

Supporting Information

Efficient Pyrrolidine Catalyzed Cycloaddition of Aziridines with Isothiocyanates, Isoselenocyanates and Carbon Disulfide “On Water”

Mani Sengoden, Murugan Vijay, Emayavaramban Balakumar and Tharmalingam Punniyamurthy*

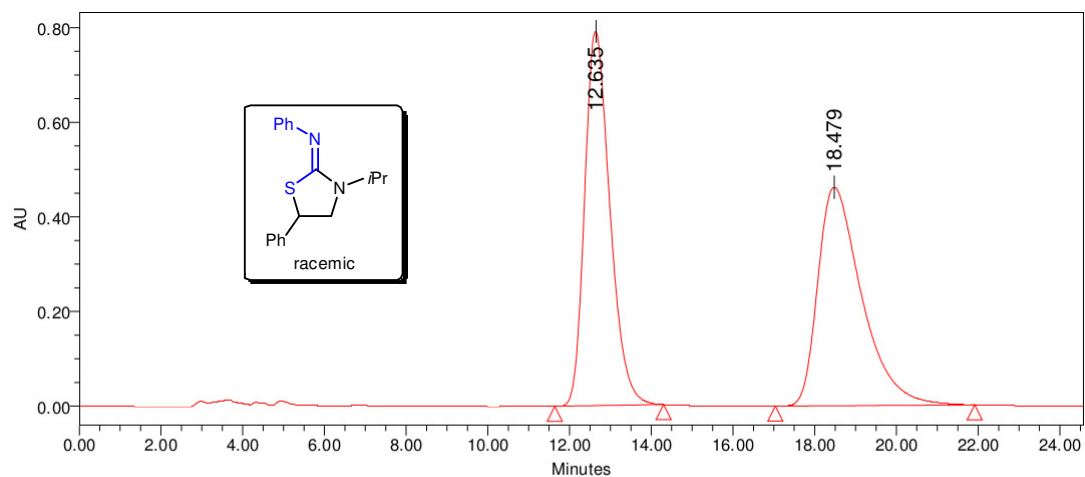
Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati-781039, India.

E-mail: tpunni@iitg.ernet.in

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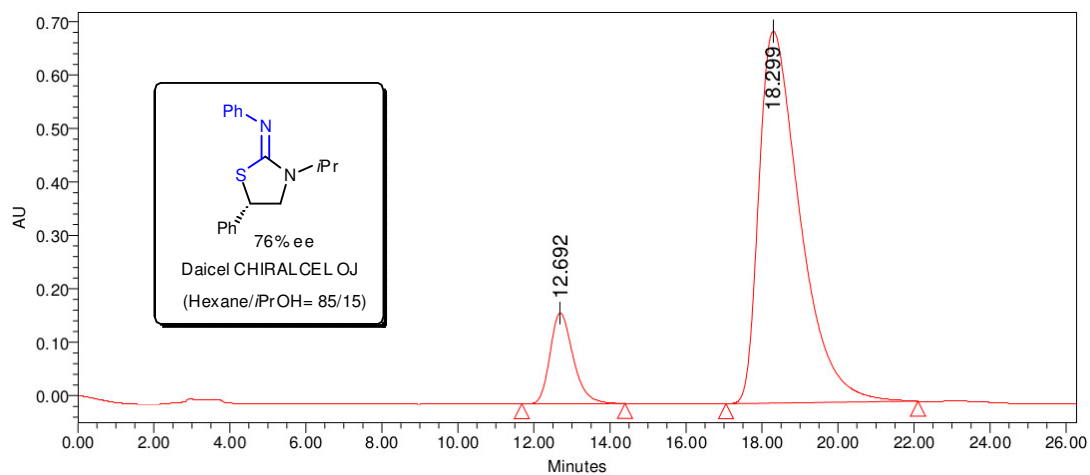
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HPLC Chromatograms:



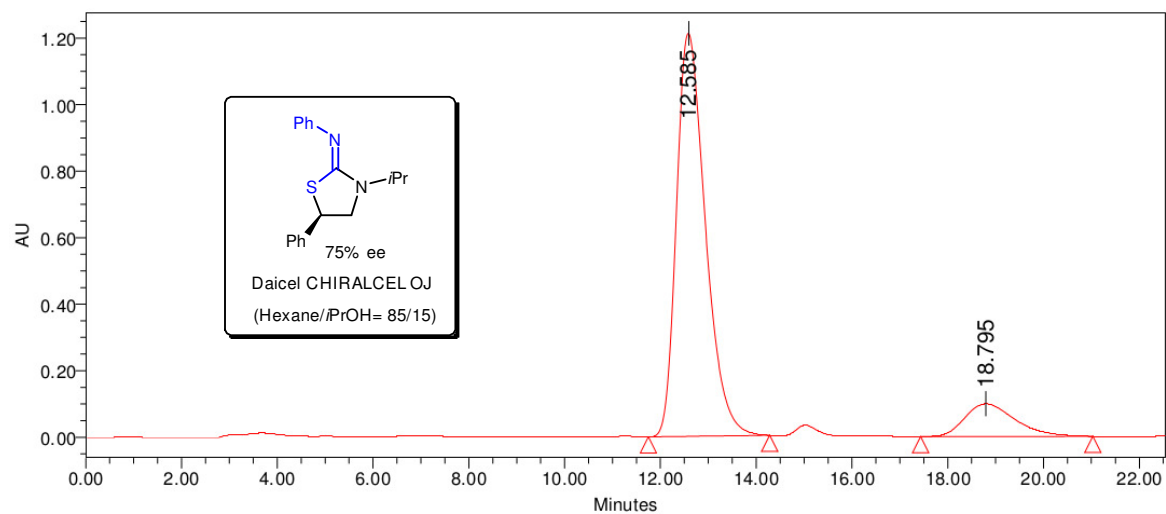
Peak Results

	RT	Height (μ V)	% Area
1	12.635	790834	49.65
2	18.479	461917	50.35



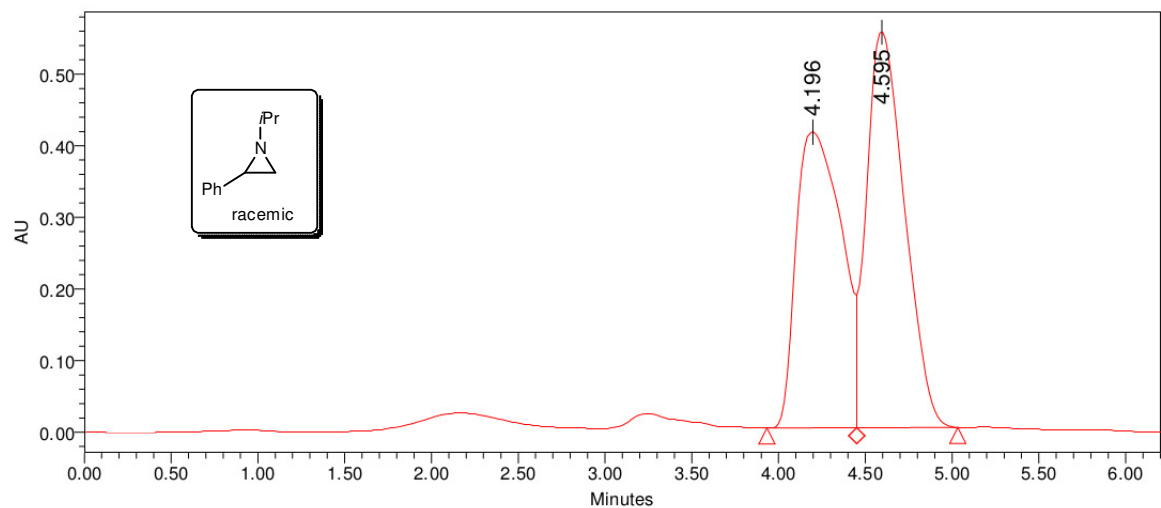
Peak Results

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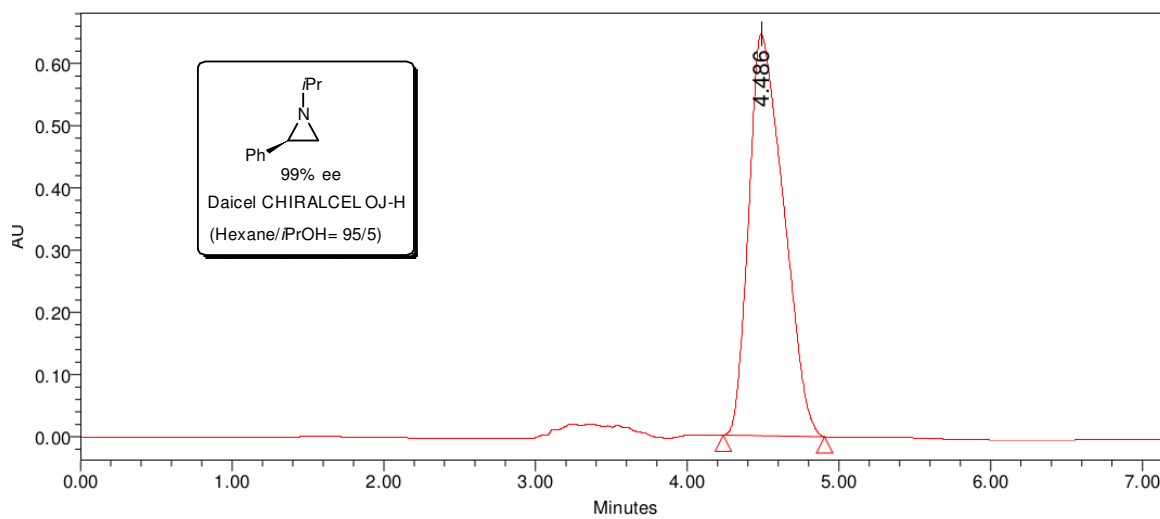
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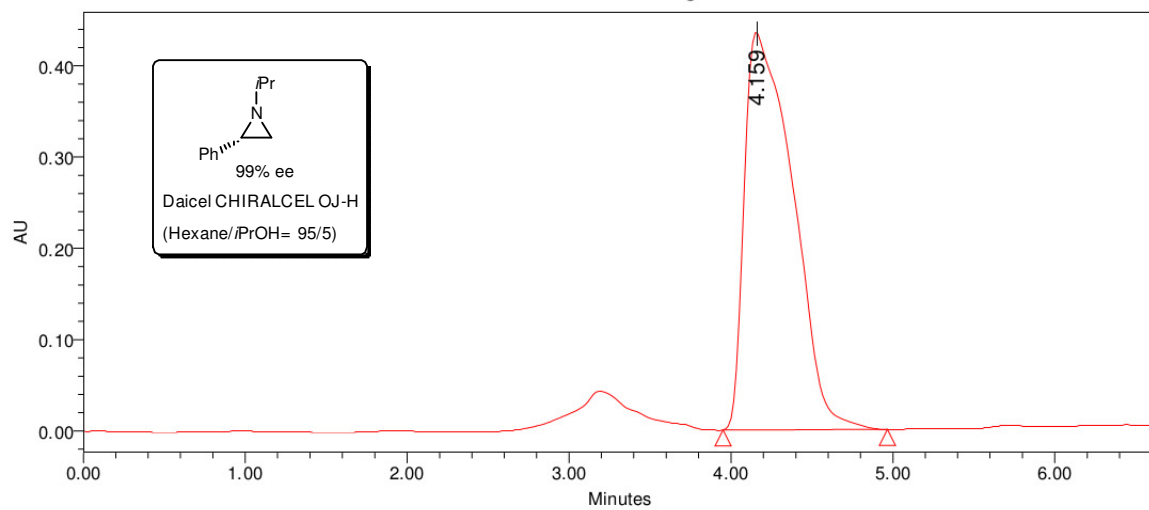
Peak Results

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Peak Results

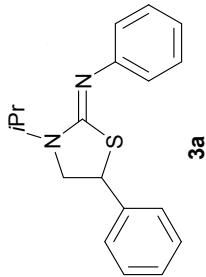
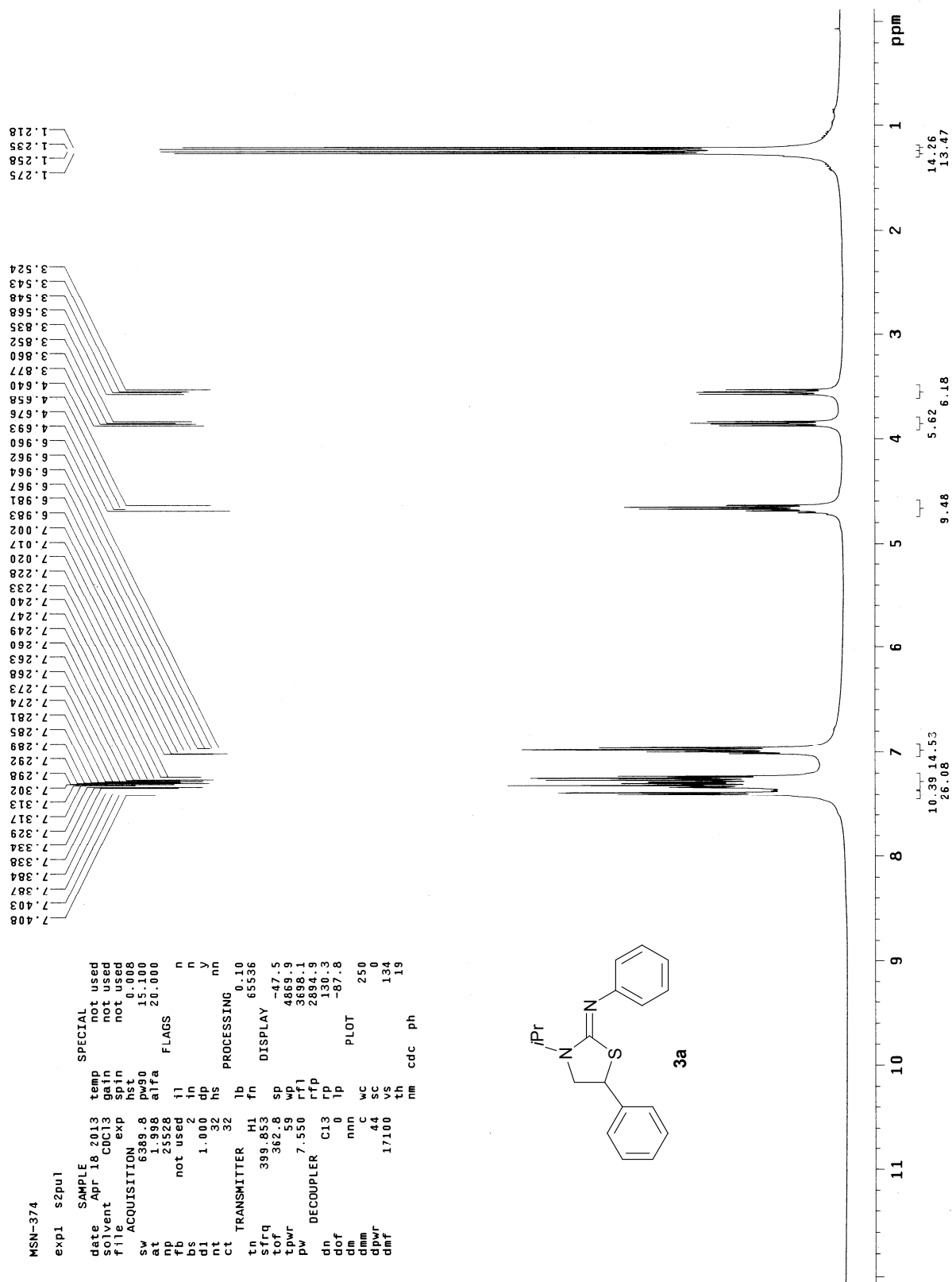
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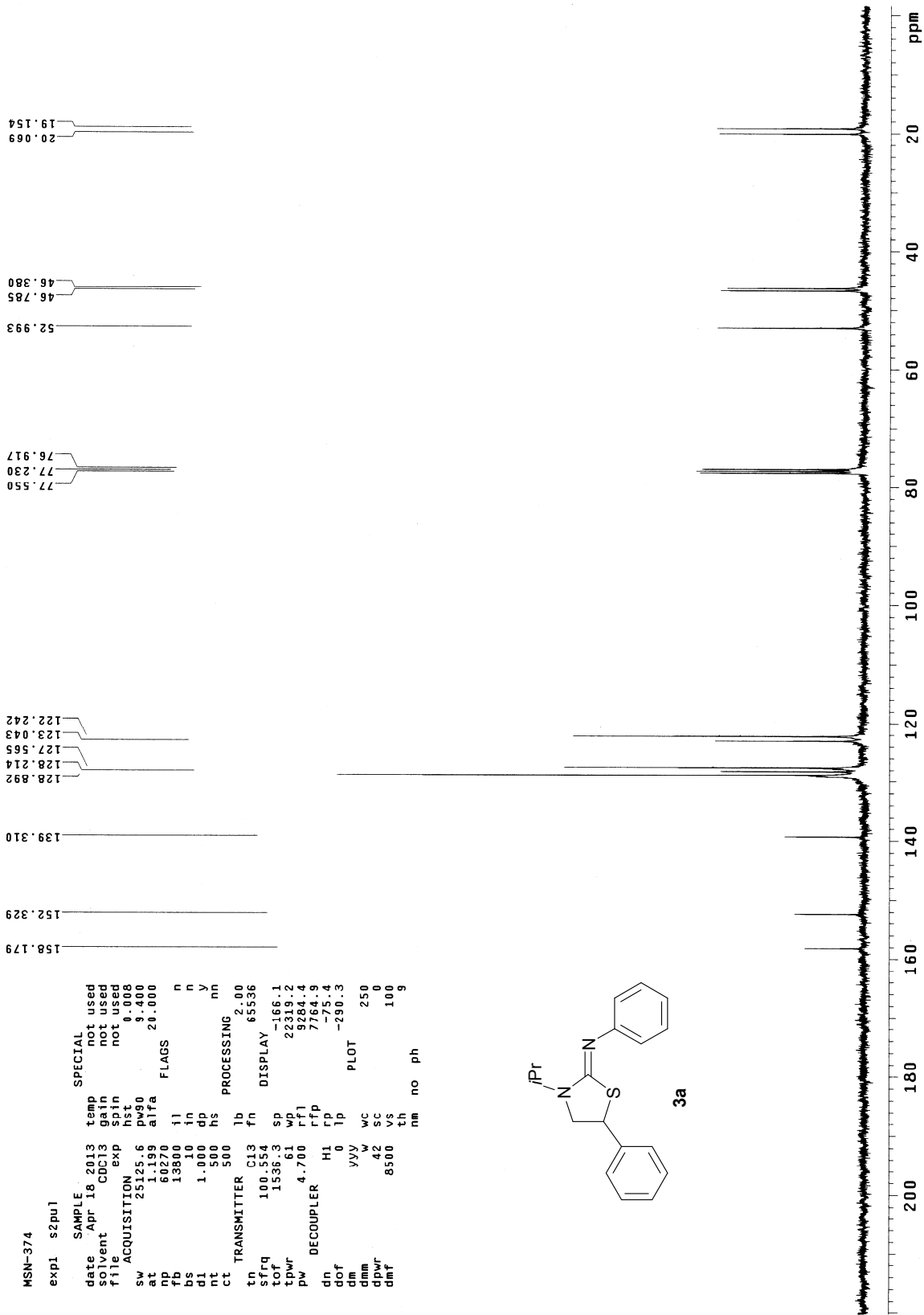


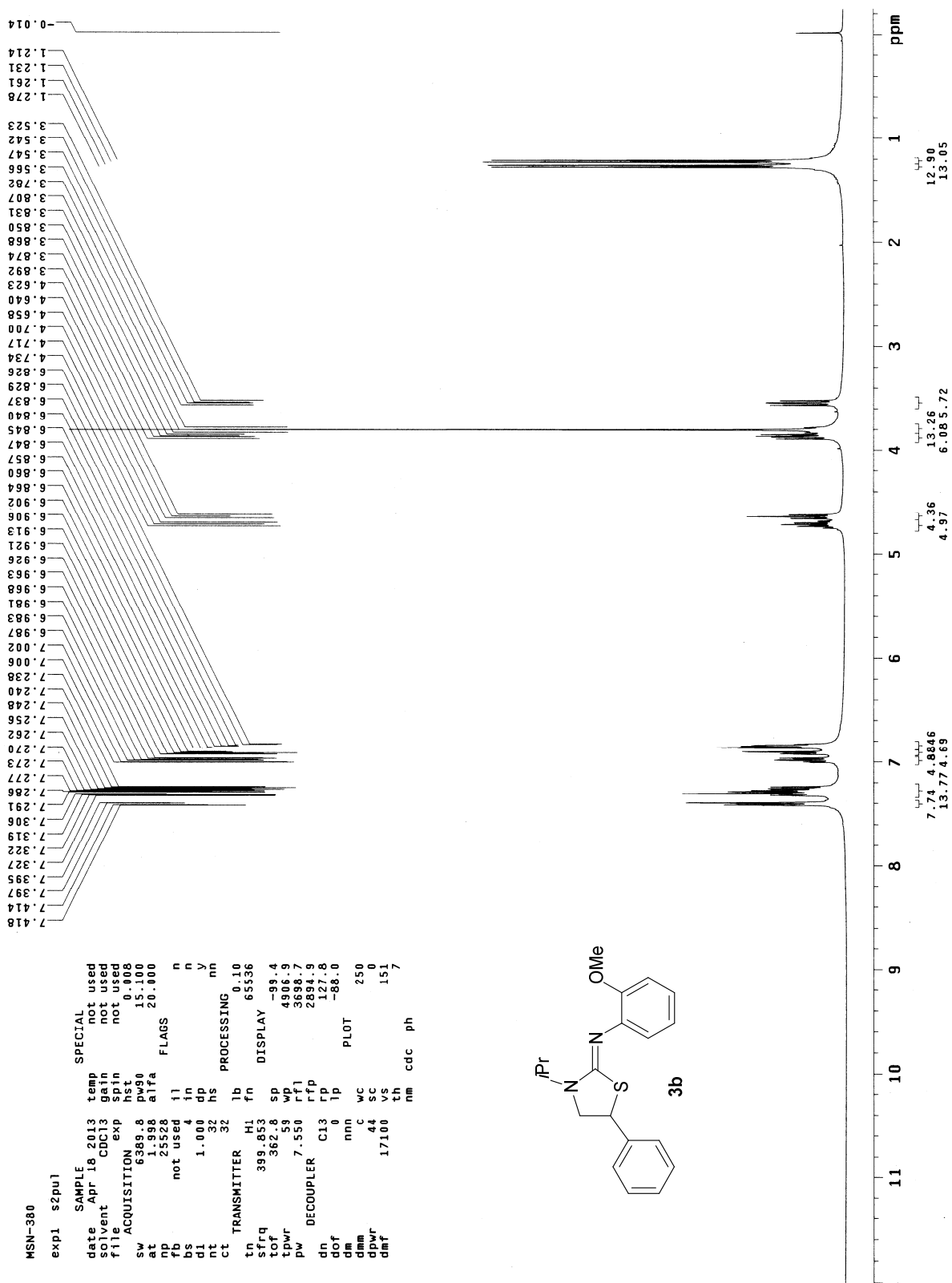
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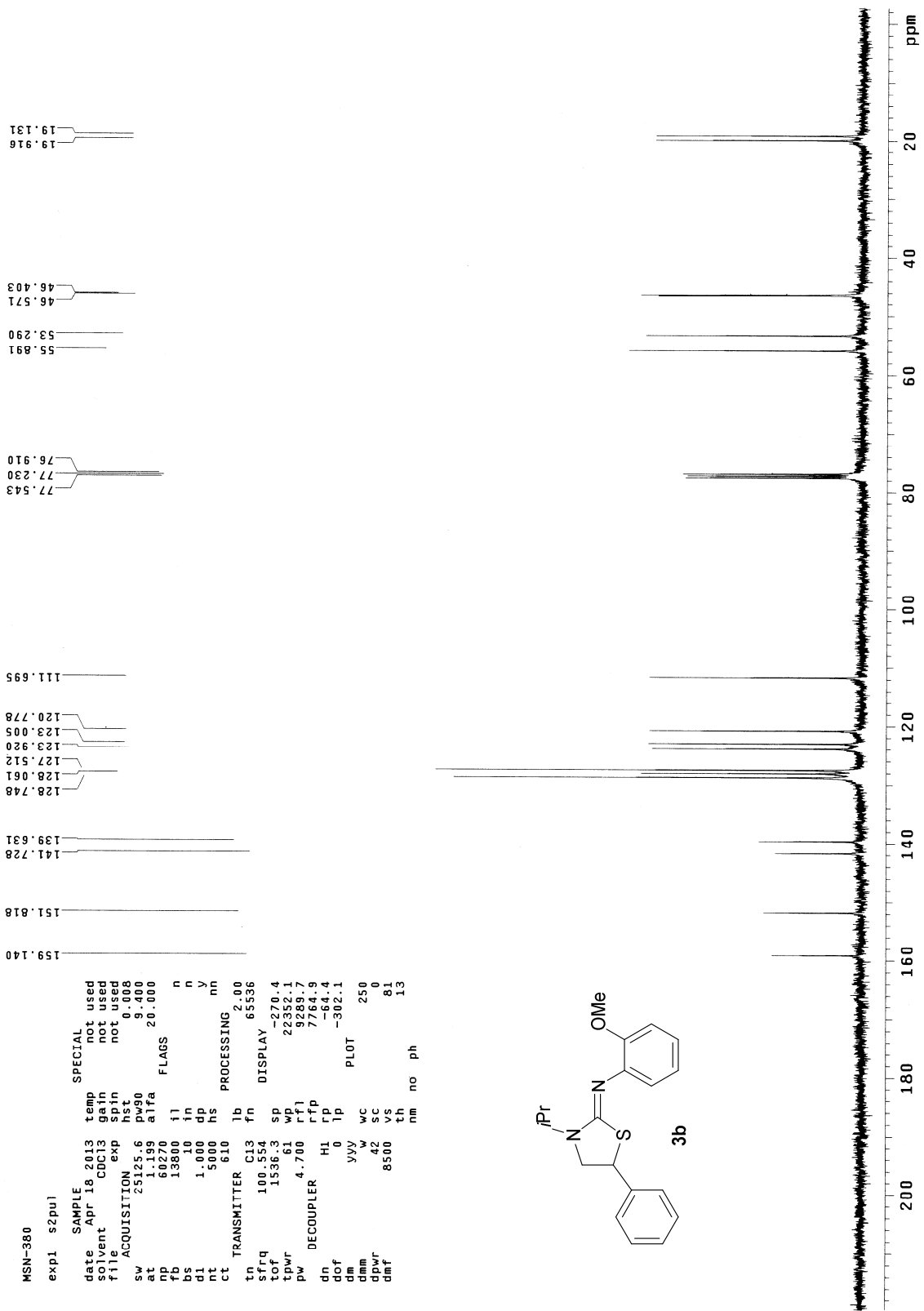
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¹H and ¹³C NMR Spectra of Cycloaddition Products and Intermediate A









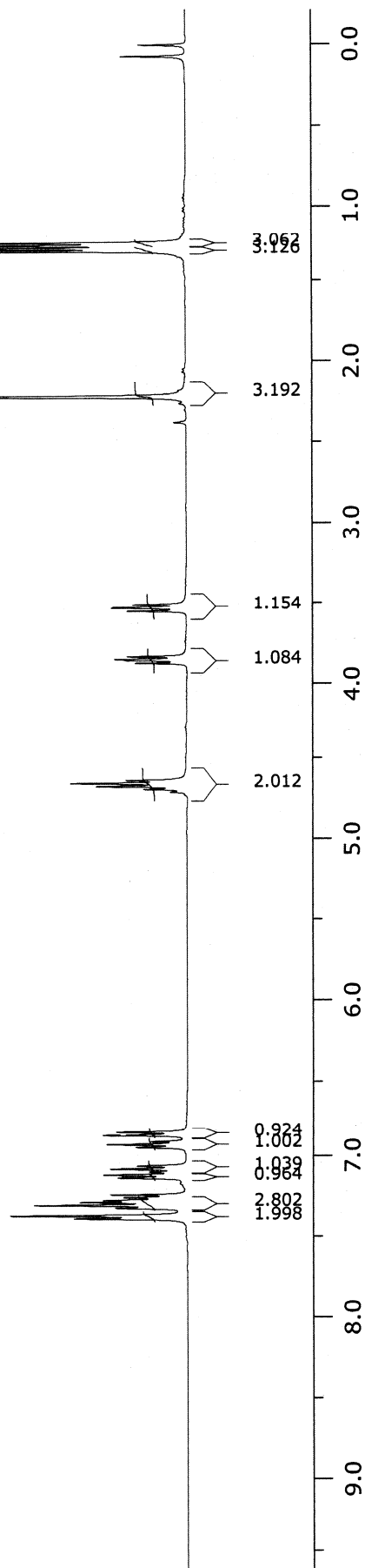
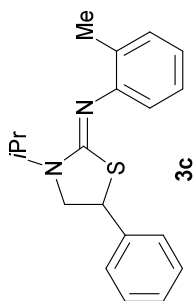
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3.8849

4.6269
4.6451
4.6643
4.6826

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6.9404
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MSN-412-A-13C



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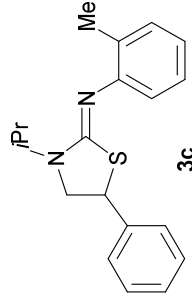
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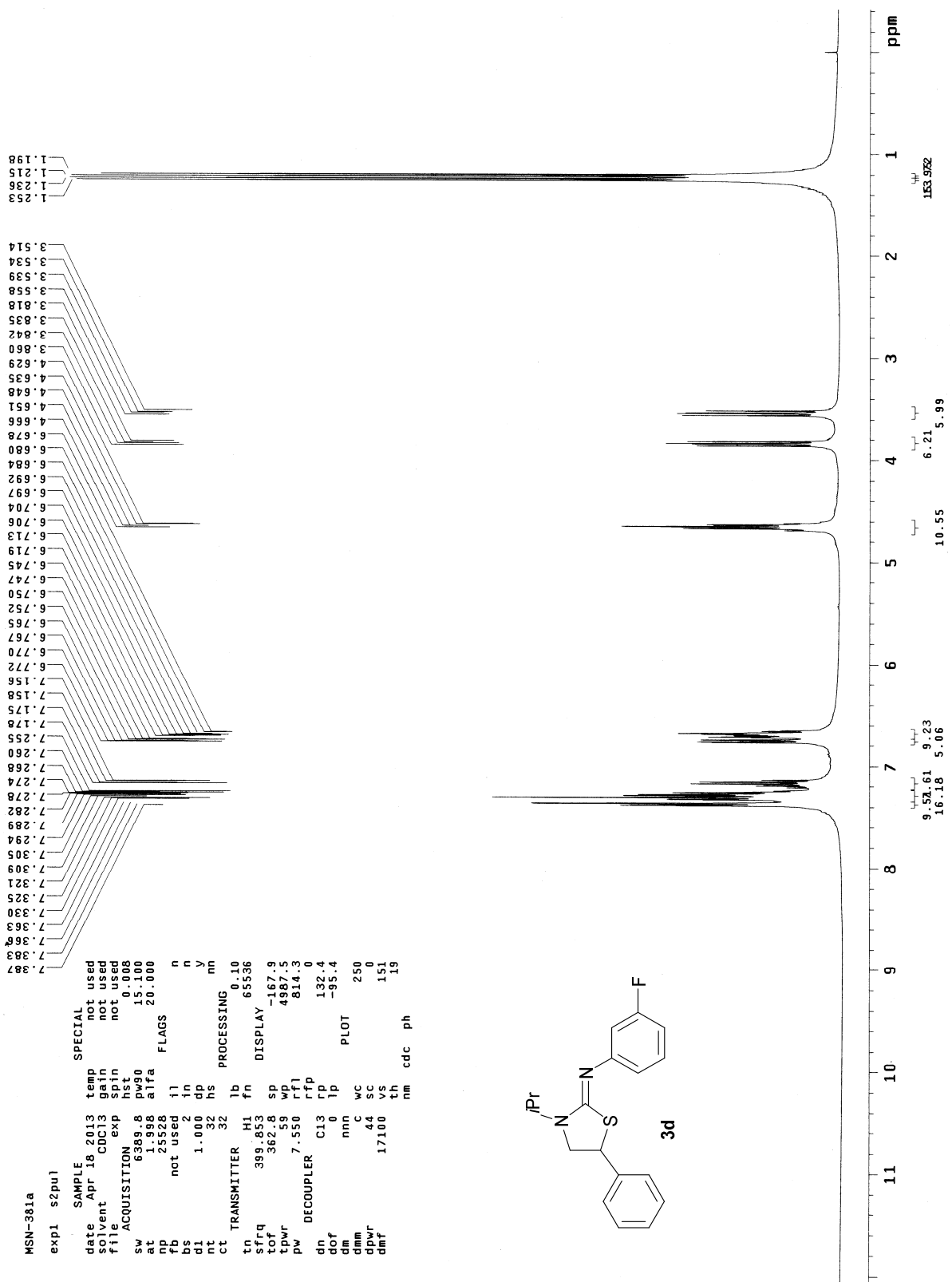
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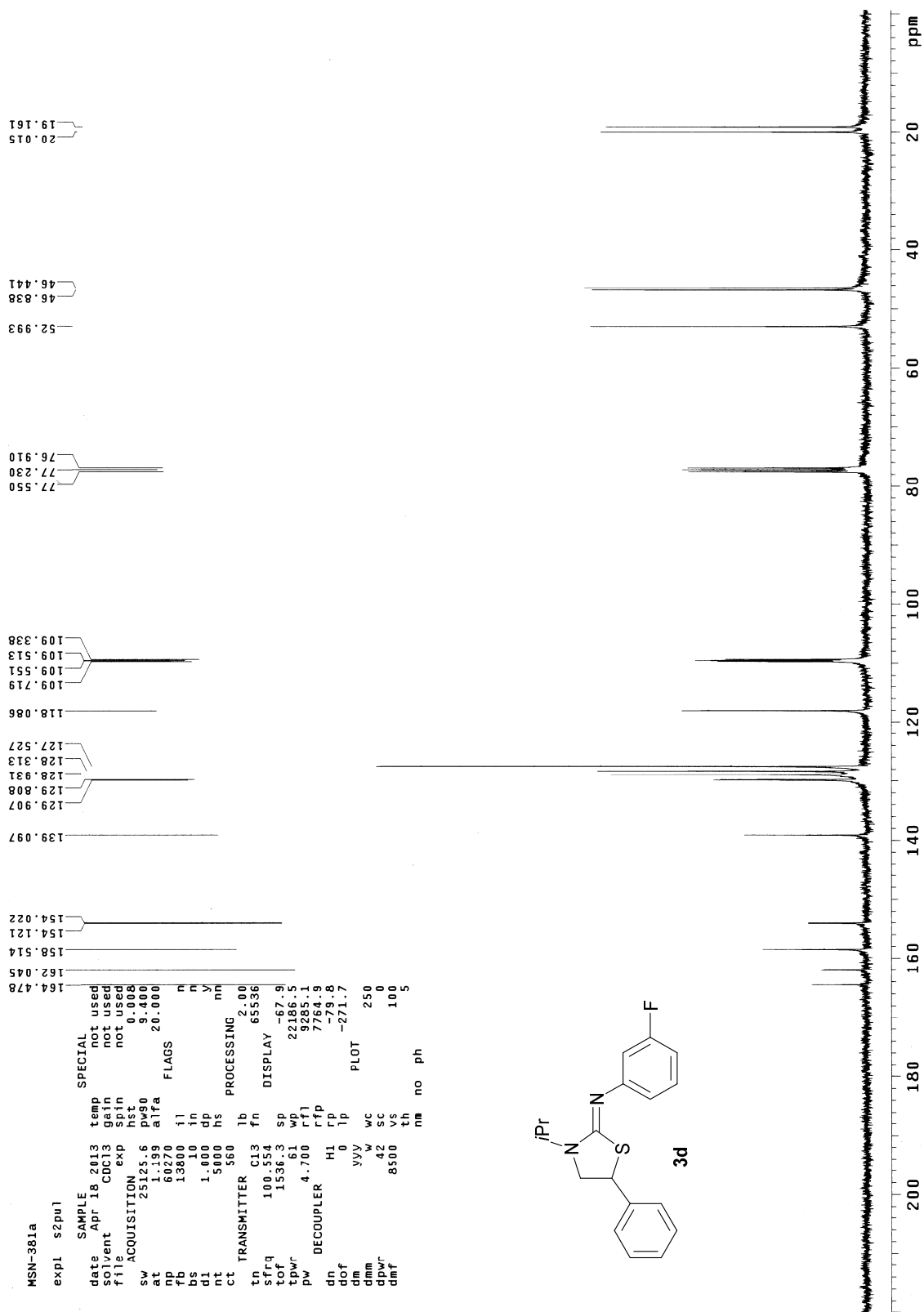
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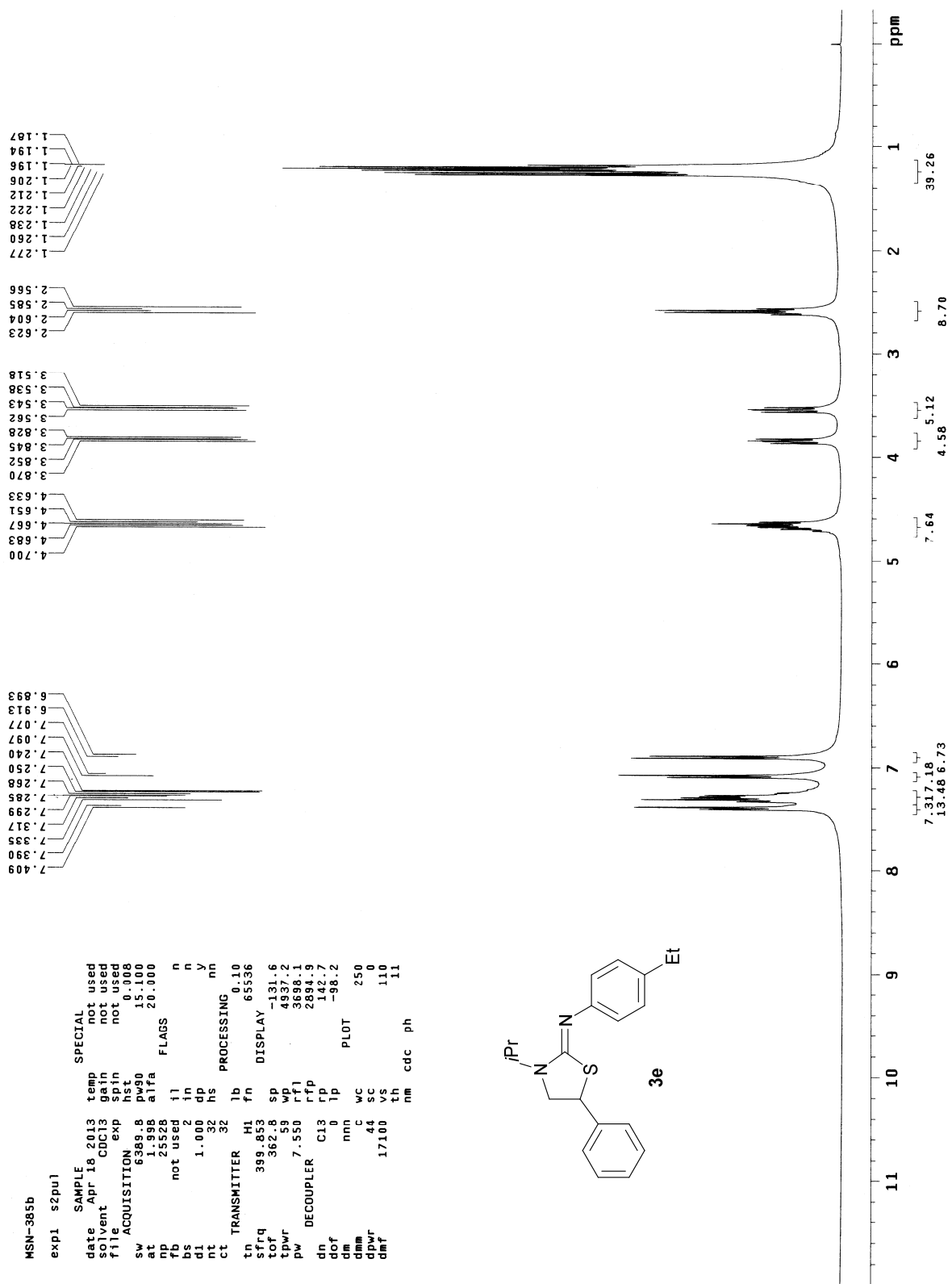
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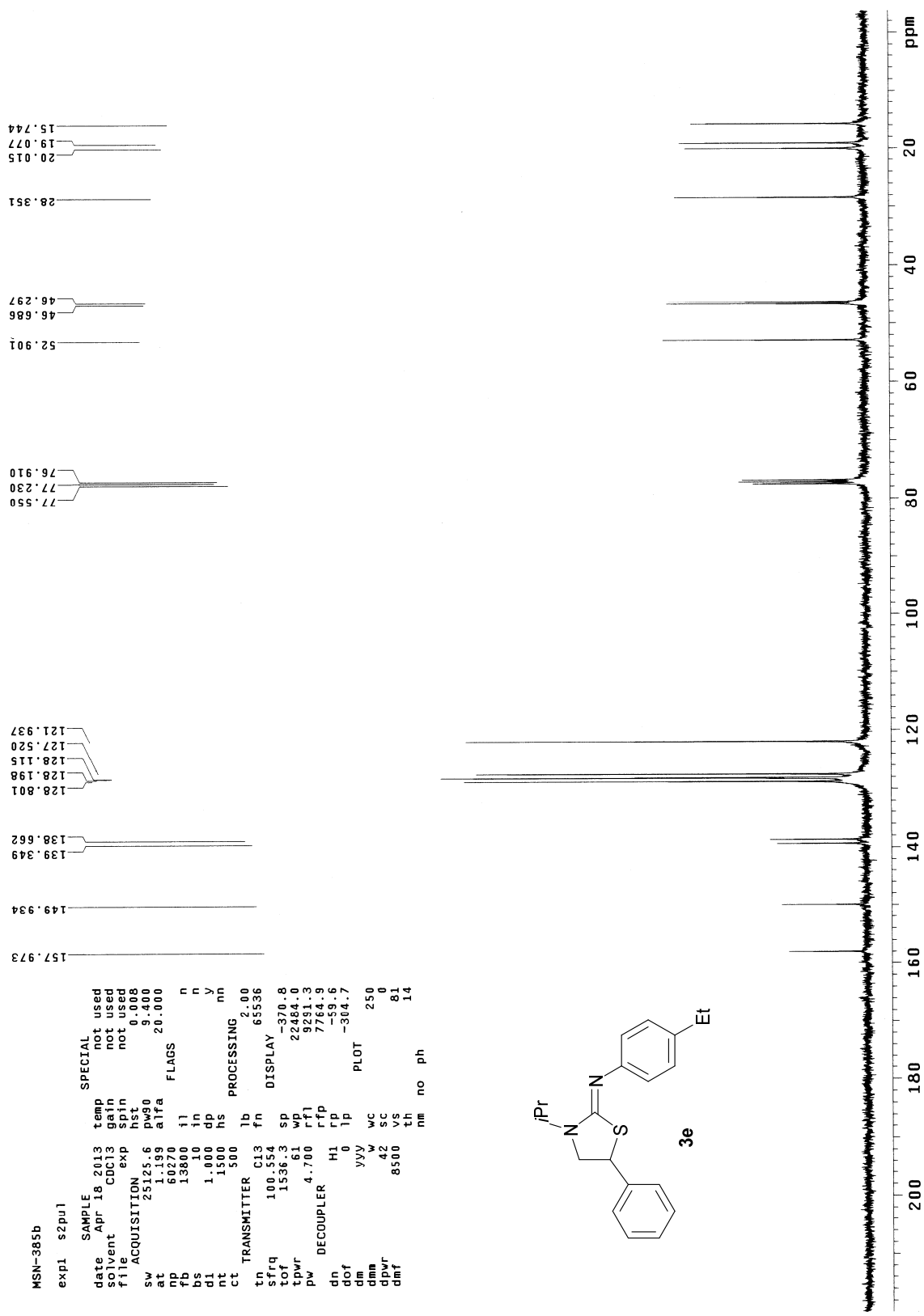
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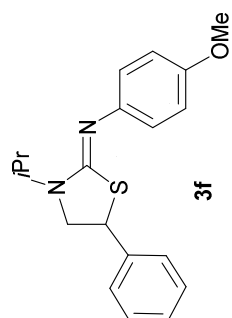
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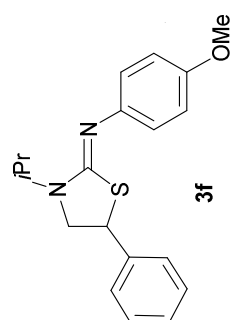
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60

80

100

120

140

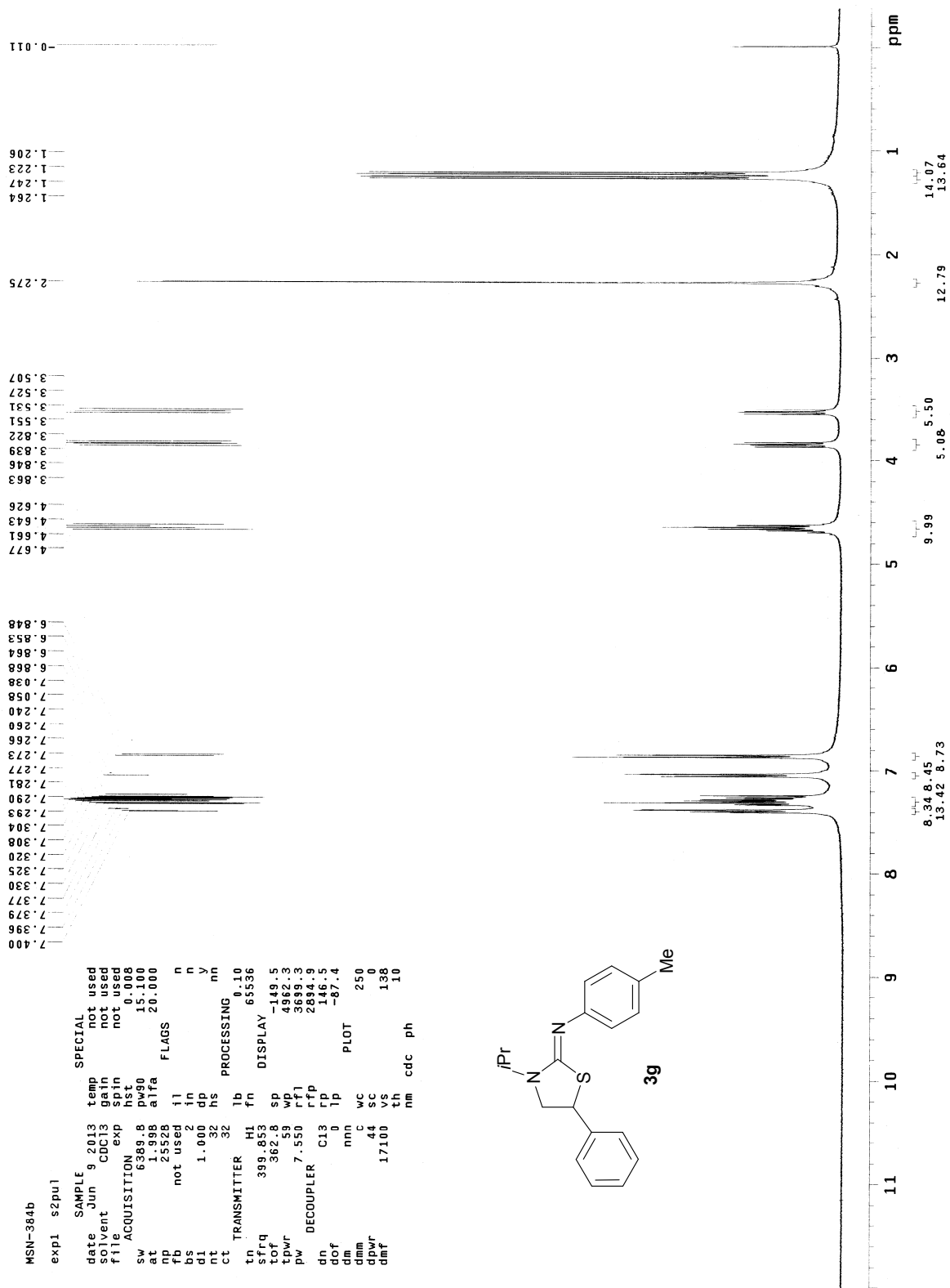
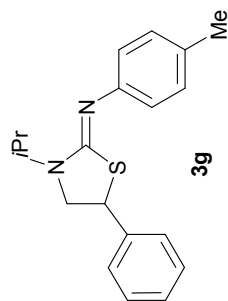
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180

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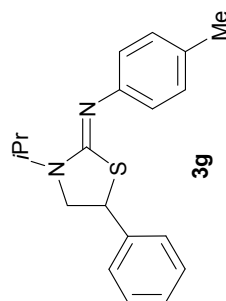
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atf	25528	alfa	FLAGS	
mp	not used	il	n	
rb	2	in	n	
nt	1.000	ds	y	
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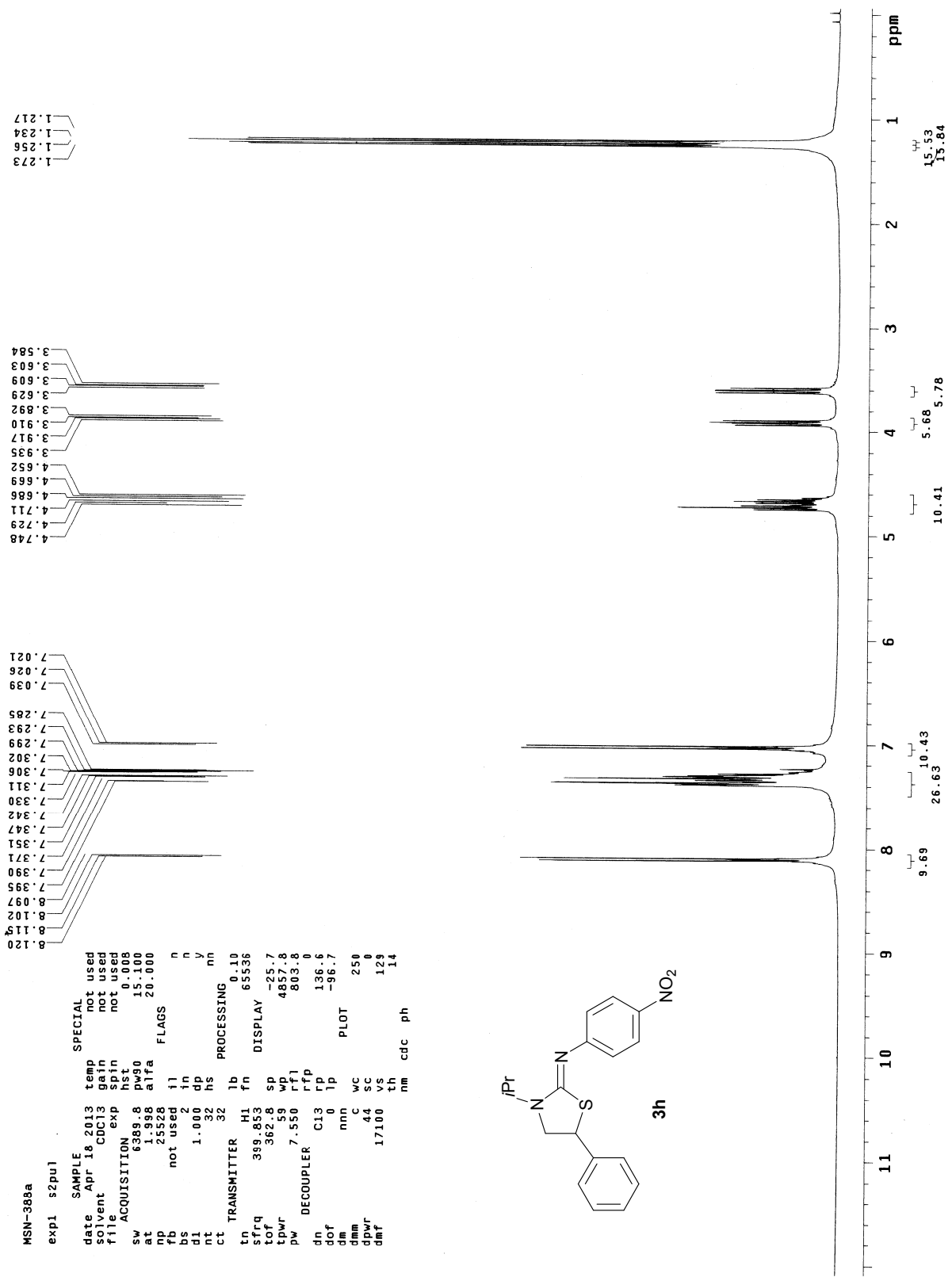


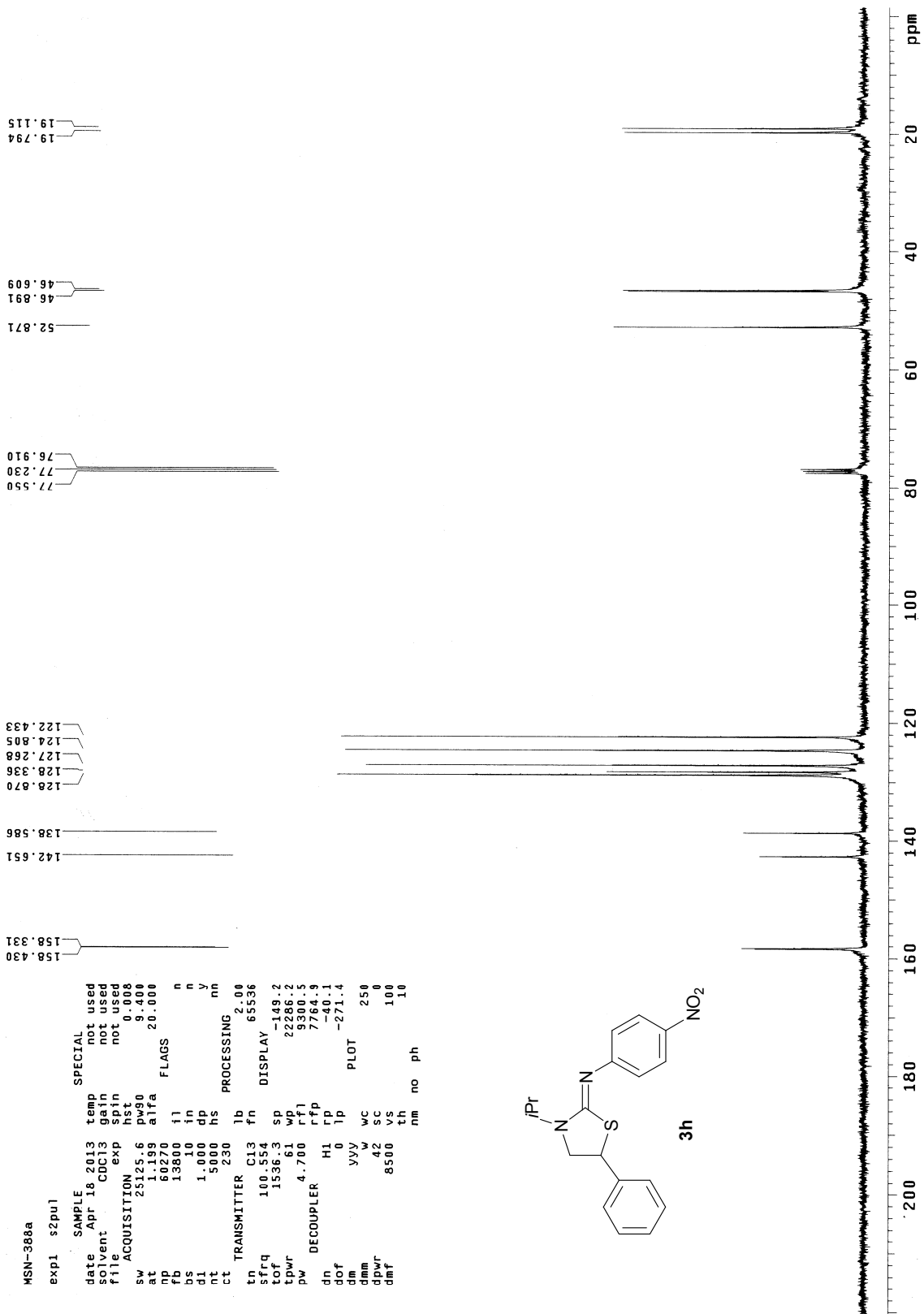
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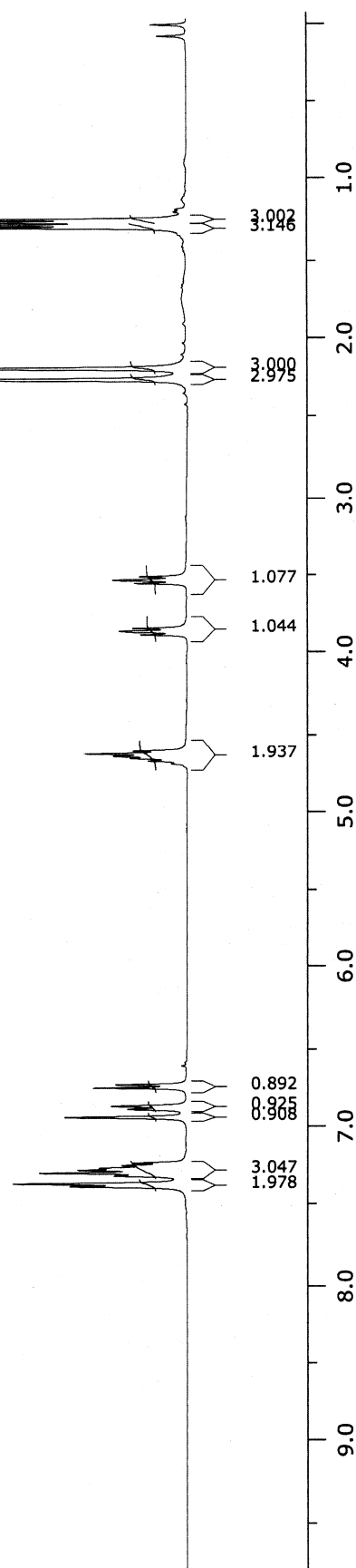
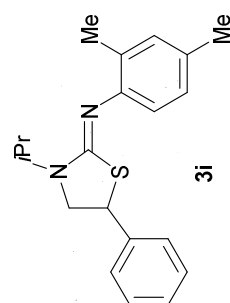
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4.6833

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6.8764
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6.9466

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MSN-423-C-13C

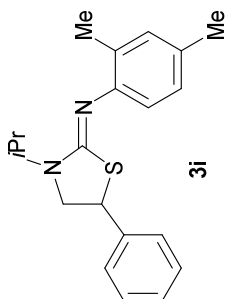


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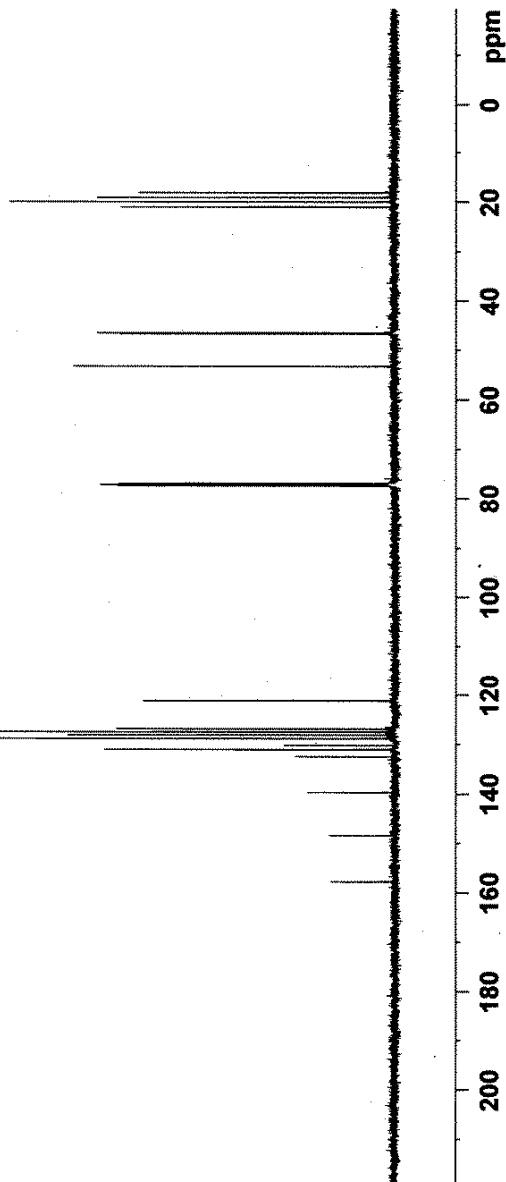
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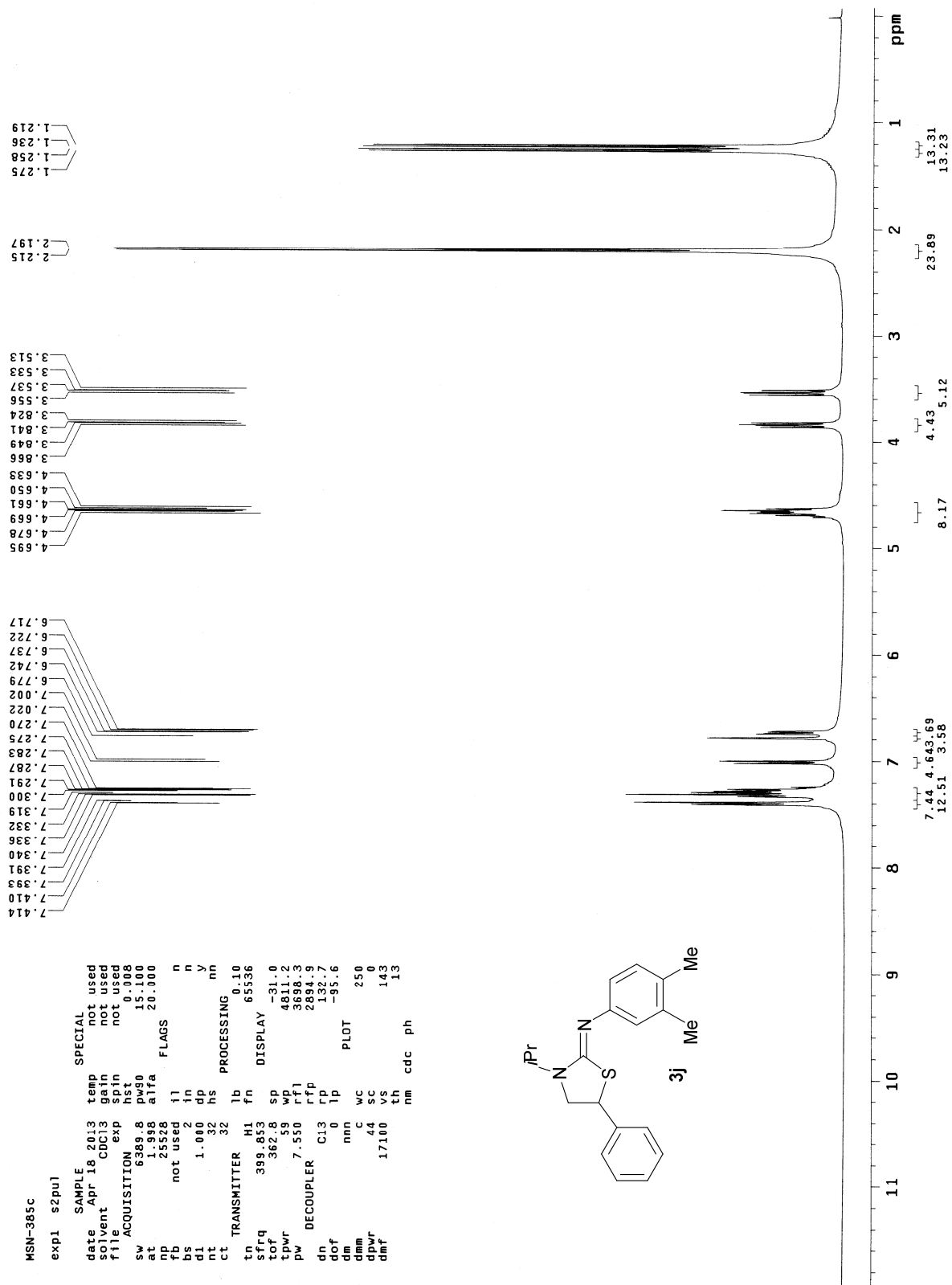
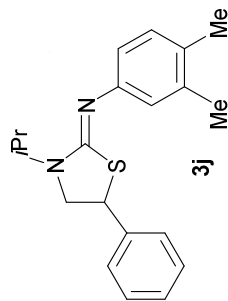
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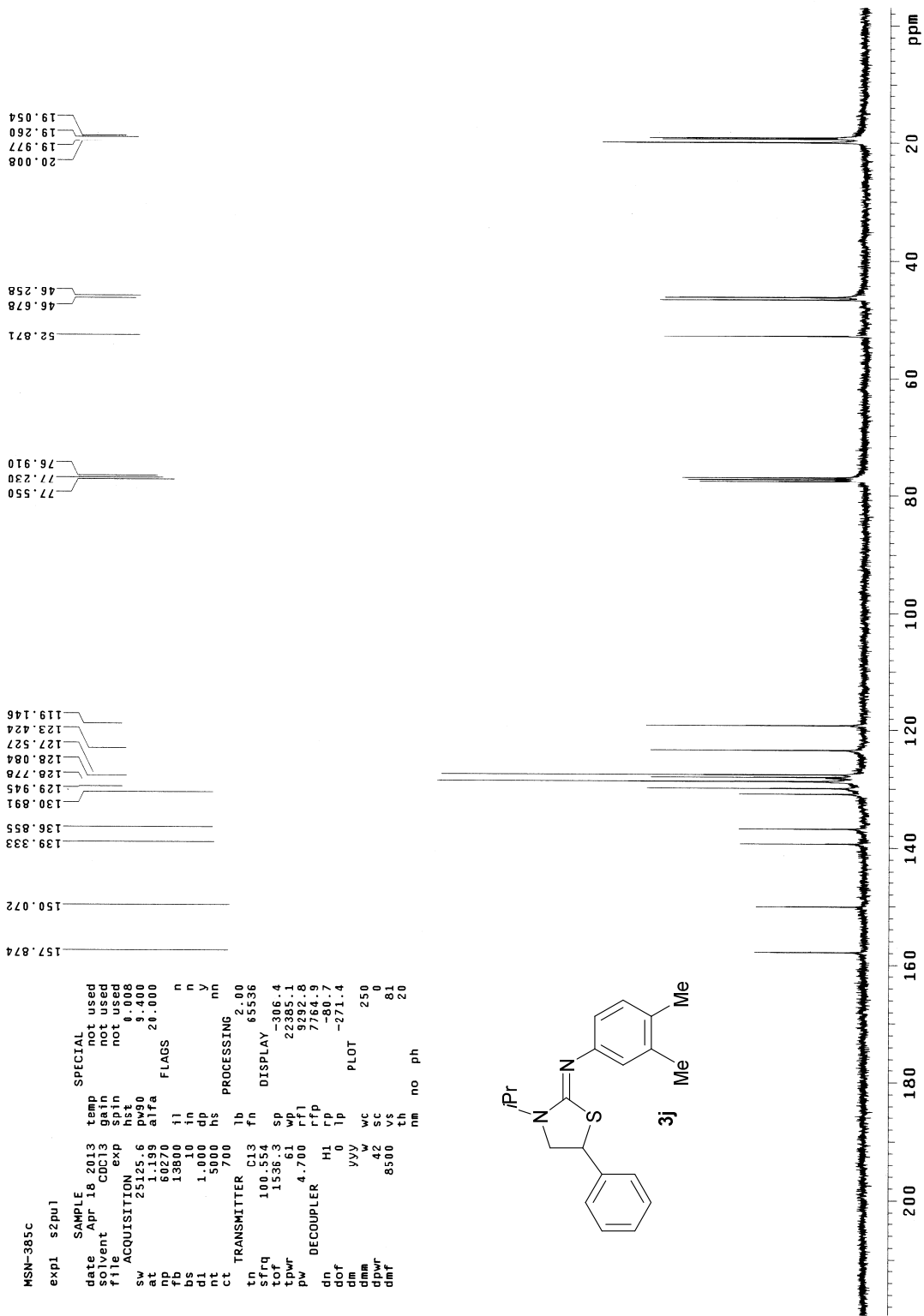


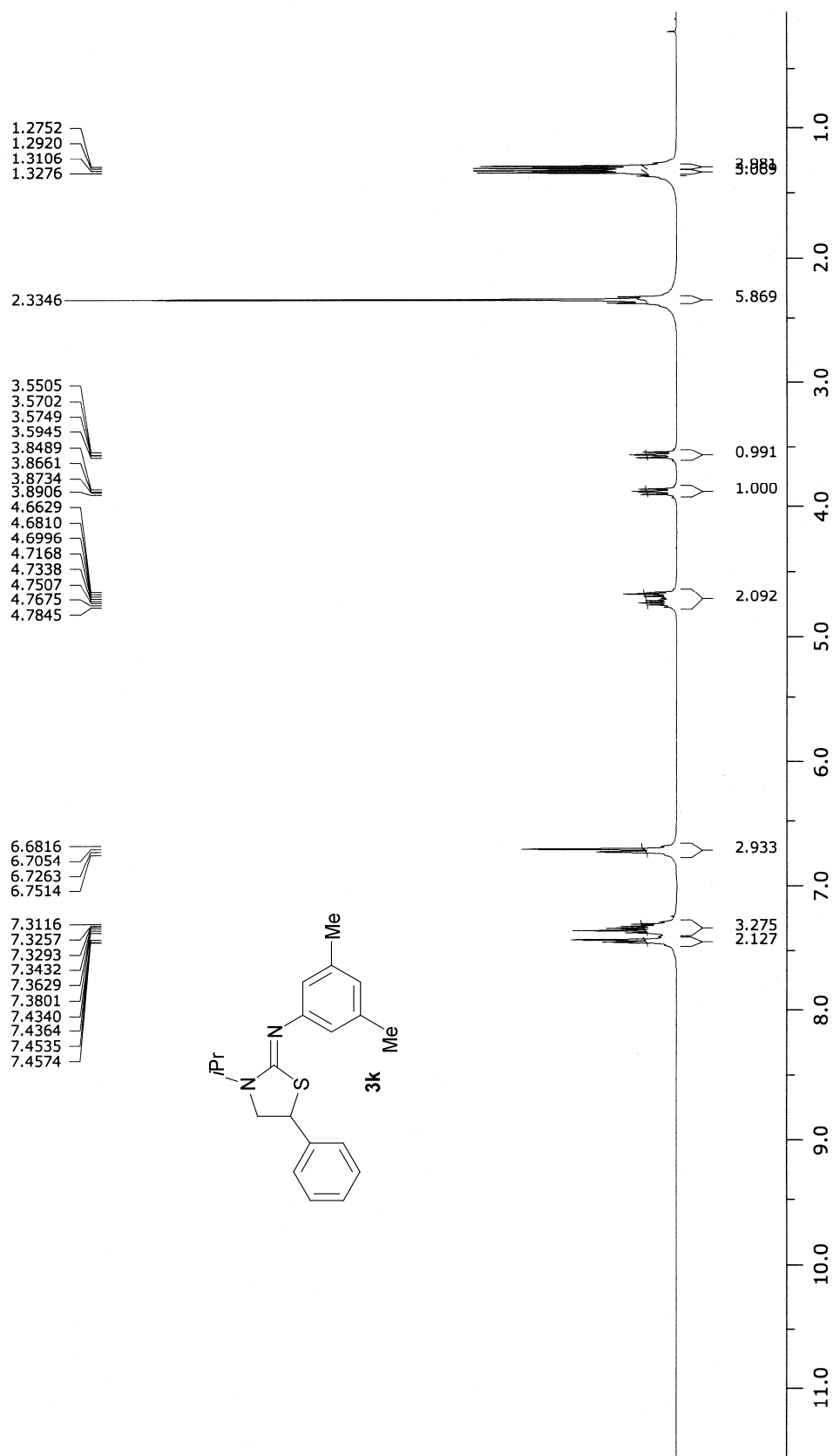
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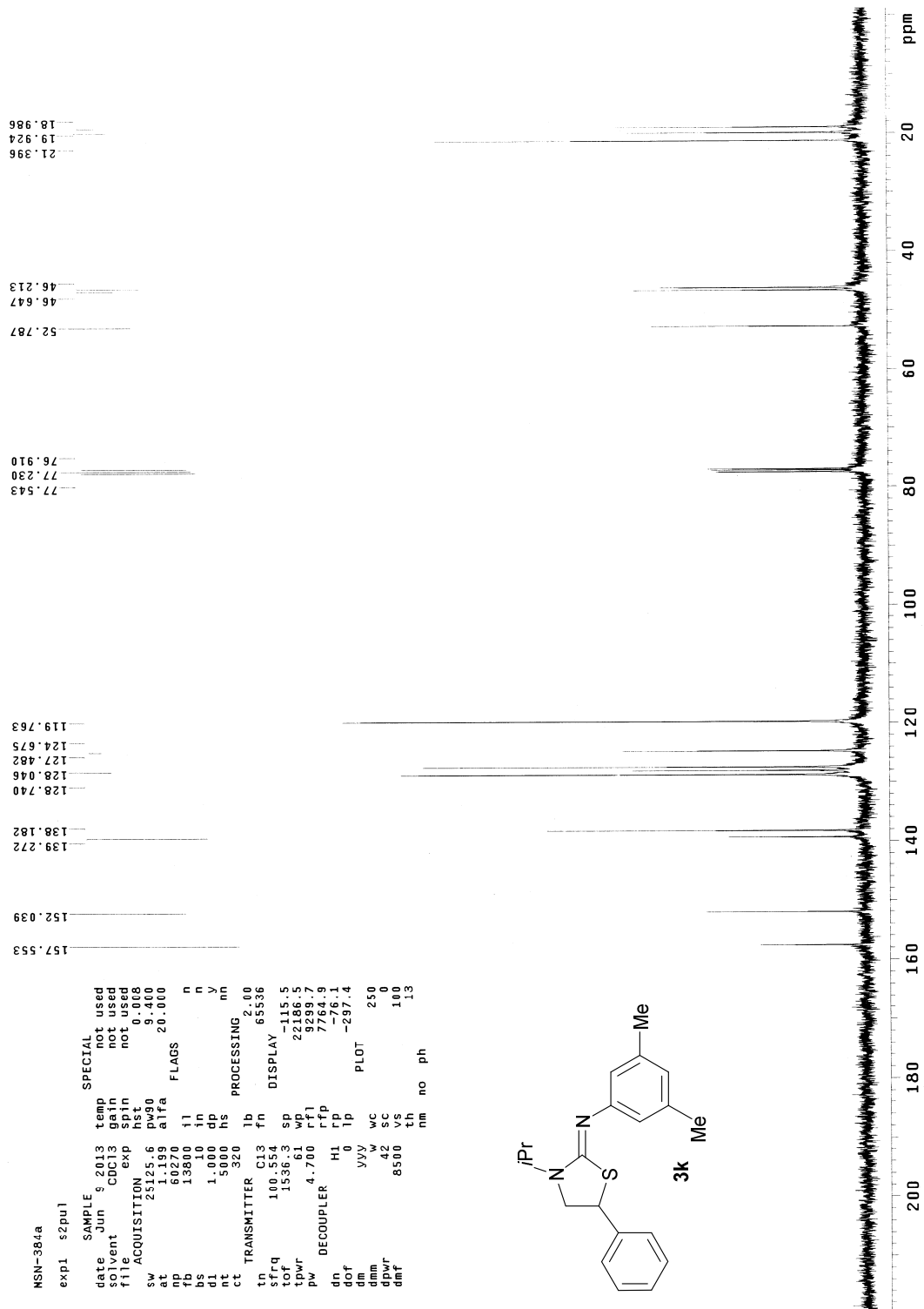
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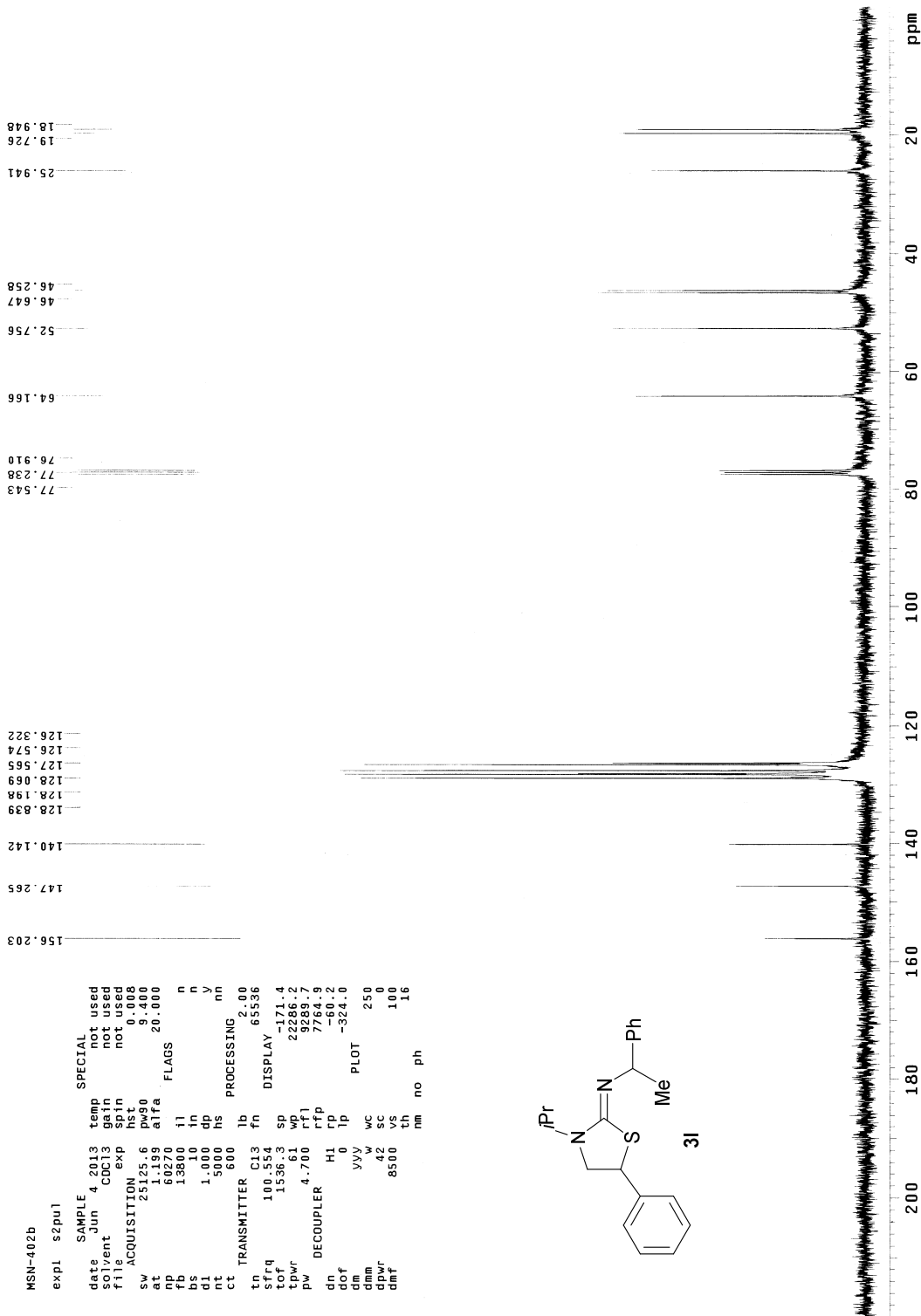
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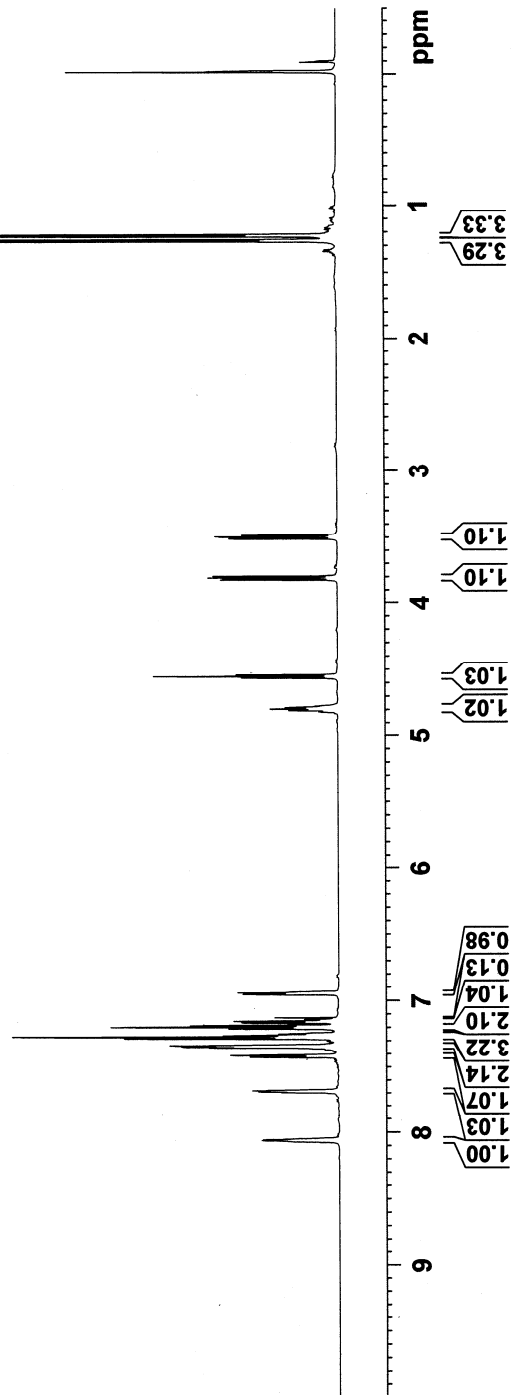
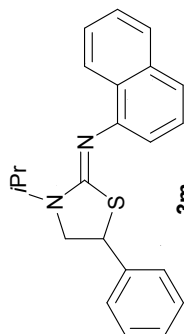


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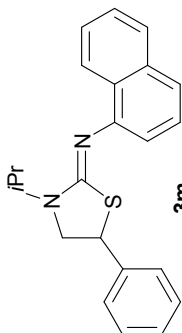


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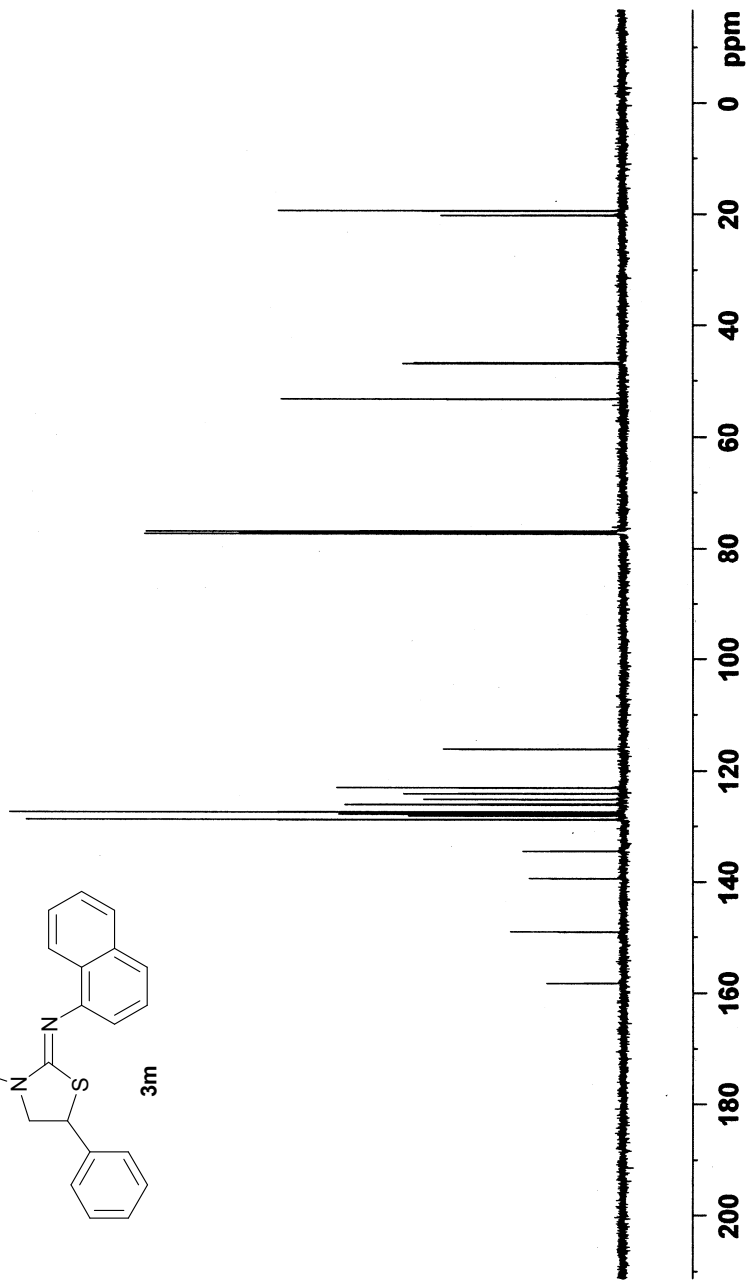
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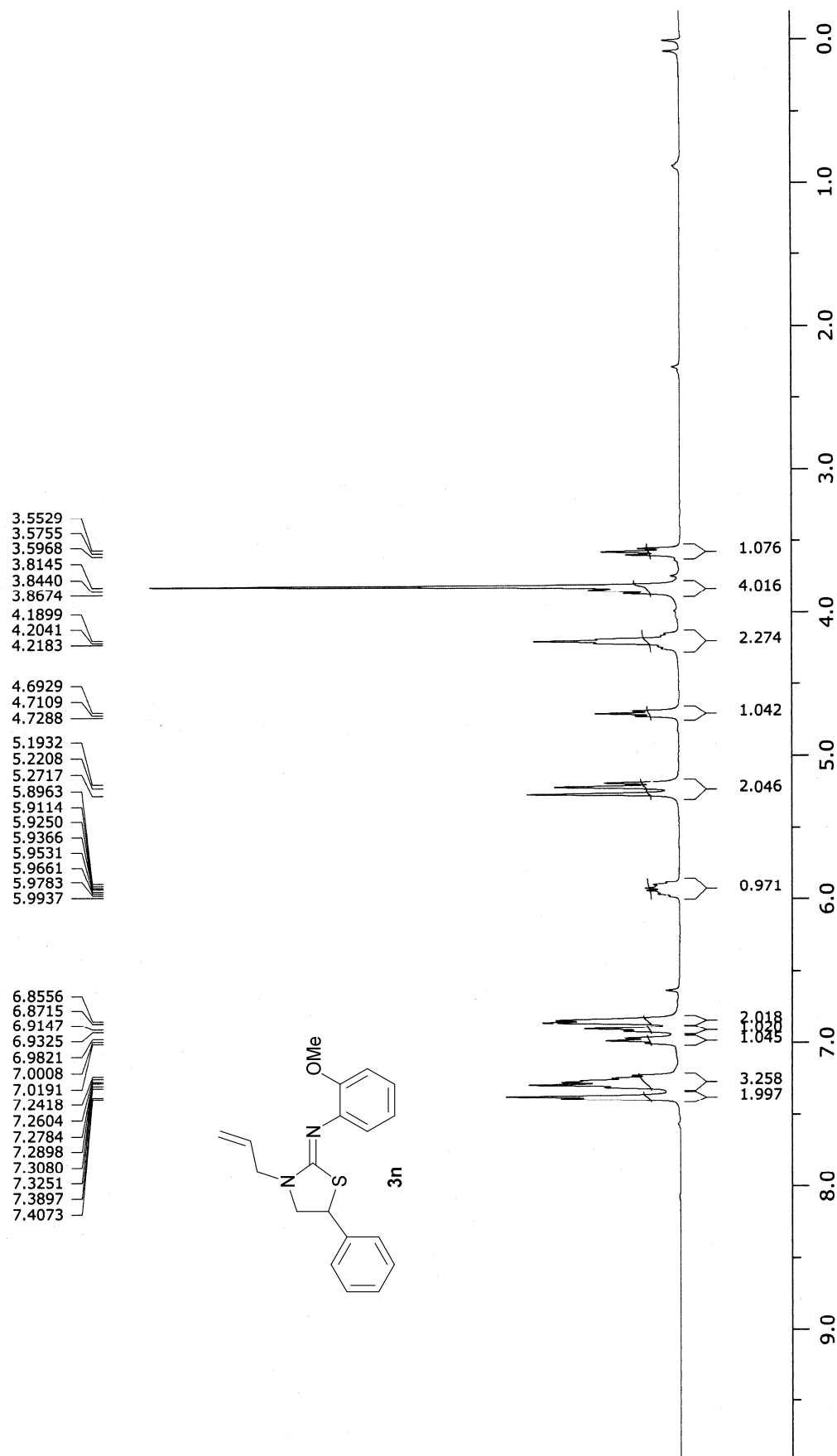
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FIDRES 1.100393 Hz
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RG 65.24
DM 13.867 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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NUC1 13C
P1 10.50 usec
PLW1 95.00000000 W

===== CHANNEL f2 =====
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NUC2 1H
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F2 - Processing parameters
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MSN_424_13C



NAME MSN_424_13C
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PROCNO 1

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Time_ 11.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 50
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 297.9 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.0000000 W

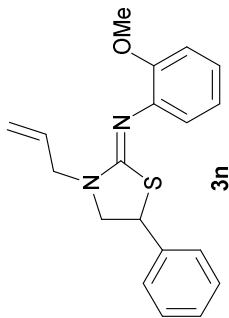
===== CHANNEL f2 =====
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 21.0000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W

F2 - Processing parameters
SI 16384
SF 150.9128630 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

58.20
55.91
49.29
46.78

77.44
77.23
77.02

159.40
151.80
141.46
139.22
133.00
128.78
128.13
127.59
124.12
122.94
120.85
118.05
111.79

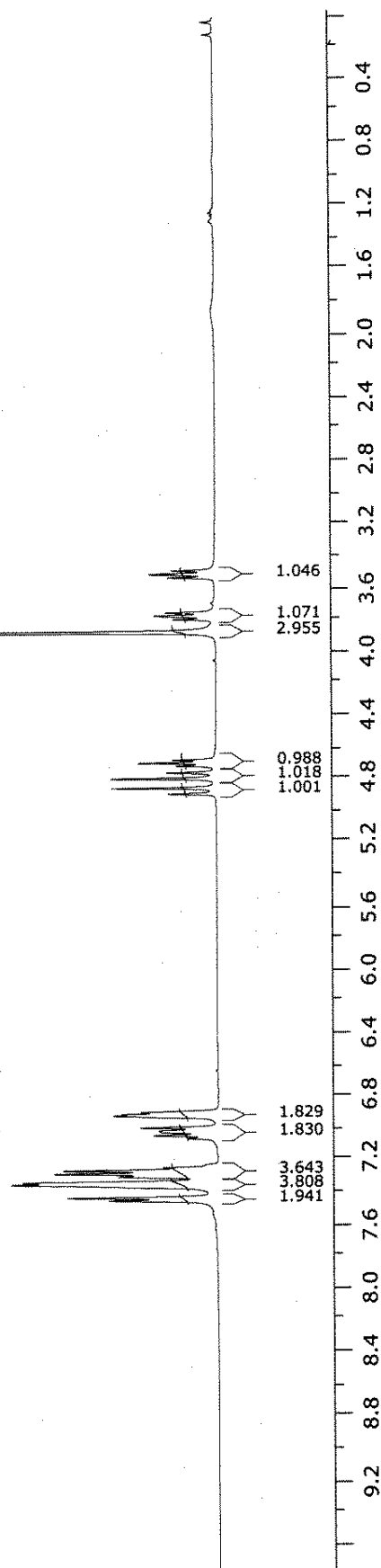
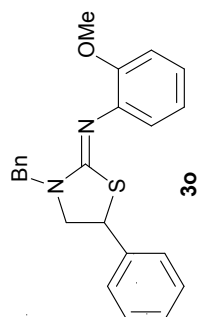


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

3.4966
3.5131
3.5193
3.5407
3.7612
3.7793
3.7844
3.8034
3.8840

4.6880
4.7062
4.7245
4.7681
4.8052
4.8653
4.9025

6.9126
6.9238
6.9323
7.0084
7.0291
7.0353
7.0571
7.2584
7.2774
7.2968
7.3170
7.3529
7.3652
7.4475
7.4657



46.8708
50.2640
56.0432
58.0094

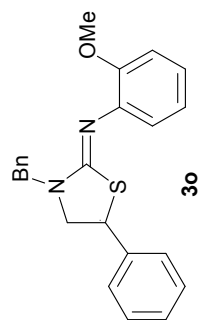
76.9139
77.2320
77.5500

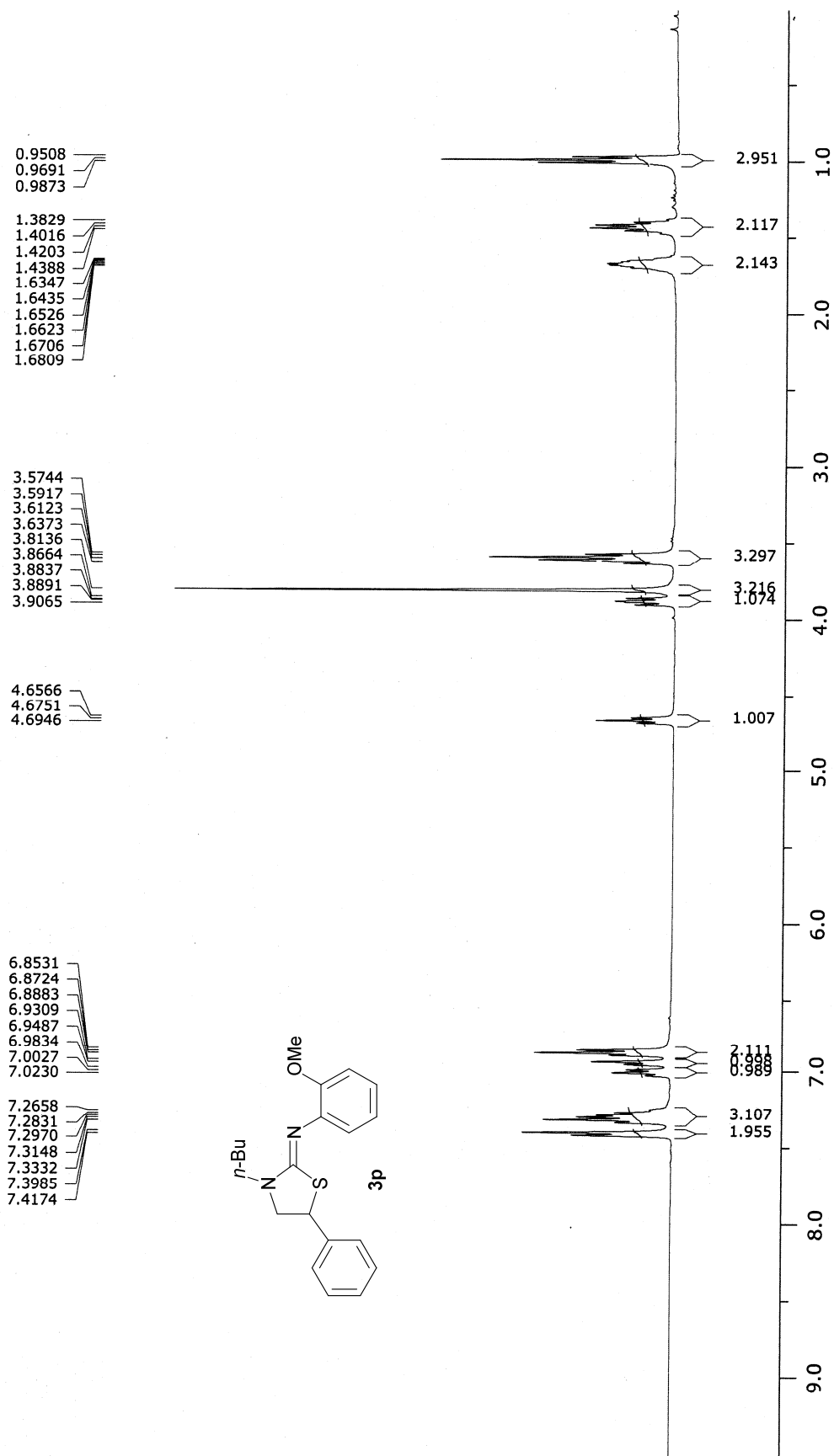
111.8734

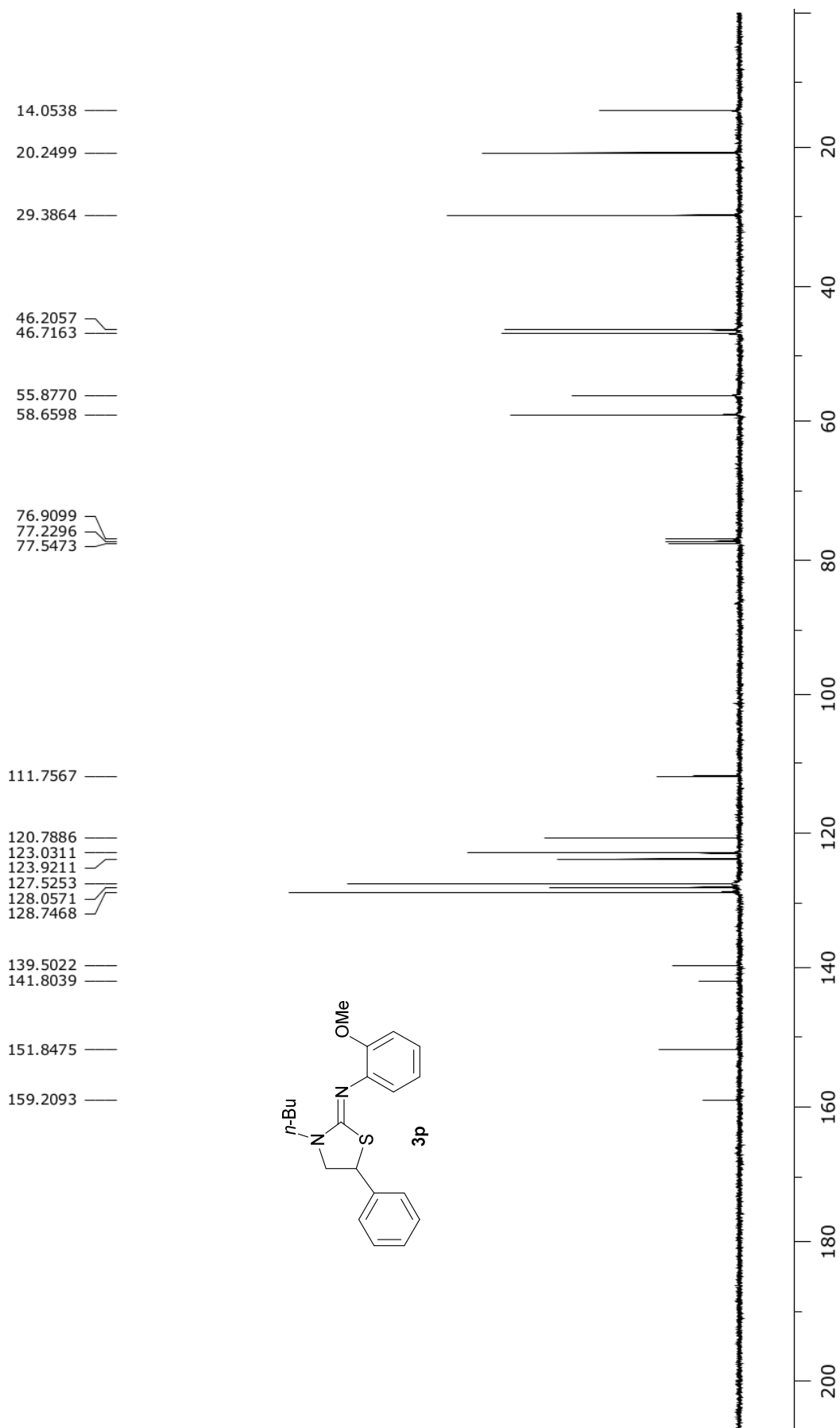
120.9706
122.9950
124.2122
127.6054
127.6558
128.1840
128.6475
128.7096
128.8259
137.2408
139.1827
141.6054

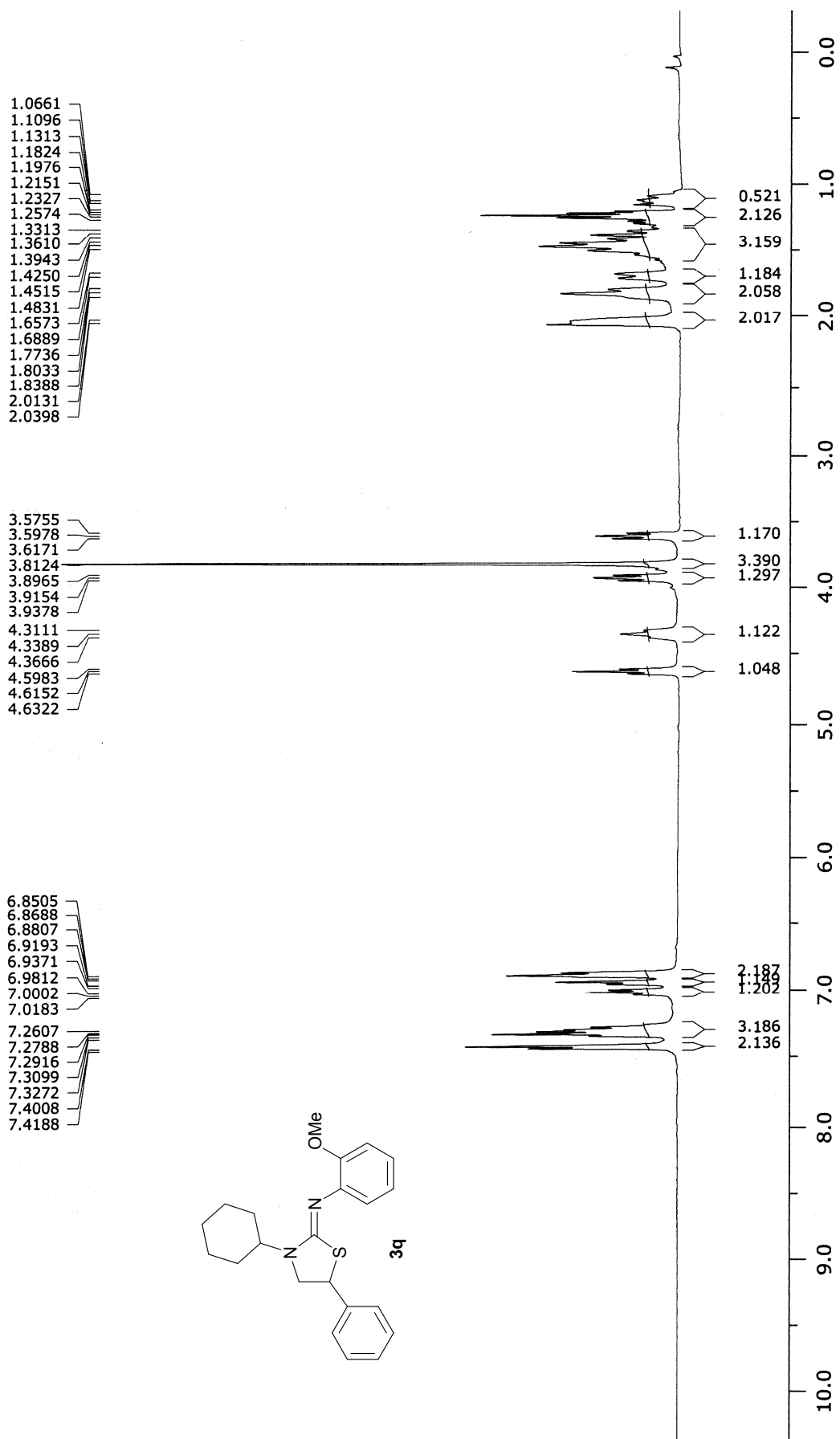
151.9668

159.7159









25.6757
25.8059
25.8521
29.7864
30.4983

46.6295
54.3268
54.5707
55.9206

76.9119
77.2300
77.5490

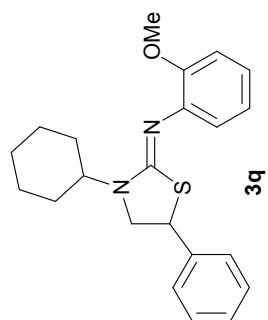
111.8734

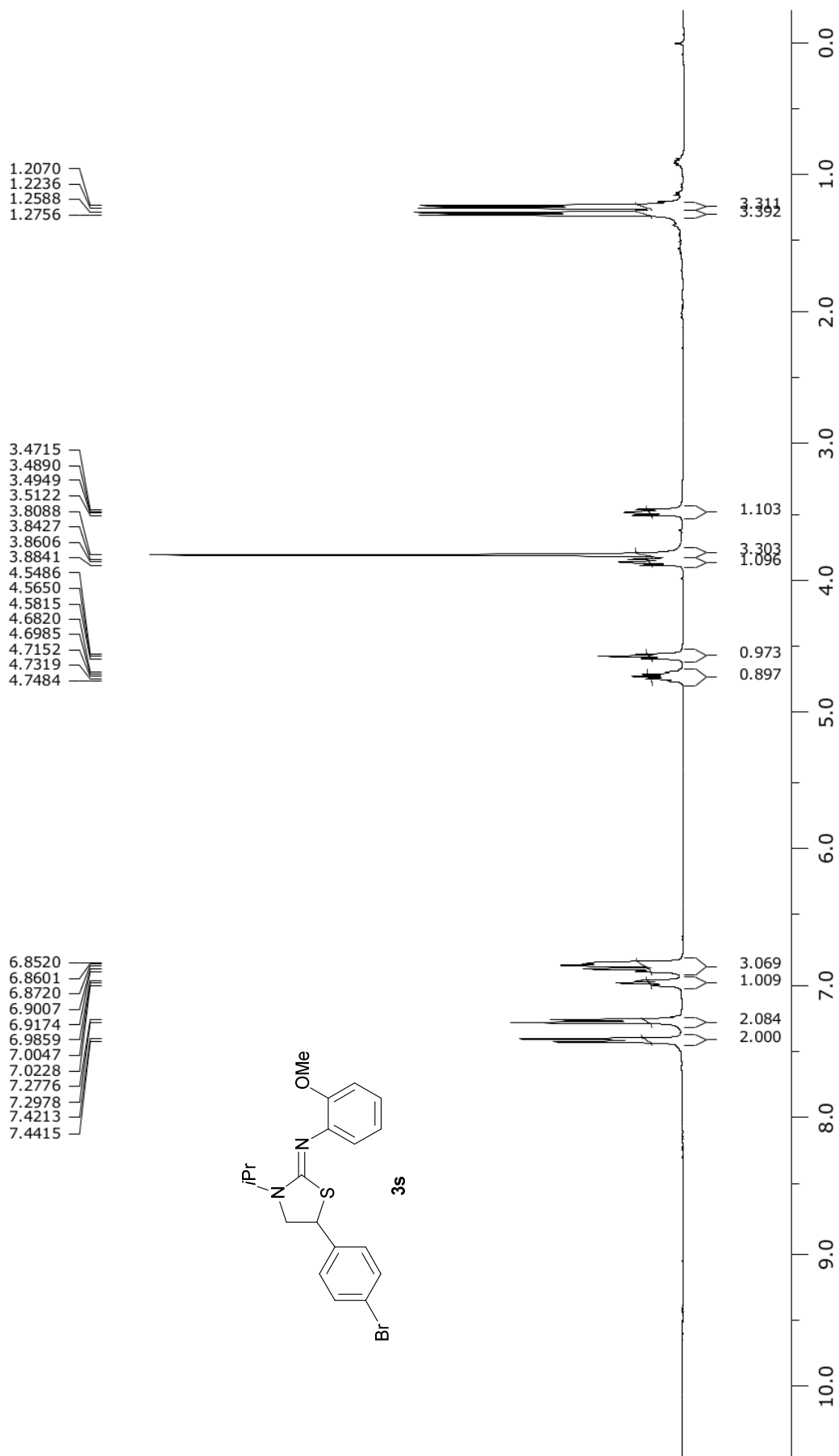
120.8271
123.3545
123.9618
127.4669
128.0237
128.7237

139.8687
141.8545

151.8469

159.3755





19.3724
19.7846

45.8796
46.5270

53.2655
55.9463

76.9119
77.2300
77.5481

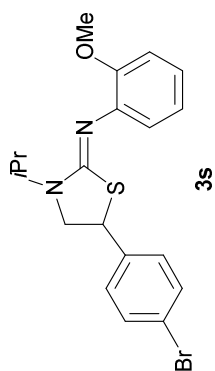
111.7763

120.8661
121.9406
123.0625
124.1354
129.2402
131.8979

139.1466
141.6001

151.7968

158.8663



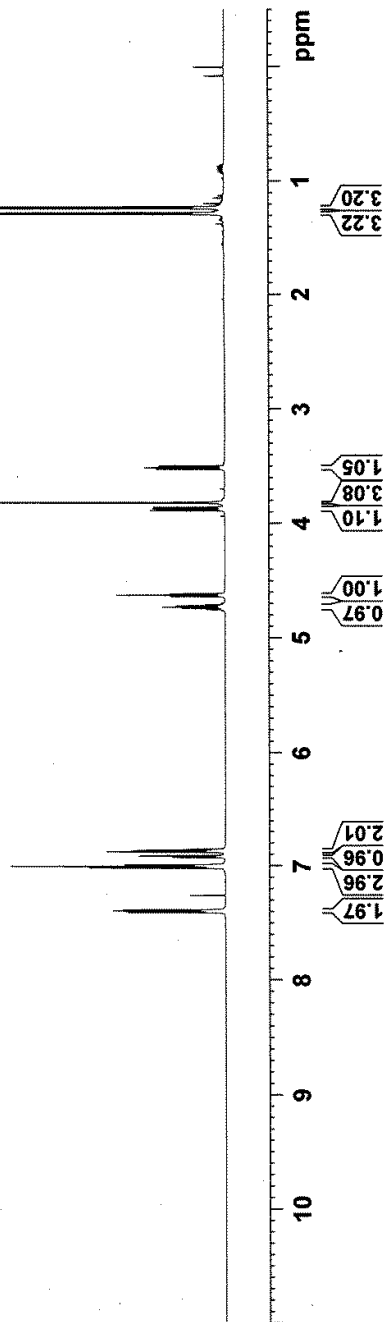
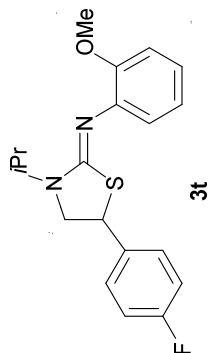


MSN-424-F_1H

Current Data Parameters
NAME: MSN-424-F_1H
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20131220
Time_: 12:34
INSTRUM: spect
PROBHD: 5 mm PABBO-BB/7
PULPROG: zg30
TD: 32768
SOLVENT: CDCl3
NS: 16
DS: 4
SWH: 12019.242 Hz
FIDRES: 0.366798 Hz
AQ: 1.3631488 sec
RG: 34.76
DW: 41.600 usec
DE: 6.50 usec
TE: 300.2 K
D1: 1.00000000 sec
TD0: 1
CHANNEL f1
SFO1: 600.1737063 MHz
NUC1: 1H
P1: 12.00 usec
PL1: 21.00000000 W
F2 - Processing parameters
SI: 16384
SF: 600.1700148 MHz
WDW: EM
SSB: 0
GB: 0
PC: 1.00

1.288
1.277
1.238
1.227

7.409
7.406
7.400
7.394
7.389
7.386
7.260
7.023
7.019
7.016
7.009
7.005
6.997
6.994
6.991
6.928
6.925
6.914
6.912
6.879
6.878
6.868
6.864
6.856
4.743
4.731
4.720
4.638
4.627
4.615
3.889
3.878
3.873
3.861
3.821
3.529
3.517
3.513
3.501



19.3006
19.9111

45.9347
46.5418

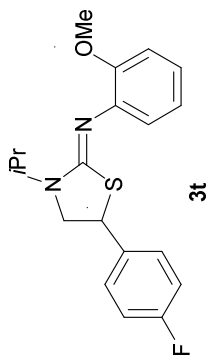
53.5445
55.9806

76.9120
77.2300
77.5480

111.8069
115.6008
115.8150
120.8901
123.1129
124.1413
129.2120
129.2929
135.6363
135.6681
141.6449

151.8648

159.0944
161.2471
163.7035



20

40

60

80

100

120

140

160

180

200

MSN-4-24-G_1H

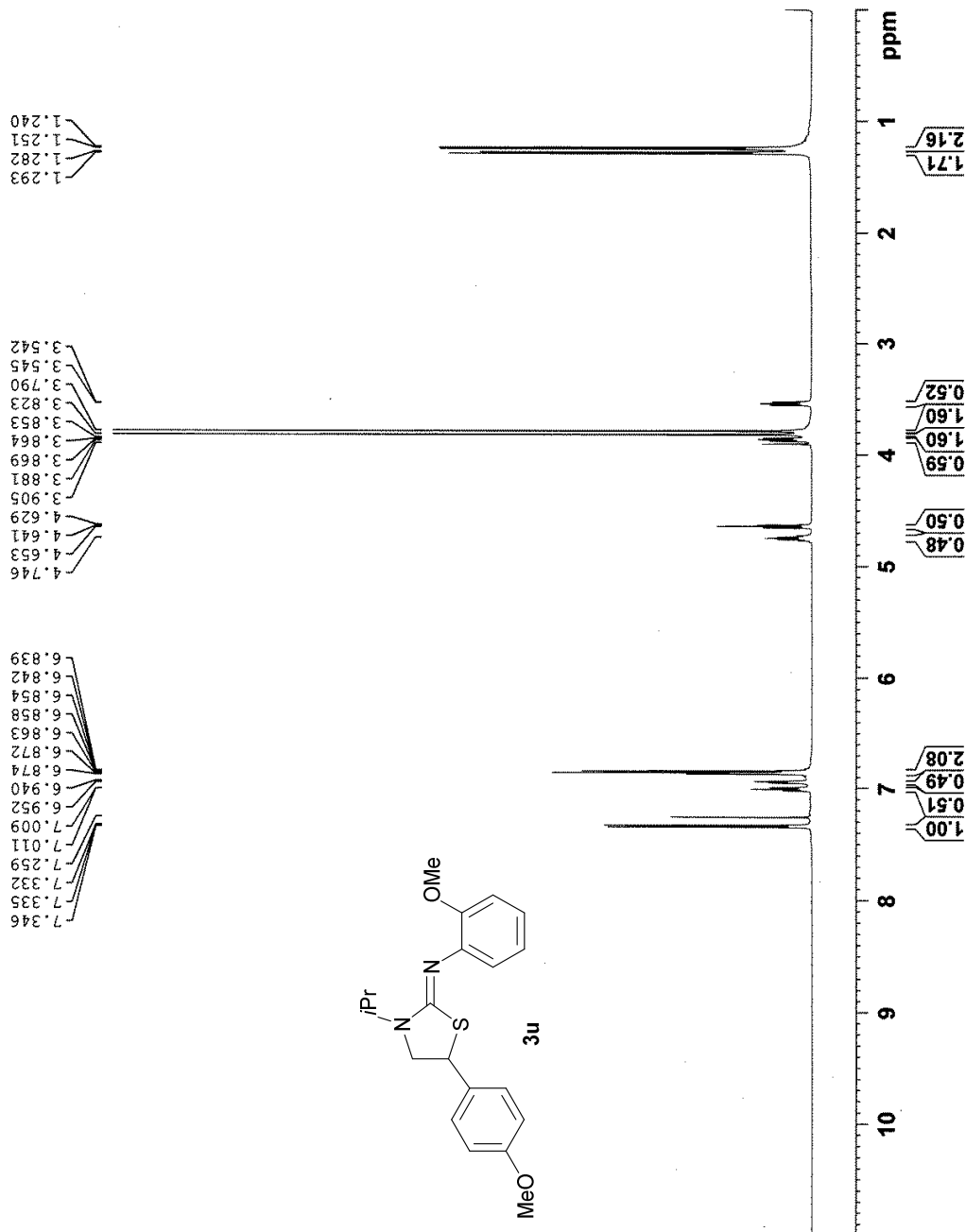


Current Data Parameters
 NAME MSN-4-24-G_1H
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131217
 Time 14:06
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 54.94
 DW 41.600 usec
 DE 2.50 usec
 TE 300.2 K
 D1 1.00000000 sec
 TDO 1

CHANNEL f1
 SFO1 600.1737063 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 21.00000000 W

F2 - Processing parameters
 SI 16384
 SF 600.1700152 MHz
 WFF 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



MSN-4-24-G_13C



Current Data Parameters
 NAME MSN-4-24-G_13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131217
 Time 14.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 98
 DS 2
 SWH 36057.691 Hz
 FIDRES 1.100393 Hz
 AQ 0.4543829 sec
 RG 65.24
 DW 13.867 usec
 DE 6.50 usec
 TE 297.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9279571 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 95.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1724007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 70.00 usec
 PLW2 21.00000000 W
 PLW12 0.61714000 W
 PLW13 0.30239999 W

F2 - Processing parameters
 SI 16384
 SF 150.9128368 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

19.26
20.15

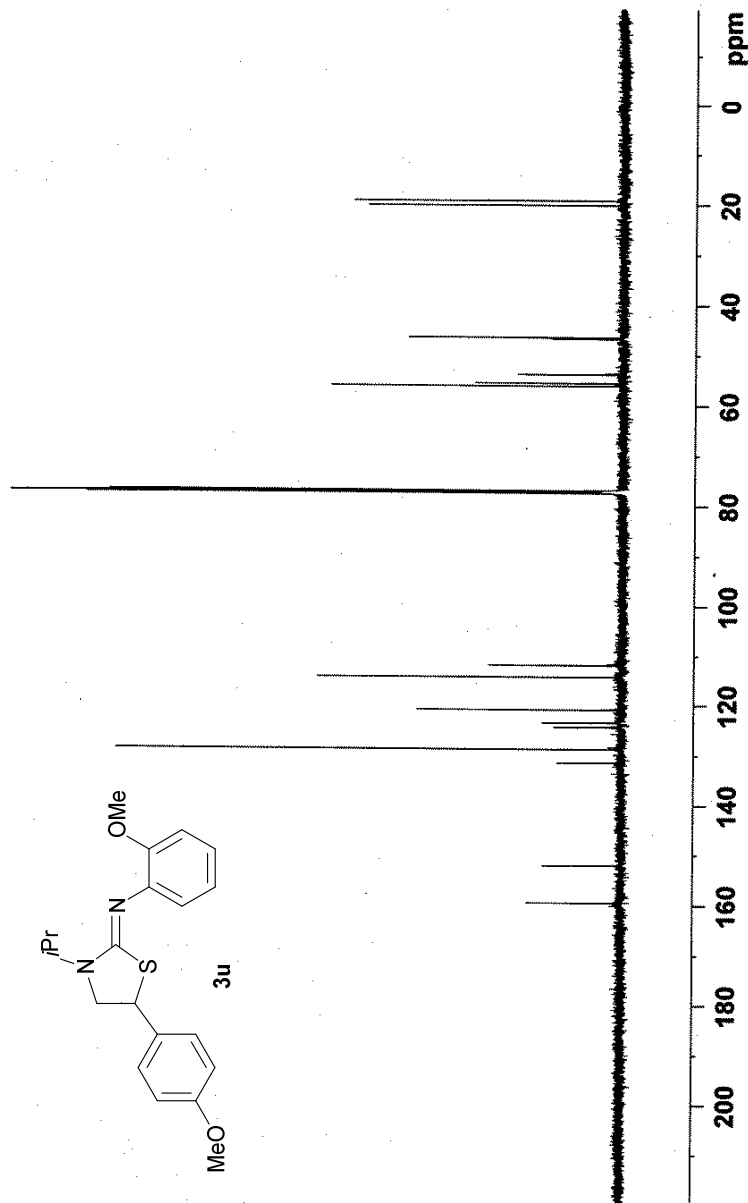
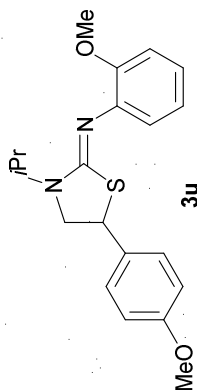
46.47
46.72

53.83
55.53
56.10

77.02
77.23
77.45

111.93
114.26
120.86
120.95
123.46
124.34
128.81
131.42

152.11
159.57



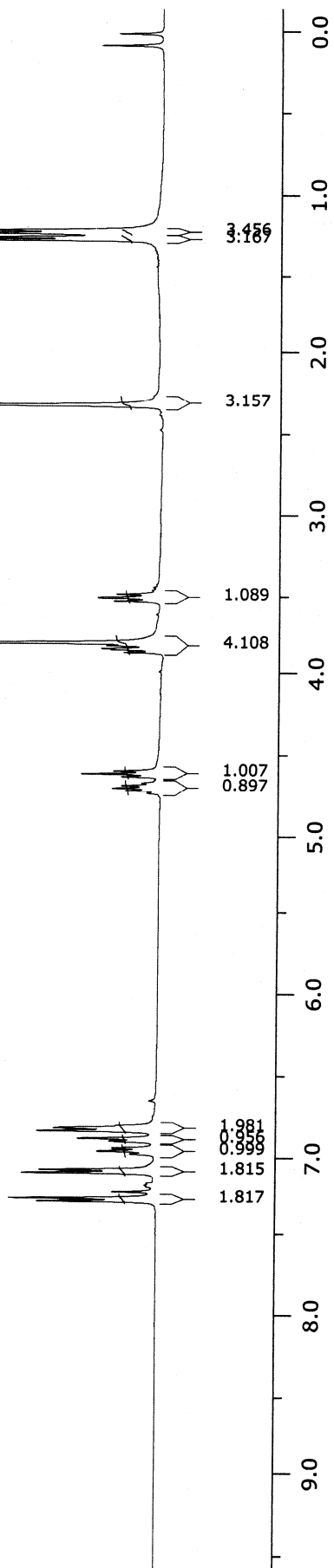
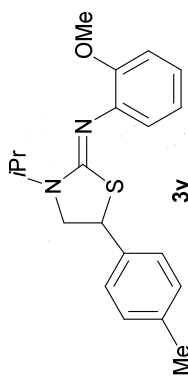
1.2091
1.2258
1.2529
1.2698

2.3070

3.4961
3.5163
3.5188
3.5394
3.8042
3.8216
3.8393
3.8457
3.8632

4.5990
4.6169
4.6349
4.6748
4.6914
4.7082
4.7250

6.8226
6.8370
6.8544
6.9014
6.9182
6.9610
6.9811
6.9988
7.0972
7.1166
7.2400
7.2788
7.2984



19.2171
20.1106
21.2787

46.5268
46.5951

53.5375
56.0559

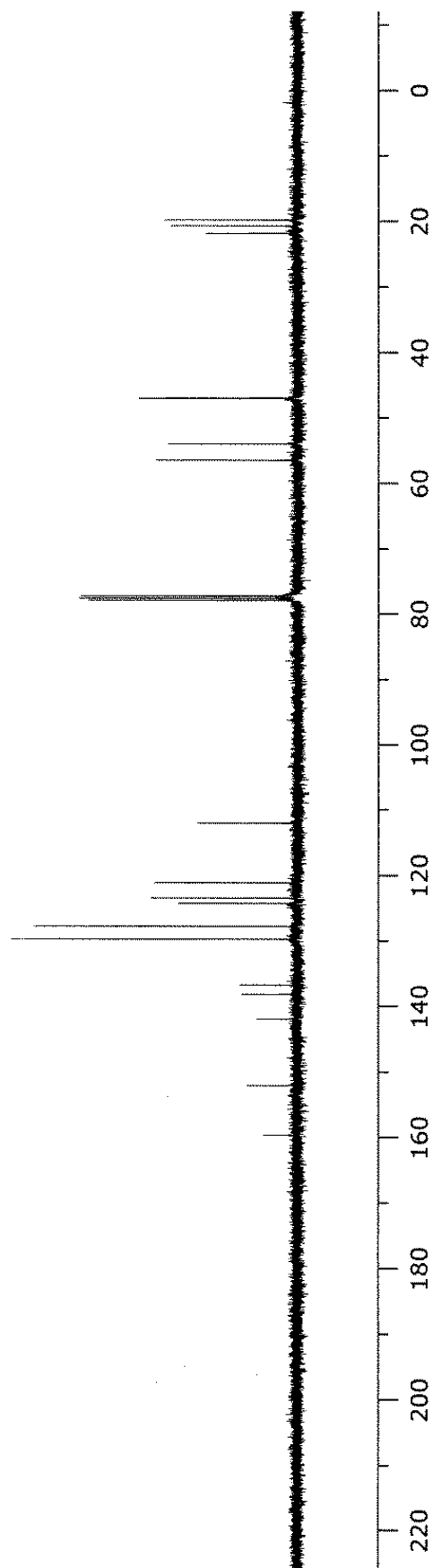
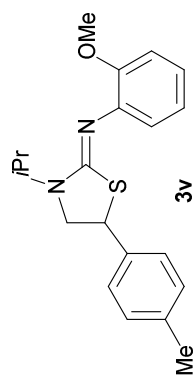
76.9116
77.2300
77.5478

111.8288

120.9019
123.2128
124.0472
127.5370
127.5672
129.4998
129.5325
136.5812
137.9944
141.7959

151.9791

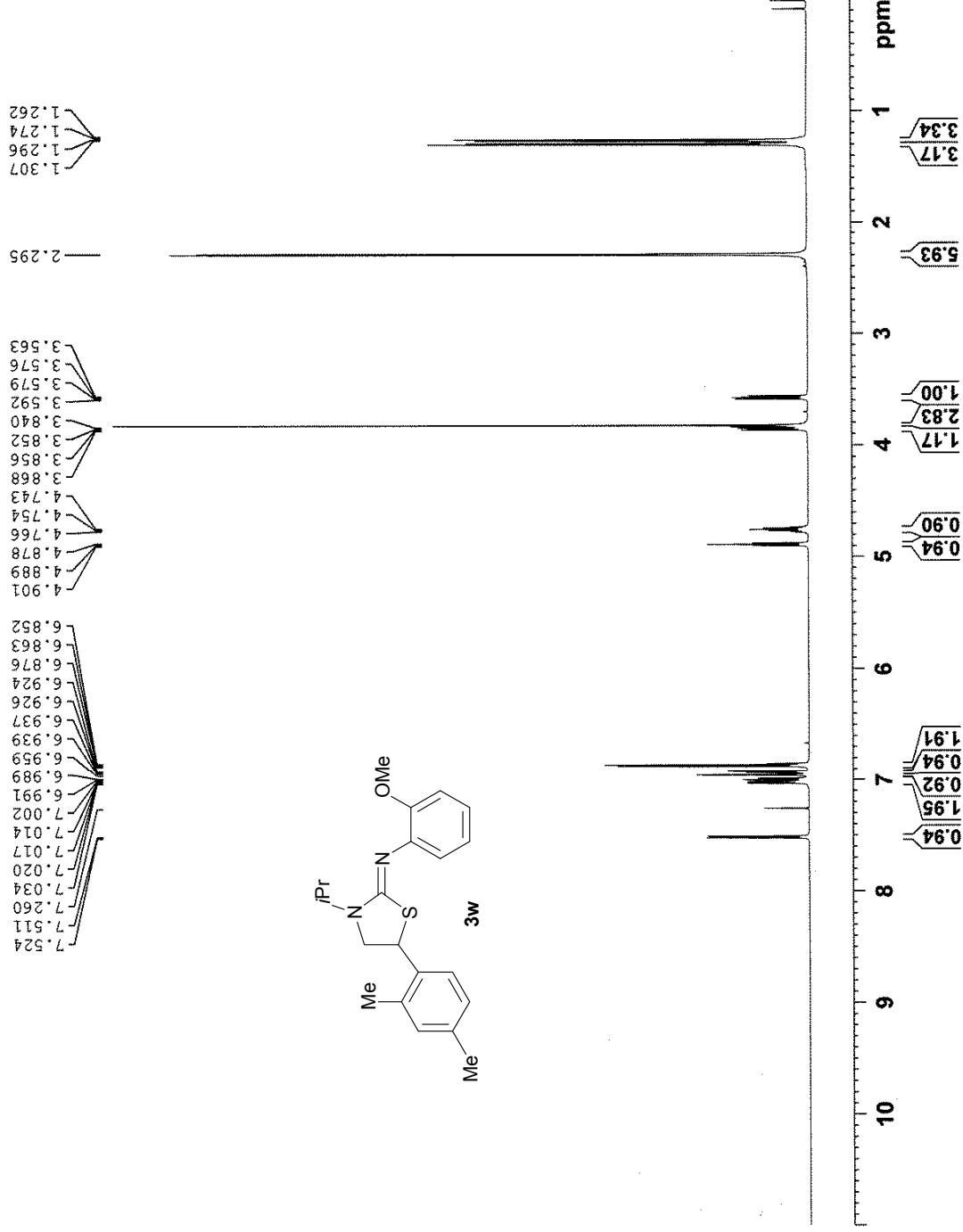
159.5762



MSN-4-24-H-1H



Current Data Parameters
 NAME MSN-4-24-H-1H
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20131217
 Time_ 14.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 12019.236 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 22.18
 DW 41.640 usec
 DE 6.50 usec
 TE 296.5 K
 D1 1.00000000 sec
 TDO 1
 CHANNEL f1
 SFO1 600.137063 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 21.00000000 W
 F2 - Processing parameters
 SI 16384
 SF 600.1700148 MHz
 SWH 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



19.2676
19.6438
19.9841
21.1217

42.4073
46.5860
52.2063
56.0122

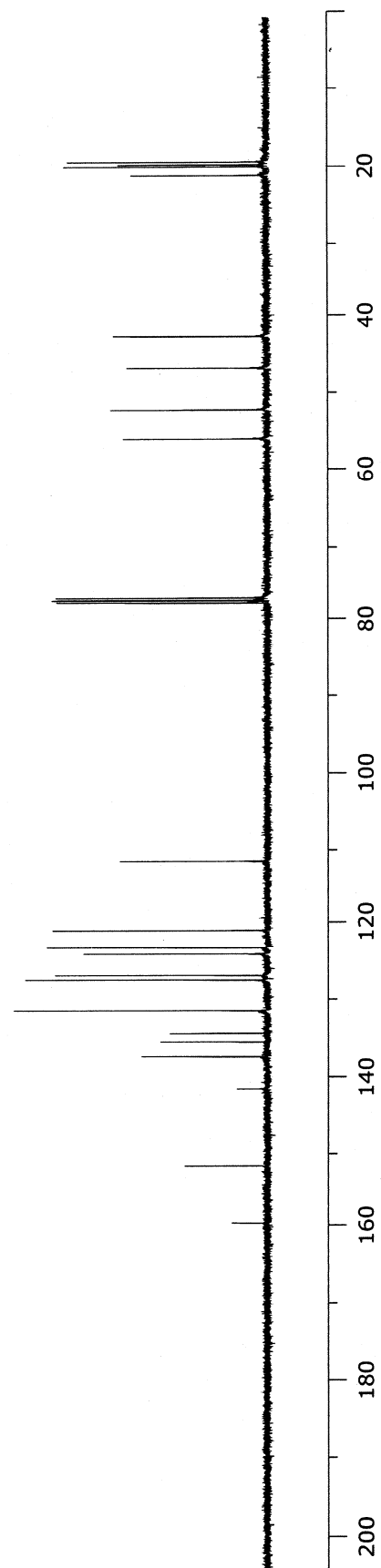
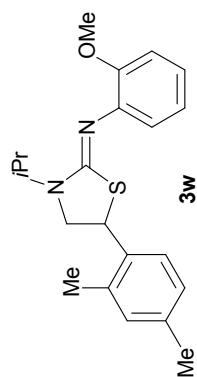
76.9121
77.2300
77.5482

111.7532

120.8534
123.1528
123.9974
126.8152
127.4139
131.4000
134.4853
135.6005
137.5398
141.7613

151.9542

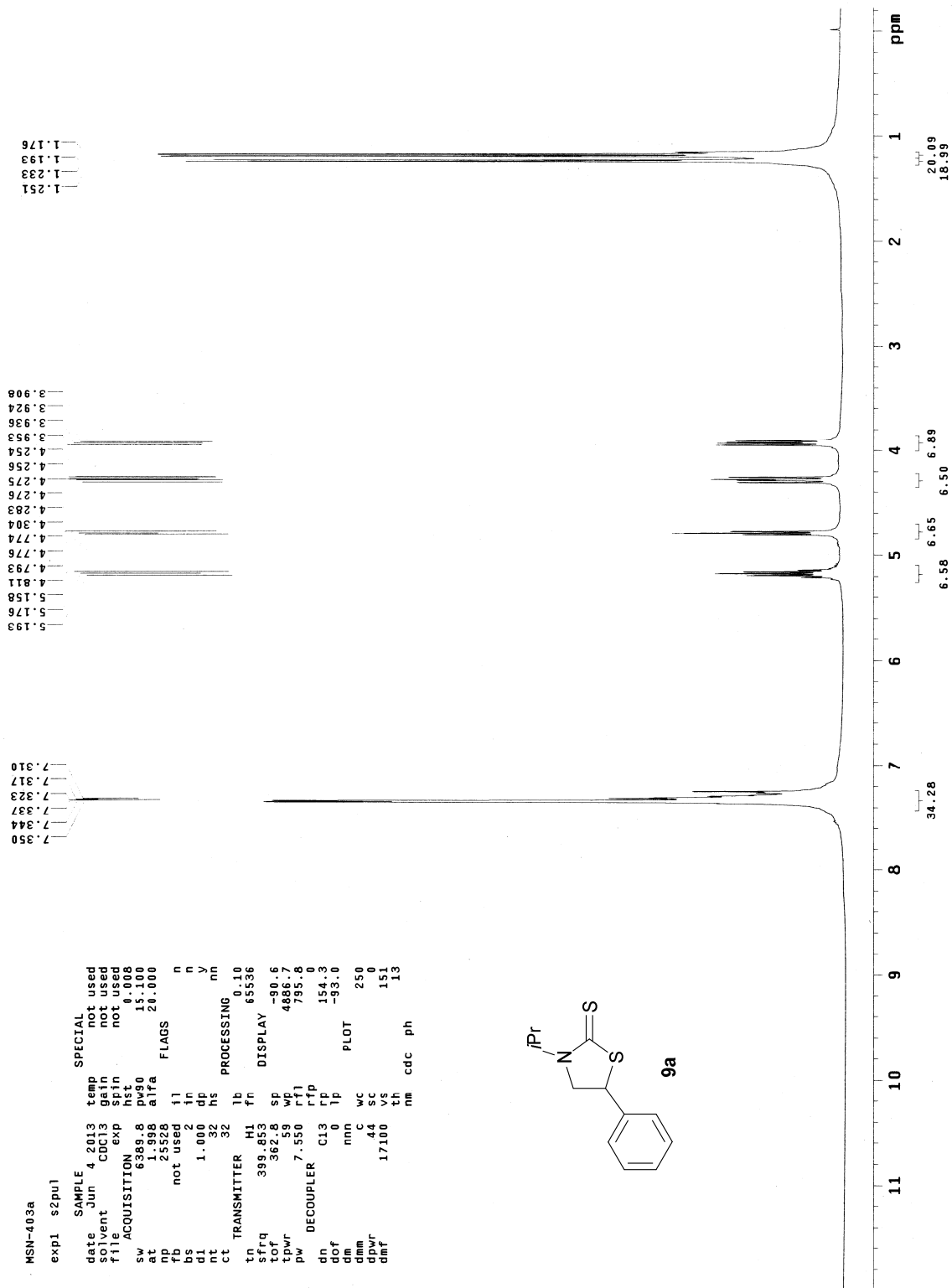
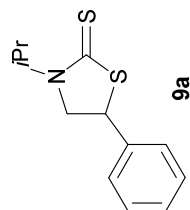
159.5704




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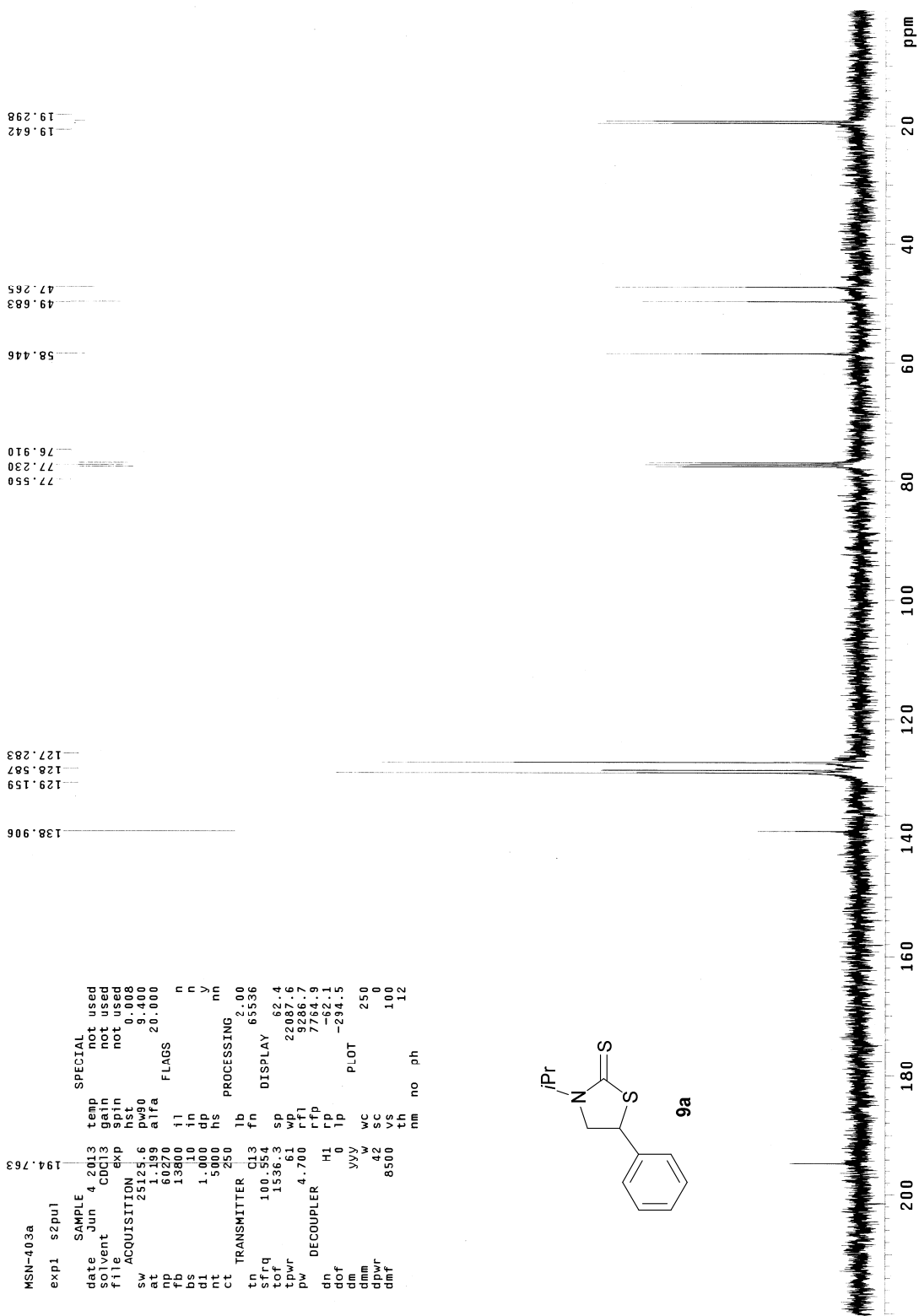
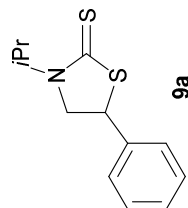
MSN-403a
exp1 s2pu1
date 4 2013 temp not used
solvent Jun CDC13 gain not used
file exp not used
ACQUISITION hst 0.008
sw 6389.8 pw90 15.100
at 1.998 alfa 20.000
np not used ll n
fb not used ll n
bs 1.002 in n
d1 32 dp y
ct 32 hs nm
tn TRANSMITTER H1 lb 0.10 PROCESSING 0.10
sfrq 399.853 fn 65536
tof 362.8 sp DISPLAY
tpwr 59 wp 4886.7
pw 7.550 rfl 795.8
DECOUPLER C13 rfp 0
dn 0 tp 154.3
dof 0 tp -95.0
dmc nmc wc 250
dmm 44 sc 0
dpwr 17100 vs 151
dmf th 13
nm cdc ph

```



MSN-403a
exp1 s2pul
194.763

SAMPLE		SPECIAL	
date	Jun 4 2013	temp	not used
solvent	CDCl3	gain	not used
file		spin	not used
sw	ACQUISITION	exp	0.008
at	25125.6	hst	9.400
fb	1025.9	pw90	20.000
fl	13800	alpha	20.000
nt	1.000	fl	20.000
bs	10	in	n
di	10	in	n
nt	5000	hs	nn
ct	250	lb	2.00
tn	100.554	fn	65536
sfrq	1536.3	sp	62.4
tof	61	wp	22087.5
tpwr	4.700	rfn	758.9
pw	DECOUPLER	rfp	-62.1
dn	H1	rfp	-234.5
dof	0	lp	PLOT
dm	yvv	wc	250
dmm	42	sc	0
dpwr	8500	vs	100
dmf		th	12
		nm	ph



1.234
1.216
1.170
1.153

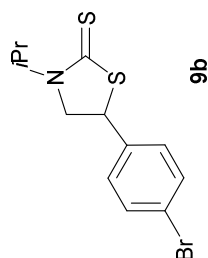
5.169
5.152
5.136
4.734
4.716
4.698
4.681
4.260
4.252
4.231
3.890
3.874
3.860
3.845

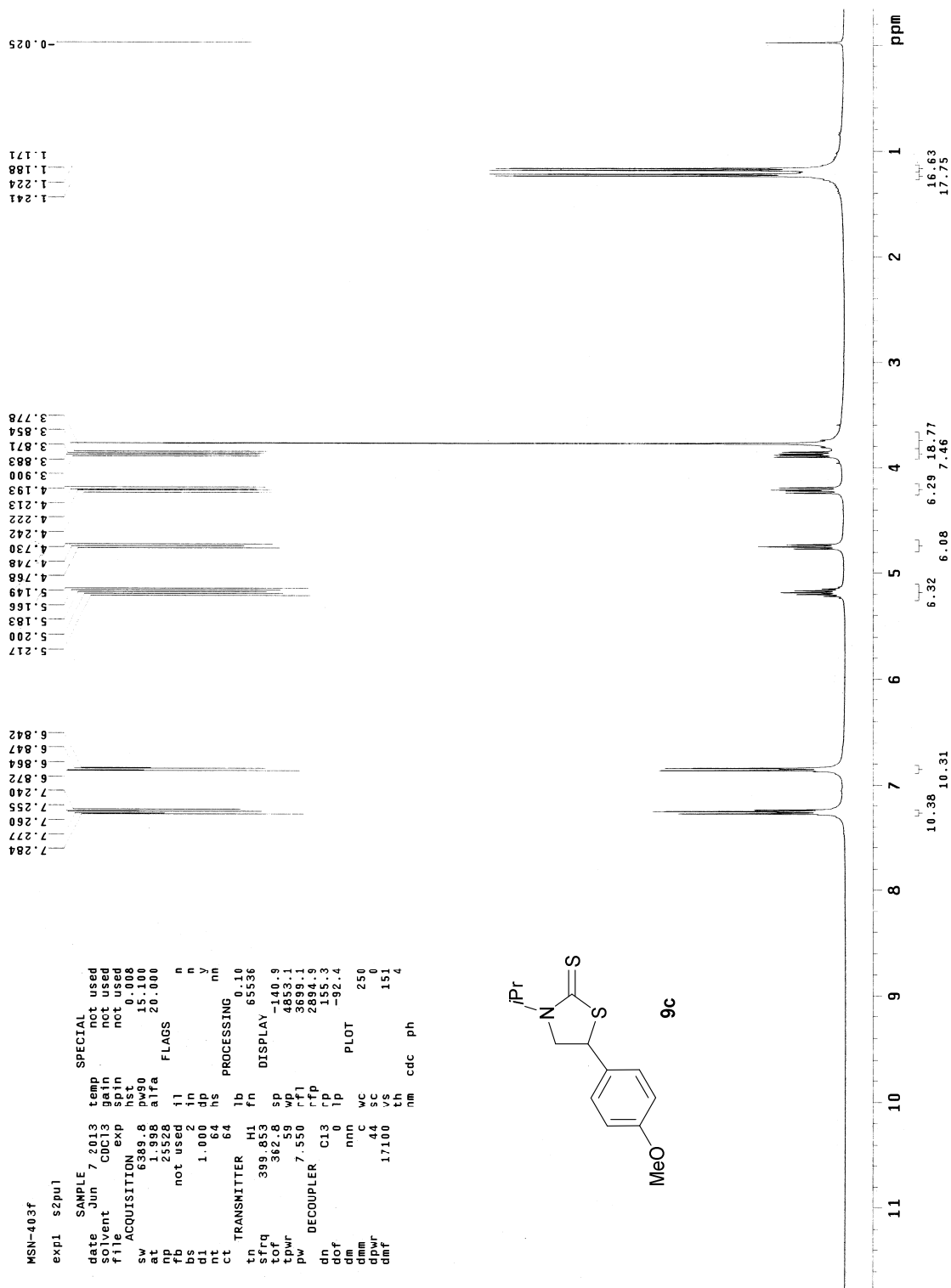
7.466
7.445
7.240
7.227
7.206

MSN-403e

exp1 s2pu1

date	Jun 9 2013	SAMPLE	temp	not used	SPECIAL
solvent	CDCl3	gain	not used		
file		spin	not used		
sw	6389.8	hst	0.008		
at	1.998	pw90	15.100		
np	25528	alfa	20.000	FLAGS	
fb	not used	fl		n	
ds	not used	tn		n	
dt	1.006	dp		y	
nt	32	hs		nn	
ct	32	hs		nn	
tn	TRANSMITTER	lb	0.10		
sfrq	399.853	fn	65536		
tor	362.8	sp	-39.7	DISPLAY	
tpwr	7.550	rfl	4911.8		
pw	7.550	rfl	803.8		
dn	DECOUPLER	C13	140.6		
dof	0	lp	-87.3		
dm	nnn	wc	250	PLOT	
dmm	c	sc	119		
dpwr	44	th	113		
dmt	17160	nm	cdc	ph	





```

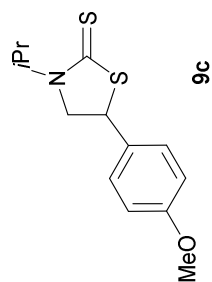
MSN-403f
exp1 s2pu1
date 9 2013 temp not used
solvent Jun CDCl3 gain not used
file exp not used
sw ACQUISITION hst 0.008
at 25125.6 pw90 9.400
np 1.199 alpha 20.000
pb 60270 il n
bs 13600 il n
qt 1.000 dp n
nt 5000 hs v
ct TRANSMITTER 410 PROCESSING nm
tn c13 fb 2.00
sfrq 100.554 fn 65536
tof 1536.3 sp DISPLAY
tpwr 61 wp -127.7
pw 4.700 rfl 22418.1
dn DECOUPLER H1 rfp 9312.0
dof 0 ip -53.6
dm yyy PLOT -286.3
dm wc 250
dmn 42 sc
dmw 8500 vs
dmf th nm no ph

```

19.032
 19.382
 46.579
 49.393
 55.182
 58.308
 76.910
 77.230
 77.543

114.173
 128.221
 130.509

159.376



200 180 160 140 120 100 80 60 40 20 ppm

