

**Enantioselective Synthesis of Cocaine C-1 Analogs using Sulfinimines (*N*-Sulfinyl
Imines)**

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Supporting Information Available – Part 2

Contents:

NMR spectra for:

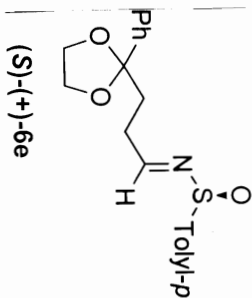
Compound	Page ¹ H	Page ¹³ C	Compound	Page ¹ H	Page ¹³ C
(<i>S</i>)-(+)- 6e	S-27	S-28	(<i>S</i> ,3 <i>S</i>)-(+)- 12c	S-39	S-40
(<i>S</i>)-(+)- 7a	S-29	S-30	(<i>S</i> ,3 <i>S</i>)-(+)- 12e	S-41	S-42
(<i>S</i>)-(+)- 7b	S-31	S-32	(<i>S</i> ,3 <i>S</i>)-(+)- 13a	S-43	S-44
(<i>S</i>)-(+)- 7d	S-33	S-34	(<i>S</i> ,3 <i>S</i>)-(+)- 12b	S-45	S-46
(<i>S</i>)-(+)- 7e	S-35	S-36	(<i>S</i> ,3 <i>S</i>)-(+)- 13d	S-47	S-48
(<i>S</i> ,3 <i>S</i>)-(+)- 12a	S-37	S-38	(<i>S</i> ,3 <i>S</i>)-(+)- 13e	S-49	S-50

8.192
8.180
8.169

7.495
7.475
7.364
7.360
7.344
7.340
7.281
7.277
7.266
7.260
7.256
7.245
7.241
7.234
7.230
7.216
7.210
7.195

3.883
3.880
3.843
3.841
3.836
3.675
3.663
3.659
3.655
3.649

2.556
2.545
2.538
2.526
2.519
2.508
2.325
2.178
2.160
2.154
2.142
2.136
2.117



22-5

9 8 7 6 5 4 3 2 PPM

1.00

2.032.03

5.45

2.032.07

2.00 2.08

3.02

TN-II-264A, proton, atm.

F1: 400.130 F2: 1.000

EX: SW1: 8013 PW: 9.8 usec

PD: 1.0 sec

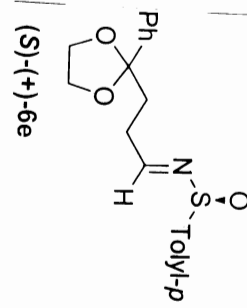
OF1: 1979.0 NA: 16

LB: 0.1

USER: temple -- DATE: Feb 2 00:01:59 2009 EST (UT-5h) templ

PTSId: 32768

WinNuts - \$naresh.1



S-28



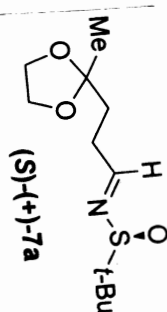
167.106
142.070
141.535
129.687
128.185
128.031
125.582
124.579
109.529
77.322
77.000
76.685
64.545
64.491
35.907
30.566
21.374

TN-II-264A, carbonOVNTE.all,
 F1: 100.613 F2: 1.000
 EX: SW1: 25126 PW: 5.7 usec PD: 2.0 sec OF1: 10021.5 NA: 6000 LB: 3.0
 USER: temple -- DATE: Feb 2 05:38:03 2009 EST (UT-5h) temp
 PTSId: 32768
 WinNuts - \$naresh.1

S-29

8.105
8.094
8.084

7.260



3.968
3.960
3.956
3.951
3.944
3.941
3.939
3.937
3.930
3.925

2.632
2.625
2.614
2.605
2.596
2.594
2.029
2.018
2.014
2.009
1.998
1.995
1.991
1.978
1.621
1.343
1.184

8.97

4.02

2.00

3.02

0.97

1.97

PPM

USER: temple -- DATE: Mar 16 05:06:09 1970 EST (UT-5h) templ

Varma-313-2-CH3 sulfimine (tBu)-column-pure, proton.atm.

F1: 400.130

F2: 1.000

SW1: 8013

OF1: 2004.3

PTSId: 32768

EX: PW: 9.8 usec

PD: 1.0 sec

NA: 16

LB: 0.1

WinNuts - \$NMR2.1

169.141

109.039

77.323

77.000

76.688

64.642

64.569

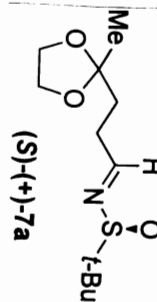
56.346

34.409

30.716

23.880

22.168



S - 30

160

140

120

100

80

60

40

20 PPM

Varma-313-3-CH3 sulfonamide (tBu)-column-pure, carbonOVNTE.all,

F1: 100.613

F2: 1.000

SW1: 25126

OF1: 10014.9

PTSID: 32768

USER: temple -- DATE: Mar 16 14:36:05 1970 EST (UT-5h) templ

EX:

PW: 5.7 usec

PD: 2.0 sec

NA: 10000

LB: 3.0

WinNuts - \$NMR2.1

8.099
8.088
8.077

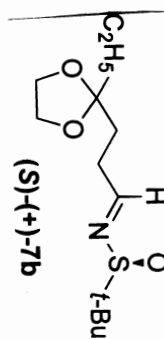
7.260
7.258

3.950
3.949
3.942

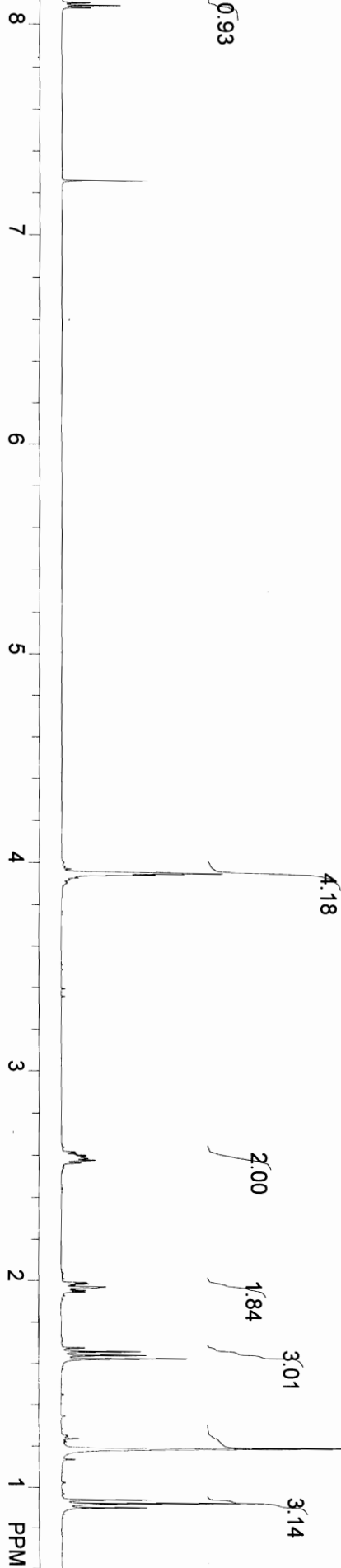
2.586
2.585
2.578

1.989
1.983
1.968
1.965
1.657
1.638
1.622

1.185
0.936
0.917
0.898

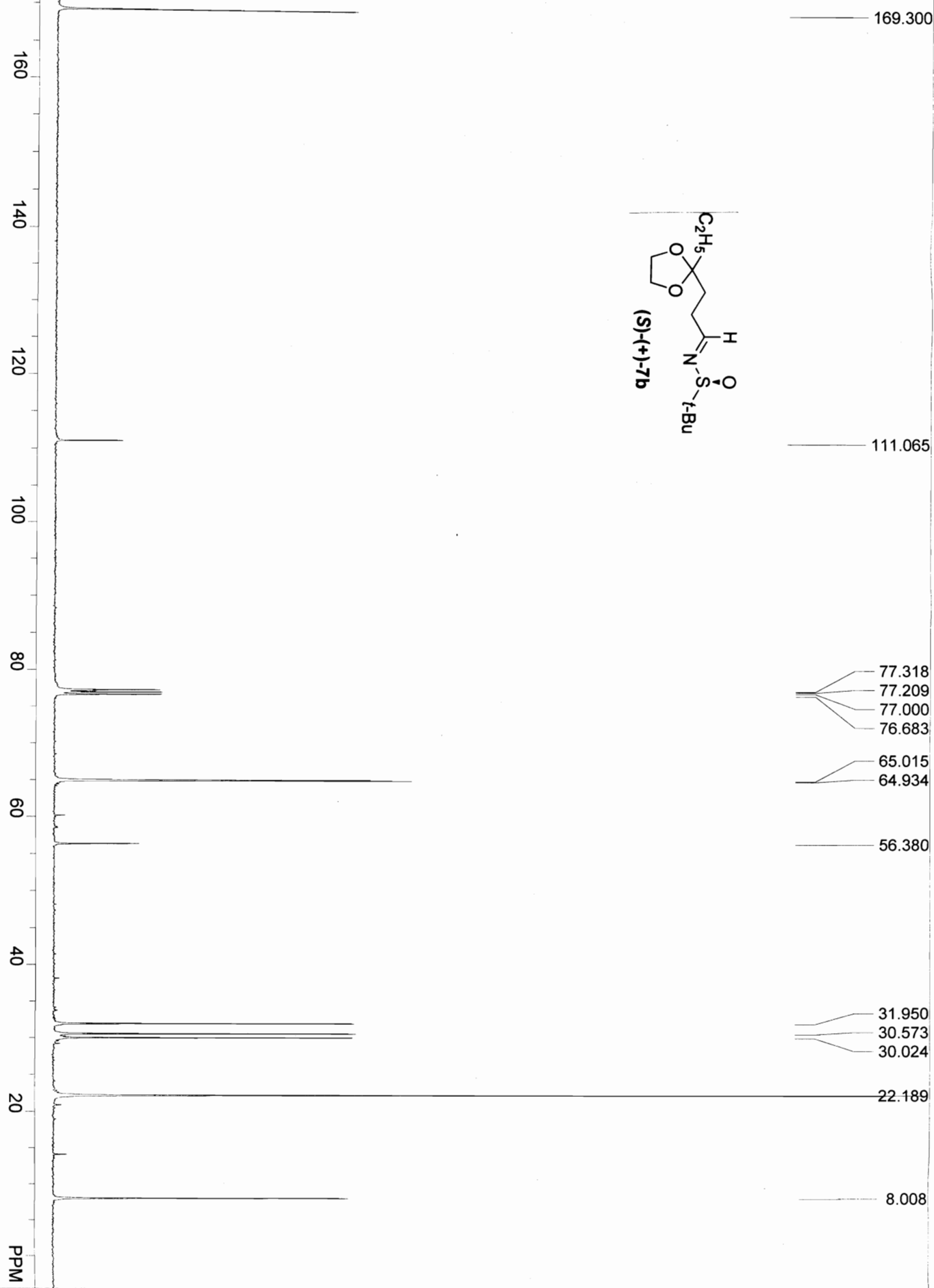
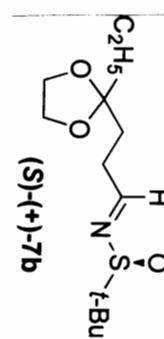


12-31



Varmu-253-2-column-re check, proton, atm, F1: 400.130 F2: 1.000 SW1: 8013 OF1: 2004.2 LB: 0.1 USER: temple -- DATE: Nov 15 09:51:17 2010 EST (UT-5h) templ
EX: PD: 1.0 sec NA: 16 PTSId: 32768 WinNuts - \$NMRL.1

5-32



Varma-253-1-column-pure, carbon1HR.atm, USER: temple -- DATE: Nov 13 15:17:44 2010 EST (UT-5h) templ

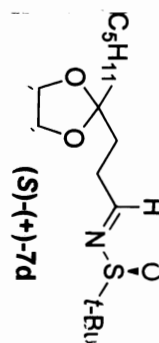
F1: 100.613 F2: 1.000 SW1: 25126 OF1: 10016.3 LB: 3.0 PTSId: 32768

EX: PW: 5.7 usec PD: 2.0 sec NA: 2050

WinNuis - \$NMR1.1

8.098
8.087
8.076

7.260



3.947
3.940
3.938
3.935

2.577
1.989
1.983
1.968
1.625
1.608
1.594
1.585
1.319
1.302
1.293
1.289
1.283
1.275
1.187
0.902
0.885
0.867

S-23

1.00

4.03

2.03

2.02

2.27

6.22

8.98

3.05

8

7

6

5

4

3

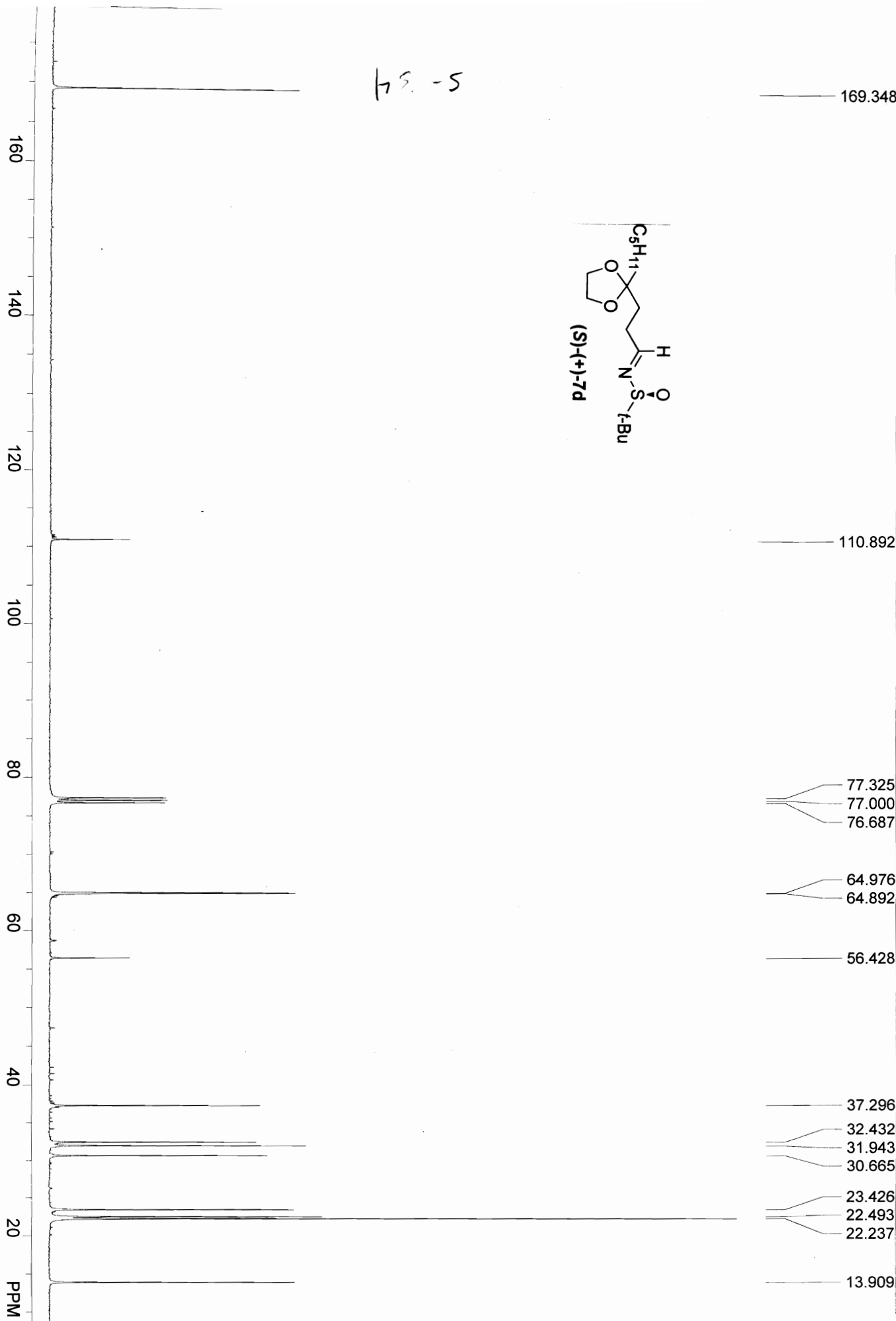
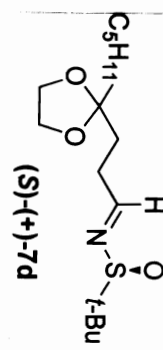
2

1

0 PPM

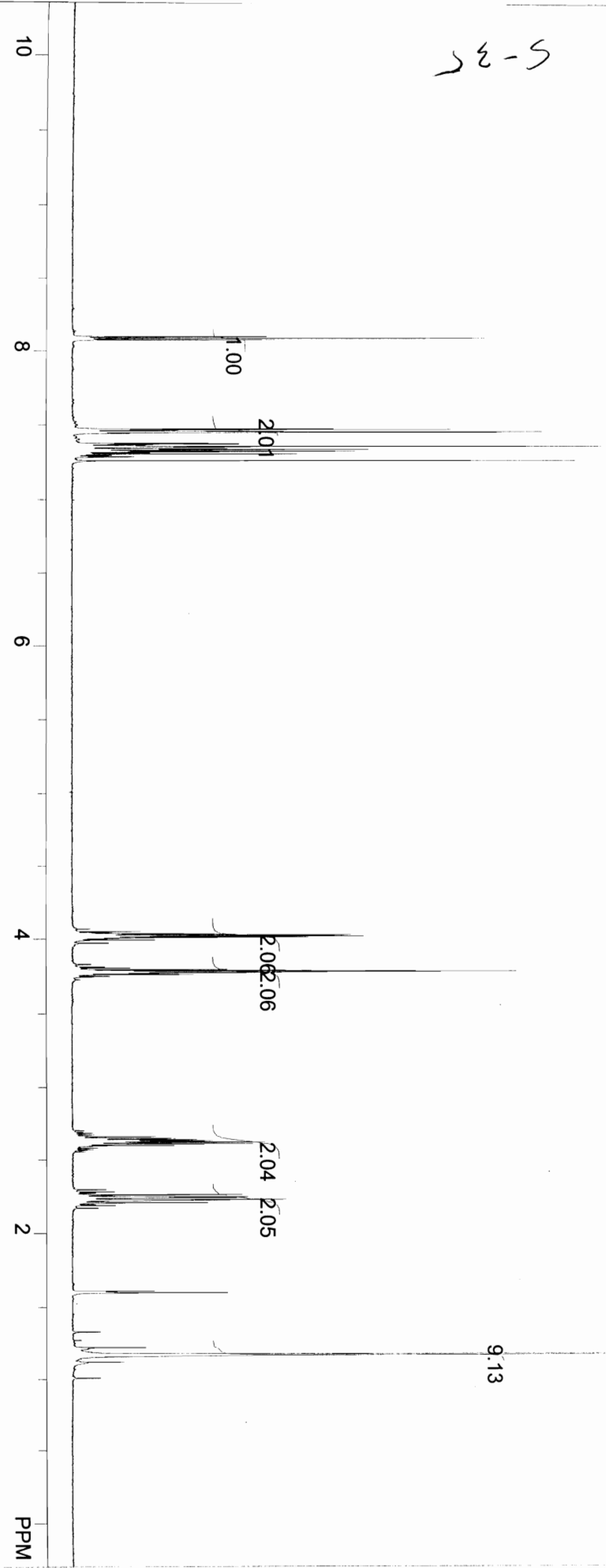
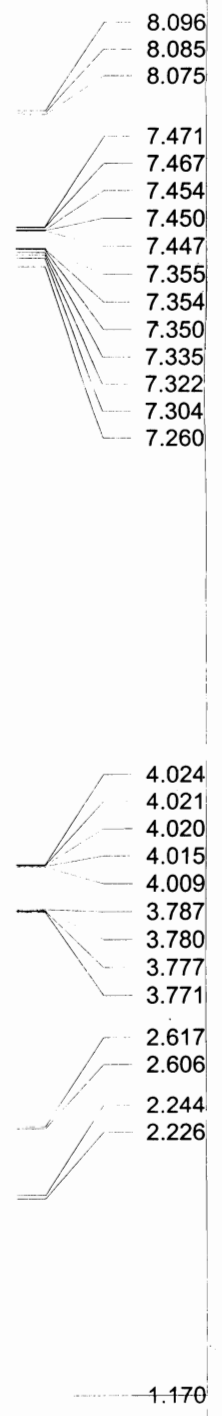
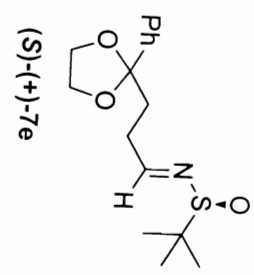
Varmas-247-3-column-pure-re check, proton, atm, USER: temple -- DATE: Nov 16 11:14:26 2010 EST (UT-5h) templ
F1: 400.130 F2: 1.000 SW1: 8013 OF1: 2004.3 PTS1d: 32768
EX: PW: 9.8 usec PD: 1.0 sec NA: 16 LB: 0.1
WinNuts - \$NMR1.1

HS-5



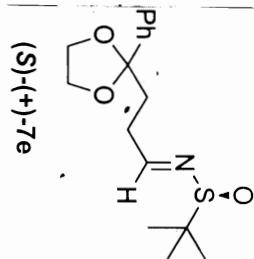
Varma-247-1-column-pure., carbon 1HR.atm,
F1: 100.613 F2: 1.000 SW1: 25126 OF1: 10018.6
EX: PW: 5.7 usec PD: 2.0 sec NA: 2050 LB: 3.0
USER: temple -- DATE: Oct 13 11:01:28 2010 EDT (UT-4h) templ
PTSId: 32768
WinNuts - \$NMRI.1

5-25

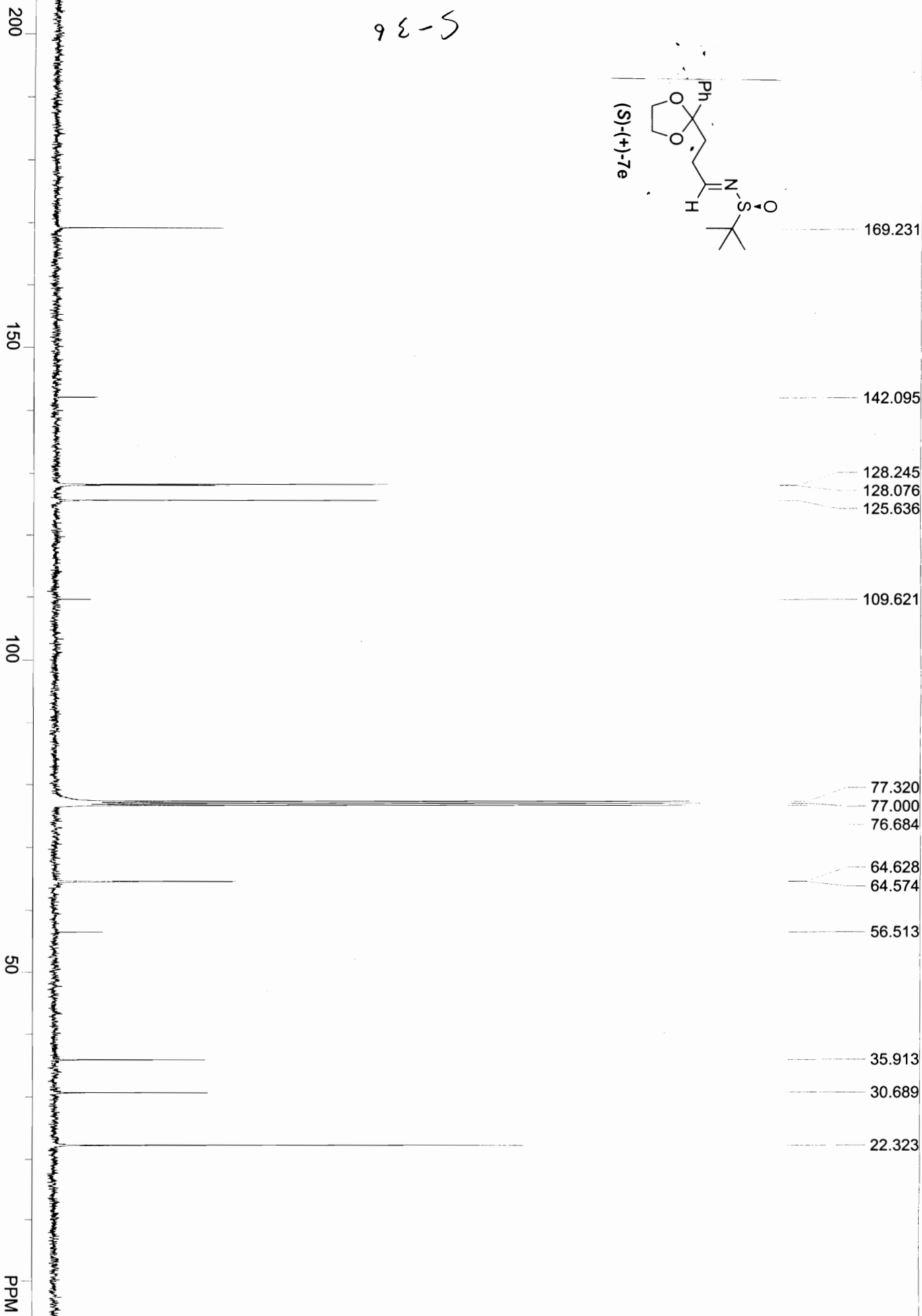


TN-IV-38, proton, atm, F1: 400.130 F2: 1.000 SW1: 8013 PW: 9.8 usec PD: 1.0 sec OF1: 2004.2 NA: 16 LB: 0.1

USER: temple -- DATE: Dec 12 15:40:52 2010 EST (UT-5h) templ PTSId: 32768 WiniNuis - \$naresh_NMR.1

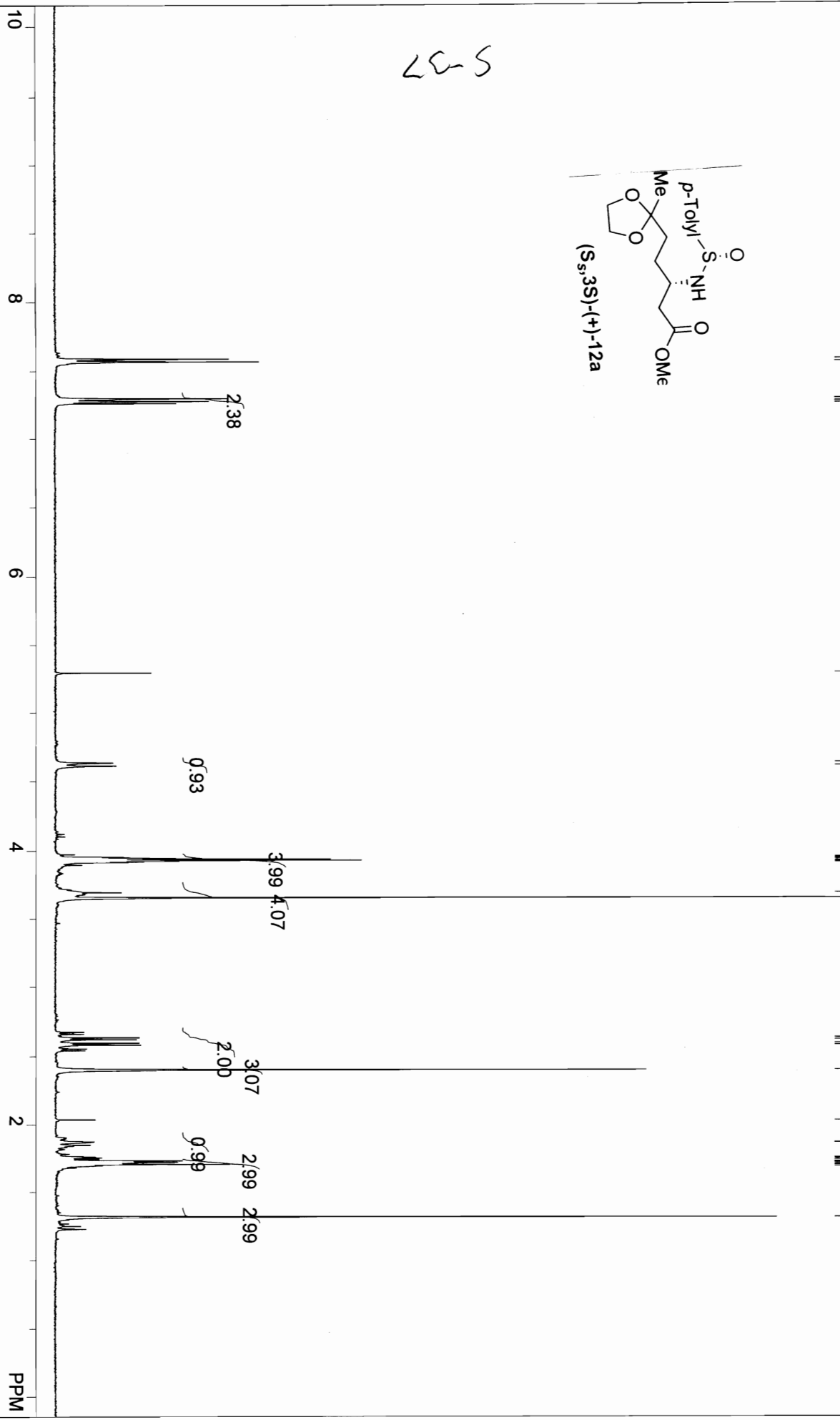
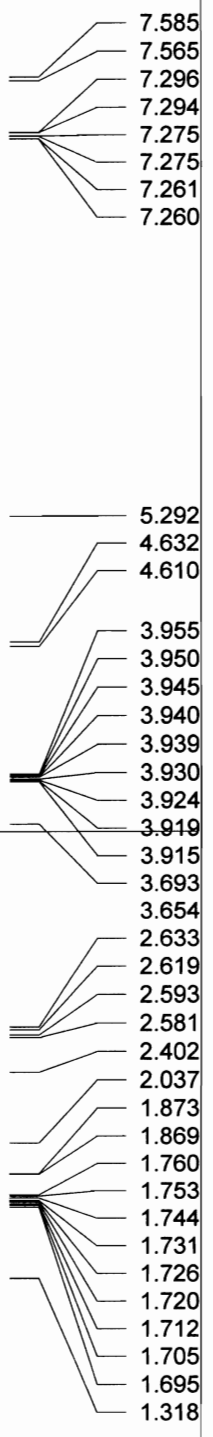
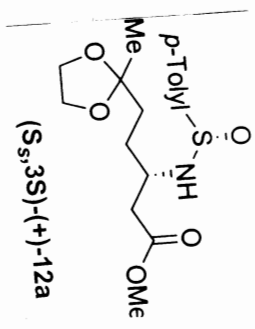


98-5



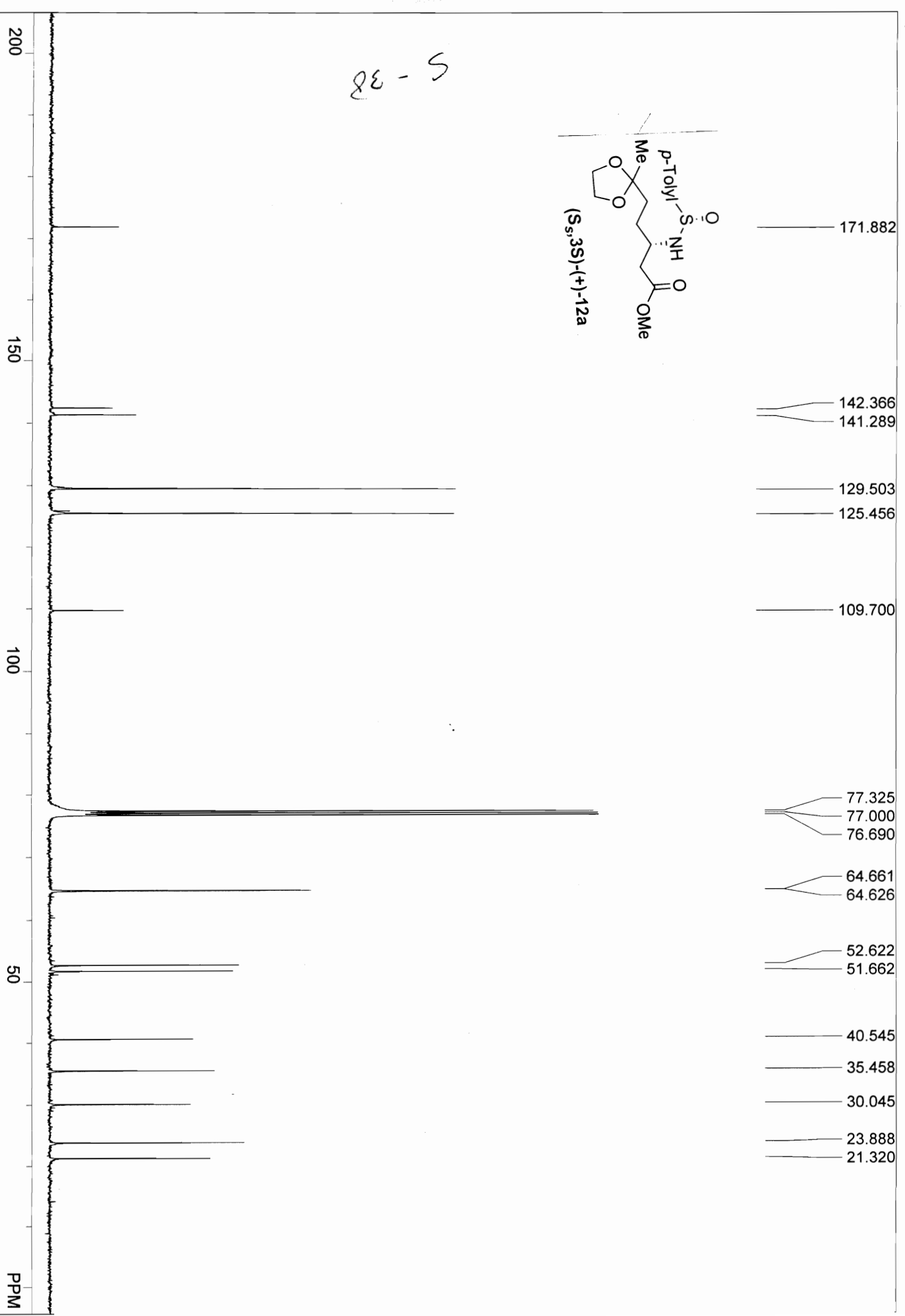
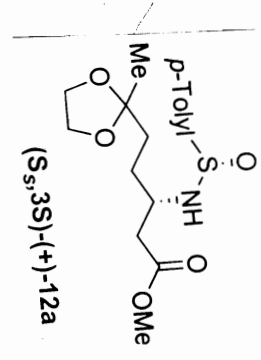
TN-IV-38, carbonOVNTE.all
 F1: 100.613 F2: 1.000 SW1: 25126 PD: 2.0 sec OF1: 10023.8 NA: 2500 LB: 3.0
 EX: USER: temple -- DATE: Dec 12 18:00:29 2010 EST (UT-5h) templ
 PTSId: 32768 W/mNuts - \$naresh_NMR.1

25-5



TN-II-153, proton, atm
F1: 400.130 F2: 1.000 SW1: 8013
EX: PW: 9.8 usec PD: 1.0 sec OF1: 2004.7
NA: 16 LB: 0.1
USER: temple -- DATE: Sep 11 16:47:41 2008 EDT (UT-4h) templ
PTSId: 32768
WinNuts - \$naresh_NMR.1

S - 38



TN-II-153, carbonOVNTE.all
F1: 100.613 F2: 1.000 SW1: 25126 PW: 5.7 usec PD: 2.0 sec OF1: 10022.6 NA: 8000 LB: 3.0
EX: USER: temple -- DATE: Sep 12 04:54:51 2008 EDT (UT-4h) templ
PTSId: 32768
WinNuts - \$naresh_NMR.1

(TN-11-153)

7.585
7.581
7.569
7.565
7.295
7.294
7.274
7.260

4.624
4.602

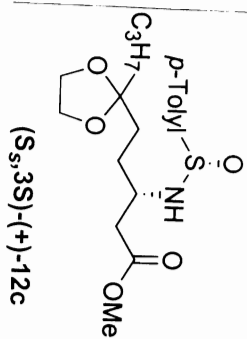
3.928

3.655

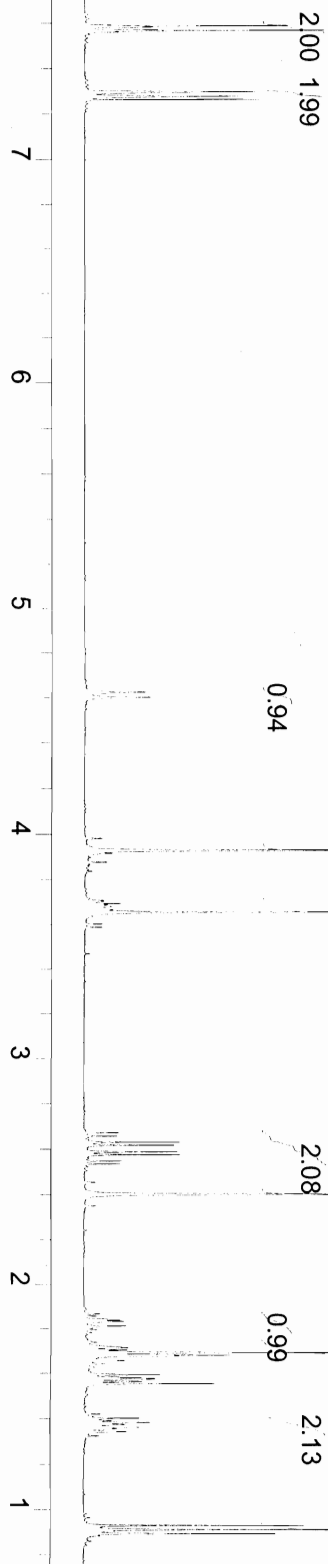
2.631
2.616
2.588
2.575
2.402

1.838
1.833
1.813
1.714
1.704
1.693
1.682
1.677
1.657

1.595
1.582
1.577
1.573
1.564
1.554
1.401
1.382
1.374
1.362
1.342
0.930
0.912
0.894



S-39

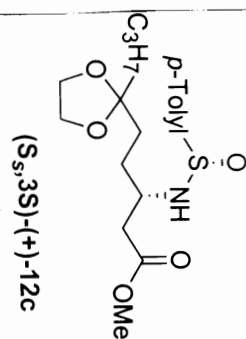
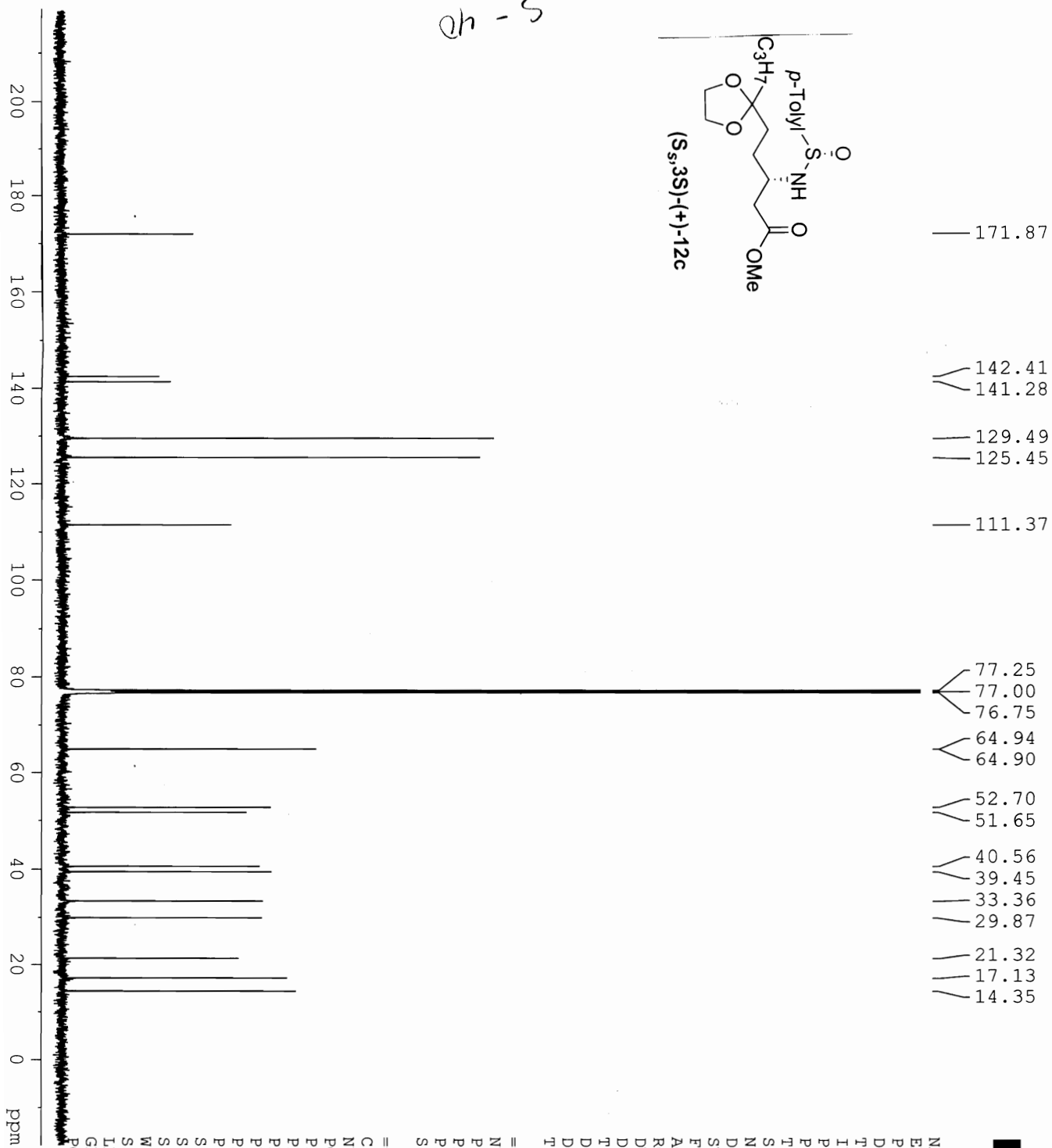


TN-III-228, proton, atm.
 F1: 400.130 F2: 1.000 SW1: 8013 PD: 1.0 sec NA: 16 LB: 0.1
 EX: USER: temple -- DATE: Apr 15 18:42:00 2010 EDT (UT-4h) templ
 PTSId: 32768 WinNuis - \$naresh_NMR.1

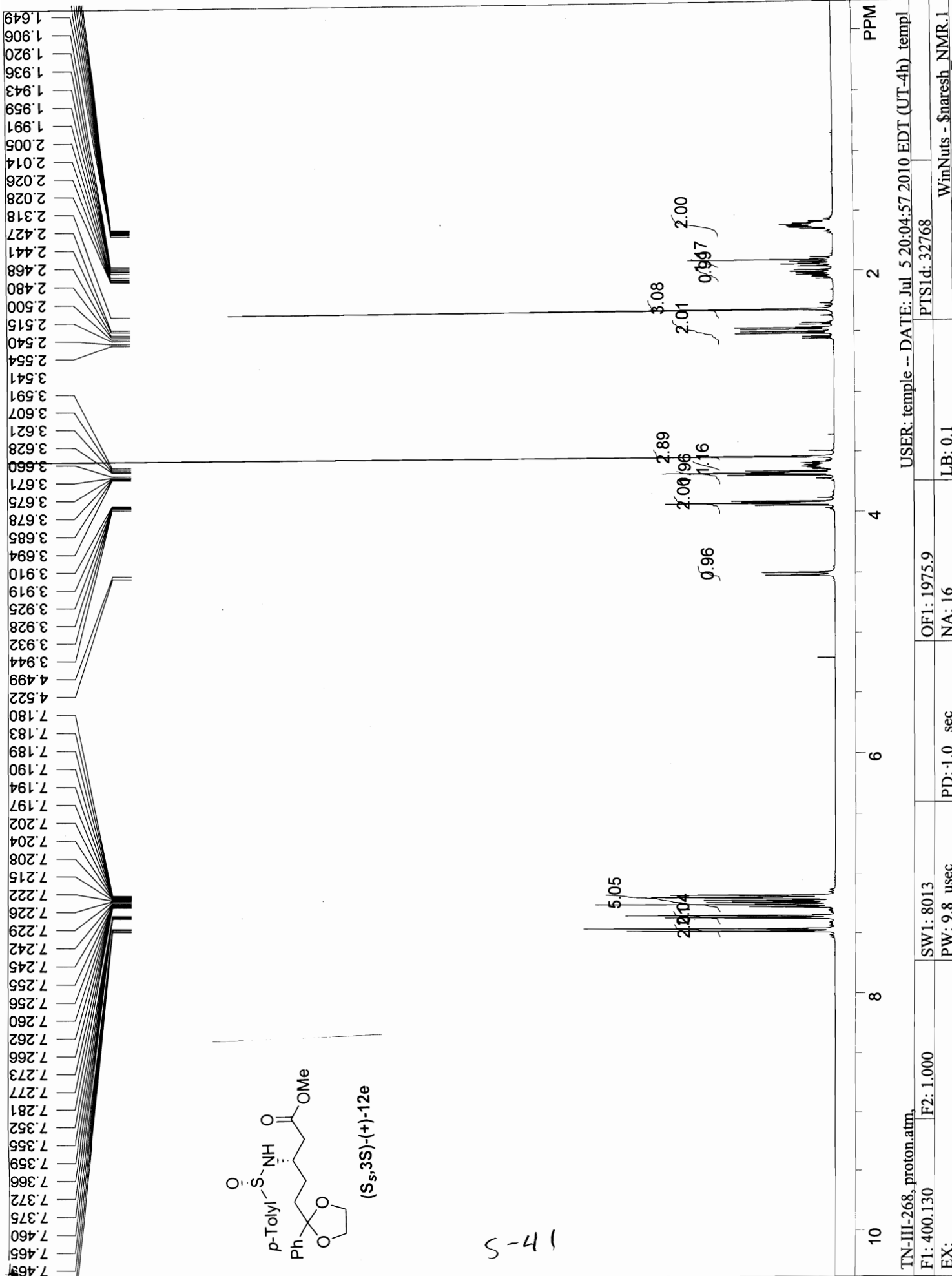
PROCNO	1
Date_	20100415
Time_	18.58
INSTRUM	5 mm PABBO BB-
PROBHD	spect
PULPROG	zgpg30
TD	65536
TD	CDC13
NS	1121
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
Rg	1150
DW	16.800 usec
DE	6.50 usec
TE	293.7 K
D1	2.0000000 sec
D11	0.0300000 sec
TD0	1

	CHANNEL f1
NUC1	13C
P1	9.00 usec
PL1	0.50 dB
PLW	85.96688843 W
SFO1	125.7703643 MHz

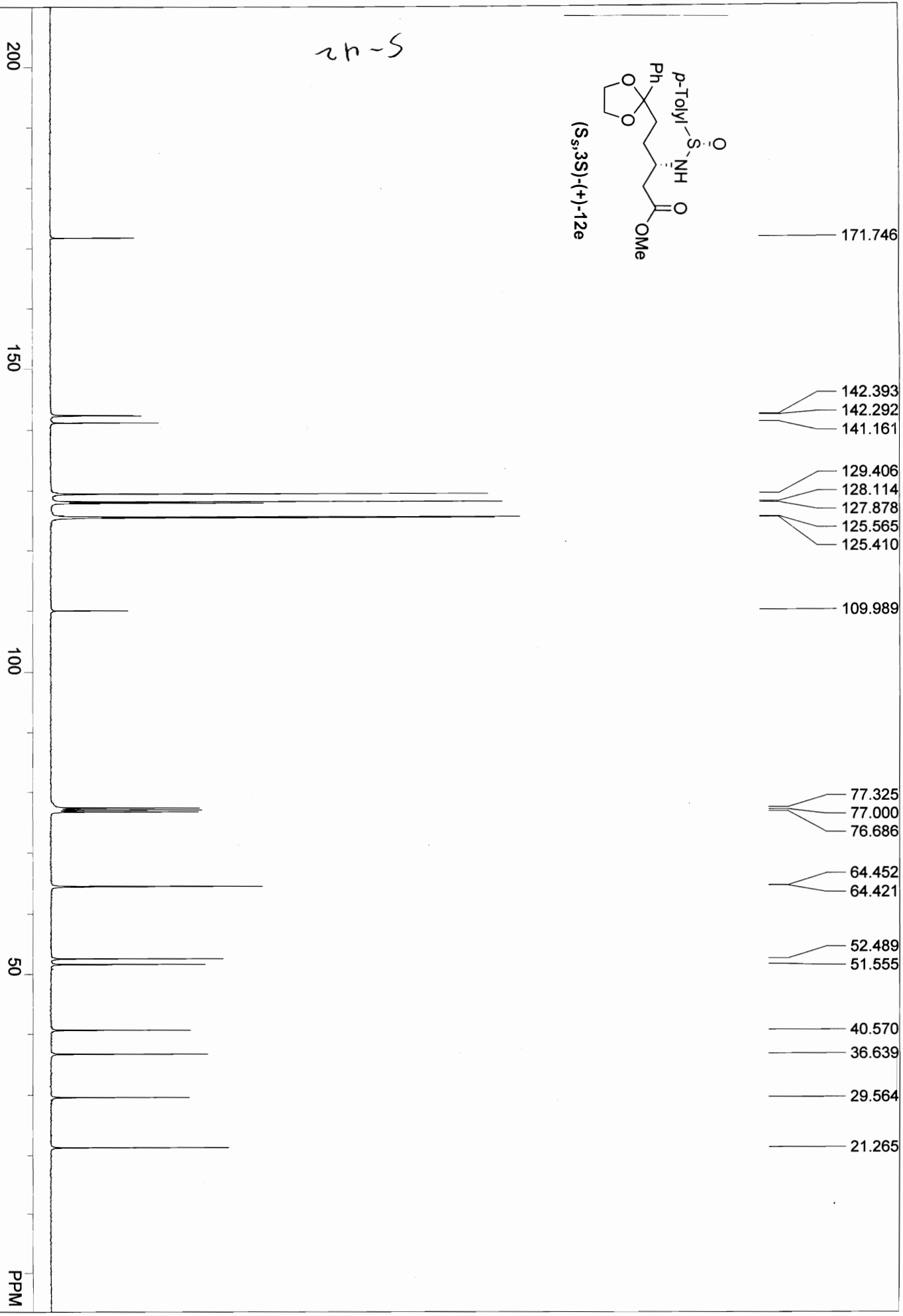
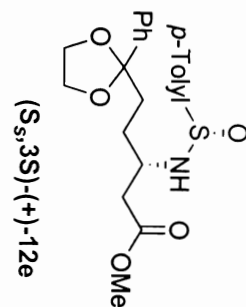
```
===== CHANNEL f2 =====
CPDPRG2          waltz16
NUC2             1H
PCPD2            80.00 usec
PL2              2.00 dB
PL12             18.68 dB
PL13             18.68 dB
PL1W             18.54325104 W
PL12W            0.39827755 W
PL13W            0.39827755 W
SFO2             500.1320005 MHz
SI               32768
SF              125.7377915 MHz
WDW             EM
SSB              0
LB              2.50 Hz
GB              0
PC              1.40
```



oh - 5

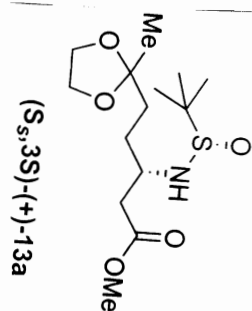


TN-III-268, proton.atm, USER: temple -- DATE: Jul 5 20:04:57 2010 EDT (UT-4h) templ
 F1: 400.130 F2: 1.000 OF1: 1975.9 PTS1d: 32768
 EX: PW: 9.8 usec PD: 1.0 sec NA: 16 LB: 0.1 WinNuts - \$naresh_NMR.1



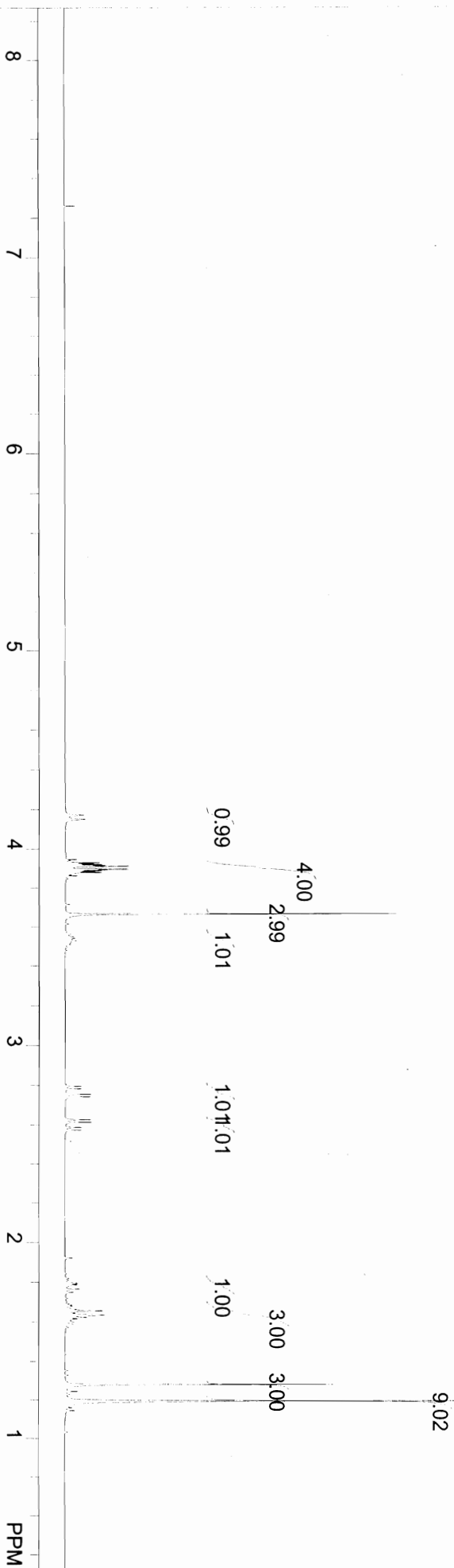
TN-III-268, carbonOVNTE, all,
 F1: 100.613 F2: 1.000 SW1: 25126 PW: 5.7 usec PD: 2.0 sec OF1: 10017.0 NA: 8000 LB: 3.0
 EX:

USER: temple -- DATE: Jul 6 03:28:28 2010 EDT (UT-4h) templ
 PTSId: 32768

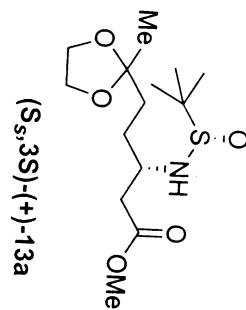


5-43

- 4.172
- 4.151
- 3.945
- 3.928
- 3.924
- 3.919
- 3.914
- 3.910
- 3.895
- 3.891
- 3.886
- 3.882
- 3.877
- 3.860
- 3.664
- 3.527
- 2.795
- 2.781
- 2.755
- 2.742
- 2.627
- 2.614
- 2.587
- 2.574
- 1.795
- 1.791
- 1.786
- 1.764
- 1.664
- 1.656
- 1.634
- 1.623
- 1.616
- 1.279
- 1.244
- 1.193



TN-IV-26, proton, atm, F1: 400.130 F2: 1.000 SW1: 8013 PW: 9.8 usec PD: 1.0 sec NA: 16 OF1: 2004.4 LB: 0.1
 USER: temple -- DATE: Nov 10 09:47:02 2010 EST (UT-5h) templ PTSId: 32768
 EX: WinNus - \$naresh_NMR.1



h-5

200

150

100

50

PPM

172.142

109.523

77.322

77.000

76.677

64.480

64.442

55.735

53.823

51.510

40.202

35.303

29.882

23.670

22.529

USER: temple -- DATE: Nov 10 20:54:03 2010 EST (UT-5h) templ

TN-IV-26, carbon 1HR, atm,
F1: 100.613 F2: 1.000

SW1: 25126

OF1: 10014.5

PTSId: 32768

EX: PW: 5.7 usec

PD: 2.0 sec

NA: 2048

LB: 3.0

WinNus - \$naresh_NMR.1

4261

7.260

4.168

3.934

3.927

3.919

3.688

2.778

2.765

2.647

2.634

2.044

1.639

1.620

1.610

1.601

1.589

1.583

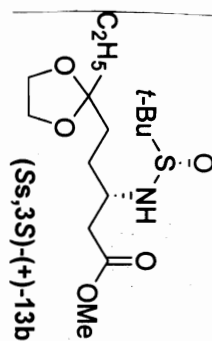
1.217

1.182

0.906

0.887

0.868



-sh-5

7

6

5

4

3

2

1

PPM

0.96

3.99

3.00

1.02

0.990.99

0.96

5.67

8.84

3.13

USER: temple -- DATE: Nov 18 19:00:10 2010 EST (UT-5h) temp1

Varma-256-1-column-pure, proton.atm,

F1: 400.130

F2: 1.000

SW1: 8013

PW: 9.8 usec

PD: 1.0 sec

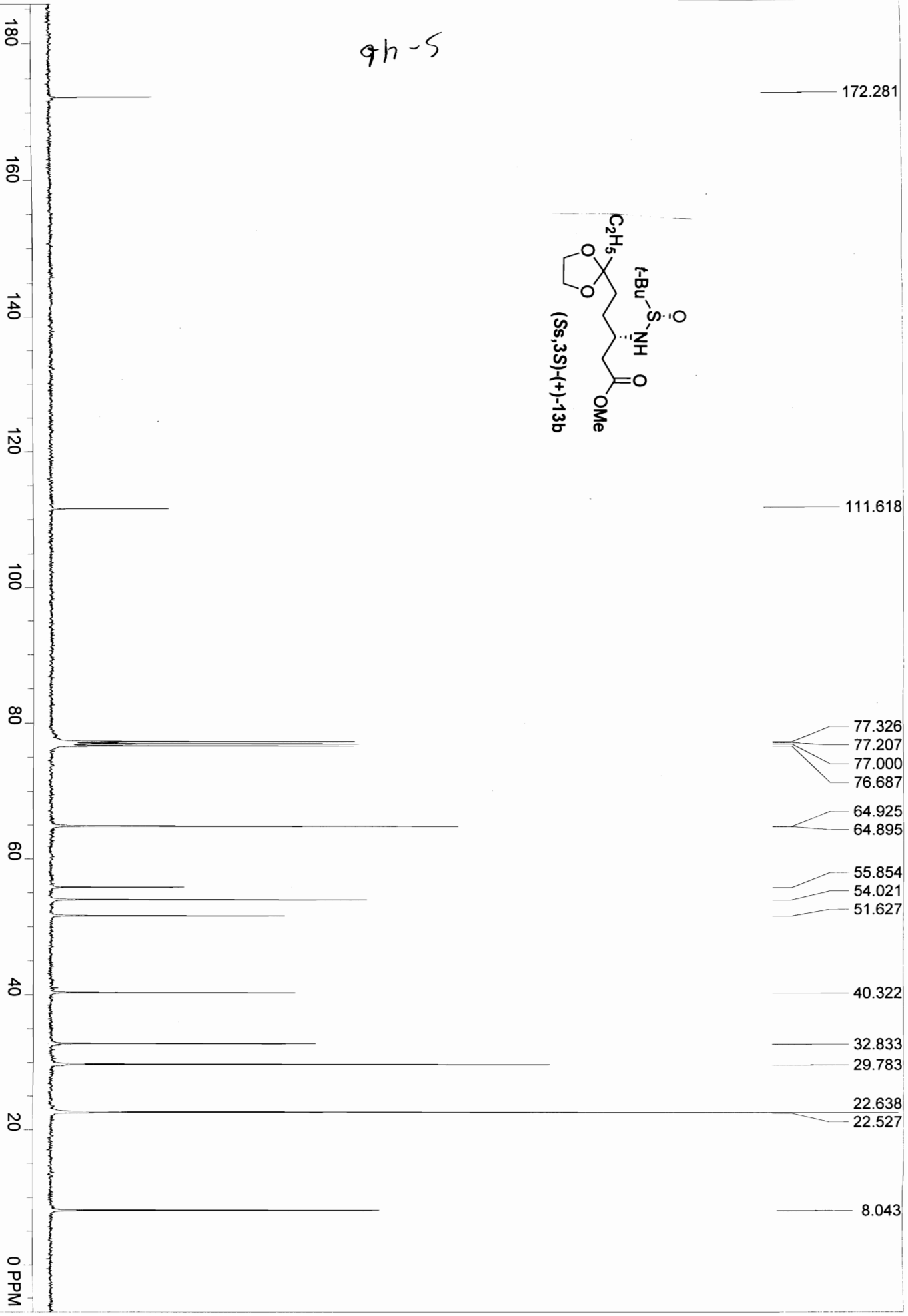
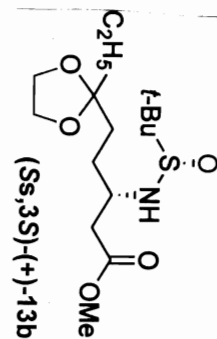
NA: 16

LB: 0.1

PTSID: 32768

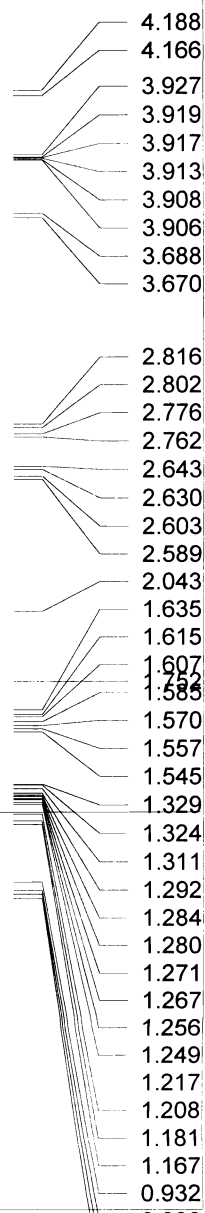
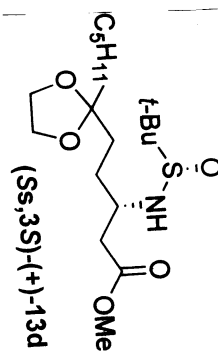
WinNuts - \$NMR1.1

gh-5



Varm-a-256-2-column-pure., carbon 1HR, atm.
F1: 100.613 F2: 1.000 SW1: 25126 OF1: 10020.9
EX: PW: 5.7 usec PD: 2.0 sec NA: 2100 LB: 3.0
USER: temple -- DATE: Nov 19 16:24:29 2010 EST (UT-5h) templ
PTSId: 32768
WinNuts - \$NMRI.1

7.260



Lh-7

7 6 5 4 3 2 1 0 PPM

4.03 3.01 0.97 0.99 0.98 0.99 5.21 6.04 9.00 3.15

Varma-248-2-column-pure, proton, atm,
F1: 400.130 F2: 1.000

SW1: 8013
PW: 9.8 usec

PD: 1.0 sec

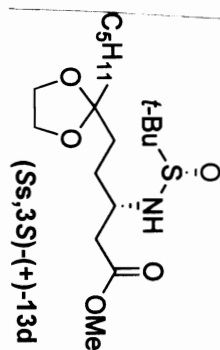
OF1: 2004.5
NA: 16

USER: temple -- DATE: Oct 18 22:28:43 2010 EDT (UT-4h) templ

PTSID: 32768

LB: 0.1
WinNuts - \$NMRI.1

8h-5



200 150 100 50 0 PPM

172.295

111.402

77.318

77.201

77.000

76.675

64.861

64.834

55.874

54.018

51.647

40.322

37.054

33.282

31.988

29.824

23.464

22.650

22.566

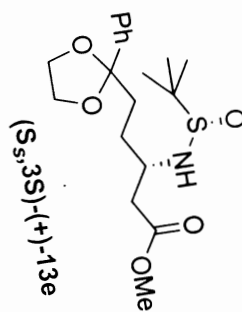
13.944

USER: temple -- DATE: Oct 21 12:01:23 2010 EDT (UT-4h) templ

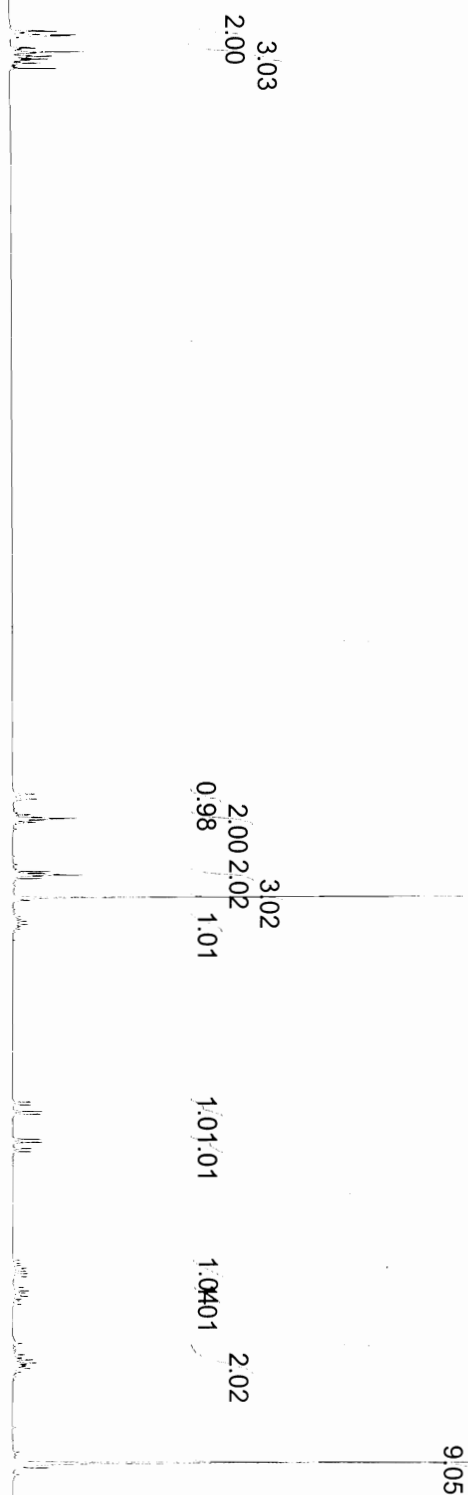
Varna-248-1-column-pure, carbon1HR.atm, SW1: 25126, OF1: 10021.3, LB: 3.0, WinNuts - \$NMR1.1
 F1: 100.613, F2: 1.000, PD: 2.0 sec, NA: 1966, PTSId: 32768

7.424
7.420
7.416
7.408
7.404
7.400
7.352
7.348
7.333
7.331
7.327
7.317
7.313
7.305
7.301
7.297
7.283
7.260

4.102
4.080
4.013
4.011
4.001
3.997
3.994
3.988
3.980
3.977
3.766
3.758
3.753
3.751
3.749
3.744
3.733
3.651
3.639
3.534
2.761
2.747
2.720
2.708
2.601
2.586
2.561
2.547
2.014
1.939
1.915
1.637
1.623
1.621
1.599
1.188
1.168



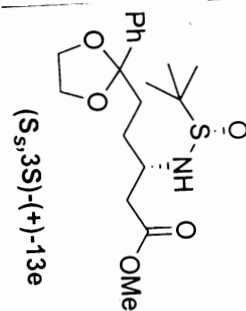
bh - S



8 7 6 5 4 3 2 1 PPM

TN-IV-40(spot-A), proton, atm.
F1: 400.130 F2: 1.000 SW1: 8013 OF1: 2004.6
EX: PW: 9.8 usec PD: 1.0 sec NA: 64 LB: 0.1

USER: temple -- DATE: Dec 16 14:35:11 2010 EST (UT-5h) templ
PTSId: 32768
WinNuts - \$nareh_NMR.1



05 - 5

200 150 100 50 PPM

172.077

142.219

128.010
127.763
125.435

109.914

77.318
77.000
76.676

64.347
64.306

55.727
53.667
51.479

40.250
36.535

29.459

22.543

TN-IV-40(Spot-A- Beta-Amino Ester), carbon1HR,atm, USER: temple -- DATE: Dec 15 18:54:39 2010 EST (UT-5h) templ
F1: 100.613 F2: 1.000 SW1: 25126 OF1: 10012.1 LB: 3.0 PTSId: 32768
EX: PW: 5.7 usec PD: 2.0 sec NA: 2048 WmNuts - \$nareh_NMR.1