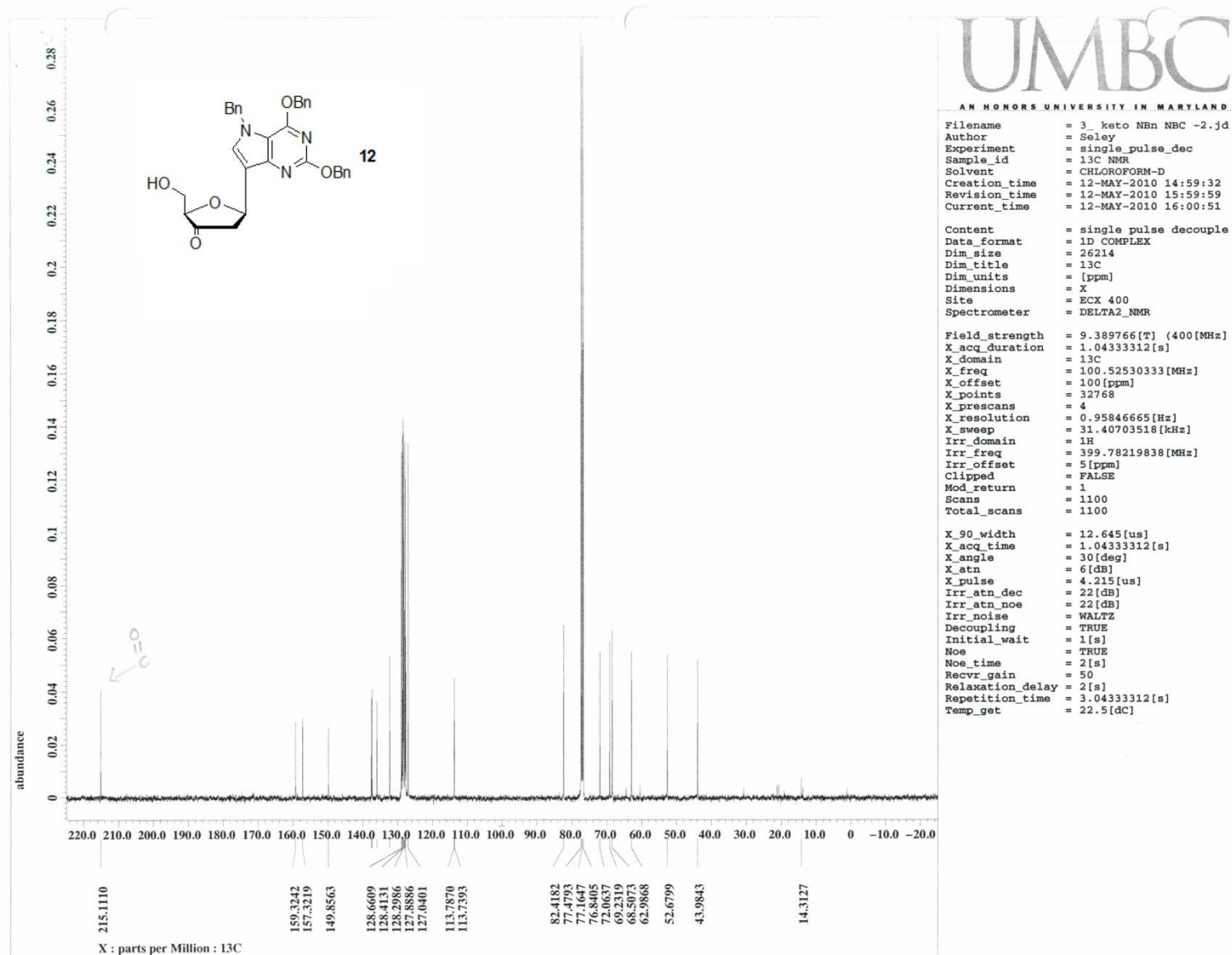


File Name : D:\VG70S Data\20100707\Kartik\KT_03_128\AccMass20PC_KT_03_128_20100708_2.ms2
Creation Date/Time : 7/8/2010 at 18:11:42
File Type : V/E raw data
File Source : Acquired on MASPEC II system [I132/1240]
File Title : FAB Accurate Mass Scan KT-3-128
Instrument : VG70S
Notes : R = 10000, 20% Sweepwidth m/z = 426-480 amu, S = 25sec/dec
Sample in mNBA matrix on slated probe tip, PEGME 550 mass ref
Gun = 28kV @ 2uA

SCAN GRAPH. Flagging=High Resolution M/z. Ctd=[Thr:10mV, Min.Wid(Mlt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
Scan 1#0:16 - 30#2:56. Entries=33. Base M/z=473.29619. 100% Int.=2.11288. POS.

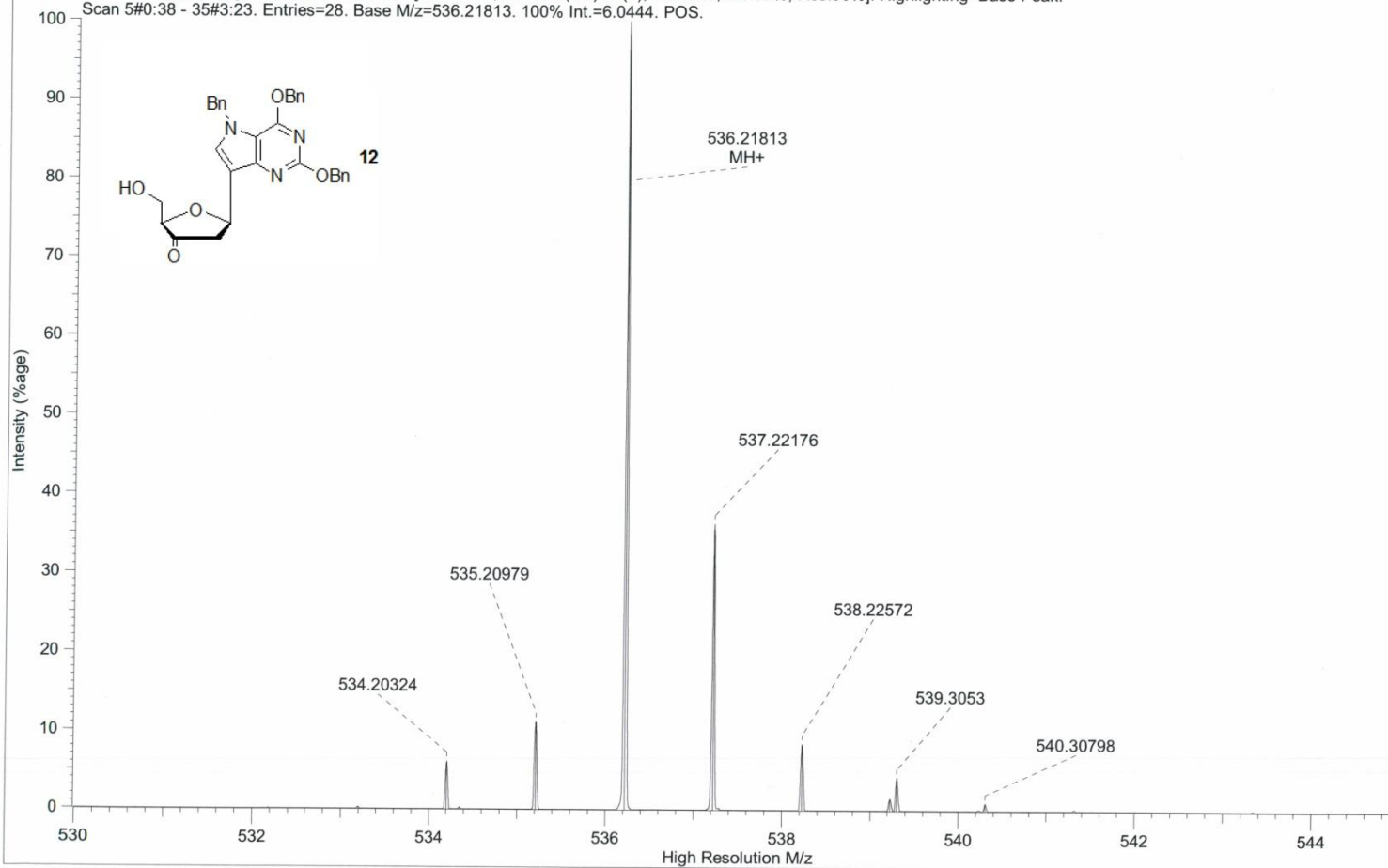


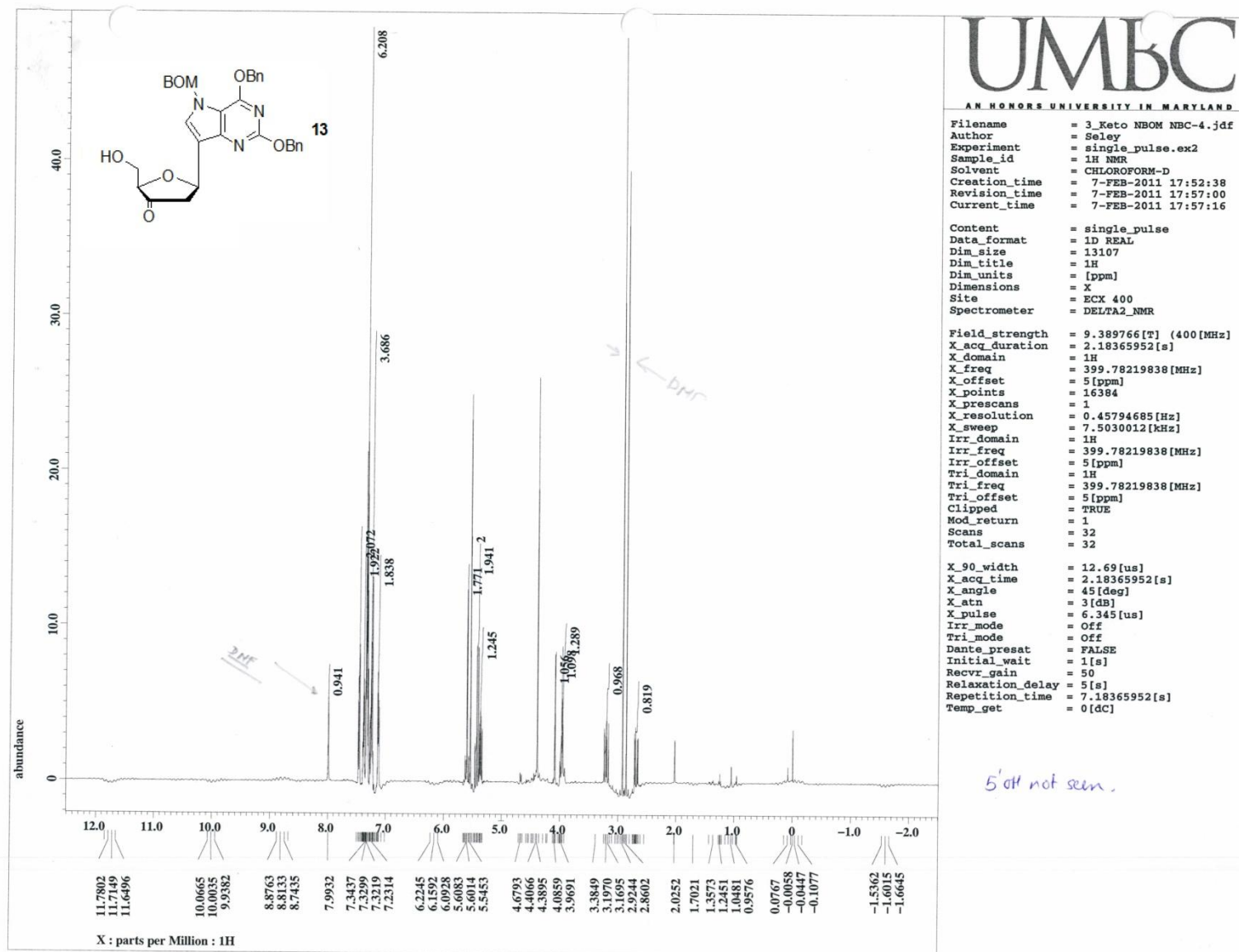


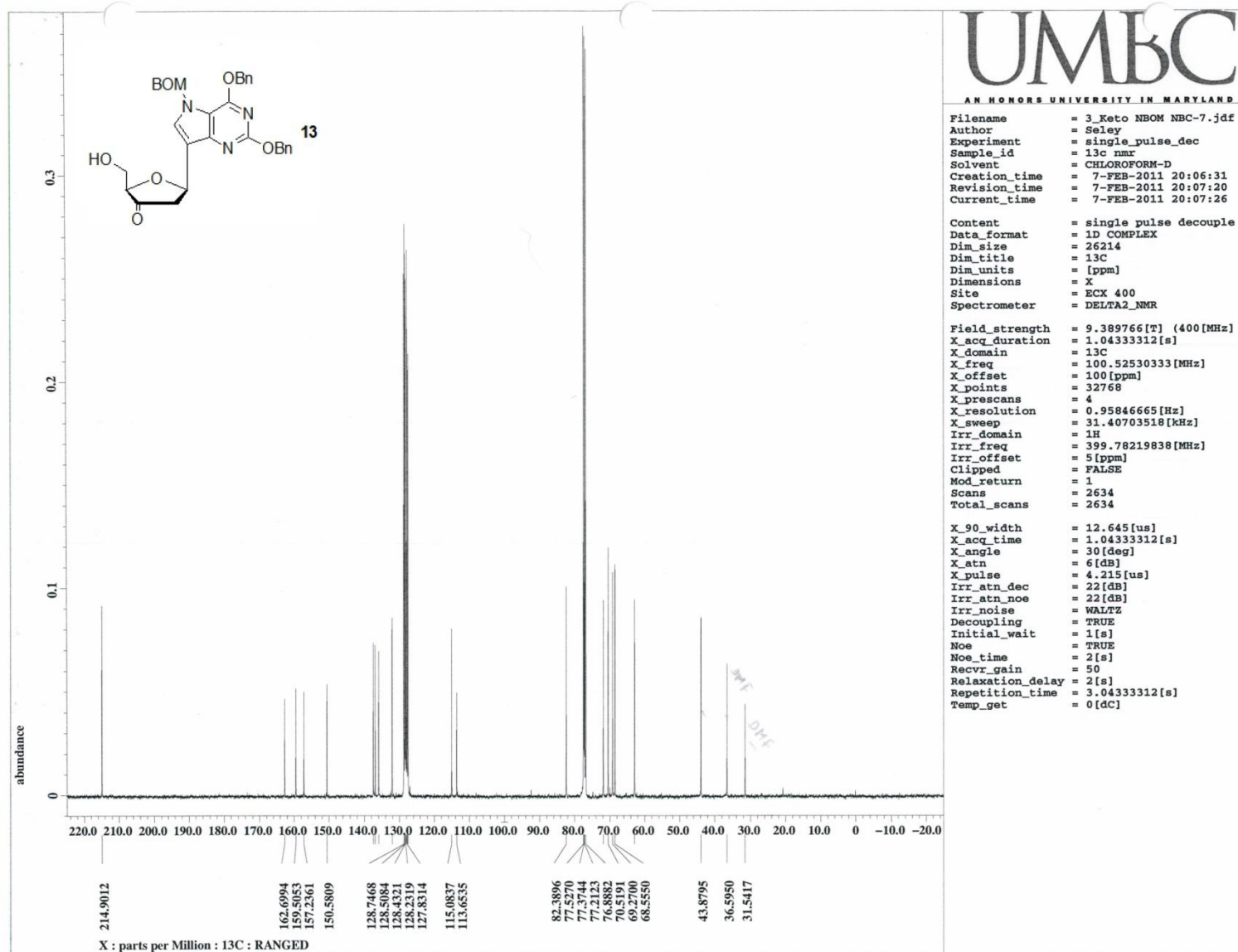


File Name : D:\VG70S Data\20100707\Kartik\KT_03_69\AccMass20PC_KT_03_69_20100708_1.ms2
Creation Date/Time : 7/8/2010 at 17:38:52
File Type : V/E raw data
File Source : Acquired on MASPEC II system [I132/1240]
File Title : FAB Accurate Mass Scan KT-3-69
Instrument : VG70S
Notes : R = 10000, 20% Sweepwidth m/z = 511-565 amu, S = 25sec/dec
Sample in mNBA matrix on slated probe tip, PEGME 550 mass ref
Gun = 28kV @ 2uA

SCAN GRAPH. Flagging=High Resolution M/z. Ctd=[Thr:10mV, Min.Wid(Mlt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
Scan 5#0:38 - 35#3:23. Entries=28. Base M/z=536.21813. 100% Int.=6.0444. POS.





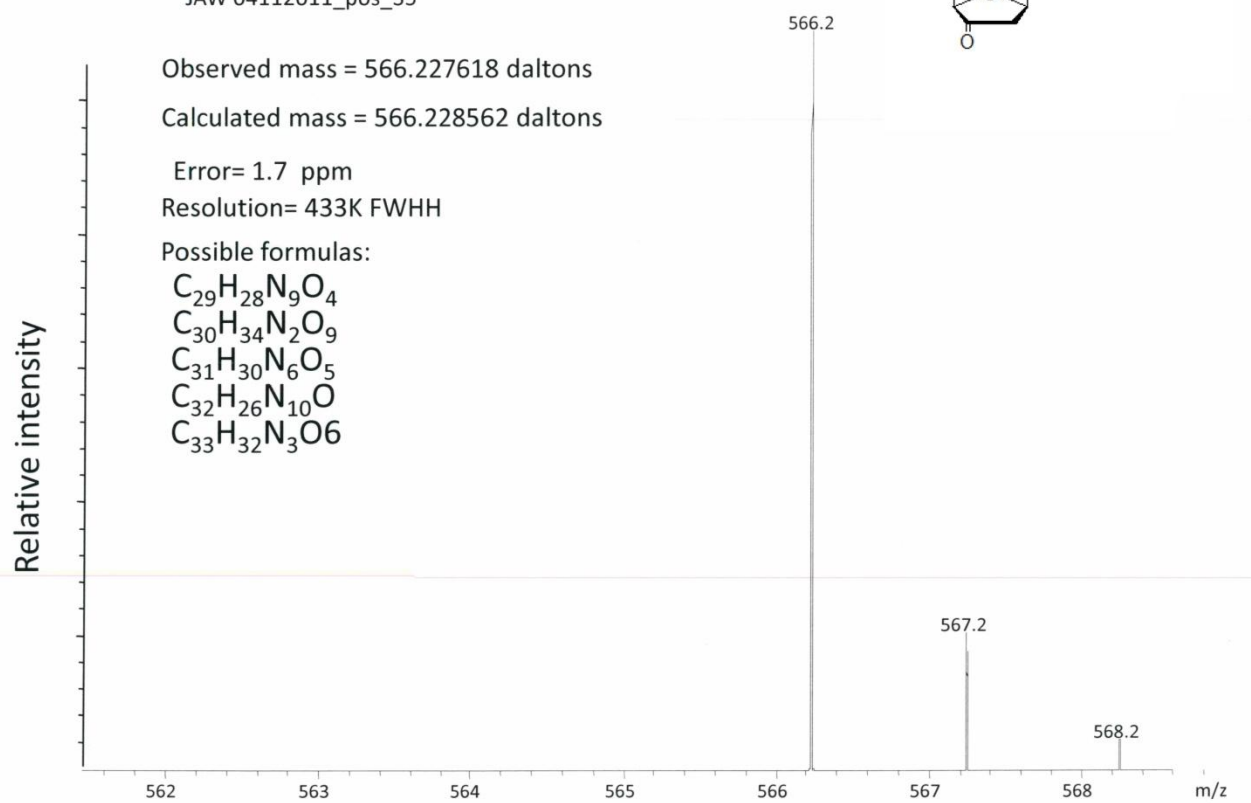
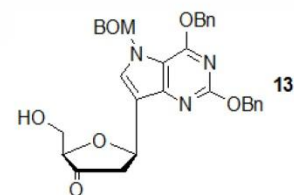


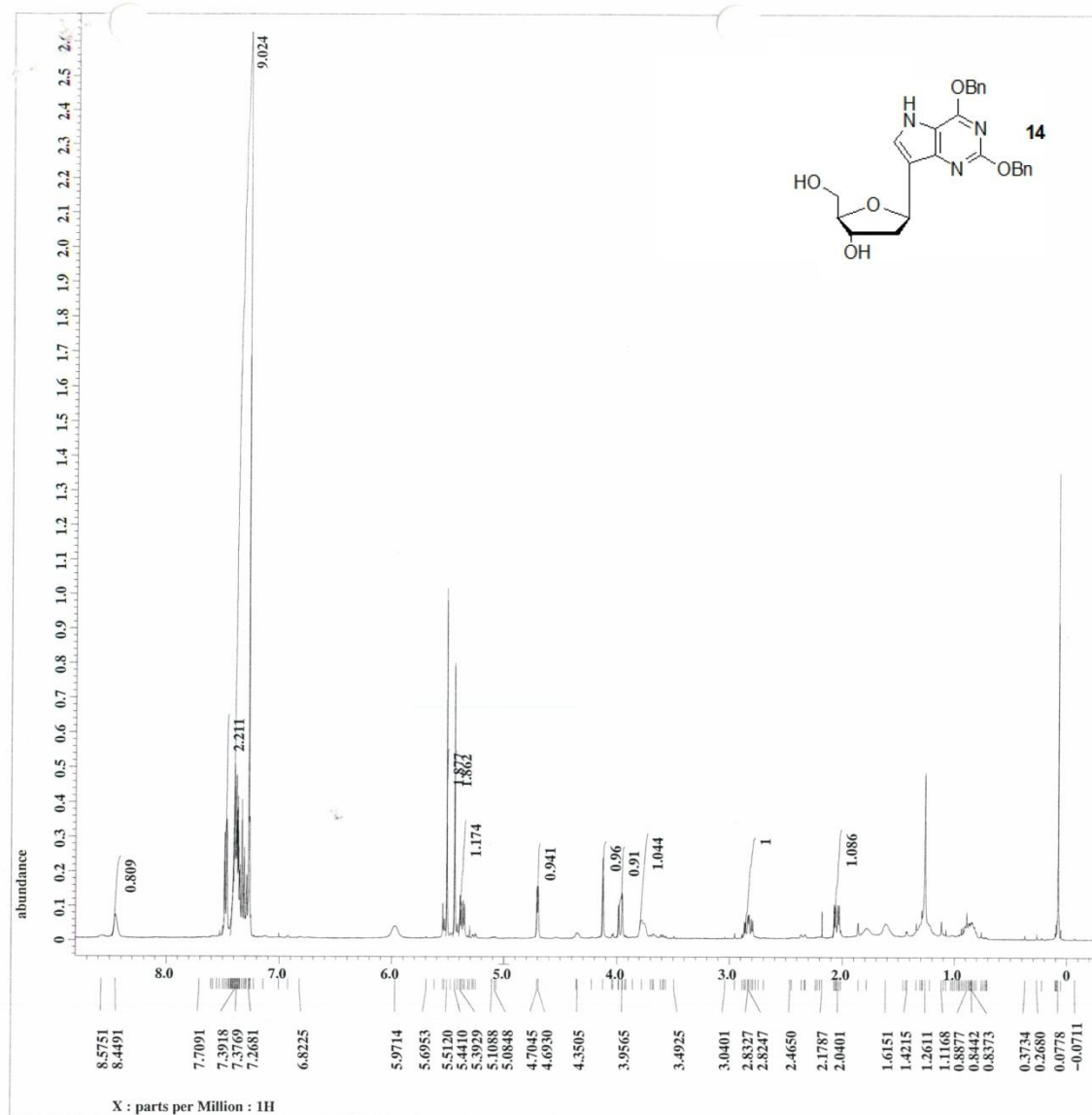
KT/03/131

Narrowband

FW= 565

JAW 04112011_pos_35





UMBC

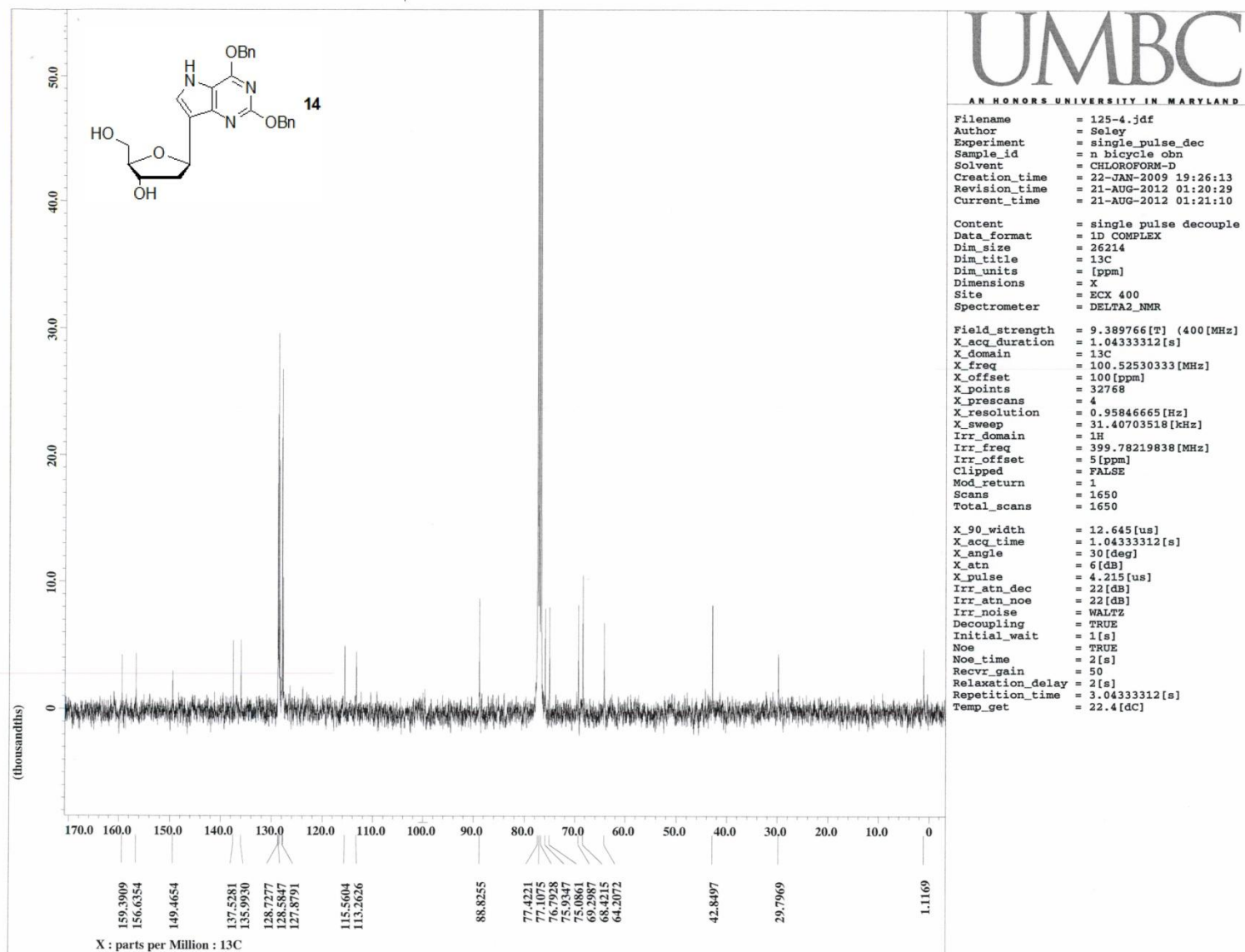
AN HONORS UNIVERSITY IN MARYLAND

Filename = 126-4.jdf
 Author = Seley
 Experiment = single_pulse.ex2
 Sample_id = n bicycle obn - purif
 Solvent = CHLOROFORM-D
 Creation_time = 22-JAN-2009 13:58:24
 Revision_time = 22-JAN-2009 13:58:50
 Current_time = 22-JAN-2009 13:59:02

Content = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = DELTA2_NMR

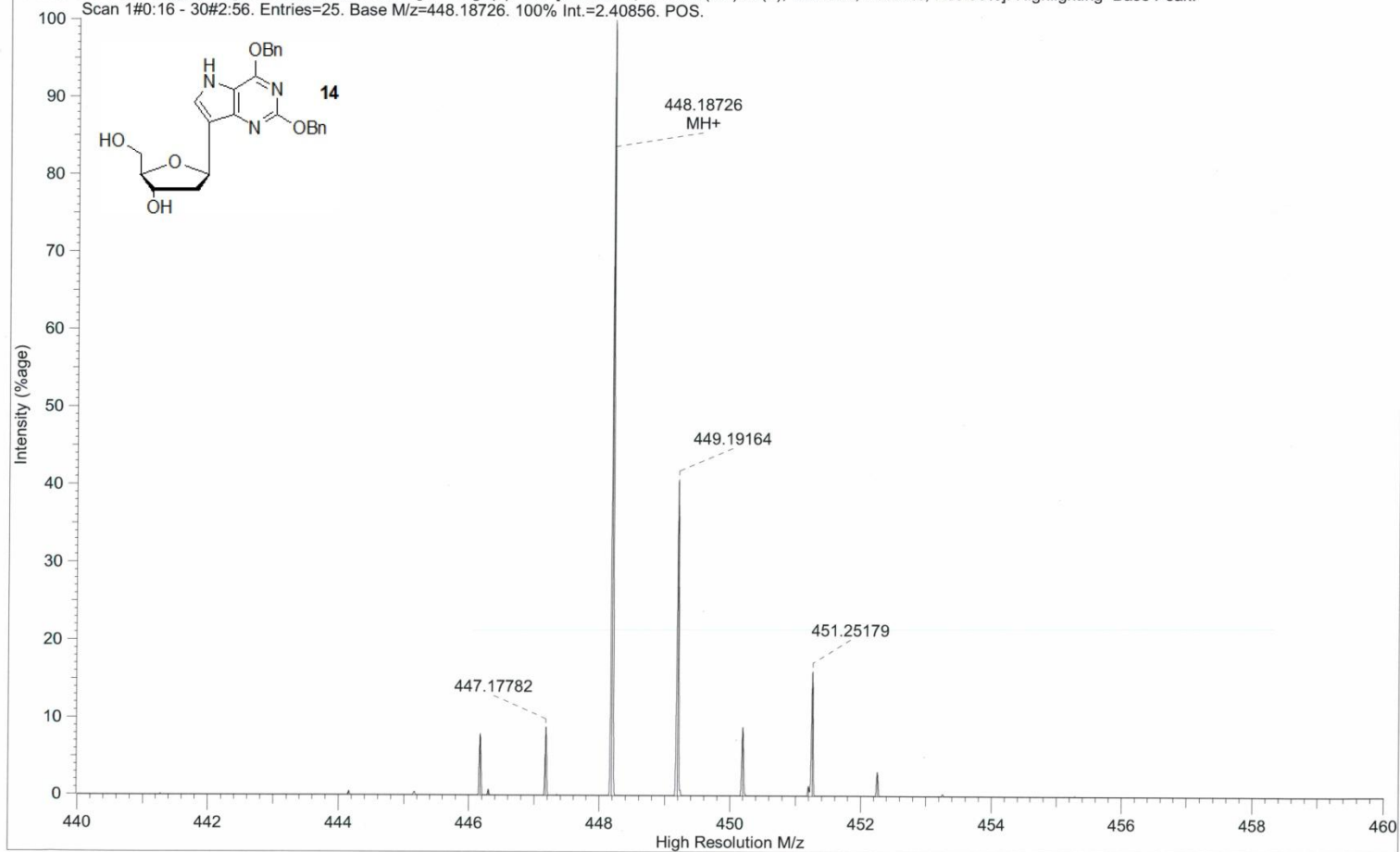
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 2.18365952[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.45794685[Hz]
 X_sweep = 7.5030012[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 72
 Total_scans = 72
 X_90_width = 12.69[us]
 X_acq_time = 2.18365952[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 6.345[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 44
 Relaxation_delay = 5[s]
 Repetition_time = 7.18365952[s]
 Temp_get = 22.3[dc]

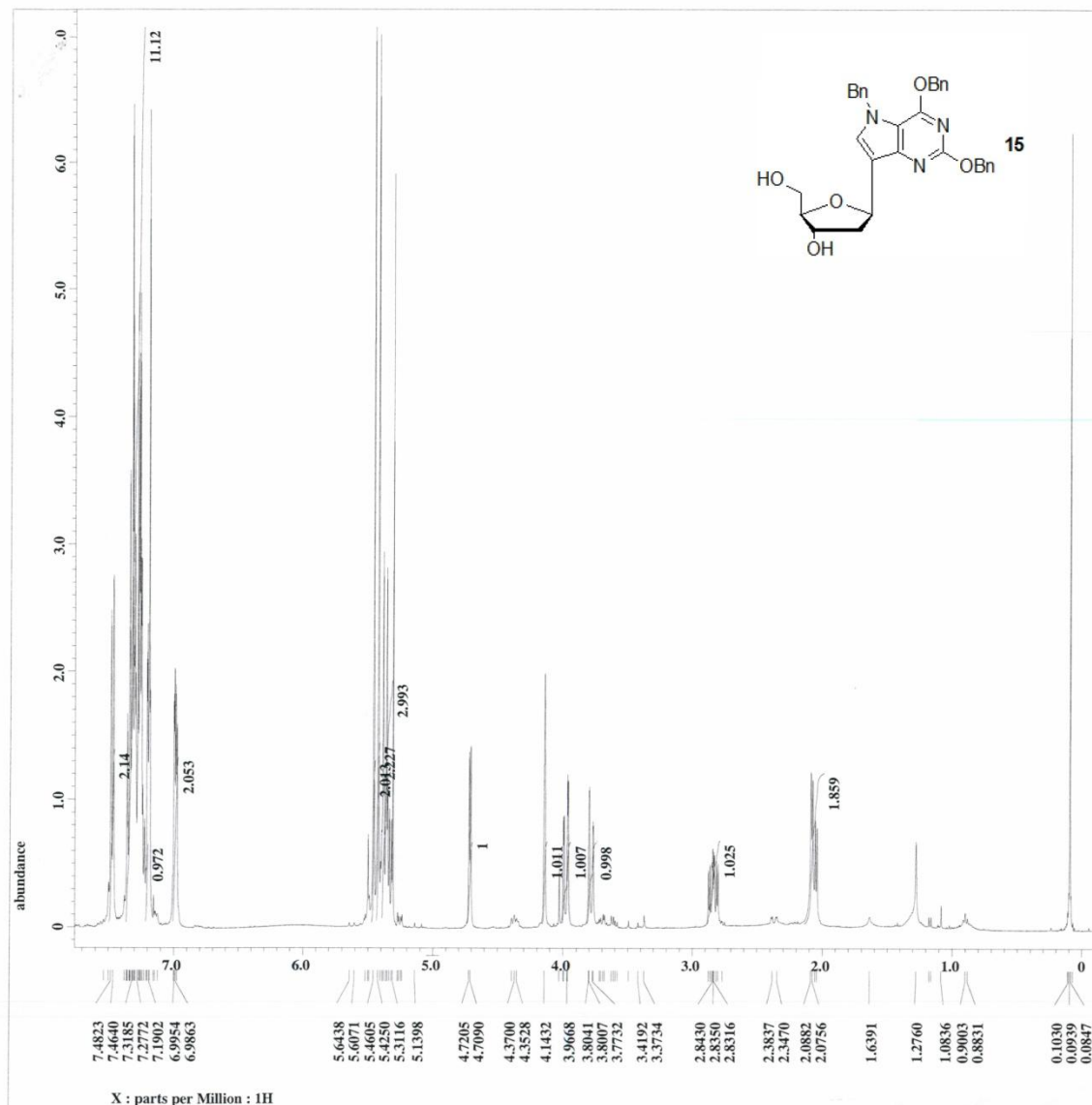
5'CH



File Name : D:\VG70S Data\20130313\Kartik\KT_02_31\AccMass20PC_KT_02_31_20130314_1.ms2
Creation Date/Time : 3/14/2013 at 18:22:39
File Type : V/E raw data
File Source : Acquired on MASPEC II system [I132/1240]
File Title : FAB Accurate Mass Scan KT-02-31
Instrument : VG70SE
Notes : R = 10000, 20% Sweepwidth m/z = 426-480 amu, S = 25sec/dec
Sample in mNBA matrix on slated probe tip, PEGMME 350 mass ref
Gun = 28kV @ 2uA

SCAN GRAPH. Flagging=High Resolution M/z. Rolling Average(5). Ctd=[Thr:10mV, Min.Wid(Mlt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
Scan 1#0:16 - 30#2:56. Entries=25. Base M/z=448.18726. 100% Int.=2.40856. POS.





UMBC

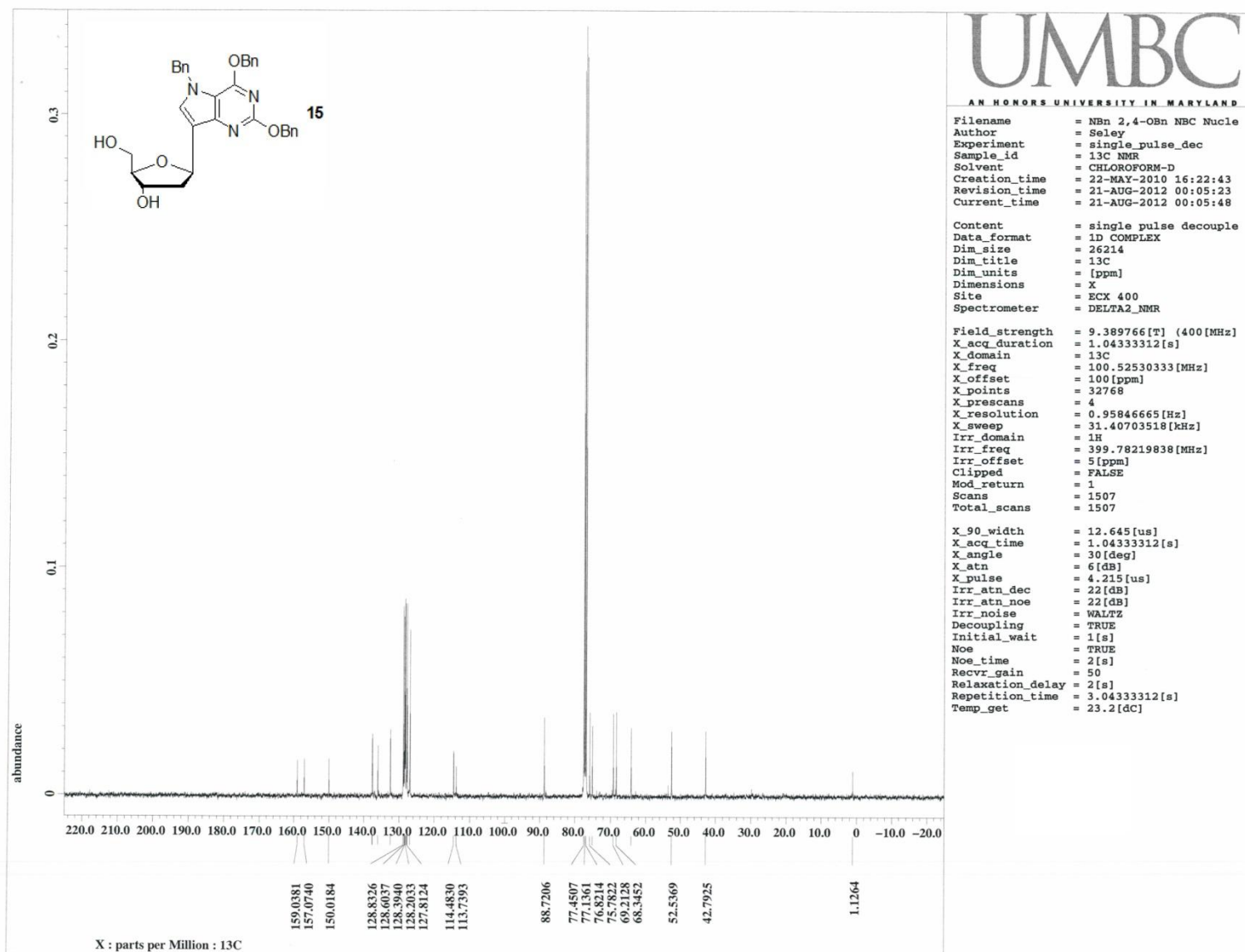
AN HONORS UNIVERSITY IN MARYLAND

Filename = Nbn NBC nucleoside-8.
 Author = Seley
 Experiment = single_pulse.ex2
 Sample_id = 1H NMR
 Solvent = CHLOROFORM-D
 Creation_time = 14-MAY-2010 10:05:27
 Revision_time = 21-AUG-2012 00:10:45
 Current_time = 21-AUG-2012 00:10:51

Content = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = DELTA2_NMR

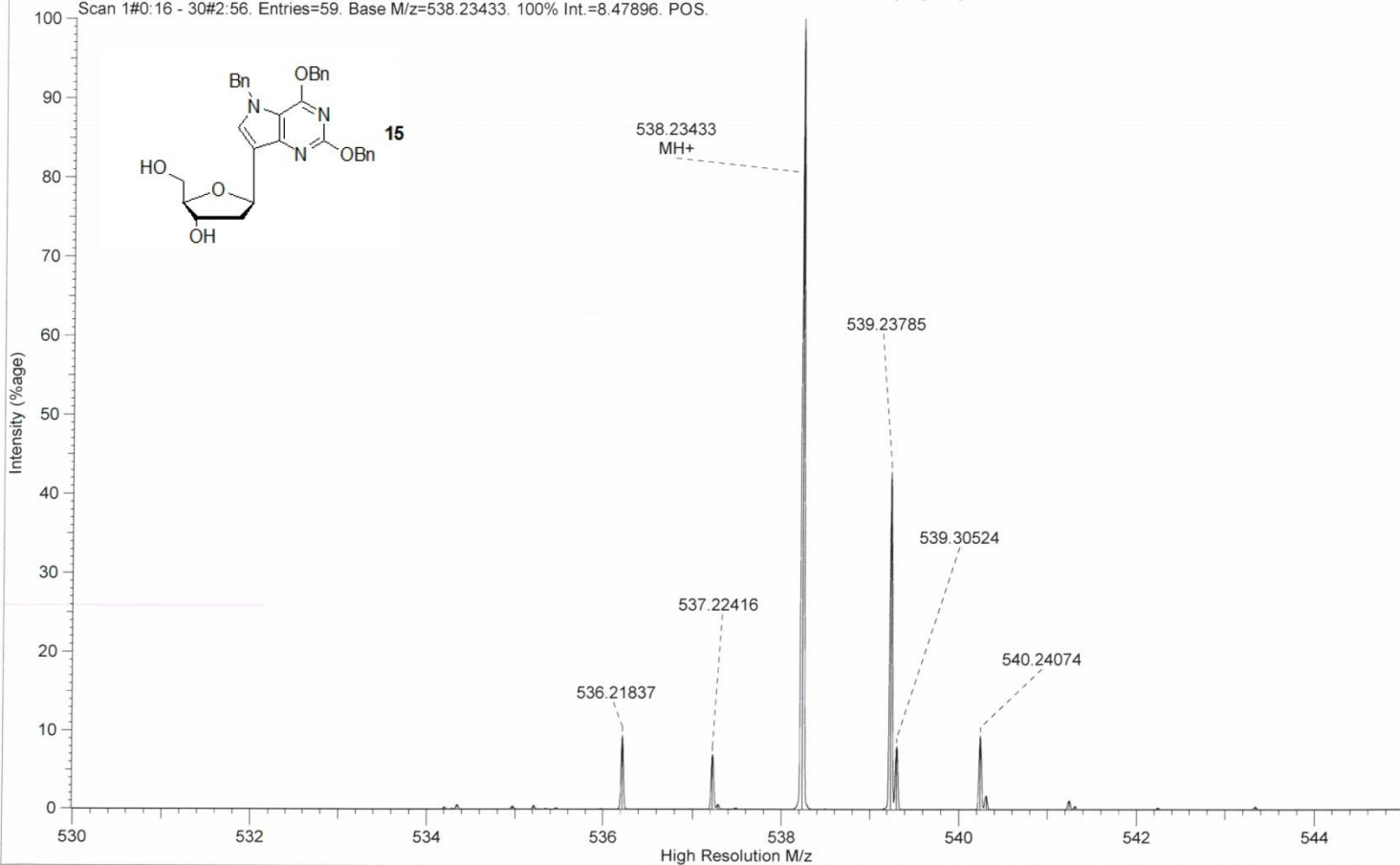
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 2.18365952[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.45794685[Hz]
 X_sweep = 7.5030012[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 32
 Total_scans = 32

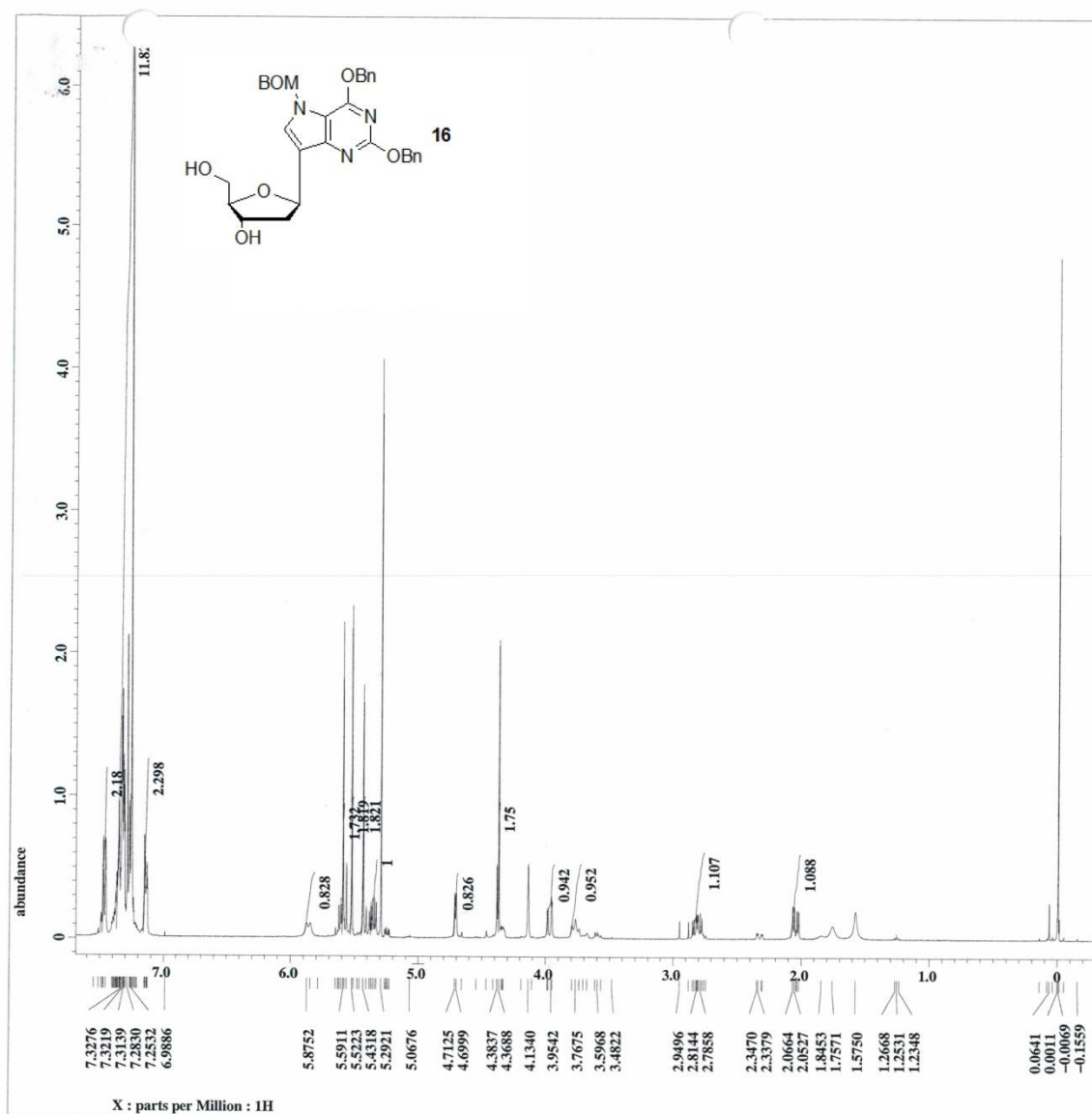
X_90_width = 12.69[us]
 X_acq_time = 2.18365952[s]
 X_angle = 45[deg]
 X_atn = 3[db]
 X_pulse = 6.345[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 7.18365952[s]
 Temp_get = 23.1[dc]



File Name : D:\VG70S Data\20100707\Kartik\KT_03_70\AccMass20PC_KT_03_70_20100708_1.ms2
Creation Date/Time : 7/8/2010 at 17:21:46
File Type : V/E raw data
File Source : Acquired on MASPEC II system [II32/1240]
File Title : FAB Accurate Mass Scan KT-3-70
Instrument : VG70S
Notes : R = 10000, 20% Sweepwidth m/z = 511-565 amu, S = 25sec/dec
Sample in mNBA matrix on slated probe tip, PEGME 550 mass ref
Gun = 28kV @ 2uA

SCAN GRAPH. Flagging=High Resolution M/z. Ctd=[Thr:10mV, Min.Wid(Mlt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
Scan 1#0:16 - 30#2:56. Entries=59. Base M/z=538.23433. 100% Int.=8.47896. POS.





UMBC

AN HONORS UNIVERSITY IN MARYLAND

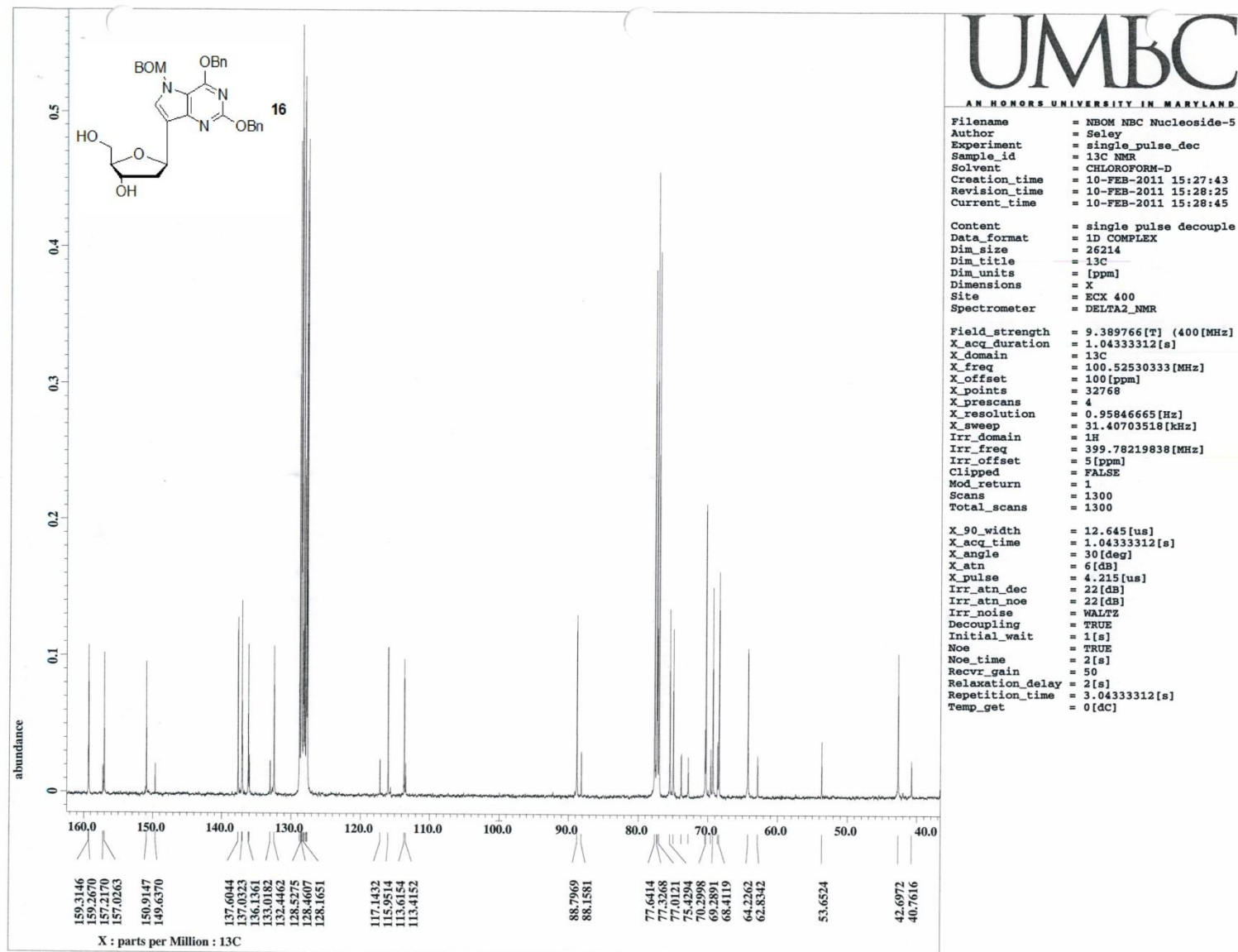
Filename = NBOM NBC Nucleoside-3
 Author = Seley
 Experiment = single_pulse.ex2
 Sample_id = 1H NMR
 Solvent = CHLOROFORM-D
 Creation_time = 10-FEB-2011 13:06:54
 Revision_time = 10-FEB-2011 13:14:22
 Current_time = 10-FEB-2011 13:14:44

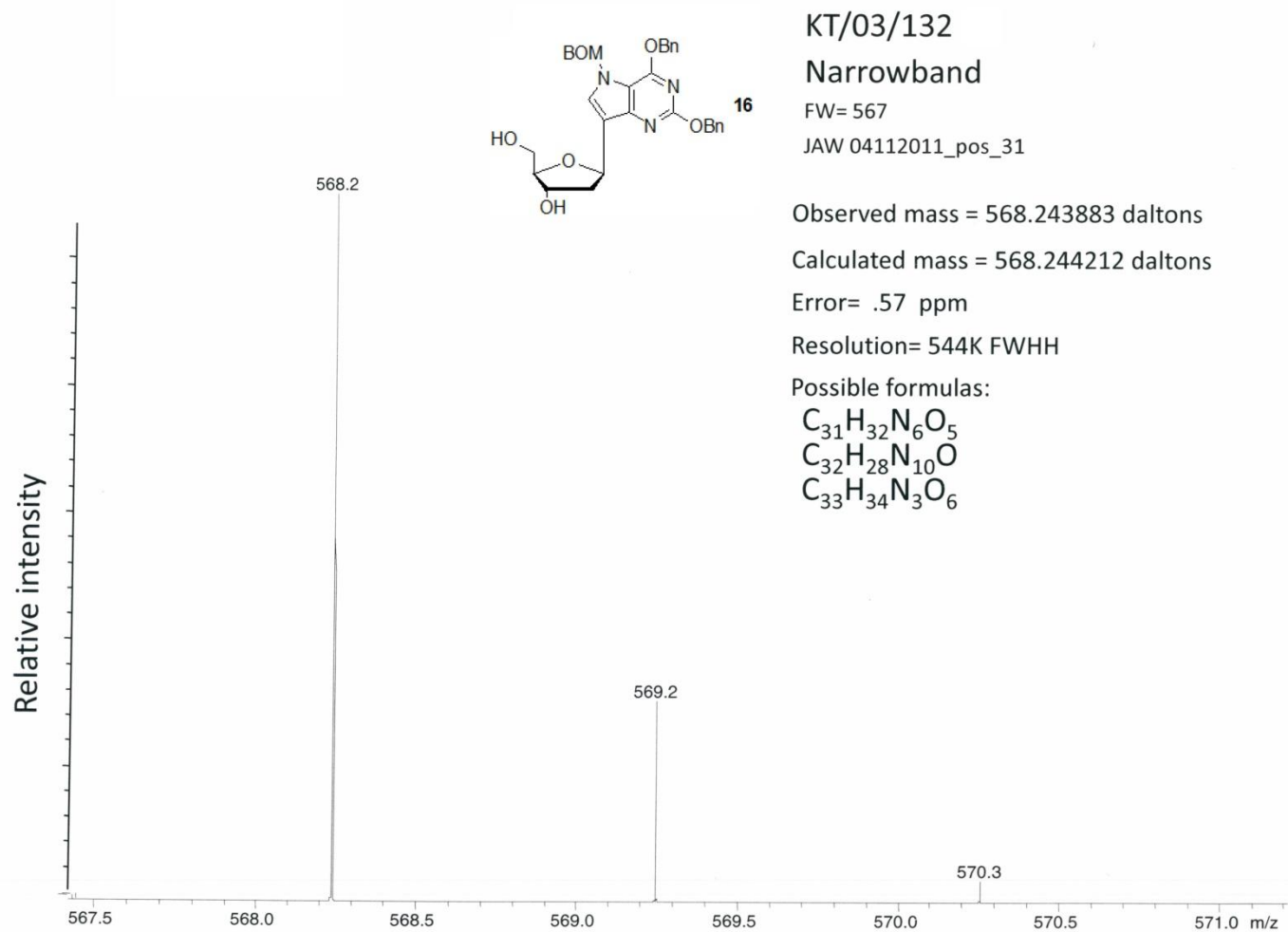
Content = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = DELTA2_NMR

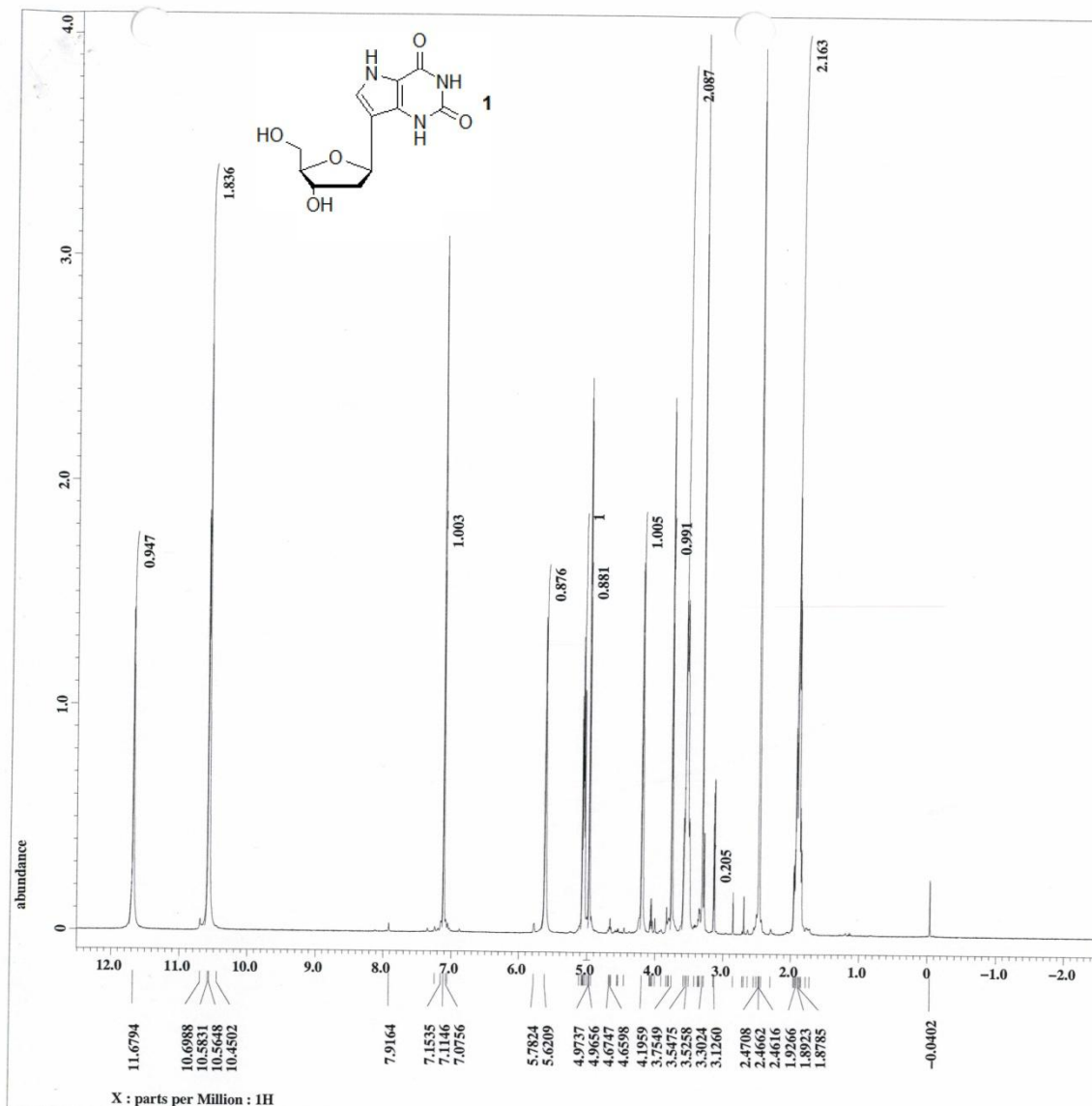
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 2.18365952[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.45794685[Hz]
 X_sweep = 7.5030012[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 32
 Total_scans = 32

X_90_width = 12.69[us]
 X_acq_time = 2.18365952[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 6.345[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 7.18365952[s]
 Temp_get = 0[dc]

s'OH not seen







UMBC

AN HONORS UNIVERSITY IN MARYLAND

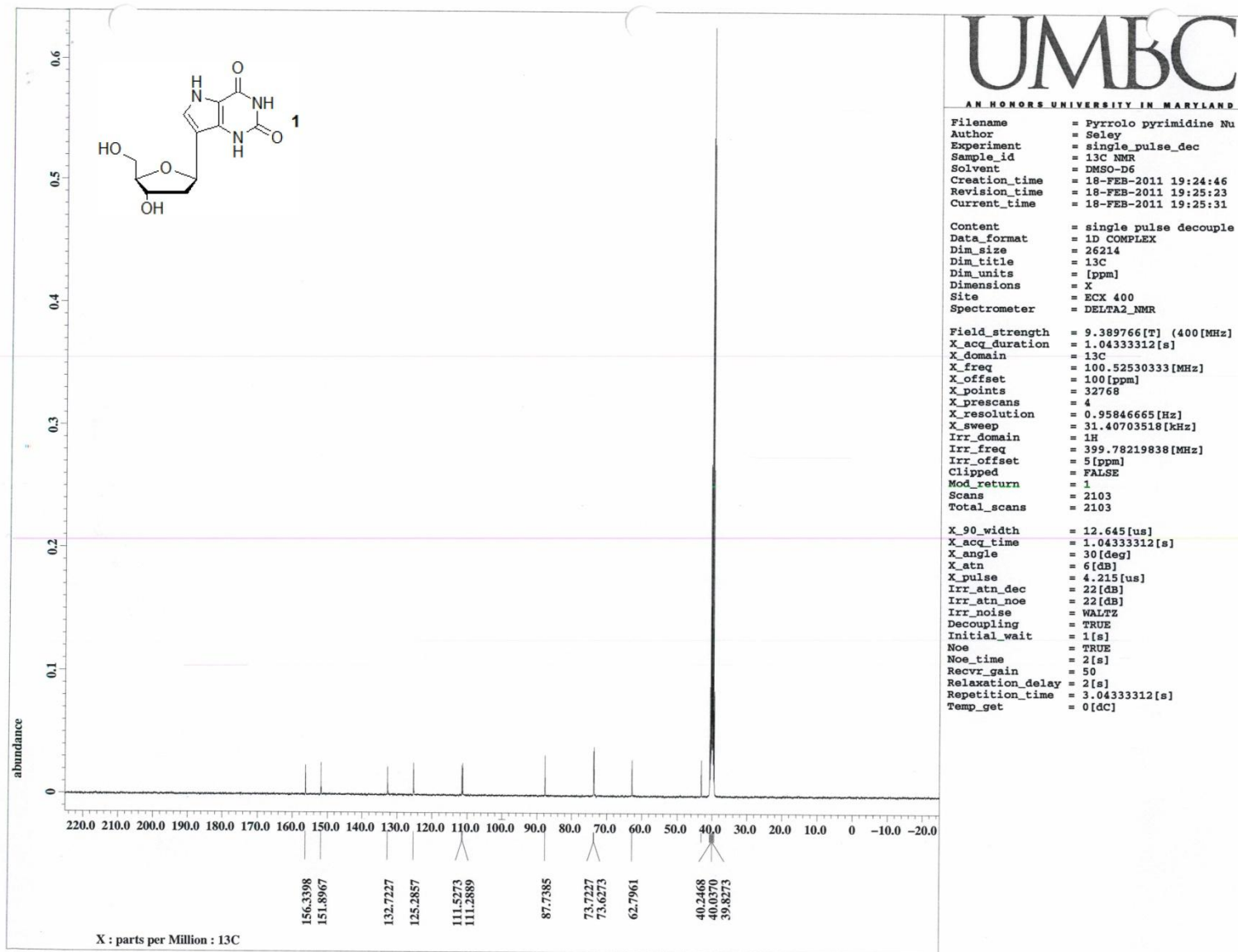
```

Filename      = Pyrrolo pyrimidine Nu
Author       = Seley
Experiment   = single_pulse.ex2
Sample_id    = 1H NMR
Solvent      = DMSO-D6
Creation_time = 18-FEB-2011 17:37:49
Revision_time = 18-FEB-2011 17:42:33
Current_time  = 18-FEB-2011 17:43:40

Content       = single_pulse
Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECX 400
Spectrometer  = DELTA2_NMR

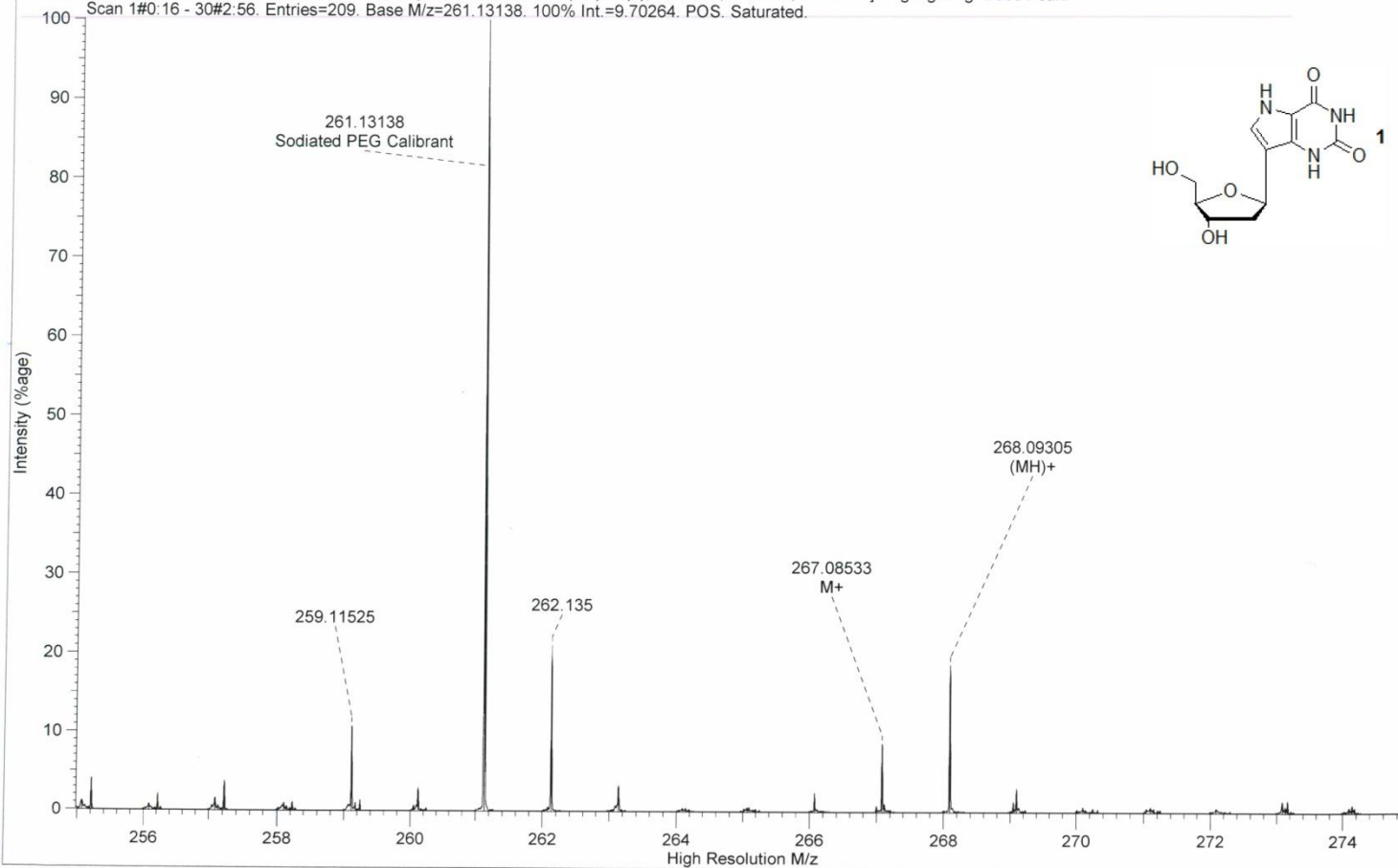
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain       = 1H
X_freq         = 399.78219838[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.45794685[Hz]
X_sweep        = 7.5030012[kHz]
Irr_domain     = 1H
Irr_freq       = 399.78219838[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 399.78219838[MHz]
Tri_offset     = 5[ppm]
Clipped        = TRUE
Mod_return     = 1
Scans          = 32
Total_scans    = 32

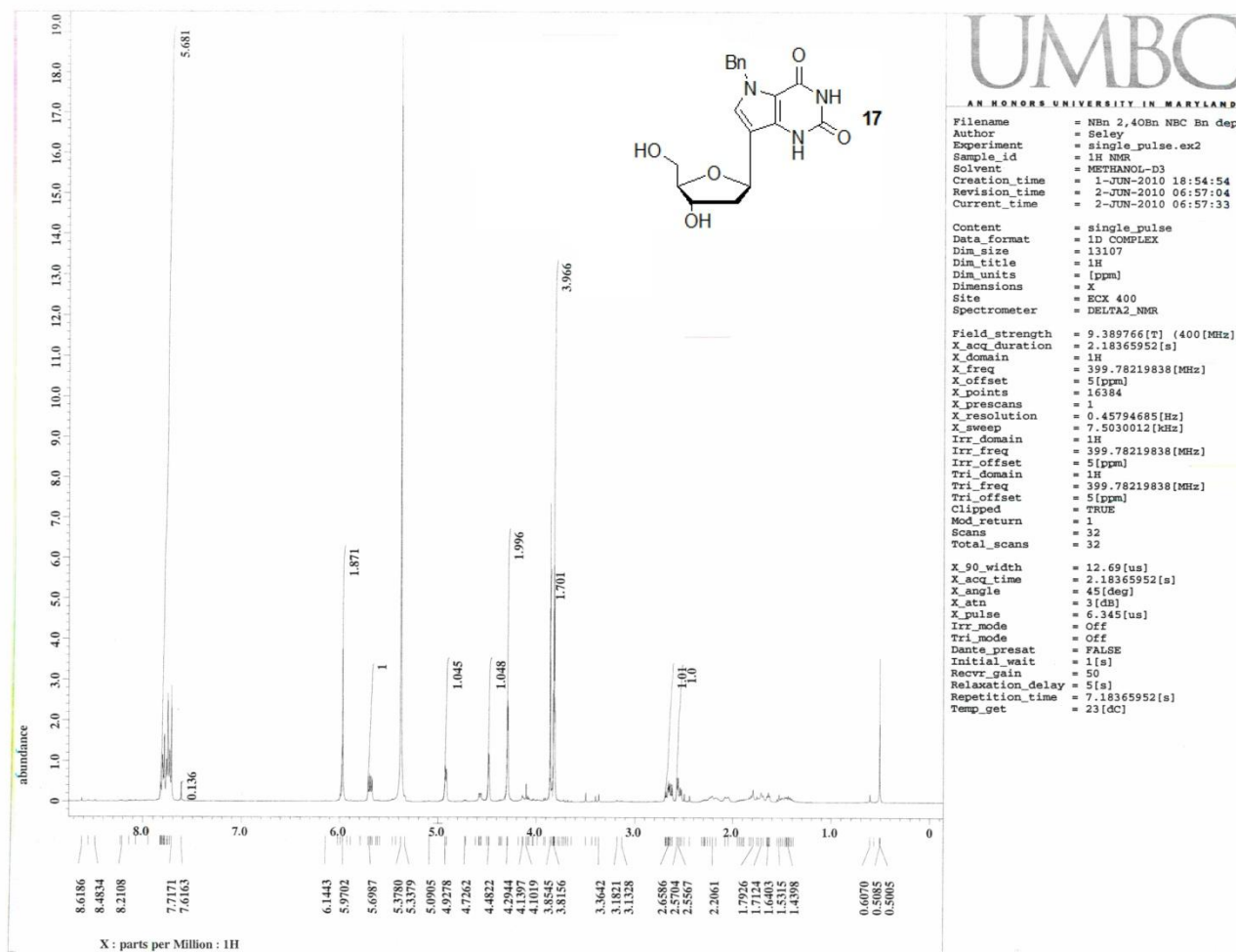
X_90_width    = 12.69[us]
X_acq_time     = 2.18365952[s]
X_angle        = 45[deg]
X_atn          = 3[dB]
X_pulse        = 6.345[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_preset   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 50
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
Temp_get       = 0[dc]
  
```

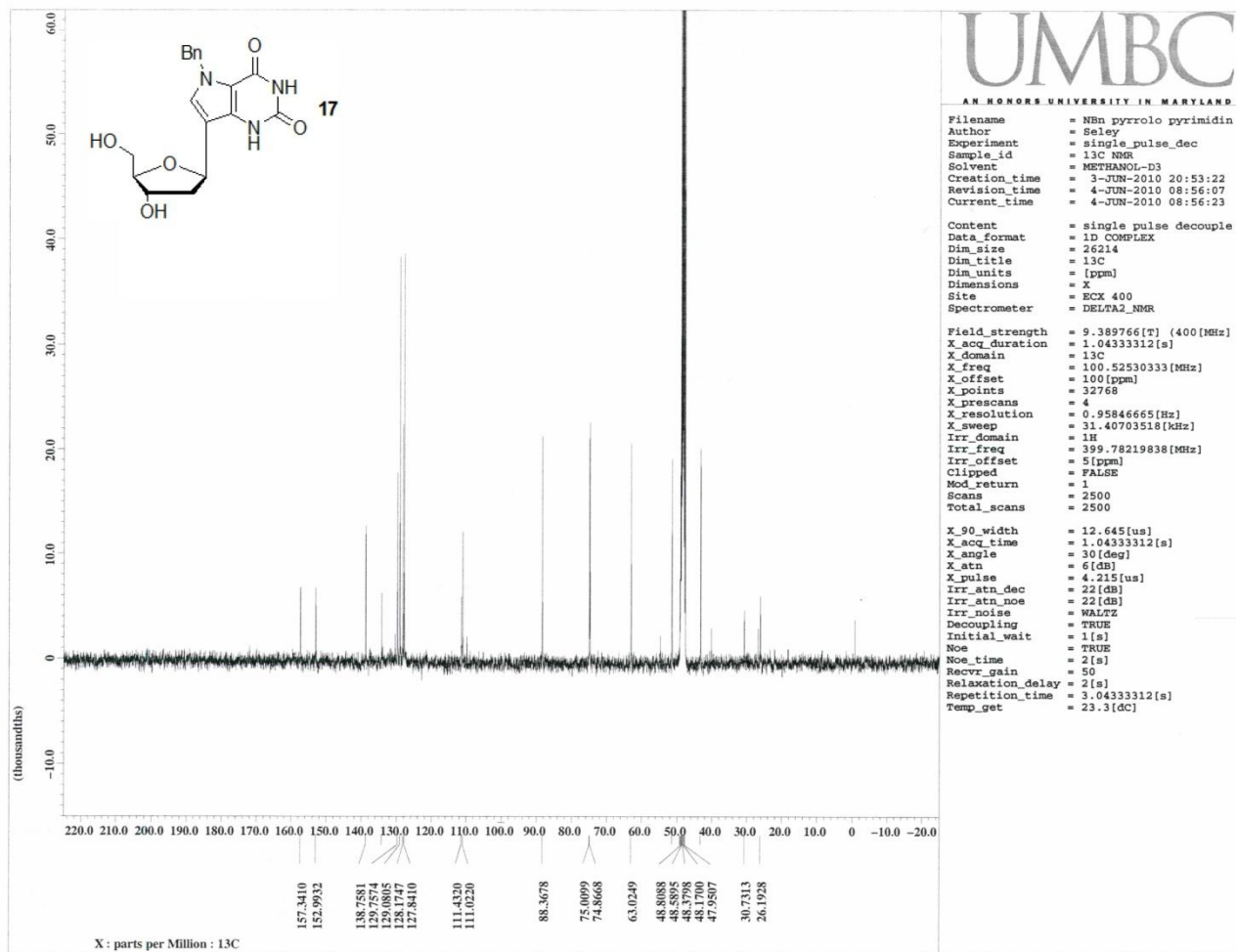


File Name : D:\VG70S Data\20090217\Kartik\KT_02_133\AccMass20PC_KT_02_133_20090217_1.ms2
Creation Date/Time : 2/17/2009 at 18:06:18
File Type : V/E raw data
File Source : Acquired on MASPEC II system [II32/1240]
File Title : FAB Accurate Mass Scan KT-02-133
Instrument : VG70SE
Notes : R = 10000, 20% Sweepwidth m/z = 236-290 amu, S = 25sec/dec
Sample in mNBA matrix on slated probe tip, PEG 200 mass ref
Gun = 28kV @ 2uA

SCAN GRAPH. Flagging=High Resolution M/z. Ctd=[Thr:10mV, Min.Wid(MIt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
Scan 1#0:16 - 30#2:56. Entries=209. Base M/z=261.13138. 100% Int.=9.70264. POS. Saturated.

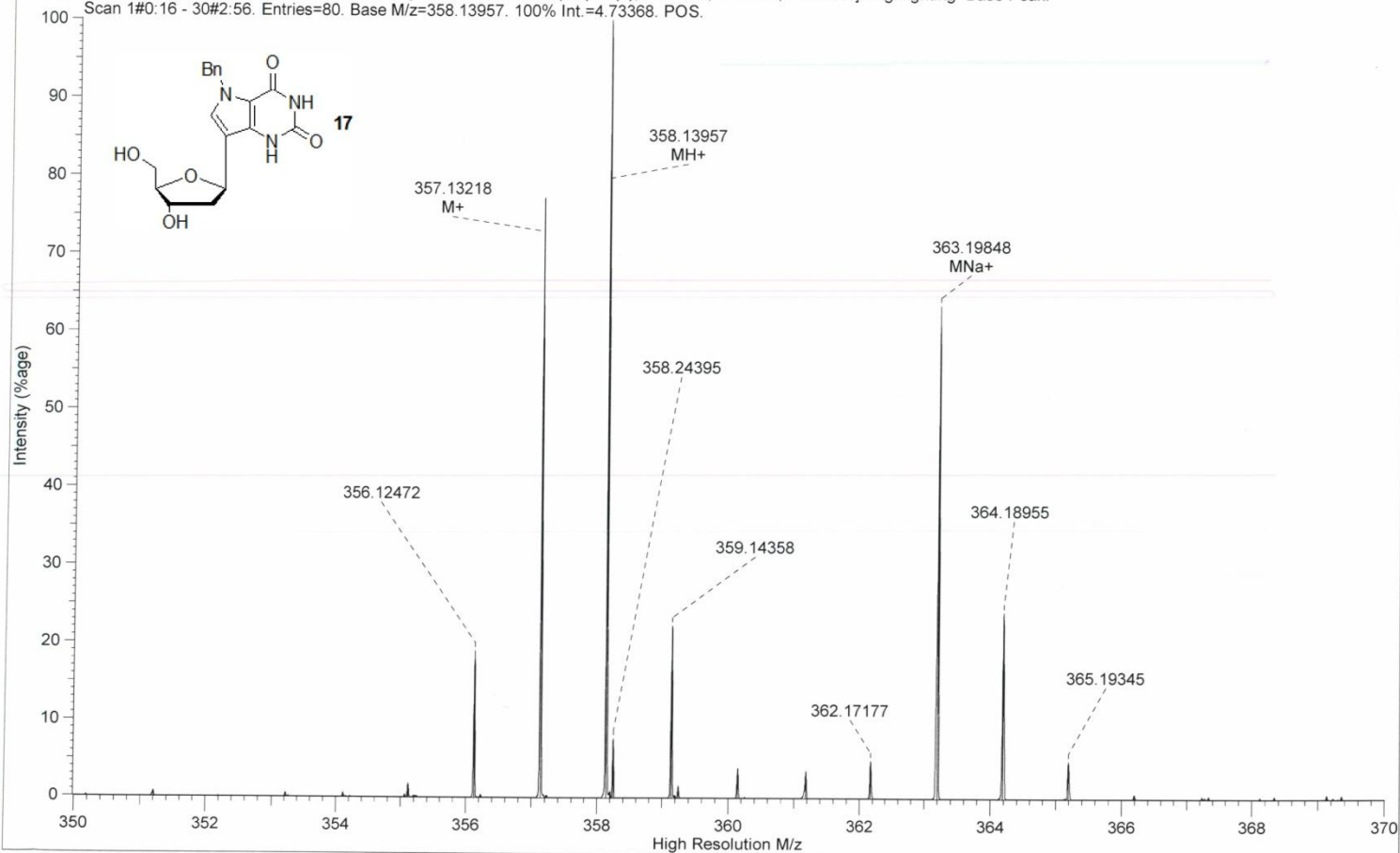


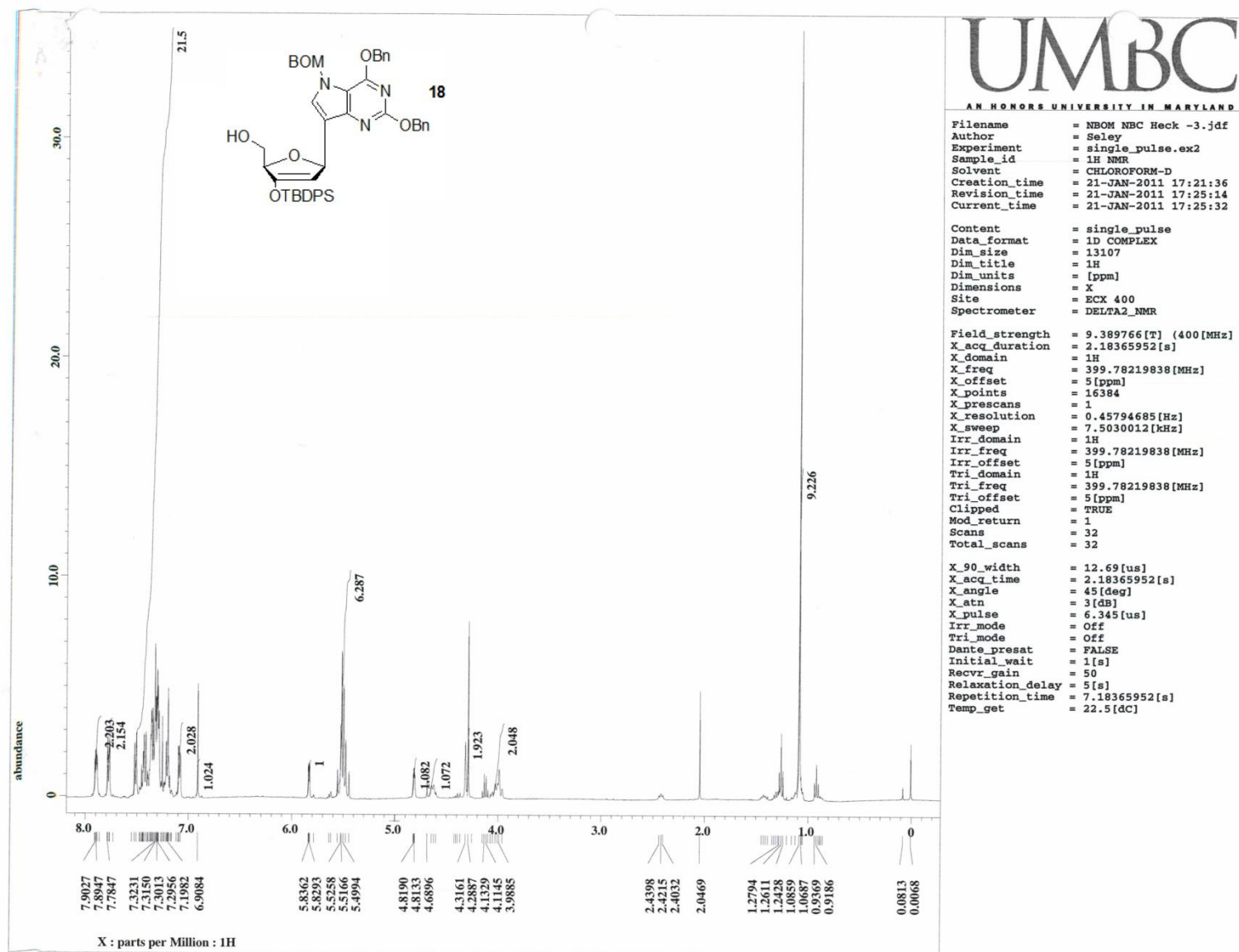


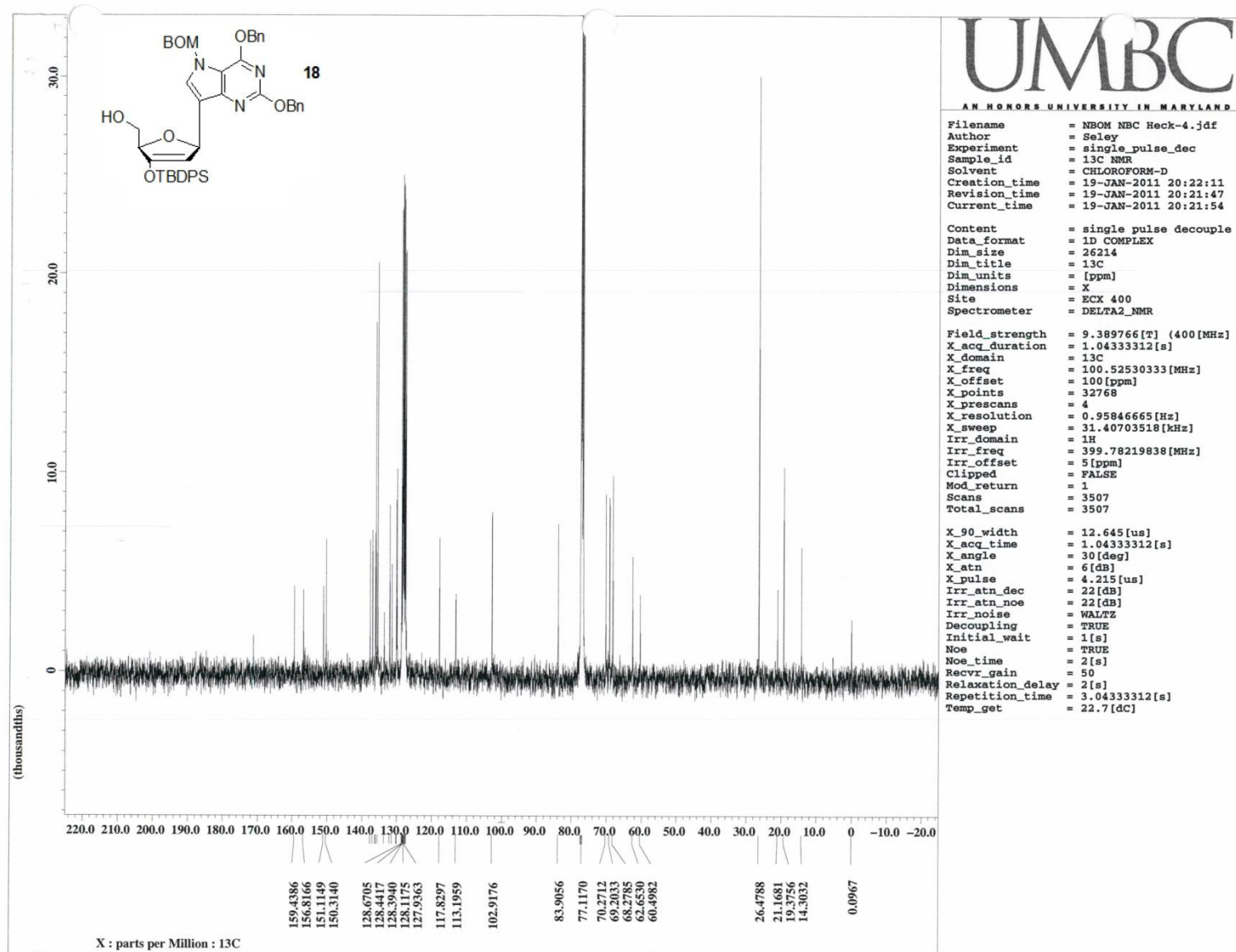


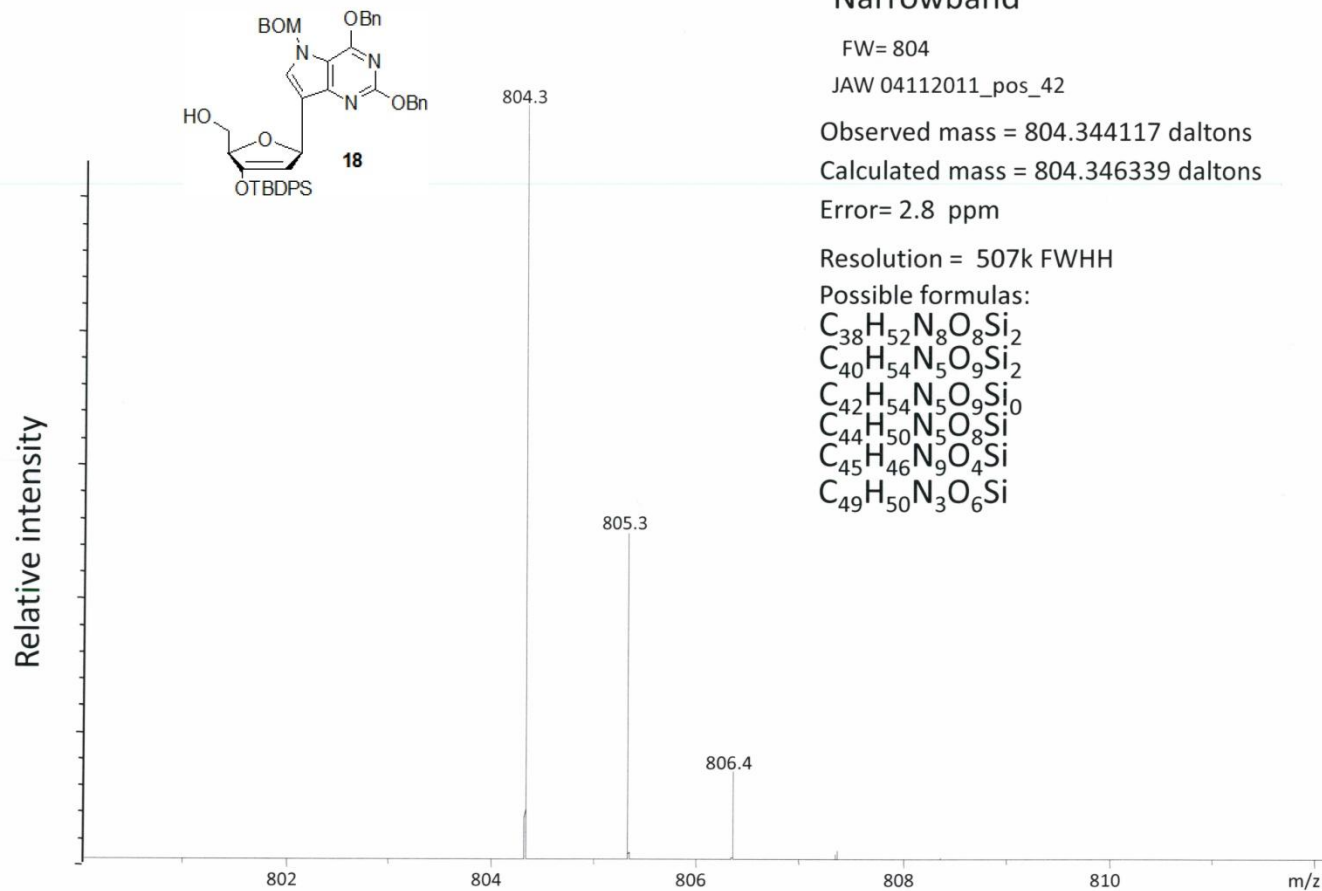
File Name : D:\VG70S Data\20100707\Kartik\KT_03_76\AccMass20PC_KT_03_76_20100709_1.ms2
 Creation Date/Time : 7/9/2010 at 13:52:16
 File Type : V/E raw data
 File Source : Acquired on MASPEC II system [I132/1240]
 File Title : FAB Accurate Mass Scan KT-3-76
 Instrument : VG70S
 Notes : R = 10000, 20% Sweepwidth m/z = 336-390amu, S = 25sec/dec
 Sample in mNBA matrix on slated probe tip, PEGME 350 mass ref
 Gun = 28kV @ 2uA

SCAN GRAPH. Flagging=High Resolution M/z. Ctd=[Thr:10mV, Min.Wid(Mit):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
 Scan 1#0:16 - 30#2:56. Entries=80. Base M/z=358.13957. 100% Int.=4.73368. POS.







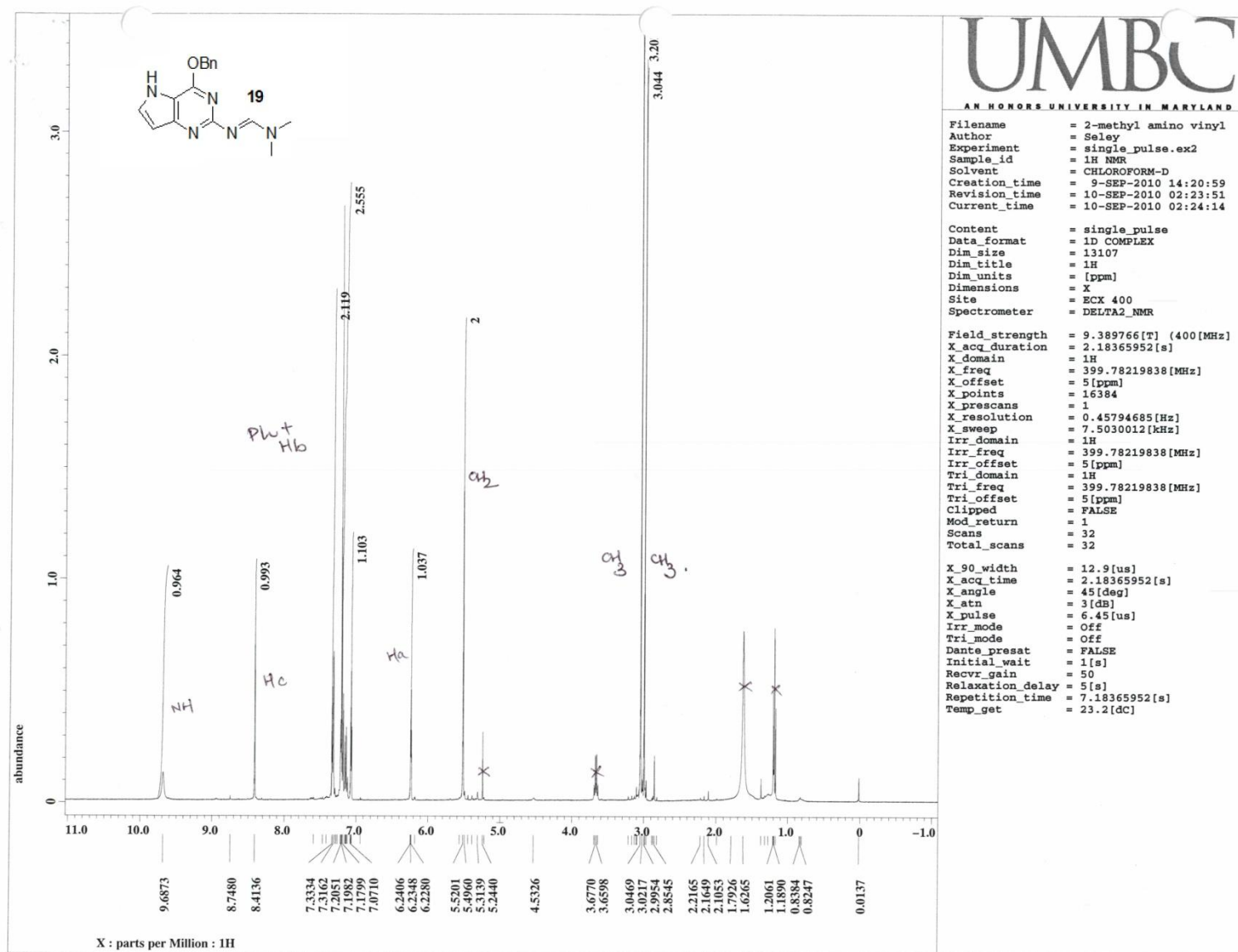


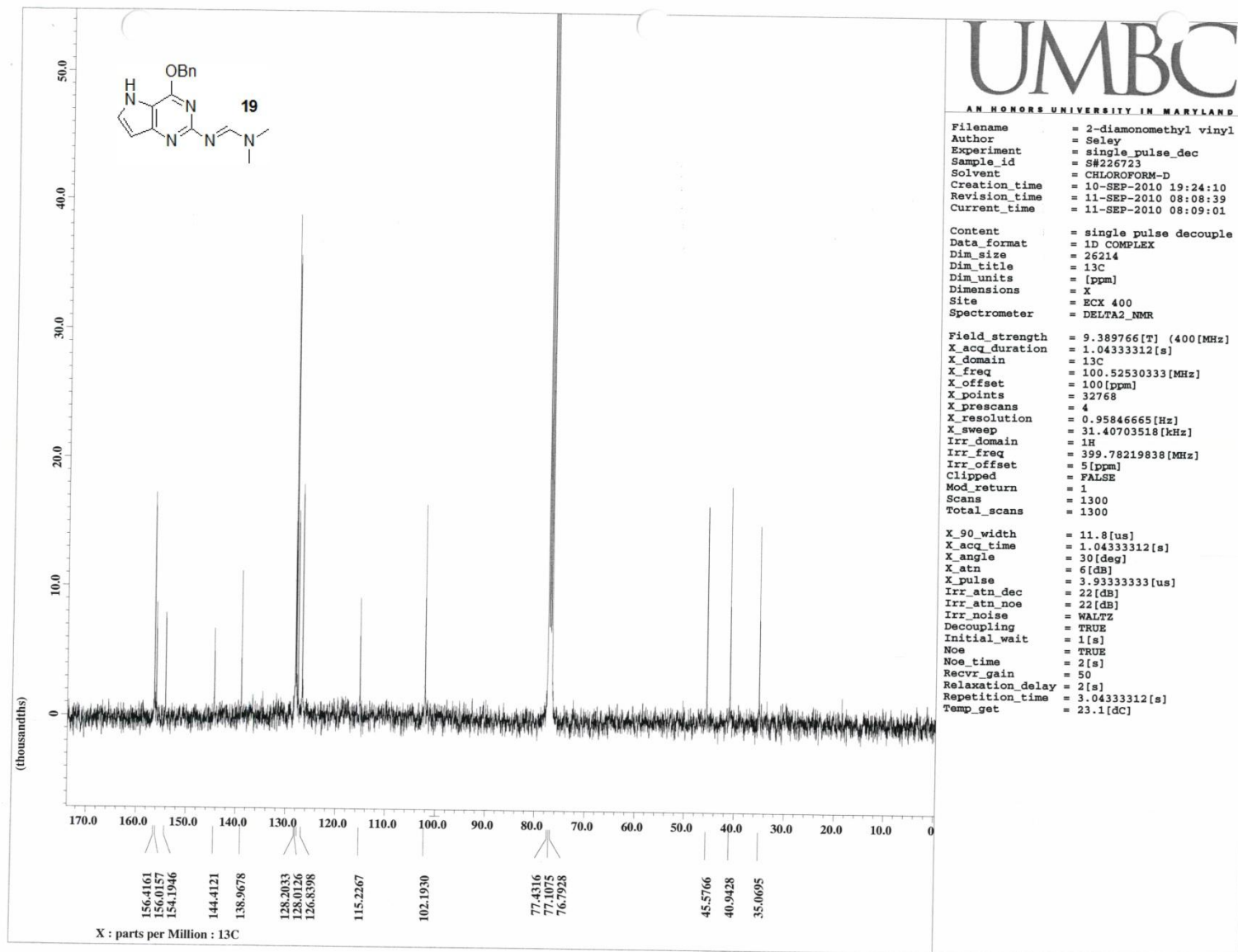
KT/03/126

Narrowband

FW= 804

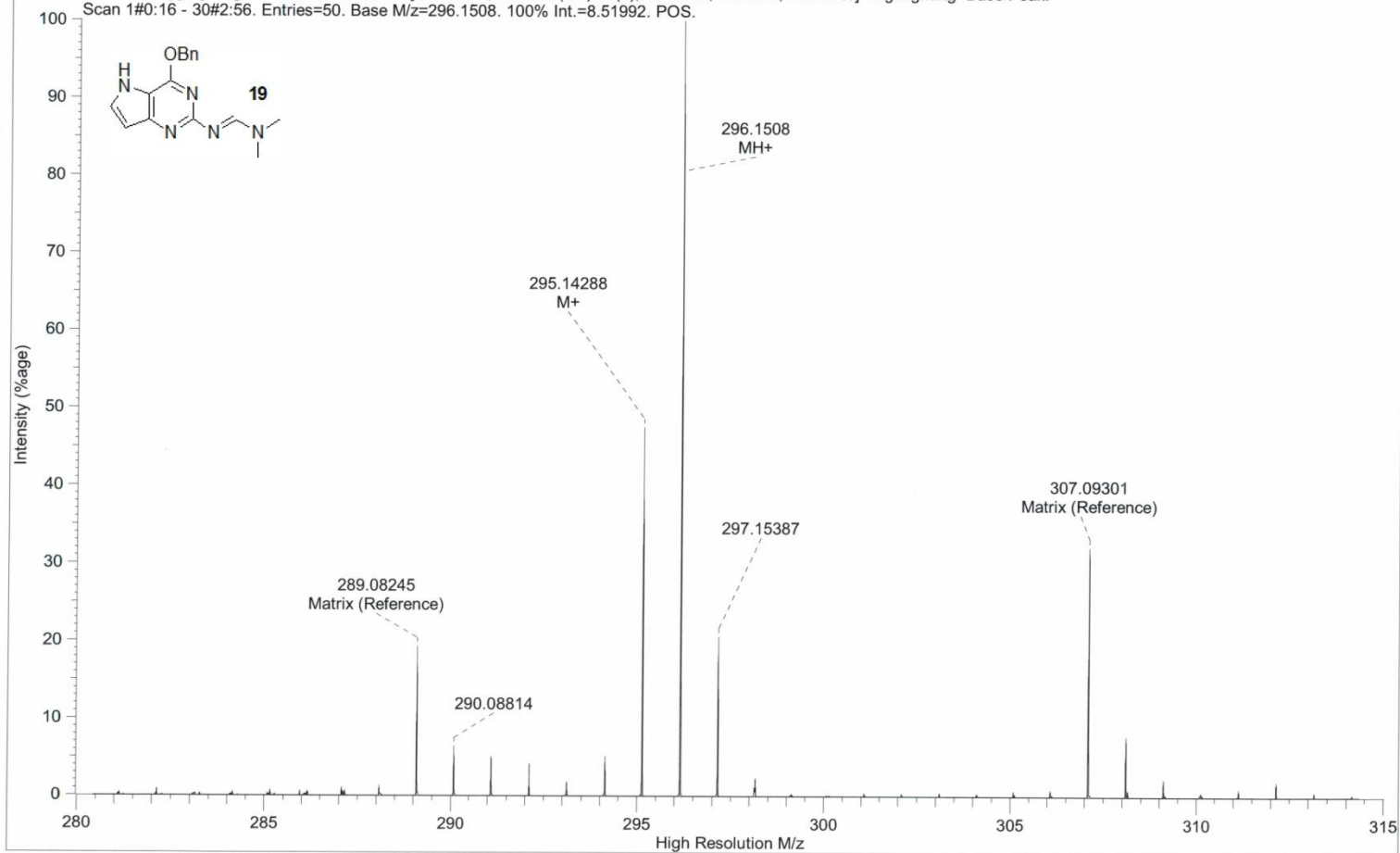
JAW 04112011_pos_42

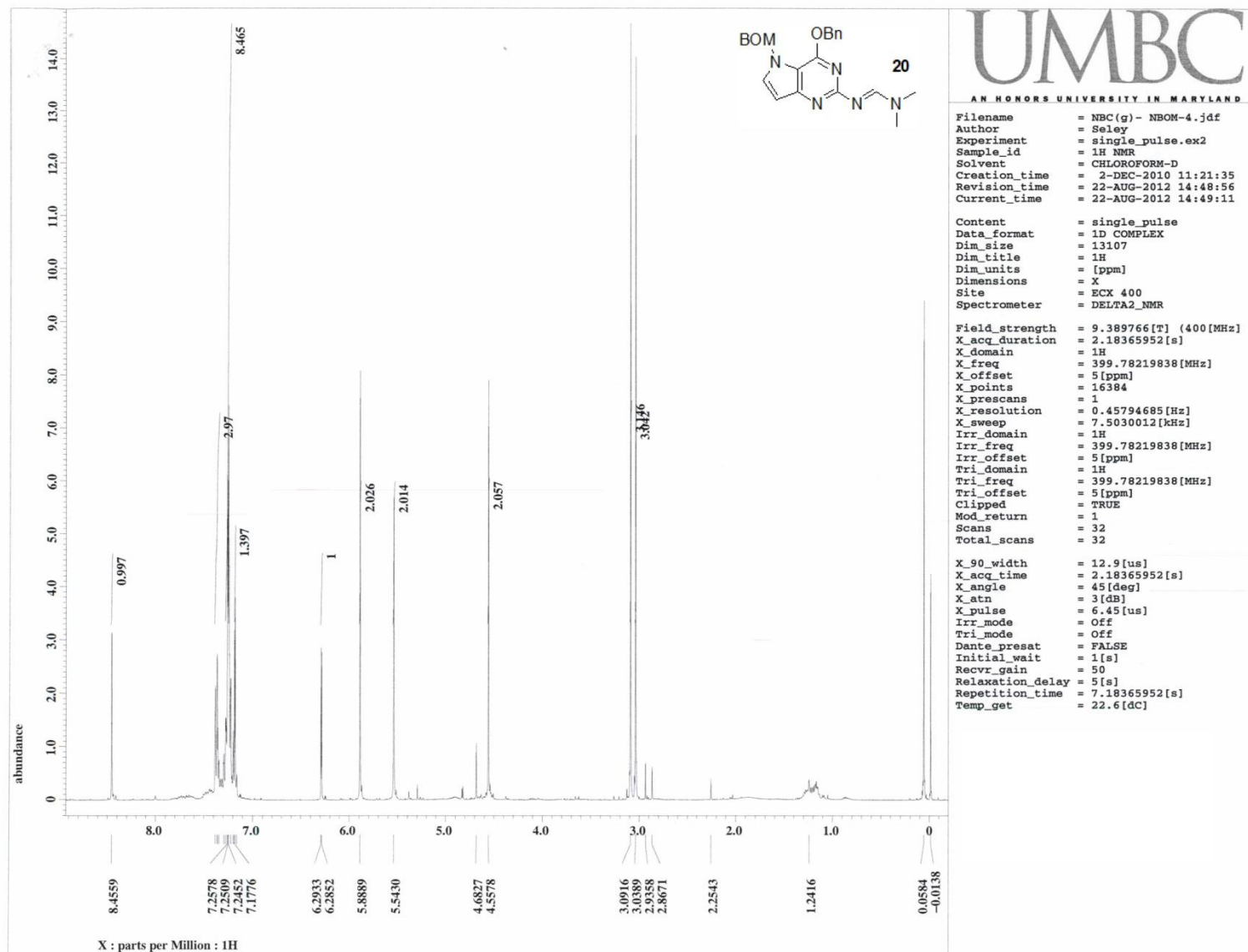


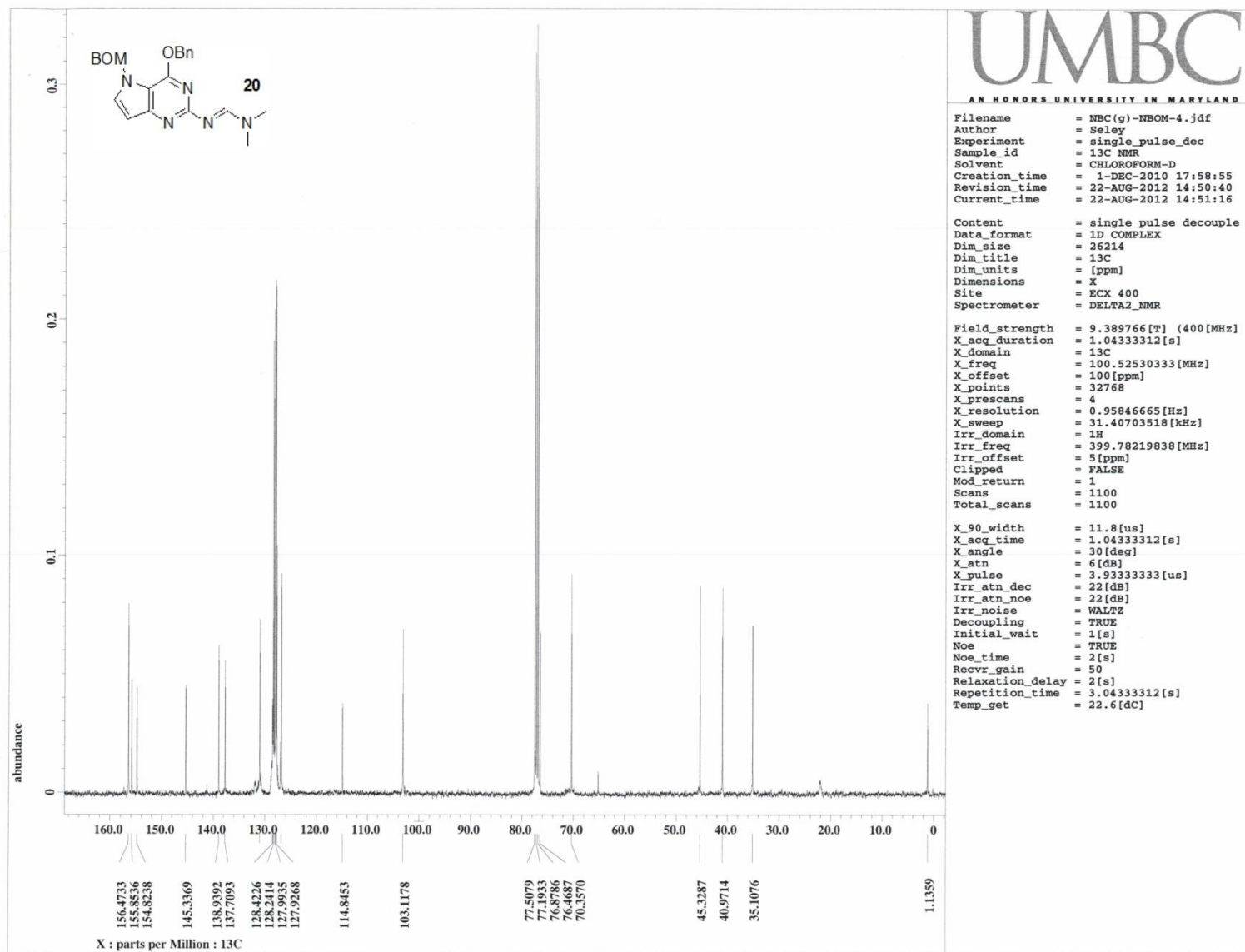


File Name : D:\VG70S Data\20101021\Kartik\KT_03_91\AccMass20PC_KT_03_91_20101022_1.ms2
Creation Date/Time : 10/22/2010 at 16:28:55
File Type : V/E raw data
File Source : Acquired on MASPEC II system [I132/1240]
File Title : FAB Accurate Mass Scan KT-03-91
Instrument : VG70SE
Notes : R = 10000, 20% Sweepwidth m/z = 281-315amu, S = 25sec/dec
Sample in mNBA matrix on slated probe tip, PEG 400 mass ref
Gun = 28kV @ 2uA

SCAN GRAPH. Flagging=High Resolution M/z. Ctd=[Thr:10mV, Min.Wid(Mlt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
Scan 1#0:16 - 30#2:56. Entries=50. Base M/z=296.1508. 100% Int.=8.51992. POS.

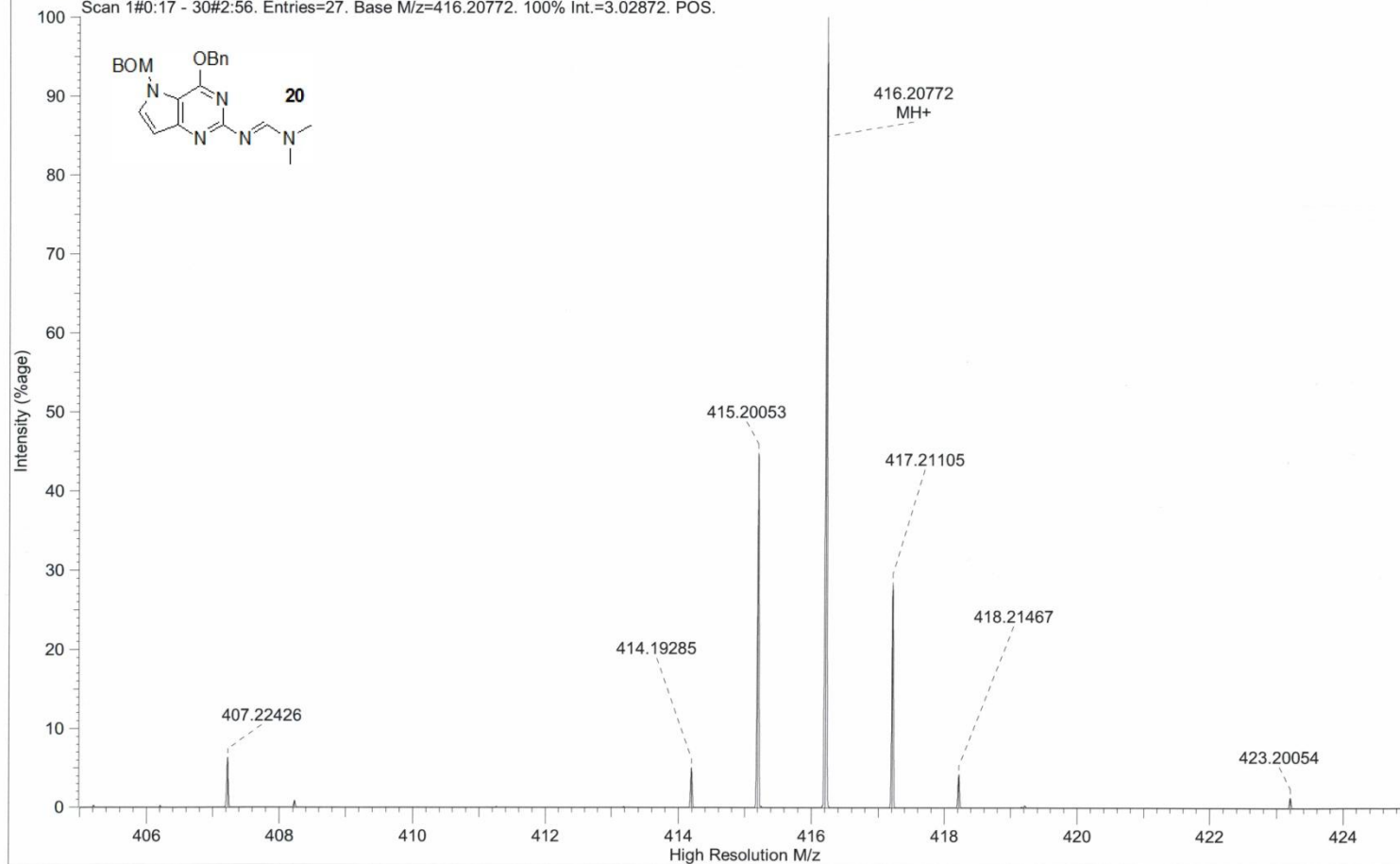


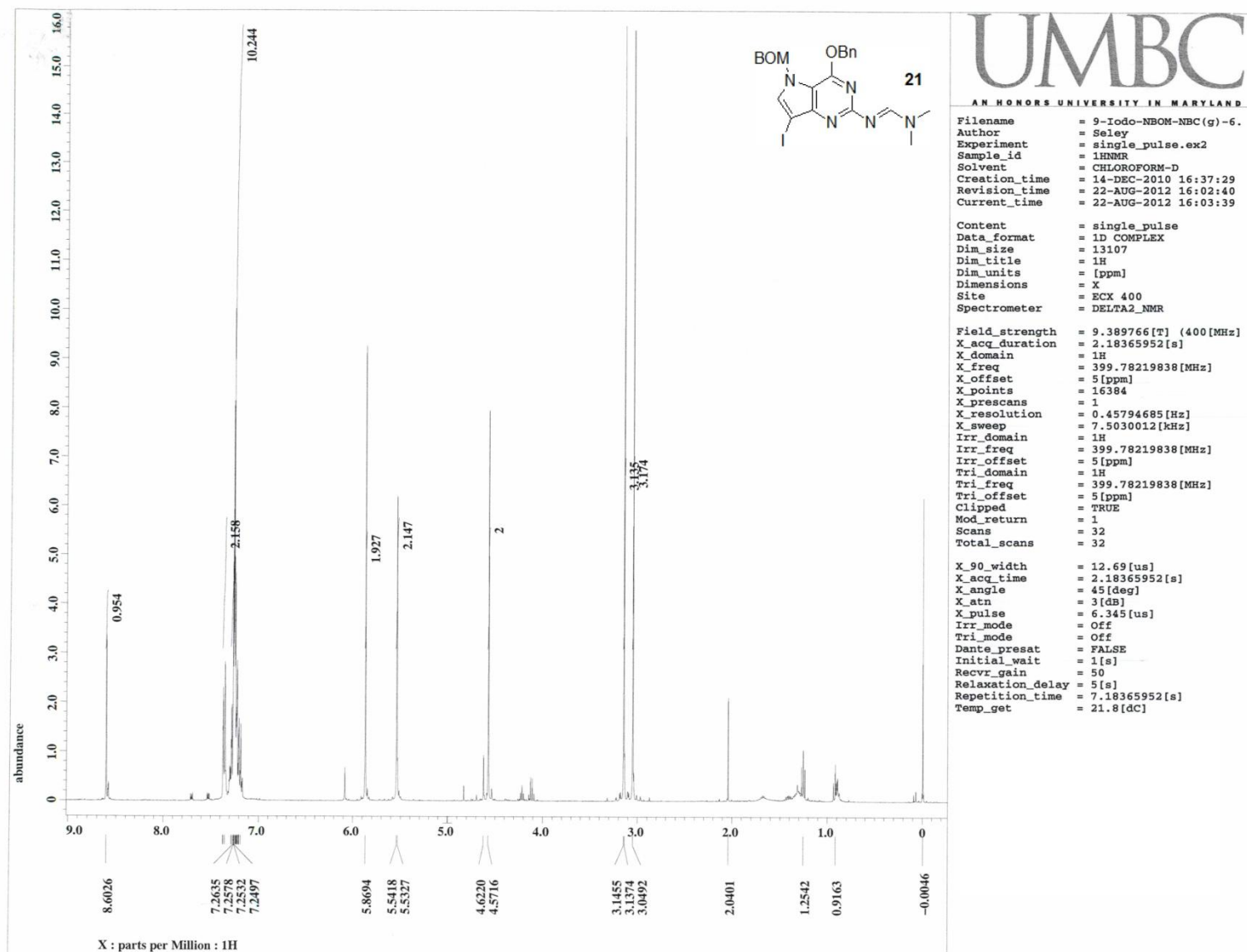


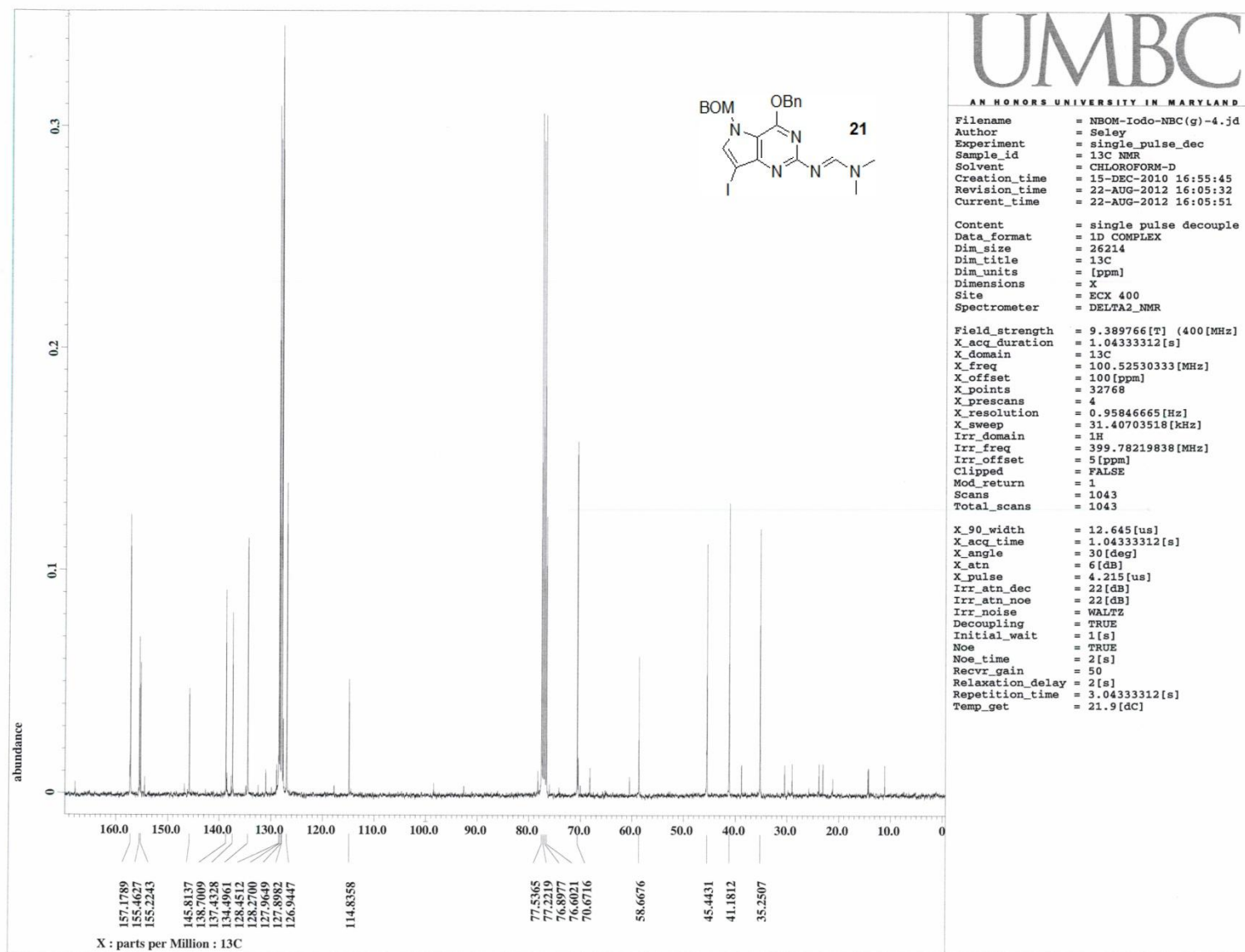


File Name : D:\VG70S Data\20130313\Kartik\KT_03_112\AccMass20PC_KT_03_112_20130314_2.ms2
Creation Date/Time : 3/14/2013 at 18:49:32
File Type : V/E raw data
File Source : Acquired on MASPEC II system [I132/1240]
File Title : FAB Accurate Mass Scan KT-03-112
Instrument : VG70SE
Notes : R = 10000, 20% Sweepwidth m/z = 381-435 amu, S = 25sec/dec
Sample in mNBA matrix on slated probe tip, PEGMME 350 mass ref
Gun = 28kV @ 2uA

SCAN GRAPH. Flagging=High Resolution M/z. Rolling Average(5). Ctd=[Thr:10mV, Min.Wid(Mlt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
Scan 1#0:17 - 30#2:56. Entries=27. Base M/z=416.20772. 100% Int.=3.02872. POS.

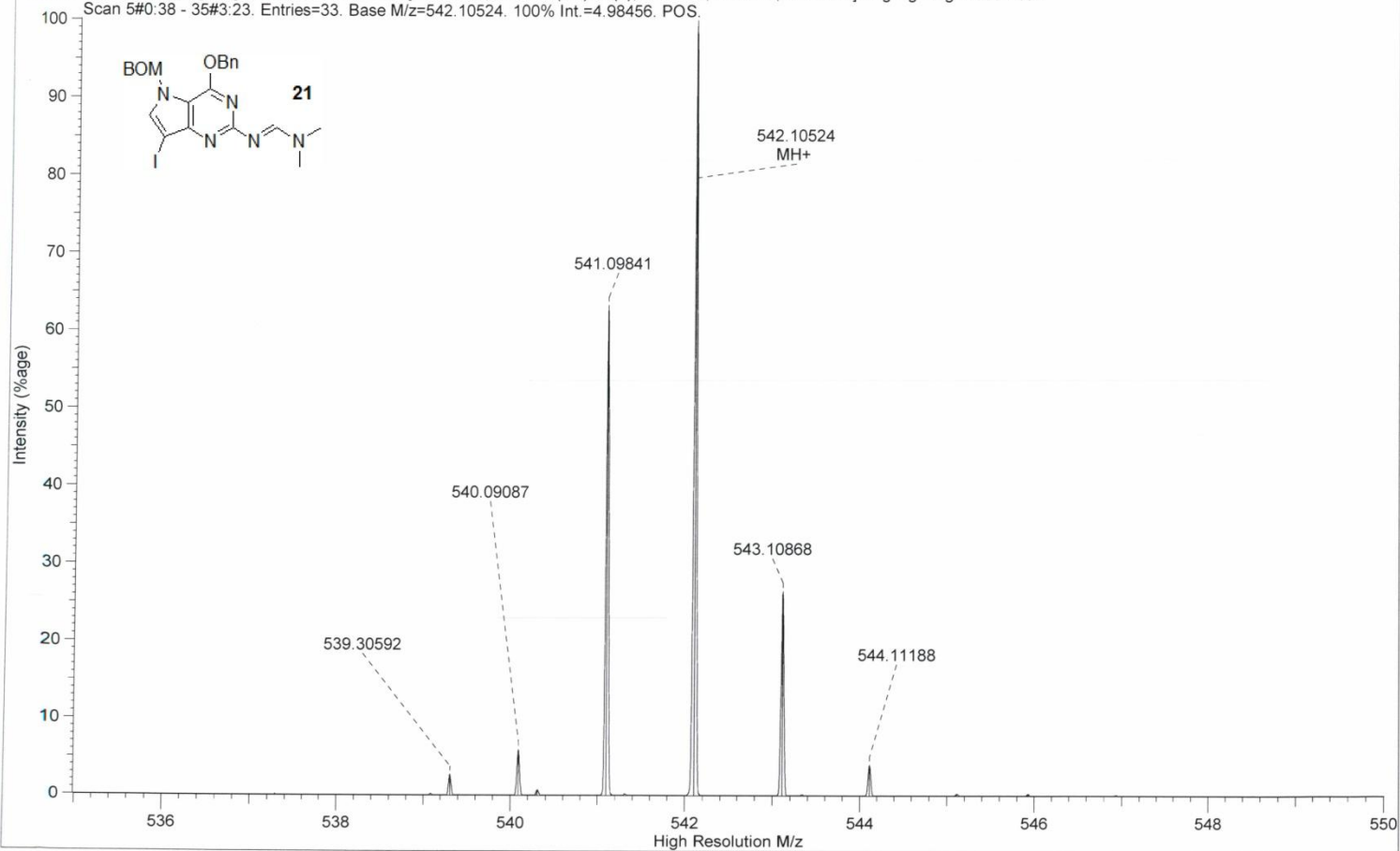


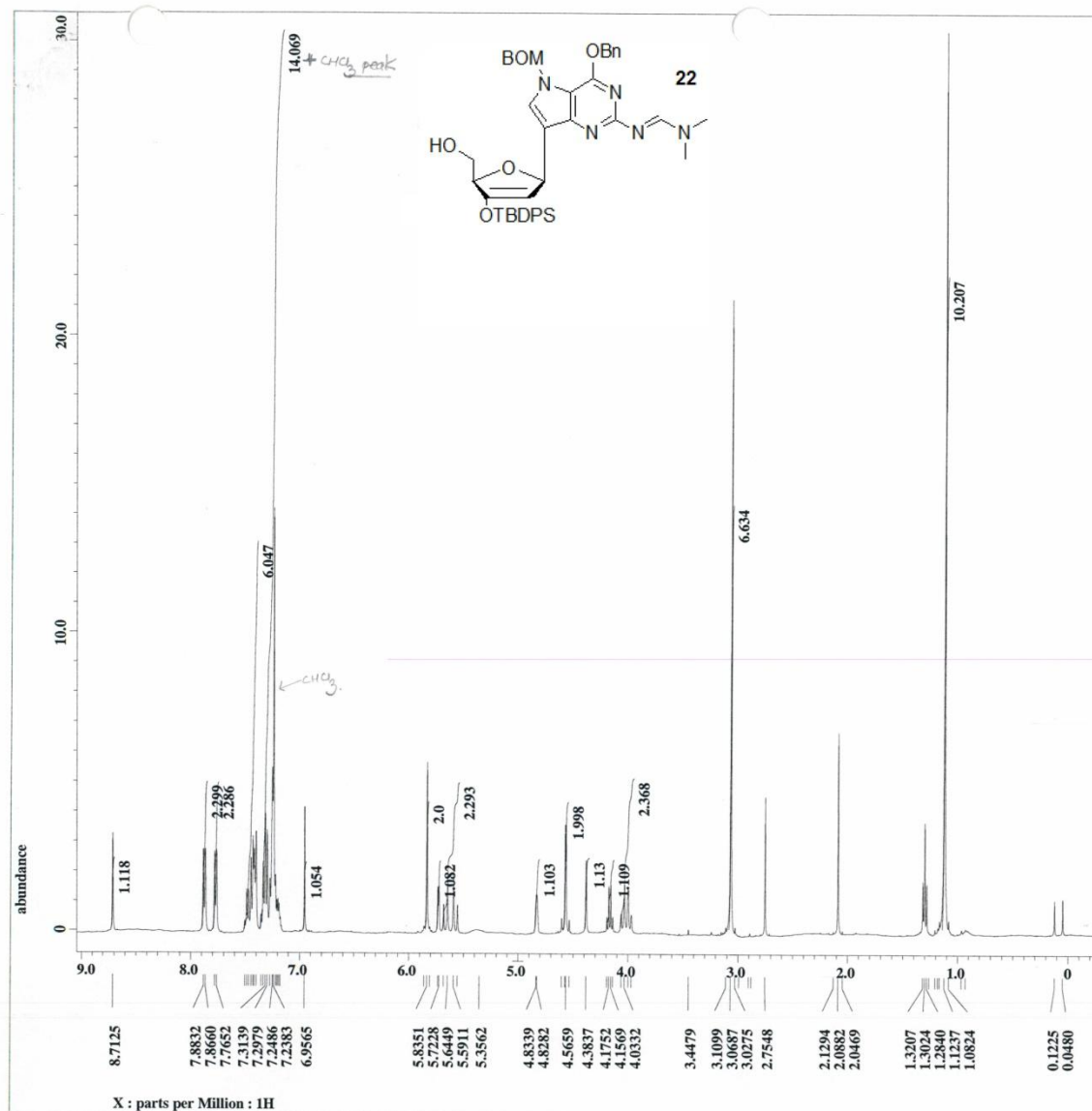




File Name : D:\VG70S Data\20101217\Kartik\KT_03_115\AccMass20PC_KT_03_115_20101217_2.ms2
 Creation Date/Time : 12/17/2010 at 17:10:30
 File Type : V/E raw data
 File Source : Acquired on MASPEC II system [II32/1240]
 File Title : FAB Accurate Mass Scan KT-03-115
 Instrument : VG70SE
 Notes : R = 10000, 20% Sweepwidth m/z = 511-565 amu, S = 25sec/dec
 Sample in mNBA matrix on slated probe tip, PEGMME 550 mass ref
 Gun = 28kV @ 2umA

SCAN GRAPH. Flagging=High Resolution M/z. Ctd=[Thr:10mV, Min.Wid(Mlt):10(7), Det:50%, Inc:50%, Res:90%]. Highlighting=Base Peak.
 Scan 5#0:38 - 35#3:23. Entries=33. Base M/z=542.10524. 100% Int.=4.98456. POS.





UMBC

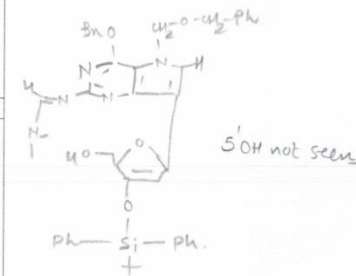
AN HONORS UNIVERSITY IN MARYLAND

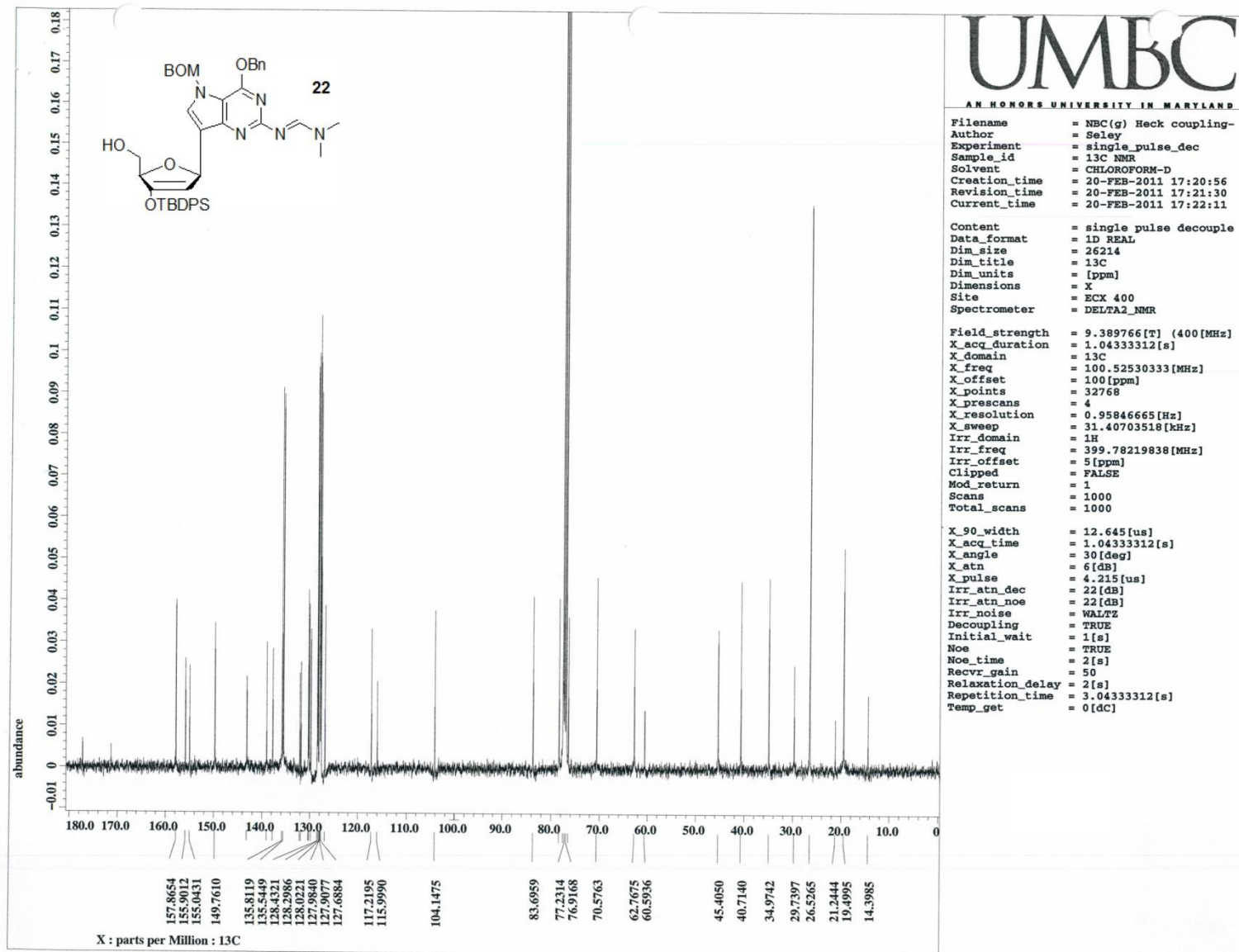
Filename = NBC(g) Heck coupling-
 Author = Seley
 Experiment = single_pulse.ex2
 Sample_id = 1H NMR
 Solvent = CHLOROFORM-D
 Creation_time = 20-FEB-2011 12:57:07
 Revision_time = 20-FEB-2011 13:02:46
 Current_time = 20-FEB-2011 13:04:06

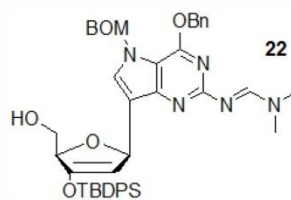
Content = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 2.18365952[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.45794685[Hz]
 X_sweep = 7.5030012[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 32
 Total_scans = 32

X_90_width = 12.69[us]
 X_acq_time = 2.18365952[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 6.345[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 7.18365952[s]
 Temp_get = 0[degC]







KT/03/134

Narrowband

FW= 767

JAW 04112011_pos_29

Observed mass = 768.358493 daltons

Calculated mass = 768.357573 daltons

Error= 1.19 ppm

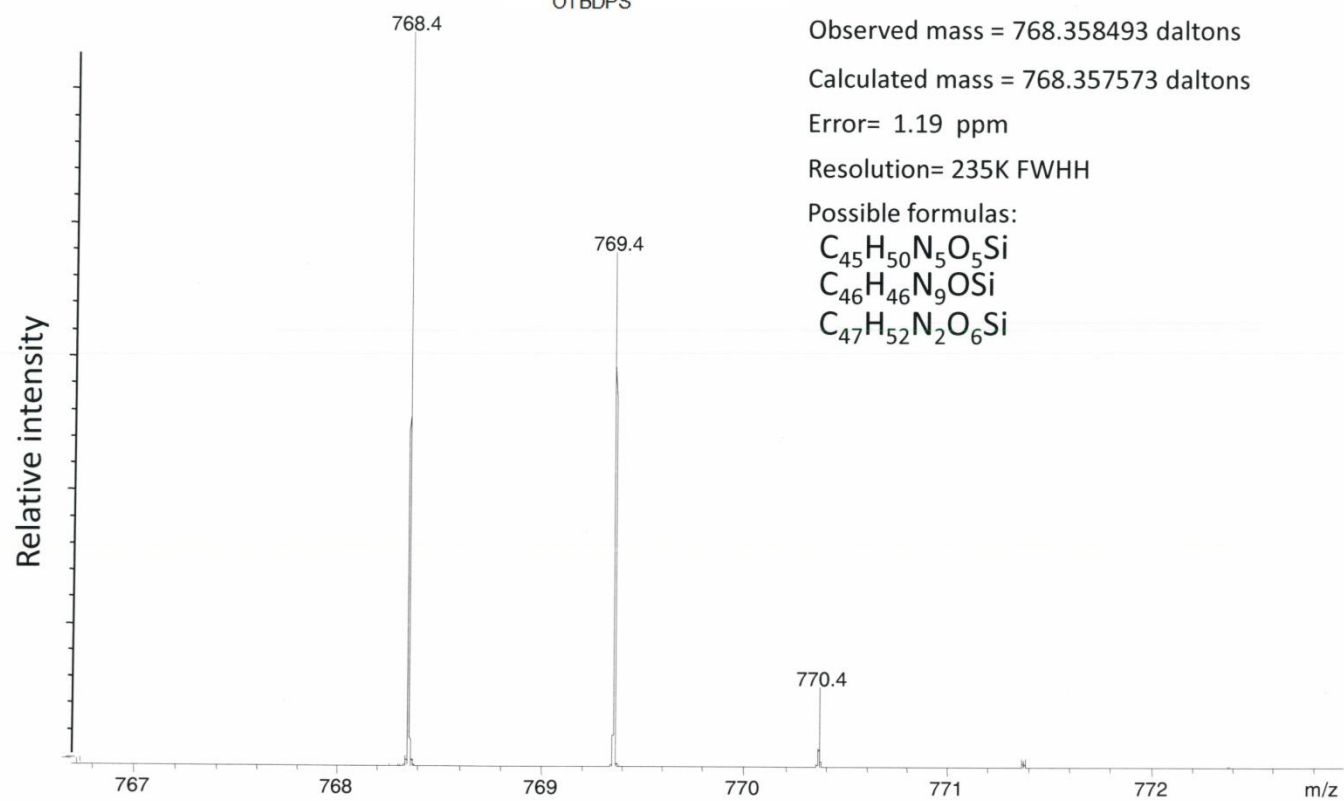
Resolution= 235K FWHH

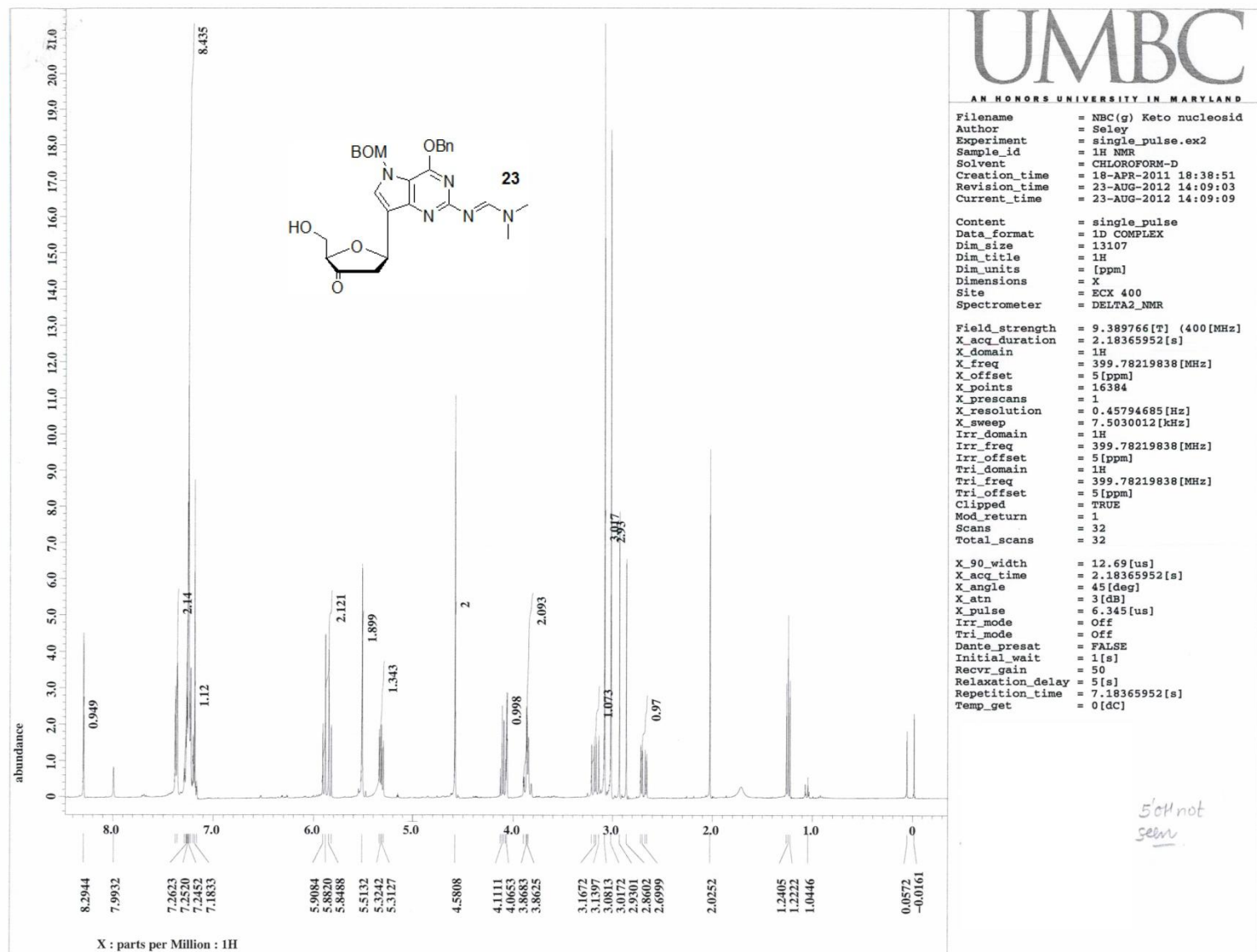
Possible formulas:

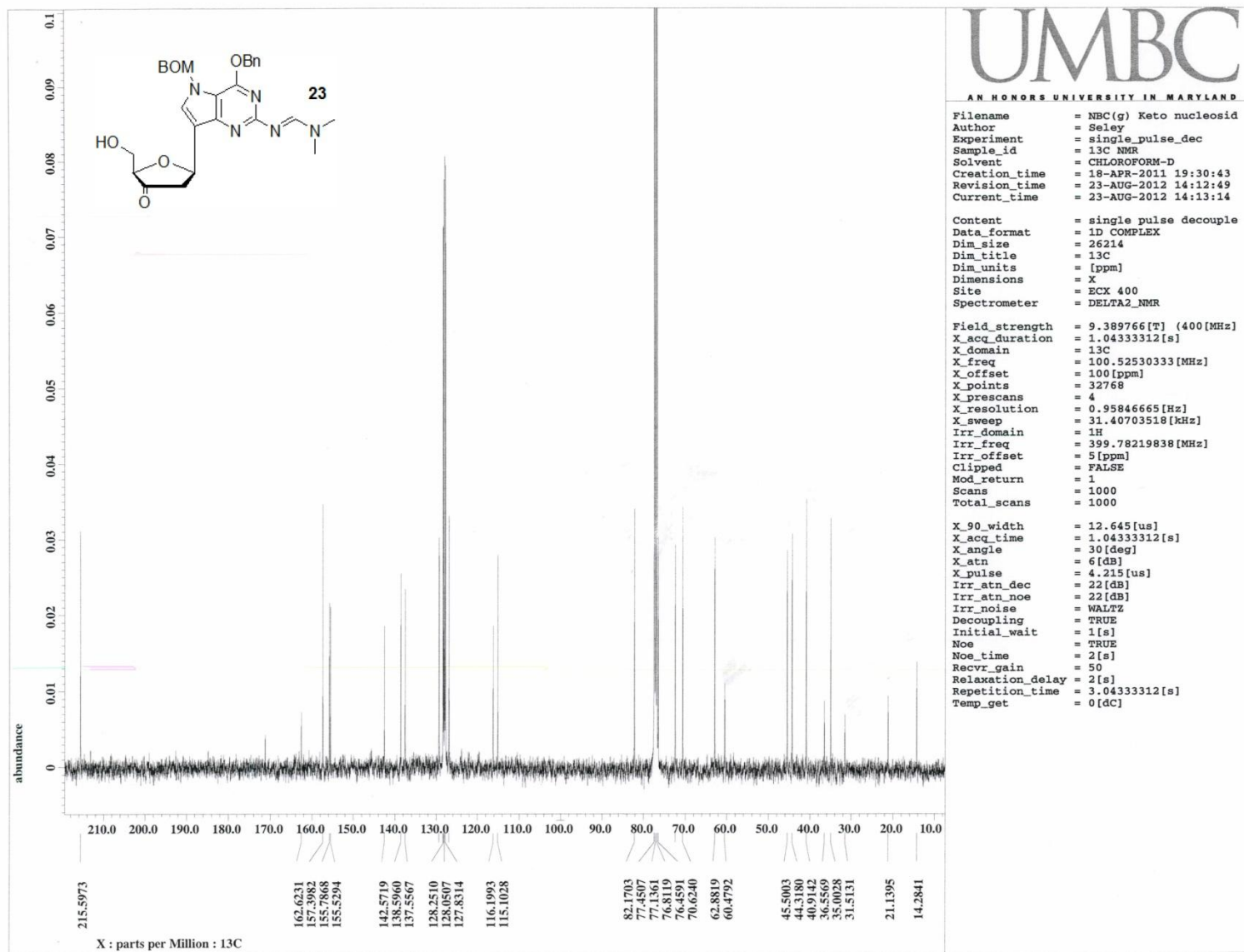
$C_{45}H_{50}N_5O_5Si$

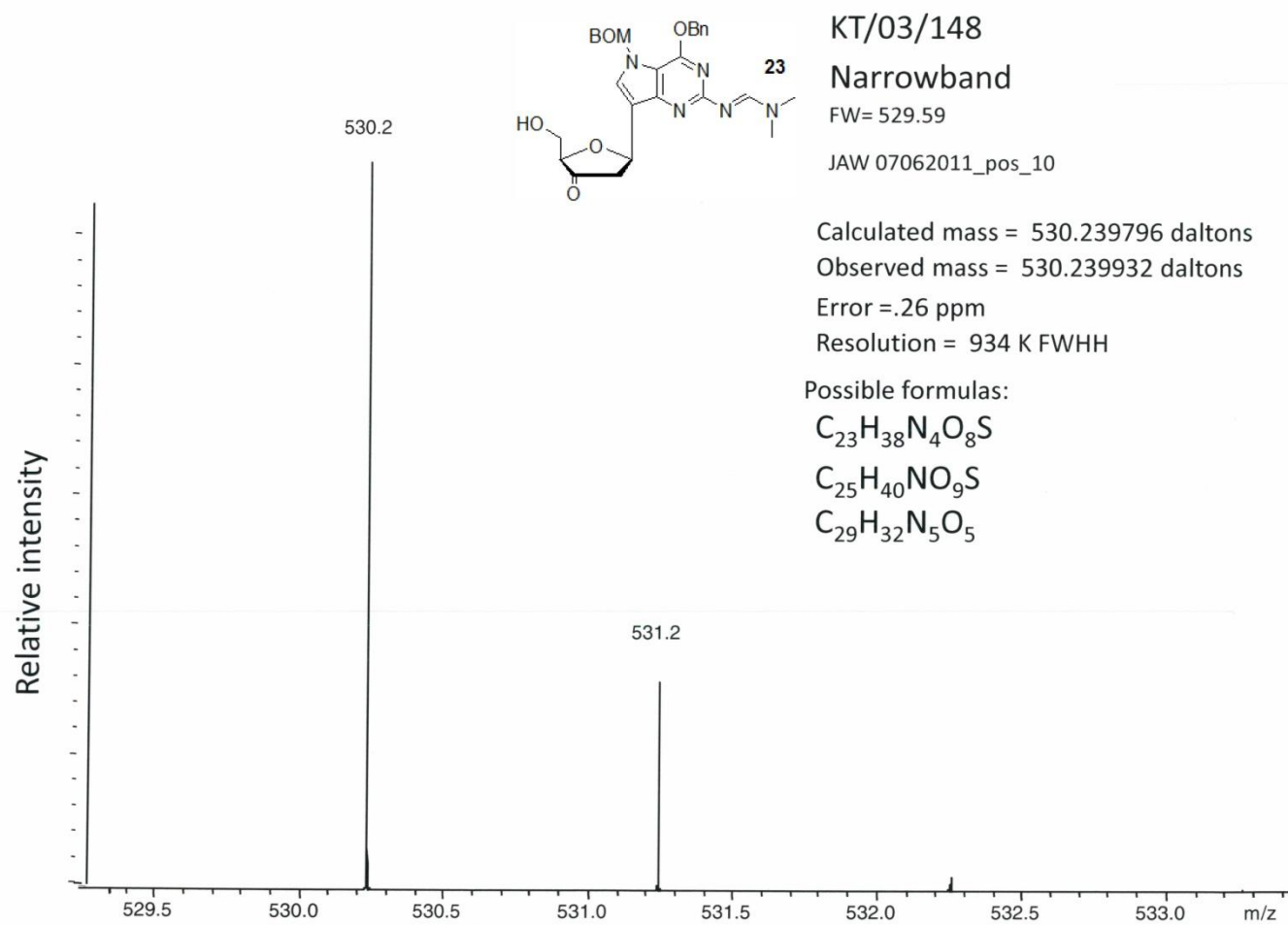
$C_{46}H_{46}N_9OSi$

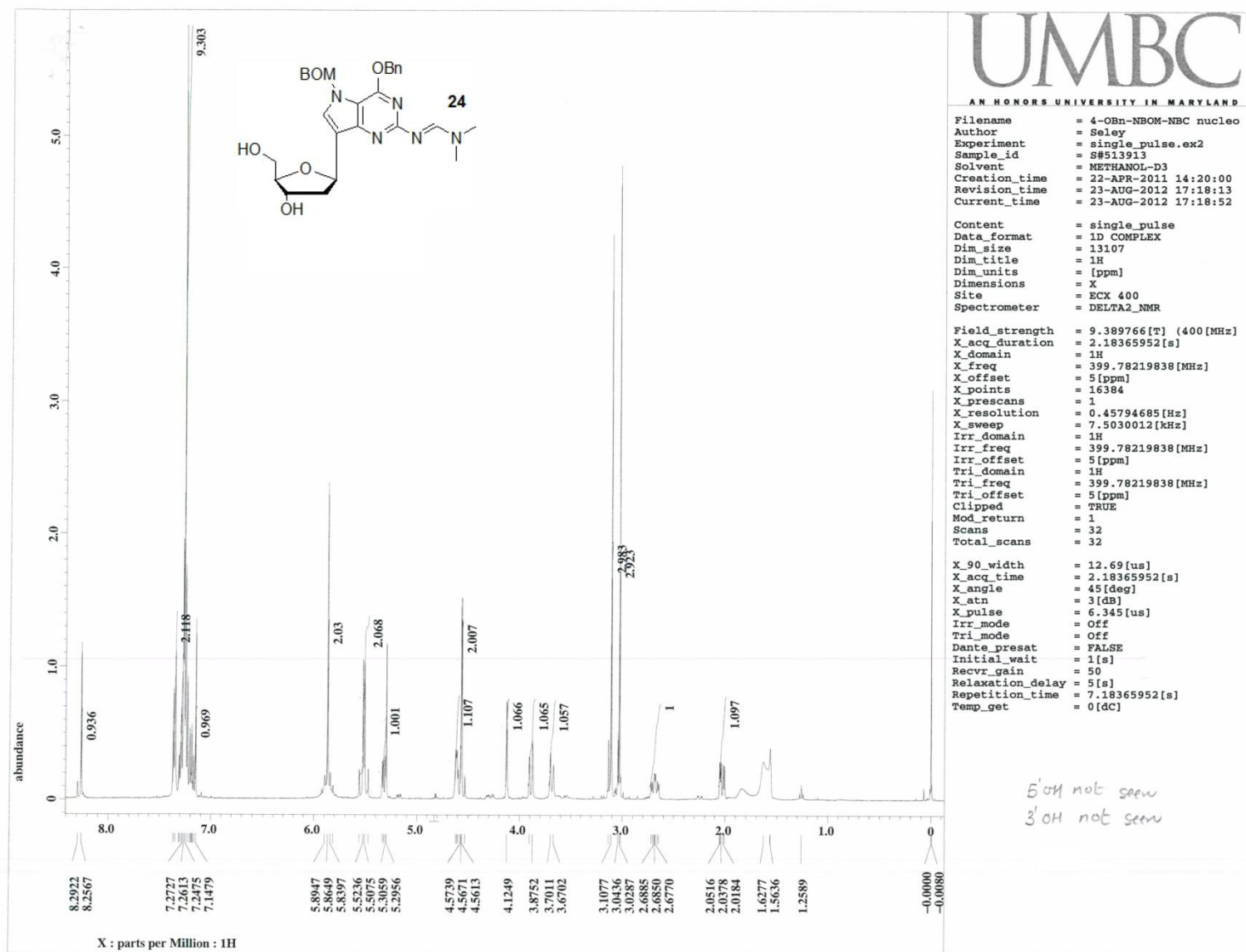
$C_{47}H_{52}N_2O_6Si$

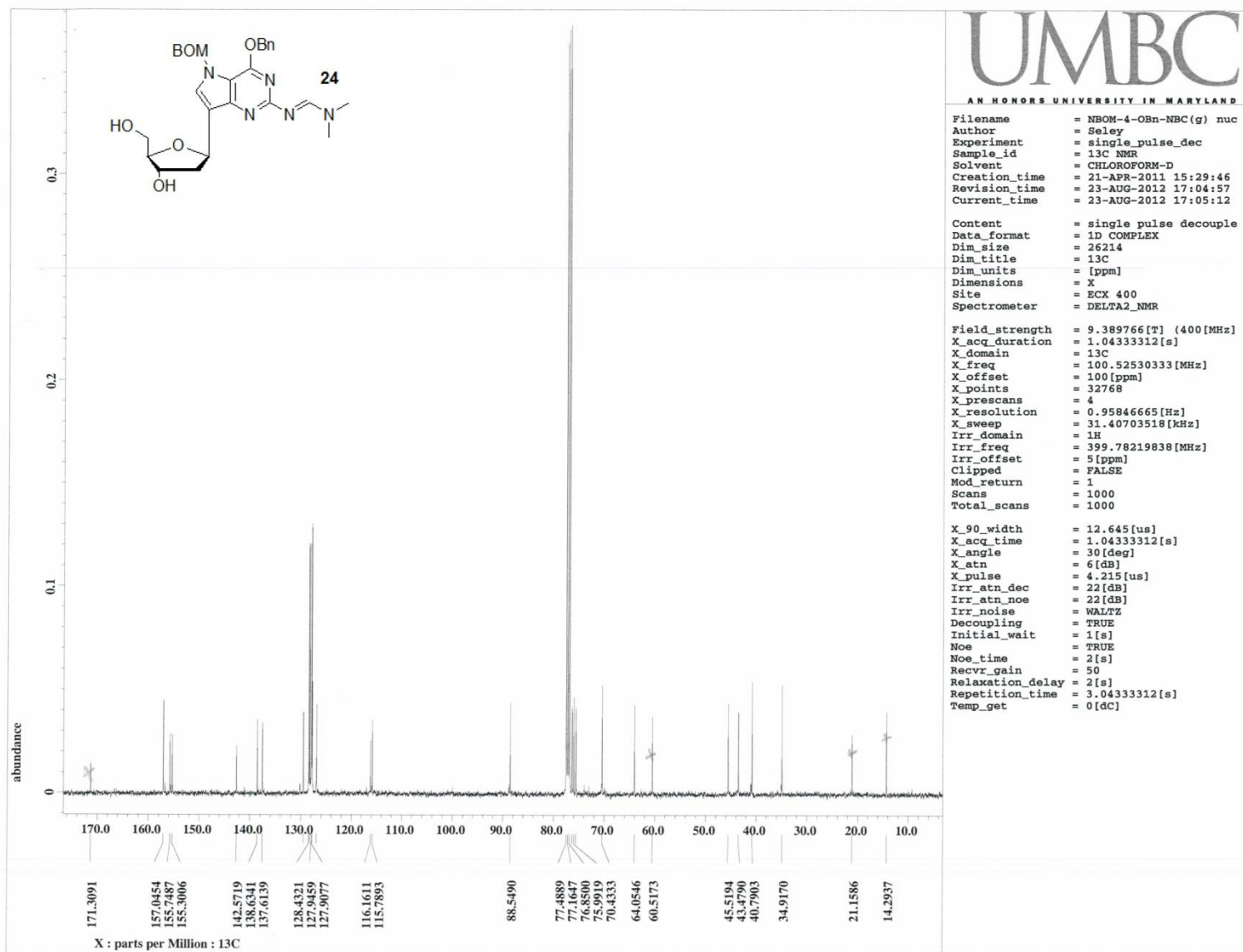


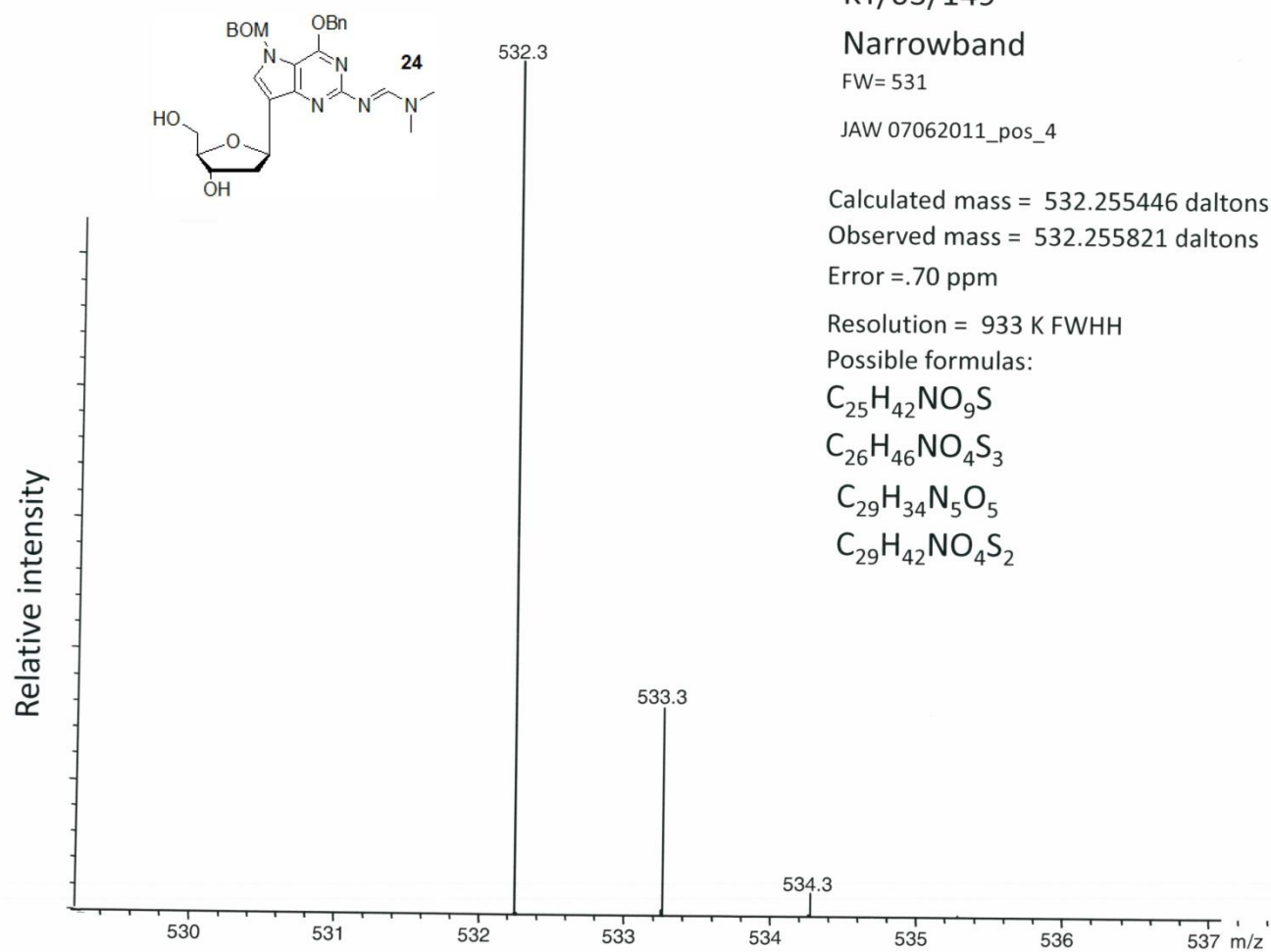


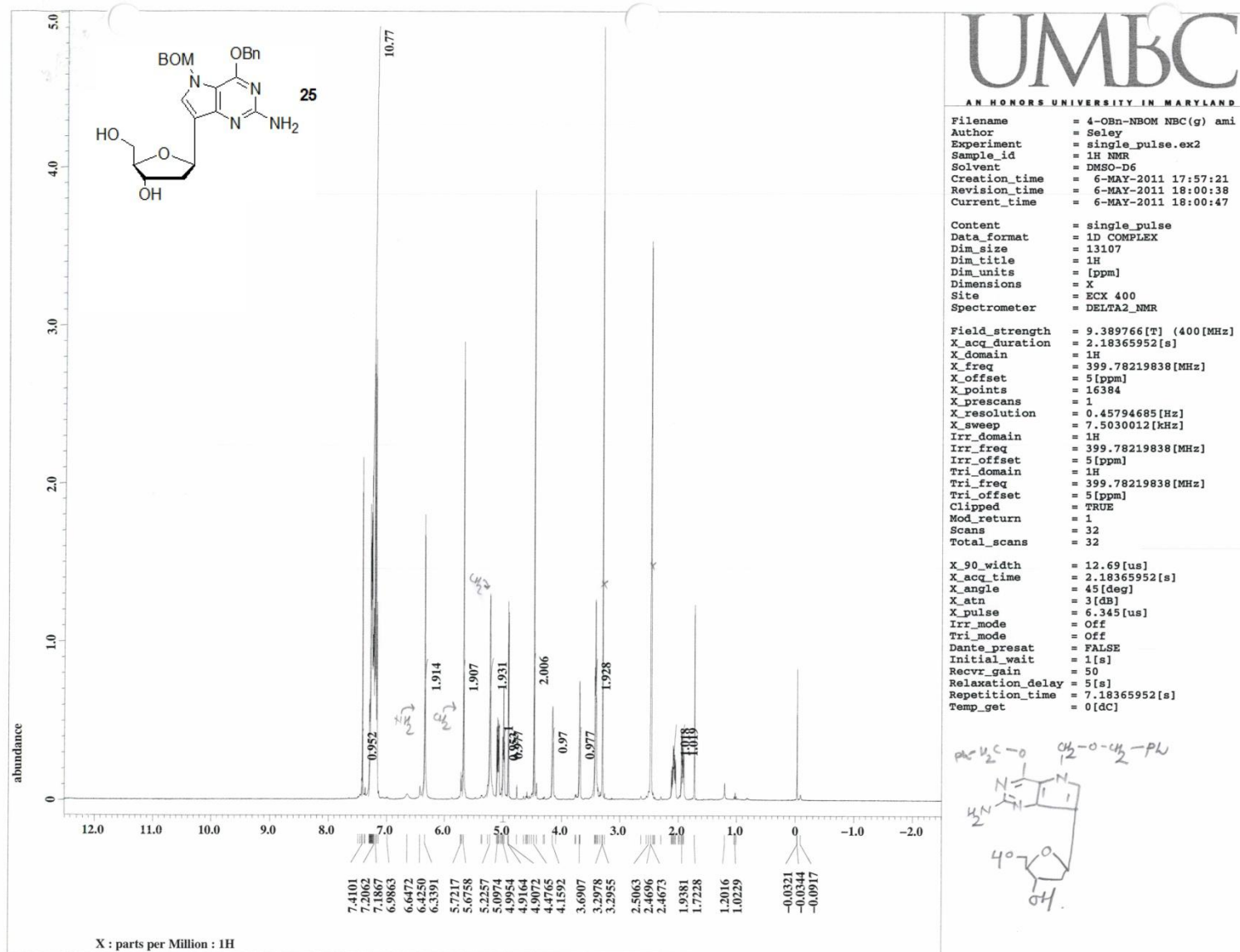


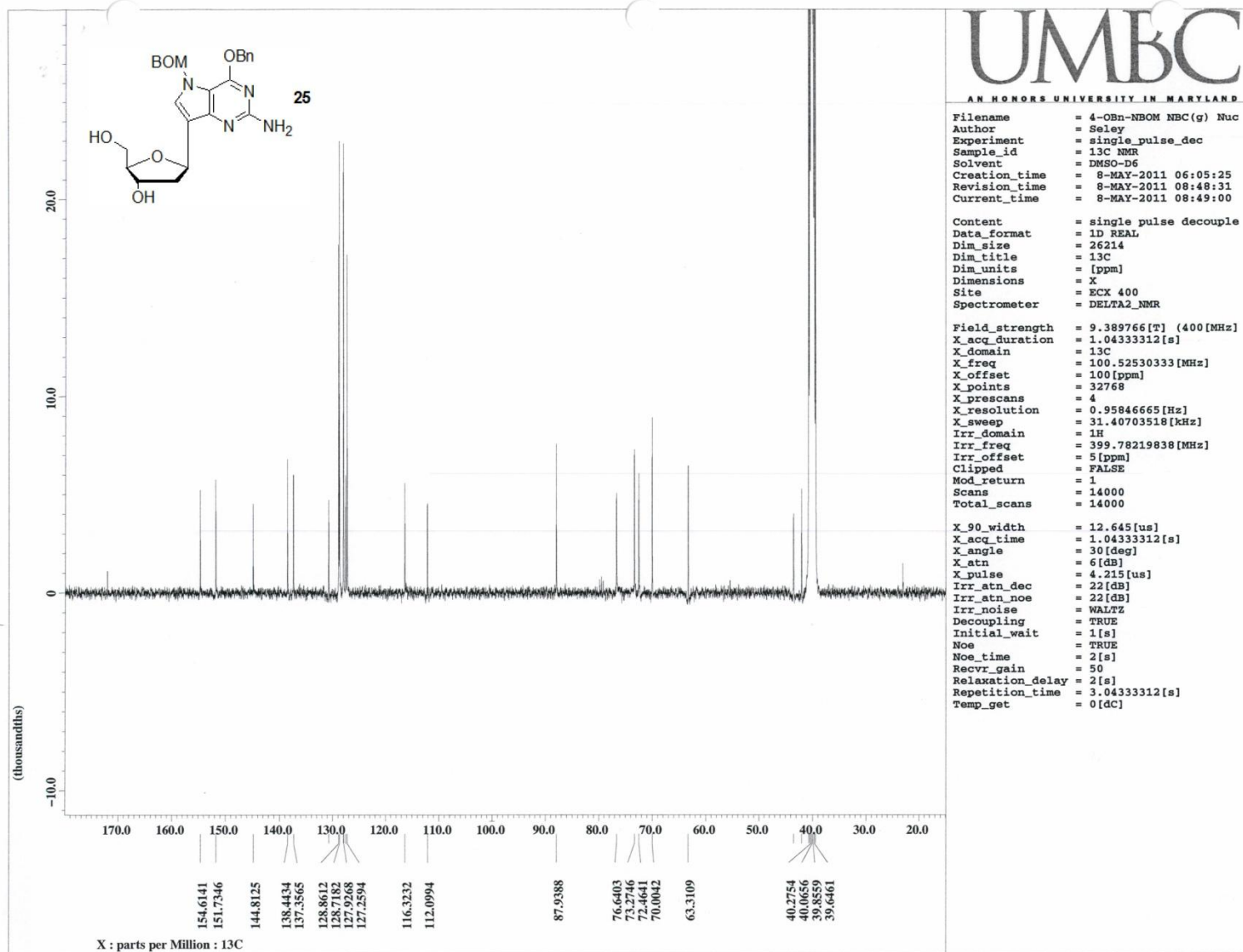


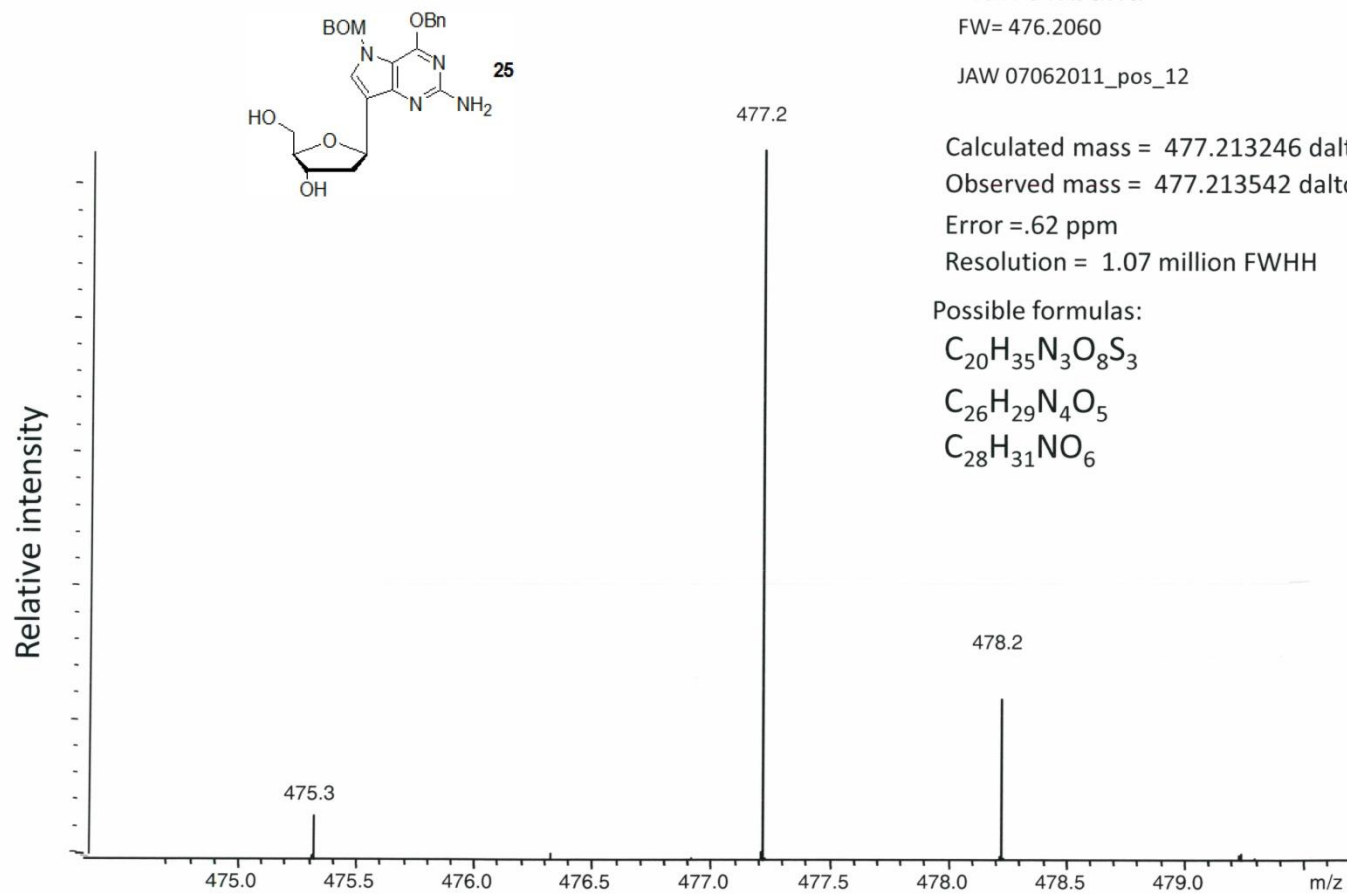












KT/03/150

Narrowband

FW= 476.2060

JAW 07062011_pos_12

Calculated mass = 477.213246 daltons

Observed mass = 477.213542 daltons

Error = .62 ppm

Resolution = 1.07 million FWHH

Possible formulas:

$C_{20}H_{35}N_3O_8S_3$

$C_{26}H_{29}N_4O_5$

$C_{28}H_{31}NO_6$

