Supporting Information

Discovery of Selective Menaquinone Biosynthesis Inhibitors against *Mycobacterium tuberculosis*

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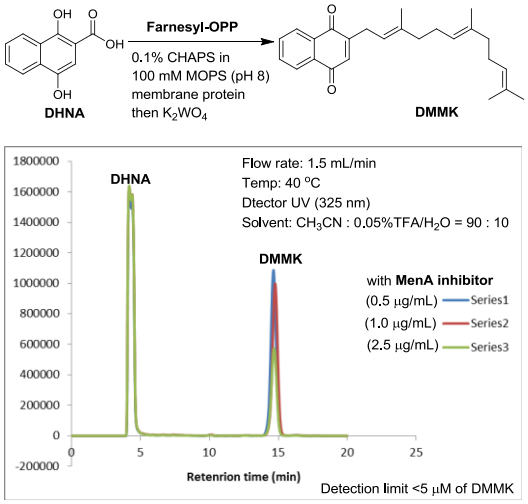
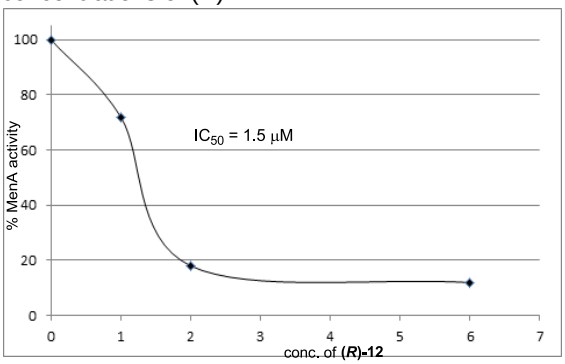
MenA Inhibitory Assay:

The substrate 1,4-dihydroxy-2-napthanoic acid (DHNA) (500 µM; 20 µl), $MgCl_2$ (5 µM; 20 µl); CHAPS (0.1%; 20 µl), Tris-buffer (pH = 8; 20 µl), membrane bound Men A (100 µl), inhibitors (0- 60 µg/ml of DMSO) and fernesylpyrophosphate (200 µM, 40 µl) were mixed together and incubated for 2 h at 37 ^{o}C. After the incubation, the reaction mixture was quenched with 0.1 M AcOH in MeOH followed by the extraction with hexane (thrice). The organic portions were then concentrated and diluted with MeOH (300 µl). From each set of enzymatic reaction mixture 20 µl was injected into the HPLC and the area of the peak for DMMK was quantified to get the IC_{50} value for different inhibitor molecules.

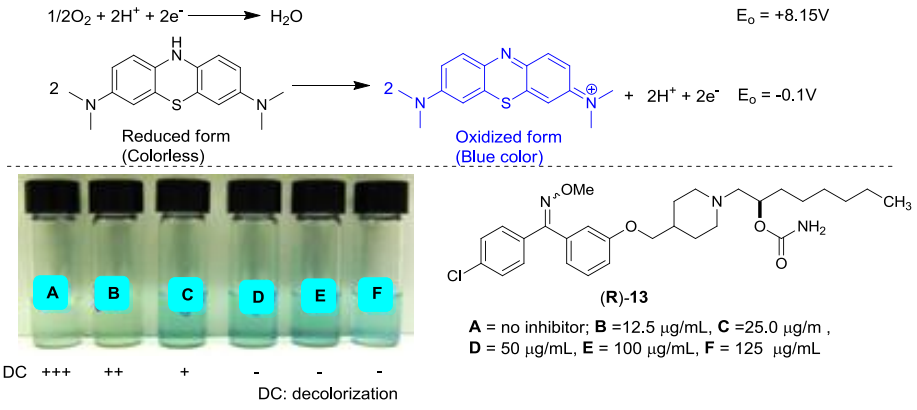


A representative MenA inhibition curve with different concentrations of (*R*)-**12**

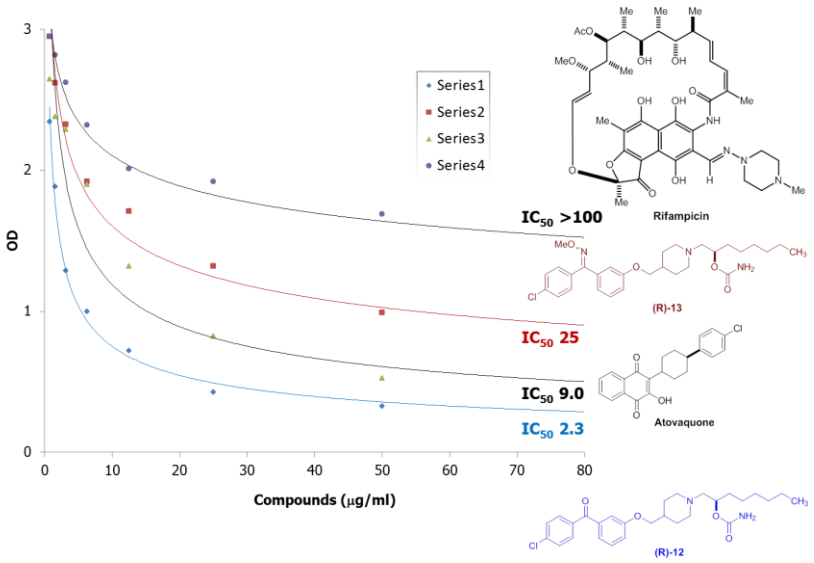


Oxygen consumption assay:

Into sterile glass vials 1.5 ml of *M. tuberculosis* (grown to 0.5 OD value) was placed. 80 µl of inhibitor molecules (total concentration ranged from 5-100 µg/ml) and 0.01% methylene blue was added. The glass vials were kept at 37 ^{o}C for 22h. The effective concentrations of the inhibitor molecule at which the electron transport systems were inhibited were determined by comparing the color intensity with the control vial (no inhibitor).



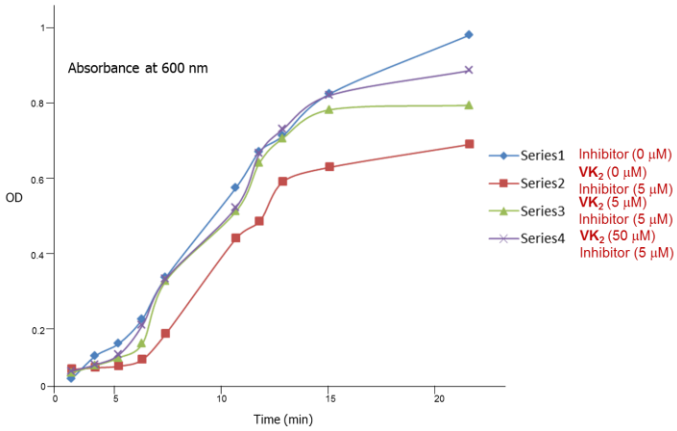
Cytotoxicities (IC_{50}) of (*R*)-12, (*R*)-13, atovaquone, and rifampin in HepG2 cells.



***E. coli* Growth Inhibitory Assays under Anaerobic Conditions:**

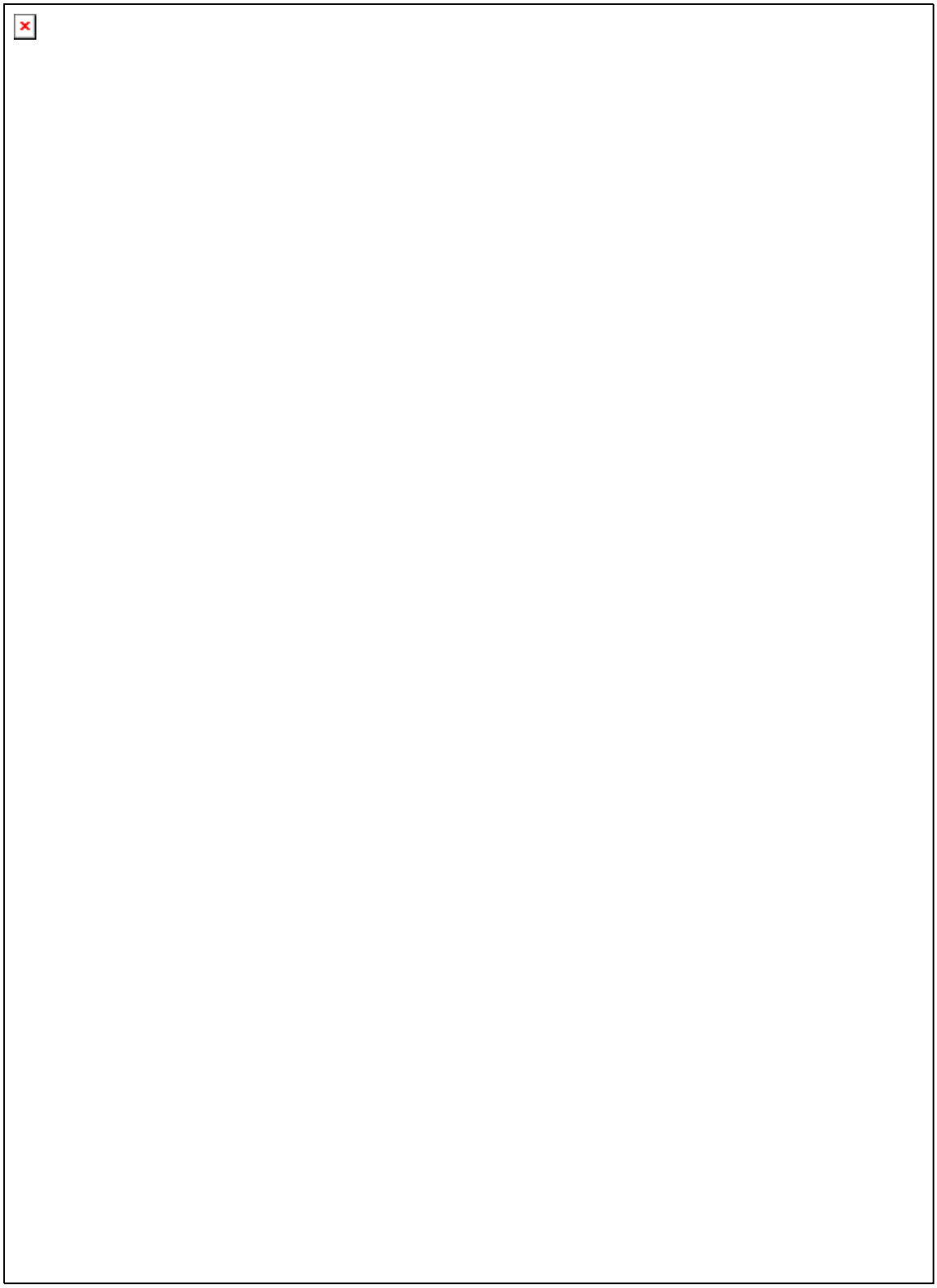
The *E. coli* was grown under anaerobic conditions using the following growth media.

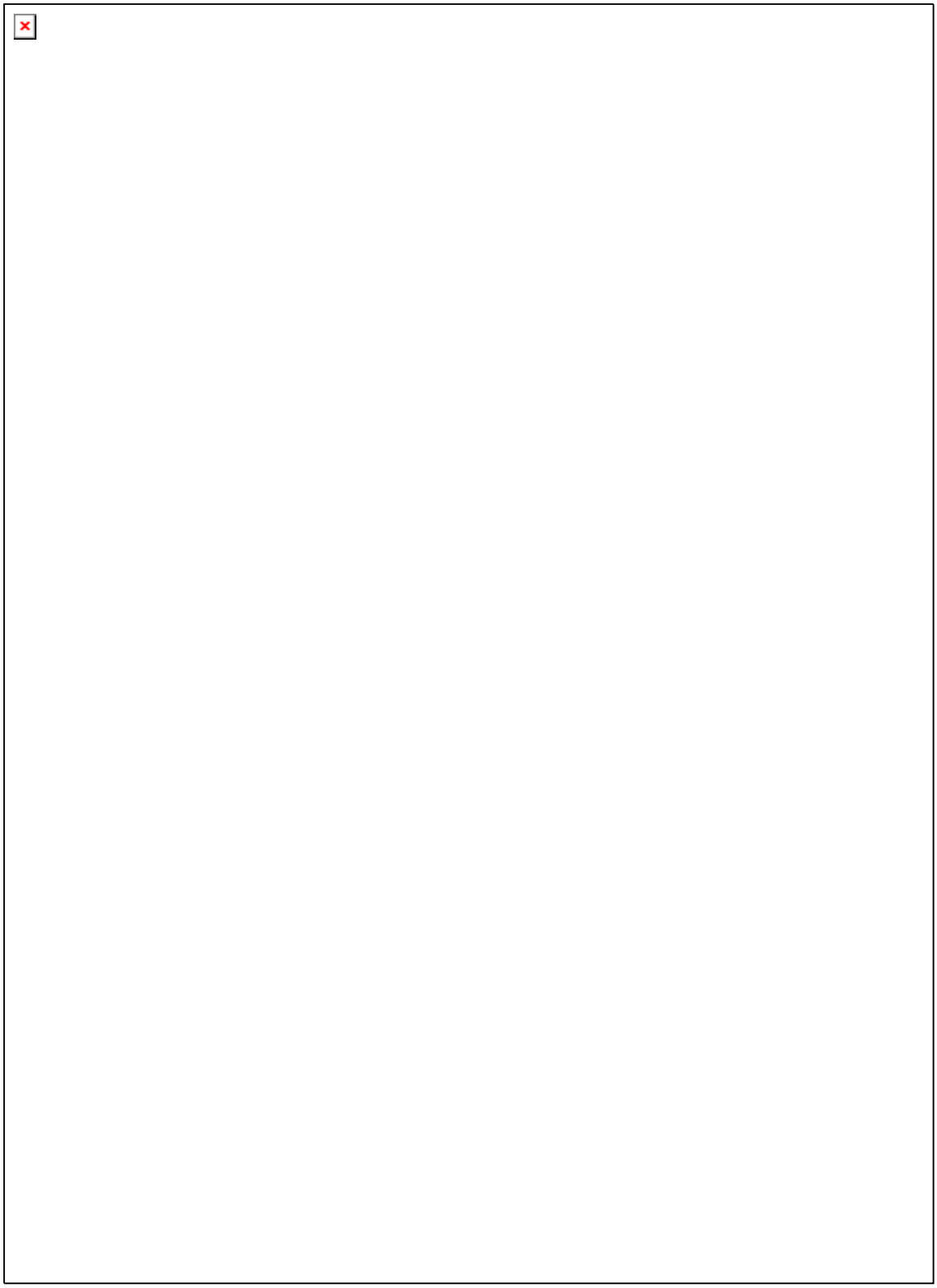
Growth Media:
Pancreatic Digest of Casein, 20.0 g
Yeast Extract, 10.0 g
Resazurin, 0.001 g
Calcium Chloride, anhydrous, 0.008 g
Magnesium Sulfate, anhydrous, 0.008 g
Potassium Phosphate, monobasic, 0.04 g
Potassium Phosphate, dibasic, 0.04 g
Sodium Chloride, 0.08 g
Sodium Bicarbonate, 0.4 g
Hemin (0.1% Soln), 5.0 mL
L-Cysteine, 0.5 g
Distilled Water, 1000.0 mL

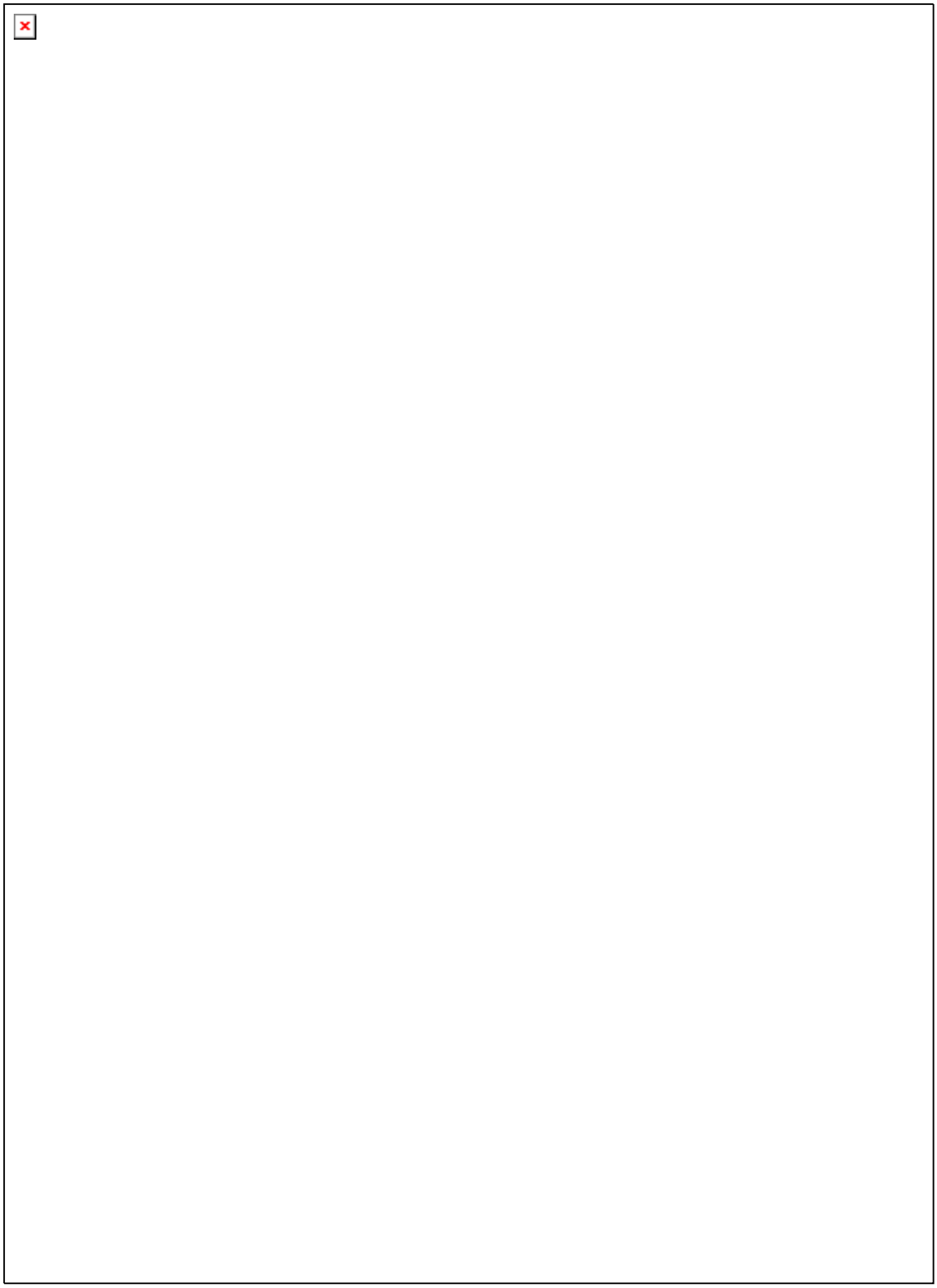


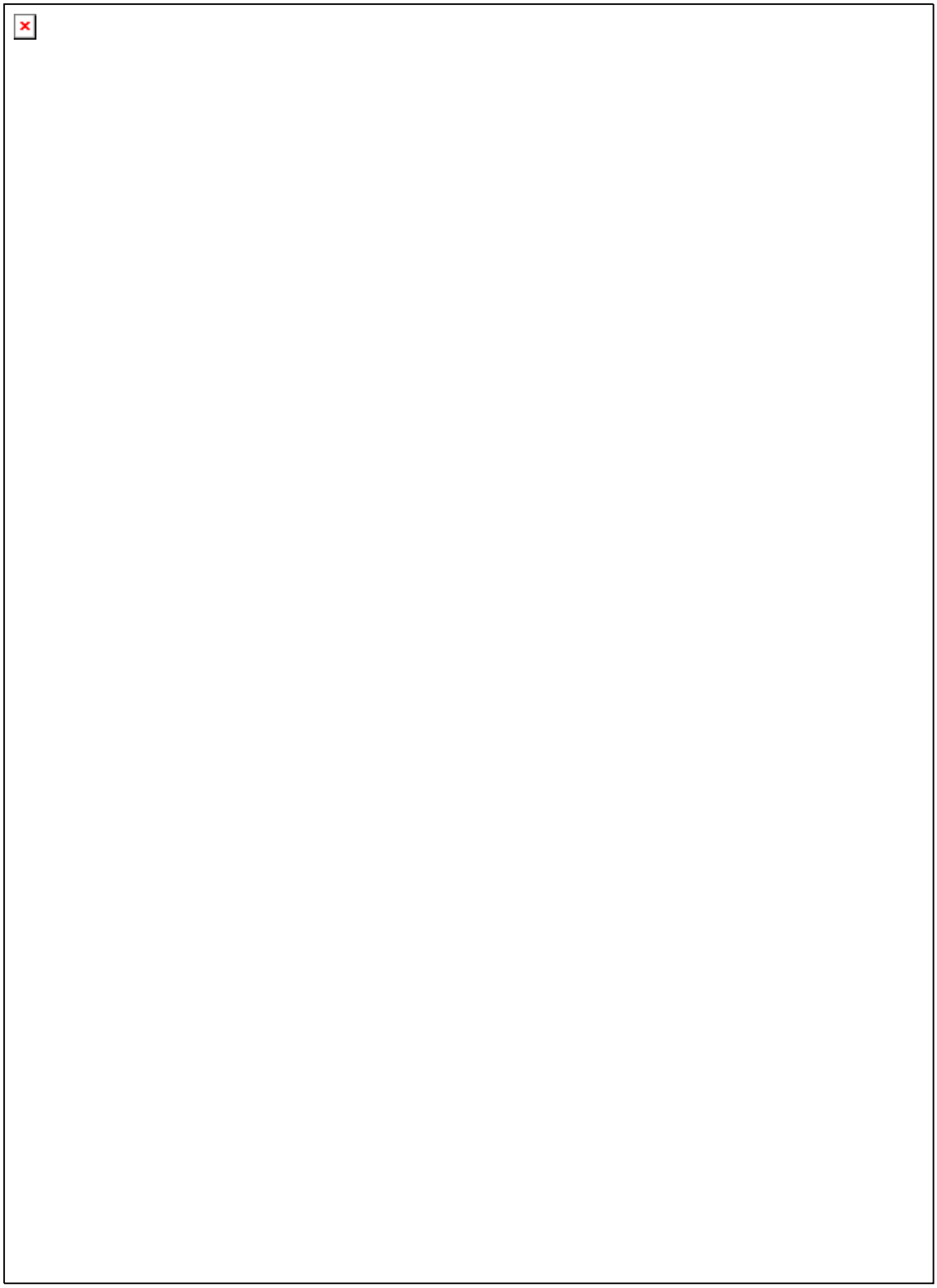
E. coli was grown with inhibitor molecule (5 µg/mL) under anaerobic conditions in the media summarized above, and the growth curve was monitored photometrically by reading the optical density at 600 nm. Similarly, *E. coli* growth rescue studies were performed by supplementing menaquinone (50 µM).

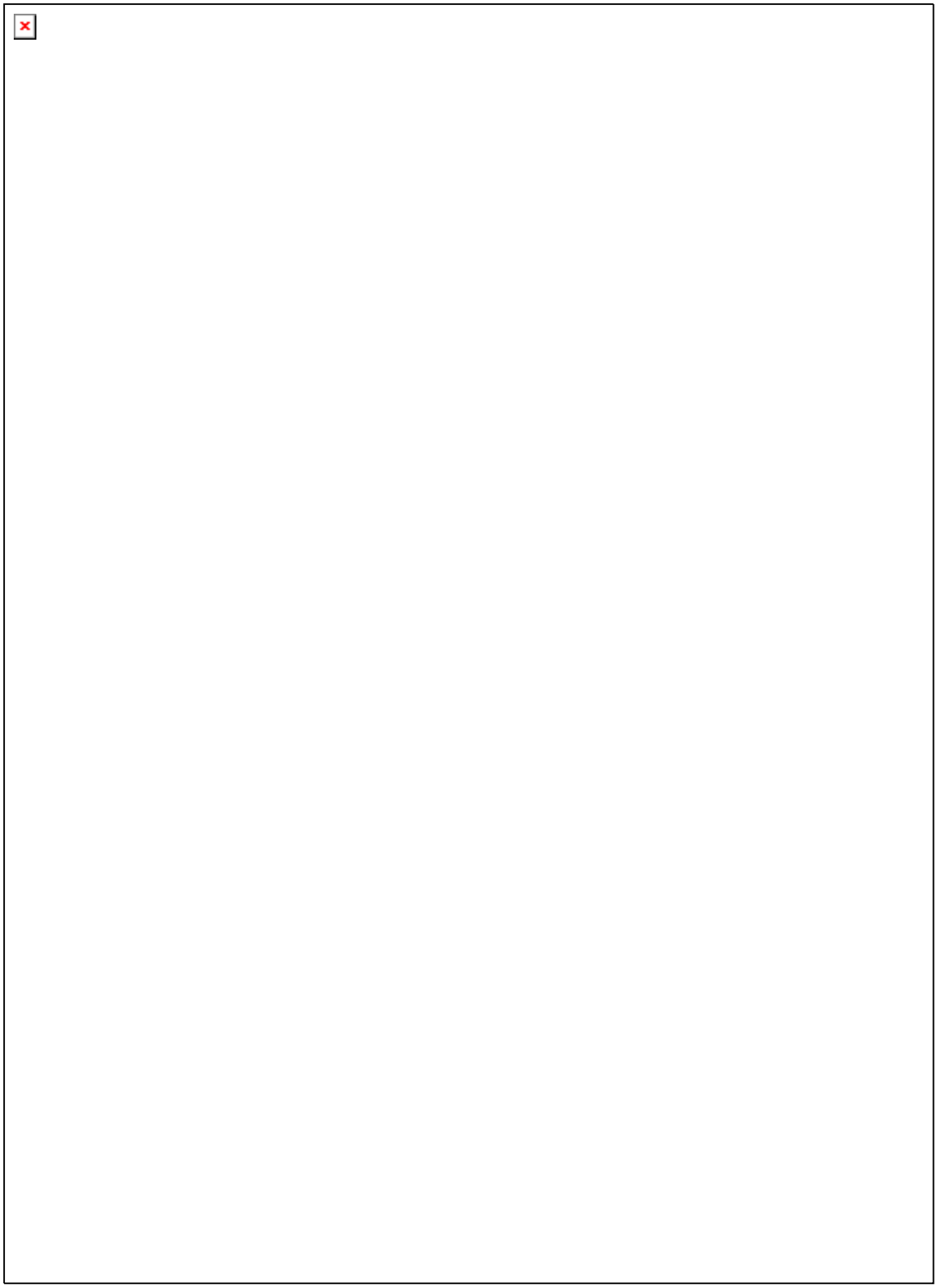
Copies of NMR Spectra and HPLC Analysis of New Compounds (follow):

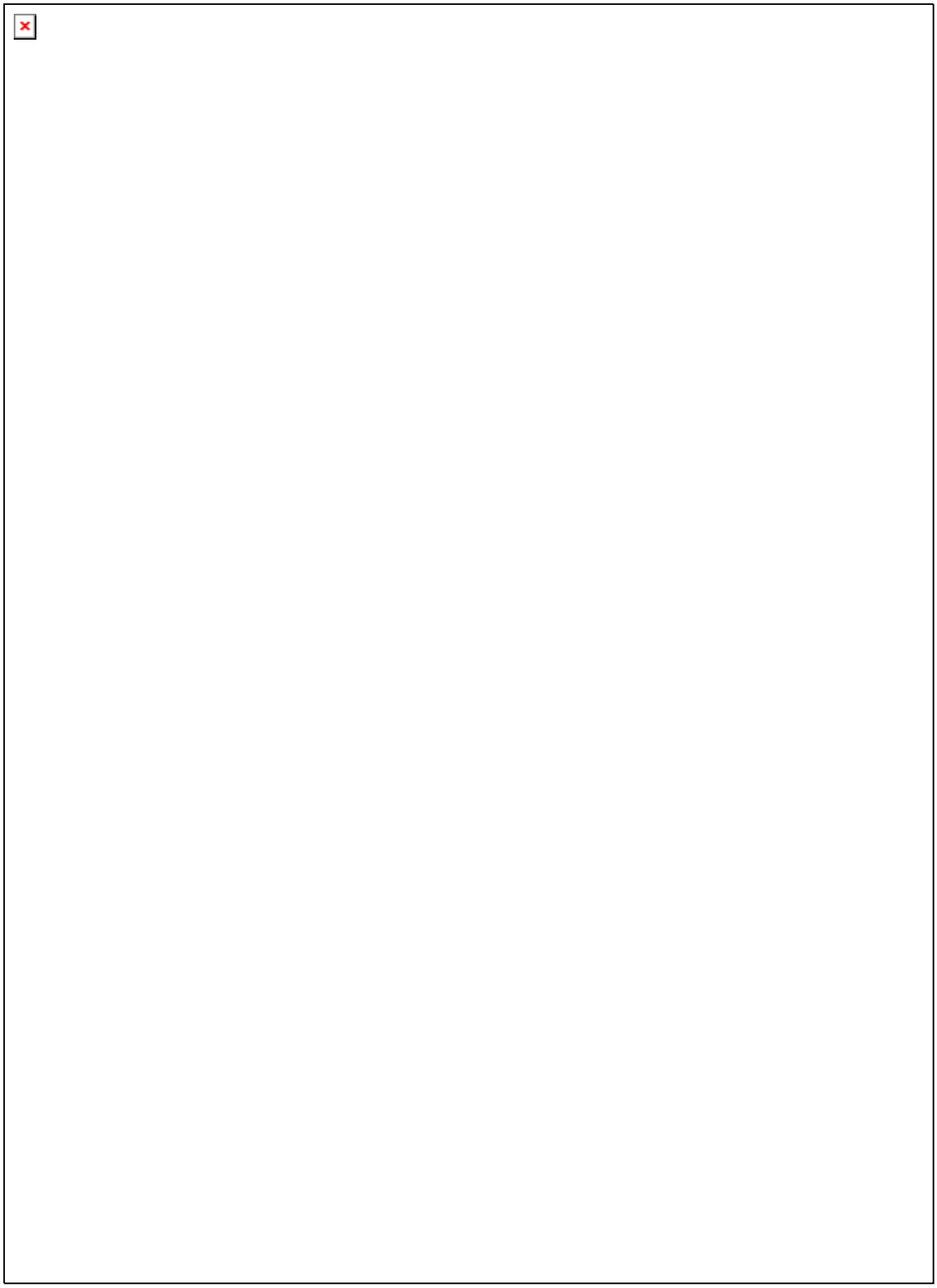


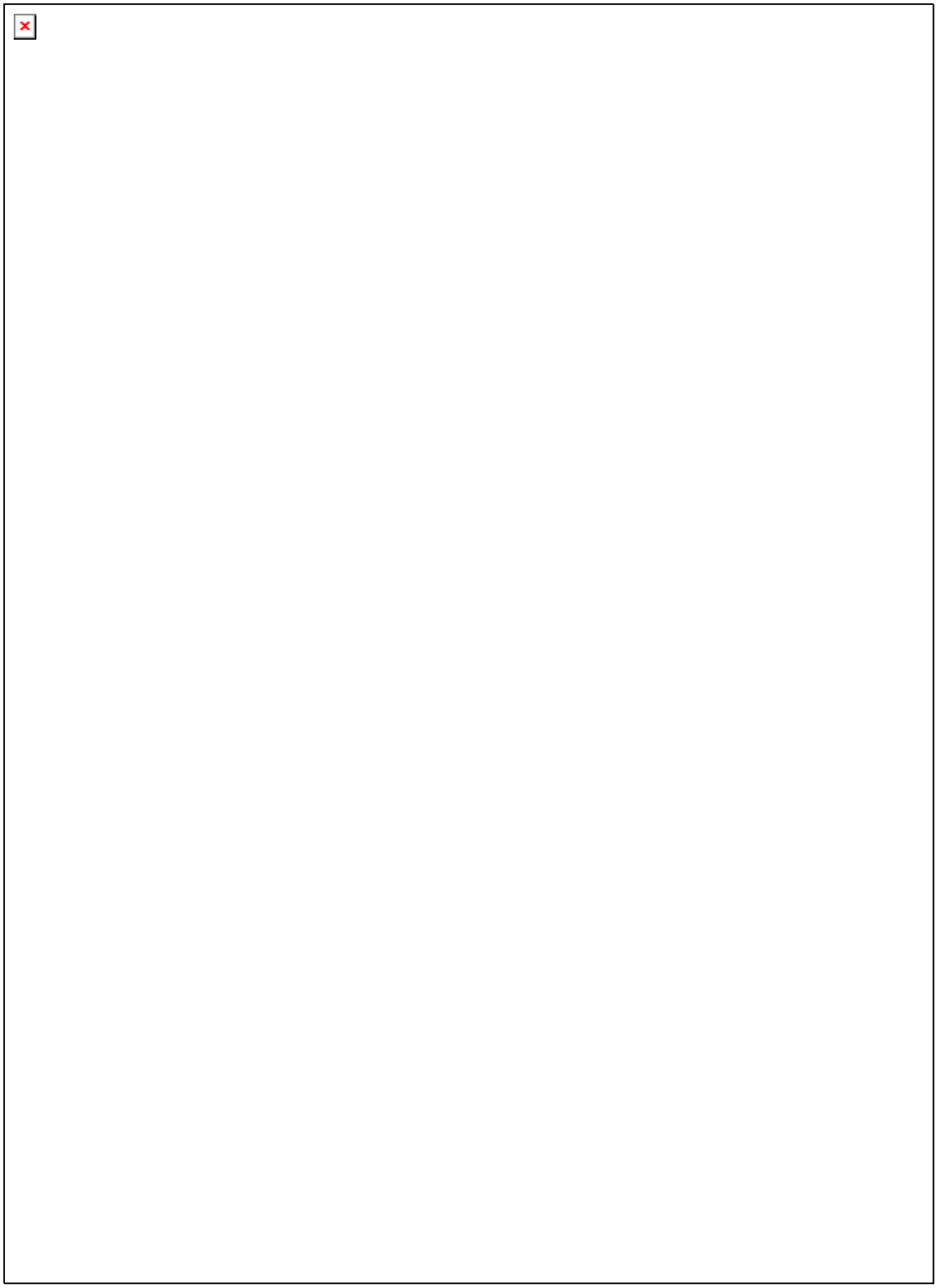


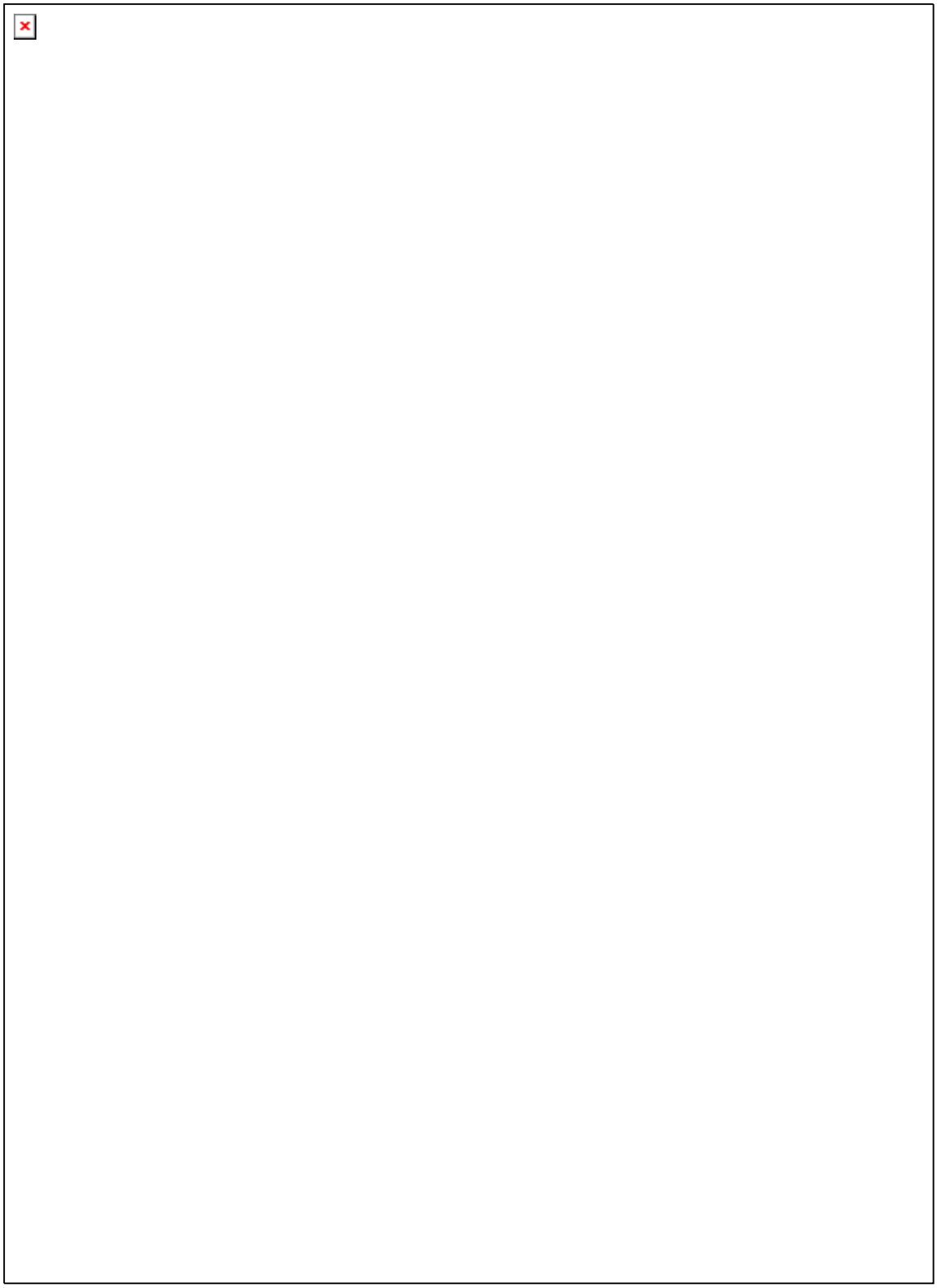


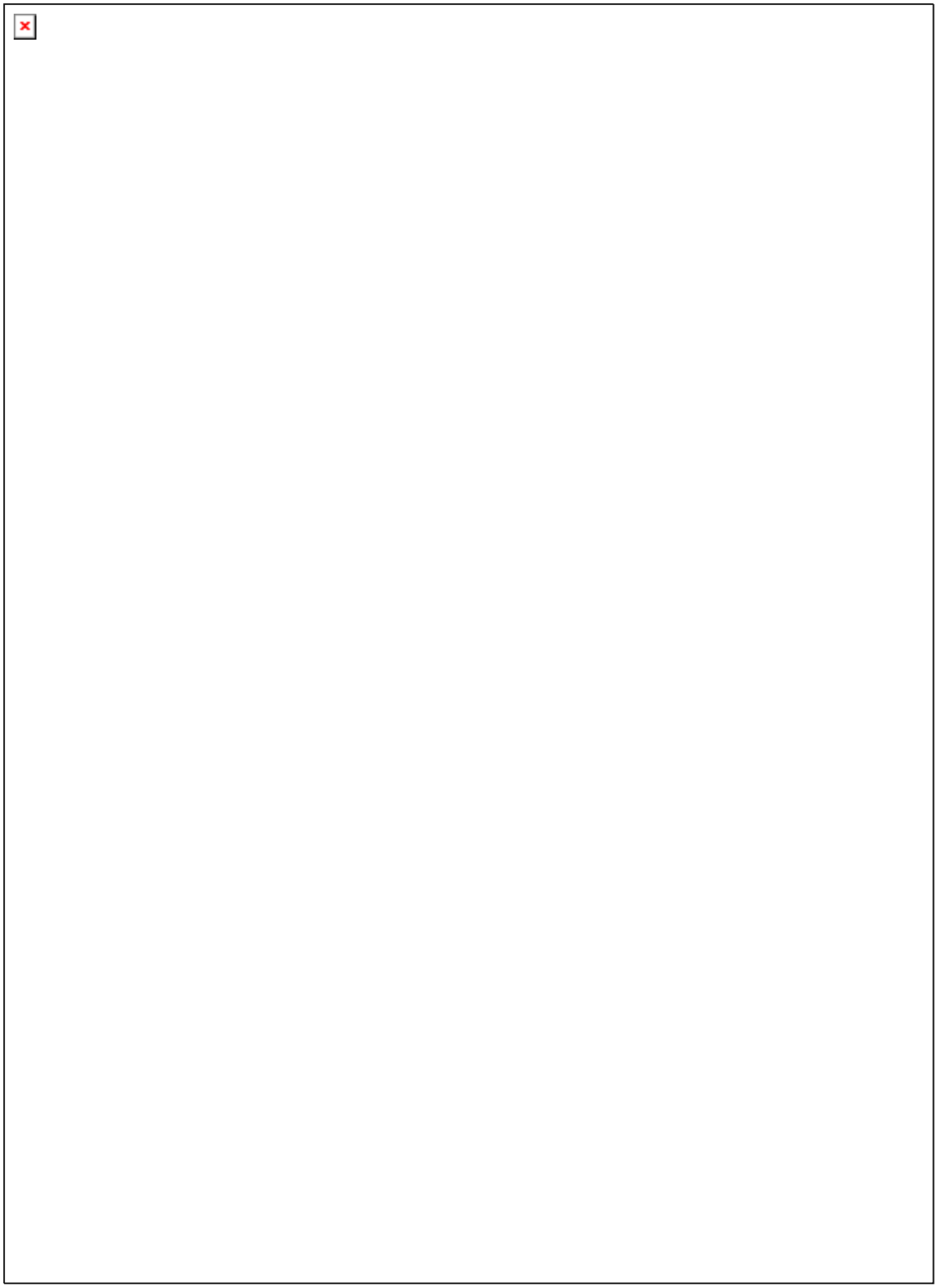


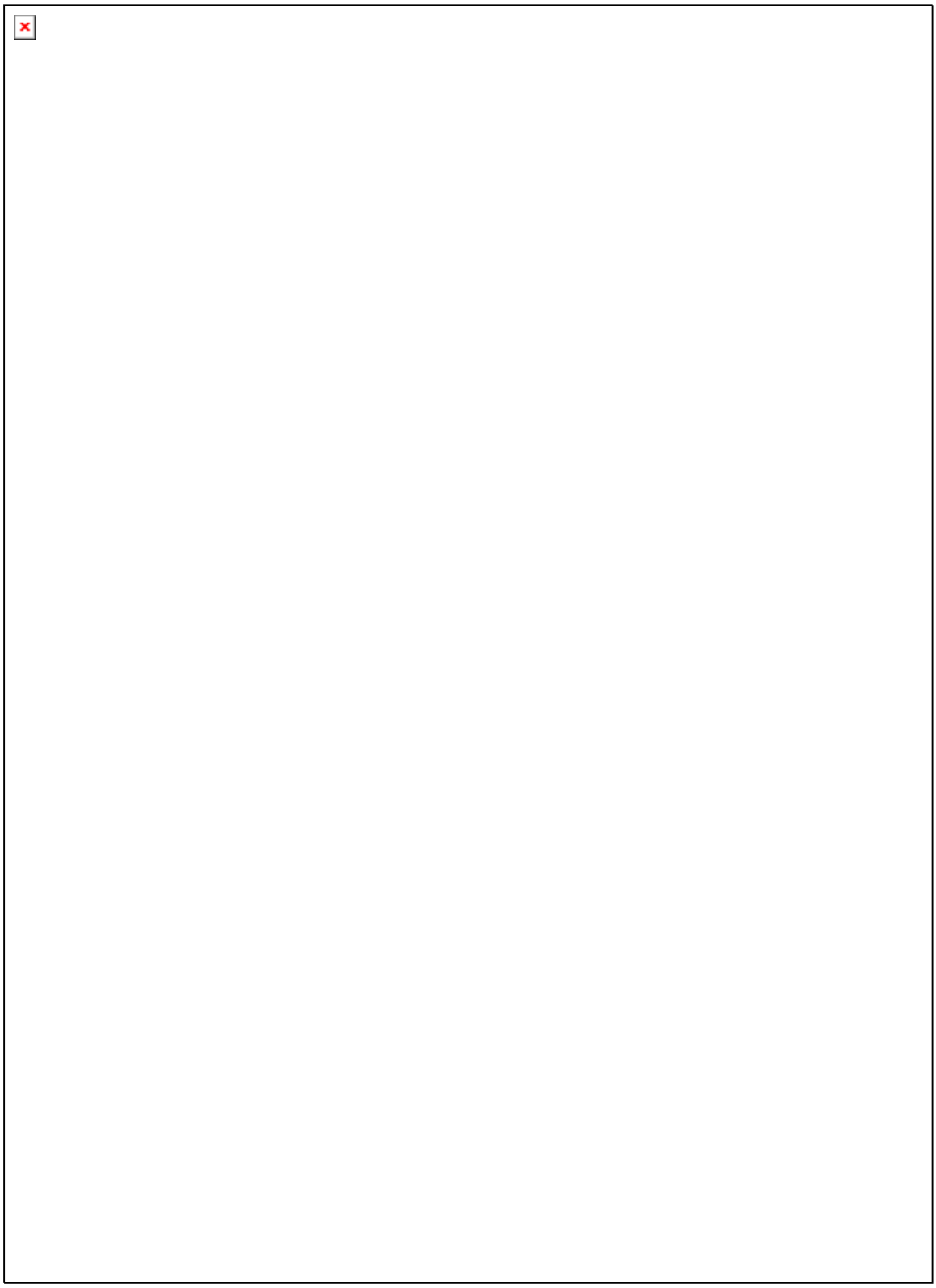


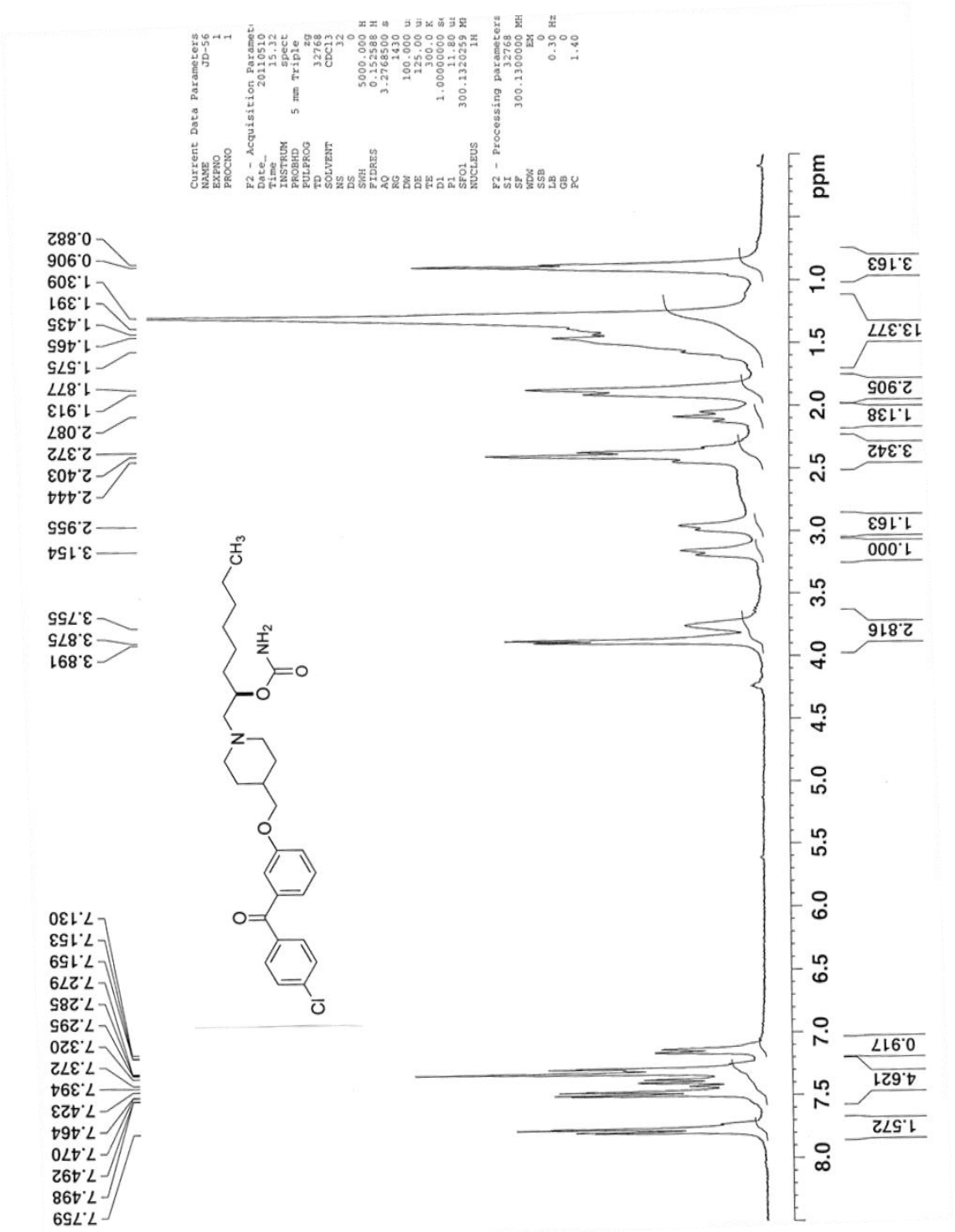








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SWH 5000.000 H
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AQ 3.2768500 s
RG 4.0
DW 100.000 u
DE 125.00 u
TE 300.0 K
D1 1.00000000 s
P1 11.80 u
SFO1 300.1320259 M
NUCLEUS 1H
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LB 0.30 Hz
GB 0
PC 1.40
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7.0
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6.0
5.5
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4.5
4.0
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7.279
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7.295
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7.372
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NH2
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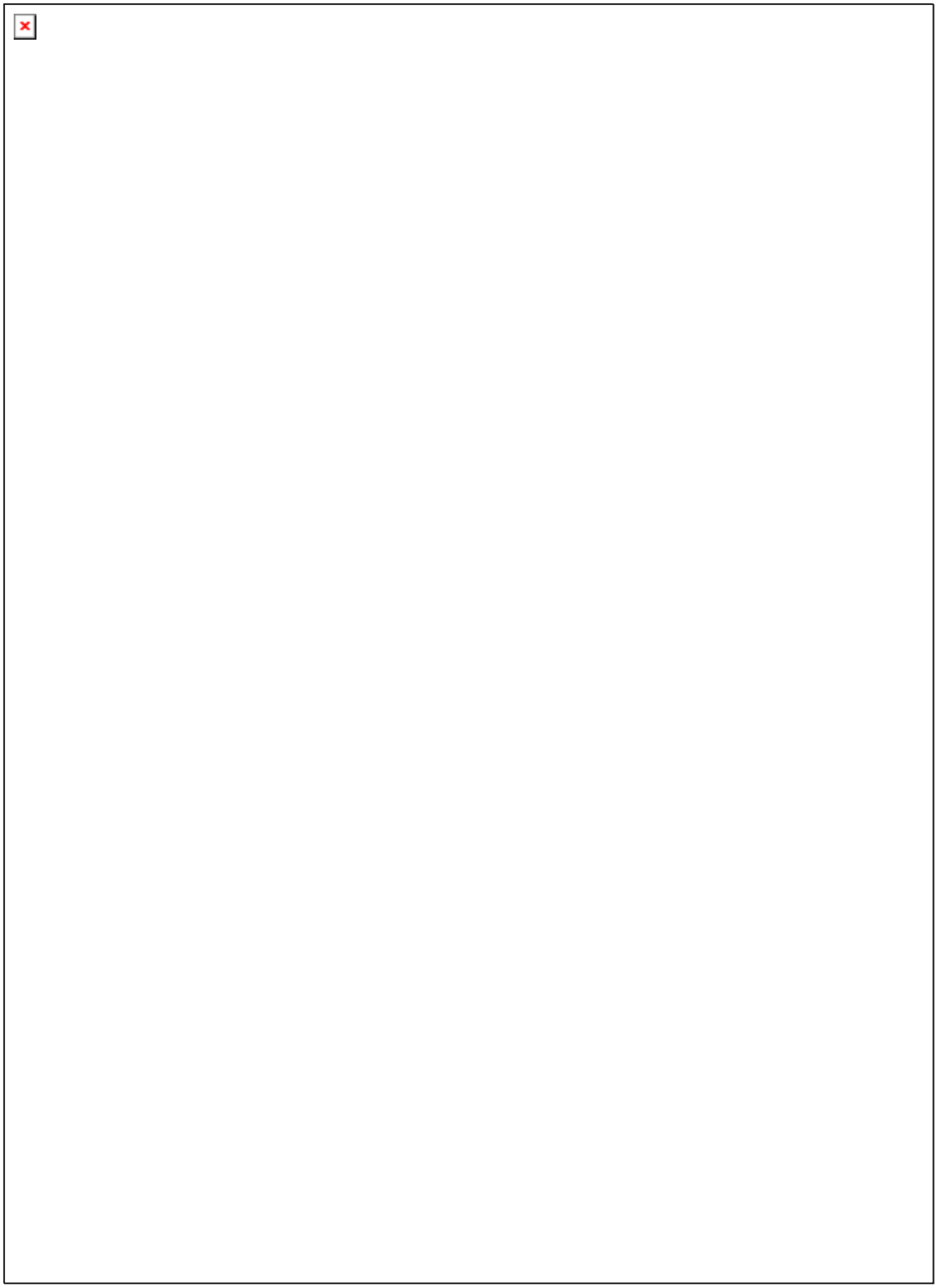
O
O
O
Cl



==== Shimadzu LabSolutions Analysis Report ====

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Vial#	: 1
Injection Volume	: 1
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Method File	: C:\LabSolutions\Data\Project1\Joy training\Mixture-235nm-62%ACN.lcm
Report Format File	: C:\LabSolutions\System\DEFAULT.lsr
Month-Day Acquired	: 10/5/2011
Month-Day Processed	: 10/5/2011

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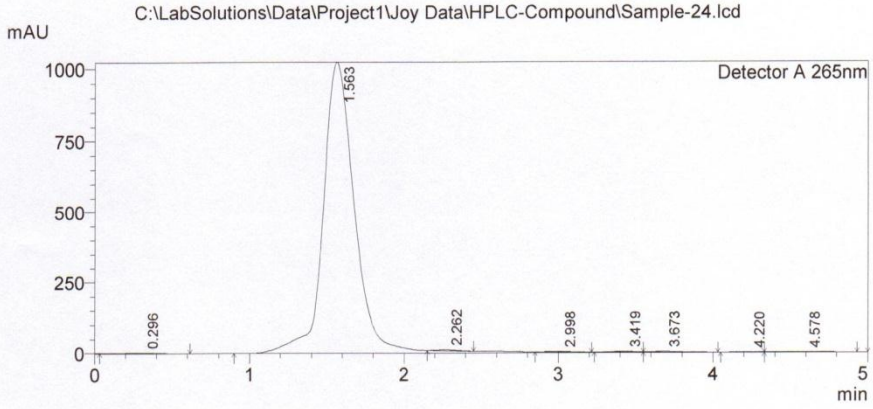
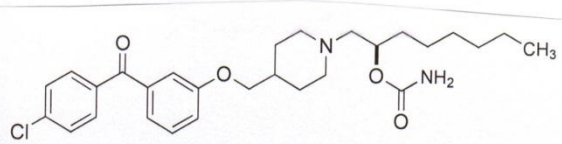
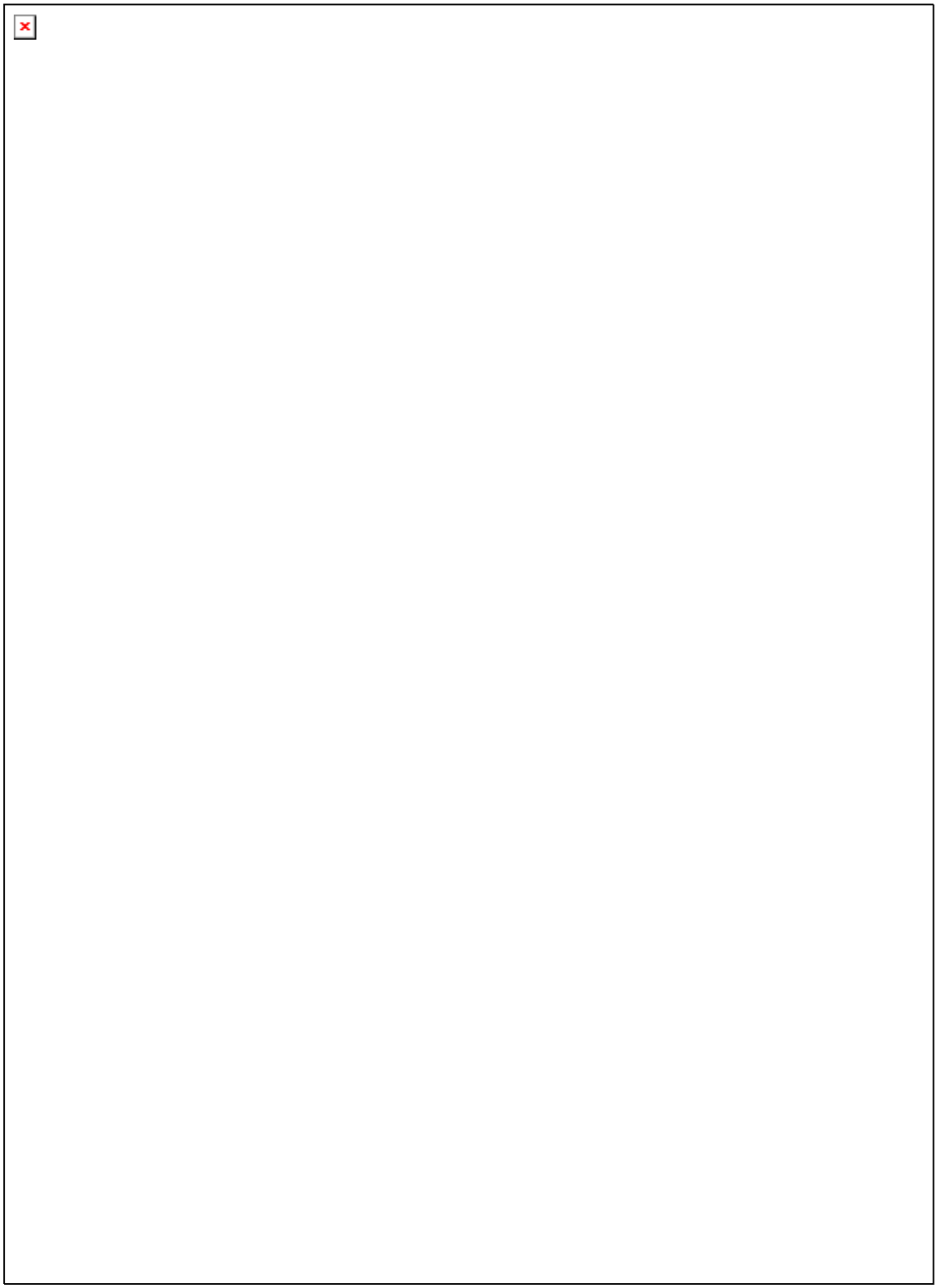
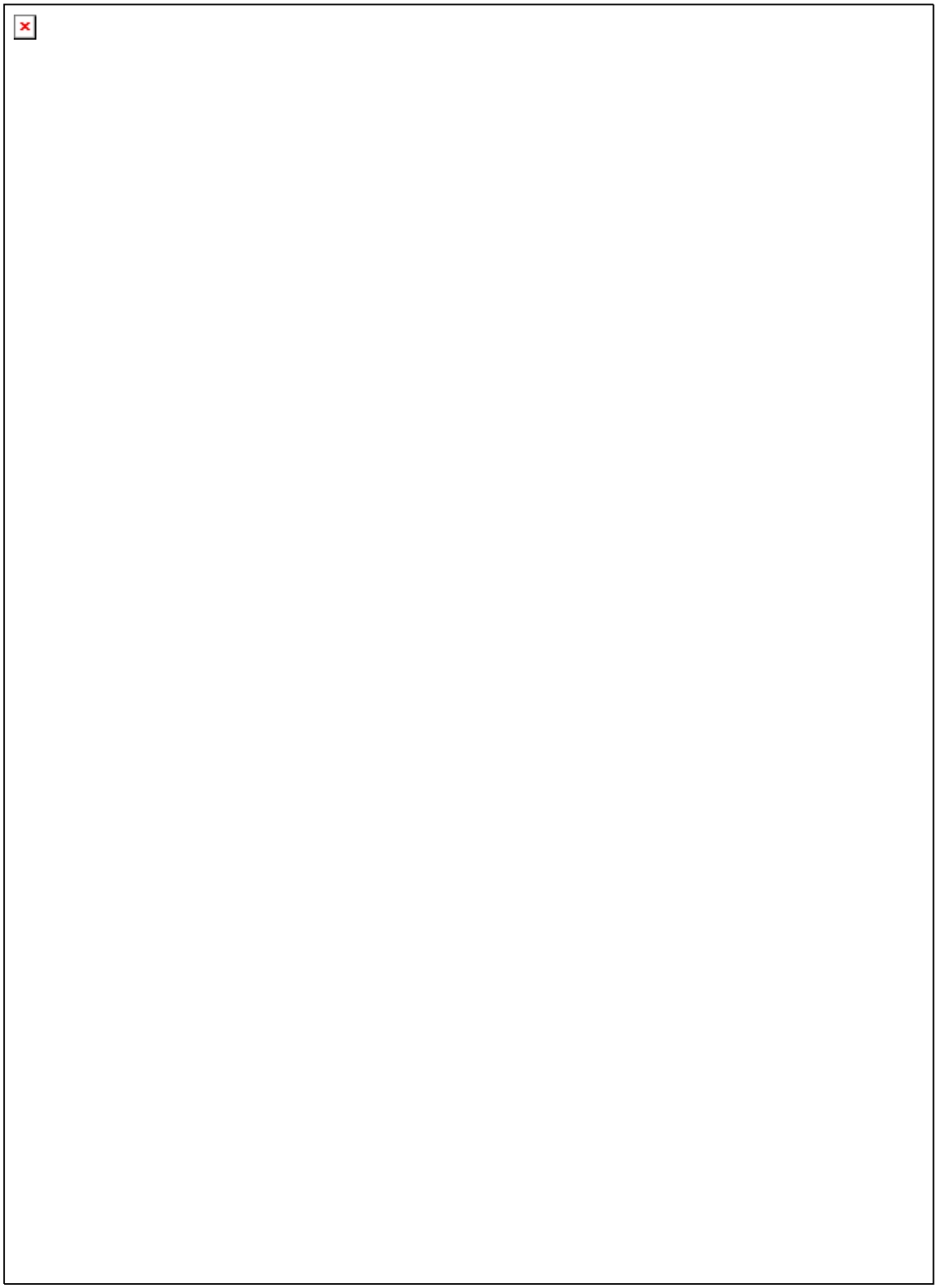


MS Chromatogram



Column: Phenominex kinetex 2.6μ C18 100A, 100 x 4.60 mm
Solvent: CH_3CN/0.05%TFA in H_2O = 25/1
flow rate: 0.5 mL/min.





==== Shimadzu LabSolutions Analysis Report ====

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Injection Volume	: 1
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Month-Day Processed	: 10/5/2011

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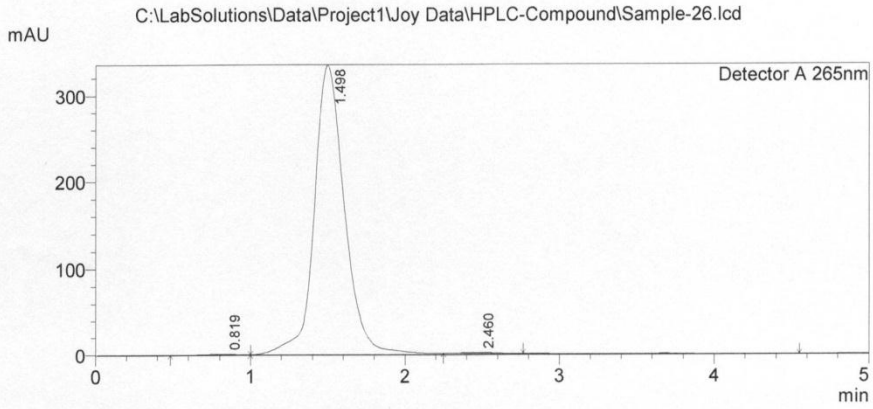
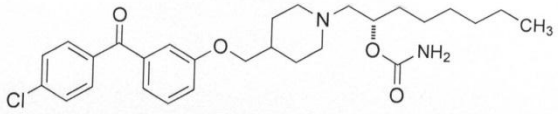
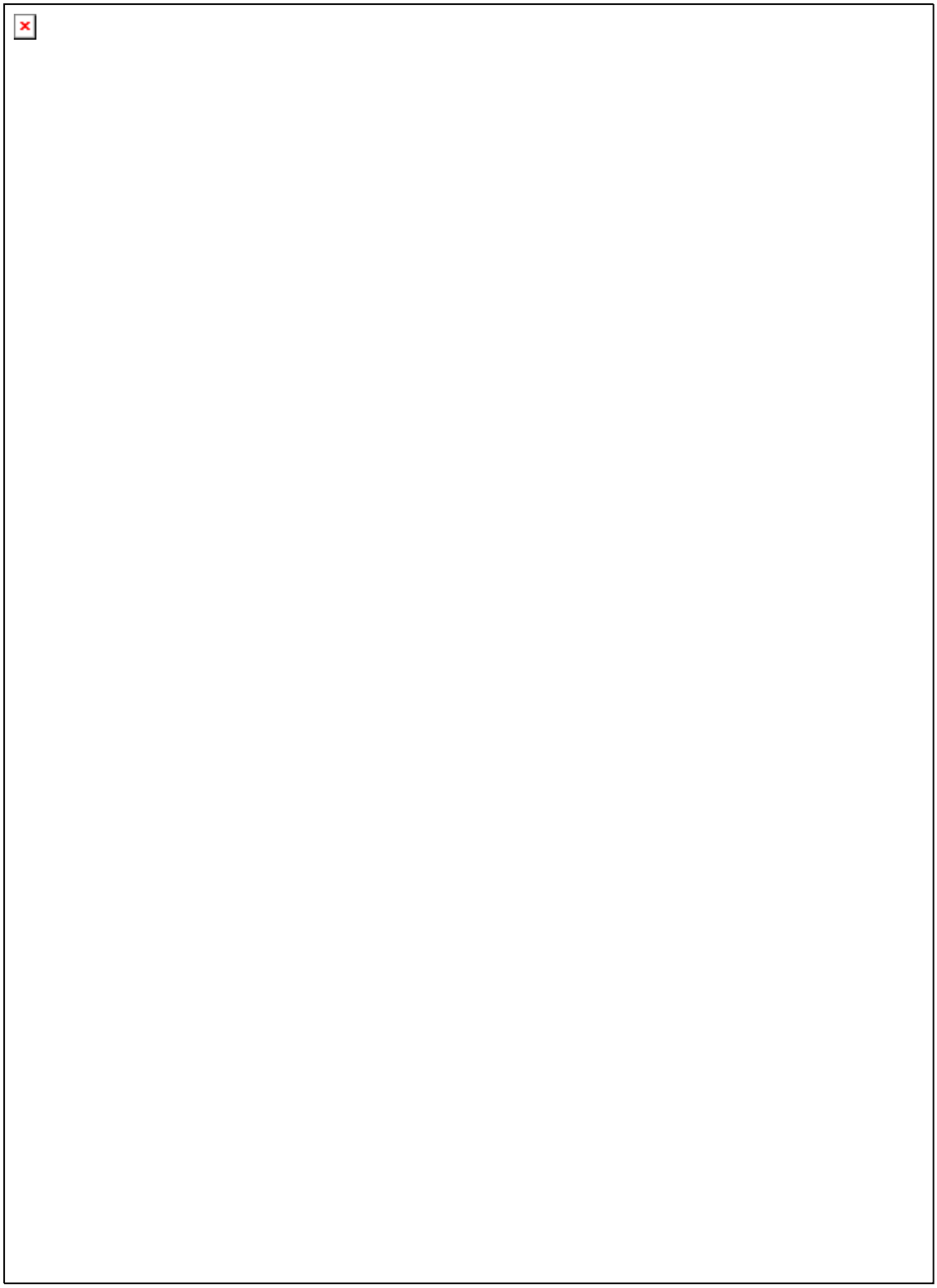
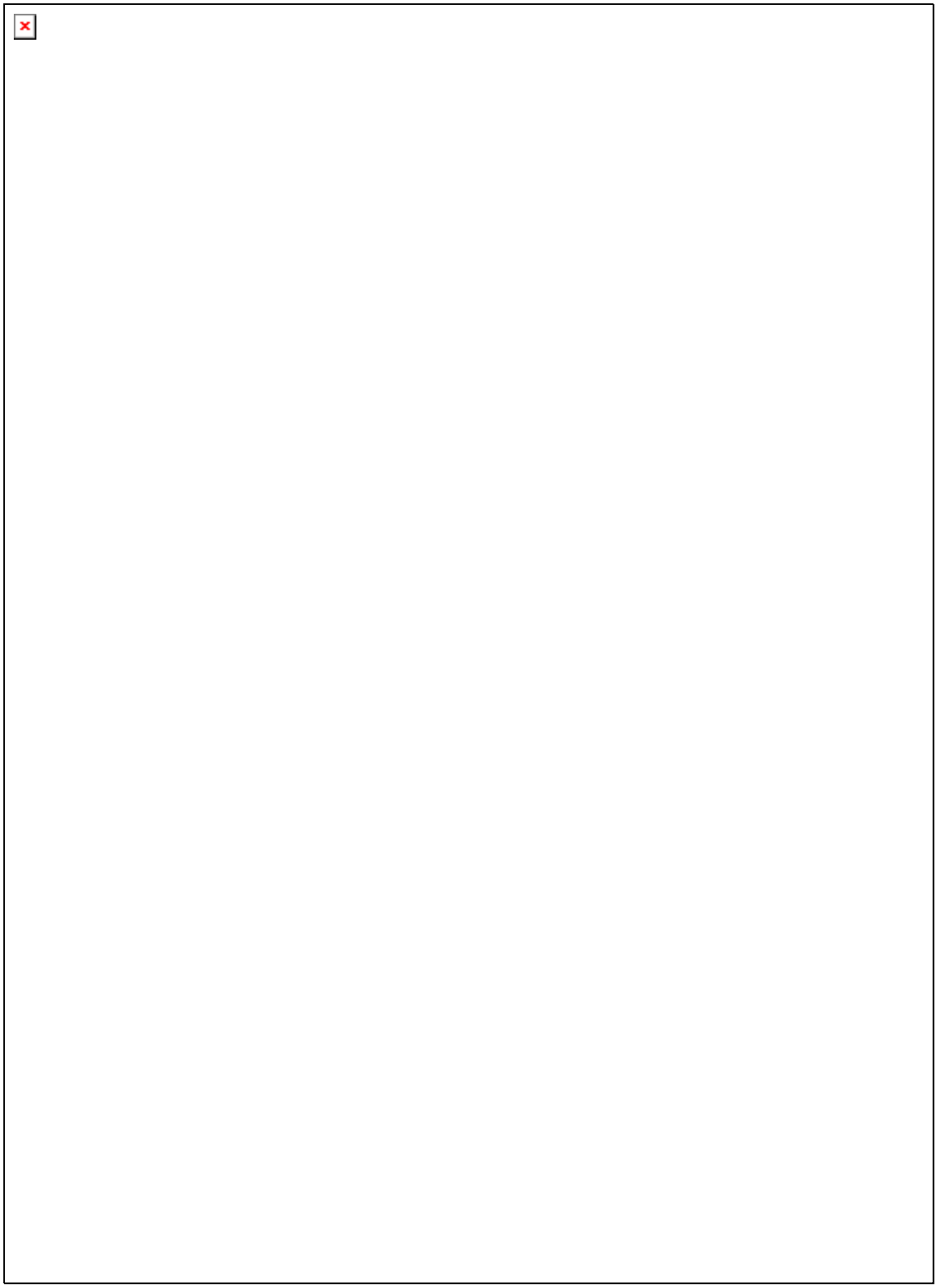


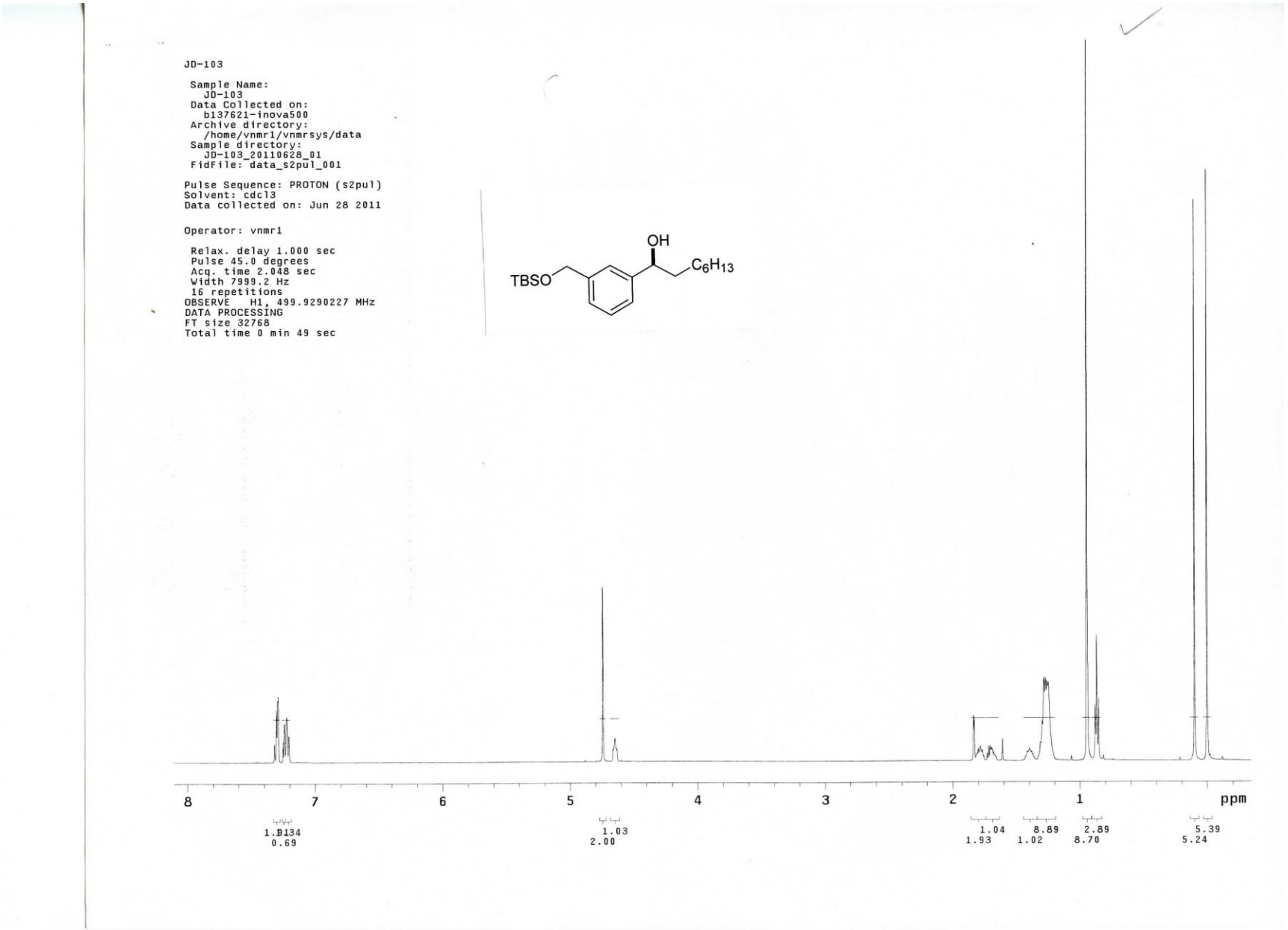
MS Chromatogram



Column: Phenominex kinetex 2.6μ C18 100A, 100 x 4.60 mm
Solvent: CH_3CN/0.05%TFA in H_2O = 25/1
flow rate: 0.5 mL/min.






JD-103
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Archive directory:
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Sample directory:
JD-103_20110628_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 28 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
16 repetitions
OBSERVE H1, 499.9290227 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec
OH
TBSO
C6H13
8
7
6
5
4
3
2
1
ppm
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1.03
2.00
1.04
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1.02
2.89
8.70
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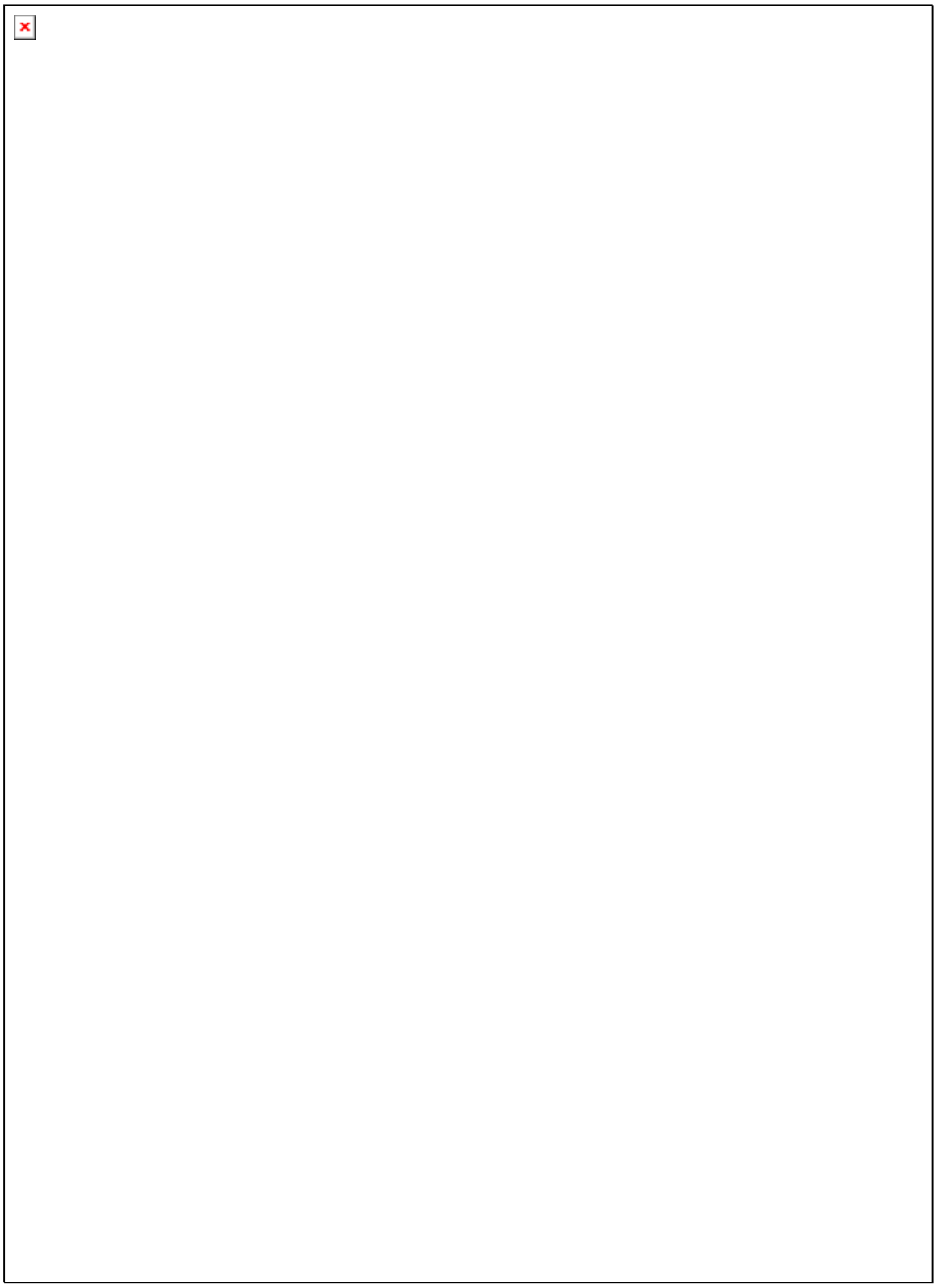
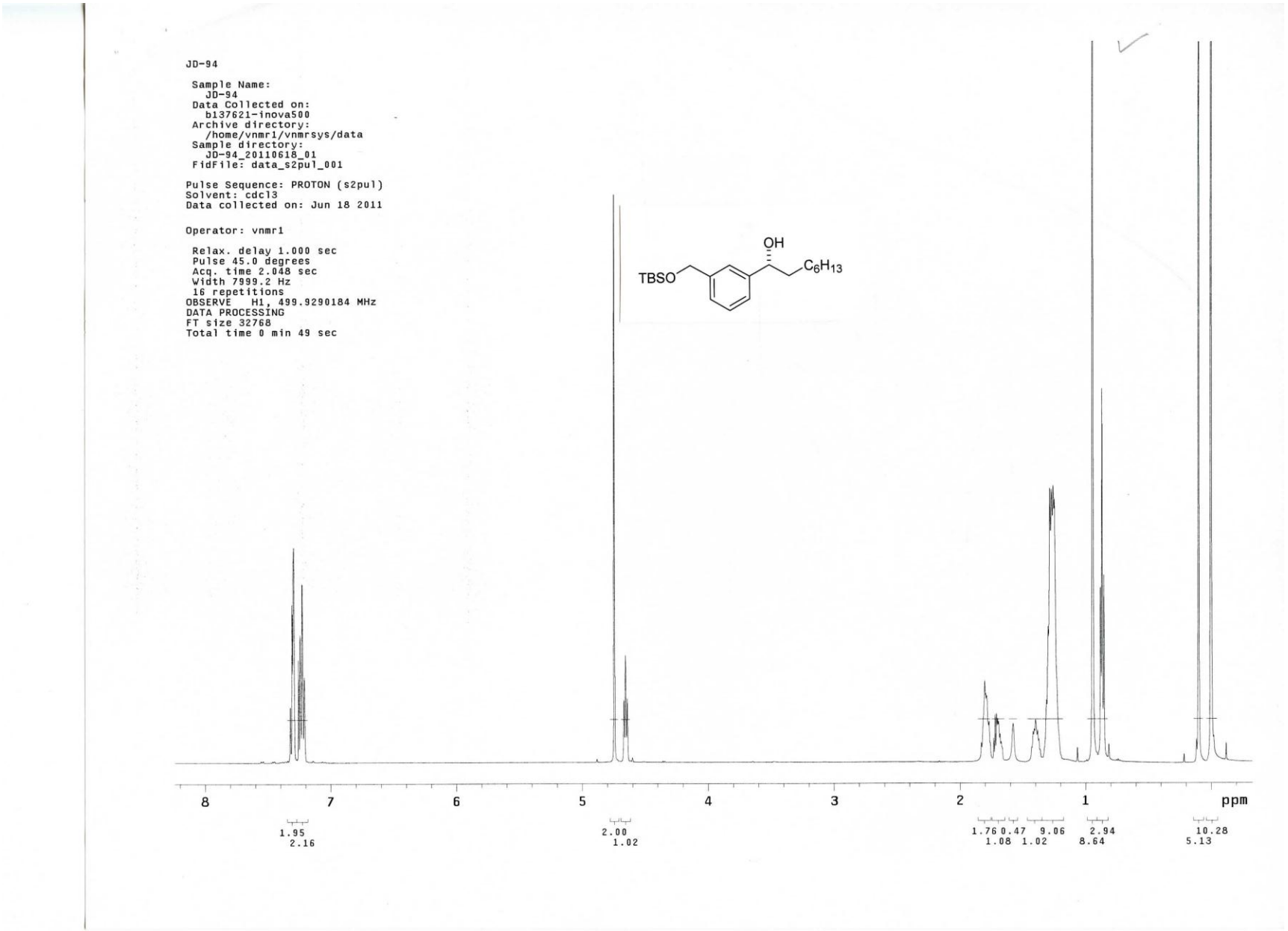
5.24

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Solvent: cdcl3
Data collected on: Jun 18 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
16 repetitions
OBSERVE H1, 499.9290184 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec
OH
TBSO
C6H13
8
7
6
5
4
3
2
1
ppm
1.95
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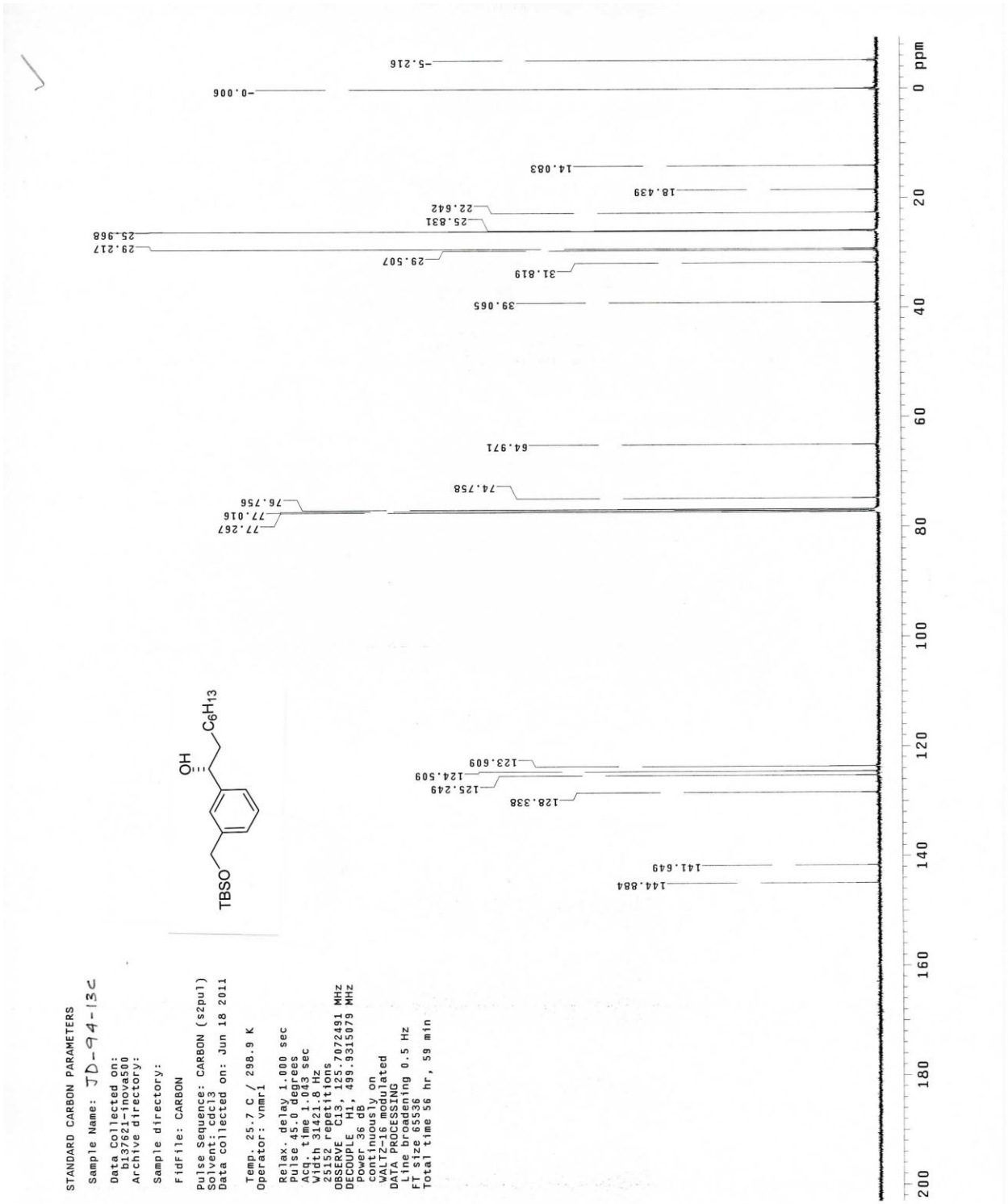
8.64
10.28
5.13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Sample directory:
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Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 18 2011
Temp. 25.7 C / 298.9 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
25152 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 59 min
OH
C6H13
TBSO
-5.216
-0.006
14.083
18.439
22.642
25.831
25.968
29.217
29.507
31.819
39.065
64.971
74.758
76.756
77.016
77.267
123.609
124.509
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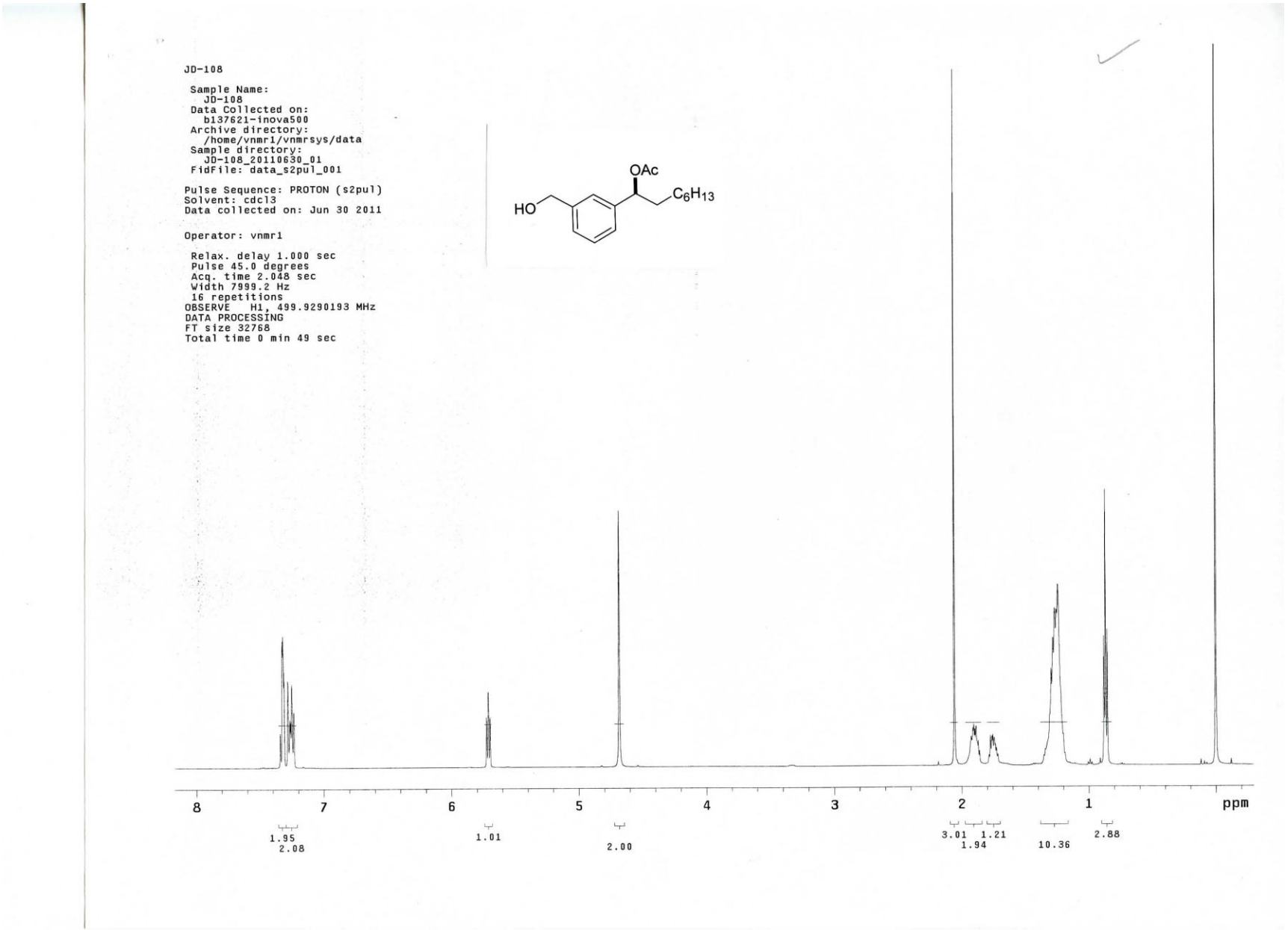
60
80
100
120
140
160
180
200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Solvent: cdcl3
Data collected on: Jun 30 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
16 repetitions
OBSERVE H1, 499.9290193 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec
OAc
HO
C6H13
8
7
6
5
4
3
2
1
ppm
1.95
2.08
1.01
2.00
3.01
1.94
1.21
10.36
2.88

STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
b137621-inova500
Archive directory:

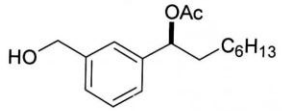
Sample directory:

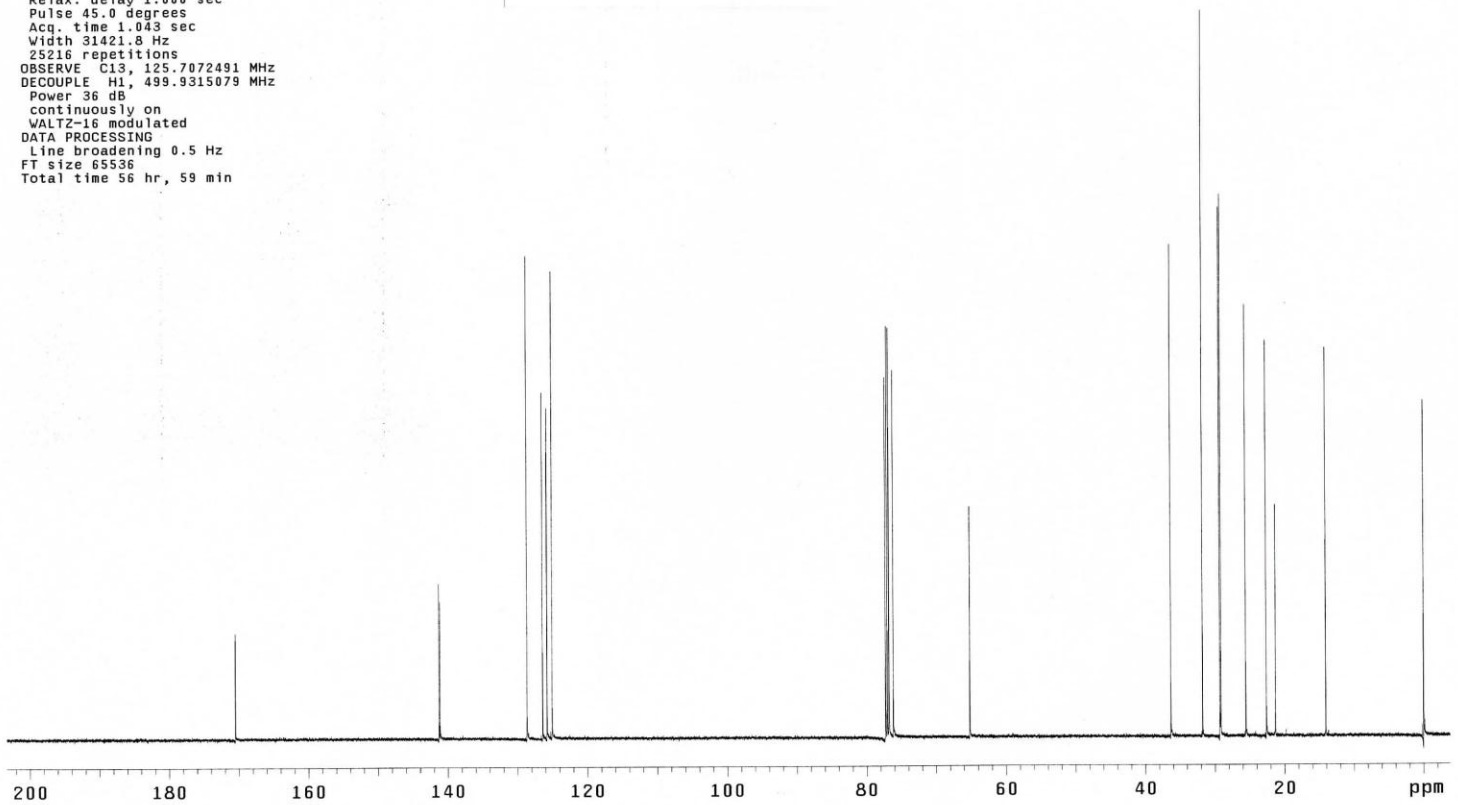
FidFile: CARBON

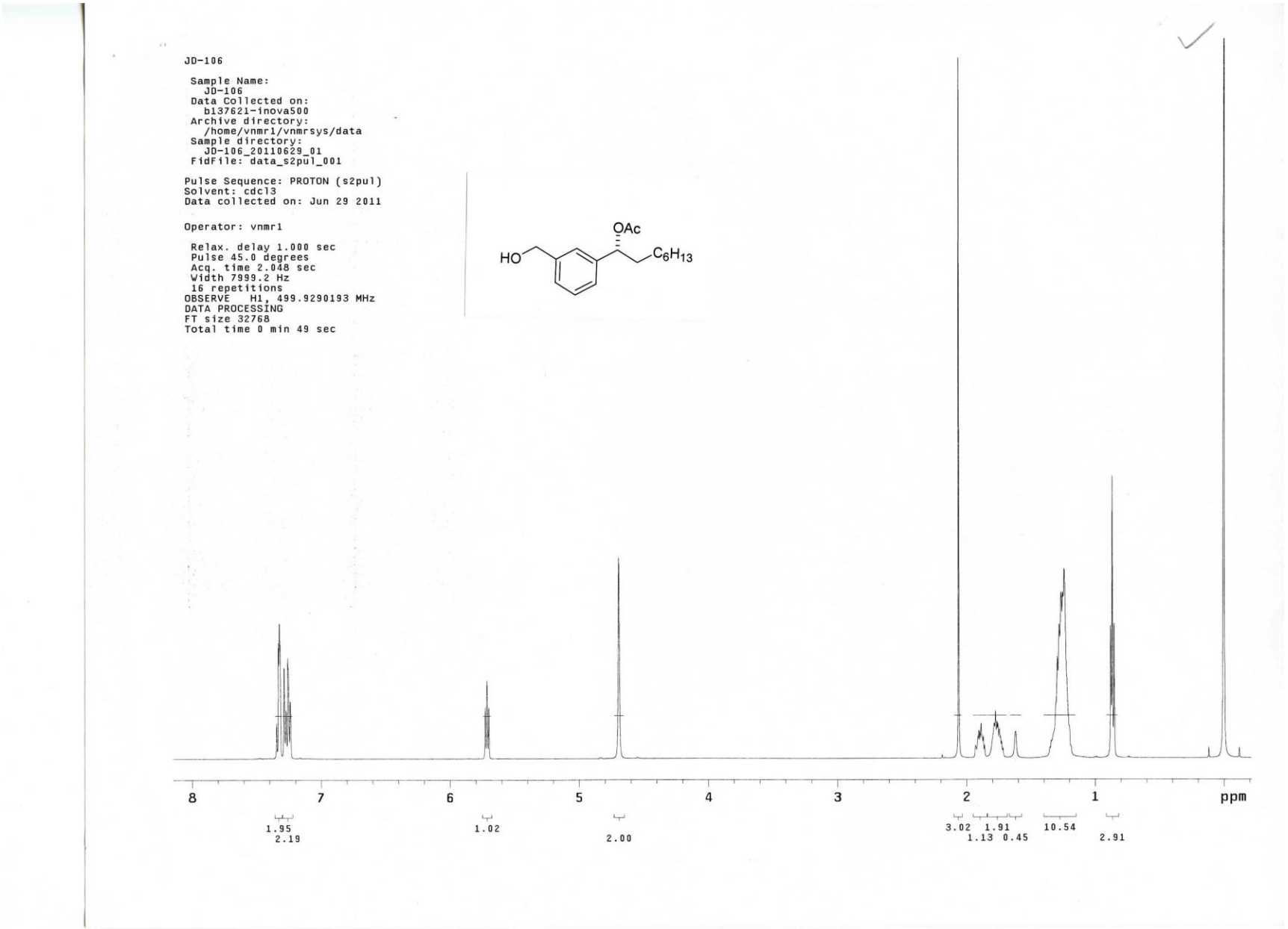
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 30 2011

Temp. 24.6 C / 297.8 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
25216 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 59 min



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Solvent: cdcl3
Data collected on: Jun 29 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
16 repetitions
OBSERVE H1, 499.9290193 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec
HO
OAc
C6H13
8
7
6
5
4
3
2
1
ppm
1.95
2.19
1.02
2.00
3.02
1.91
1.13
0.45
10.54
2.91

JD-103-13C ⟶ It should be JD-106-13C

Sample Name:
JD-103-13C
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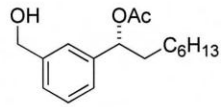
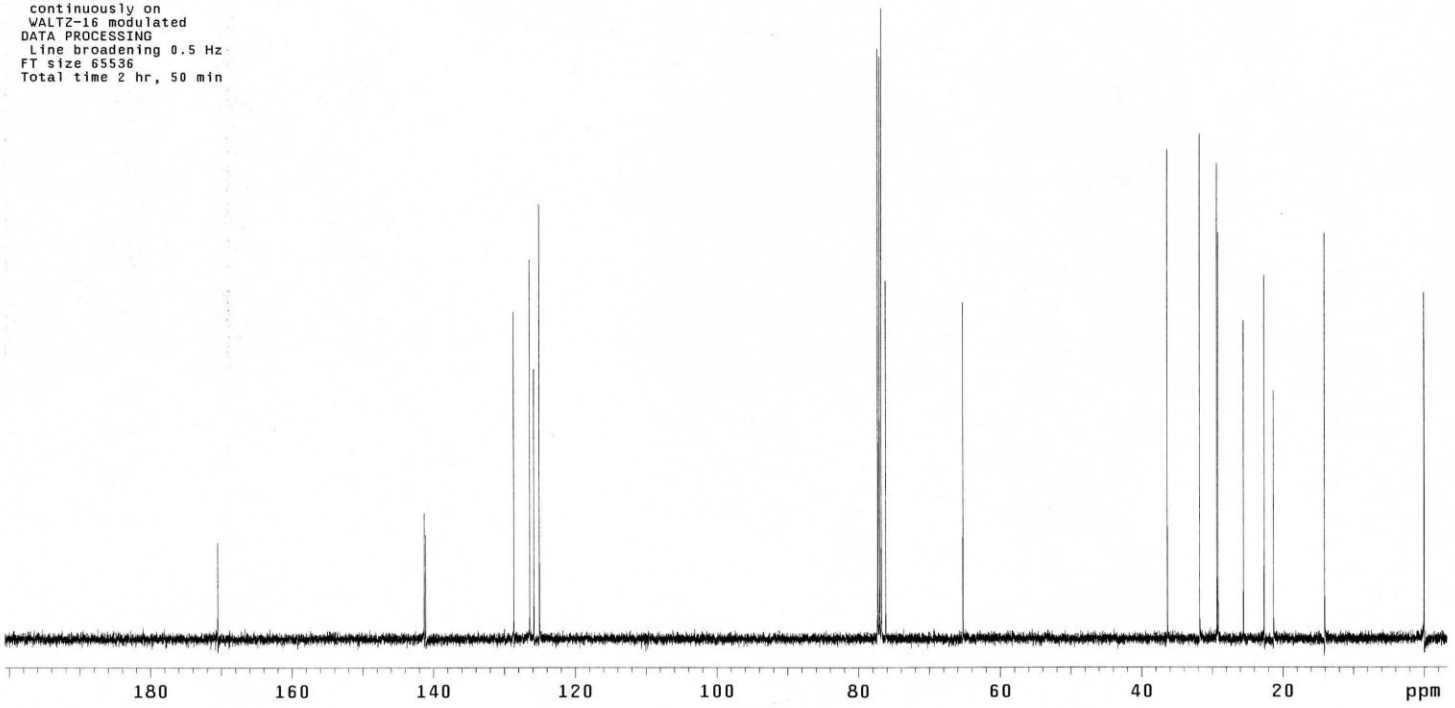
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-103-13C_20110629_01
FidFile: CARBON

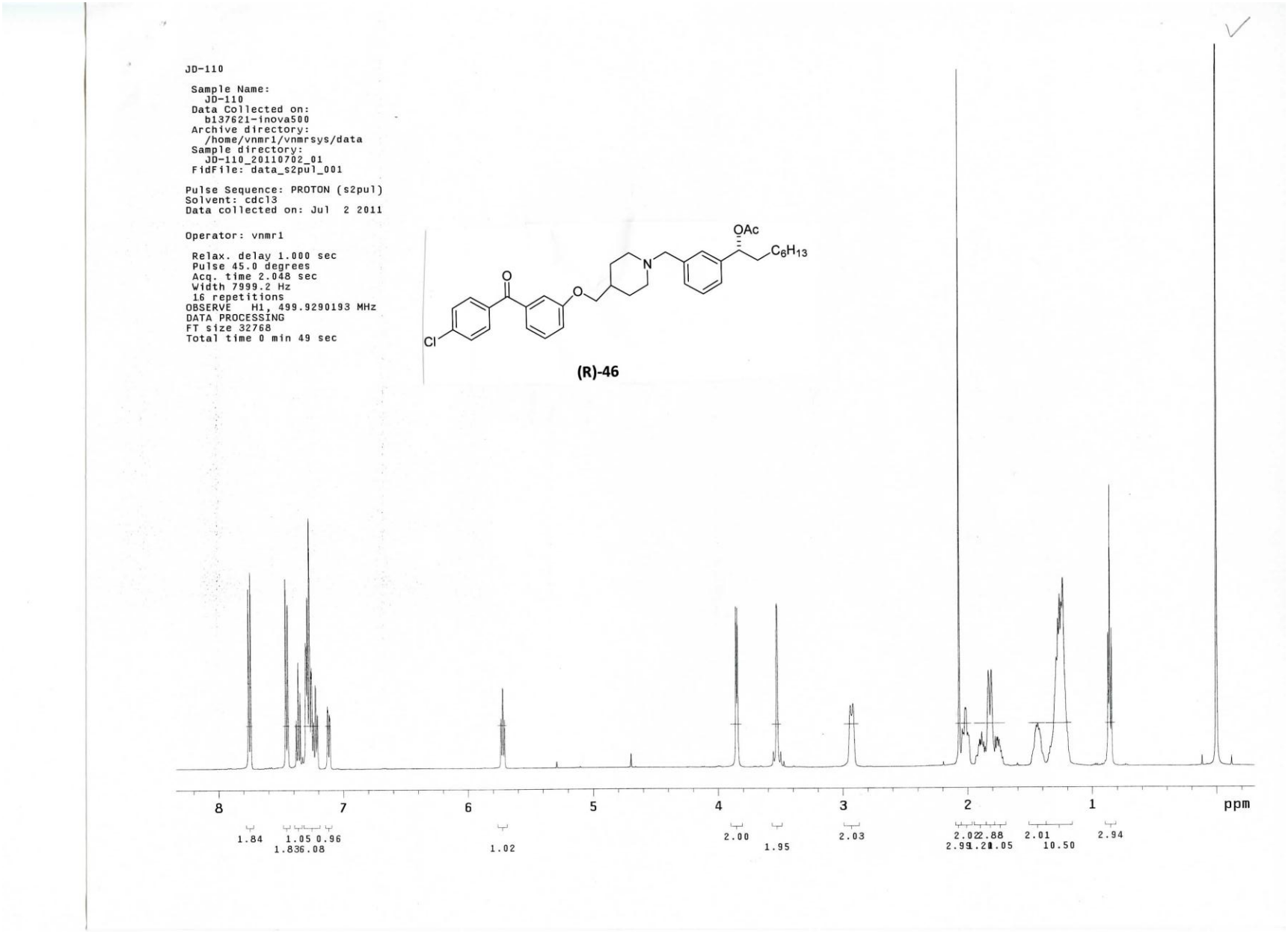
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 29 2011

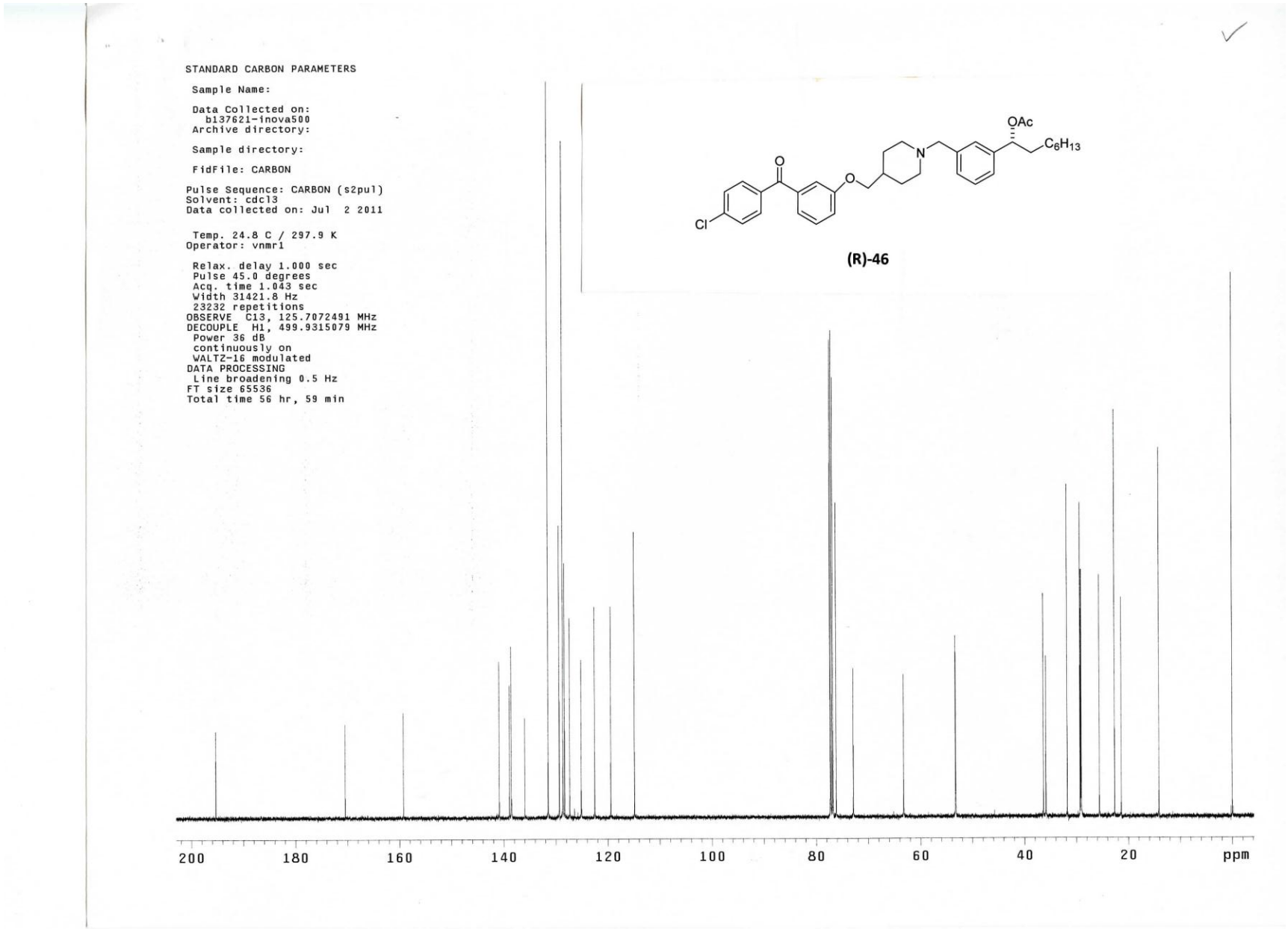
Temp. 24.8 C / 297.9 K
Operator: vnmr1

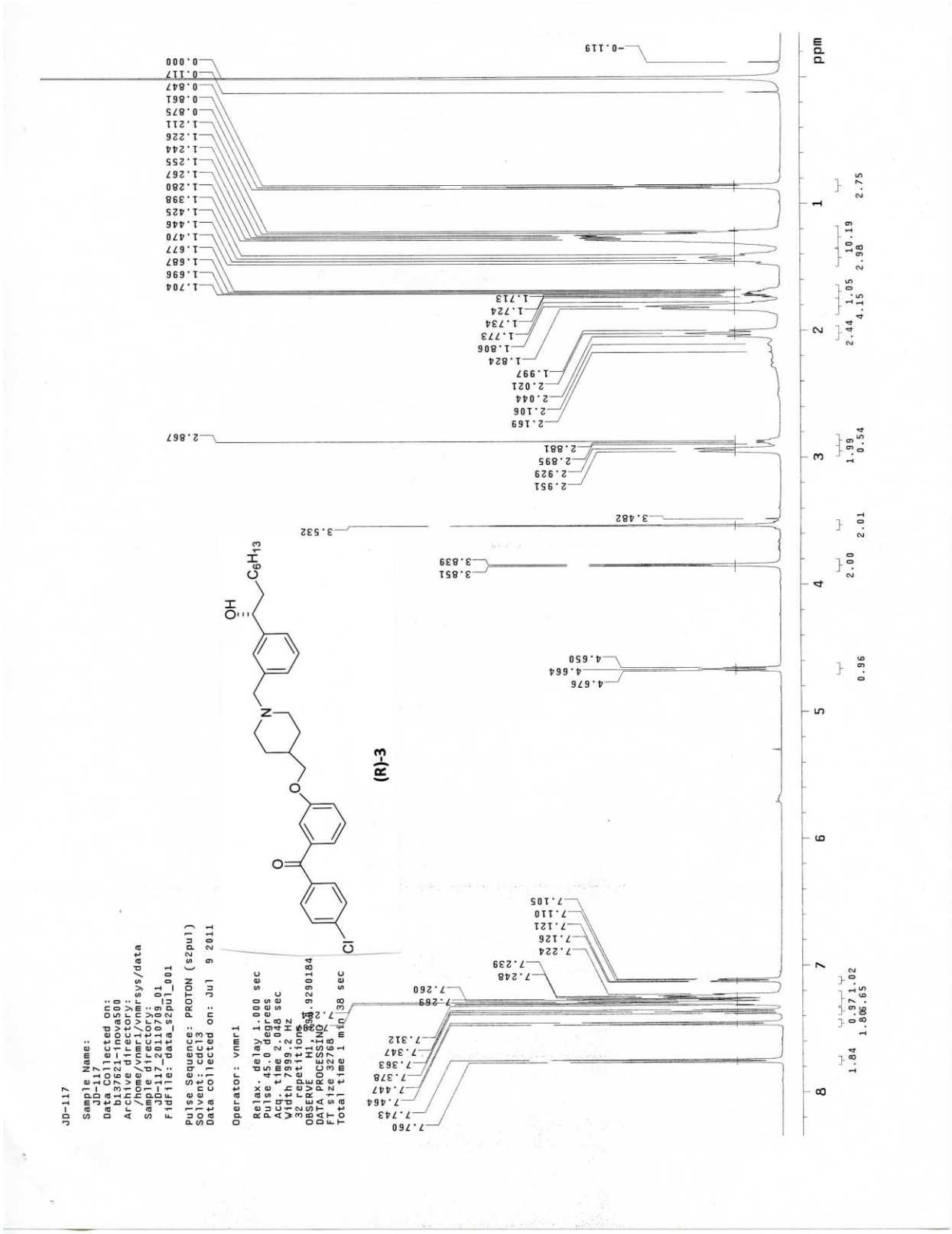
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
4544 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 2 hr, 50 min

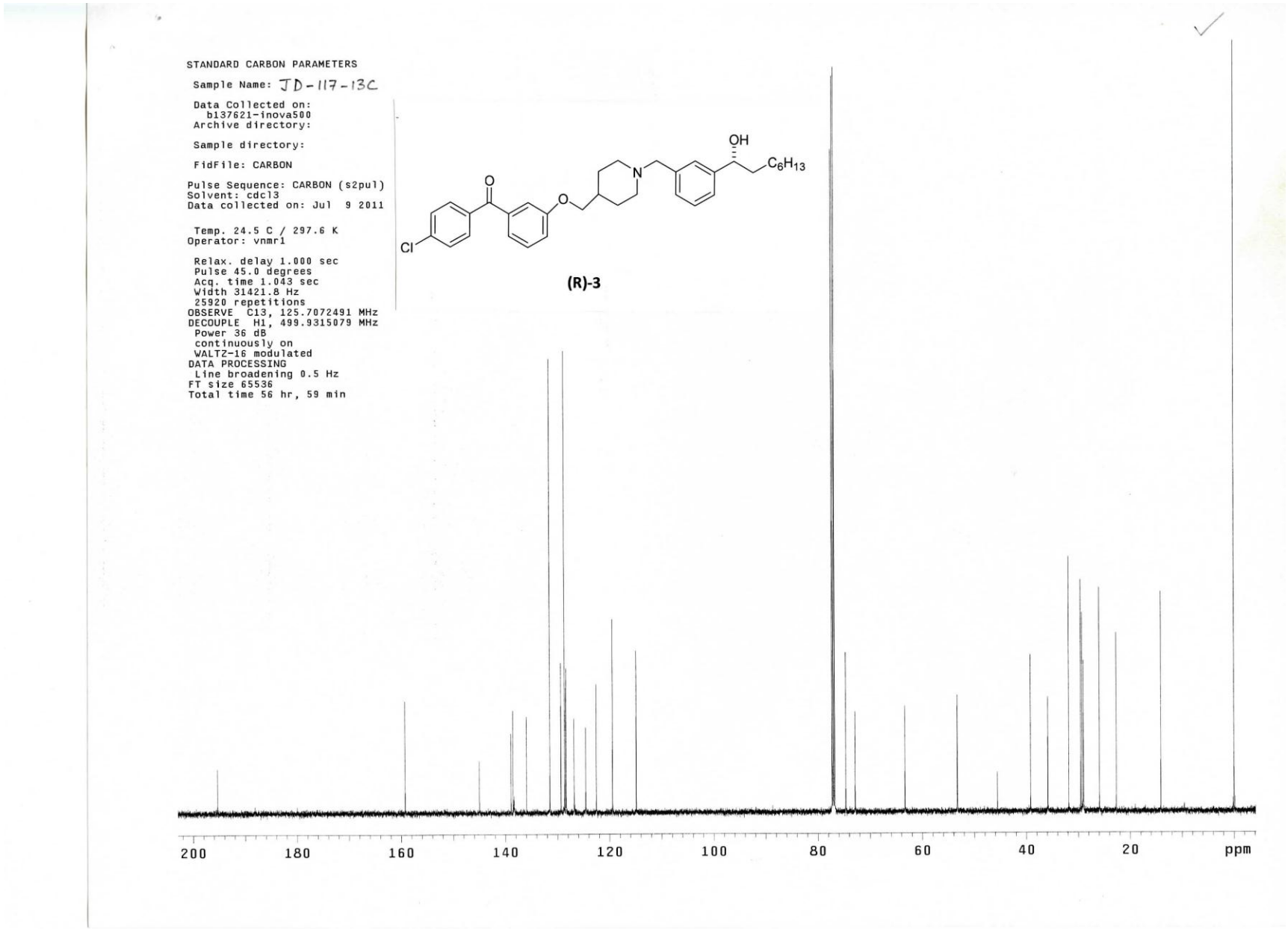





JD-110
Sample Name:
JD-110
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-110_20110702_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 2 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
16 repetitions
OBSERVE H1, 499.9290193 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec
OAc
C6H13
N
O
O
Cl
(R)-46
8
7
6
5
4
3
2
1
ppm
1.84
1.05
0.96
1.83
6.08
1.02
2.00
1.95
2.03
2.02
2.88
2.99
1.21
1.05
2.01
10.50
2.94


STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
b137621-inova500
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 2 2011
Temp. 24.8 C / 297.9 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
23232 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 59 min
OAc
C6H13
O
O
N
Cl
(R)-46
200
180
160
140
120
100
80
60
40
20
ppm


JD-117
Sample Name:
JD-117
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-117_20110709_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 9 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
32 repetitions
OBSERVE H1, 399.9290184
DATA PROCESSING
FT size 32768
Total time 1 min, 38 sec
(R)-3
ppm

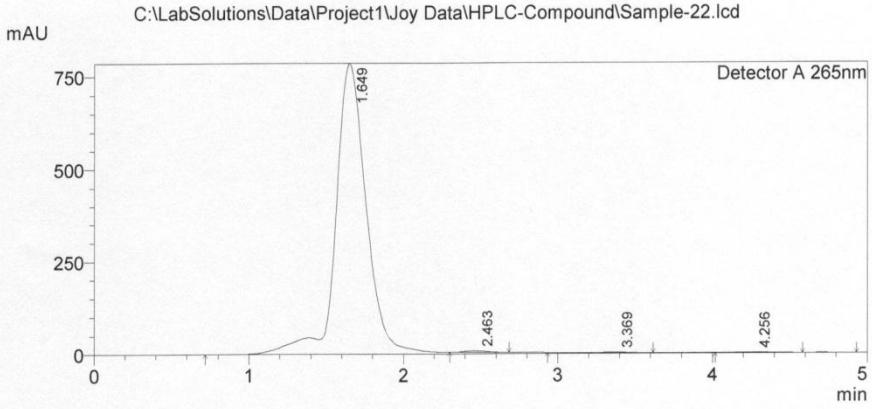

STANDARD CARBON PARAMETERS
Sample Name: JD-117-13C
Data Collected on:
b137621-inova500
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 9 2011
Temp. 24.5 C / 297.6 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
25920 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 59 min
OH
C6H13
N
O
O
Cl
(R)-3
200
180
160
140
120
100
80
60
40
20
ppm

==== Shimadzu LabSolutions Analysis Report ====

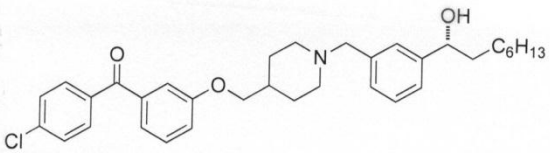
C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-22.lcd

Acquired by	: System Administrator
Sample Name	: JD-07-16-2011
Sample ID	:
Tray#	: 1
Vial#	: 1
Injection Volume	: 1
Data File	: C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-22.lcd
Method File	: C:\LabSolutions\Data\Project1\Joy training\Mixture-235nm-62%ACN.lcm
Report Format File	: C:\LabSolutions\System\DEFAULT.lsr
Month-Day Acquired	: 10/5/2011
Month-Day Processed	: 10/5/2011

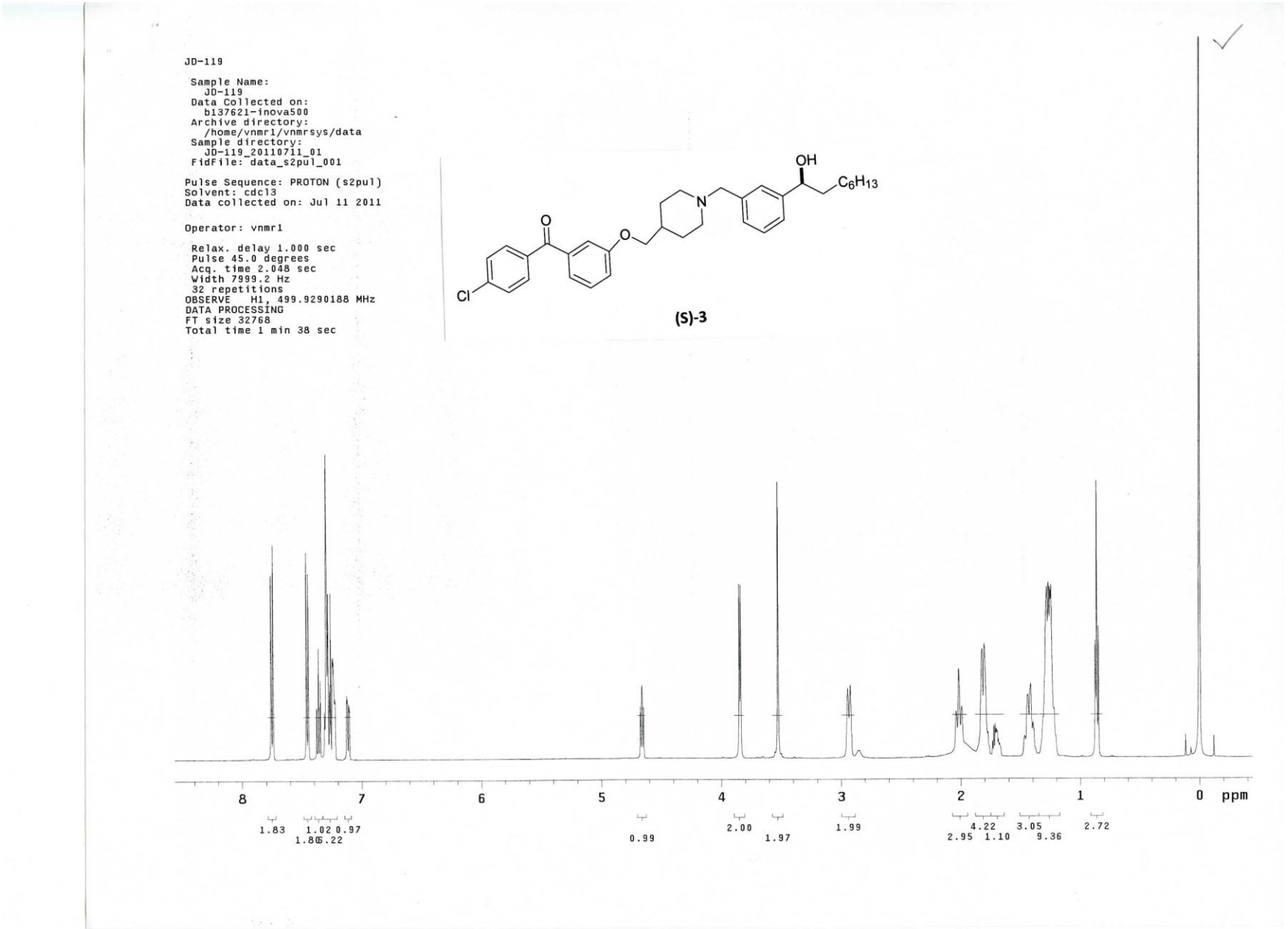
<Chromatogram>

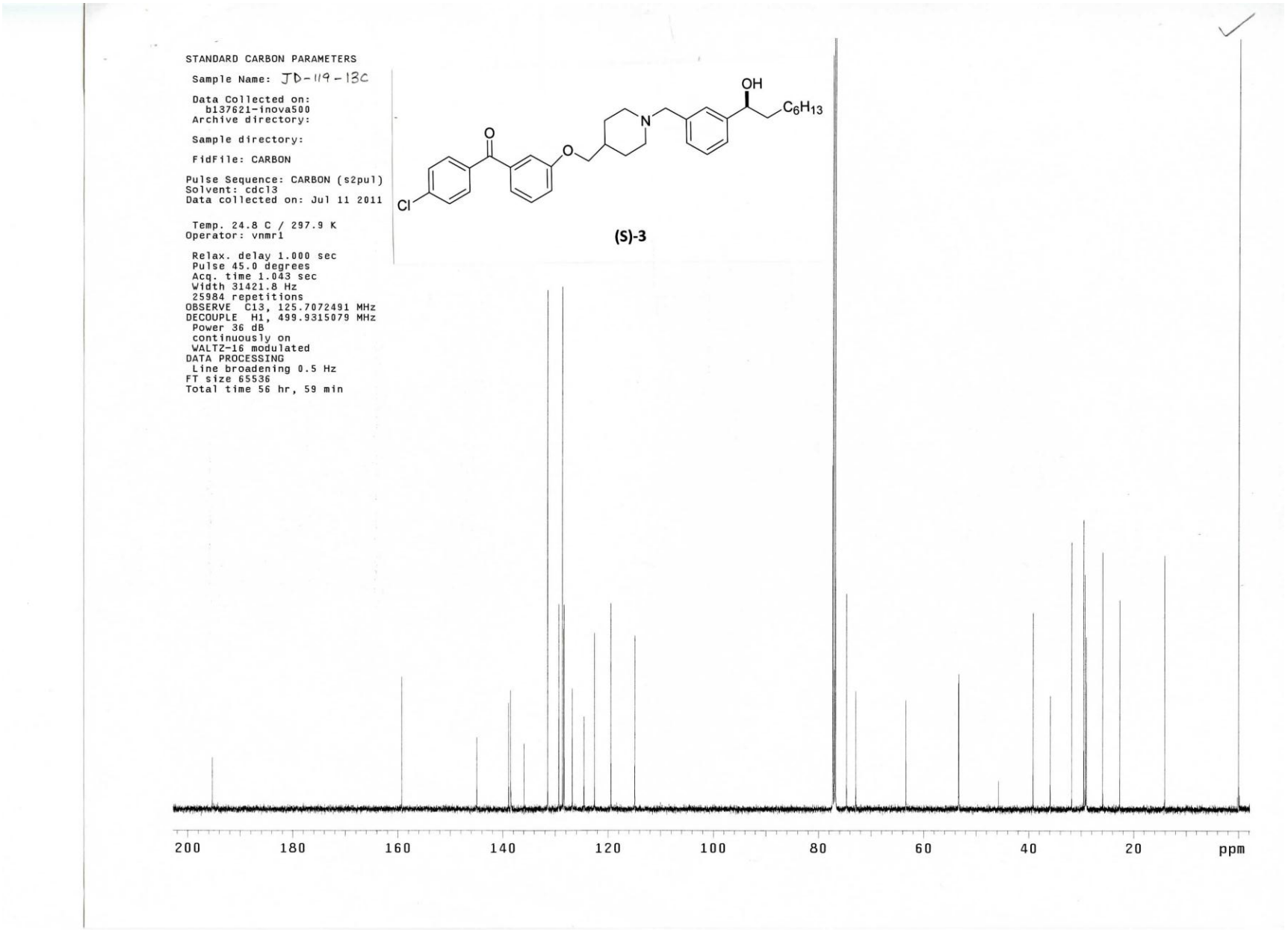


MS Chromatogram



Column: Phenominex kinetex 2.6μ C18 100A, 100 x 4.60 mm
Solvent: CH_3CN/0.05%TFA in H_2O = 25/1
flow rate: 0.5 mL/min.


JD-119
Sample Name:
JD-119
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-119_20110711_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 11 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
32 repetitions
OBSERVE H1, 499.9290188 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 38 sec
OH
C6H13
N
O
O
Cl
(S)-3
8
7
6
5
4
3
2
1
0
ppm
1.83
1.02
0.97
1.86
6.22
0.99
2.00
1.97
1.99
2.95
4.22
1.10
3.05
9.36
2.72

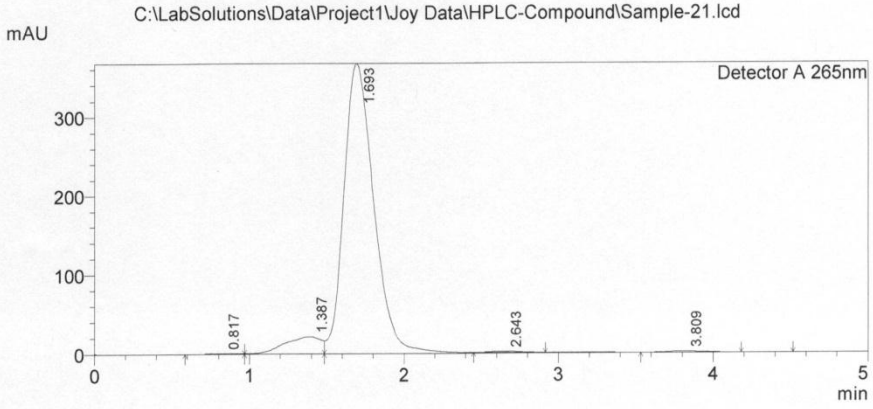

STANDARD CARBON PARAMETERS
Sample Name: JD-119-13C
Data Collected on:
b137621-inova500
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 11 2011
Temp. 24.8 C / 297.9 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
25984 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 59 min
OH
C6H13
N
O
O
Cl
(S)-3
200
180
160
140
120
100
80
60
40
20
ppm

==== Shimadzu LabSolutions Analysis Report ====

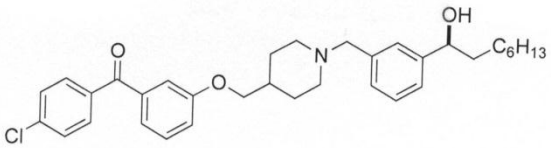
C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-21.lcd

Acquired by	: System Administrator
Sample Name	: JD-07-16-2011
Sample ID	:
Tray#	: 1
Vial#	: 1
Injection Volume	: 1
Data File	: C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-21.lcd
Method File	: C:\LabSolutions\Data\Project1\Joy training\Mixture-235nm-62%ACN.lcm
Report Format File	: C:\LabSolutions\System\DEFAULT.lsr
Month-Day Acquired	: 10/5/2011
Month-Day Processed	: 10/5/2011

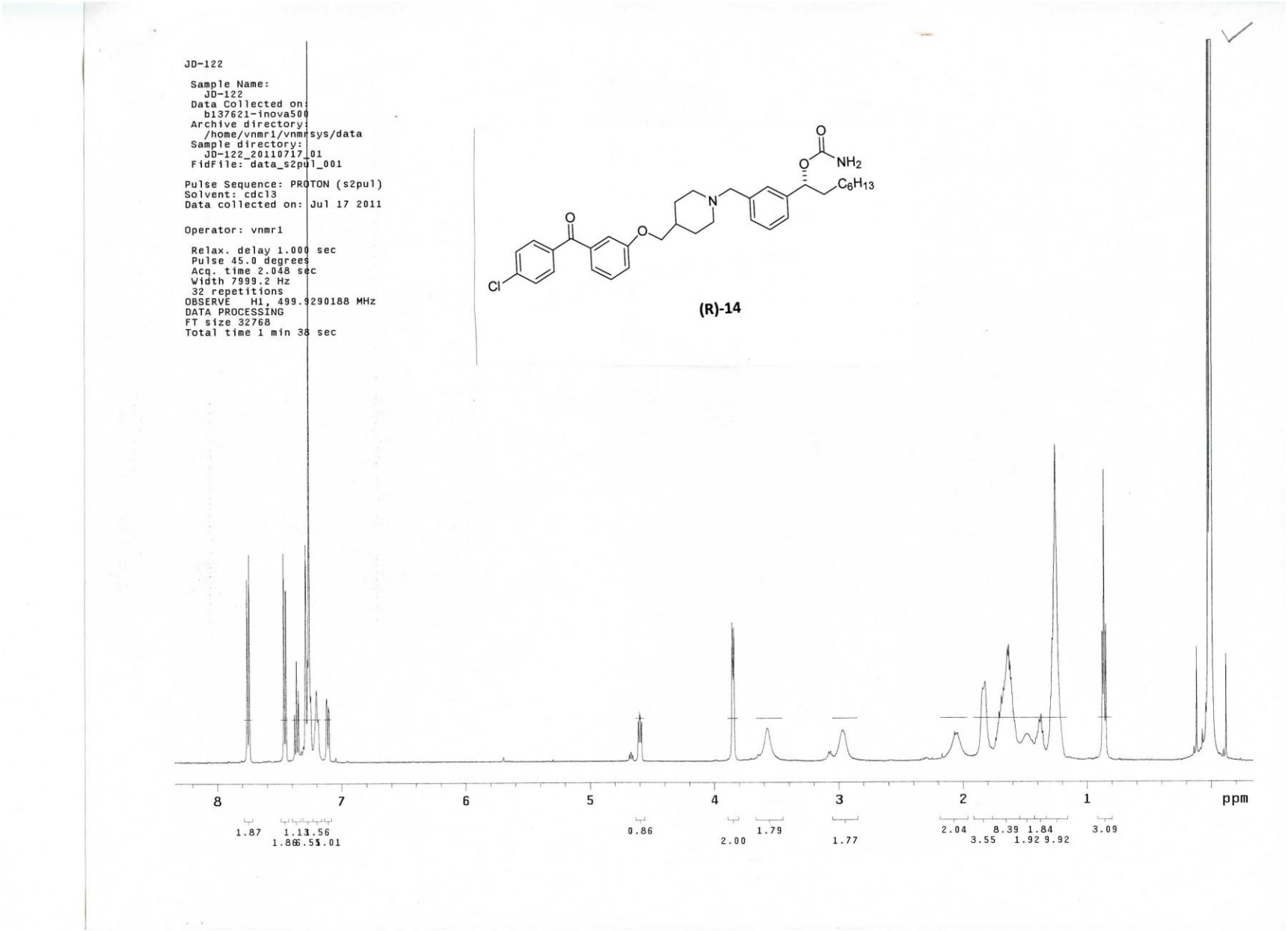
<Chromatogram>



MS Chromatogram



Column: Phenominex kinetex 2.6μ C18 100A, 100 x 4.60 mm
Solvent: CH_3CN/0.05%TFA in H_2O = 25/1
flow rate: 0.5 mL/min.


JD-122
Sample Name:
JD-122
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-122_20110717_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 17 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
32 repetitions
OBSERVE H1, 499.9290188 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 38 sec
O
O
NH2
C6H13
N
O
O
Cl
(R)-14
8
7
6
5
4
3
2
1
ppm
1.87
1.86
1.13
6.55
3.56
1.01
0.86
2.00
1.79
1.77
2.04
3.55
8.39
1.92
1.84
9.92
3.09

STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
b137621-inova500
Archive directory:

Sample directory:

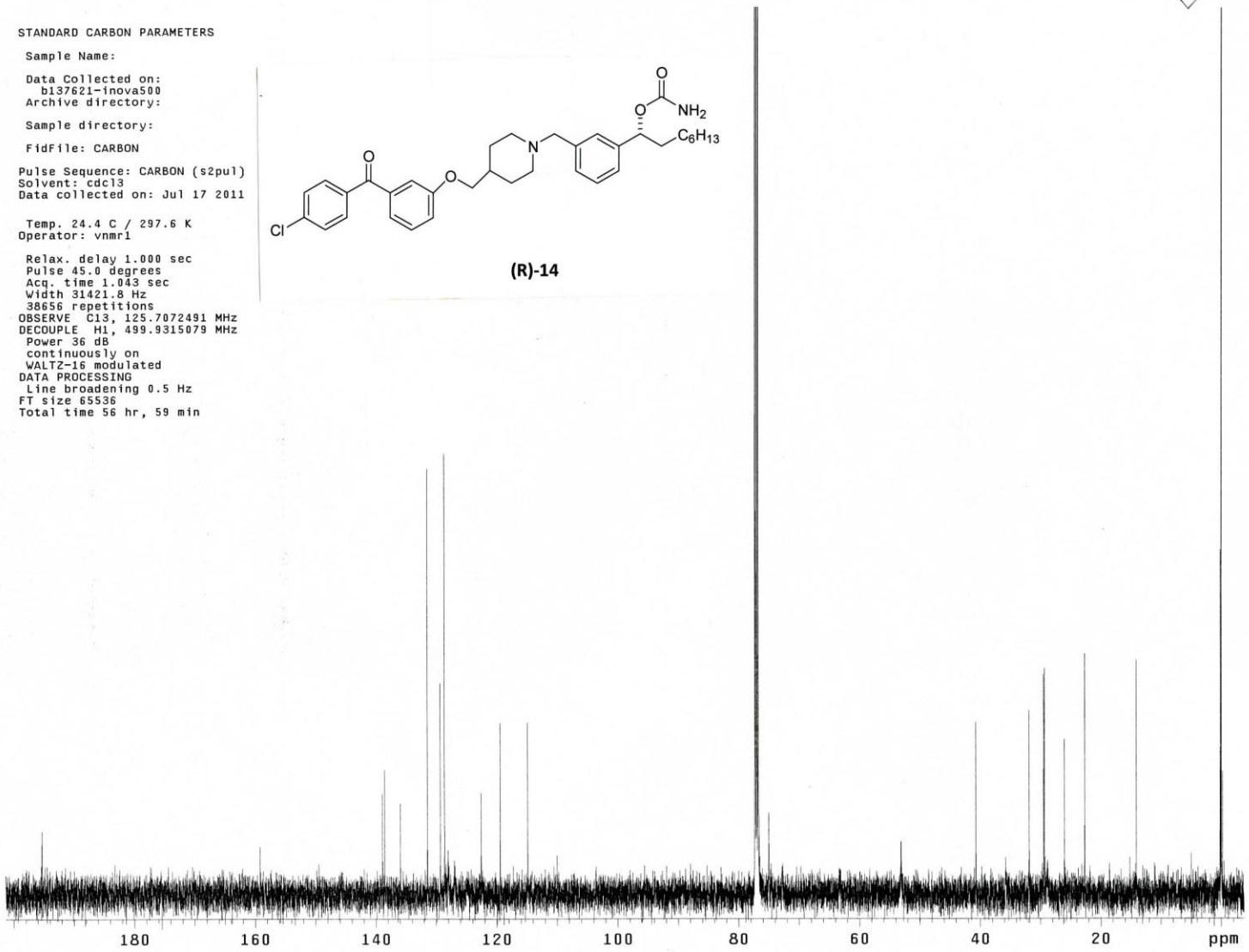
FidFile: CARBON

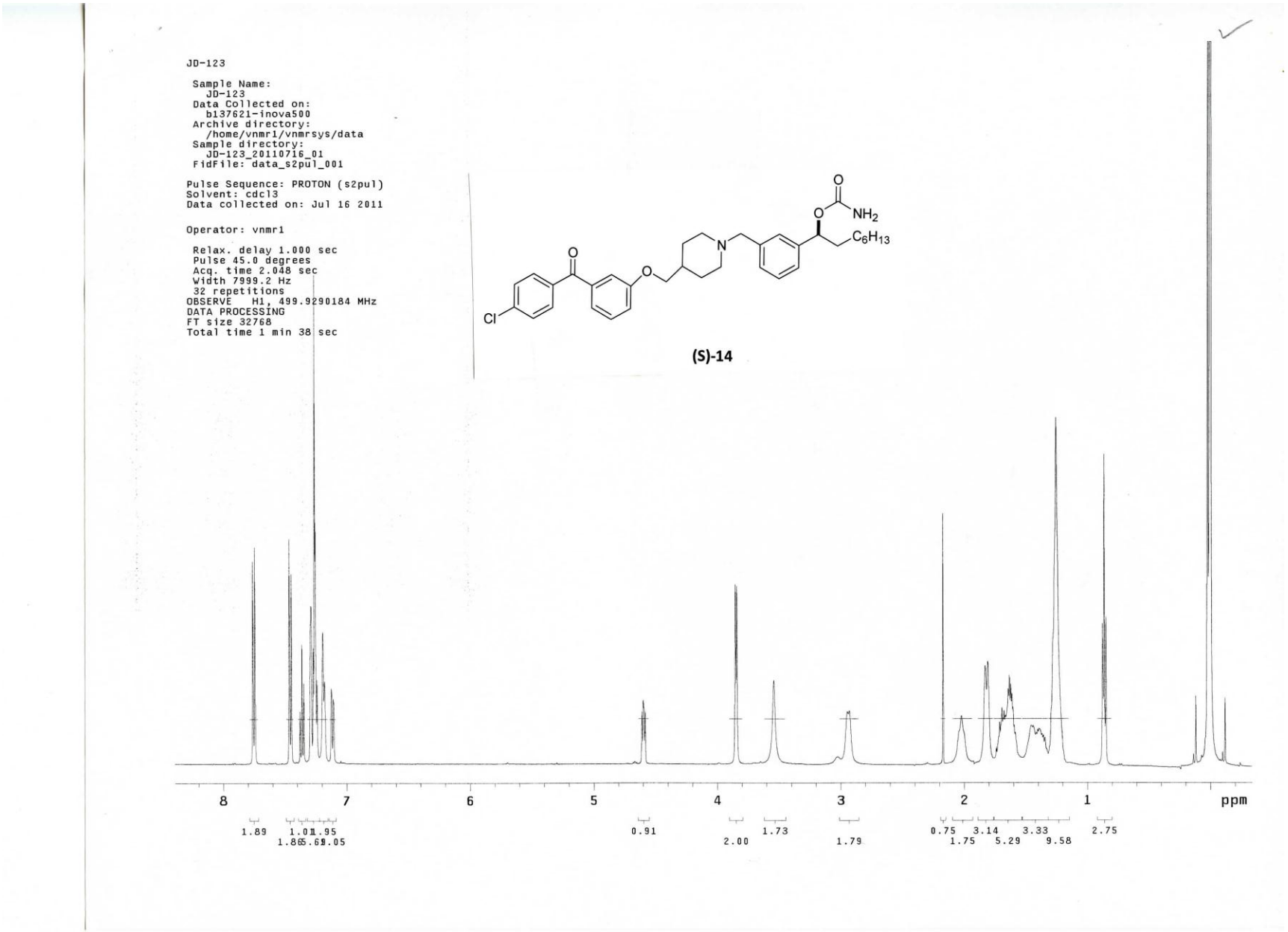
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 17 2011

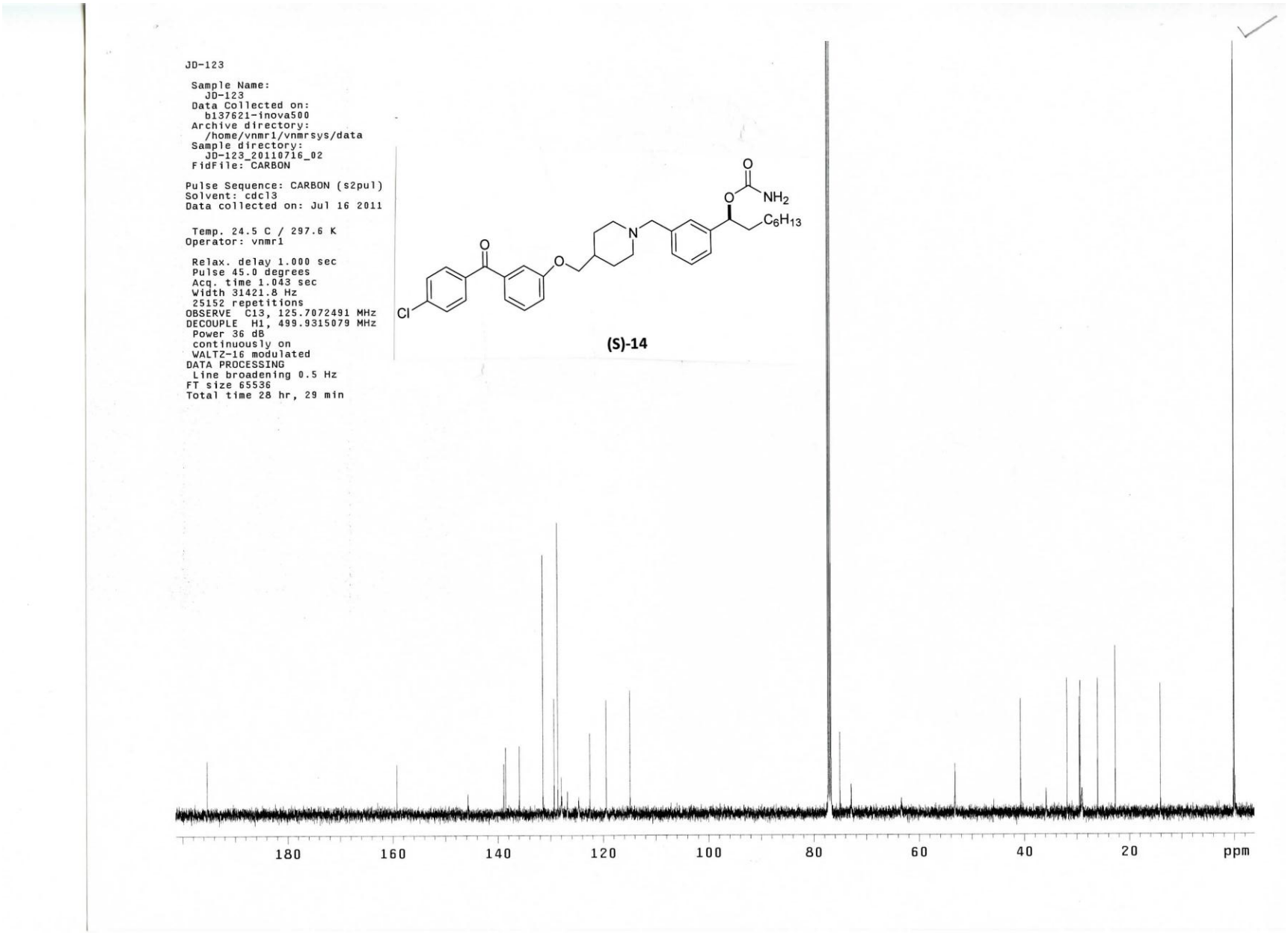
Temp. 24.4 C / 297.6 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
38656 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 59 min

(R)-14




JD-123
Sample Name:
JD-123
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-123_20110716_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 16 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
32 repetitions
OBSERVE H1, 499.9290184 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 38 sec
(S)-14
8
7
6
5
4
3
2
1
ppm
1.89
1.01
1.95
1.86
5.61
1.05
0.91
2.00
1.73
1.79
0.75
3.14
3.33
2.75
1.75
5.29
9.58


JD-123
Sample Name:
JD-123
Data Collected on:
bi37621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-123_20110716_02
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 16 2011
Temp. 24.5 C / 297.6 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
25152 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 28 hr, 29 min
O
O
NH2
C6H13
N
O
O
Cl
(S)-14
180
160
140
120
100
80
60
40
20
ppm

JD-72

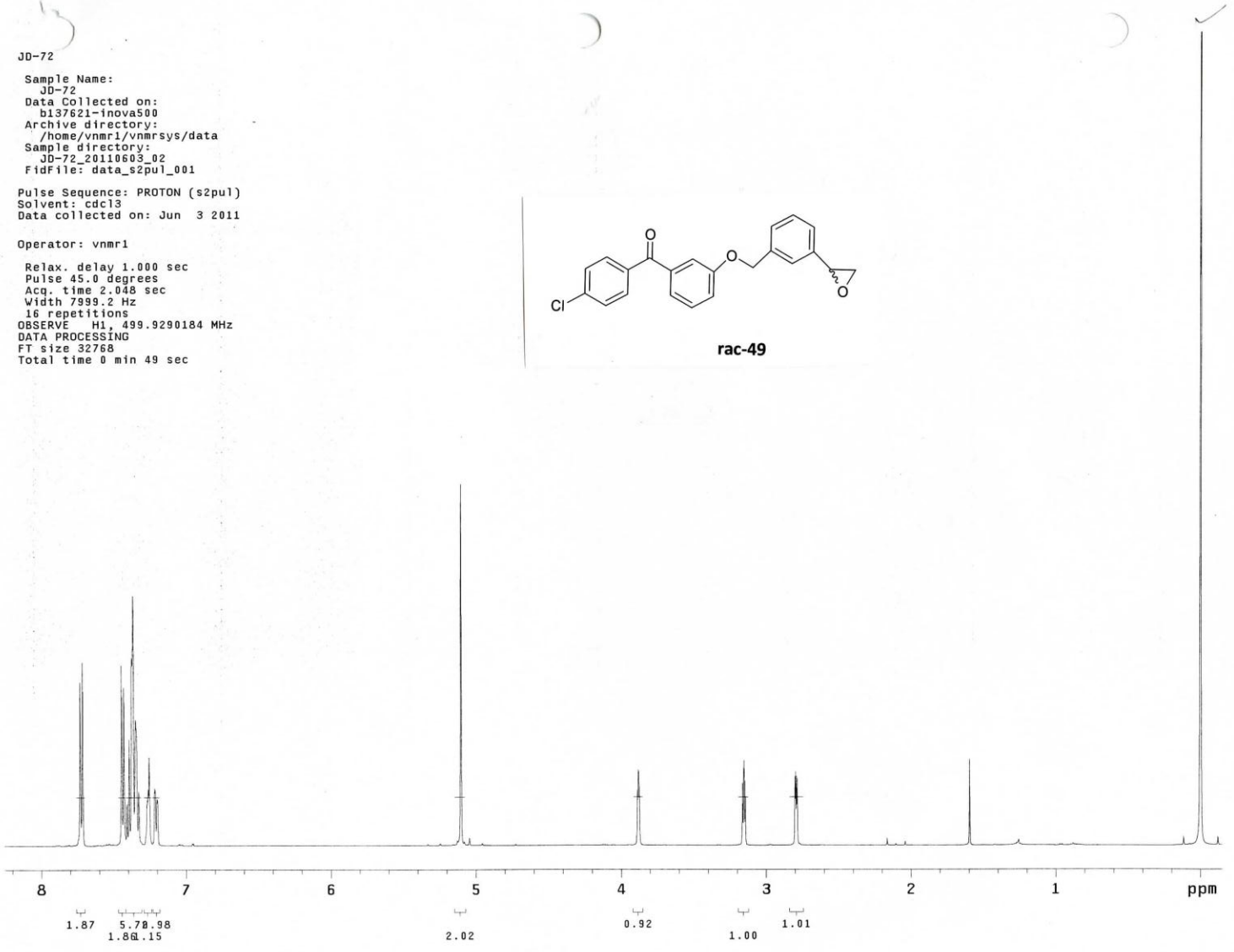
Sample Name:
JD-72
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-72_20110603_02
FidFile: data_s2pul_001

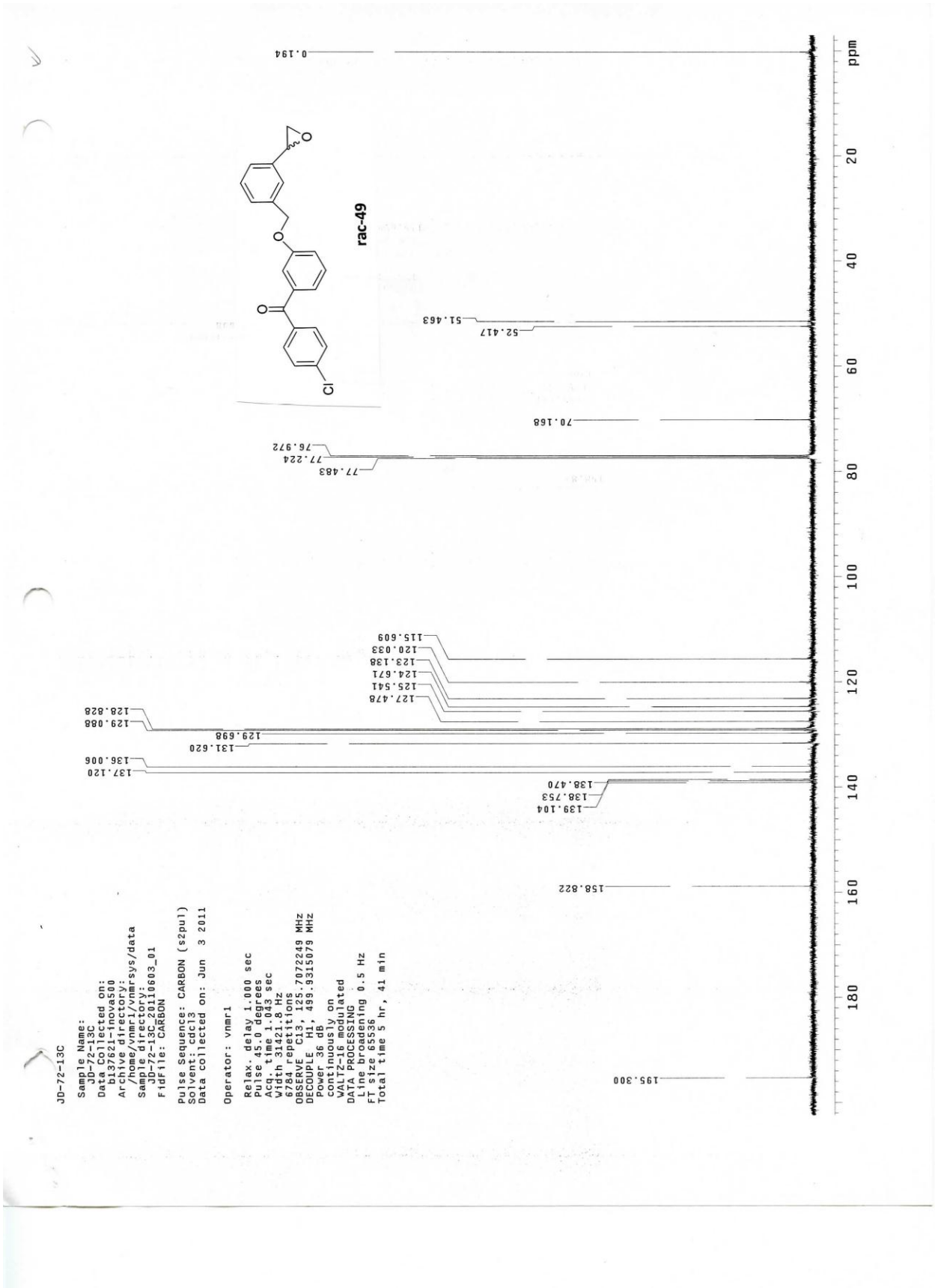
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 3 2011

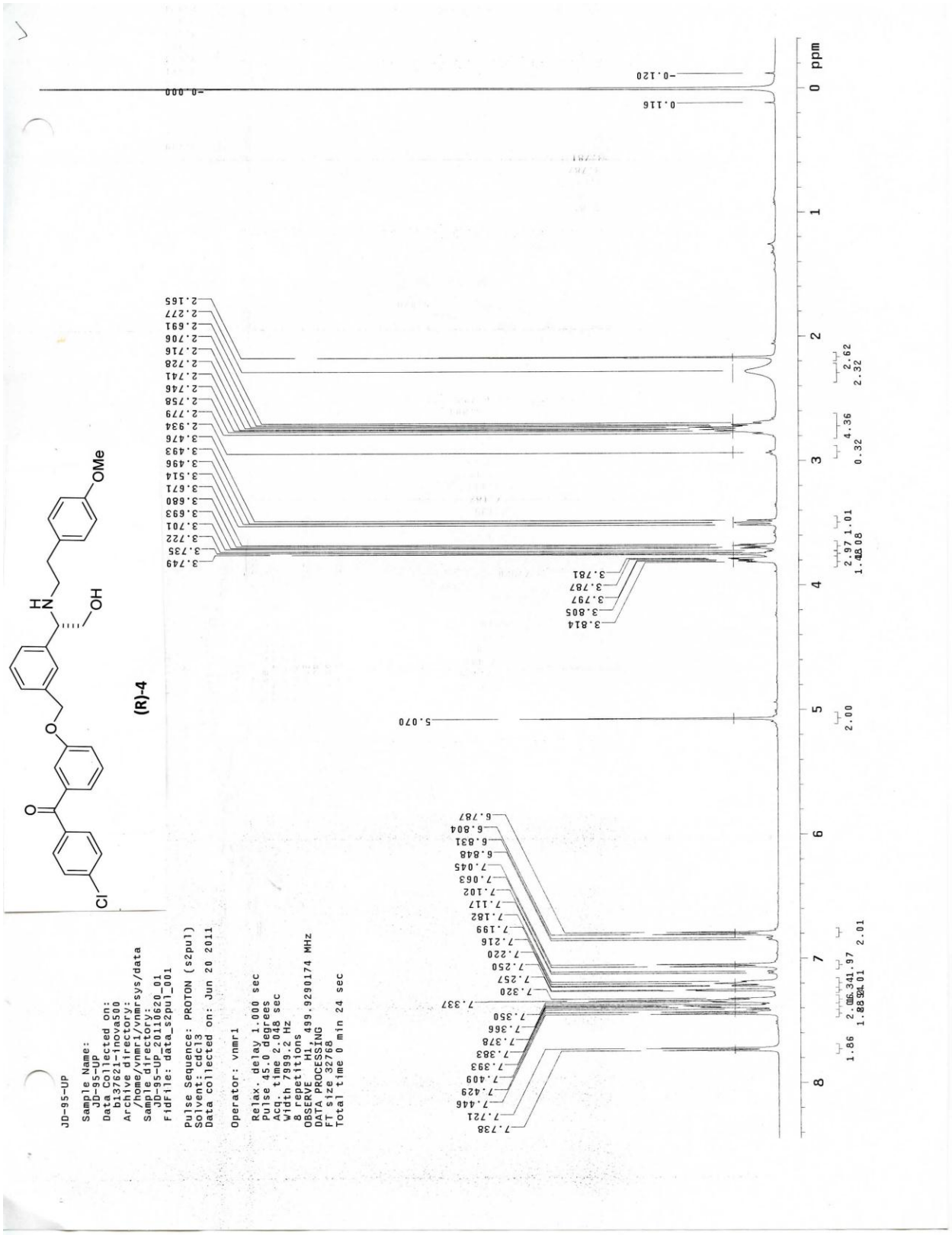
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
16 repetitions
OBSERVE H1, 499.9290184 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec

rac-49




JD-72-13C
Sample Name:
JD-72-13C
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-72-13C_20110603_01
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 3 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
6784 repetitions
OBSERVE C13, 125.7072249 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 41 min
rac-49
Cl
0.194
51.463
52.417
70.168
76.972
77.224
77.483
115.609
120.033
123.138
124.671
125.541
127.478
128.828
129.088
129.698
131.620
136.006
137.120
138.470
138.753
139.104
158.822
195.300
ppm
20
40
60
80
100
120
140
160
180


JD-95-UP
Sample Name:
JD-95-UP
Data Collected on:
bl37621-inova500
Archive directory:
/home/vnmrj/vnmrsys/data
Sample directory:
JD-95-UP_20110620_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 20 2011
Operator: vnmrj
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
8 repetitions
OBSERVE H1, 499.9290174 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
(R)-4
OMe
OH
N
O
Cl
0 ppm

STANDARD CARBON PARAMETERS

Sample Name: JD-95-UP-13C

Data Collected on:
b137621-inova500
Archive directory:

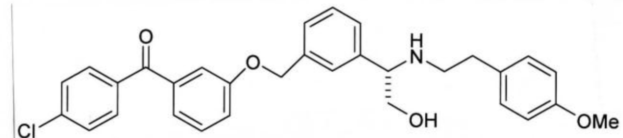
Sample directory:

FidFile: CARBON

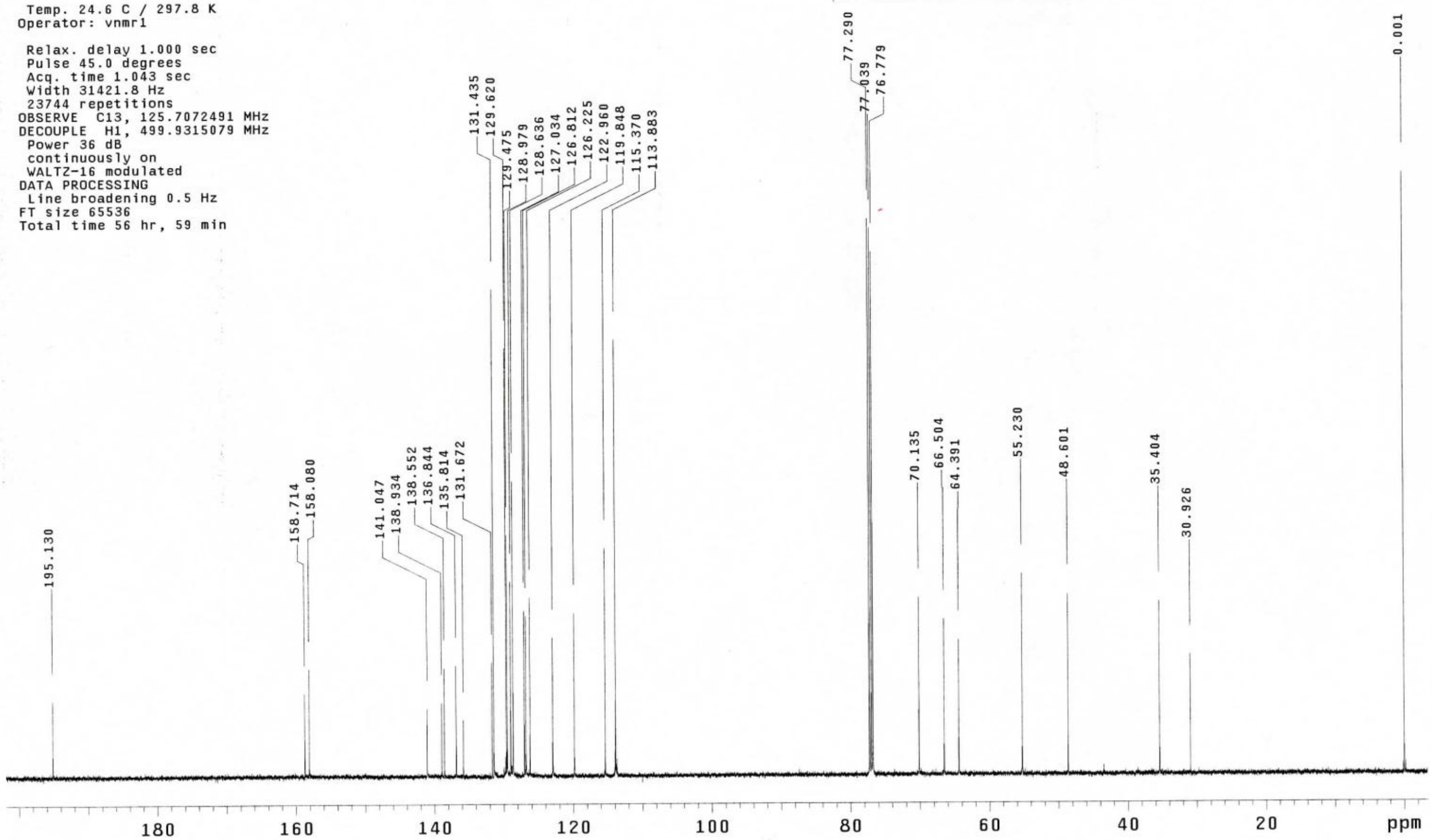
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 20 2011

Temp. 24.6 C / 297.8 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
23744 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 59 min



(R)-4

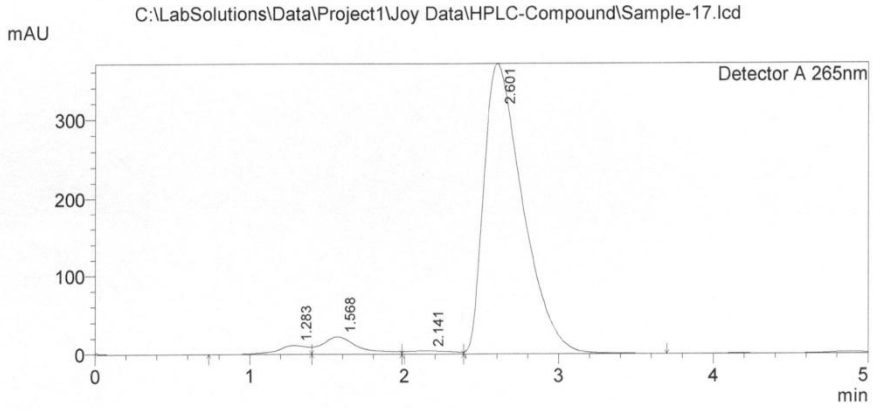


==== Shimadzu LabSolutions Analysis Report ====

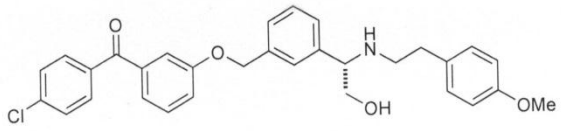
C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-17.lcd

Acquired by	: System Administrator
Sample Name	: JD-07-16-2011
Sample ID	:
Tray#	: 1
Vial#	: 1
Injection Volume	: 1
Data File	: C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-17.lcd
Method File	: C:\LabSolutions\Data\Project1\Joy training\Mixture-235nm-62%ACN.lcm
Report Format File	: C:\LabSolutions\System\DEFAULT.lsr
Month-Day Acquired	: 10/5/2011
Month-Day Processed	: 10/5/2011

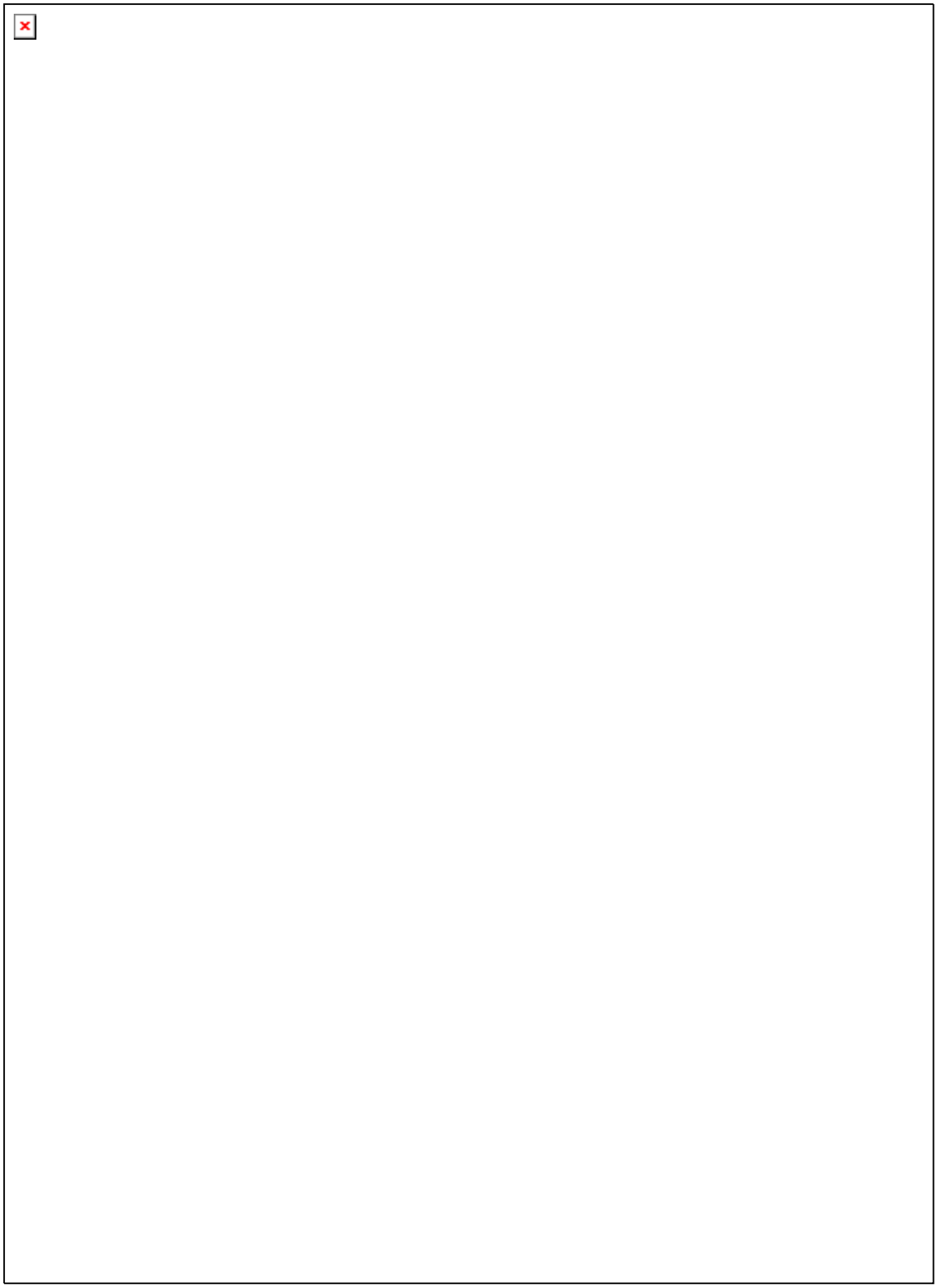
<Chromatogram>

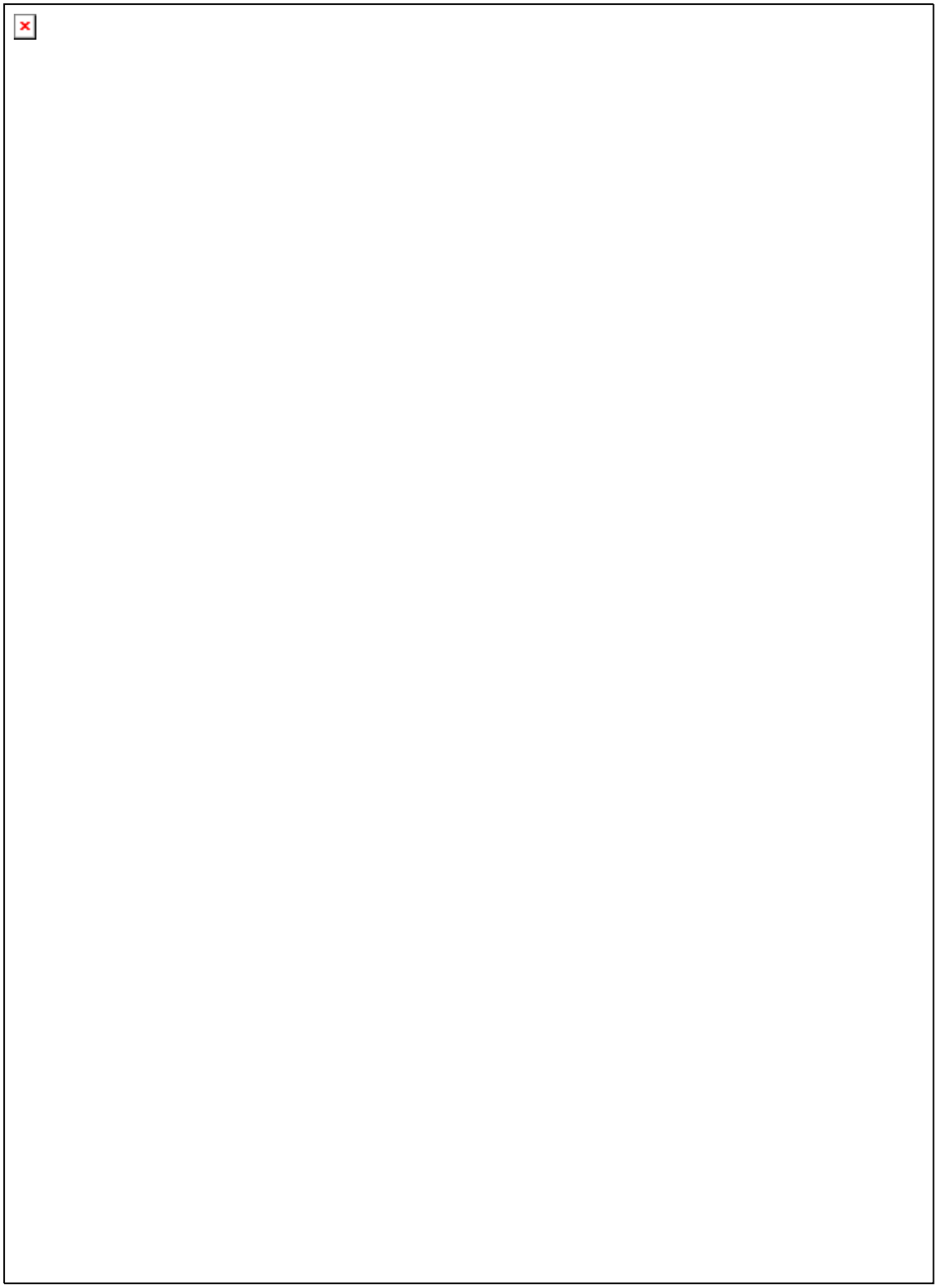


MS Chromatogram



Column: Phenominex kinetex 2.6μ C18 100A, 100 x 4.60 mm
Solvent: CH_3CN/0.05%TFA in H_2O = 25/1
flow rate: 0.5 mL/min.



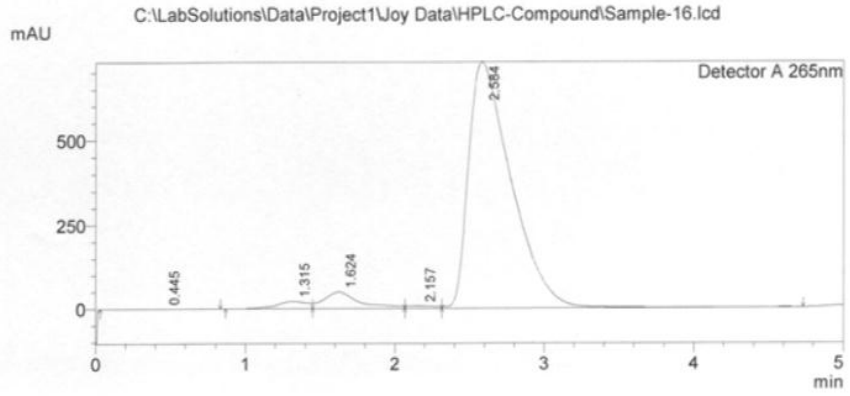


==== Shimadzu LabSolutions Analysis Report ====

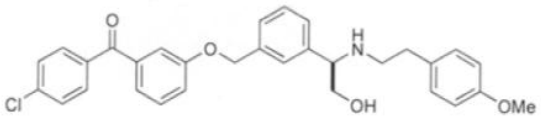
C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-16.lcd

Acquired by	: System Administrator
Sample Name	: JD-07-16-2011
Sample ID	:
Tray#	: 1
Vial#	: 1
Injection Volume	: 1
Data File	: C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-16.lcd
Method File	: C:\LabSolutions\Data\Project1\Joy training\Mixture-235nm-62%ACN.lcm
Report Format File	: C:\LabSolutions\System\DEFAULT.lsr
Month-Day Acquired	: 10/5/2011
Month-Day Processed	: 10/5/2011

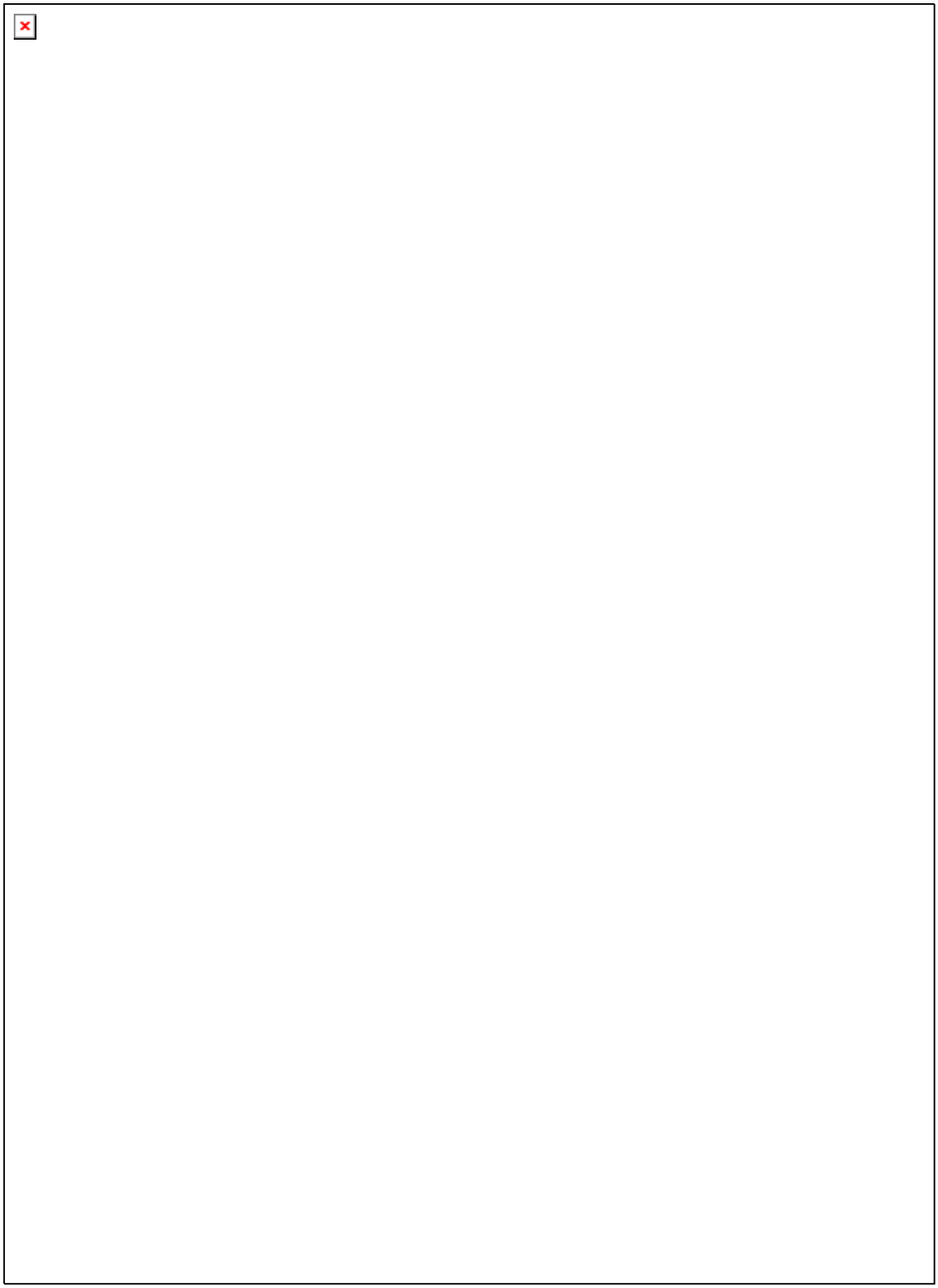
<Chromatogram>

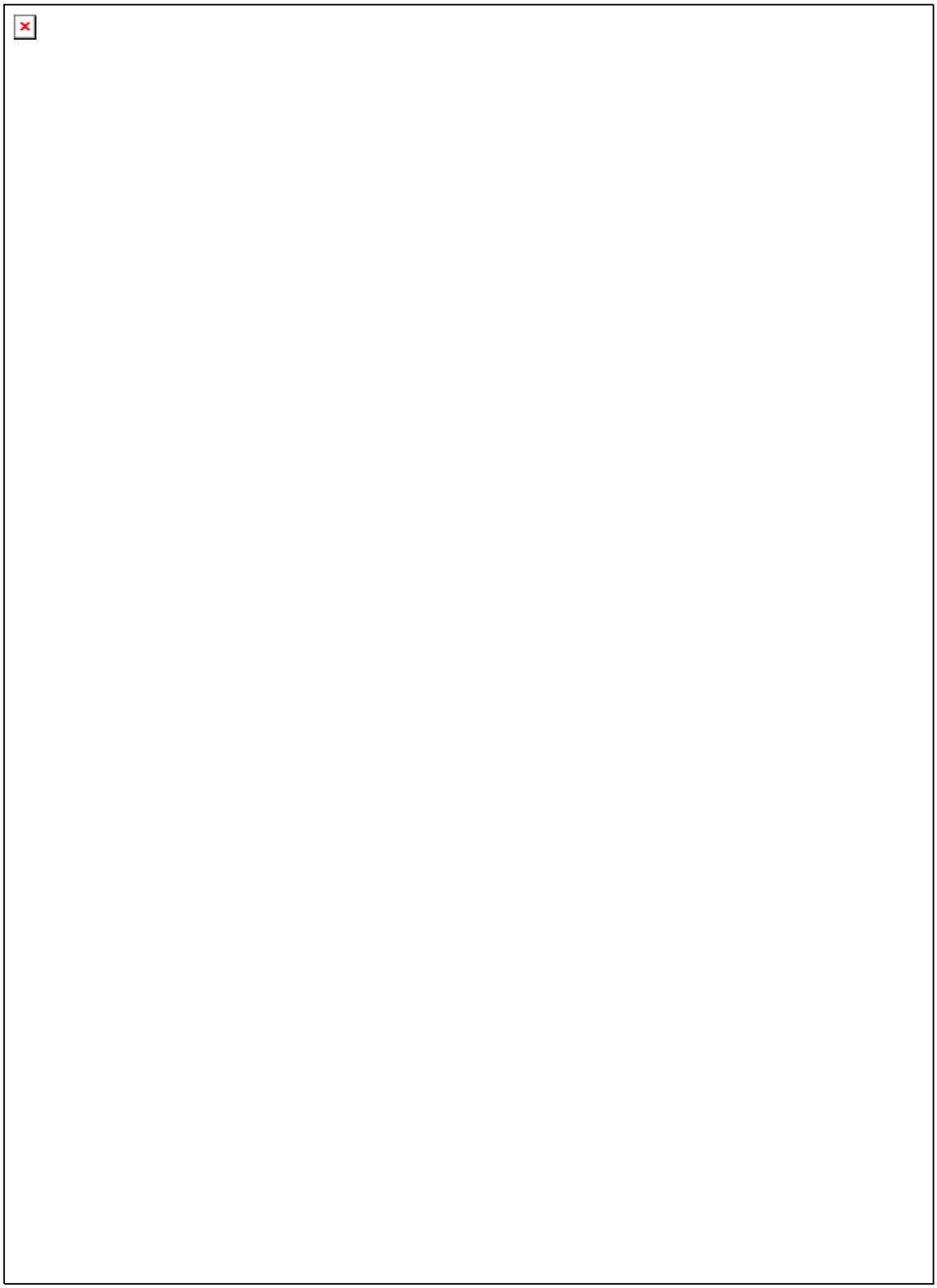


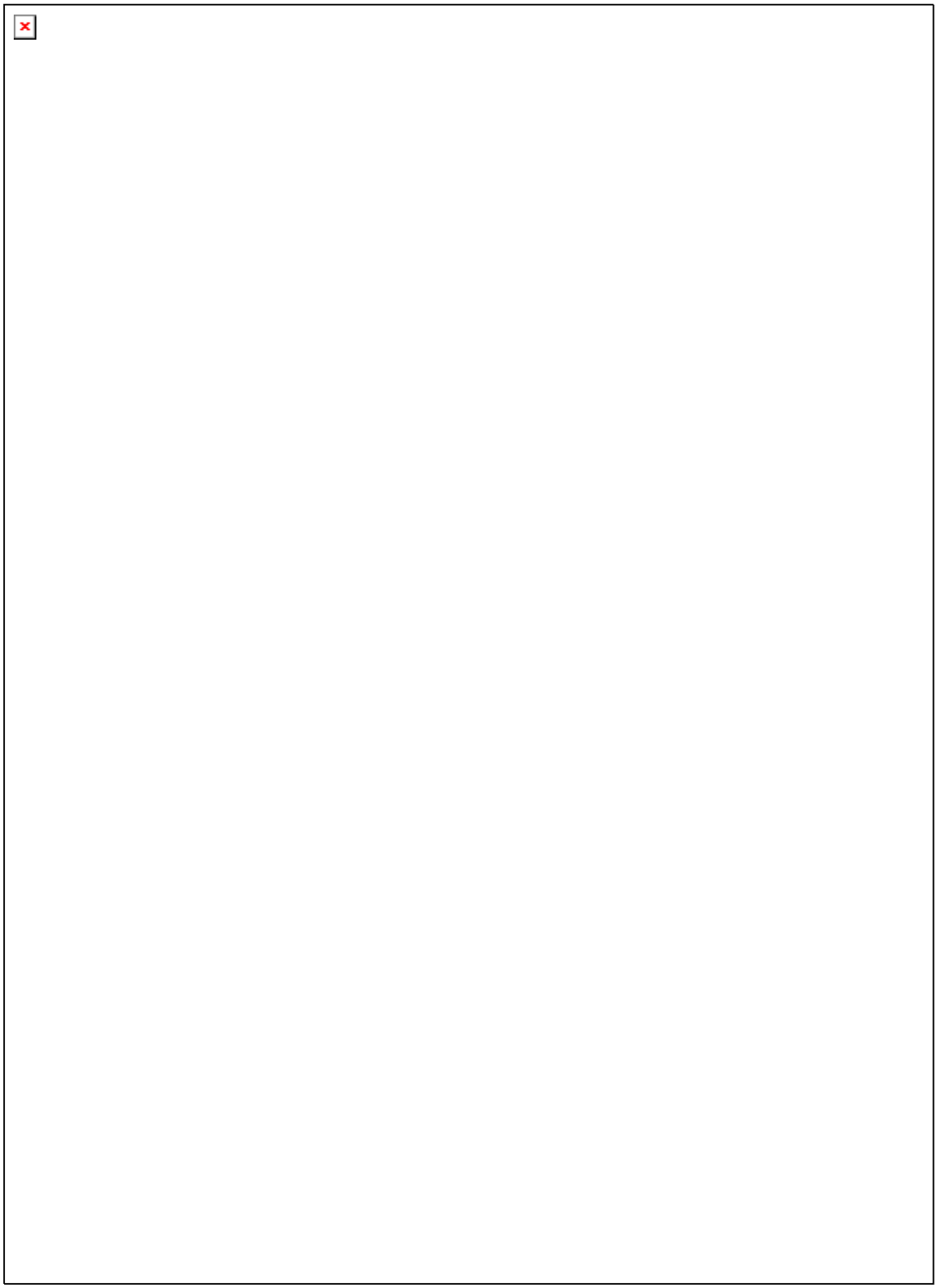
MS Chromatogram



Column: Phenominex kinetex 2.6μ C18 100A, 100 x 4.60 mm
Solvent: CH_3CN/0.05%TFA in H_2O = 25/1
flow rate: 0.5 mL/min.







STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
b137621-inova500
Archive directory:

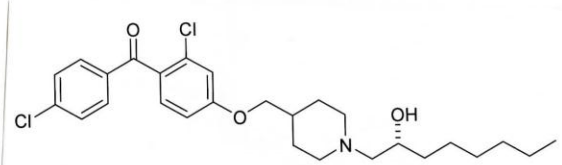
Sample directory:

FidFile: CARBON

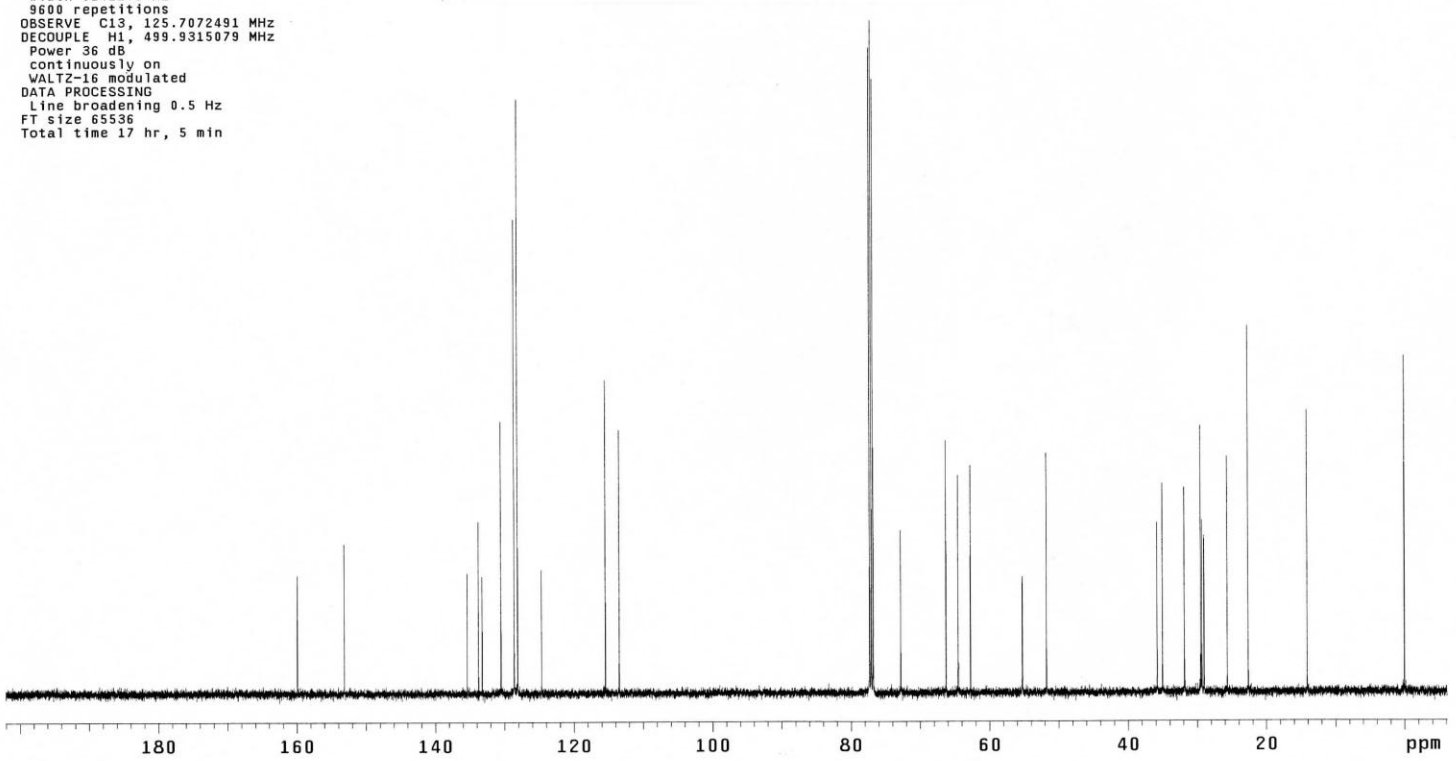
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 17 2011

Temp. 24.2 C / 297.4 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
9600 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 17 hr, 5 min



(R)-16

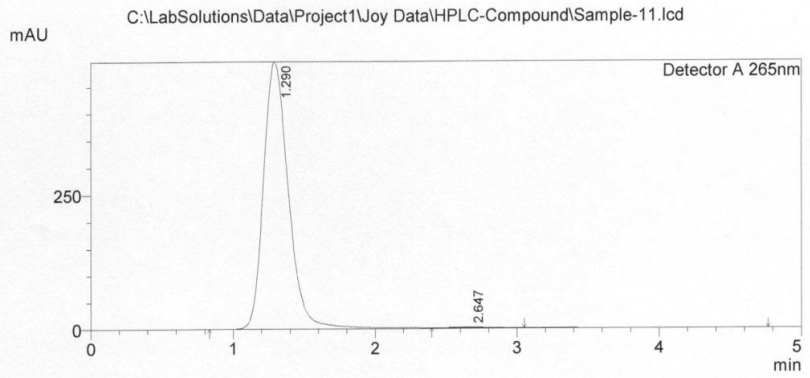


==== Shimadzu LabSolutions Analysis Report ====

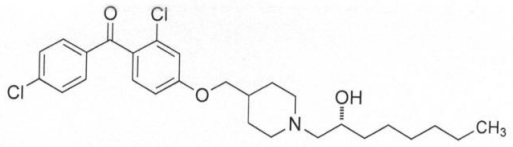
C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-11.lcd

Acquired by	: System Administrator
Sample Name	: JD-07-16-2011
Sample ID	:
Tray#	: 1
Vial#	: 1
Injection Volume	: 1
Data File	: C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-11.lcd
Method File	: C:\LabSolutions\Data\Project1\Joy training\Mixture-235nm-62%ACN.lcm
Report Format File	: C:\LabSolutions\System\DEFAULT.lsr
Month-Day Acquired	: 10/5/2011
Month-Day Processed	: 10/5/2011

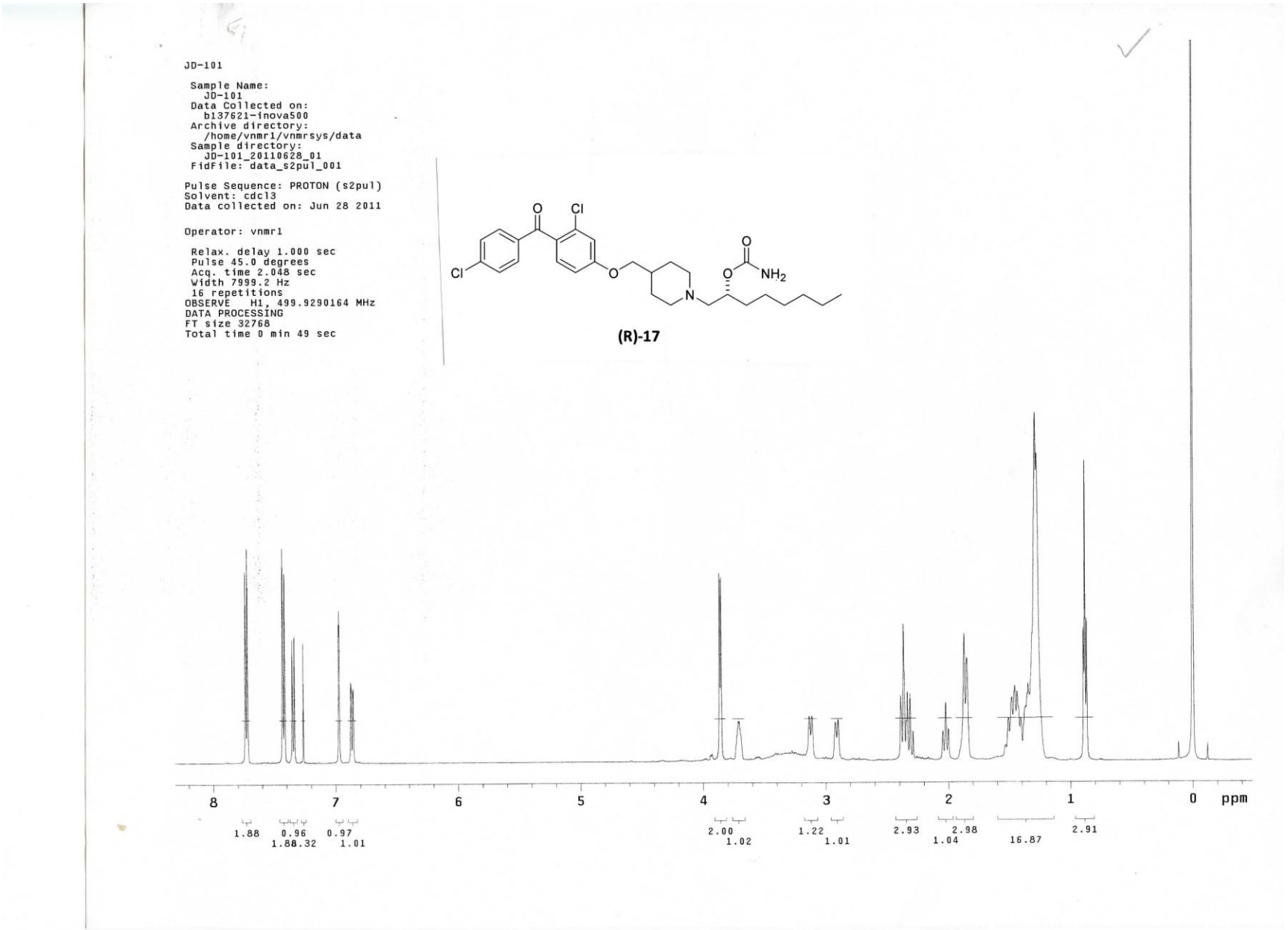
<Chromatogram>

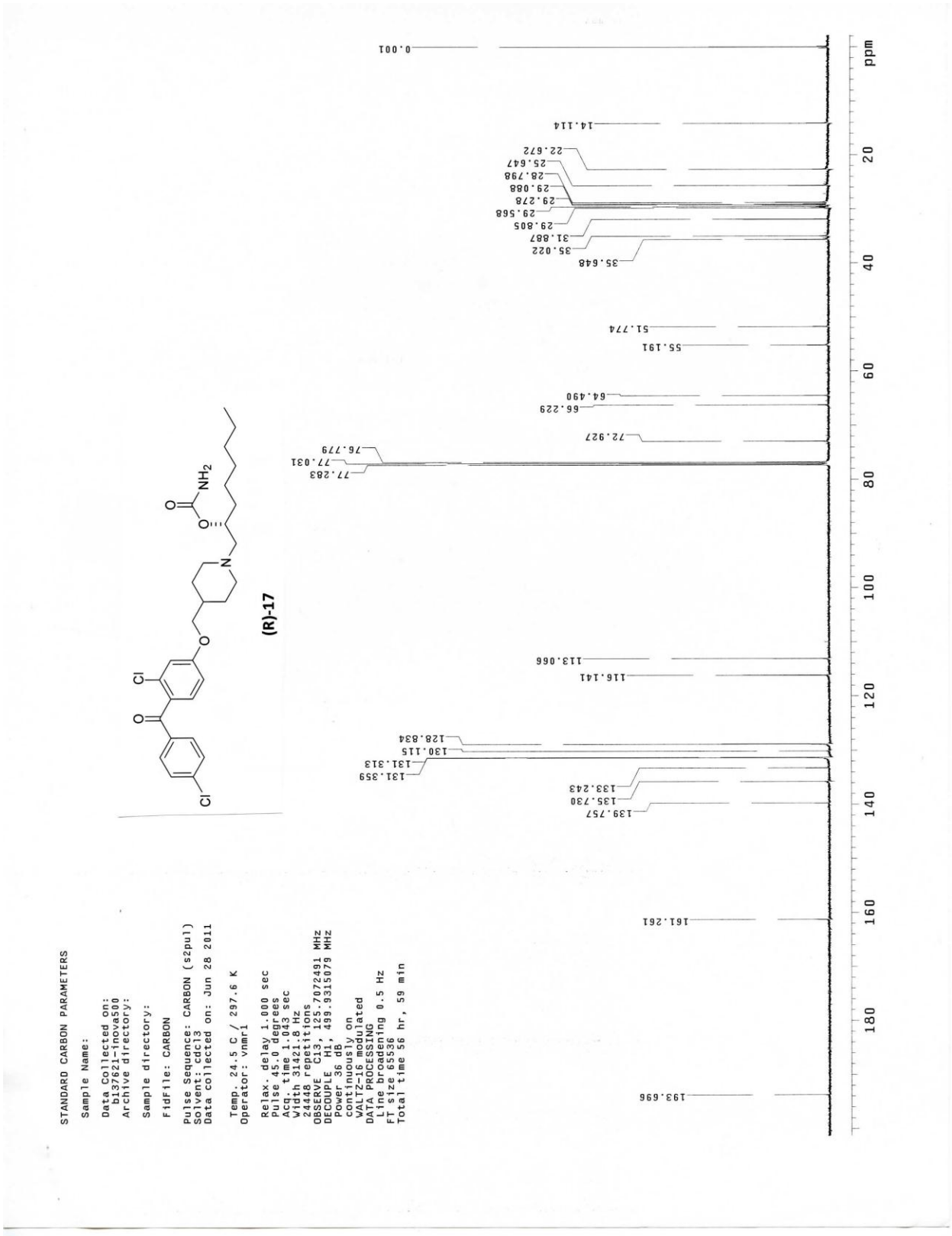


MS Chromatogram



Column: Phenominex kinetex 2.6μ C18 100A, 100 x 4.60 mm
Solvent: CH_3CN/0.05%TFA in H_2O = 25/1
flow rate: 0.5 mL/min.

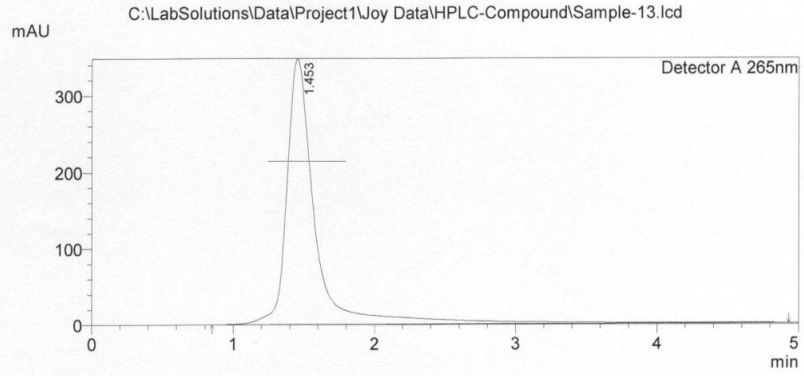

JD-101
Sample Name:
JD-101
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-101_20110628_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 28 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
16 repetitions
OBSERVE H1, 499.9290164 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec
(R)-17
8
7
6
5
4
3
2
1
0
ppm
1.88
0.96
1.88.32
0.97
1.01
2.00
1.02
1.22
1.01
2.93
2.98
1.04
16.87
2.91


STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
b13621-inova500
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 28 2011
Temp. 24.5 C / 297.6 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
24448 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 59 min
(R)-17
0.001
14.114
22.672
25.647
28.798
29.088
29.278
29.568
29.805
31.887
35.022
35.648
51.774
55.191
64.490
66.229
72.927
76.779
77.031
77.283
113.066
116.141
128.834
130.115
131.313
131.359
133.243
135.730
139.757
161.261
193.696
ppm
20
40
60
80
100
120
140
160
180

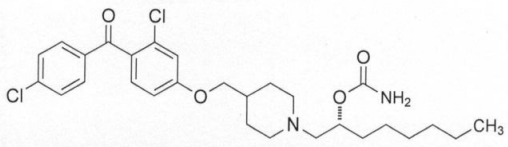
==== Shimadzu LabSolutions Analysis Report ====

C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-13.lcd
Acquired by : System Administrator
Sample Name : JD-07-16-2011
Sample ID :
Tray# : 1
Vial# : 1
Injection Volume : 1
Data File : C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-13.lcd
Method File : C:\LabSolutions\Data\Project1\Joy training\Mixture-235nm-62%ACN.lcm
Report Format File : C:\LabSolutions\System\DEFAULT.lsr
Month-Day Acquired : 10/5/2011
Month-Day Processed : 10/5/2011

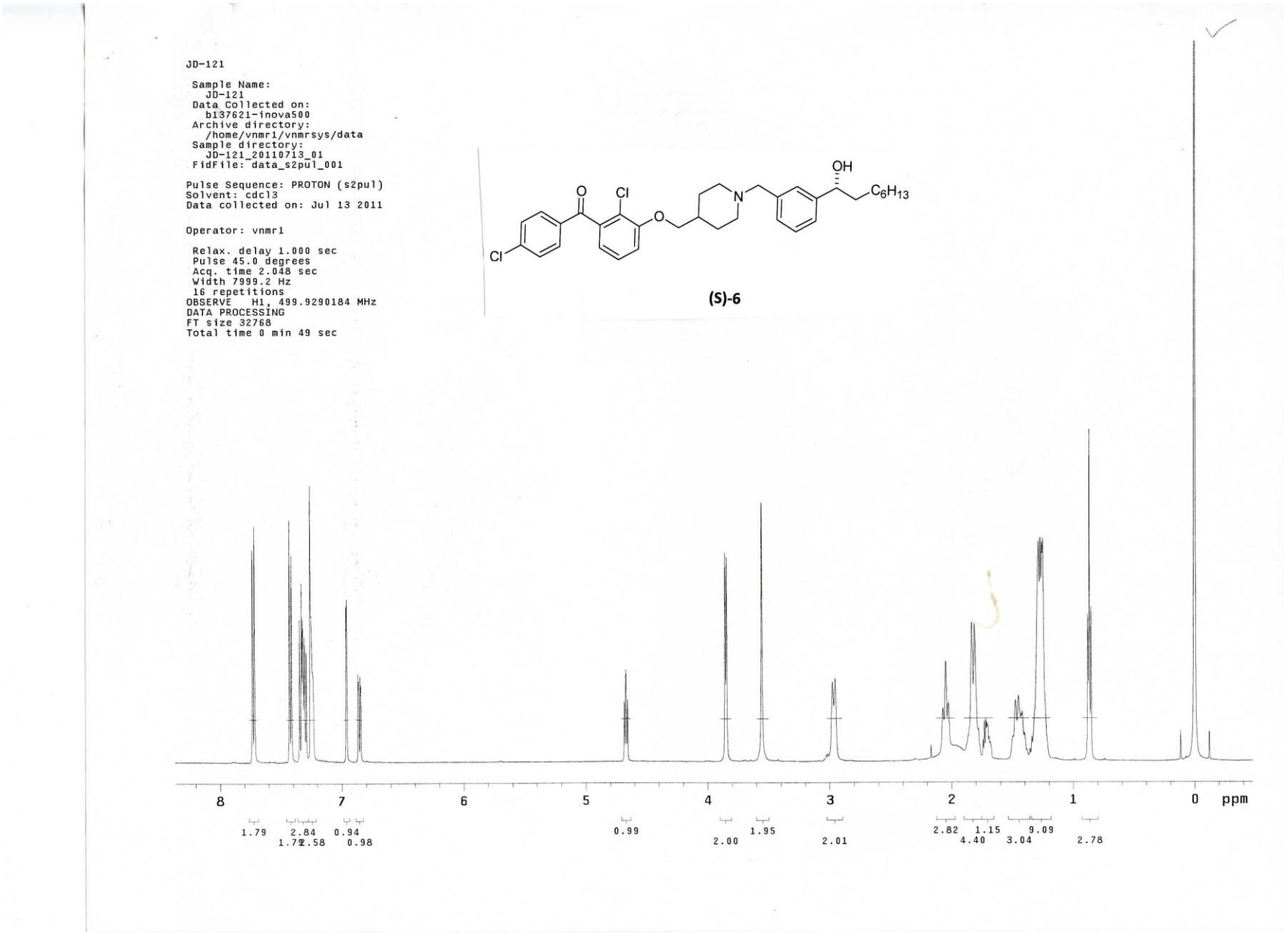
<Chromatogram>



MS Chromatogram



Column: Phenominex kinetex 2.6μ C18 100A, 100 x 4.60 mm
Solvent: CH_3CN/0.05%TFA in H_2O = 25/1
flow rate: 0.5 mL/min.


JD-121
Sample Name:
JD-121
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-121_20110713_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 13 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
16 repetitions
OBSERVE H1, 499.9290184 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec
O
Cl
OH
N
O
Cl
C6H13
(S)-6
8
7
6
5
4
3
2
1
0
ppm
1.79
2.84
1.72
2.58
0.94
0.98
0.99
2.00
1.95
2.01
2.82
4.40
1.15
3.04
9.09
2.78

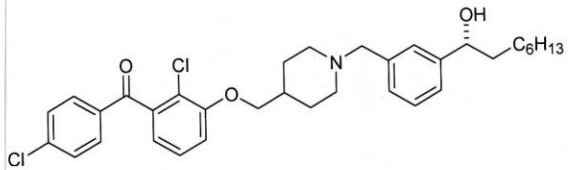
JD-121-13C

Sample Name:
JD-121-13C
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-121-13C_20110714_02
FidFile: data_s2pul_001

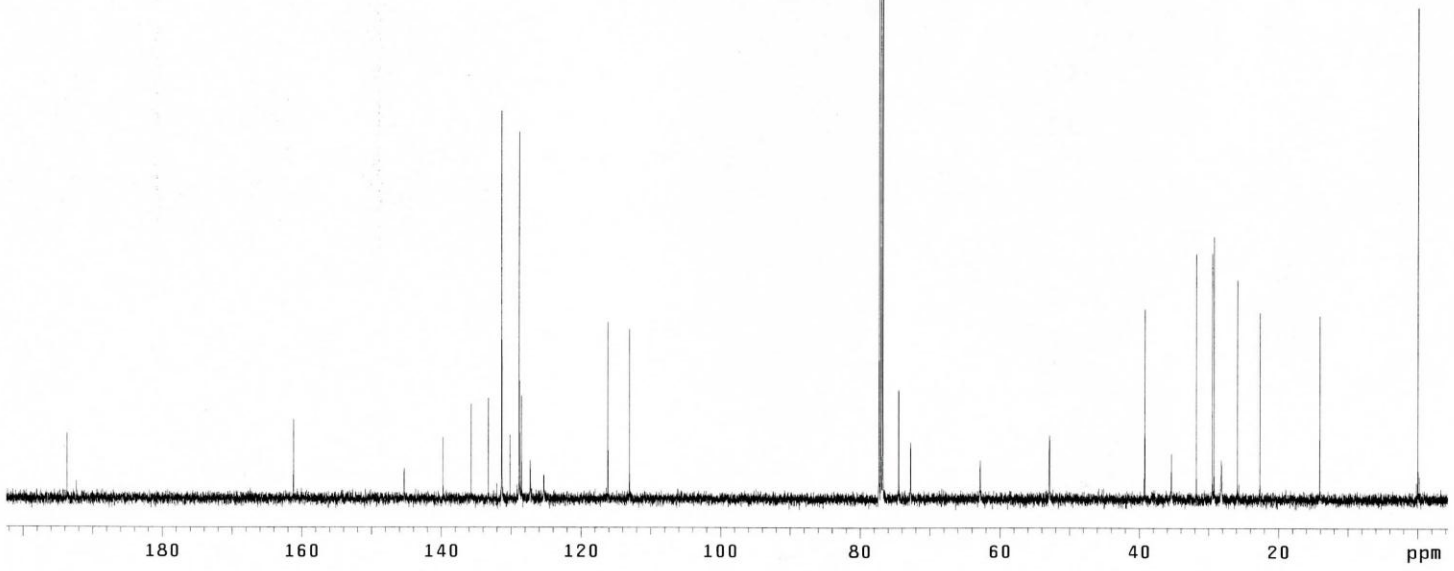
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 14 2011

Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
10000 repetitions
OBSERVE C13, 125.7072493 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 41 min



(S)-6

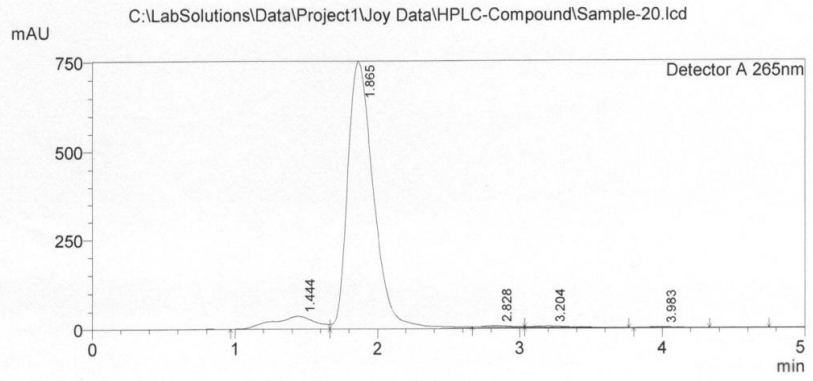


==== Shimadzu LabSolutions Analysis Report ====

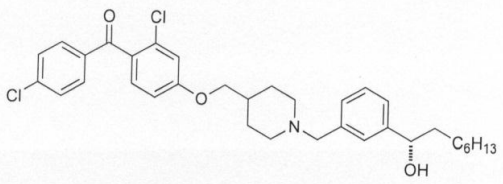
C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-20.lcd

Acquired by	: System Administrator
Sample Name	: JD-07-16-2011
Sample ID	:
Tray#	: 1
Vial#	: 1
Injection Volume	: 1
Data File	: C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-20.lcd
Method File	: C:\LabSolutions\Data\Project1\Joy training\Mixture-235nm-62%ACN.lcm
Report Format File	: C:\LabSolutions\System\DEFAULT.lsr
Month-Day Acquired	: 10/5/2011
Month-Day Processed	: 10/5/2011

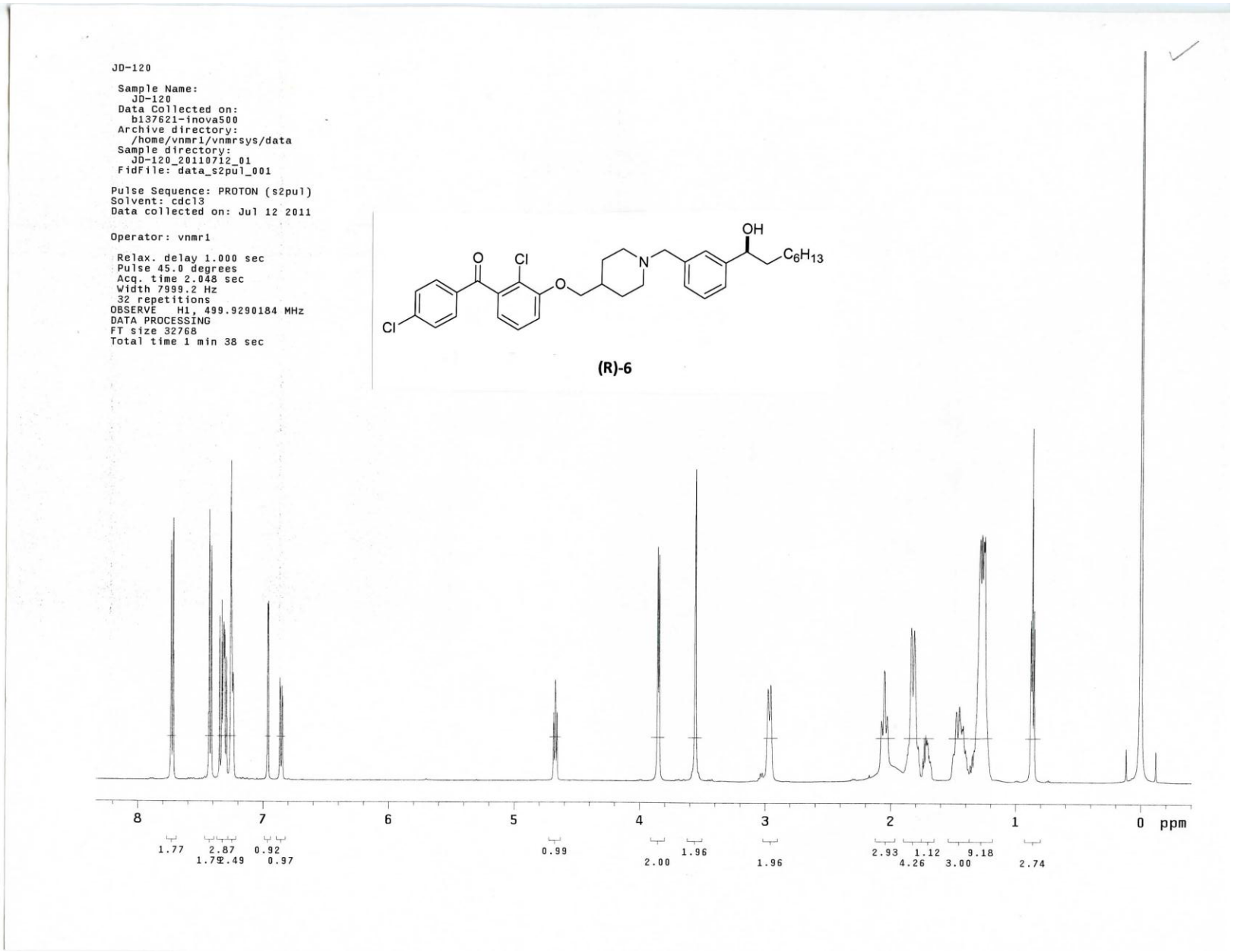
<Chromatogram>

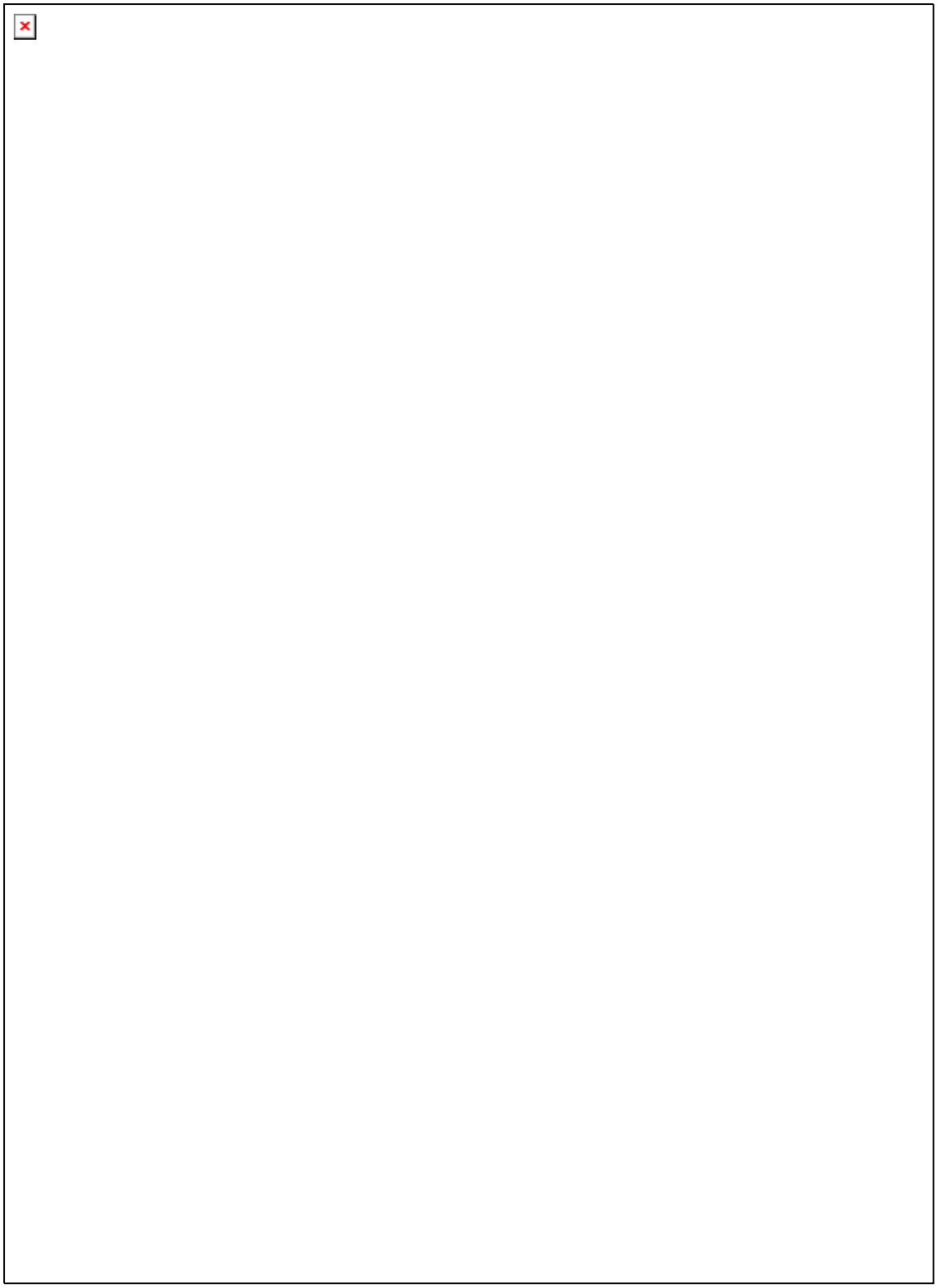


MS Chromatogram



Column: Phenominex kinetex 2.6μ C18 100A, 100 x 4.60 mm
Solvent: CH_3CN/0.05%TFA in H_2O = 25/1
flow rate: 0.5 mL/min.


JD-120
Sample Name:
JD-120
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-120_20110712_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 12 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
32 repetitions
OBSERVE H1, 499.9290184 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 38 sec
O
Cl
OH
N
O
Cl
C6H13
(R)-6
8
7
6
5
4
3
2
1
0 ppm
1.77
2.87
0.92
1.79
2.49
0.97
0.99
2.00
1.96
1.96
2.93
1.12
9.18
4.26
3.00
2.74

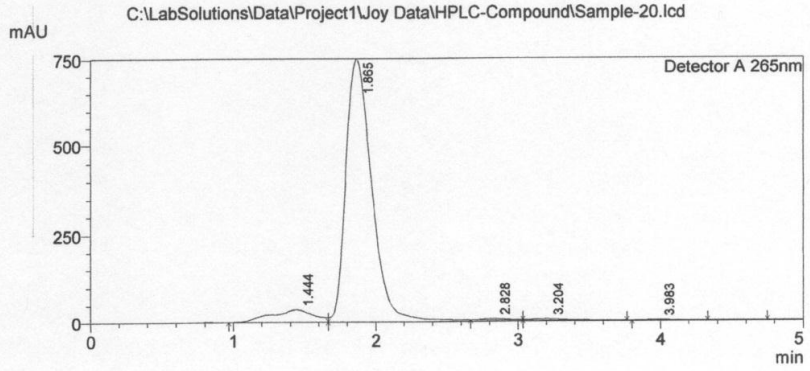


==== Shimadzu LabSolutions Analysis Report ====

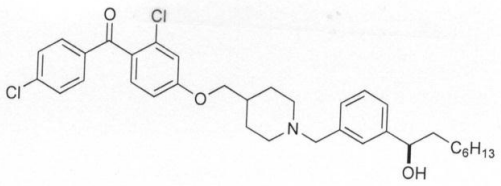
C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-20.lcd
Acquired by : System Administrator
Sample Name : JD-07-16-2011
Sample ID :
Tray# : 1
Vial# : 1
Injection Volume : 1
Data File : C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-20.lcd
Method File : C:\LabSolutions\Data\Project1\Joy training\Mixture-235nm-62%ACN.lcm
Report Format File : C:\LabSolutions\System\DEFAULT.lsr
Month-Day Acquired : 10/5/2011
Month-Day Processed : 10/5/2011

<Chromatogram>

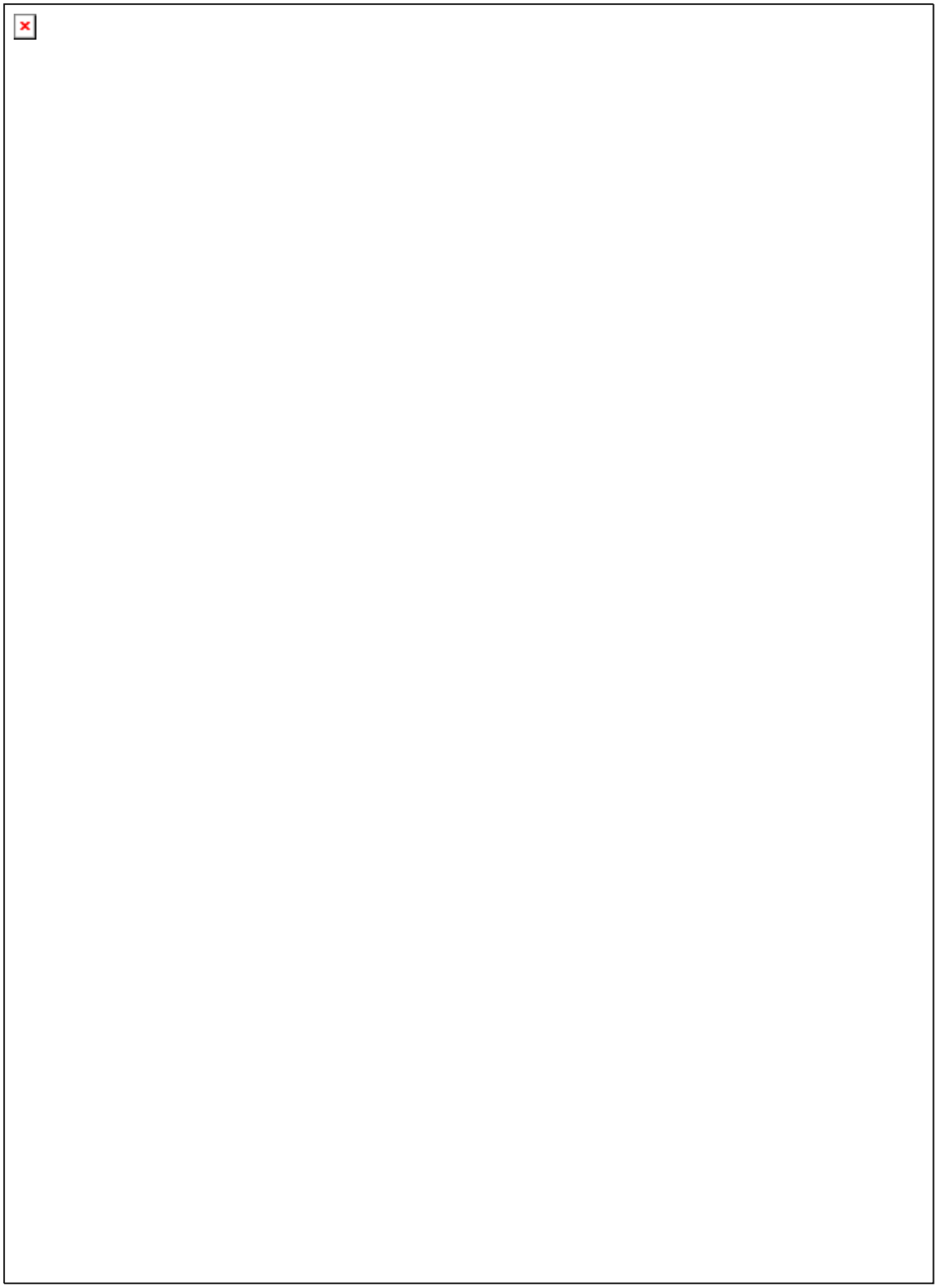
C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-20.lcd

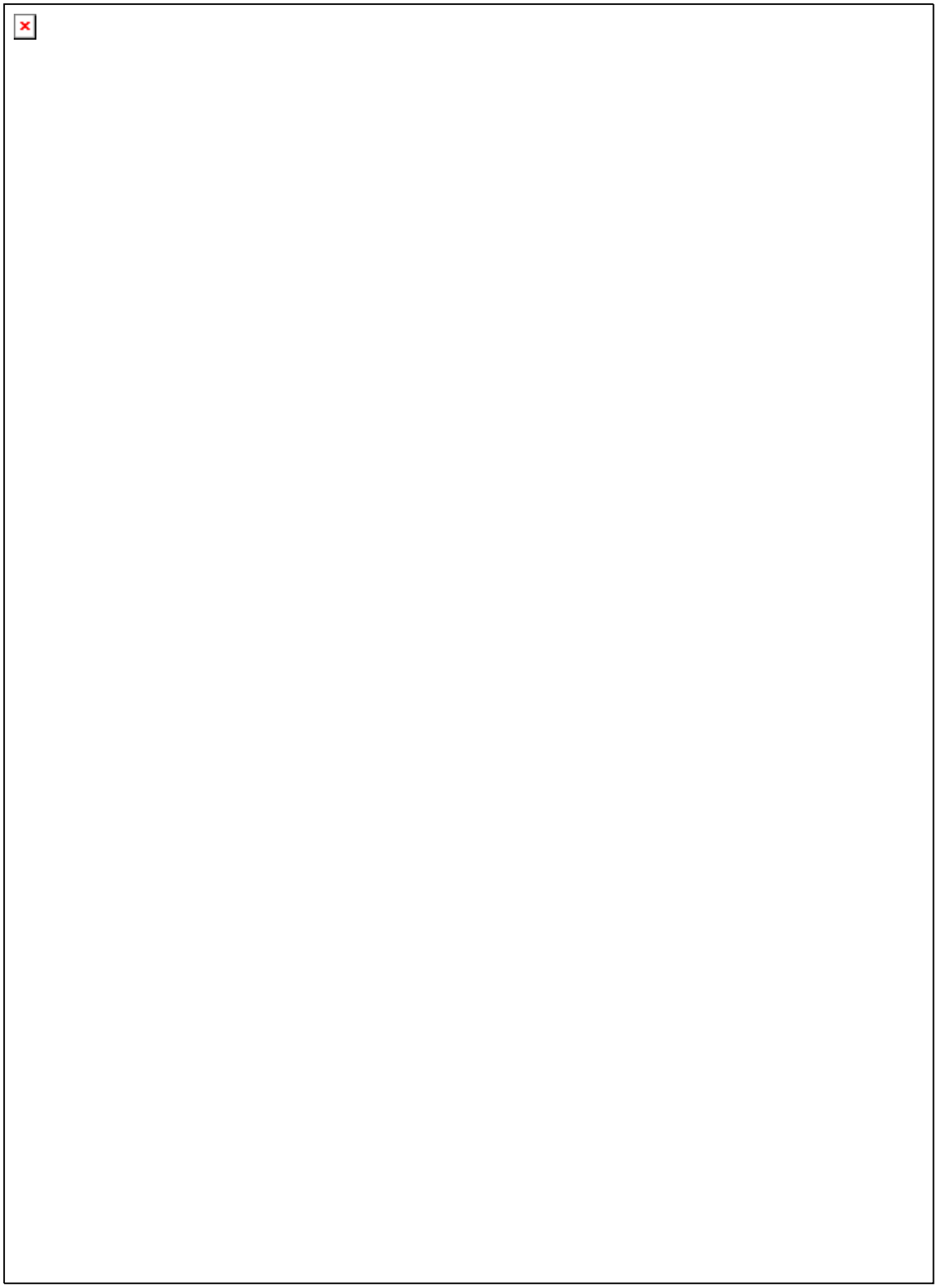


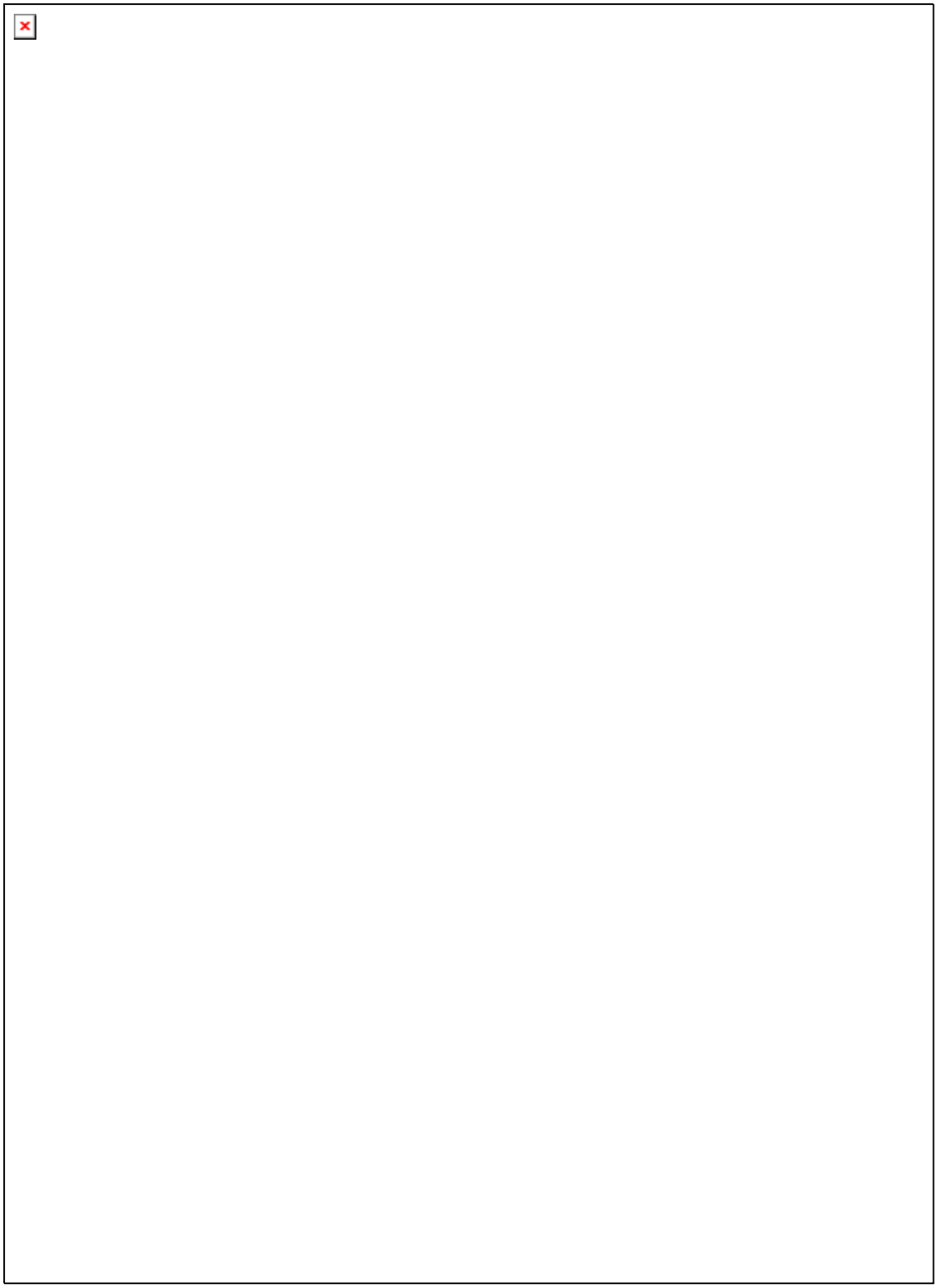
MS Chromatogram

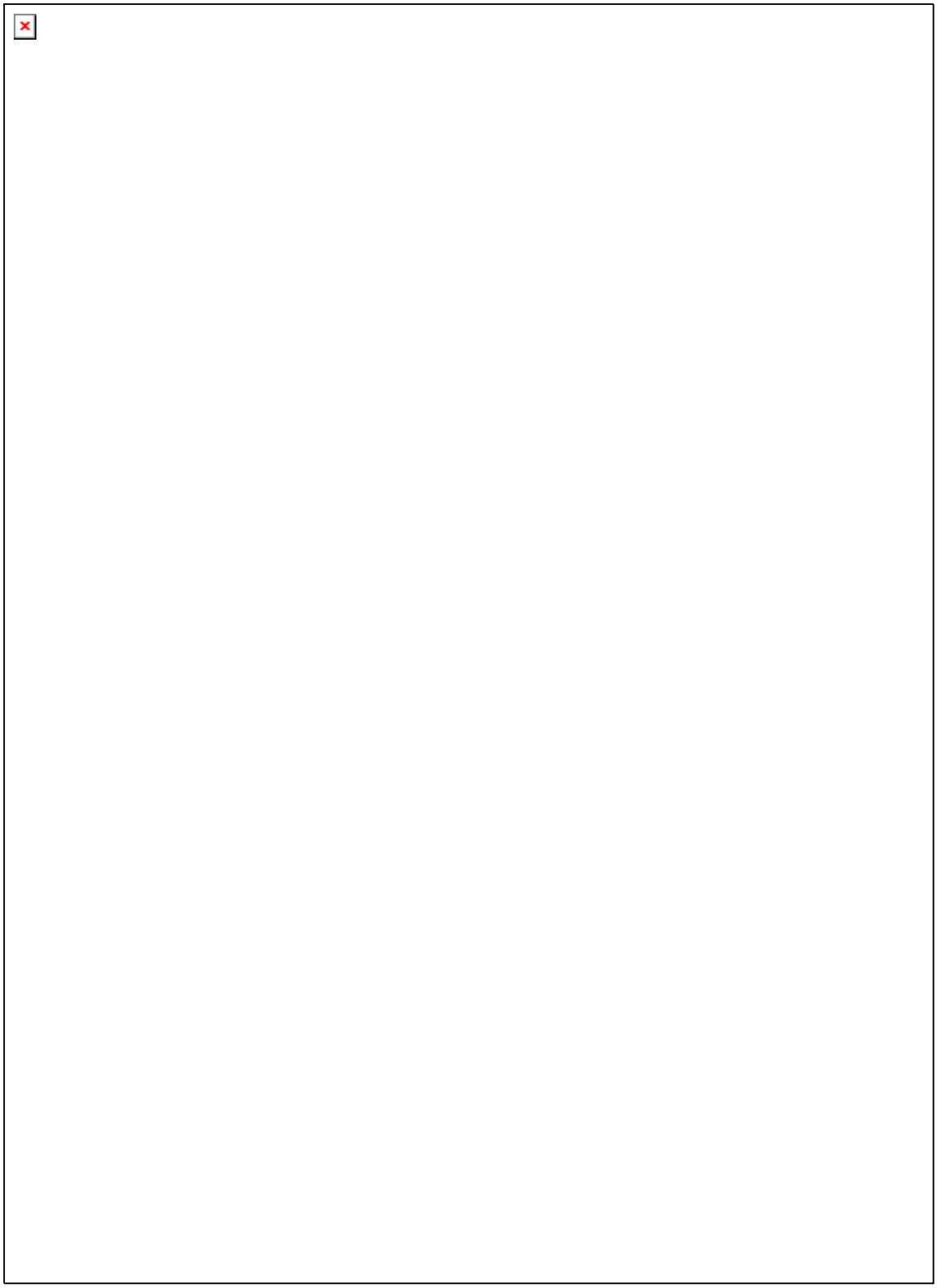


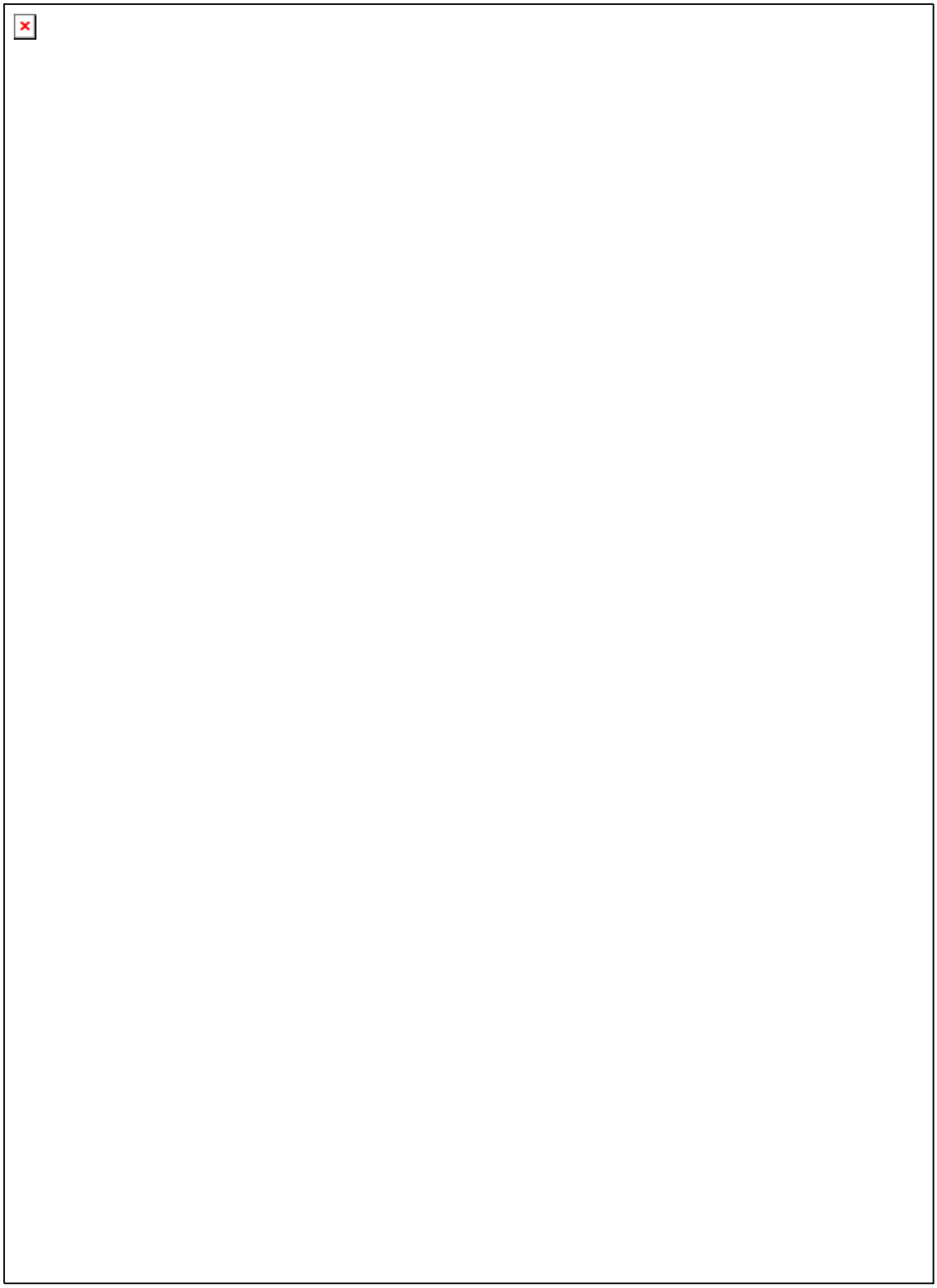
Column: Phenominex kinetex 2.6μ C18 100A, 100 x 4.60 mm
Solvent: CH_3CN/0.05%TFA in H_2O = 25/1
flow rate: 0.5 mL/min.

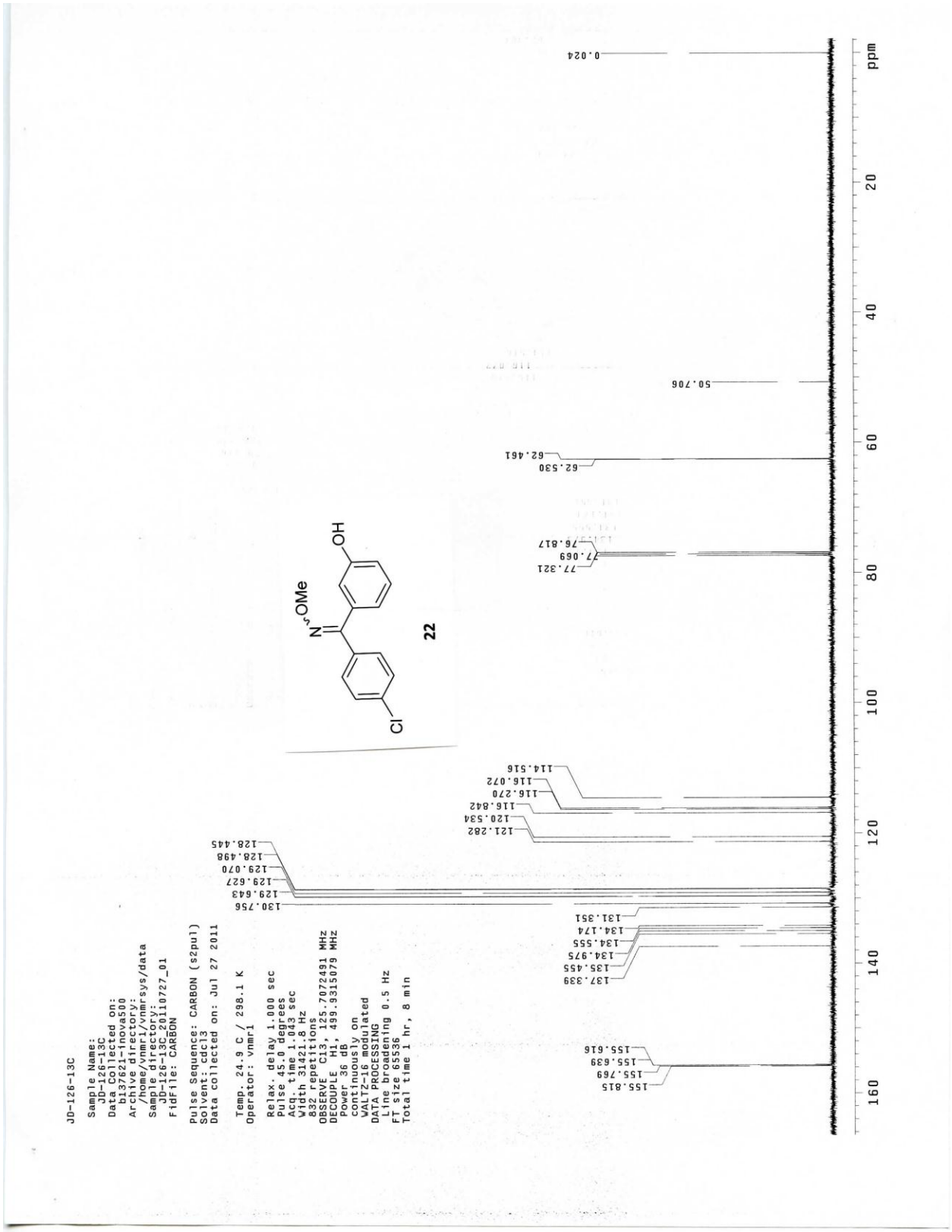











JD-126-13C
Sample Name:
JD-126-13C
Data Collected on:
b137621-1nova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-126-13C_20110727_01
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2011
Temp. 24.9 C / 298.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
832 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 8 min
0.024
50.706
62.461
62.530
76.817
77.069
77.321
114.516
116.072
116.270
116.842
120.534
121.282
128.445
128.498
129.070
129.627
129.643
130.756
131.351
134.174
134.555
134.975
135.455
137.339
155.615
155.639
155.769
155.815
OMe
N
OH
Cl
22
ppm
160
140
120
100
80
60
40
20

JD-129

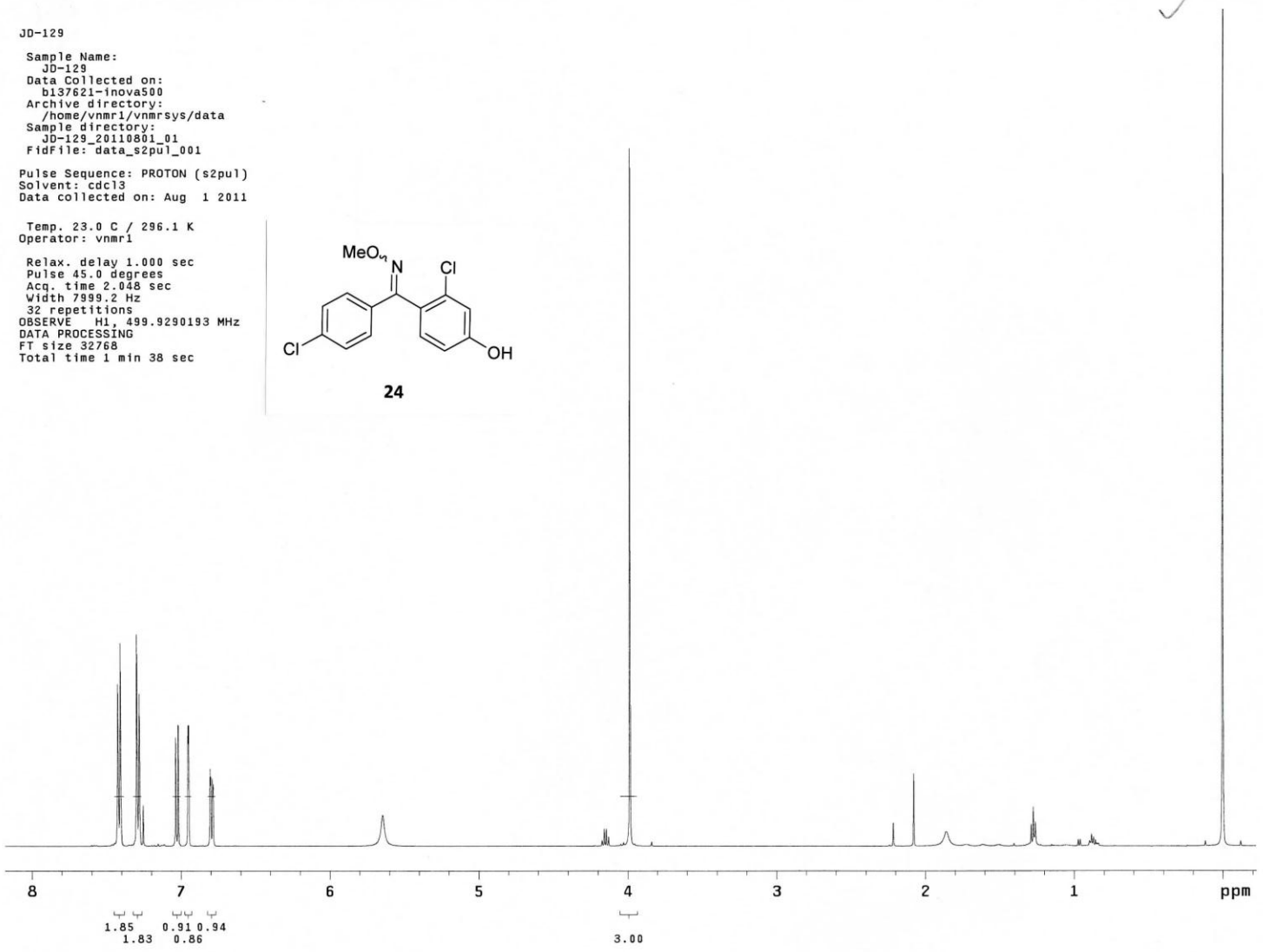
Sample Name:
JD-129
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-129_20110801_01
FidFile: data_s2pul_001

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 1 2011

Temp. 23.0 C / 296.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
32 repetitions
OBSERVE H1, 499.9290193 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 38 sec

24



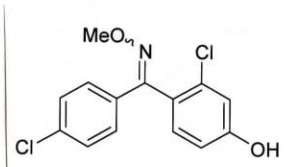
JD-129-13C

Sample Name:
JD-129-13C
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-129-13C_20110801_01
FidFile: data_s2pul_001

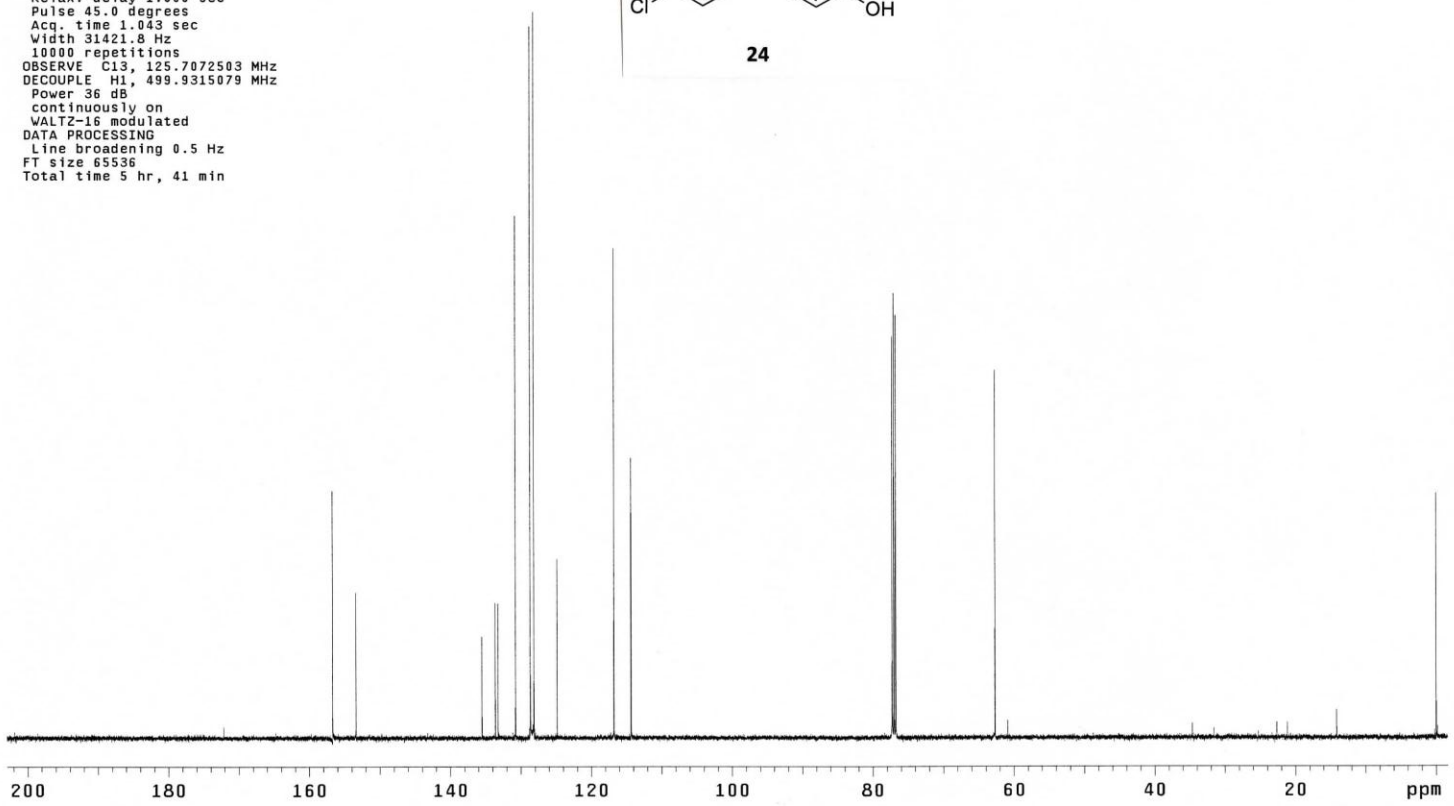
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 1 2011

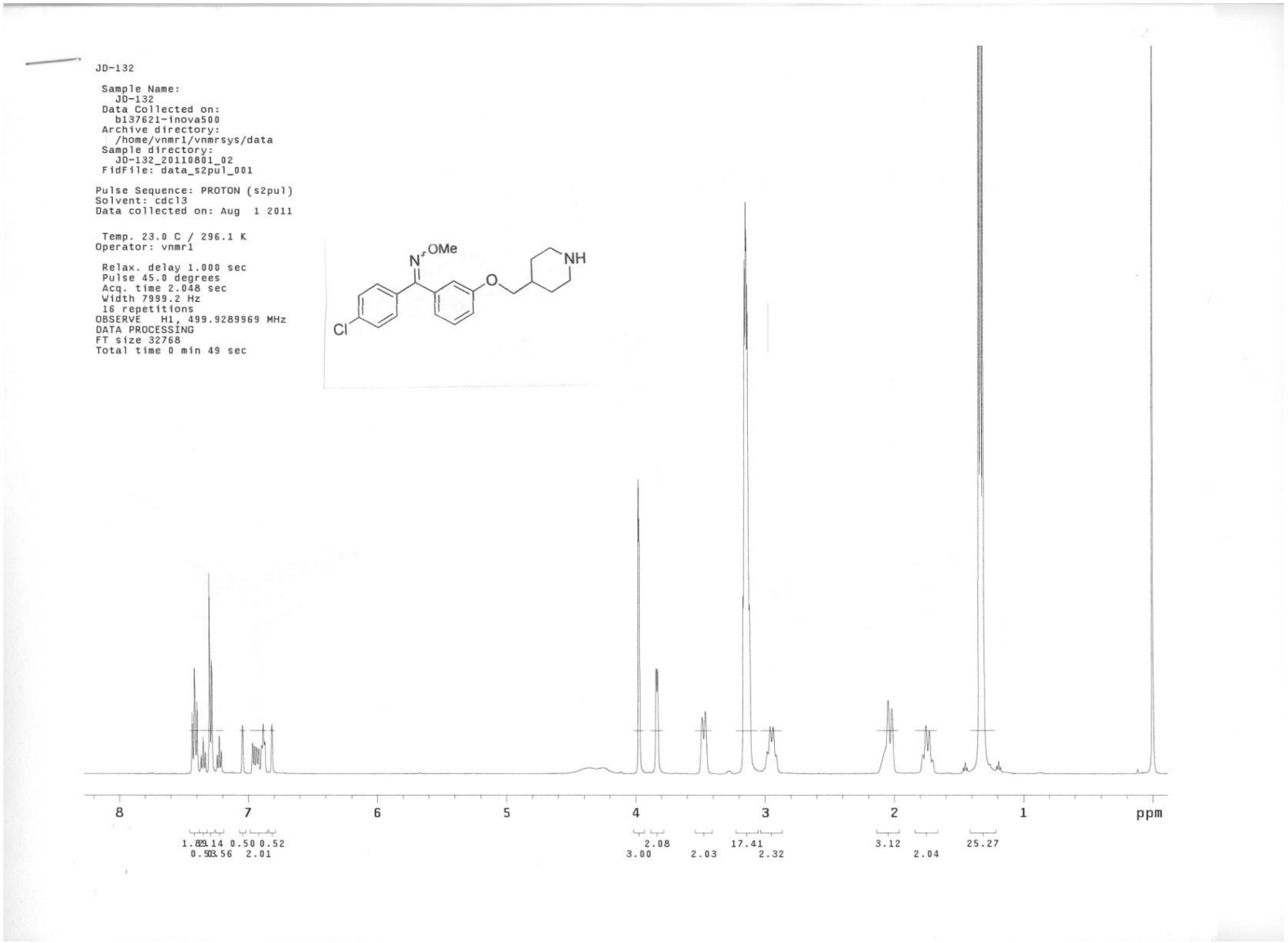
Temp. 23.0 C / 296.1 K
Operator: vnmr1

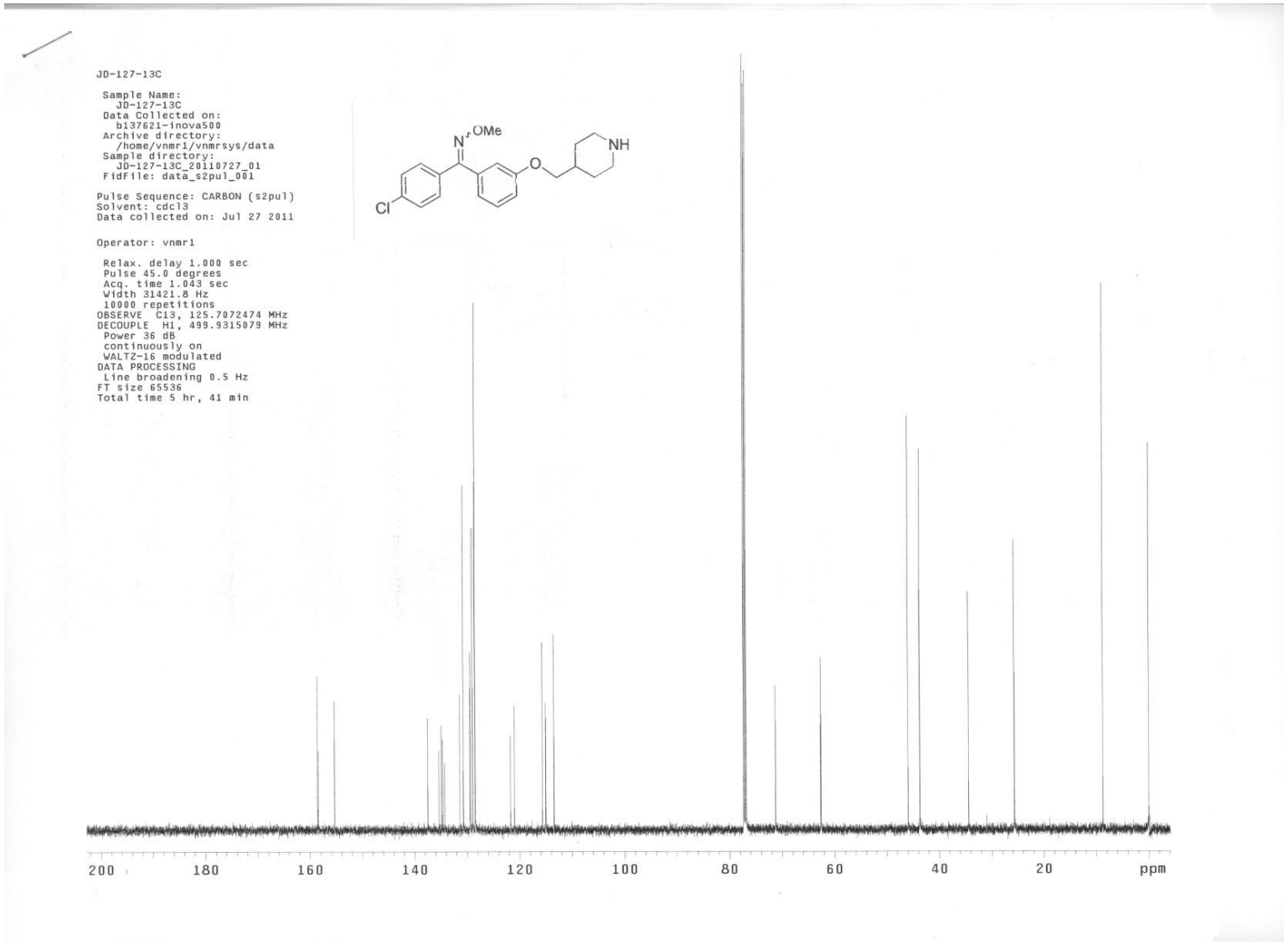
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
10000 repetitions
OBSERVE C13, 125.7072503 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 41 min

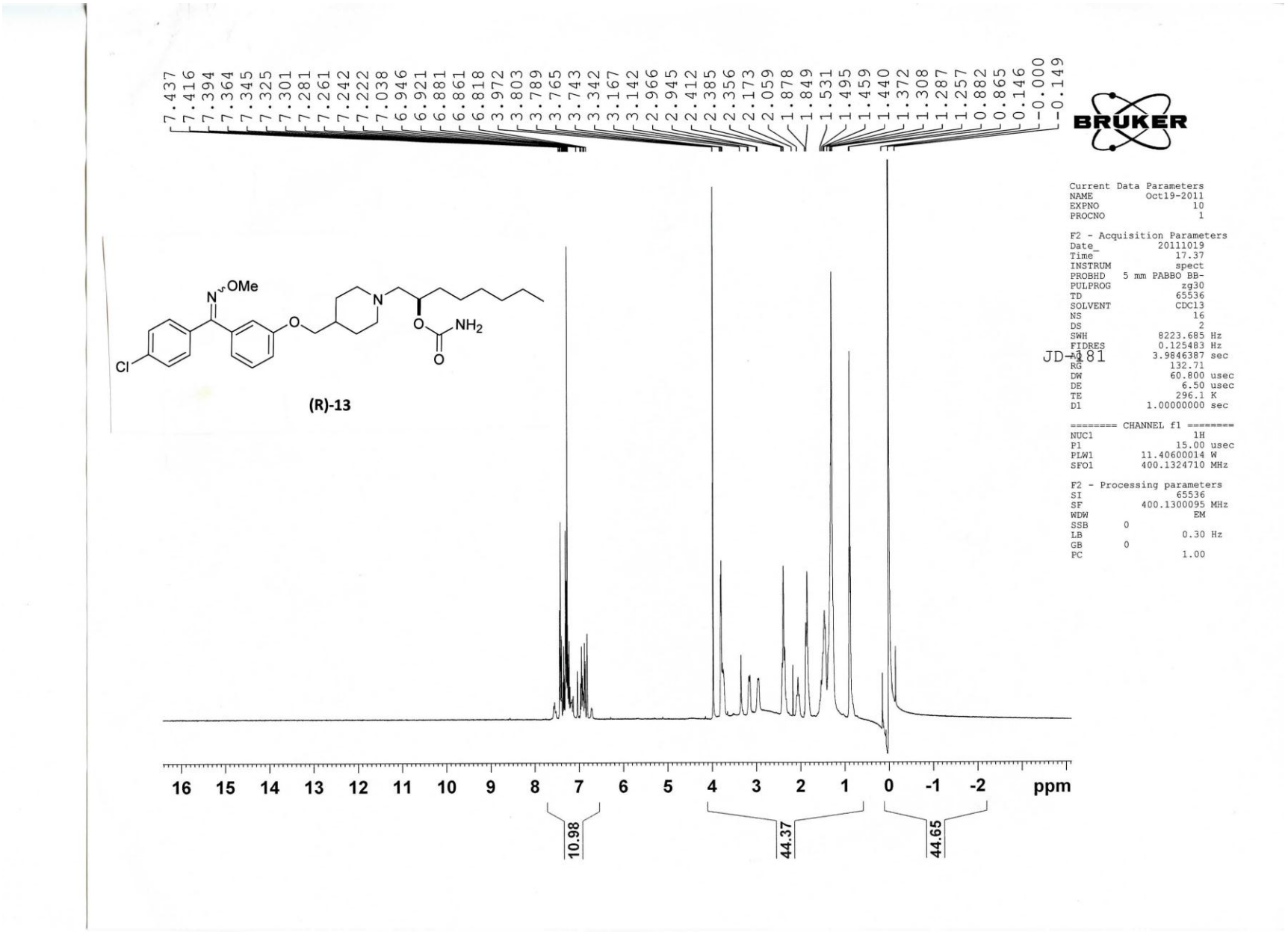


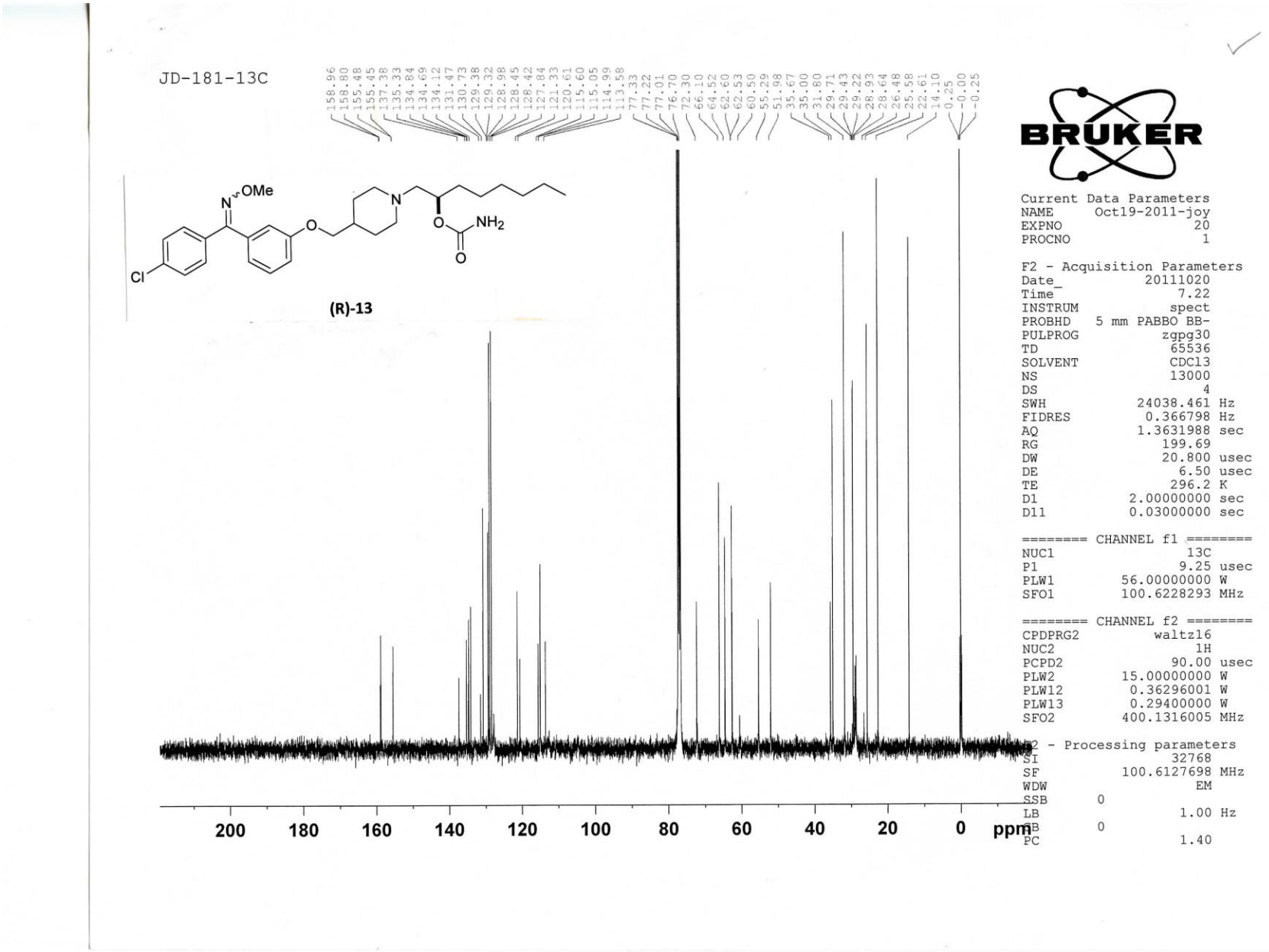
24

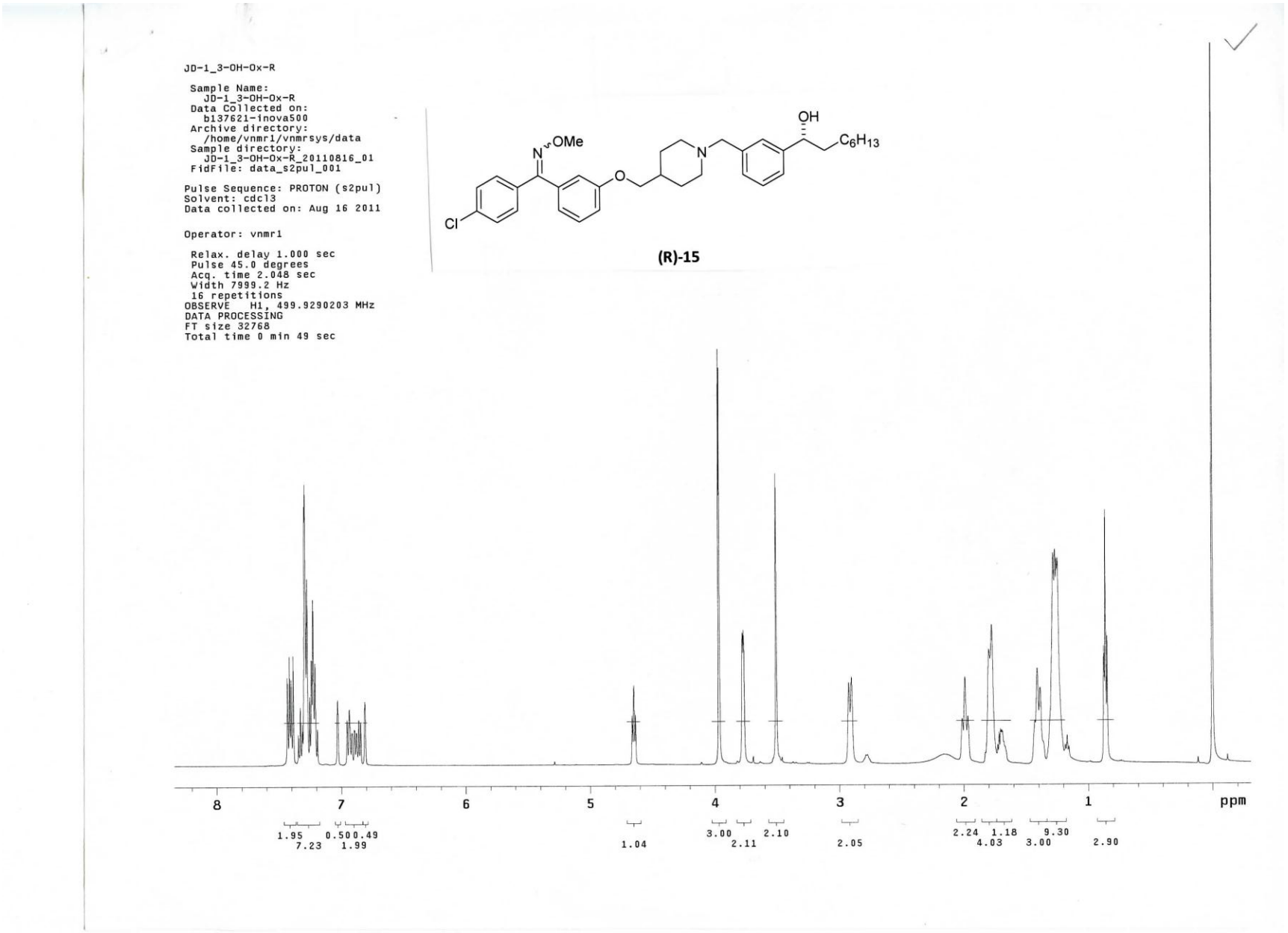


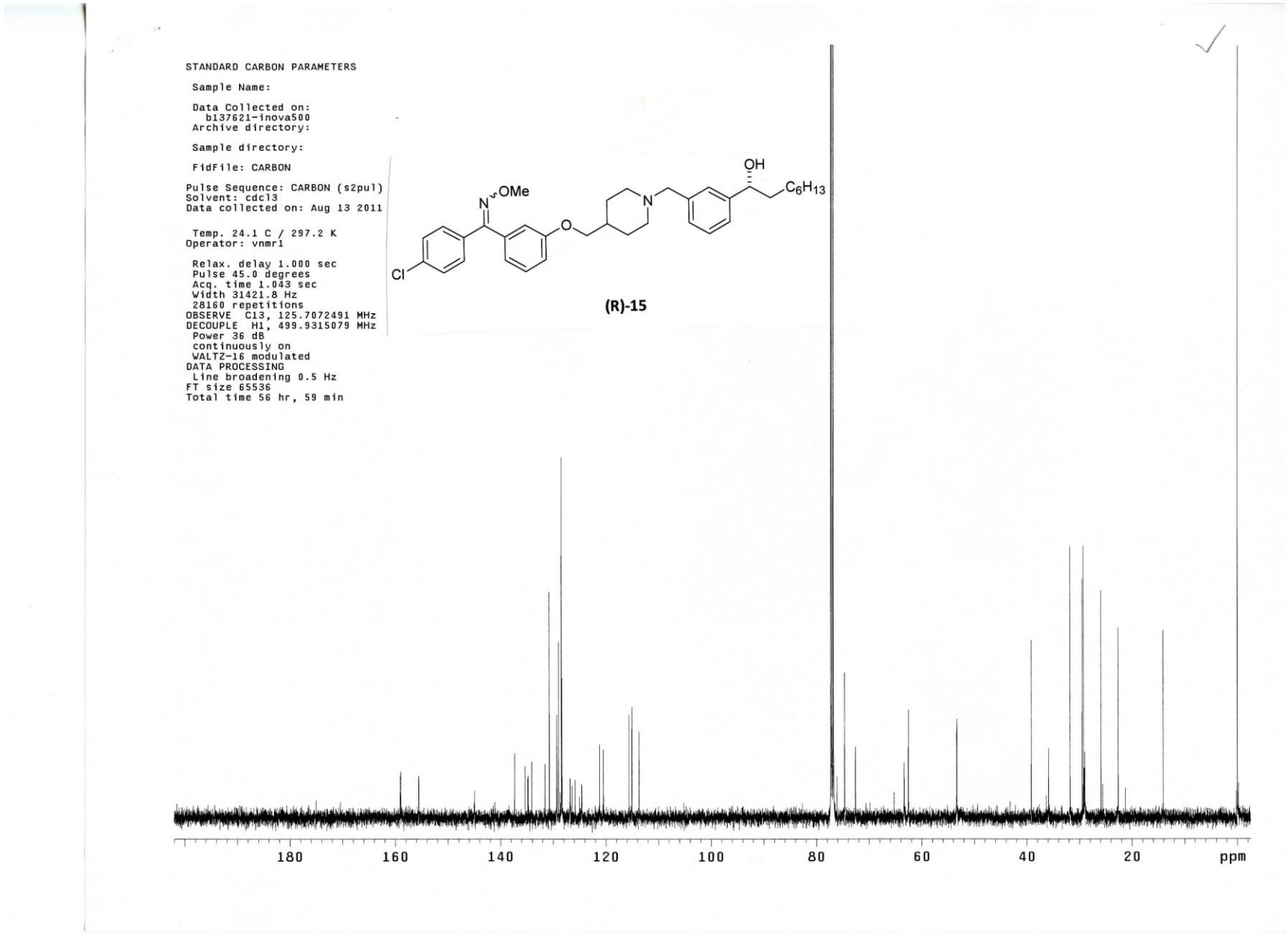

JD-132
Sample Name:
JD-132
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-132_20110801_02
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 1 2011
Temp. 23.0 C / 296.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
16 repetitions
OBSERVE H1, 499.9289969 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec
N
OMe
O
NH
Cl
8
7
6
5
4
3
2
1
ppm
1.84 2.14 0.50 0.52
0.98 3.56 2.01
2.08
3.00
2.03
17.41
2.32
3.12
2.04
25.27


JD-127-13C
Sample Name:
JD-127-13C
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-127-13C_20110727_01
FidFile: data_s2pul_001
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
10000 repetitions
OBSERVE C13, 125.7072474 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 41 min
N
OMe
NH
O
Cl
200
180
160
140
120
100
80
60
40
20
ppm


7.437
7.416
7.394
7.364
7.345
7.325
7.301
7.281
7.261
7.242
7.222
7.038
6.946
6.921
6.881
6.861
6.818
3.972
3.803
3.789
3.765
3.743
3.342
3.167
3.142
2.966
2.945
2.412
2.385
2.356
2.173
2.059
1.878
1.849
1.531
1.495
1.459
1.440
1.372
1.308
1.287
1.257
0.882
0.865
0.146
-0.000
-0.149
BRUKER
Current Data Parameters
NAME Oct19-2011
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111019
Time 17.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 132.71
DW 60.800 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 11.40600014 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
JD-181
OMe
N
O
N
O
NH2
O
Cl
(R)-13
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
10.98
44.37
44.65


JD-181-13C
158.96
158.80
155.48
155.45
137.38
135.33
134.84
134.69
134.12
131.47
130.73
129.38
129.32
128.98
128.45
128.42
127.84
121.33
120.61
115.60
115.05
114.99
113.58
77.33
77.22
77.01
76.70
72.30
66.10
64.52
62.60
62.53
60.50
55.29
51.98
35.67
35.00
31.80
29.71
29.43
29.22
28.93
28.64
26.48
25.58
22.61
14.10
0.25
-0.00
-0.25
N
OMe
O
N
O
NH2
O
Cl
(R)-13
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME Oct19-2011-joy
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111020
Time 7.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 13000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 199.69
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.36296001 W
PLW13 0.29400000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127698 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

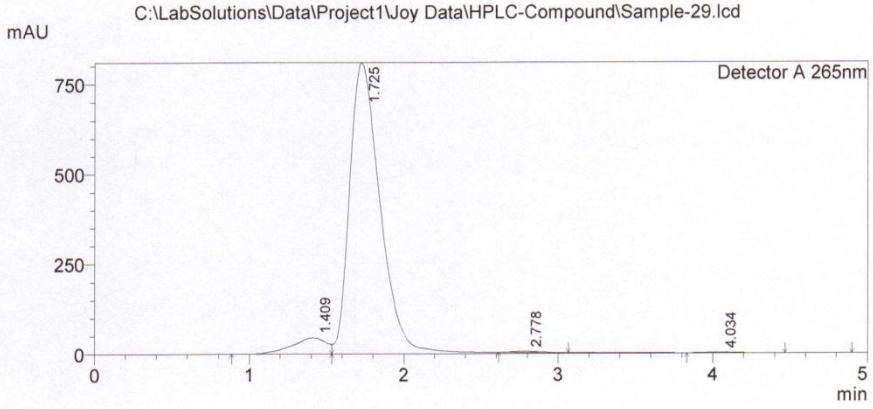

JD-1_3-OH-Ox-R
Sample Name:
JD-1_3-OH-Ox-R
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-1_3-OH-Ox-R_20110816_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 16 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
16 repetitions
OBSERVE H1, 499.9290203 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec
N
OMe
O
N
OH
C6H13
Cl
(R)-15
8
7
6
5
4
3
2
1
ppm
1.95
7.23
0.50
1.99
0.49
1.04
3.00
2.11
2.10
2.05
2.24
4.03
1.18
3.00
9.30
2.90


STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
b137621-inova500
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 13 2011
Temp. 24.1 C / 297.2 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
28160 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 59 min
N
OMe
O
N
OH
C6H13
Cl
(R)-15
180
160
140
120
100
80
60
40
20
ppm

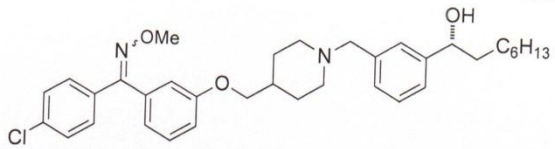
==== Shimadzu LabSolutions Analysis Report ====

C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-29.lcd
Acquired by : System Administrator
Sample Name : JD-07-16-2011
Sample ID :
Tray# : 1
Vial# : 1
Injection Volume : 1
Data File : C:\LabSolutions\Data\Project1\Joy Data\HPLC-Compound\Sample-29.lcd
Method File : C:\LabSolutions\Data\Project1\Joy training\Mixture-235nm-62%ACN.lcm
Report Format File : C:\LabSolutions\System\DEFAULT.lsr
Month-Day Acquired : 10/5/2011
Month-Day Processed : 10/5/2011

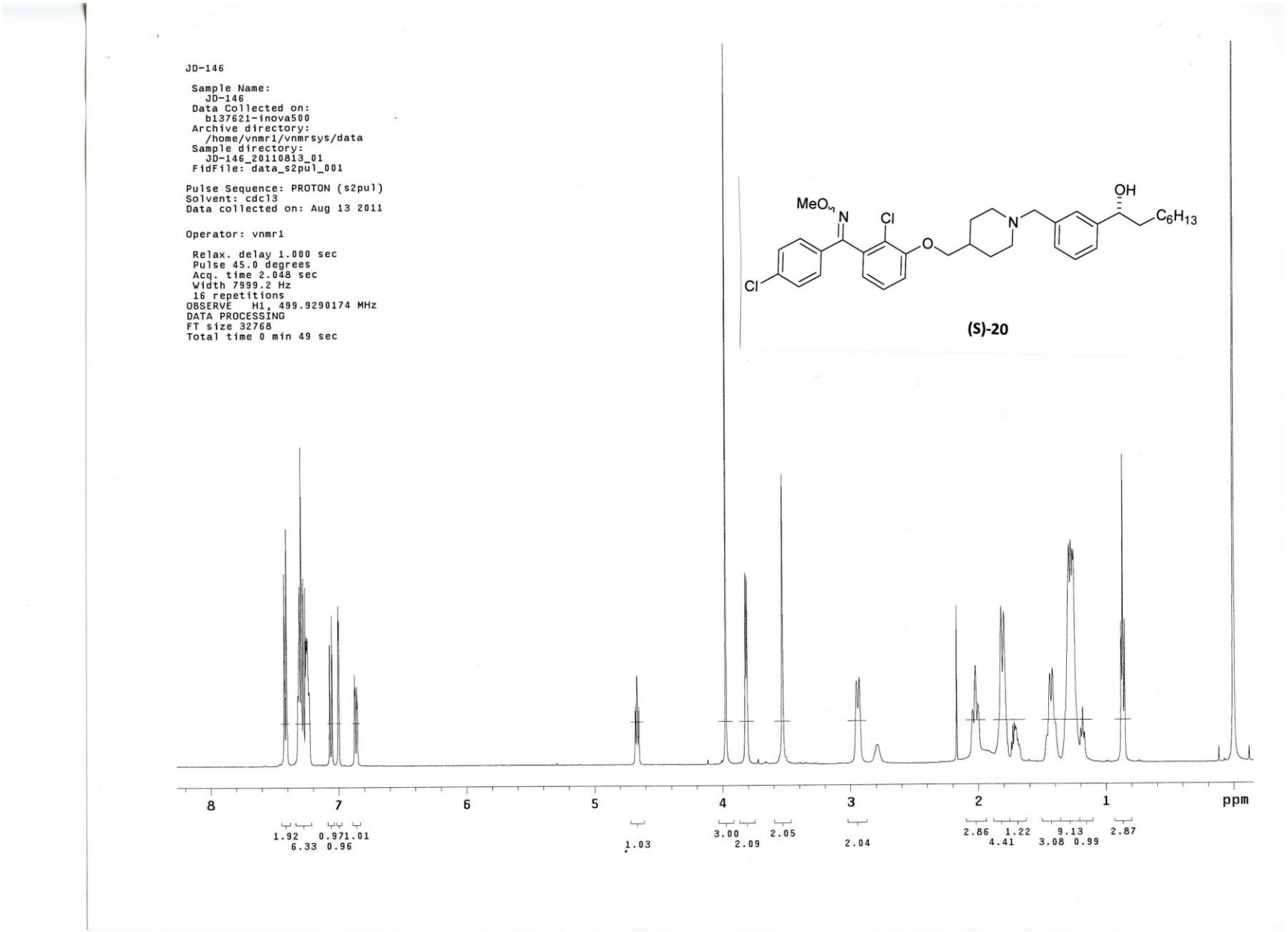
<Chromatogram>



MS Chromatogram



Column: Phenominex kinetex 2.6μ C18 100A, 100 x 4.60 mm
Solvent: CH_3CN/0.05%TFA in H_2O = 25/1
flow rate: 0.5 mL/min.


JD-146
Sample Name:
JD-146
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-146_20110813_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 13 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
16 repetitions
OBSERVE H1, 499.9290174 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec
MeO
N
Cl
O
N
OH
C6H13
Cl
(S)-20
8
7
6
5
4
3
2
1
ppm
1.92
6.33
0.971.01
0.96
1.03
3.00
2.09
2.05
2.04
2.86
4.41
1.22
9.13
3.08
0.99
2.87

STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
b137621-inova500
Archive directory:

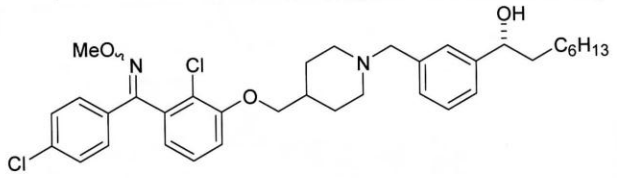
Sample directory:

FidFile: CARBON

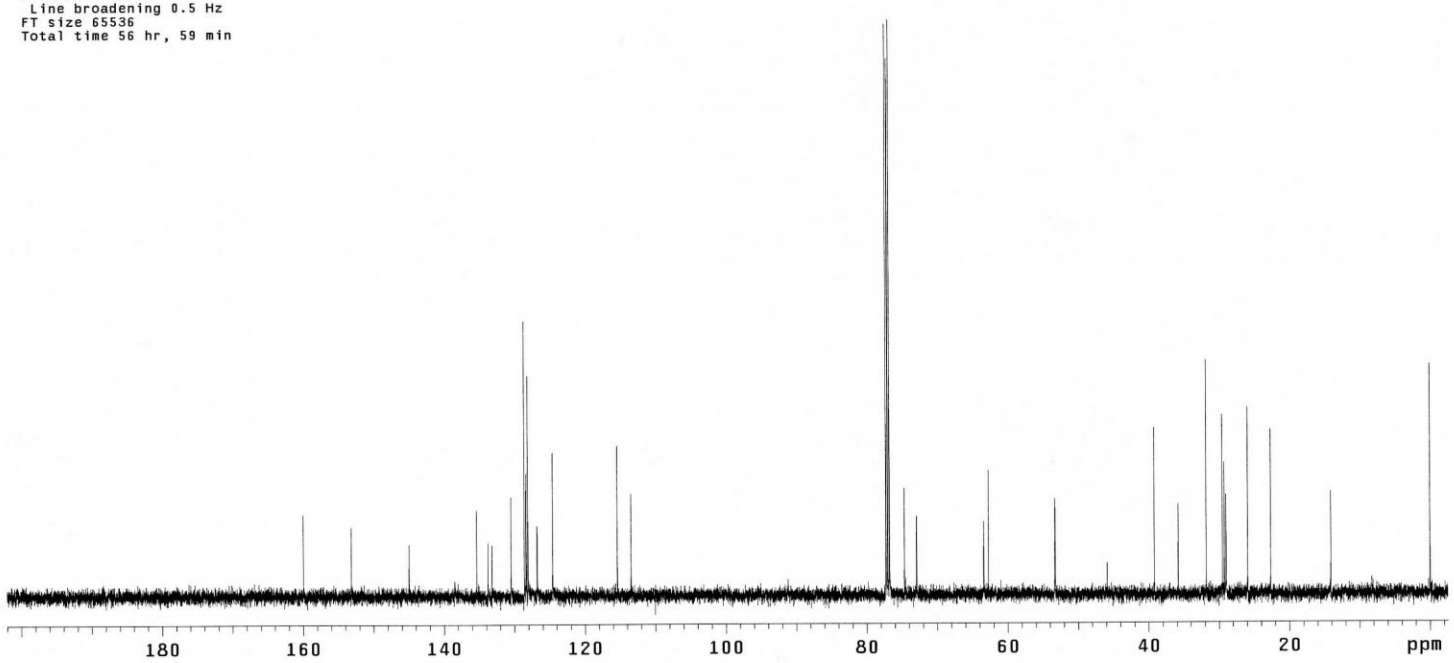
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 13 2011

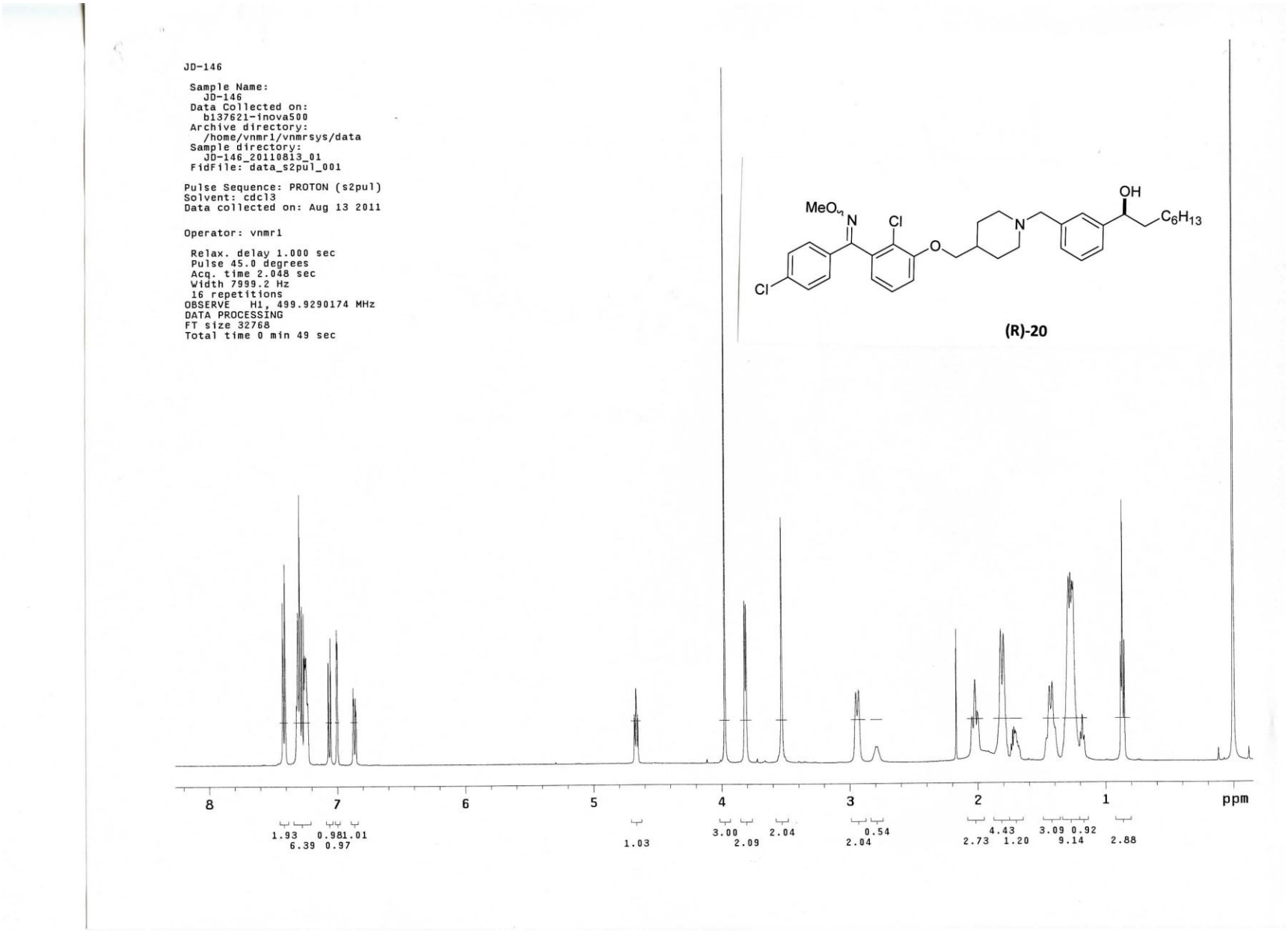
Temp. 24.3 C / 297.4 K
Operator: vnmr1

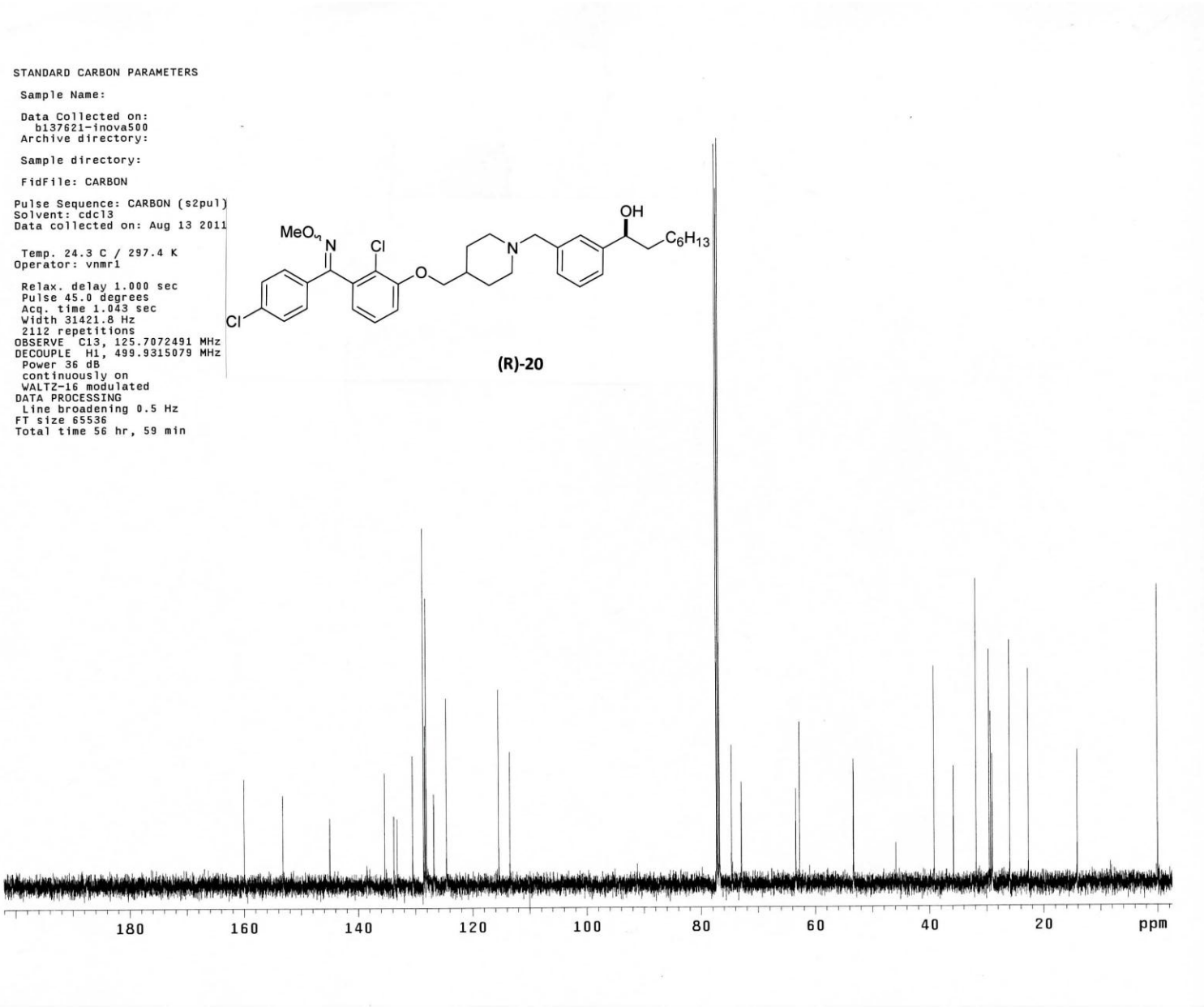
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
2048 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 59 min



(S)-20




JD-146
Sample Name:
JD-146
Data Collected on:
b137621-inova500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
JD-146_20110813_01
FidFile: data_s2pul_001
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 13 2011
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 7999.2 Hz
16 repetitions
OBSERVE H1, 499.9290174 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec
MeO
N
Cl
O
N
OH
C6H13
Cl
(R)-20
8
7
6
5
4
3
2
1
ppm
1.93
6.39
0.98
0.97
1.01
1.03
3.00
2.09
2.04
2.04
0.54
2.73
4.43
1.20
3.09
9.14
0.92
2.88


STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
b137621-inova500
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 13 2011
Temp. 24.3 C / 297.4 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31421.8 Hz
2112 repetitions
OBSERVE C13, 125.7072491 MHz
DECOUPLE H1, 499.9315079 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 59 min
MeO
N
Cl
O
N
OH
C6H13
Cl
(R)-20
180
160
140
120
100
80
60
40
20
ppm