

A Concise Asymmetric Synthesis of *cis*-2,6-Disubstituted *N*-Aryl Piperazines via Pd-Catalyzed Carboamination Reactions

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Supporting Information (continued).

¹H and ¹³C NMR spectra for new compounds in Schemes 2–3 and Tables 1–2

JSNVII-192-2-chiral

File: Proton

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnsakha

INOVA-500 "Sn.Chem.LSA,UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

20 repetitions

OBSERVE H1, 499.9042604 MHz

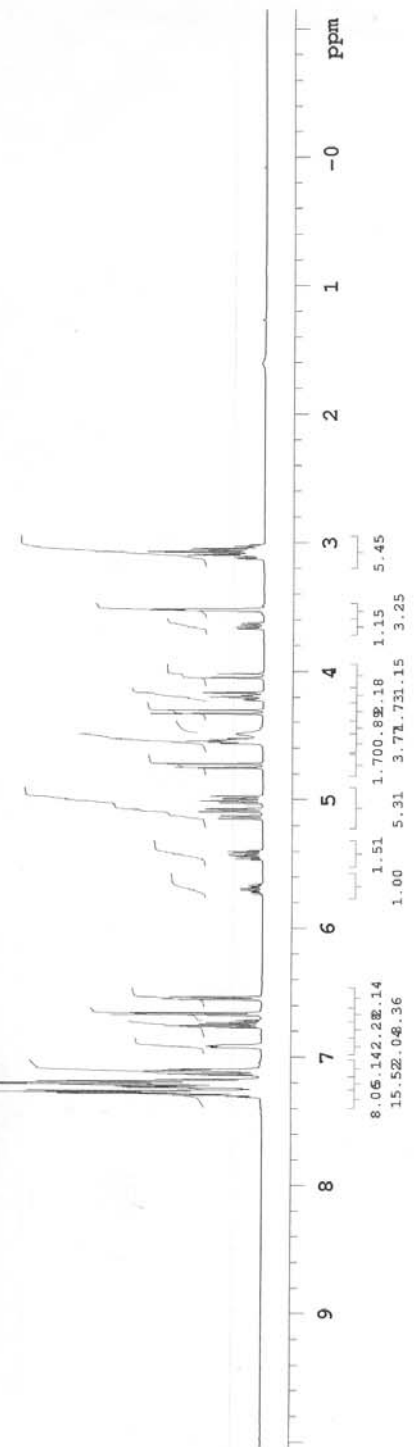
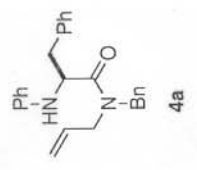
DATA PROCESSING

Line broadening 0.2 Hz

Ft size 65536

Total time 1 min, 8 sec

Acquisition date: Dec 7 2006



Standard Carbon

File: J5NVII-192-2-2-chiral-C13

Pulse Sequence: s2pnl

Solvent: cdcl3

Ambient temperature

Operator: Jnakhla

File: J5NVII-192-2-2-chiral-C13

INOVA-500 "Dy.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30165.9 Hz

260 repetitions

OBSERVE C13, 125.7010267 MHz

DECOUPLE H1, 499.9067532 MHz

Power 31 dB

continuously on

WALTZ-16 modulated

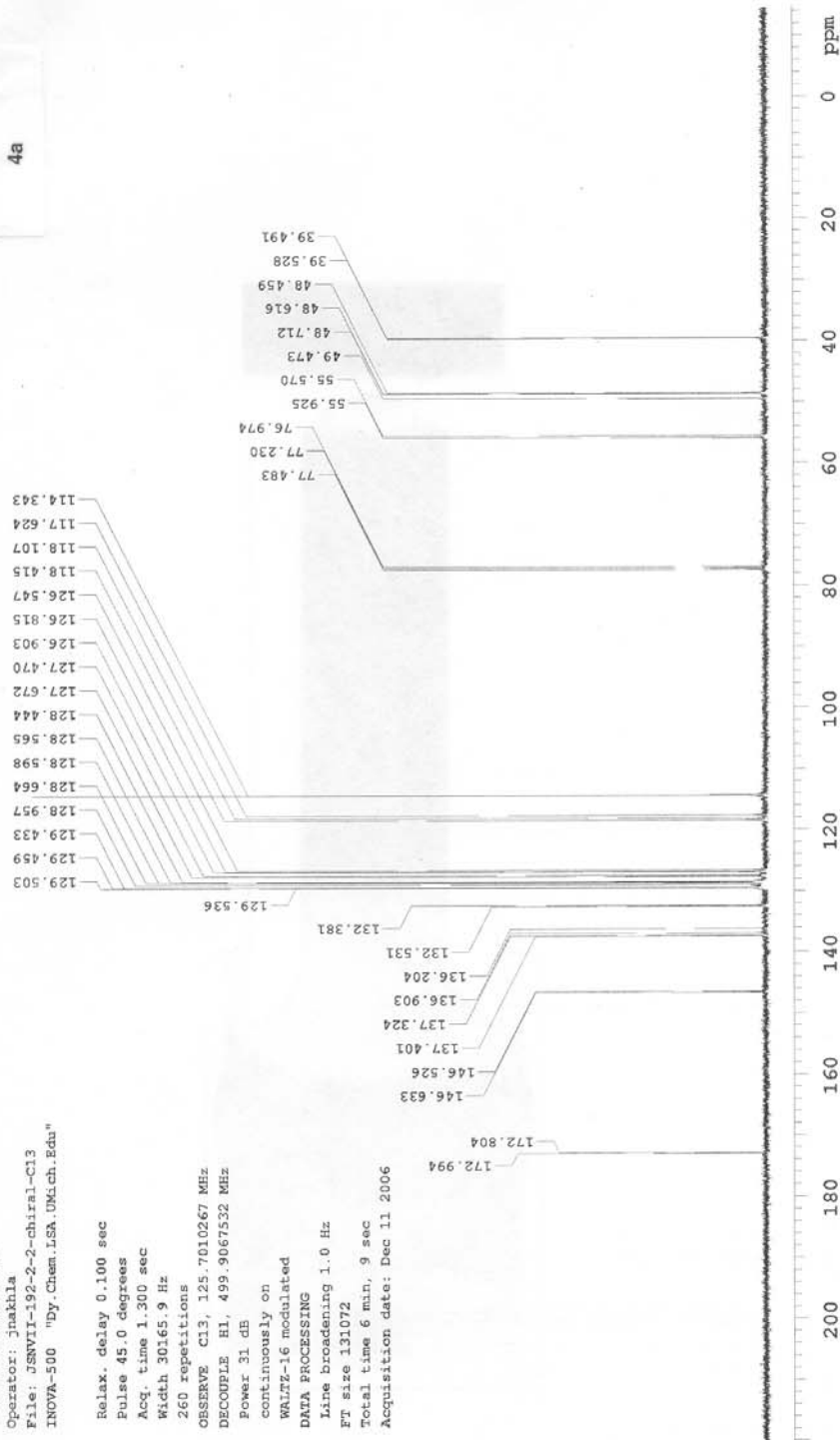
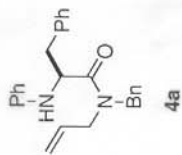
DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 6 min, 9 sec

Acquisition date: Dec 11 2006



JSNVII-186-chiral-HI

File: Proton

Pulse Sequence: #2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

INOVA-500 "Sn.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

48 repetitions

OBSERVE H1, 499.9042710 MHz

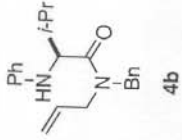
DATA PROCESSING

Line broadening 0.2 Hz

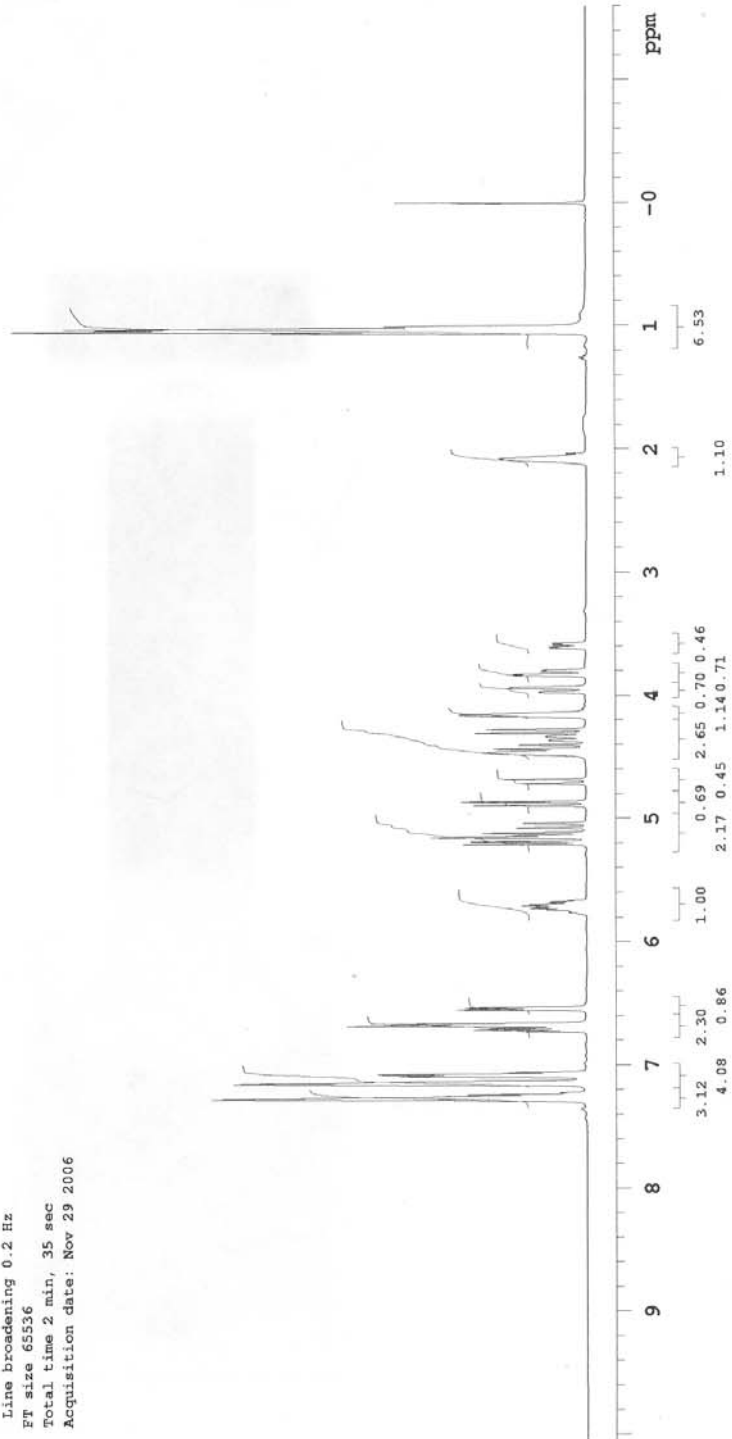
FT size 65536

Total time 2 min, 35 sec

Acquisition date: Nov 29 2006



4b



Standard Carbon

File: JSNVII-186-2-chiral-C13

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: Jnakhla

File: JSNVII-186-2-chiral-C13

INOVA-500 "Dy. Chem. LSA, UMich. Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30165.9 Hz

676 repetitions

OBSERVE C13, 125.7010350 MHz

DECOUPLE H1, 499.9067532 MHz

Power 31 dB

continuously on

WALTZ-16 modulated

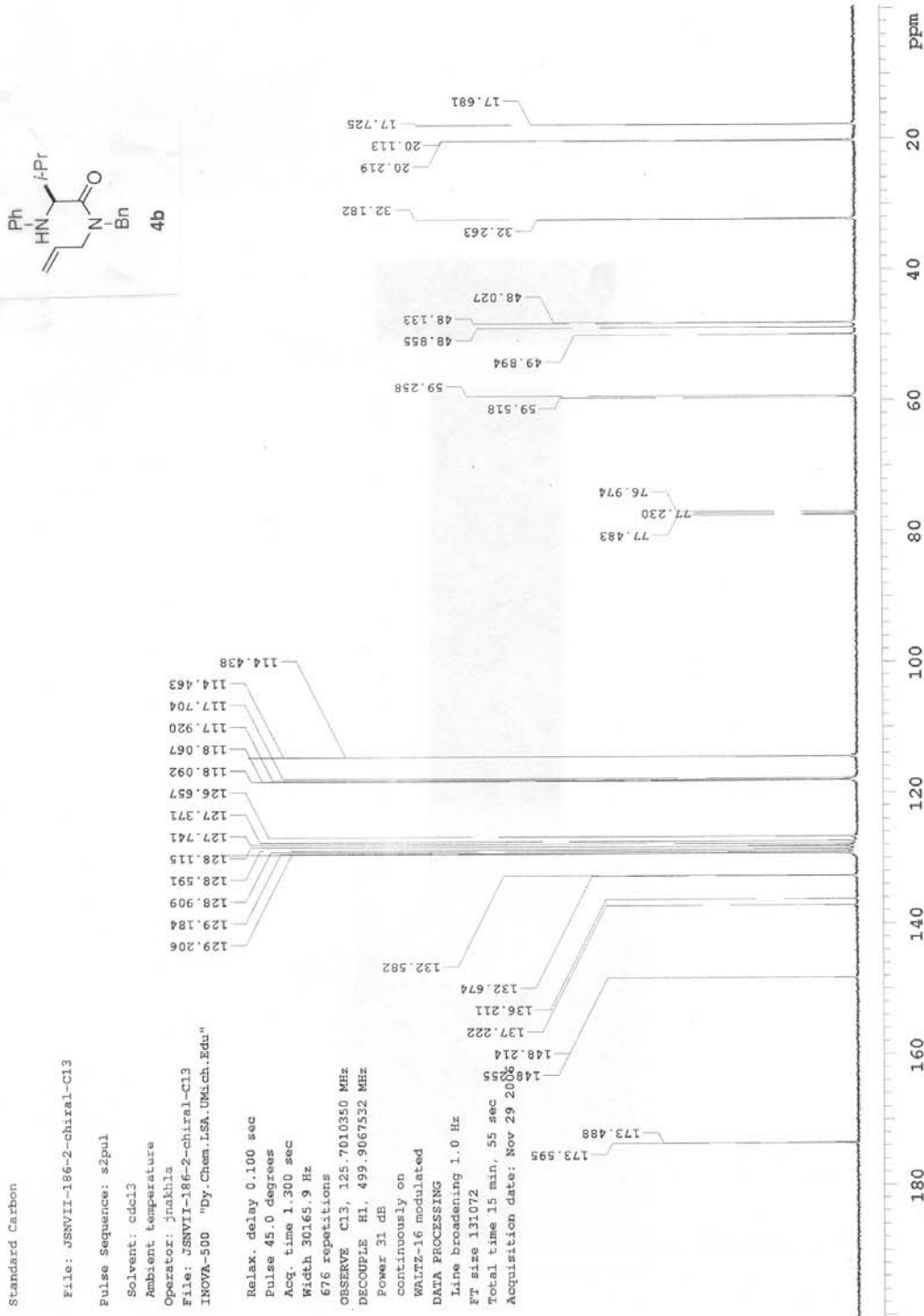
DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 15 min, 55 sec

Acquisition date: Nov 29 2006



J5NVII-204-2-chiral

File: Proton

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

INOVA-400 "Zr.Chem.LSA,UMich.Edu"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6399.5 Hz

8 repetitions

OBSERVE HI, 399.9649493 MHz

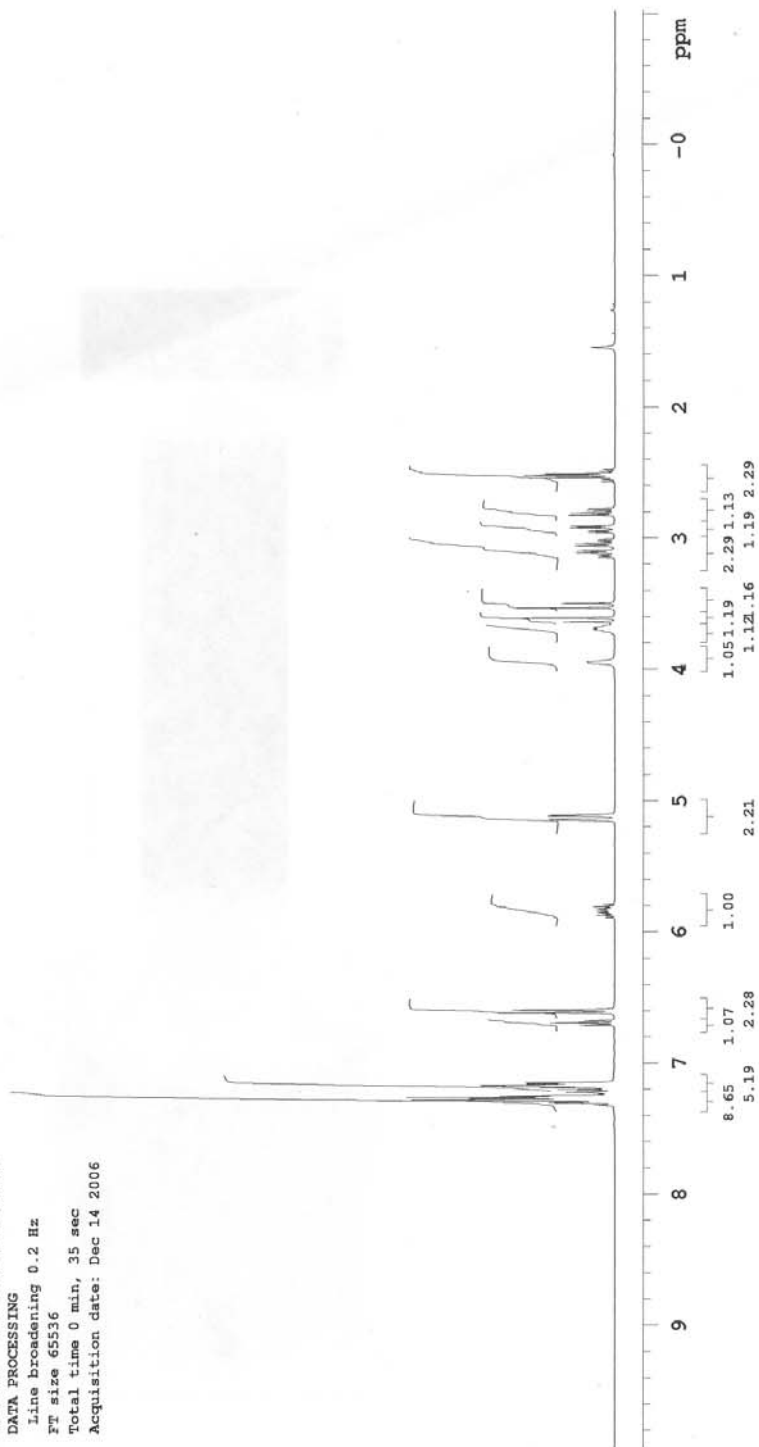
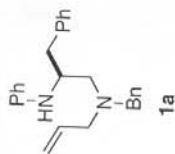
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min, 35 sec

Acquisition date: Dec 14 2006



JSNVII-204-2-C13-chiral

File: Carbon

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

INOVA-400 "Zr.Chem.USA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

292 repetitions

OBSERVE C13, 100.5712674 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

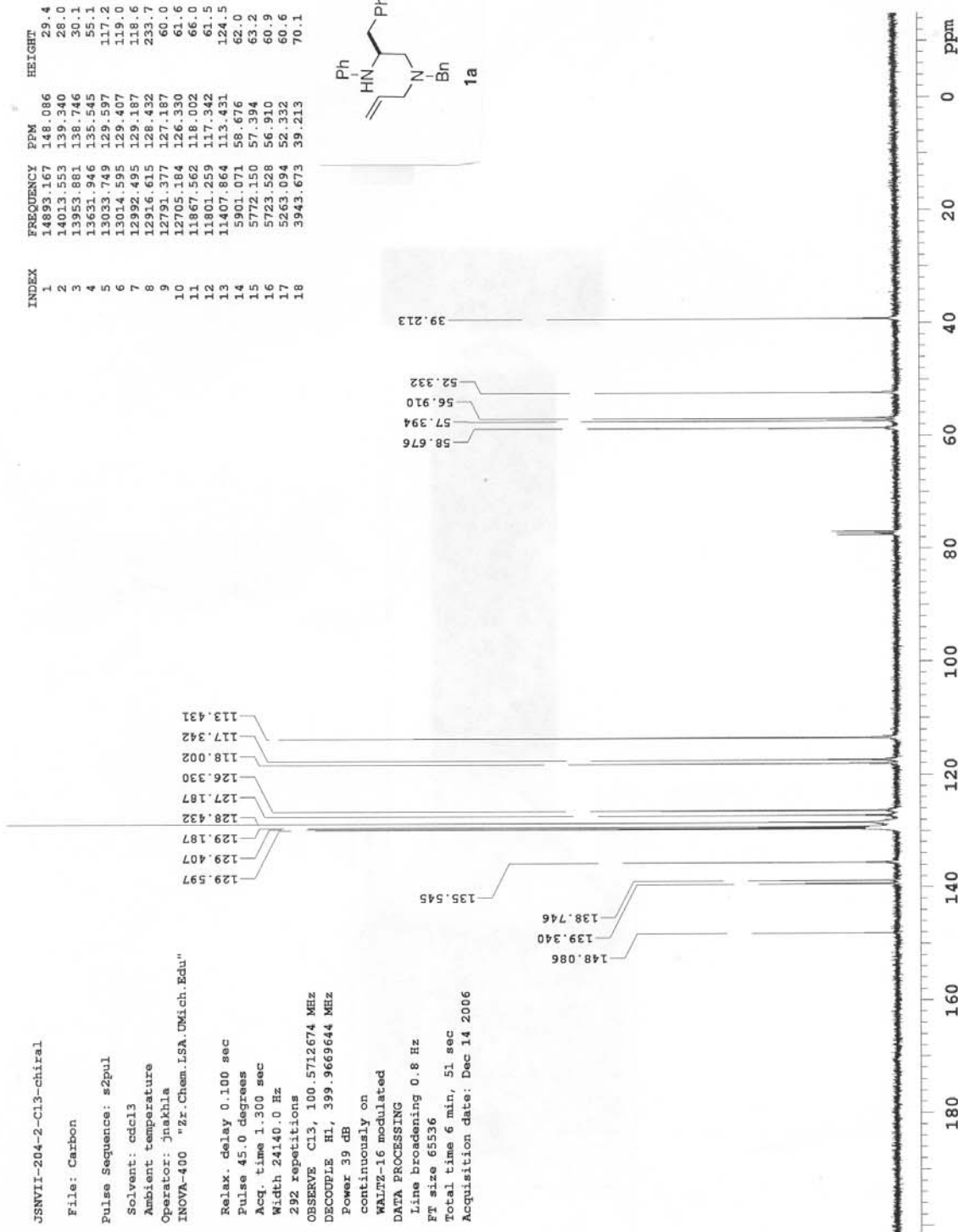
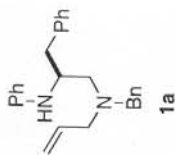
Line broadening 0.8 Hz

FT size 65536

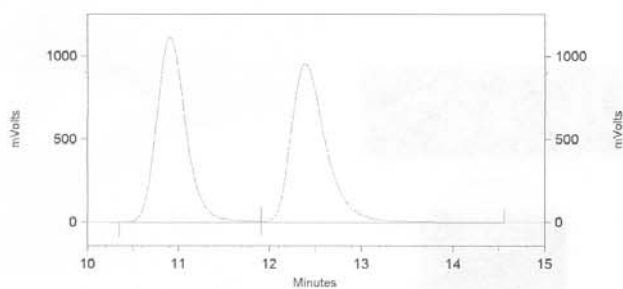
Total time 6 min, 51 sec

Acquisition date: Dec 14 2006

INDEX	FREQUENCY PPM	HEIGHT
1	14893.167	148.086
2	14013.553	139.340
3	13953.881	138.746
4	13631.946	135.545
5	13033.749	129.597
6	13014.595	129.407
7	12992.495	129.187
8	12916.615	128.432
9	12791.377	127.187
10	12705.184	126.330
11	11867.562	118.002
12	11801.259	117.342
13	11407.864	113.431
14	5901.071	58.676
15	5772.150	57.394
16	5723.528	56.910
17	5263.094	52.332
18	3943.673	39.213



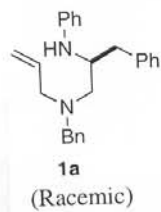
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVII-198-2-rac-jan1807-3.dat



OD-H
0.5% IPA/Hex
0.5 mL/min

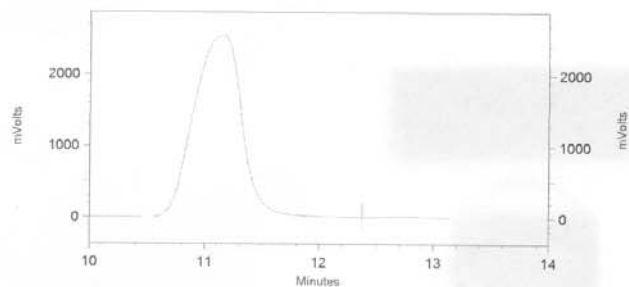
Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
10.908	24925024	49.652
12.383	25274013	50.348
Totals	50199037	100.000



OD-H
0.5% IPA/Hex
0.5 mL/min

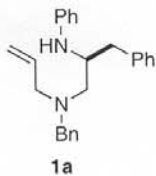
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Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
11.150	73900303	98.912
12.717	812861	1.088
Totals	74713164	100.000

OD-H
0.5% IPA/Hex
0.5 mL/min



OD-H
0.5% IPA/Hex
0.5 mL/min

Standard Proton

File: JSNVII-189-2-chiral

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jmkhla

File: JSNVII-189-2-chiral

INOVA-500 "Py. Chem. ISA, UM.Ch. Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

8 repetitions

OBSERVE H1, 499.9042606 MHz

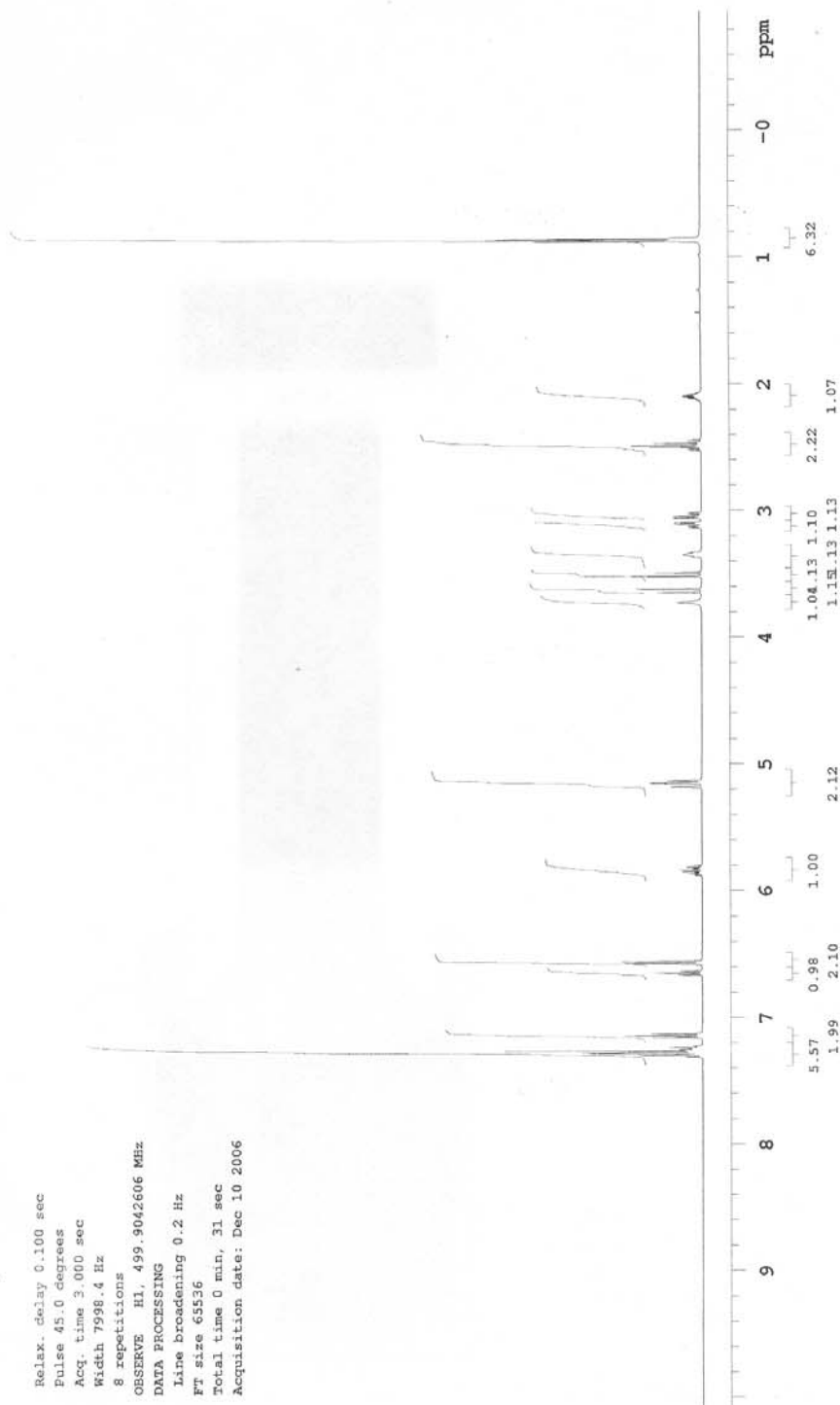
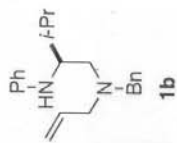
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65136

Total time 0 min, 31 sec

Acquisition date: Dec 10 2006



Std Carbon

File: JSNVII-41-2-C13

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

File: JSNVII-41-2-C13

INOVA-400 "Dy.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

440 repetitions

OBSERVE C13, 100.5712512 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

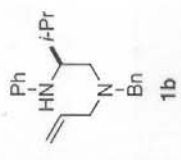
DATA PROCESSING

Line broadening 0.8 Hz

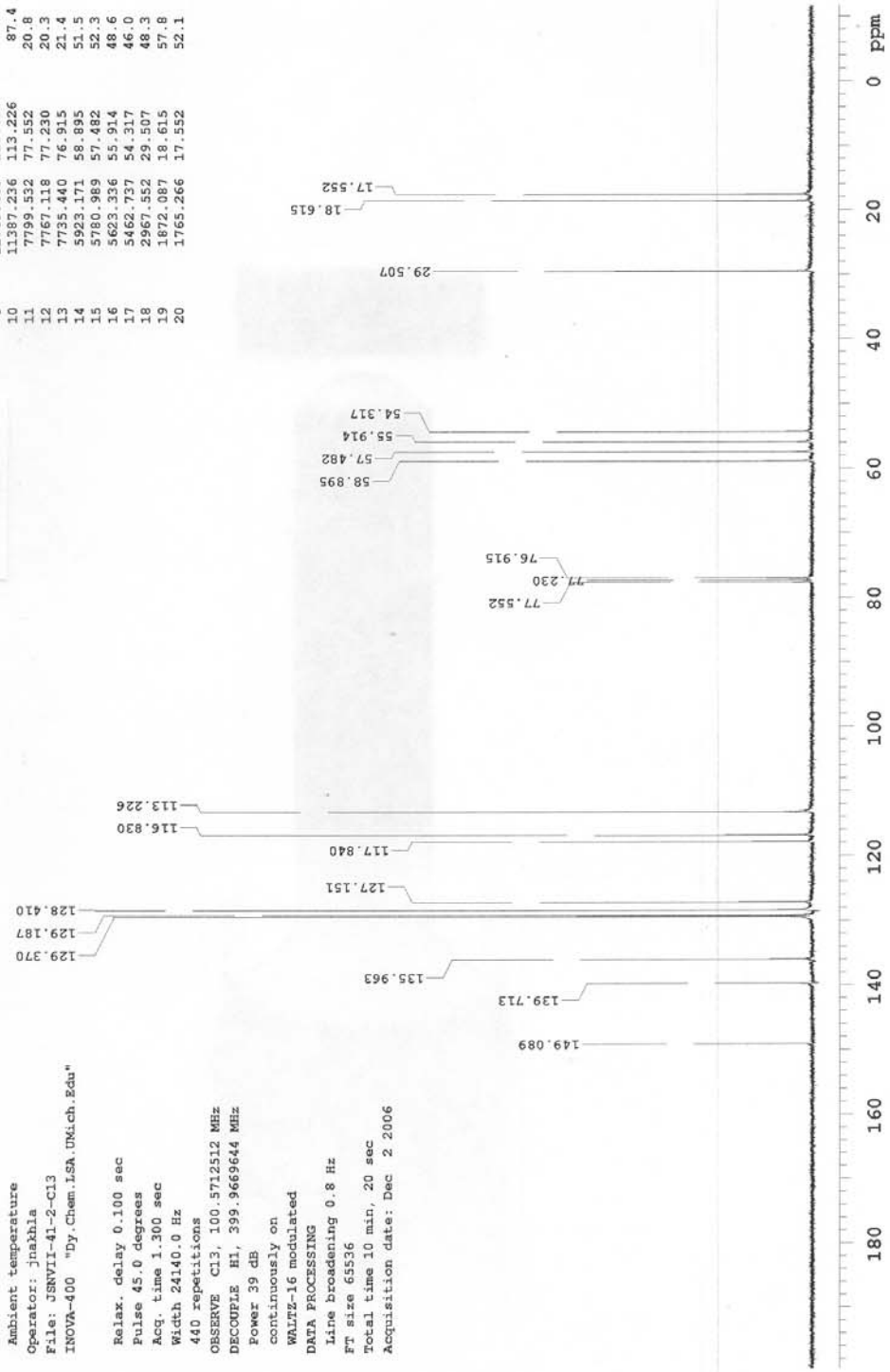
FT size 65536

Total time 10 min, 20 sec

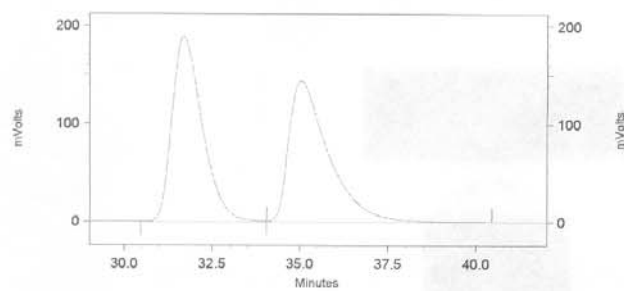
Acquisition date: Dec 2 2006



INDEX	FREQUENCY PPM	HEIGHT
1	14994.093	149.089
2	14051.124	139.713
3	13673.936	135.963
4	13010.911	129.370
5	12992.493	129.187
6	12914.404	128.410
7	12787.692	127.151
8	11851.353	117.840
9	11749.689	116.830
10	11387.236	113.226
11	7799.532	77.552
12	7767.118	77.230
13	7735.440	76.915
14	5923.171	58.895
15	5780.989	57.482
16	5623.336	55.914
17	5462.737	54.317
18	2967.552	29.507
19	1872.087	18.615
20	1765.266	17.552



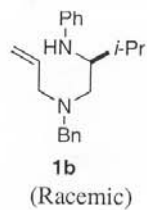
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OD-H
0.1% IPA/Hex
0.2 mL/min

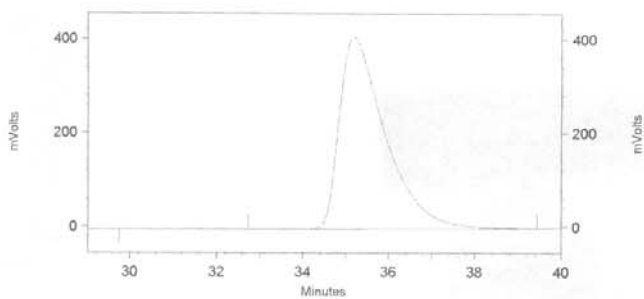
Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
31.683	11357604	49.645
35.008	11428075	50.155
Totals	22785679	100.000



OD-H
0.1% IPA/Hex
0.2 mL/min

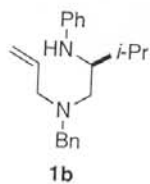
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OD-H
0.1% IPA/Hex
0.2 mL/min

Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
31.650	11634	0.038
35.175	30236956	99.962
Totals	30248590	100.000



OD-H
0.1% IPA/Hex
0.2 mL/min

Std proton

File: JSNVIII-96-2-H1

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: Jnakhla

File: JSNVIII-96-2-H1

INOVA-400 "Py.Chem.USA,UMich.Edu"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6399.5 Hz

8 repetitions

OBSERVE H1, 399.9649481 MHz

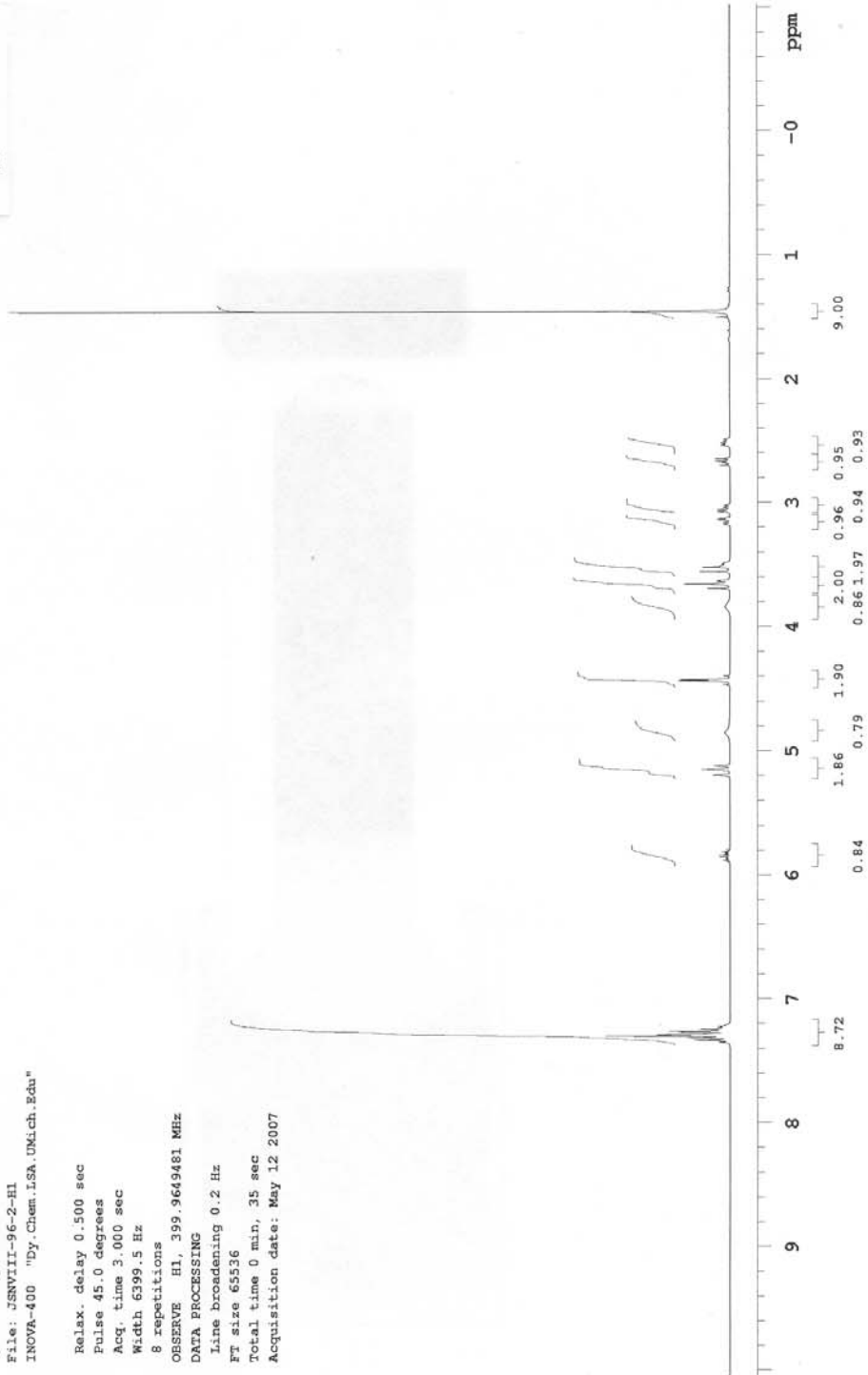
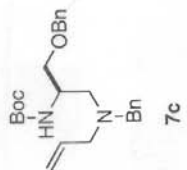
DATA PROCESSING

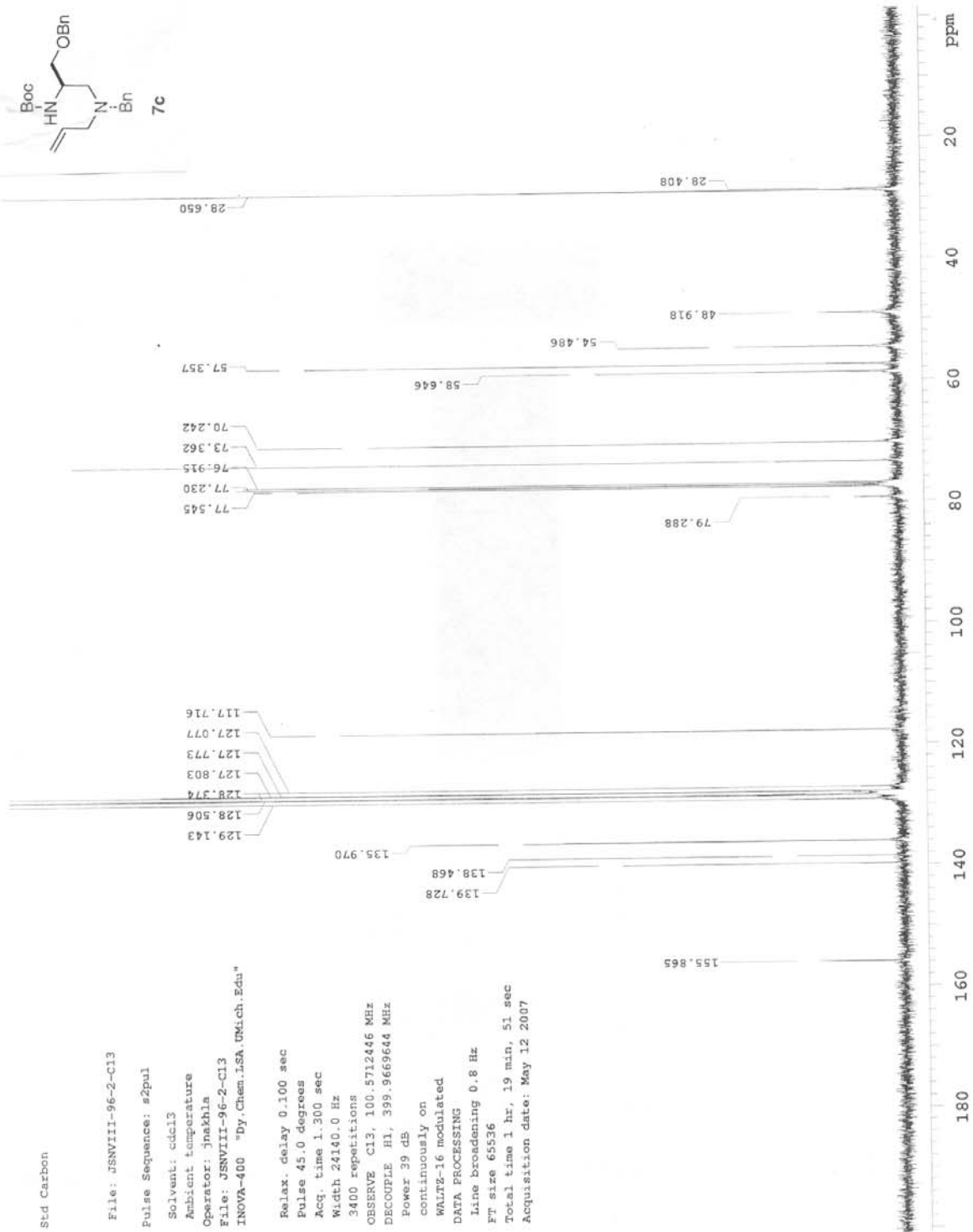
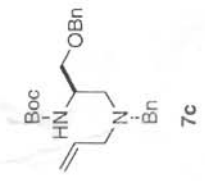
Line broadening 0.2 Hz

FT size 65536

Total time 0 min, 35 sec

Acquisition date: May 12 2007





Std Carbon

File: JSNVIII-96-2-C13

Pulse Sequence: #2pul

Solvent: cdcl3

Ambient temperature

Operator: jnaxhla

File: JSNVIII-96-2-C13

INOVA-400 "Dy.Chem.LSA,UMi.ch.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

3400 repetitions

OBSERVE C13, 100.5712446 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 1 hr, 19 min, 51 sec

Acquisition date: May 12 2007

JENVIII-147-2-bocaminechiral

File: Proton

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

INOVA-500 "Sn.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

24 repetitions

OBSERVE H1, 499.9042604 MHz

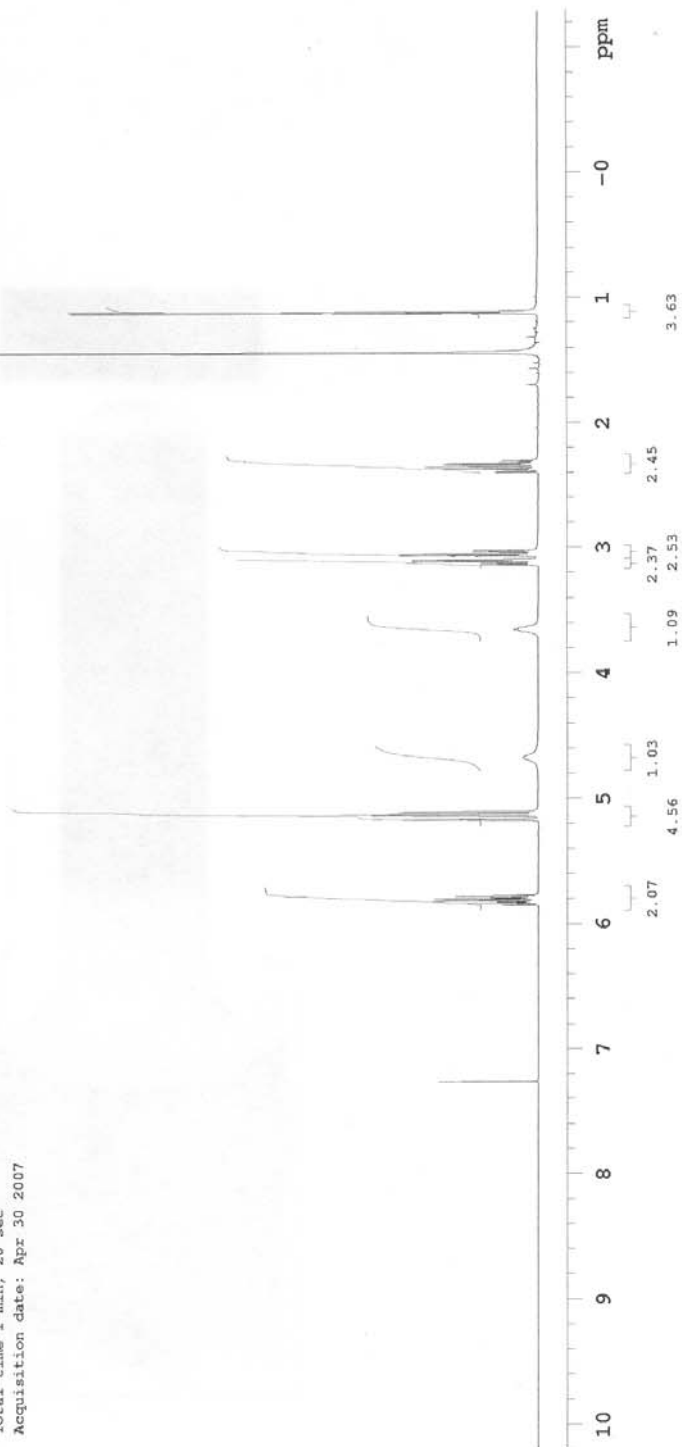
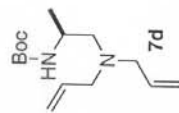
DATA PROCESSING

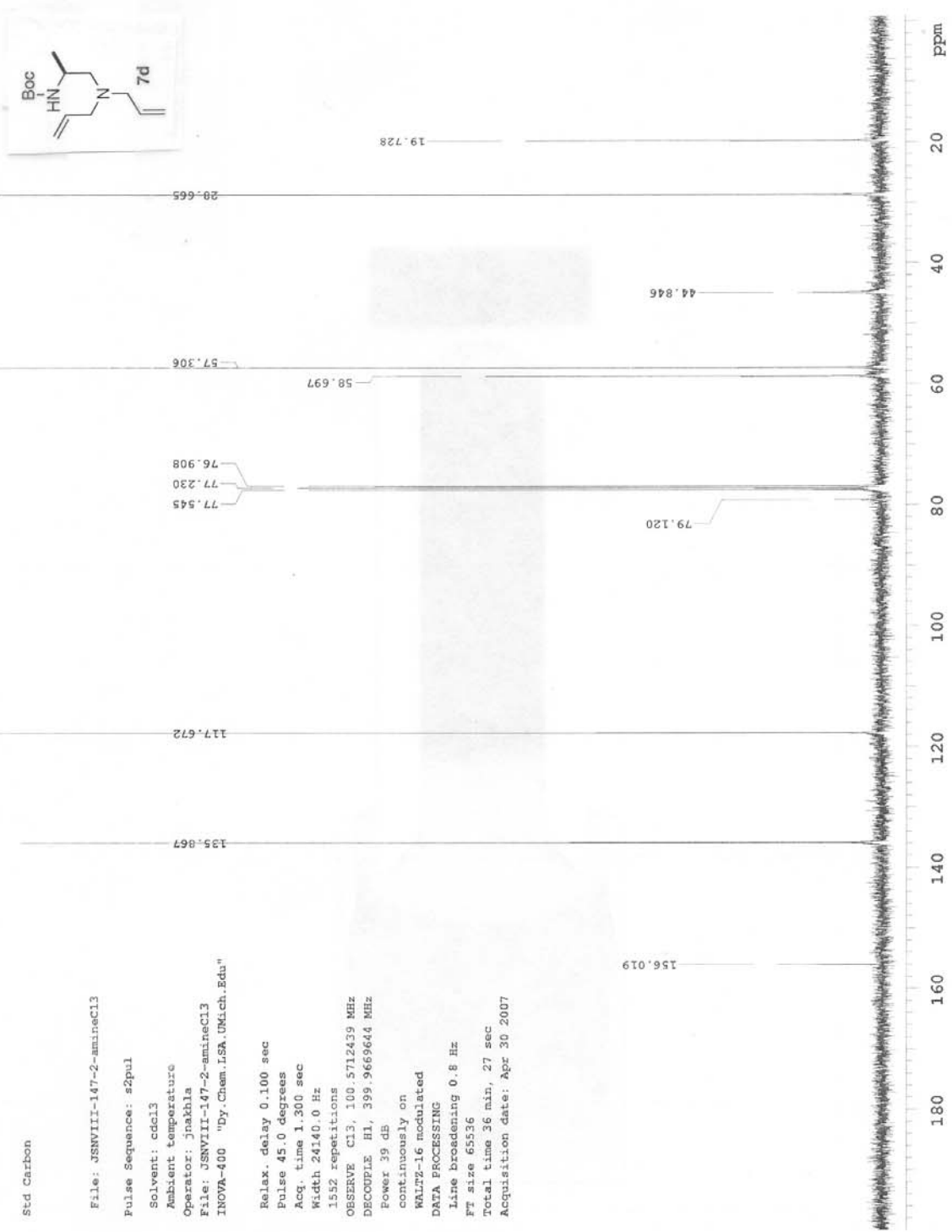
Line broadening 0.2 Hz

FT size 65536

Total time 1 min, 20 sec

Acquisition date: Apr 30 2007





Std Carbon

File: JSNVIII-147-2-amineCl3

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: Jnakhla

File: JSNVIII-147-2-amineCl3

INOVA-400 "Dy.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

1552 repetitions

OBSERVE C13, 100.5712439 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

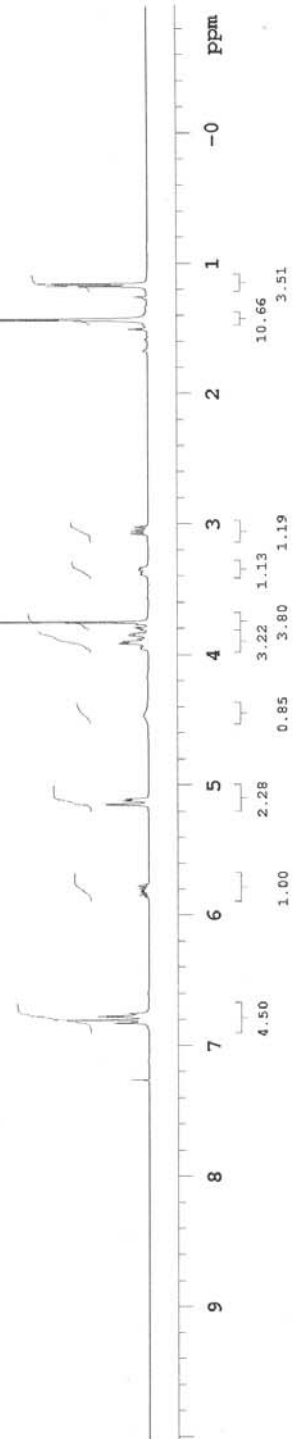
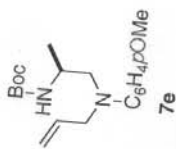
Total time 36 min, 27 sec

Acquisition date: Apr 30 2007

Std proton

File: JSNVIII-143-2
 Pulse Sequence: s2pul
 Solvent: cdcl3
 Ambient temperature
 Operator: jnakhla
 File: JSNVIII-143-2
 INOVA-400 "Kr.chem.lsa.umich.edu"

Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 3.000 sec
 Width 6399.5 Hz
 4 repetitions
 OBSERVE H1, 399.9649484 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 65536
 Total time 0 min, 21 sec
 Acquisition date: Apr 26 2007



Std Carbon

File: JSNVIII-143-2-C13

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

File: JSNVIII-143-2-C13

INOVA-400 "Dy.Chem.LSA,UMich.Eds"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

856 repetitions

OBSERVE C13, 100.5712461 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

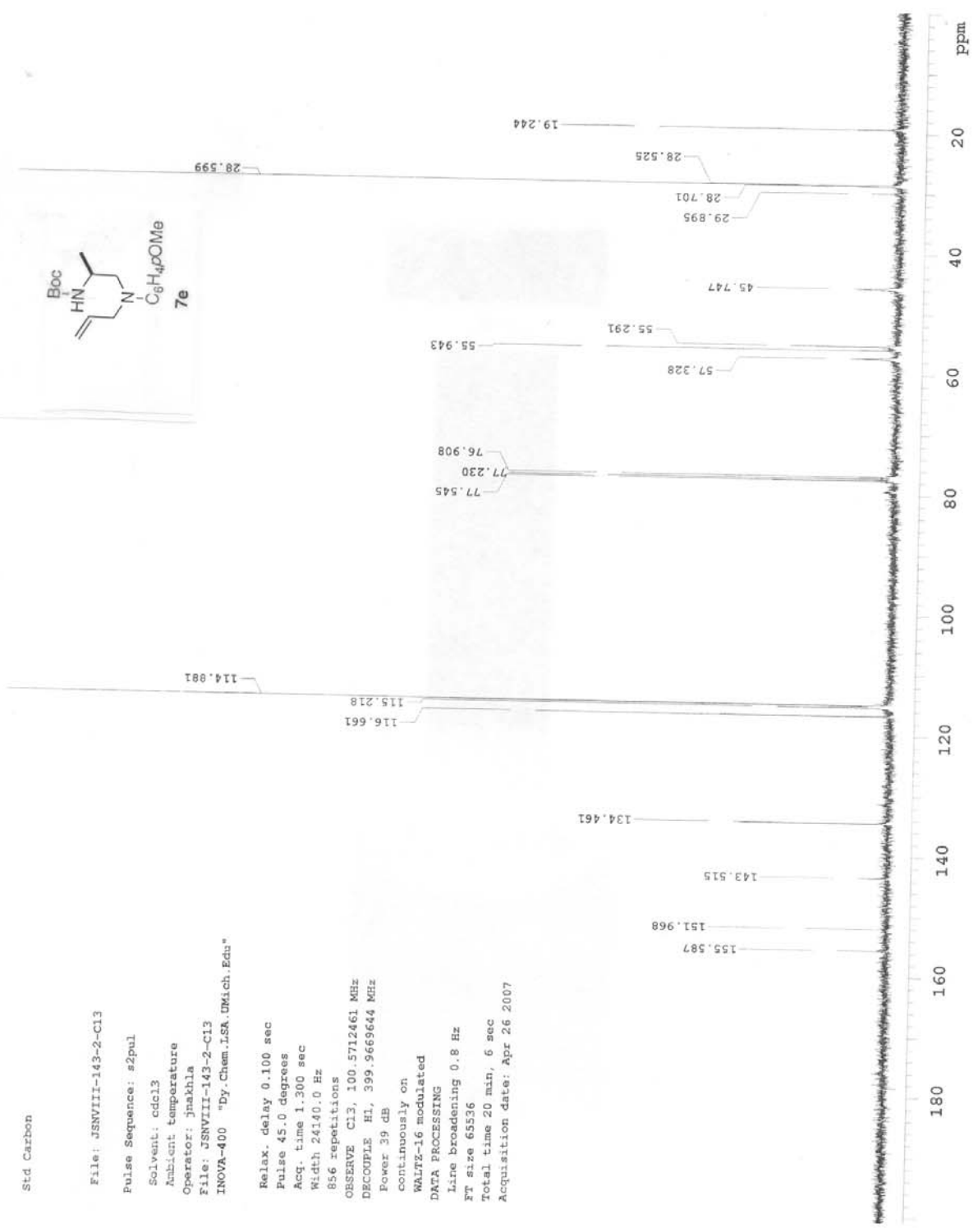
DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 20 min, 6 sec

Acquisition date: Apr 26 2007



J5NVIII-98-2-2-H1

File: Proton

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

INOVA-500 "Sn.Chem.LSA,UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. Time 3.000 sec

Width 7998.4 Hz

8 repetitions

OBSERVE H1, 499.9042581 MHz

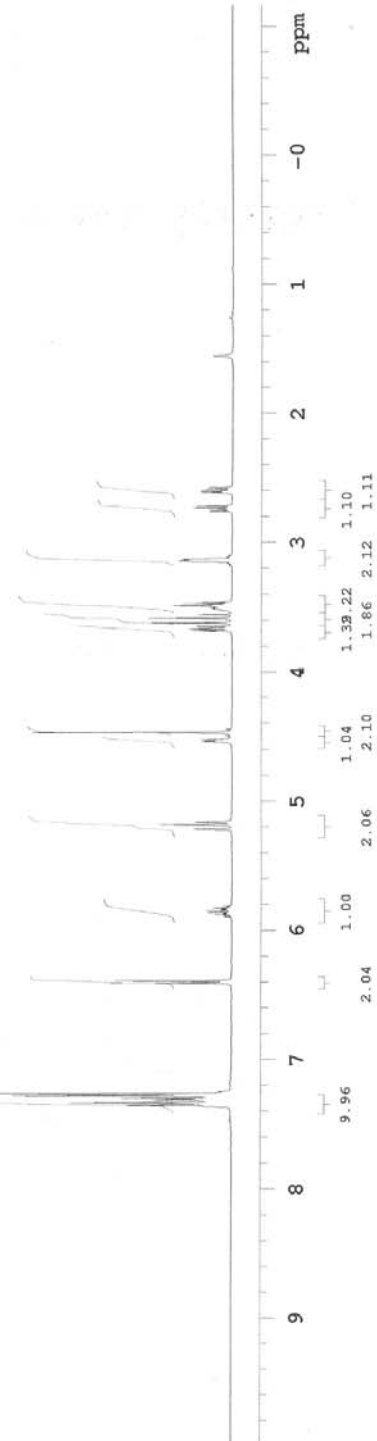
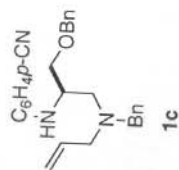
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total Time 0 min, 31 sec

Acquisition date: Mar 15 2007



JSNVIII-98-2-2-C13

File: Carbon

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

INOVA-400 "Zr.Chem.USA,UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

1232 repetitions

OBSERVE C13, 100.5712520 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

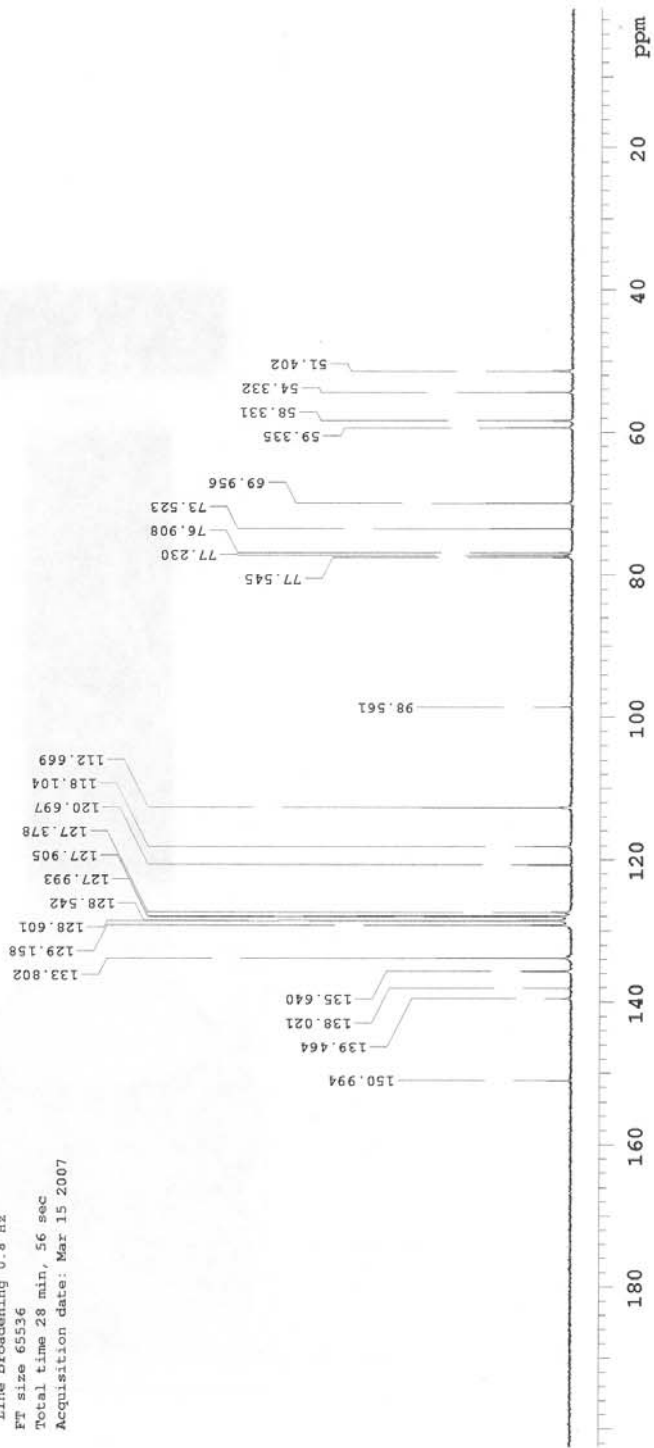
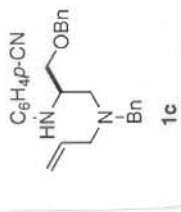
Line broadening 0.8 Hz

FT size 65536

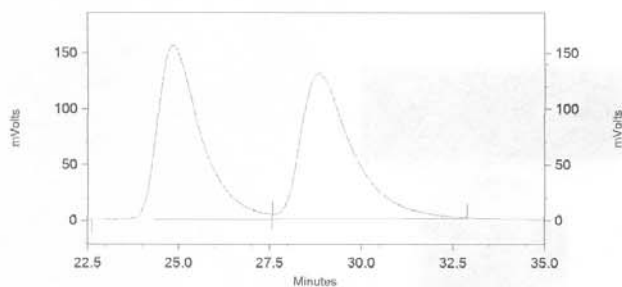
Total time 28 min, 56 sec

Acquisition date: Mar 15 2007

INDEX	FREQUENCY PPM	HEIGHT
1	15185.633	9.9
2	14026.076	4.5
3	13880.947	8.3
4	13641.521	135.640
5	13456.611	133.802
6	12989.547	129.158
7	12933.558	128.601
8	12927.664	128.542
9	12872.412	127.993
10	12863.572	127.905
11	12810.530	127.378
12	12138.664	120.697
13	11877.874	118.104
14	11331.247	112.669
15	9912.373	98.561
16	7798.796	77.545
17	7767.118	77.230
18	7734.703	76.908
19	7394.350	73.523
20	7035.580	69.956
21	5967.373	59.335
22	5866.445	58.331
23	5464.210	54.332
24	5169.532	51.402



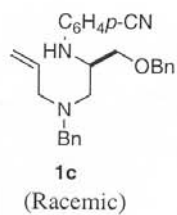
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-99-2-racAD0.7mLperpen-2.dat



AD
0.7% IPA/Hex
1 mL/min

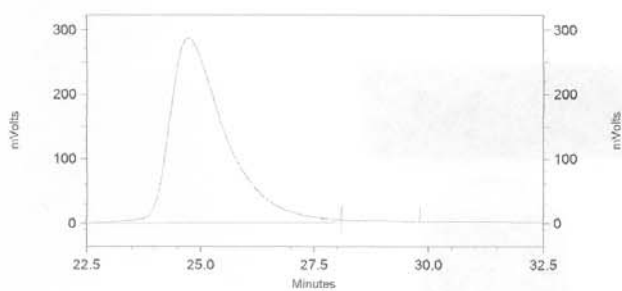
Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
24.842	12928286	50.095
28.825	12879138	49.905
Totals	25807424	100.000



AD
0.7% IPA/Hex
1 mL/min

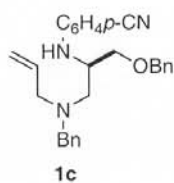
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New
Folder\JSNVIII-98-2-2-racAD0.7pelmlpermin2.dat



AD
0.7% IPA/Hex
1 mL/min

Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
24.750	24428409	99.251
28.100	184284	0.749
Totals	24612693	100.000



AD
0.7% IPA/Hex
1 mL/min

J5NVIII-150-2

File: Proton

Pulse Sequence: s2pul

Solvent: cdc13

Ambient temperature

Operator: jmakhsa

INOVA-500 "Sn. Chem. USA. UMich. Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

24 repetitions

OBSERVE H1, 499.9042614 MHz

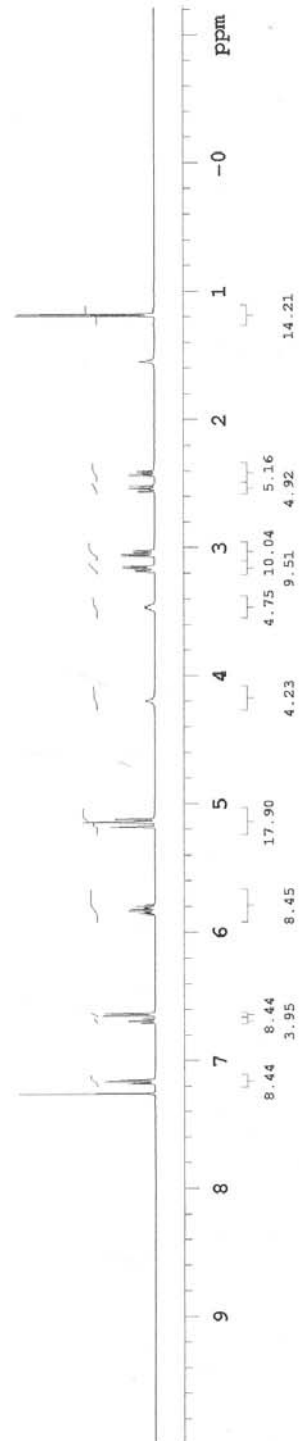
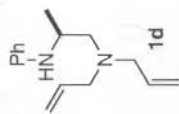
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min, 20 sec

Acquisition date: May 1 2007



JSNVIII-150-2-C13

File: Carbon

Pulse Sequence: szpul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

INOVA-400 "Zi.Chem.I.SA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

144 repetitions

OBSERVE C13, 100.5712571 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

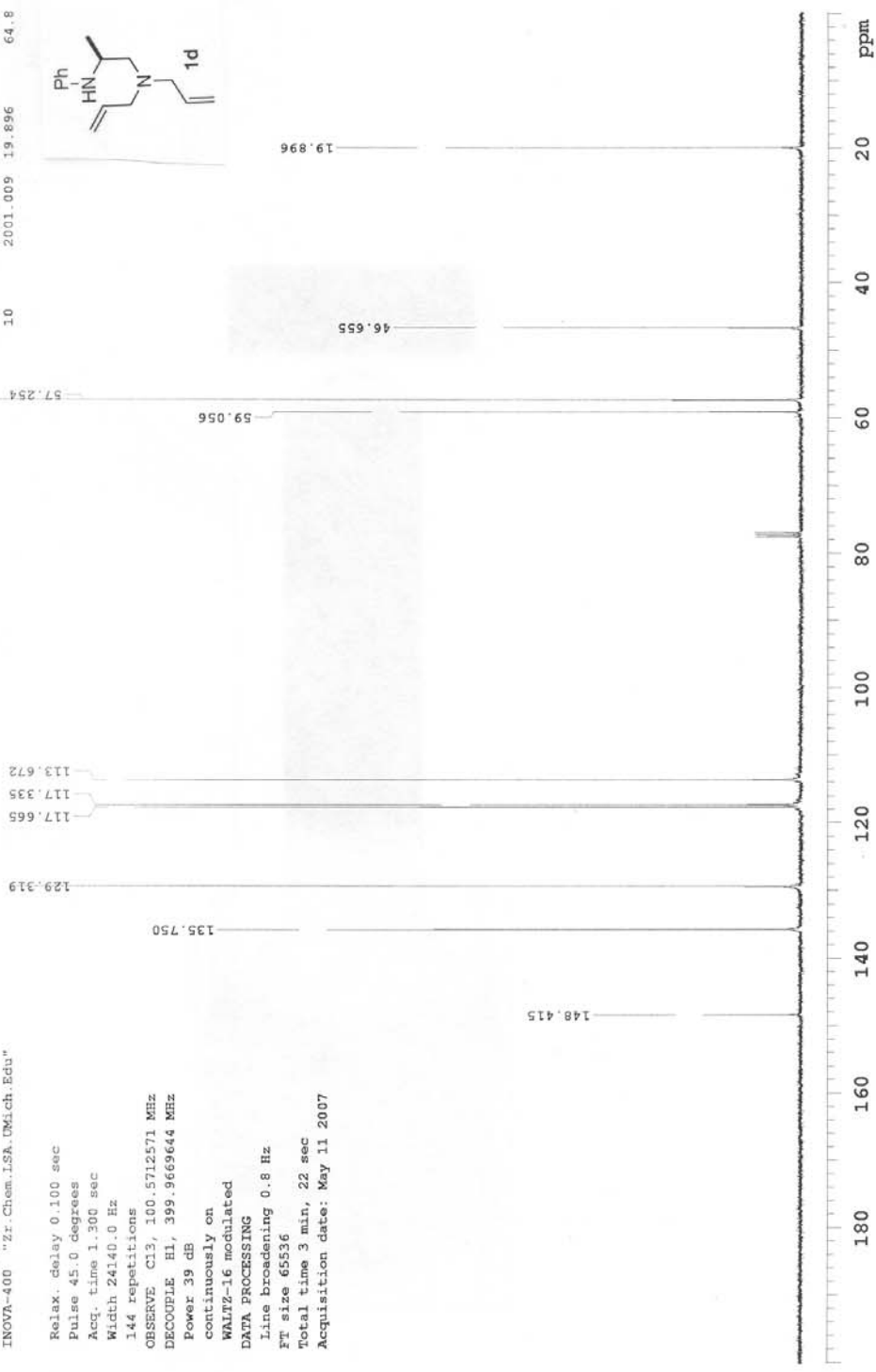
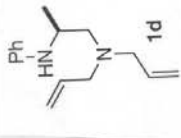
Line broadening 0.8 Hz

FT size 65536

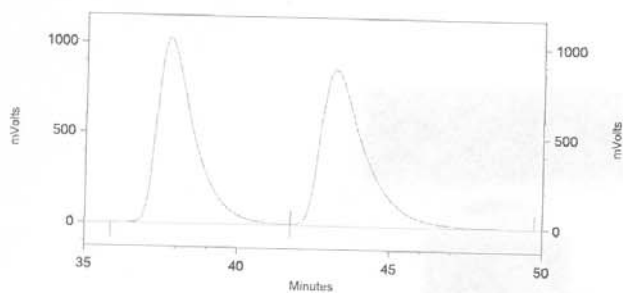
Total time 3 min, 22 sec

Acquisition date: May 11 2007

INDEX	FREQUENCY PPM	HEIGHT
1	14926.317	148.415
2	13652.572	135.750
3	13005.754	129.319
4	11833.673	117.665
5	11800.522	117.335
6	11432.174	113.672
7	5939.379	59.056
8	5756.152	57.254
9	4692.154	46.655
10	2001.009	19.896



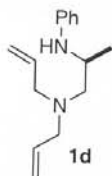
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-118-2-rac-OJH4.dat



OJ-H
1% IPA/Hex
0.2 mL/min

Detector 1 Ch2-254nm
Results

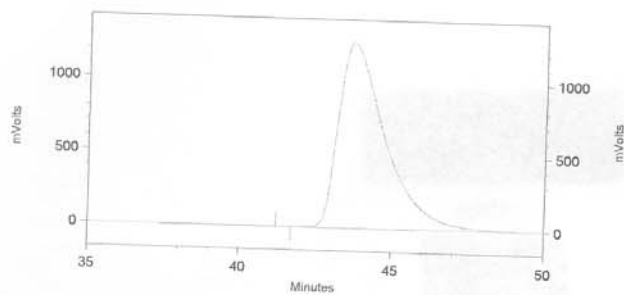
Retention Time	Area	Area Percent
37.733	86677422	49.766
43.175	87493951	50.234
Totals	174171373	100.000



(Racemic)

OJ-H
1% IPA/Hex
0.2 mL/min

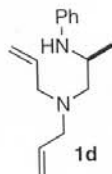
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-150-2-chiralc-OJH-1per.dat



OJ-H
1% IPA/Hex
0.2 mL/min

Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
38.708	270174	0.200
43.683	134817201	99.800
Totals	135087375	100.000

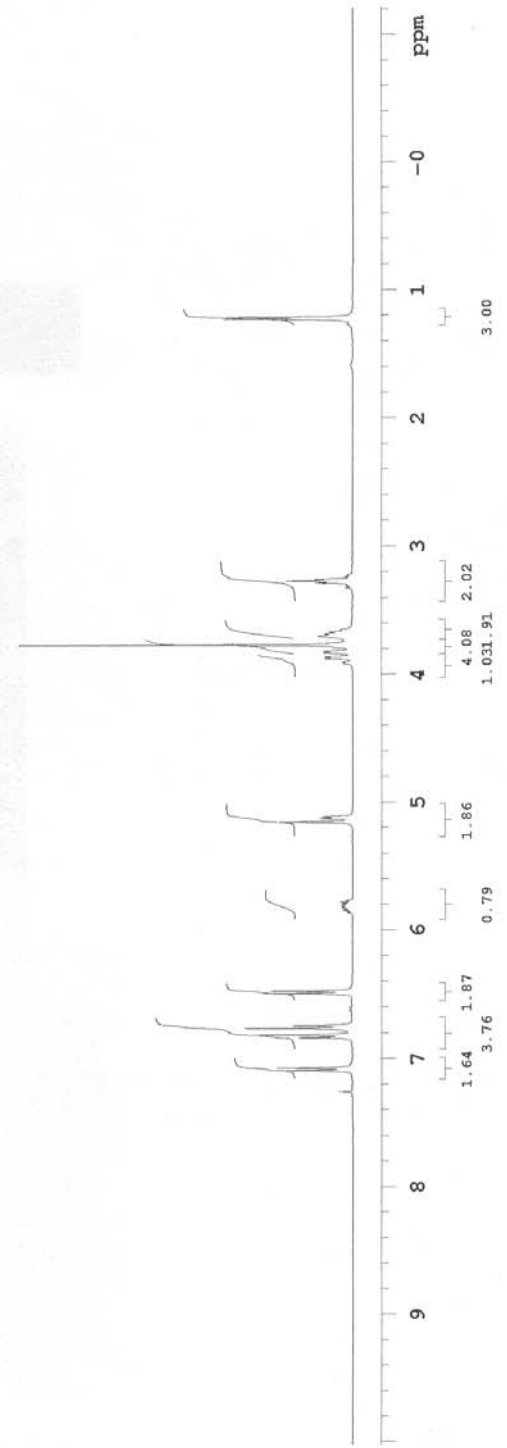
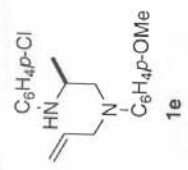


OJ-H
1% IPA/Hex
0.2 mL/min

JSNVII-141-2-HI400-withBINAP

File: Proton
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: jnakhla
INOVA-400 "Zr.Chem.USA,UMich.Edu"

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 6399.5 Hz
8 repetitions
OBSERVE HI, 399.9649486 MHz
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 0 min, 35 sec
Acquisition date: Apr 25 2007



JSNVIII-141-2-withBINAP-Cl3

File: Carbon

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

INOVA-400 "Sr.Chem.LSA,UMich,Edh"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

92 repetitions

OBSERVE C13, 100.5712475 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

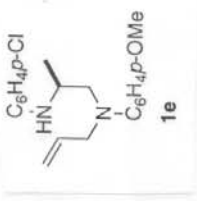
DATA PROCESSING

Line broadening 0.8 Hz

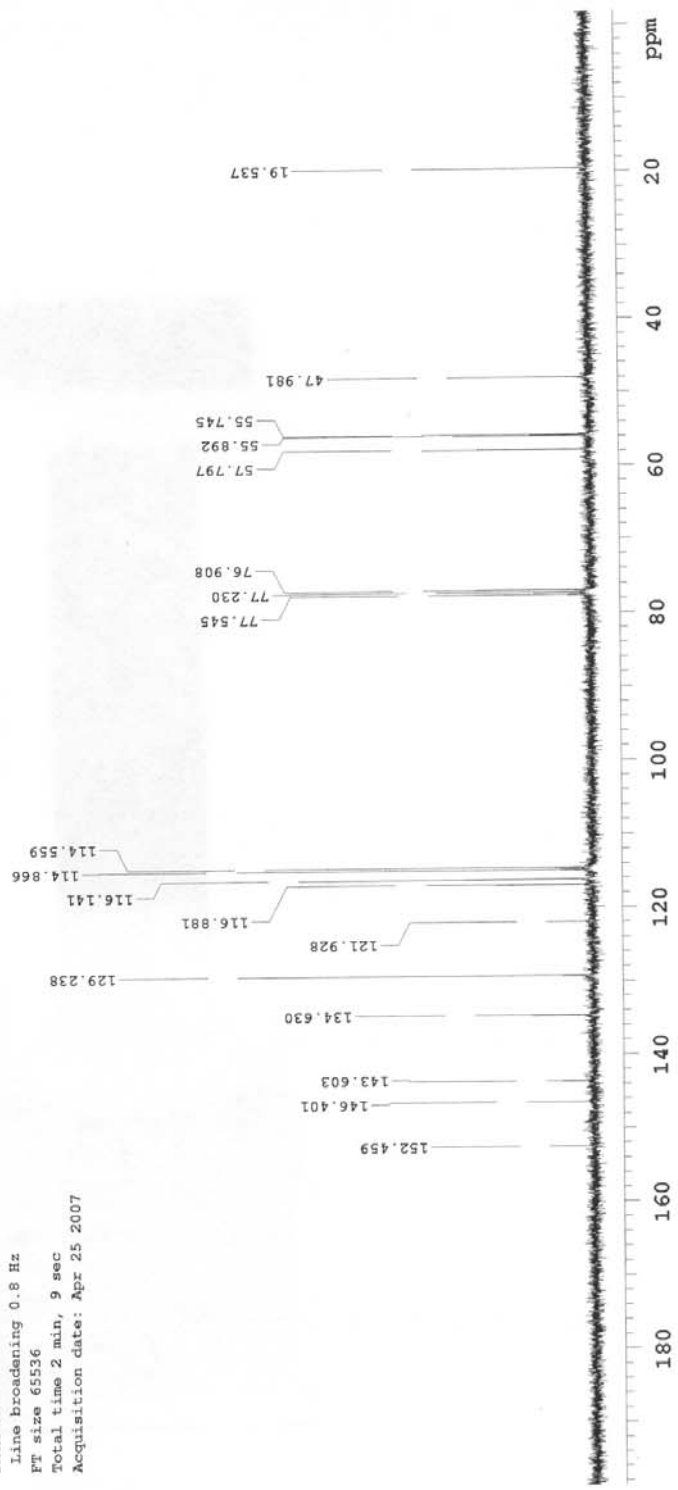
FT size 65536

Total time 2 min, 9 sec

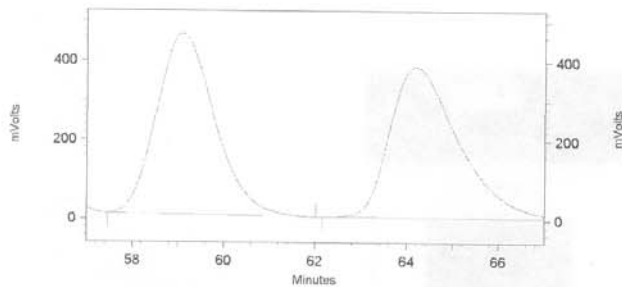
Acquisition date: Apr 25 2007



INDEX	FREQUENCY	PPM	HEIGHT
1	15352.972	152.459	7.6
2	14723.726	146.401	11.5
3	14442.308	143.603	8.1
4	13539.857	134.630	20.1
5	12997.650	129.238	59.4
6	12262.429	121.928	8.0
7	11754.846	116.881	28.2
8	11680.440	116.141	49.2
9	11552.255	114.866	59.5
10	11521.314	114.559	54.8
11	7798.795	77.545	27.3
12	7767.117	77.230	26.0
13	7734.703	76.908	28.2
14	5812.666	57.797	28.2
15	5621.126	55.892	22.9
16	5606.392	55.745	28.2
17	4825.495	47.981	23.8
18	1964.910	19.537	29.3



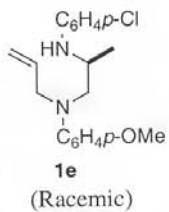
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-135-2-OD18.dat



OD
1% IPA/Hex
0.2 mL/min

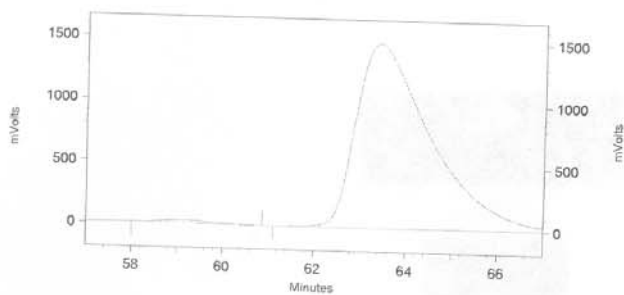
Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
59.092	40209739	50.254
64.175	39803931	49.746
Totals	80013670	100.000



OD
1% IPA/Hex
0.2 mL/min

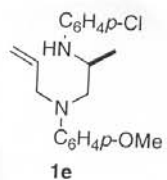
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-141-2-OD4.dat



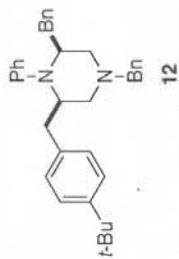
OD
1% IPA/Hex
0.2 mL/min

Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
59.142	1818825	1.065
63.375	169040764	98.935
Totals	170859589	100.000



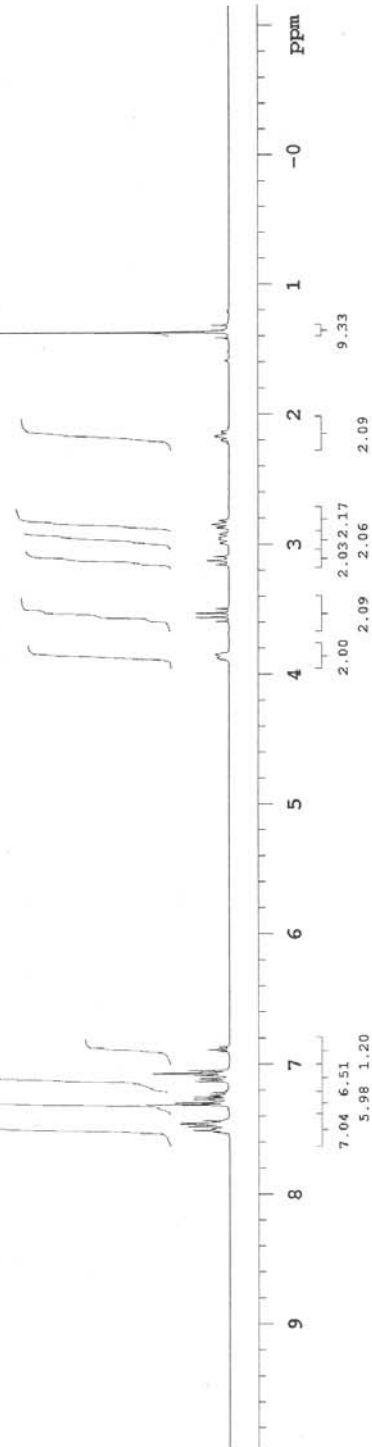
OD
1% IPA/Hex
0.2 mL/min



```

exp1 Proton
SAMPLE
date Dec 17 2006 temp not used
solvent cdcl3 gain not used
file /home/jnkhla- spin 20
/vmrzsys/data/Inov- hat 0.008
a.400/JSNVII-206-2~ pw90 13.800
-2.fid alfa 6.600
ACQUISITION FLAGS
SW 6399.5 il n
at 3.000 in n
np 38396 dp y
fb 4000 hs nn
bs 4 PROCESSING
ss 2 lb 0.20
dl 0.500 in not used
nt 1000 DISPLAY
ct 16 sp -463.1
TRANSMITTER
tn H1 xel 4454.5
sfrq 399.967 rfp 3670.3
tof 399.9 xp 2903.7
tpwr 59 lp -1.4
PW 6.900 MC 250
DECOUPLER
dn CL3 sc 0
dof 0 vs 26
da nnn th 13
dmm c ai cdc ph
dpwr 32
dmf 29412

```



Std Carbon

File: JSNVIII-54-2-C13

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnaakha

File: JSNVIII-54-2-C13

INOVA-400 "Dy.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

4616 repetitions

OBSERVE C13, 100.5712468 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

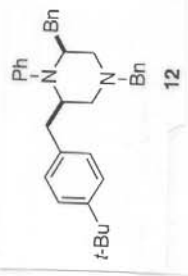
DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 1 hr, 48 min, 25 sec

Acquisition date: May 12 2007



31.609
34.576
36.942

37.513

54.530
55.540
55.584
63.232

54.119

76.915
77.230
77.552

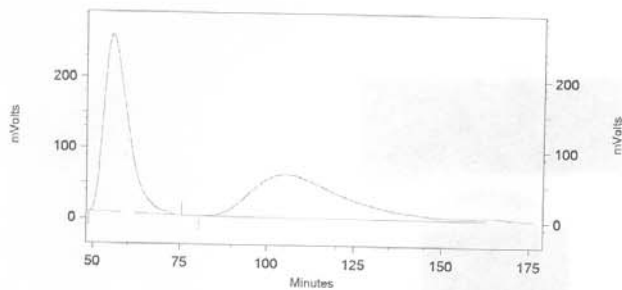
113.548
117.401

125.576
126.220
127.473
128.586
128.682
129.143
129.524
129.919
130.088

137.267
138.966
140.394
147.068
149.031

ppm
20
40
60
80
100
120
140
160
180

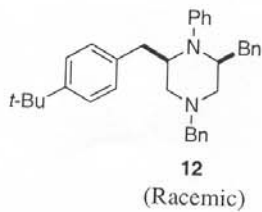
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New
Folder\JSNVII-206-2-racFeb107.dat



OJ-H
2% IPA/Hex
0.1 mL/min

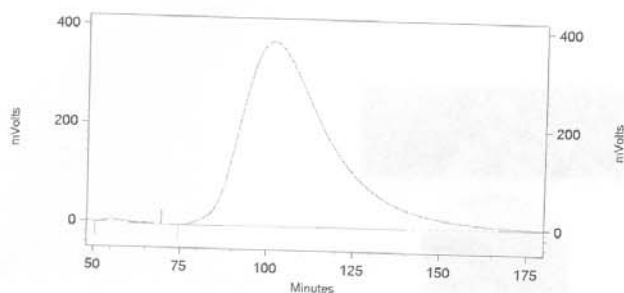
Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
55.425	121188913	51.231
105.233	115365613	48.769
Totals	236554526	100.000



OJ-H
2% IPA/Hex
0.1 mL/min

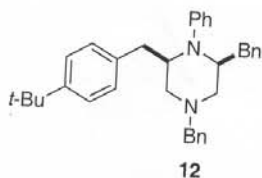
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-53-2-chiral-5.dat



OJ-H
2% IPA/Hex
0.1 mL/min

Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
55.133	2368950	0.355
101.142	664080657	99.645
Totals	666449607	100.000



OJ-H
2% IPA/Hex
0.1 mL/min

J5NVIII-47-2

File: J5NVIII-47-2

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnaakha

File: J5NVIII-47-2

INOVA-400 "2F.Chem.LSA.UMich.Edu"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6399.5 Hz

28 repetitions

OBSERVE F1, 399.9649490 MHz

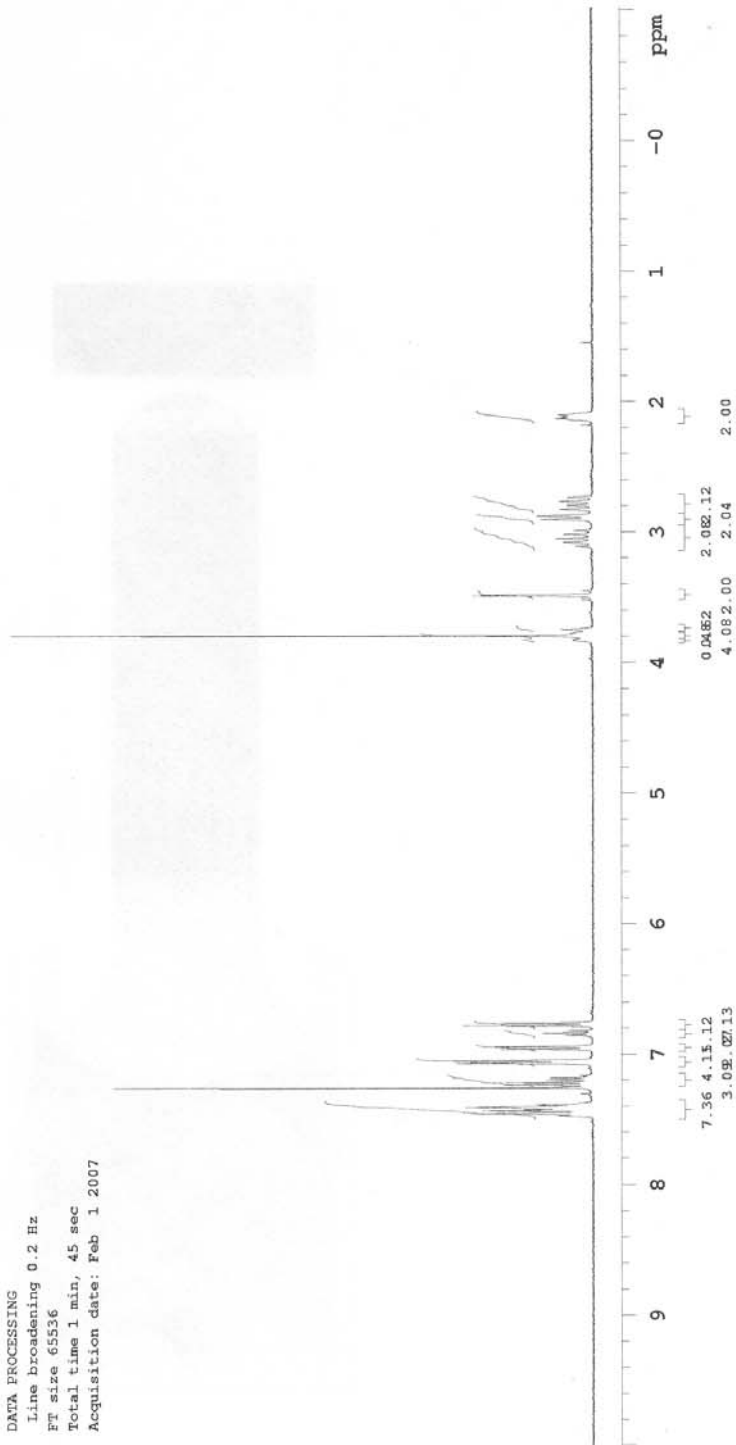
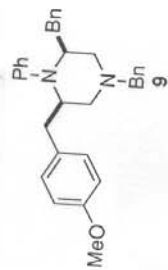
DATA PROCESSING

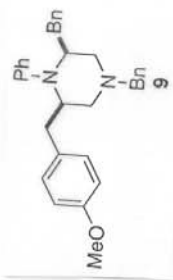
Line broadening 0.2 Hz

FT size 65836

Total time 1 min, 45 sec

Acquisition date: Feb 1 2007





Std Carbon

File: JSNVIII-47-2-C13

Pulse Sequence: s2pdl

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

File: JSNVIII-47-2-C13

INOVA-400 "Md.Chem.LSA,UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

836 repetitions

OBSERVE C13, 100.5712527 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

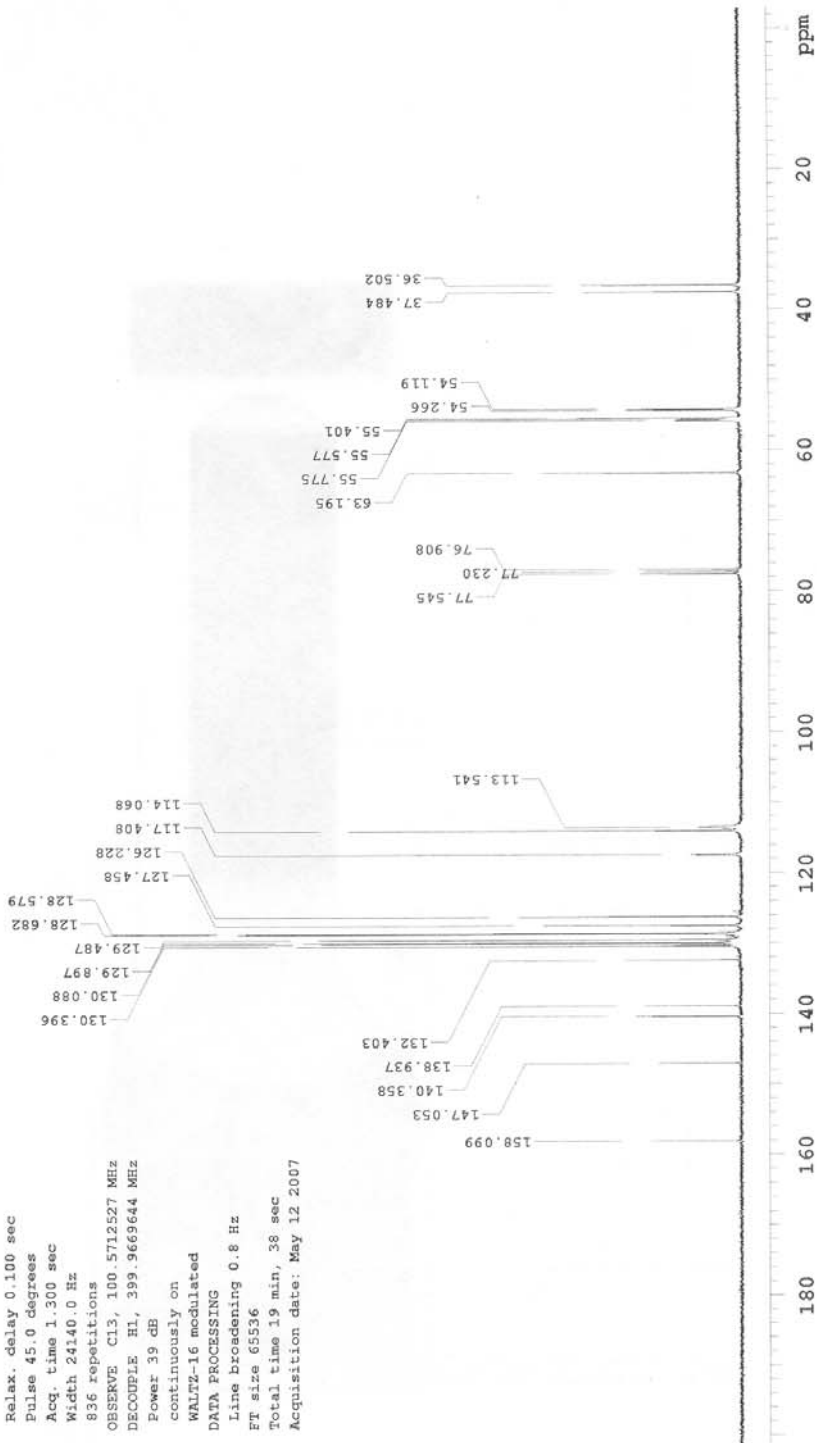
DATA PROCESSING

Line broadening 0.8 Hz

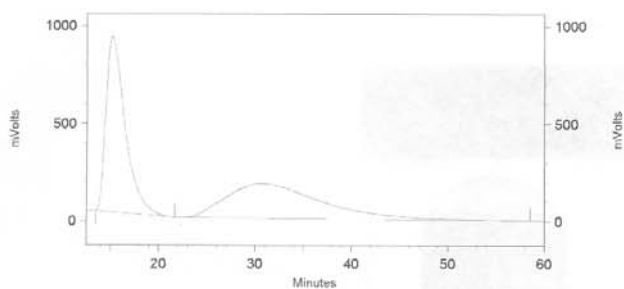
FT size 65536

Total time 19 min, 38 sec

Acquisition date: May 12 2007



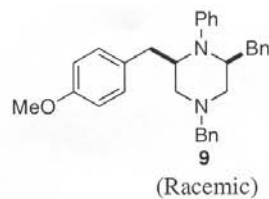
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-2-2-rac-5.dat



OJ-H
10% IPA/Hex
0.5 mL/min

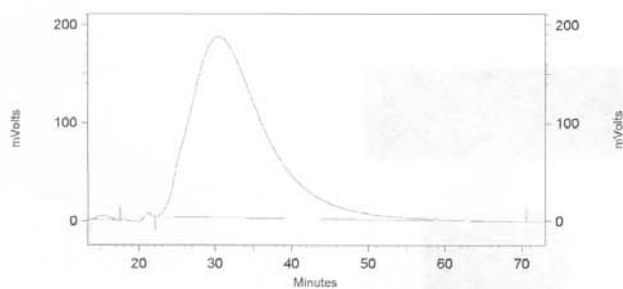
Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
15.175	158185551	51.428
30.725	149403298	48.572
Totals	307588849	100.000



OJ-H
10% IPA/Hex
0.5 mL/min

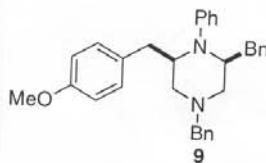
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-39-2-chiral-8.dat



OJ-H
10% IPA/Hex
0.5 mL/min

Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
15.125	498271	0.398
30.500	124736349	99.602
Totals	125234620	100.000



OJ-H
10% IPA/Hex
0.5 mL/min

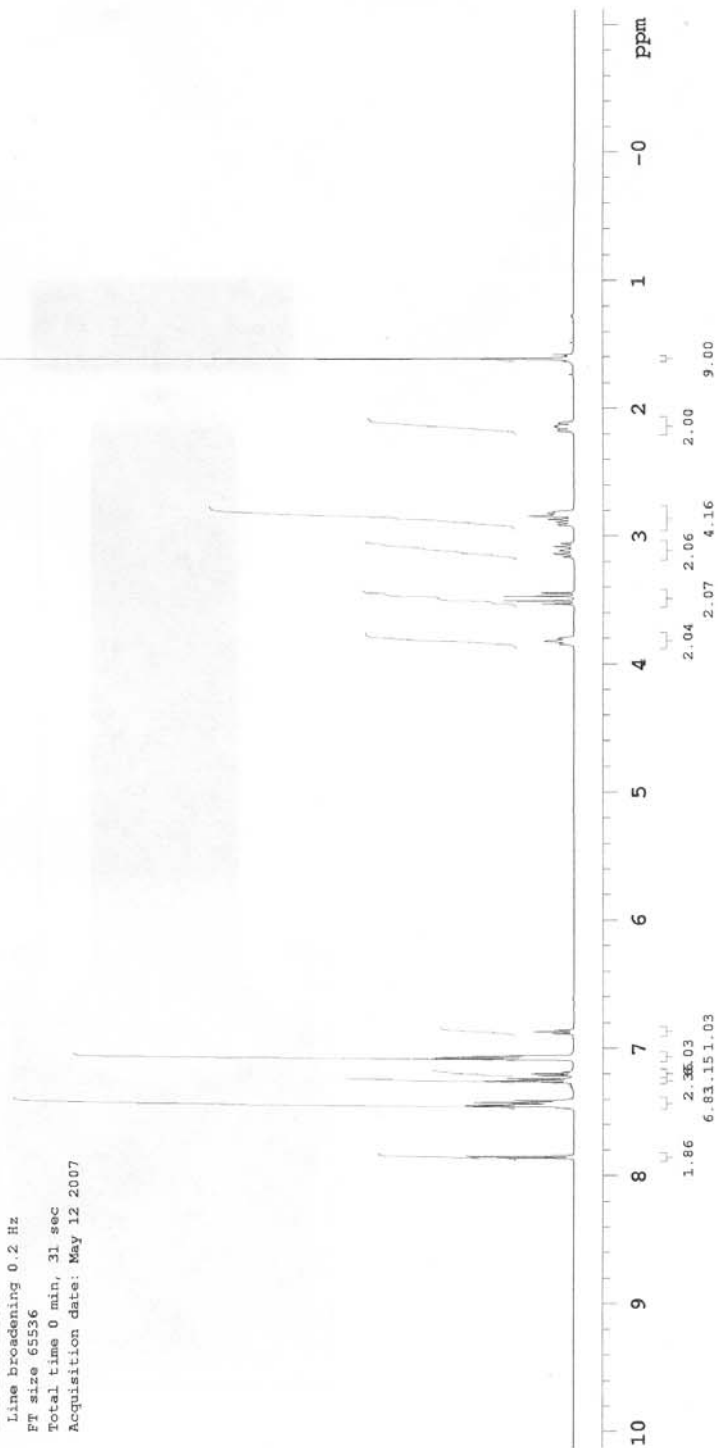
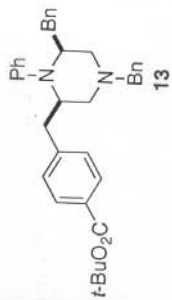
Standard Proton

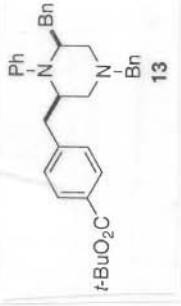
File: Proton
 Pulse Sequence: s2pul
 Solvent: cdcl3
 Ambient temperature
 Operator: Jnakhia
 INOVA-500 "En.Chem.LSA.DMich.Edu"

Relax. delay 0.100 sec
 Pulse 45.0 degrees
 Acq. time 3.000 sec
 Width 8003.2 Hz
 8 repetitions

OBSERVE H1, 499.9042612 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 65536

Total time 0 min, 31 sec
 Acquisition date: May 12 2007





Std Carbon

File: JSNVIII-42-C13

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

File: JSNVIII-42-C13

INOVA-400 "Dy. Chem. I.S.A. UMich. Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

1016 repetitions

OBSERVE C13, 100.5712527 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

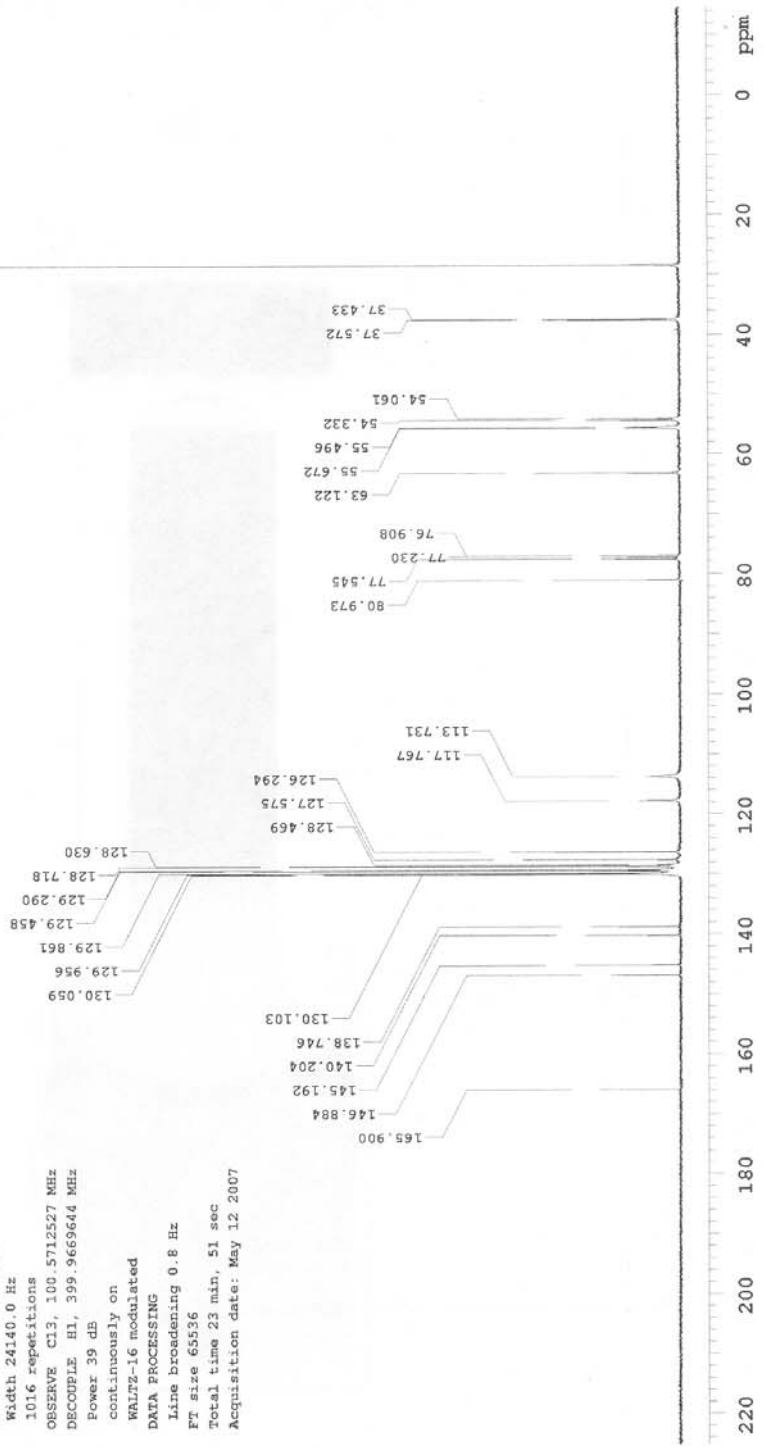
DATA PROCESSING

Line broadening 0.8 Hz

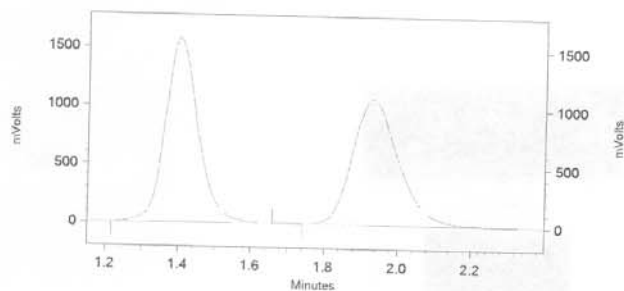
FT size 65536

Total time 23 min, 51 sec

Acquisition date: May 12 2007



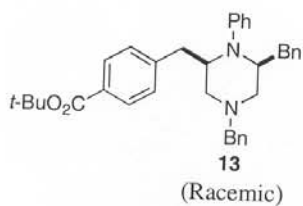
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVII-208-2-rac-12.dat



OD-H
5% IPA/Hex
2 mL/min

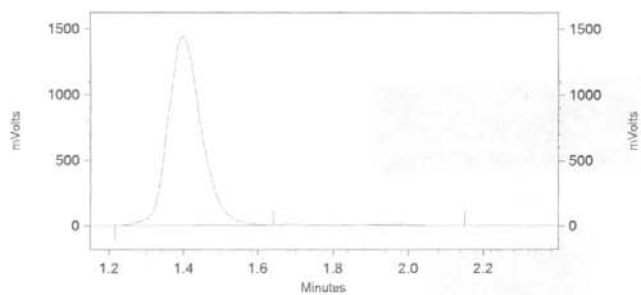
Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
1.400	9803626	51.113
1.925	9376659	48.887
Totals	19180285	100.000



OD-H
5% IPA/Hex
2 mL/min

Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-42-2-1chiral.dat

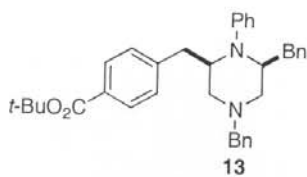


OD-H
5% IPA/Hex
2 mL/min

Detector 1 Ch2-254nm

Results

Retention Time	Area	Area Percent
1.400	8916087	99.285
1.942	64232	0.715
Totals	8980319	100.000



OD-H
5% IPA/Hex
2 mL/min

Std proton

File: JSNVIII-74-2-H1

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jna@hls

File: JSNVIII-74-2-H1

INOVA-400 "2: Chem.LSA.UWich.Edh"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6399.5 Hz

4 repetitions

OBSERVE H1, 399.9649491 MHz

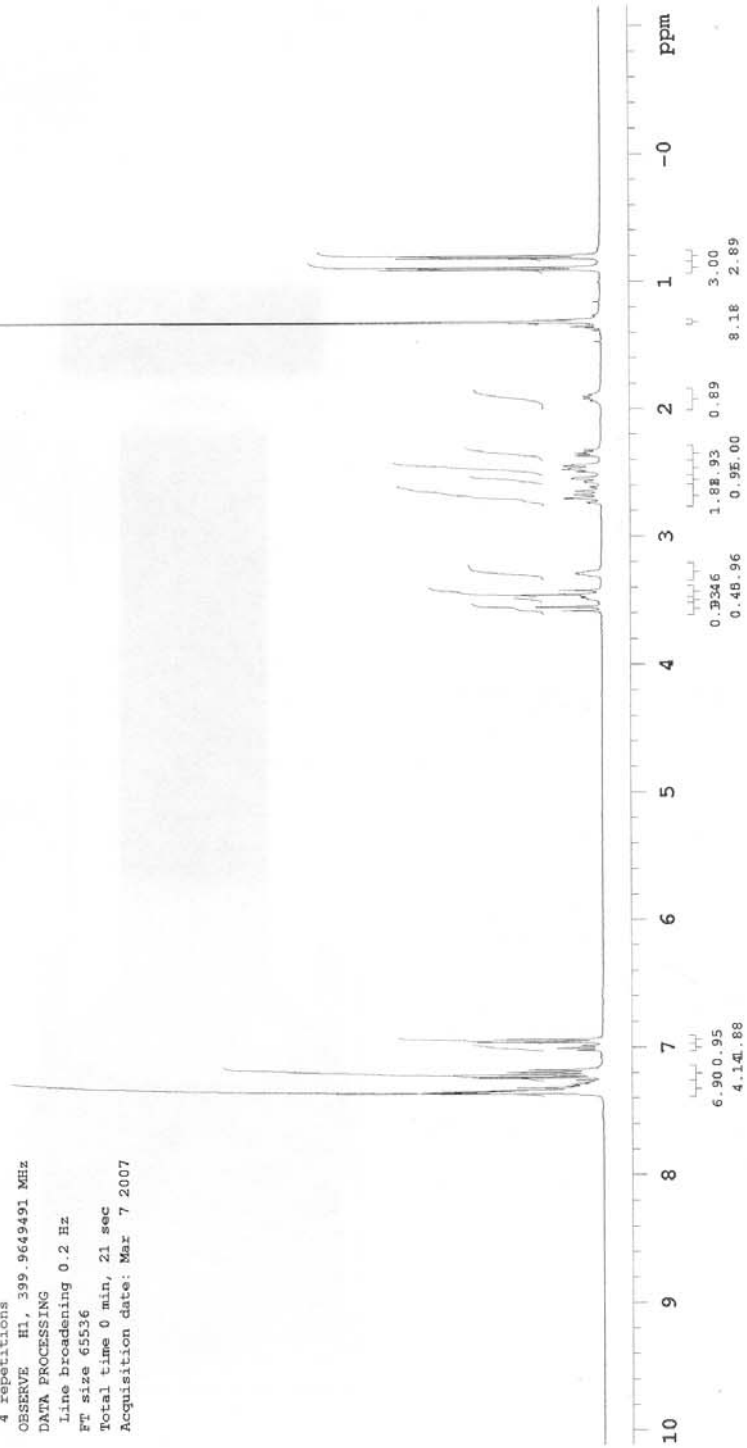
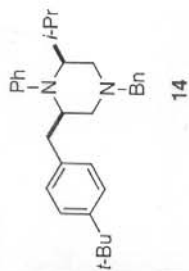
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min, 21 sec

Acquisition date: Mar 7 2007



Std Carbon

File: JSNVII-197-2-Cl3-chiral

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhia

File: JSNVII-197-2-Cl3-chiral

INOVA-400 "Ma.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

316 repetitions

OBSERVE C13, 100.5712542 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

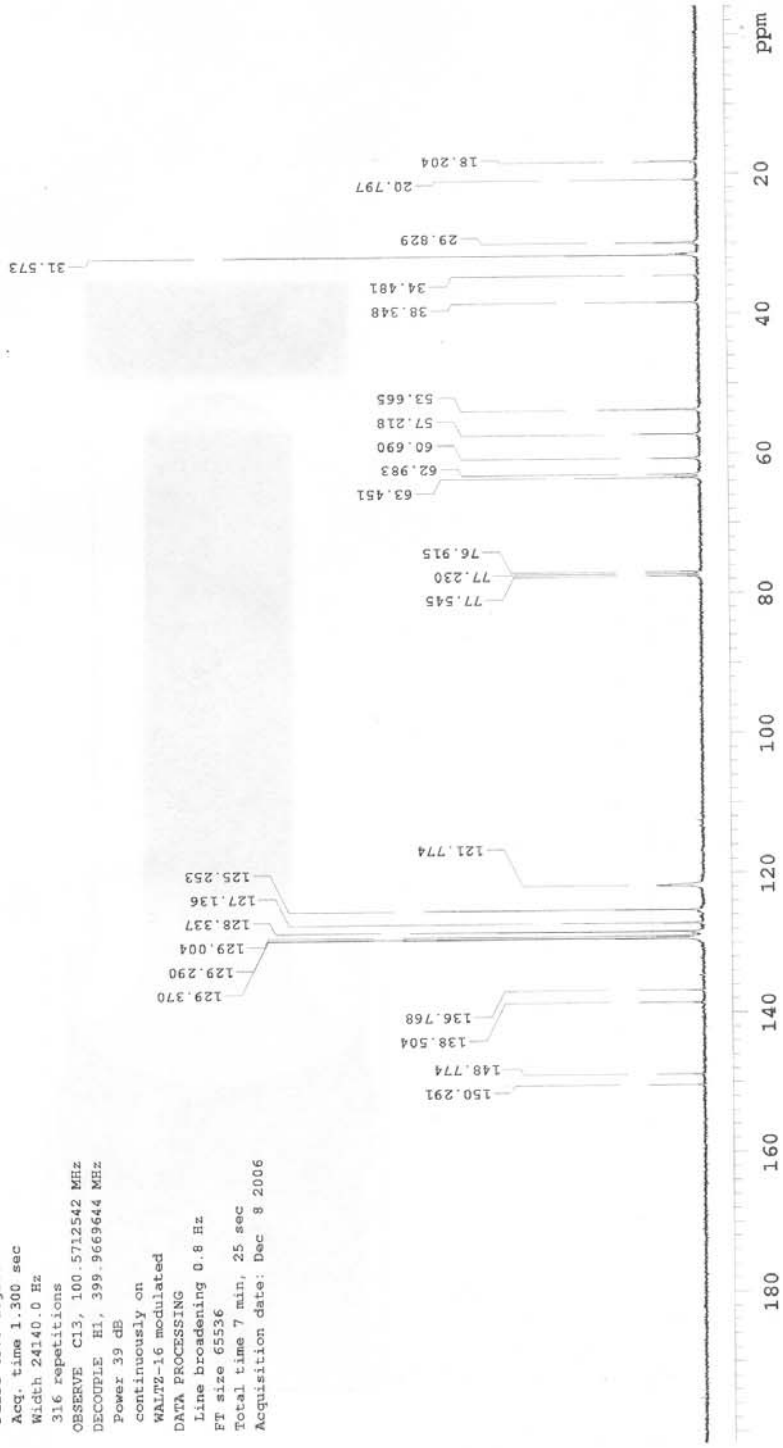
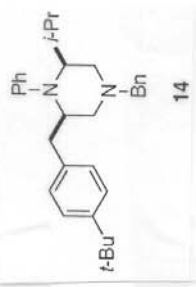
DATA PROCESSING

Line broadening 0.8 Hz

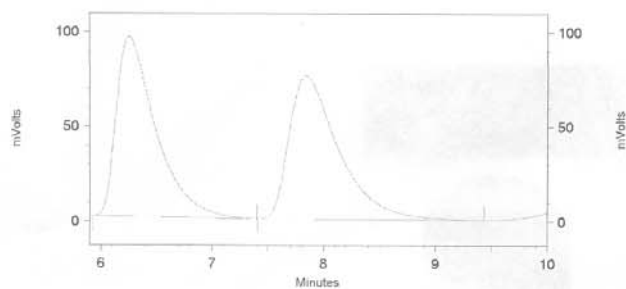
FT size 65536

Total time 7 min, 25 sec

Acquisition date: Dec 8 2006



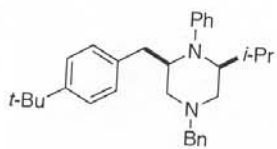
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-66-2-may16071mLpermindillhex.dat



OD-H
100% Hex
1 mL/min

Detector 1 Ch2-254nm
Results

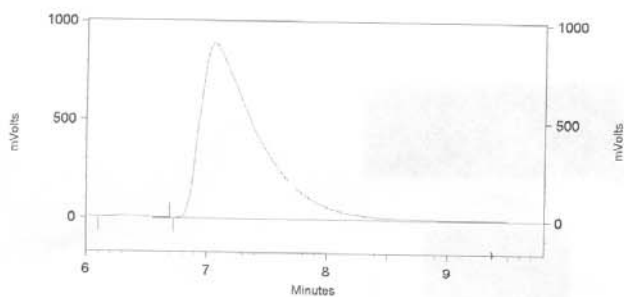
Retention Time	Area	Area Percent
6.250	2334202	50.007
7.842	2333531	49.993
Totals	4667733	100.000



14
(Racemic)

OD-H
100% Hex
1 mL/min

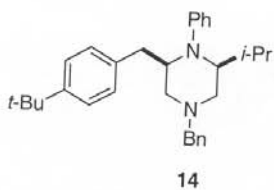
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-59-2-chiralhexanes.dat



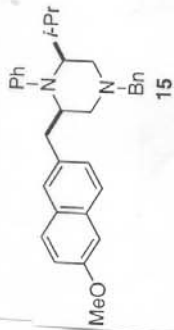
OD-H
100% Hex
1 mL/min

Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
6.292	92296	0.312
7.058	29526566	99.688
Totals	29618862	100.000



OD-H
100% Hex
1 mL/min



Standard Proton

File: J5NVIII-61-2H1

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

File: J5NVIII-61-2H1

INVA-500 "Py, Chem. Lab, UGA, ch., Edu"

Pulsx, delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

8 repetitions

OBSERVE H1, 499.9042611 MHz

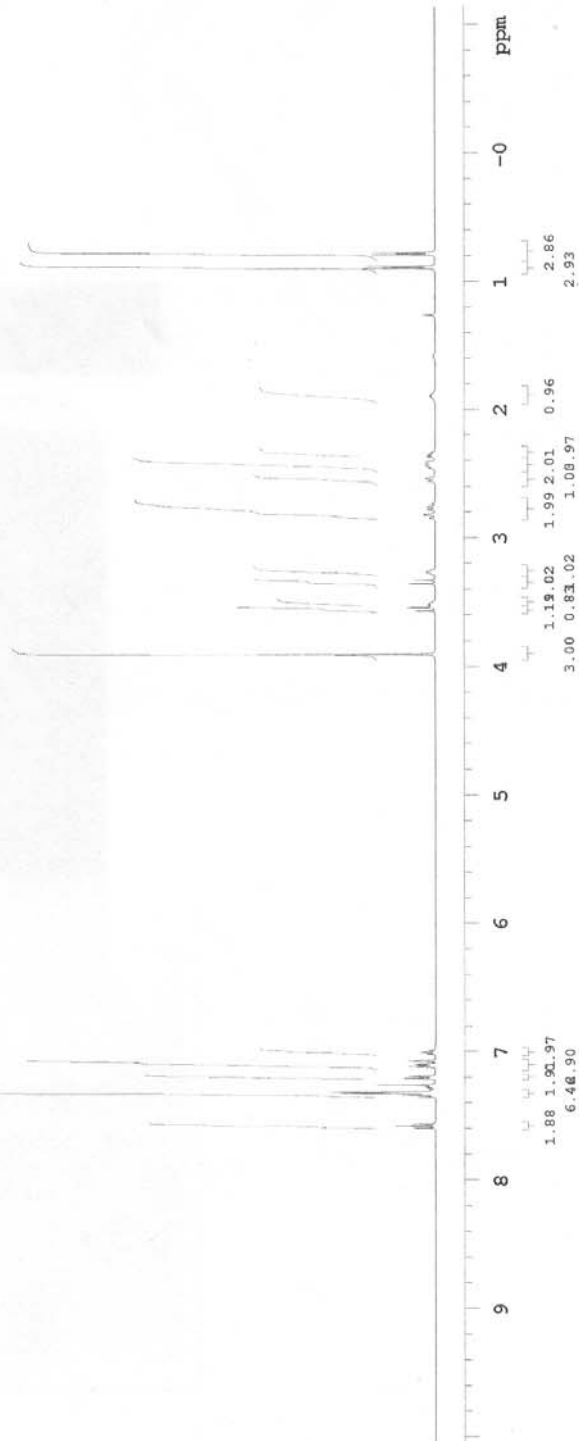
DATA PROCESSING

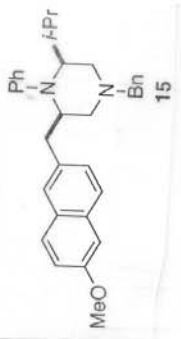
Line broadening 0.2 Hz

FT size 65536

Total time 0 min, 31 sec

Acquisition date: Mar 9 2007





Std Carbon

File: JSNVIII-61-2-C13

Pulse Sequence: #2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

File: JSNVIII-61-2-C13

INOVA-400 "Md.Chem.LSA.DMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

1208 repetitions

OBSERVE C13, 100.5712425 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

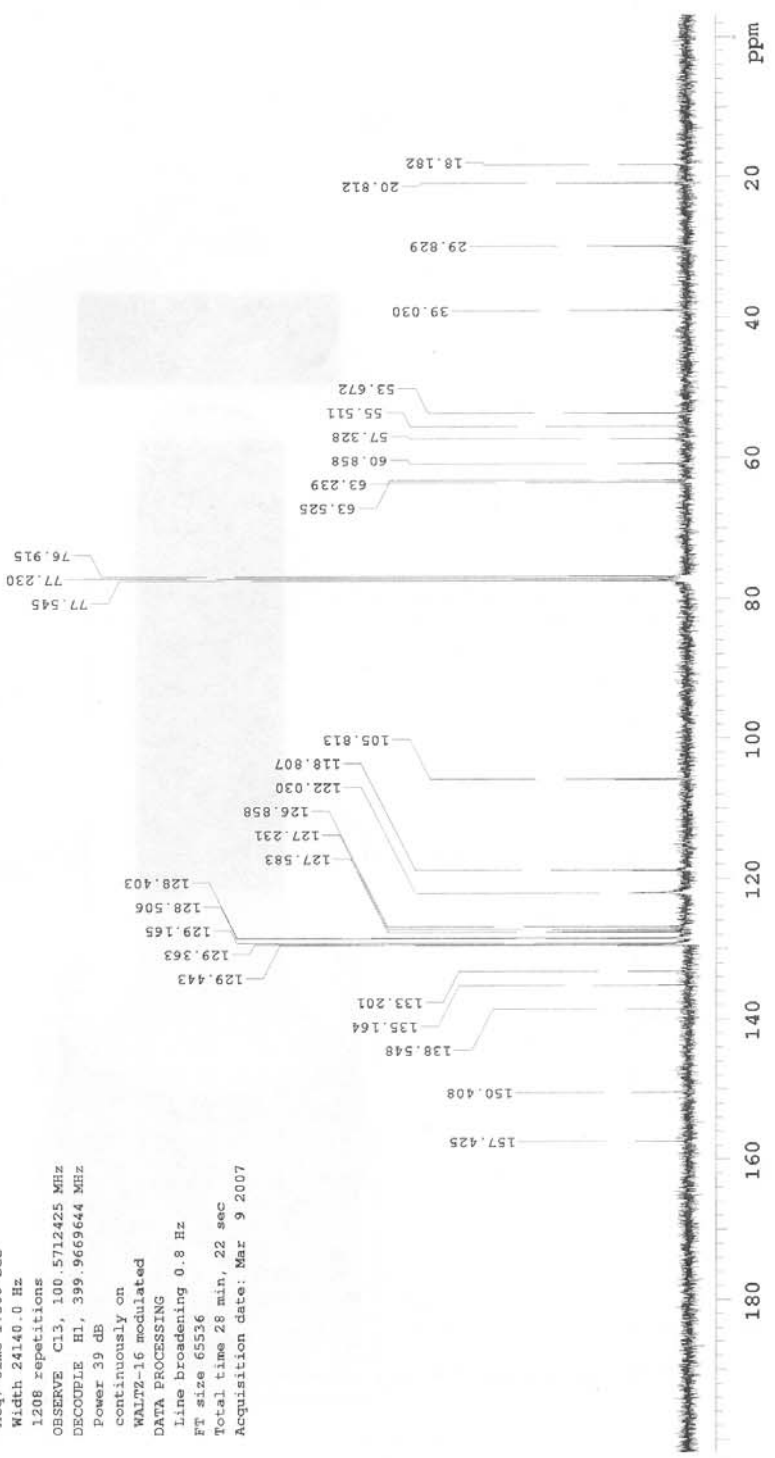
DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 28 min, 22 sec

Acquisition date: Mar 9 2007



Standard Proton

File: JSNVIII-61-2-cosy

Pulse Sequence: gCOSY

Solvent: cd3od

Ambient temperature

Operator: jmkhla

File: JSNVIII-61-2-cosy

INOVA-500 "Md.Chem.USA,UMich.Edu"

Relax. delay 1.301 sec

Acq. time 0.206 sec

Width 4970.2 Hz

2D Width 4970.2 Hz

2 repetitions

200 increments

OBSERVE H1, 499.9062312 MHz

DATA PROCESSING

Sine bell 0.103 sec

F1 DATA PROCESSING

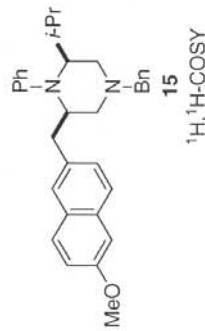
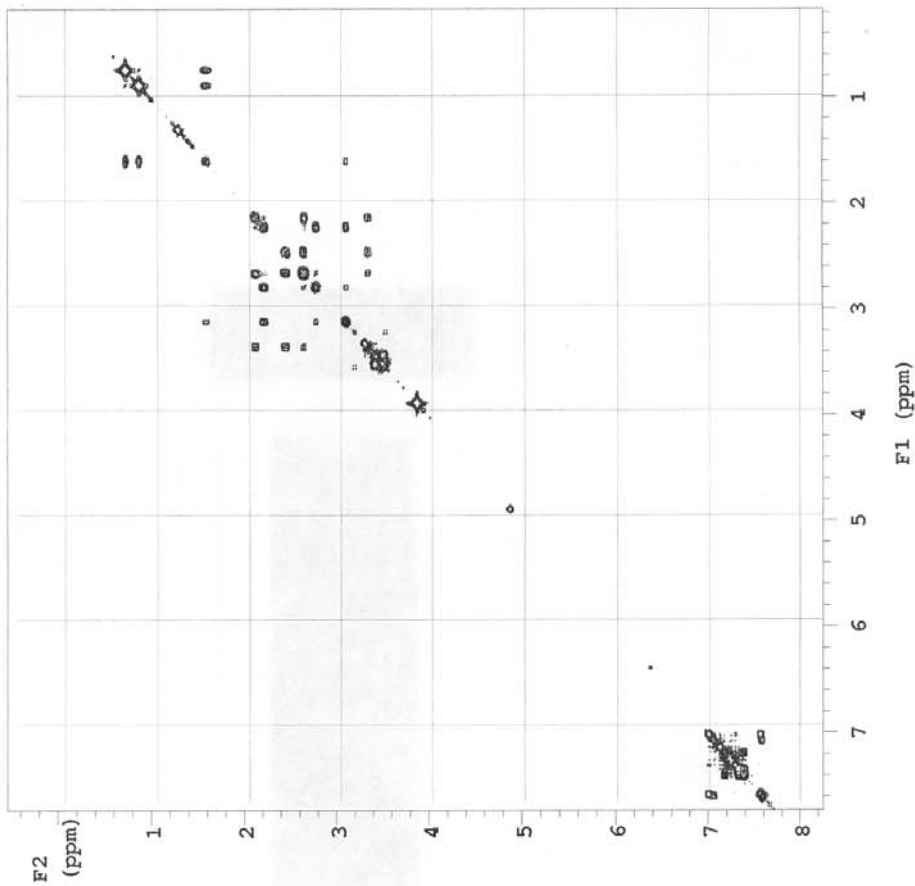
Sine bell 0.080 sec

FT size 4096 x 4096

Total time 10 min, 40 sec

Acquisition date: Mar 9 2007

In MeOH



In MeOH

Std proton

File: Noesy

Pulse Sequence: NOESY

Solvent: cd3cd

Ambient temperature

Operator: jnakhla

INOVA-400 "Zr.Chem.LSA.UMich.Edu"

Relax. delay 1.000 sec

Mixing 0.500 sec

Acq. time 0.229 sec

Width 4474.8 Hz

2D Width 4474.8 Hz

8 repetitions

2 x 200 increments

OBSERVE H1, 399.9665404 MHz

DATA PROCESSING

Gauss apodization 0.106 sec

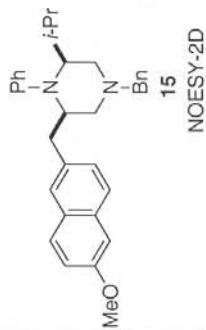
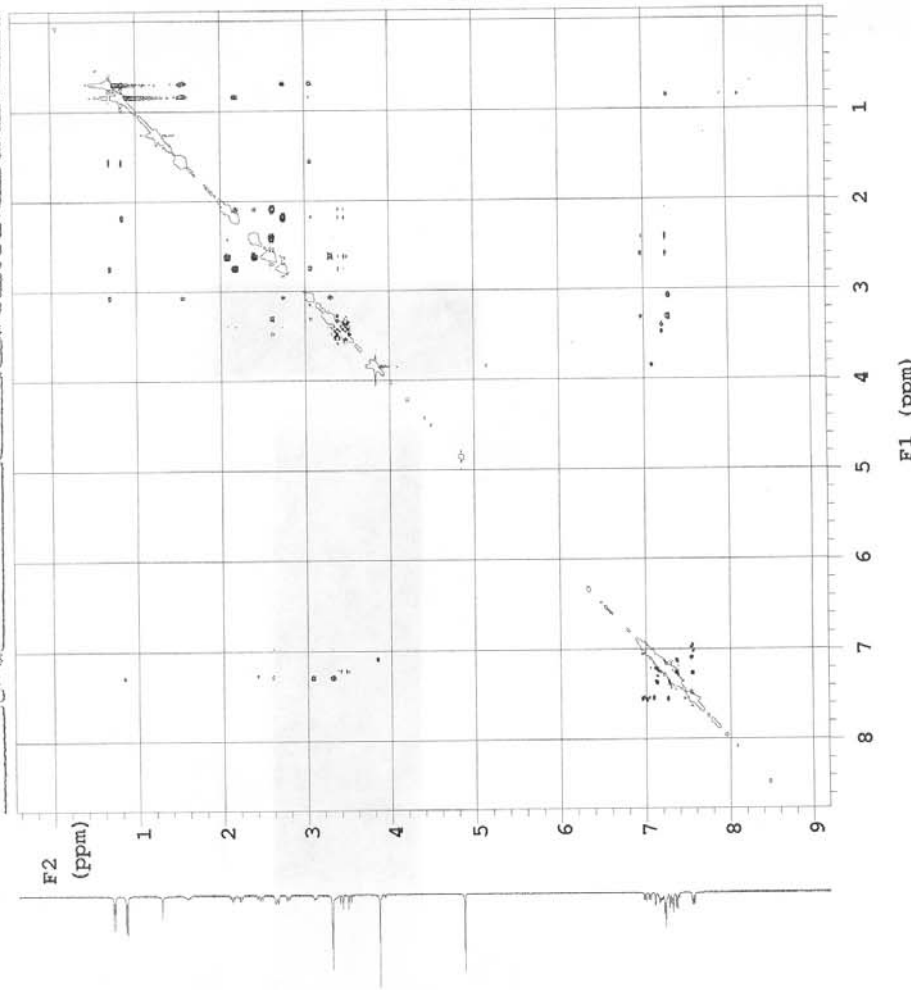
F1 DATA PROCESSING

Gauss apodization 0.082 sec

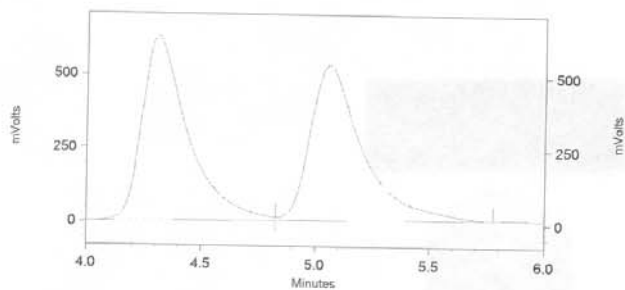
FT size 4096 x 4096

Total time 1 hr, 35 min, 15 sec

Acquisition date: Mar 10 2007



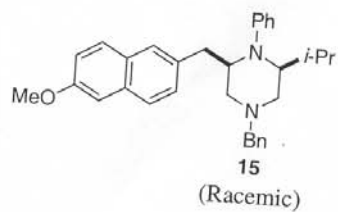
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-67-2-rac30AD.dat



AD
5% IPA/Hex
0.9 mL/min

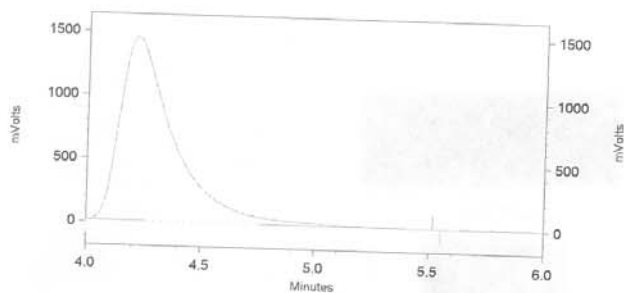
Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
4.308	8690072	50.871
5.058	8392403	49.129
Totals	17082475	100.000



AD
5% IPA/Hex
0.9 mL/min

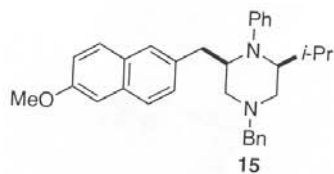
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-61-2-chiral-feb1307dii2.dat



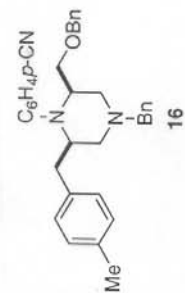
AD
5% IPA/Hex
0.9 mL/min

Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
4.217	23659024	99.580
5.775	99800	0.420
Totals	23758824	100.000



AD
5% IPA/Hex
0.9 mL/min



Standard Proton

File: JSNVIII-105-2

Pulse Sequence: #2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

File: JSNVIII-105-2

INOVA-500 "Dy.Chem.LSA,UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7988.4 Hz

8 repetitions

OBSERVE H1, 499.9042609 MHz

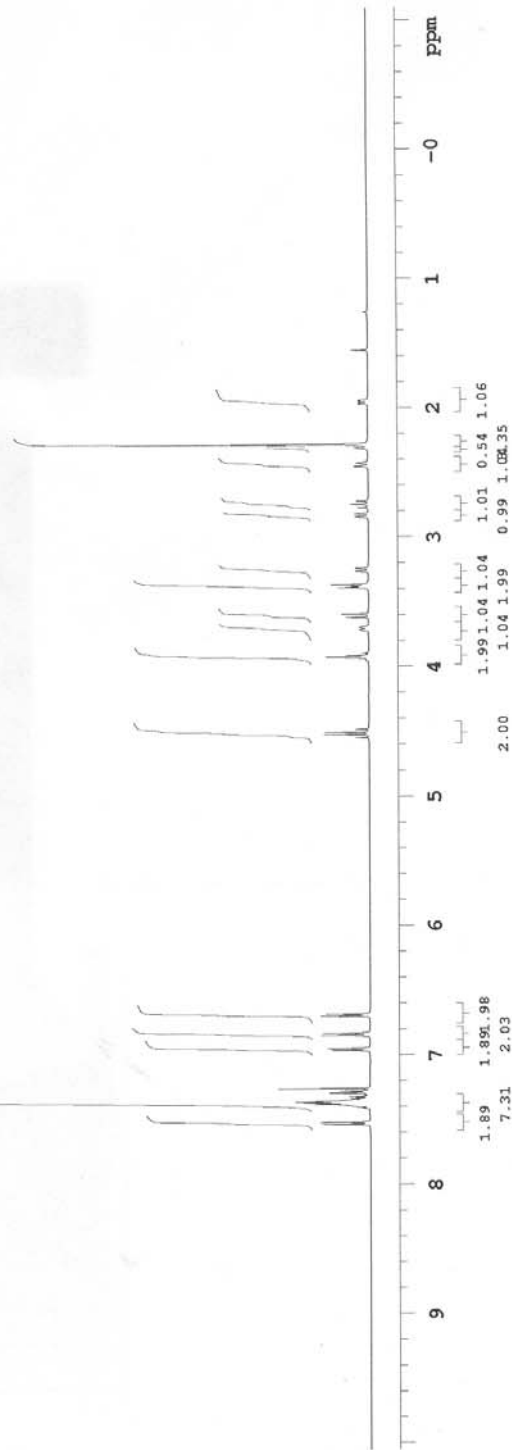
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min, 31 sec

Acquisition date: Mar 8 2007



Standard Carbon

File: JSNVIII-105-2-C13

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

File: JSNVIII-105-2-C13

INOVA-500 "Dy.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acc. time 1.300 sec

Width 30165.9 Hz

17420 repetitions

OBSERVE C13, 125.7010001 MHz

DECOUPLE H1, 499.9067532 MHz

Power 31 dB

continuously on

WALTZ-16 modulated

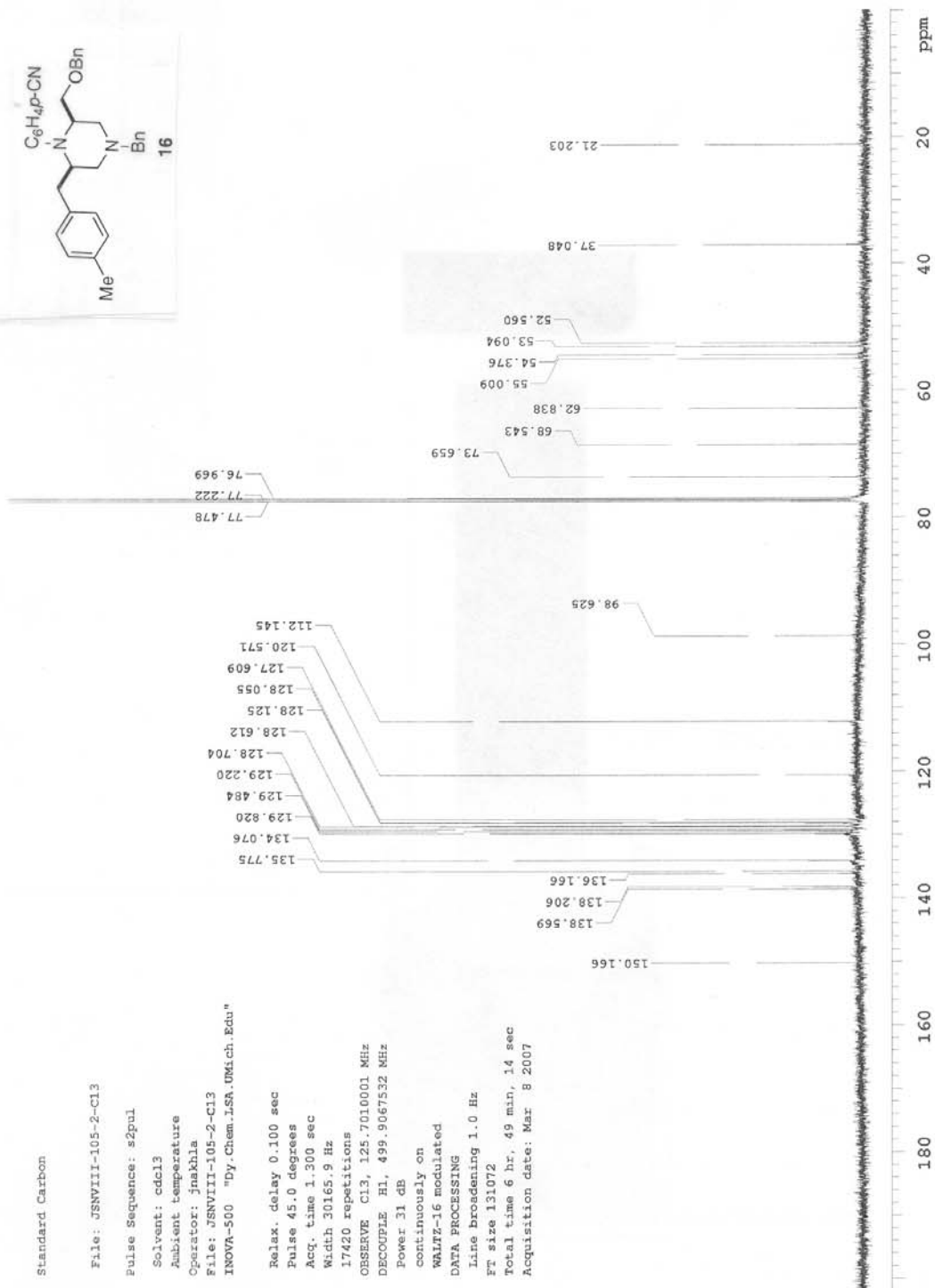
DATA PROCESSING

Line broadening 1.0 Hz

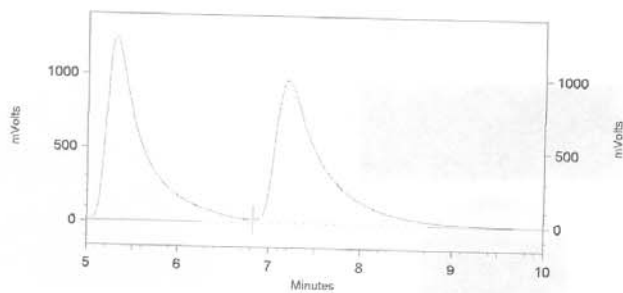
FT size 131072

Total time 6 hr, 49 min, 14 sec

Acquisition date: Mar 8 2007



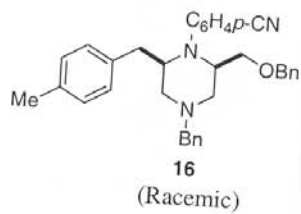
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-108-2AD2.dat



AD
10% IPA/Hex
1 mL/min

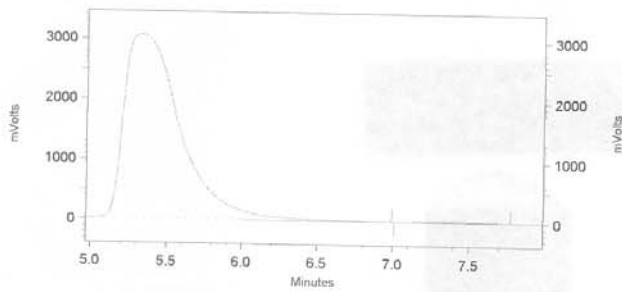
Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
5.308	5057835	48.766
7.192	5313778	51.234
Totals	10371613	100.000



AD
10% IPA/Hex
1 mL/min

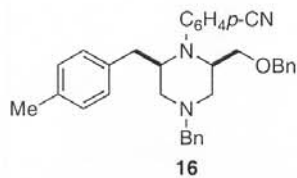
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New
Folder\JSNVIII-105-2AD.dat



AD
10% IPA/Hex
1 mL/min

Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
5.317	16510652	98.561
7.408	241039	1.439
Totals	16751691	100.000



AD
10% IPA/Hex
1 mL/min

Standard Proton

File: JSNVIII-106-2-H1

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

File: JSNVIII-106-2-H1

INOVA-500 "Md.Chem.LSA,UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

8 repetitions

OBSERVE H1, 499.9042609 MHz

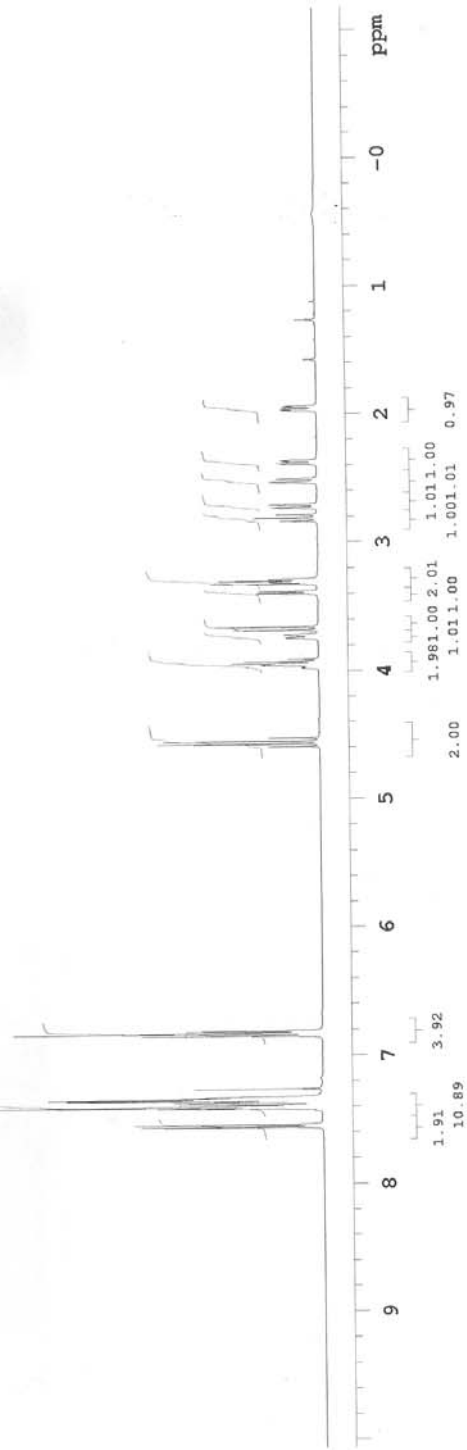
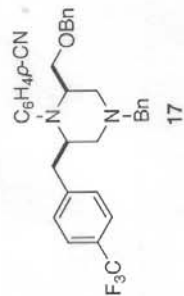
DATA PROCESSING

Line broadening 0.2 Hz

Ft size 65536

Total time 0 min, 31 sec

Acquisition date: Mar 7 2007



Standard Carbon

File: JSNVIII-106-2-C13

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jrnathla

File: JSNVIII-106-2-C13

INOVA-500 "Md.Chem.LSA.UMi.Ch.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30165.9 Hz

1232 repetitions

OBSERVE C13, 125.7010010 MHz

DECOUPLE H1, 499.9067532 MHz

Power 31 dB

continuously on

WALTZ-16 modulated

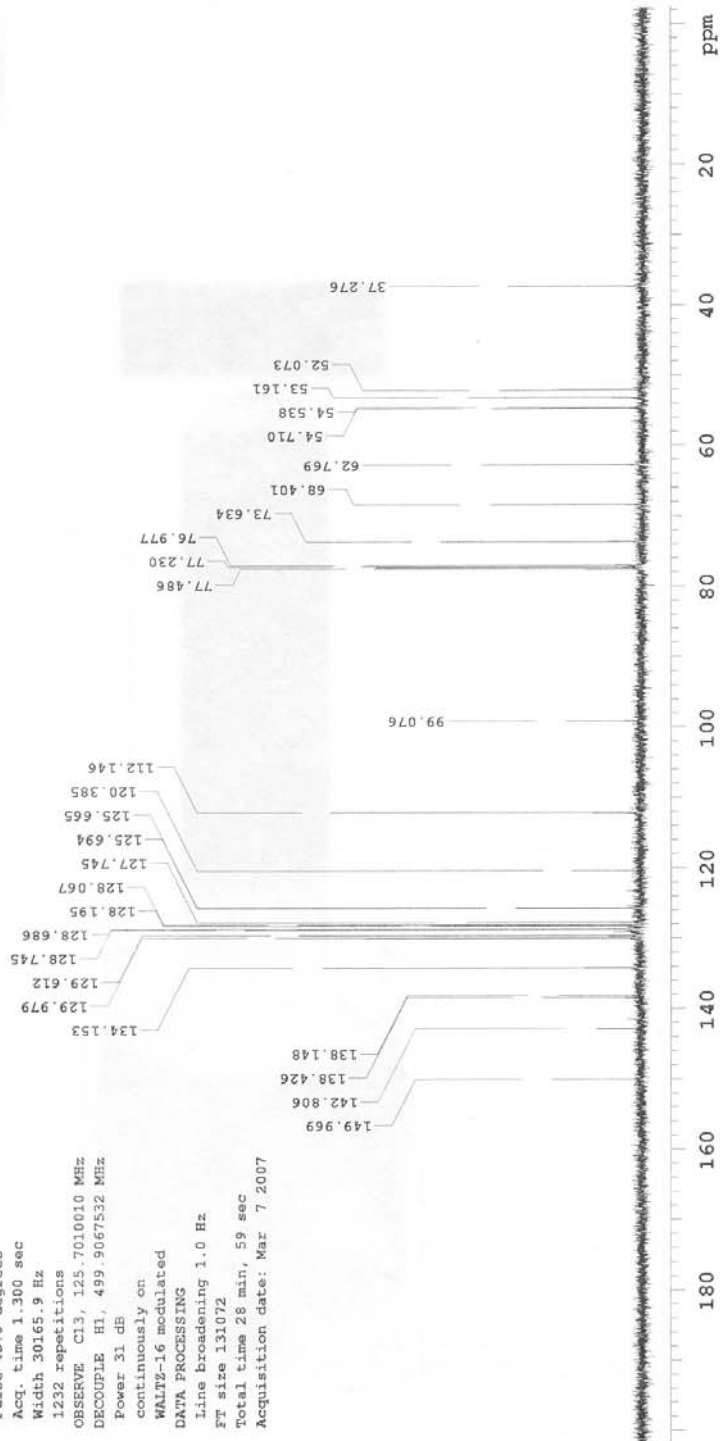
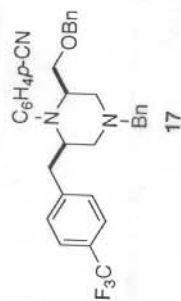
DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 28 min, 59 sec

Acquisition date: Mar 7 2007



Standard Proton

File: JSNVIII-106-2-COSYinCH3CN

Pulse Sequence: gCOSY

Solvent: c6d6

Ambient temperature

Operator: jnakhla

File: JSNVIII-106-2-COSYinCH3CN

INOVA-500 "Md.Chem.USA.UMich.Edu"

Relax. delay 1.301 sec

Acq. time 0.128 sec

Width 7998.4 Hz

2D Width 7998.4 Hz

2 repetitions

200 increments

OBSERVE H1, 499.9070426 MHz

DATA PROCESSING

Sine bell 0.064 sec

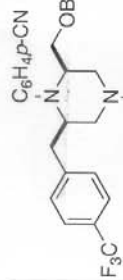
F1 DATA PROCESSING

Sine bell 0.050 sec

FF size 4096 x 4096

Total time 10 min, 4 sec

Acquisition date: Mar 8 2007



17

$^1\text{H}, ^1\text{H-COSY}$

F2
(ppm)

1

2

3

4

5

6

7

8

F1 (ppm)

2

3

4

5

6

7

8

Standard Proton

File: JSNVIII-106-2-HSQC

Pulse Sequence: gHSQC

Solvent: cdcl3

Ambient temperature

Operator: jmakhla

File: JSNVIII-106-2-HSQC

INOVA-500 "Md.Chem.USA,UMi.ch.Edu"

Relax. delay 1.301 sec

Acq. time 0.199 sec

Width 7998.4 Hz

2D Width 21367.5 Hz

4 repetitions

2 x 256 increments

OBSERVE H1, 499.9042609 MHz

DECOUPLE C13, 125.7104522 MHz

Power 40 dB

on during acquisition

off during delay

W40 id modulated

DATA PROCESSING

Gauss apodization 0.092 sec

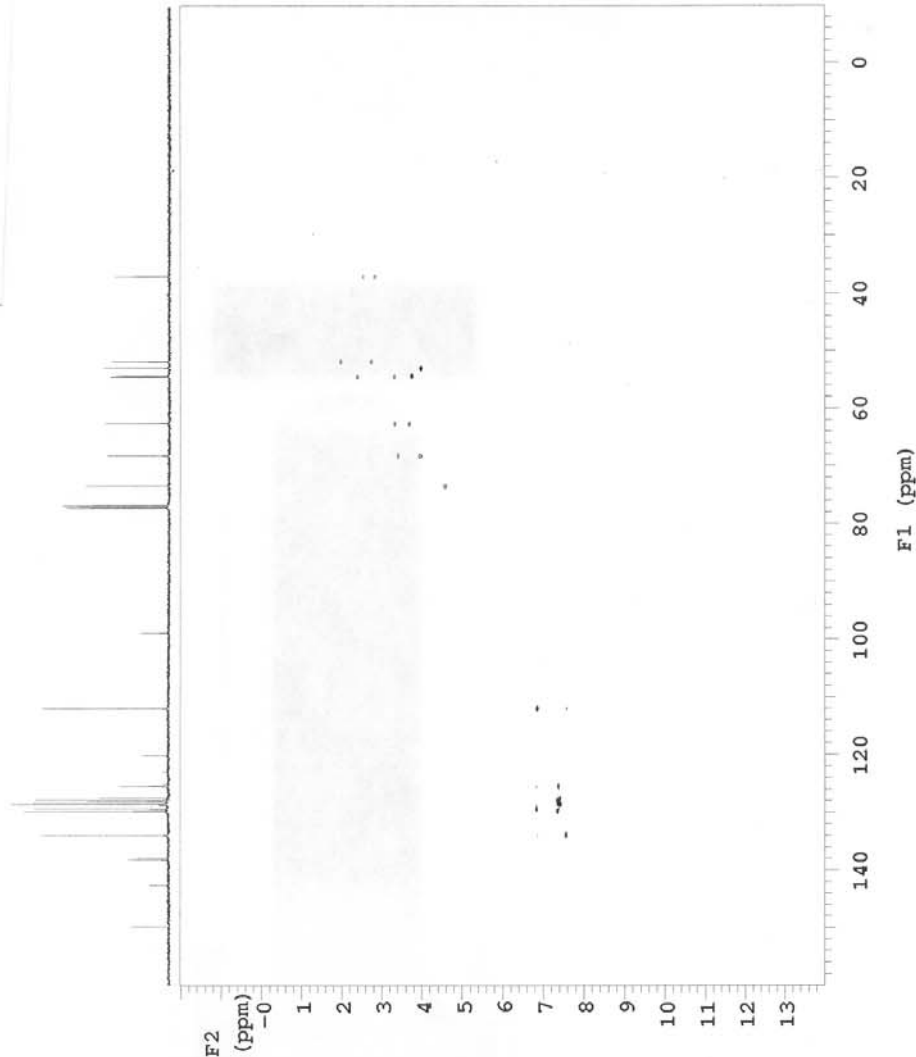
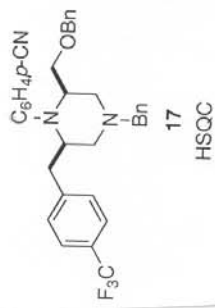
F1 DATA PROCESSING

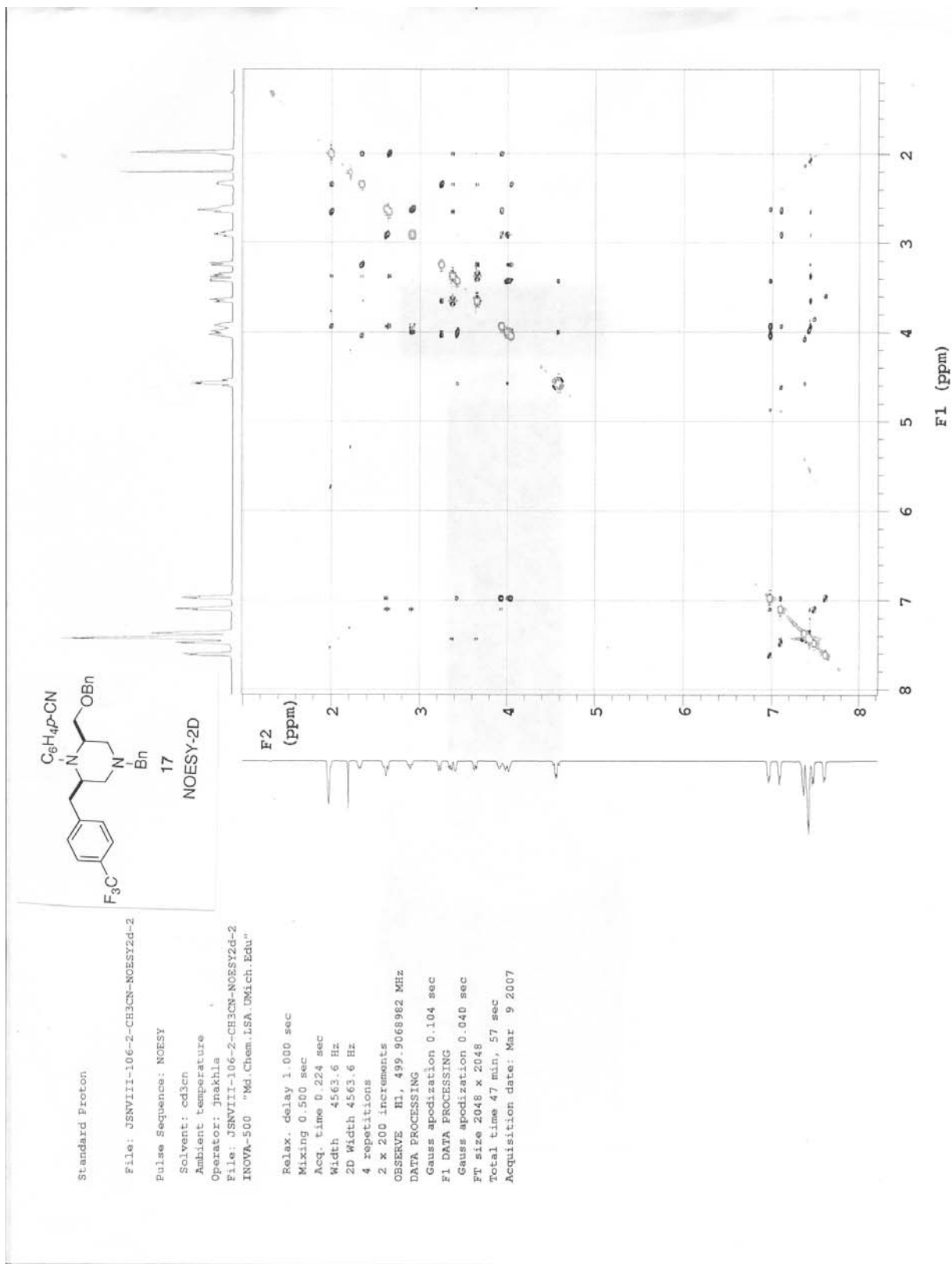
Gauss apodization 0.011 sec

FT size 8192 x 2048

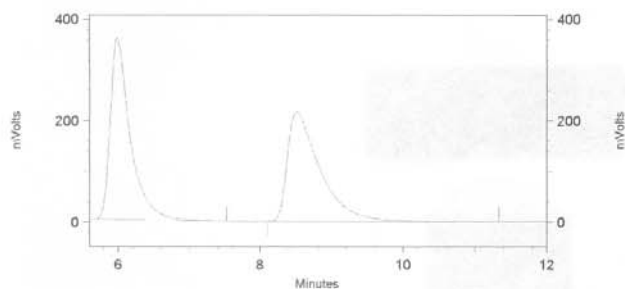
Total time 53 min, 53 sec

Acquisition date: Mar 8 2007





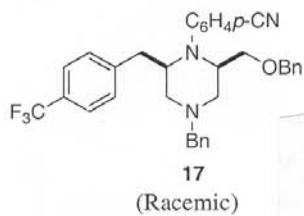
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New
Folder\JSNVIII-109-2-AD.dat



AD
10% IPA/Hex
1 mL/min

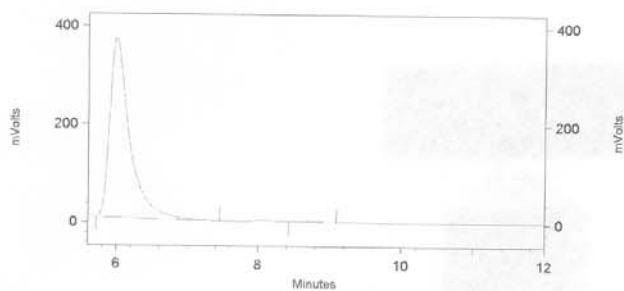
Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
5.983	6965137	50.378
8.508	6860614	49.622
Totals	13825751	100.000



AD
10% IPA/Hex
1 mL/min

Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-106-2-AD.dat

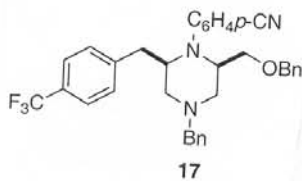


AD
10% IPA/Hex
1 mL/min

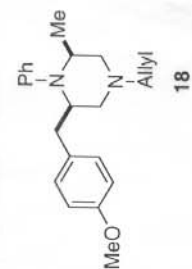
Detector 1 Ch2-254nm

Results

Retention Time	Area	Area Percent
5.992	7074994	99.686
8.675	22274	0.314
Totals	7097268	100.000



AD
10% IPA/Hex
1 mL/min



File: JSNVIII-152-2-reaction2-major1diastereomer

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhle

File: JSNVIII-152-2-reaction2-major1diastereomer

INOVA-500 "MD.Chem.USA.DMICH.EDU"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

4 repetitions

OBSERVE H1, 499.9042609 MHz

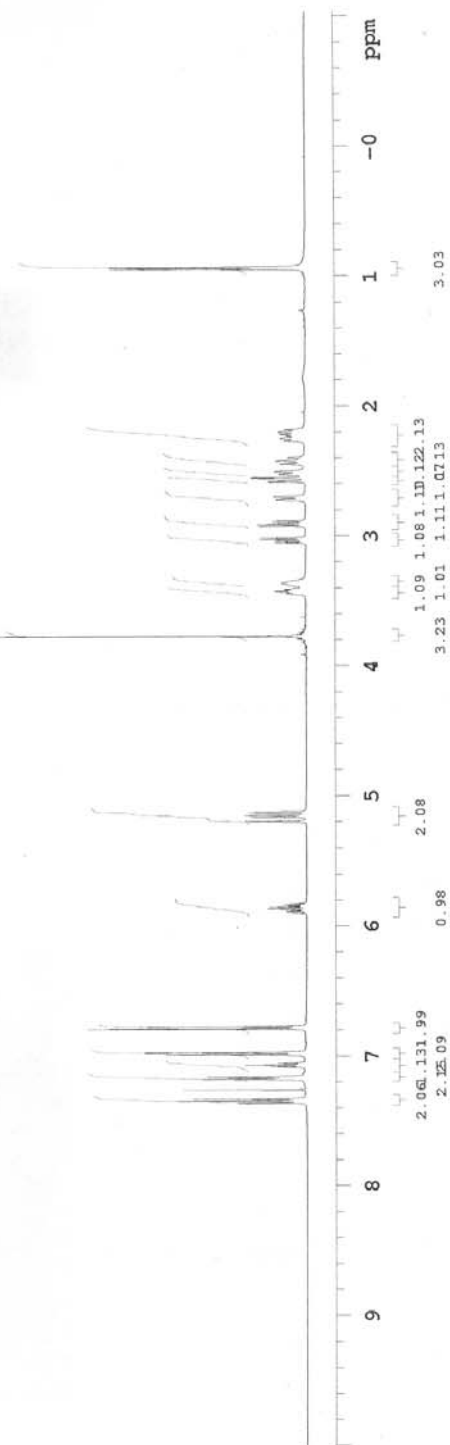
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min, 18 sec

Acquisition date: May 2 2007



Std Carbon

File: JSNVIII-152-2-C13

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jhakhia

File: JSNVIII-152-2-C13

INOVA-400 "Md.Chem.LSA,DMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

1140 repetitions

OBSERVE C13, 100.5712453 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

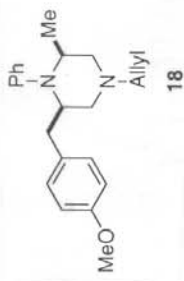
Line broadening 0.8 Hz

FT size 65536

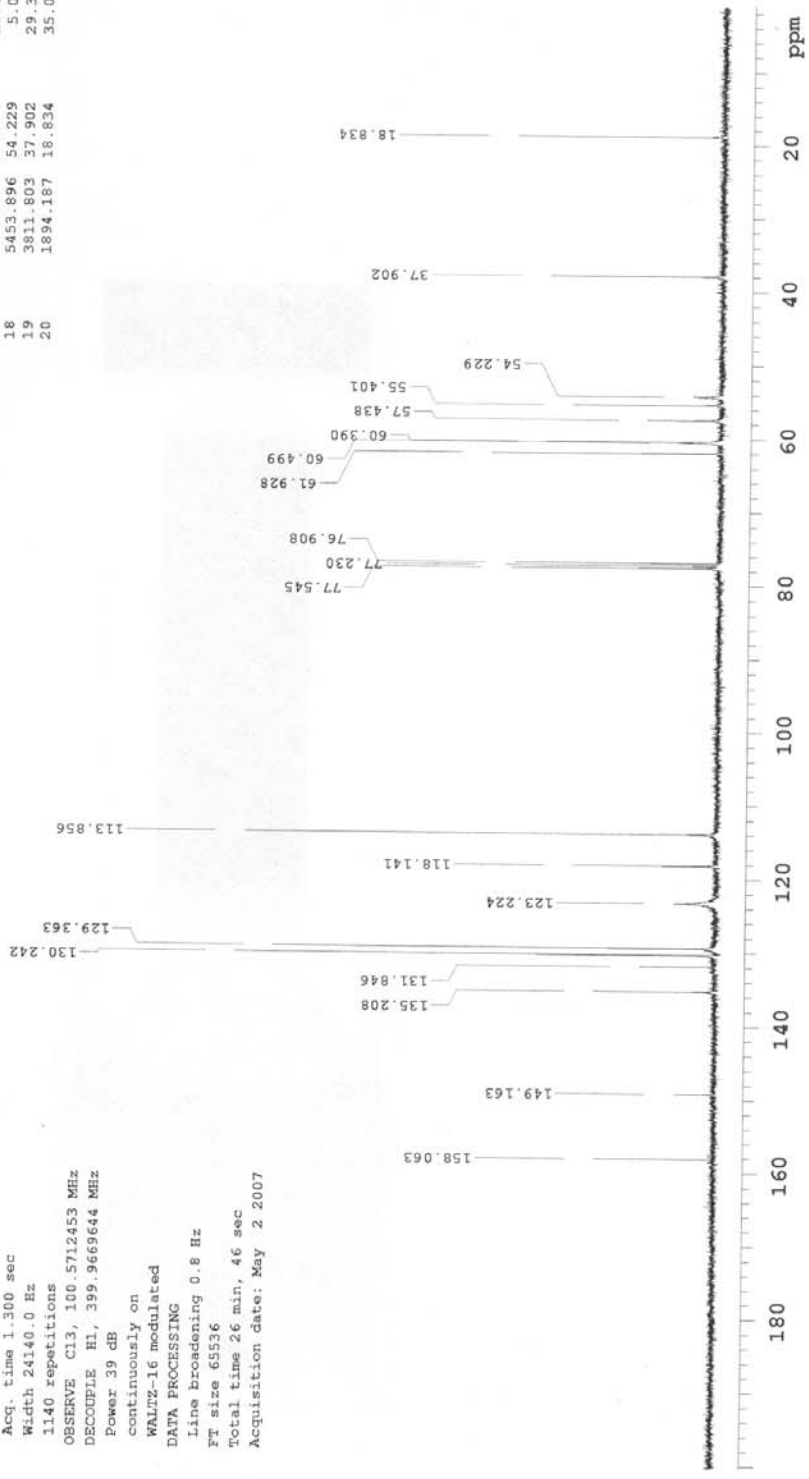
Total time 26 min, 46 sec

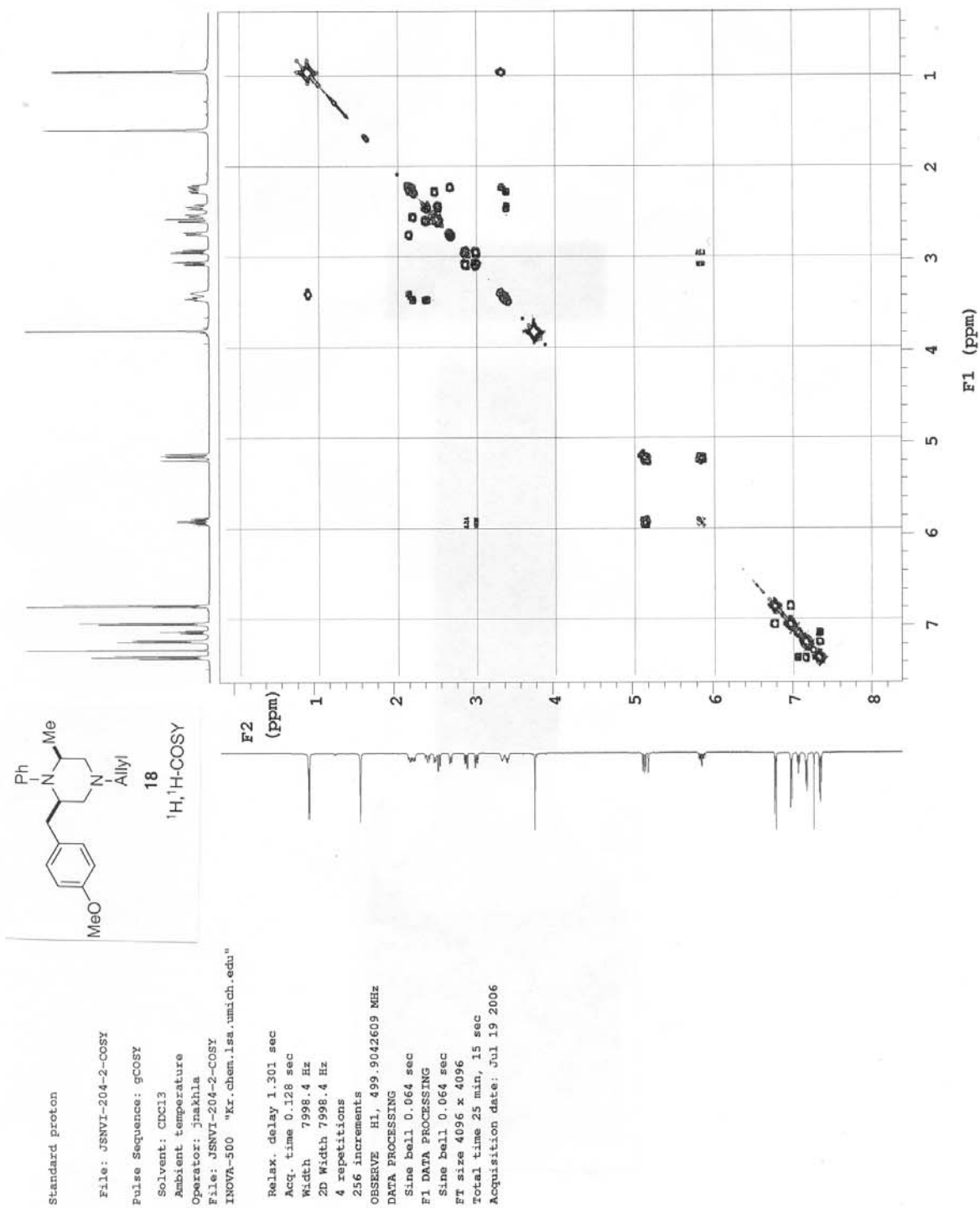
Acquisition date: May 2 2007

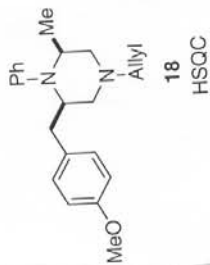
INDEX	FREQUENCY PPM	HEIGHT
1	15896.543	158.063
2	15001.459	149.163
3	13598.056	135.208
4	13259.913	131.846
5	13098.577	130.242
6	13010.173	129.363
7	12392.823	123.224
8	11881.557	118.141
9	11450.591	113.856
10	7798.795	77.545
11	7767.117	77.230
12	7734.703	76.908
13	6228.162	61.928
14	6084.507	60.499
15	6073.456	60.390
16	5776.568	57.438
17	5571.767	55.401
18	5453.896	54.229
19	3811.803	37.902
20	1894.187	18.834



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File: JSNVI-204-2-HSQC

Pulse Sequence: gHSQC

Solvent: CDCl3

Ambient temperature

Operator: jnakkla

File: JSNVI-204-2-HSQC

INOVA-500 "Kr.chem.isa.umich.edu"

Relax. delay 1.301 sec

Acq. time 0.199 sec

Width 4282.0 Hz

2D Width 21367.5 Hz

4 repetitions

2 x 200 increments

OBSERVE H1, 499.9042607 MHz

DECOUPLE C13, 125.7104522 MHz

Power 41 dB

on during acquisition

off during delay

W40_id modulated

DATA PROCESSING

Gauss apodization 0.092 sec

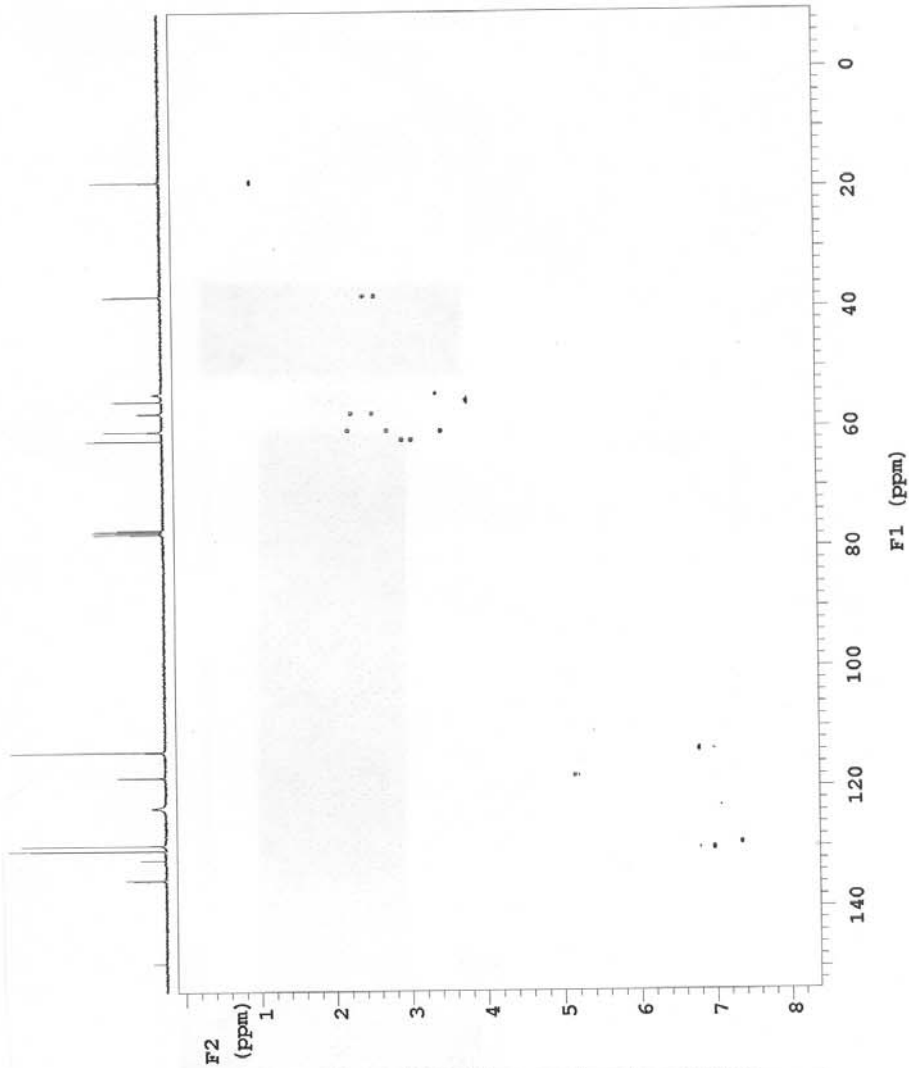
F1 DATA PROCESSING

Gauss apodization 0.009 sec

FT size 4096 x 2048

Total time 42 min, 15 sec

Acquisition date: Aug 2 2006



Standard proton

File: JENVI-204-2-NOESY2D

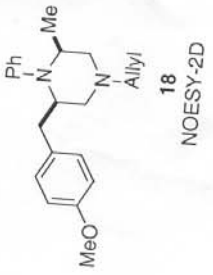
Pulse Sequence: NOESY

Solvent: CDCl3

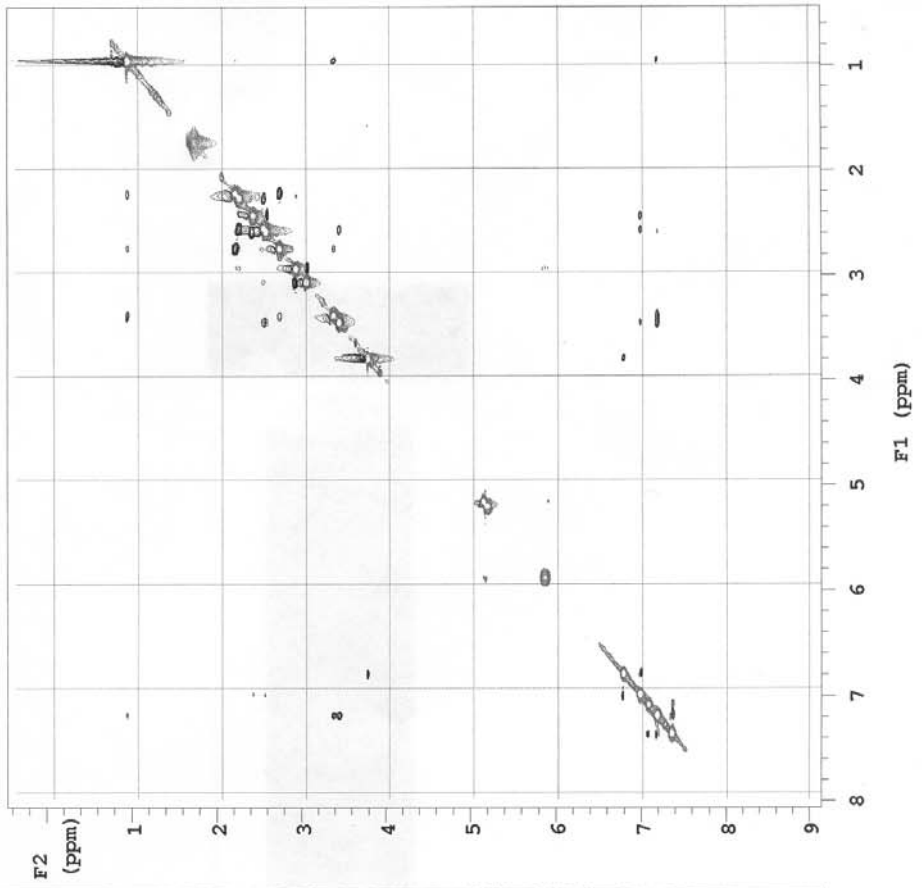
Ambient temperature

Operator: Jnakhla

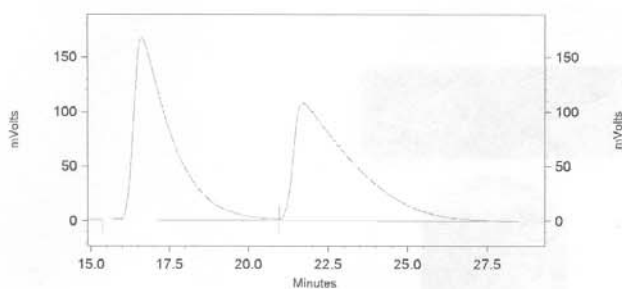
File: JENVI-204-2-NOESY2D
INOVA-500 "Kr.chem.1sa.umich.edu"



Relax. delay 1.000 sec
 Mixing 0.400 sec
 Acq. time 0.128 sec
 Width 7998.4 Hz
 2D Width 7998.4 Hz
 4 repetitions
 2 x 128 increments
 OBSERVE H1, 499.9042537 MHz
 DATA PROCESSING
 Gauss apodization 0.059 sec
 F1 DATA PROCESSING
 Gauss apodization 0.030 sec
 FT size 2048 x 2048
 Total time 27 min, 20 sec
 Acquisition date: Jul 31 2006



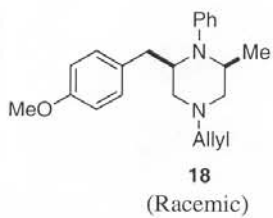
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-127-2-rachexODH3.dat



OD-H
100% Hex
1 mL/min

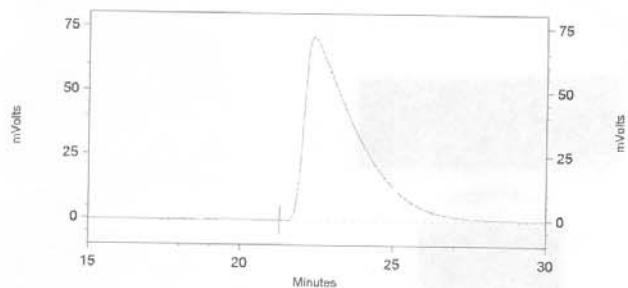
Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
16.600	13692114	49.687
21.708	13864520	50.313
Totals	27556634	100.000



OD-H
100% Hex
1 mL/min

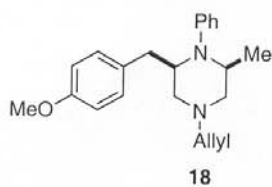
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-152-2-ODHhexanes.dat



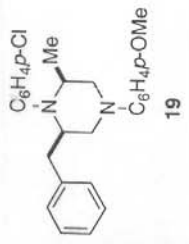
OD-H
100% Hex
1 mL/min

Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
19.750	30013	0.351
22.392	8511817	99.649
Totals	8541830	100.000



OD-H
100% Hex
1 mL/min



File: JSNVIII-146-2-smallerscale

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

File: JSNVIII-146-2-smallerscale

INOVA-500 "Dy.Chem.LSA,UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

44 repetitions

OBSERVE H1, 499.9042614 MHz

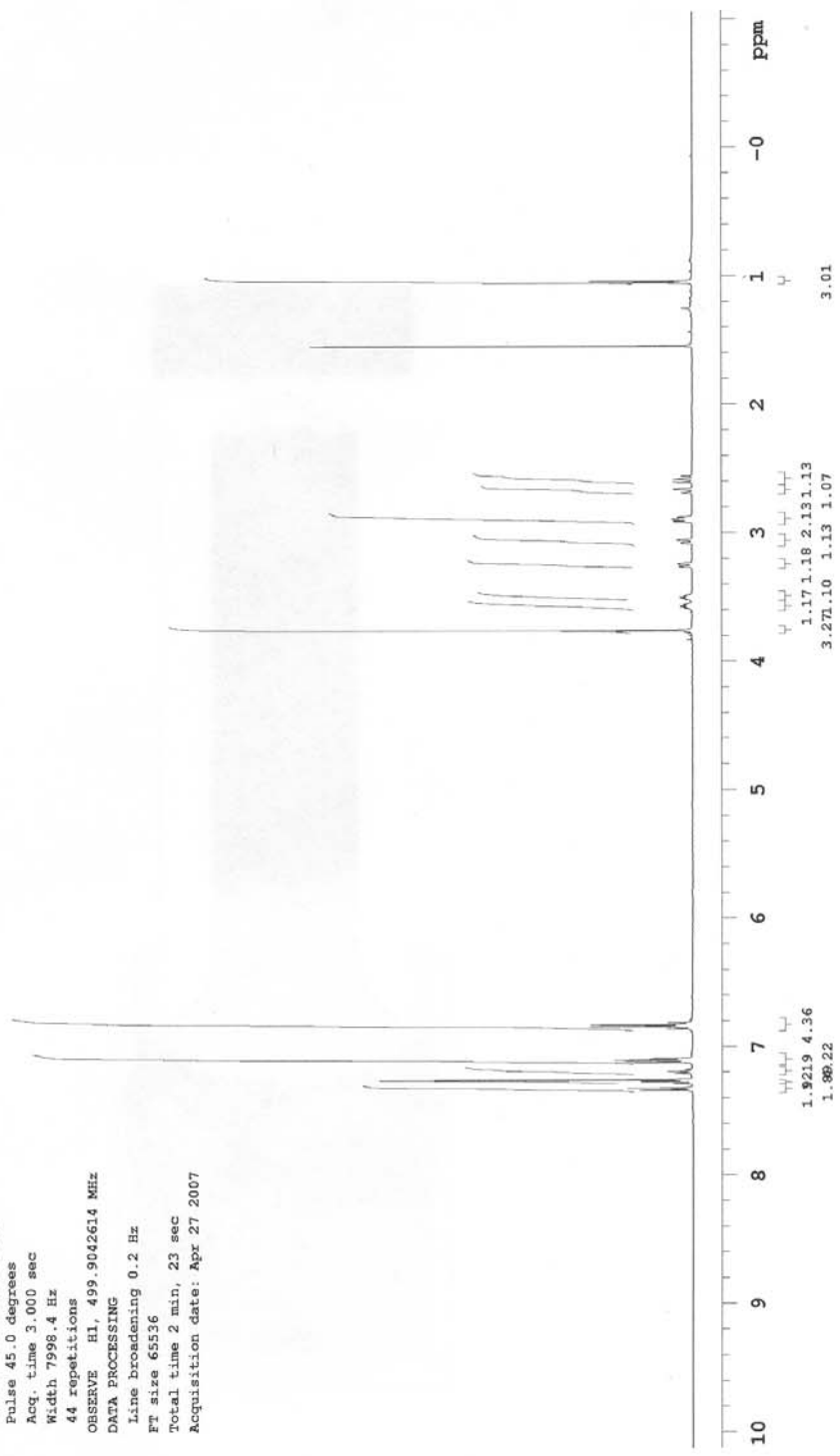
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min, 23 sec

Acquisition date: Apr 27 2007



Standard Carbon

File: JSNVIII-146-2-C13

Pulse Sequence: szpul

Solvent: cdcl3

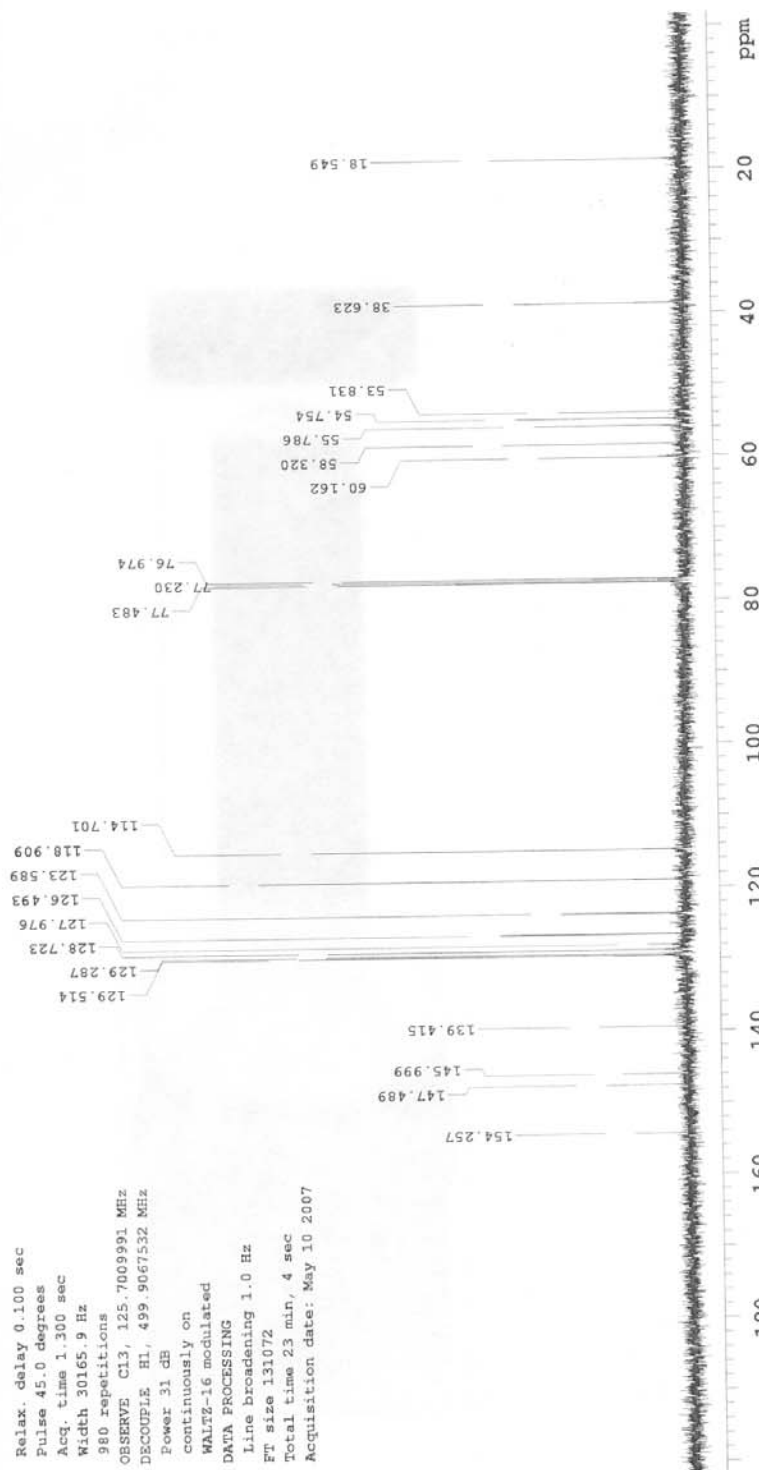
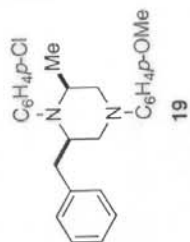
Ambient temperature

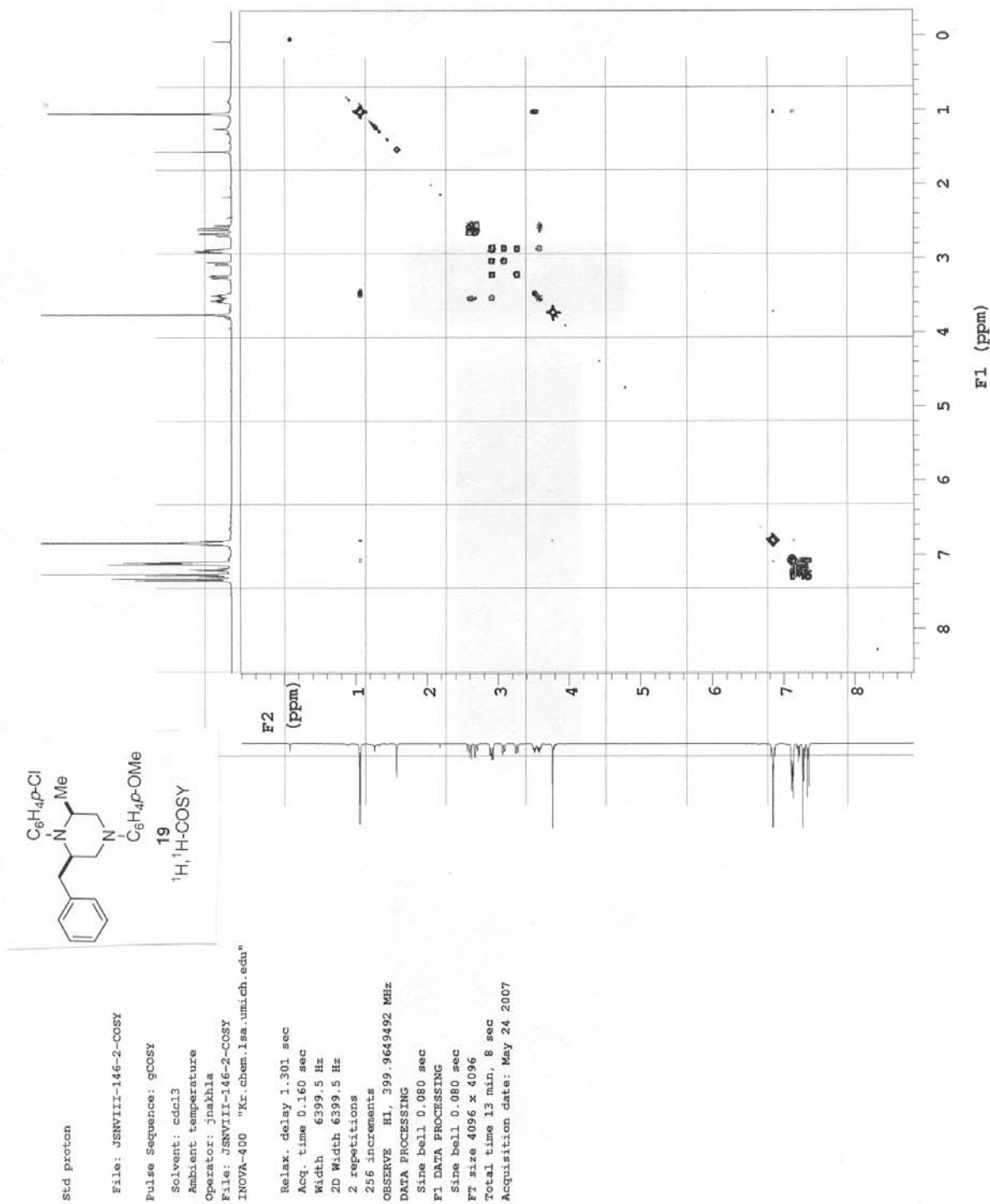
Operator: jnakhla

File: JSNVIII-146-2-C13

INOVA-500 "Md.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 30165.9 Hz
 980 repetitions
 OBSERVE C13, 125.7009991 MHz
 DECOUPLE H1, 499.9067532 MHz
 Power 31 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 131072
 Total time 23 min, 4 sec
 Acquisition date: May 10 2007





Std proton

File: JSNVIII-146-2-COSY

Pulse Sequence: gCOSY

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

File: JSNVIII-146-2-COSY

INOVA-400 "Kr.chem.lsa.umich.edu"

Relax. delay 1.301 sec

Acq. time 0.160 sec

Width 6399.5 Hz

2D Width 6399.5 Hz

2 repetitions

256 increments

OBSERVE H1, 399.9649492 MHz

DATA PROCESSING

Sine bell 0.080 sec

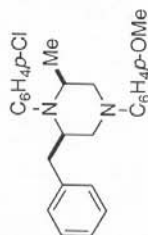
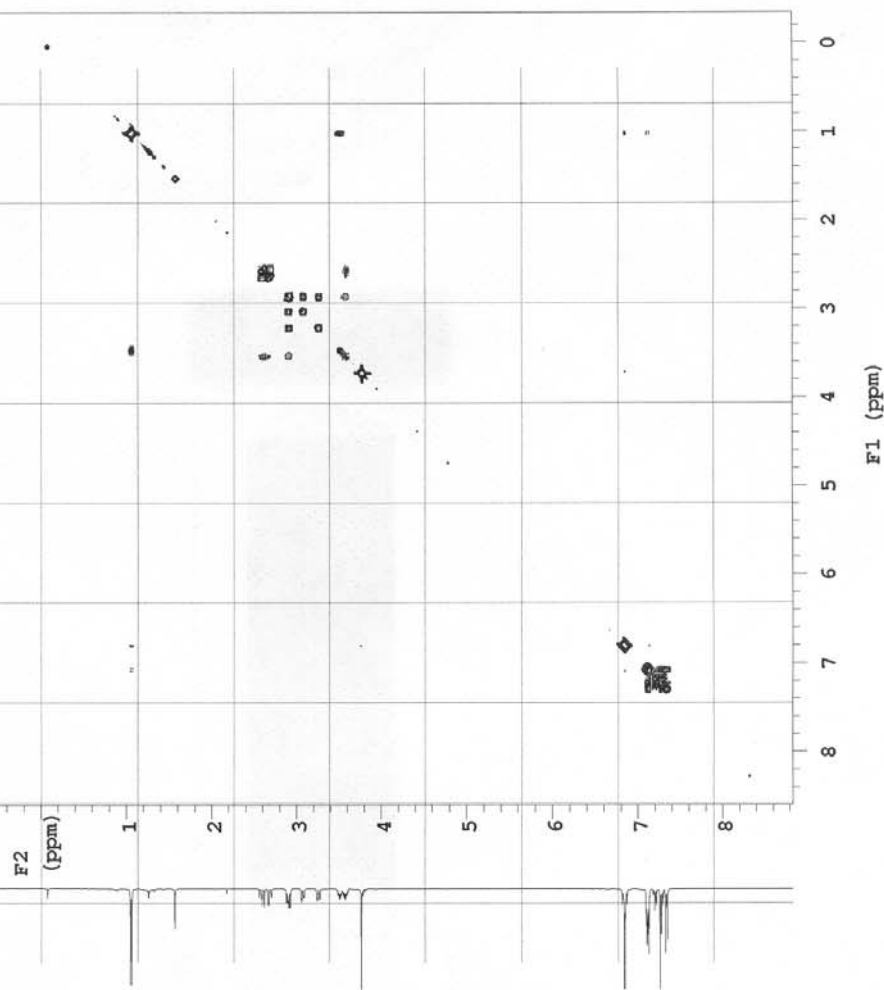
F1 DATA PROCESSING

Sine bell 0.080 sec

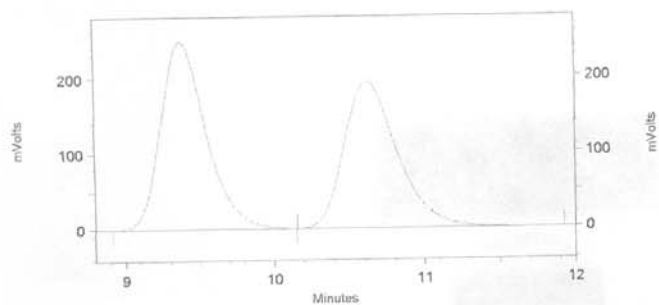
FT size 4096 x 4096

Total time 13 min, 8 sec

Acquisition date: May 24, 2007

¹H, ¹H-COSY

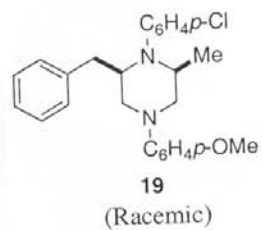
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-139-2-ODH4a.dat



OD-H
1% IPA/Hex
0.5 mL/min

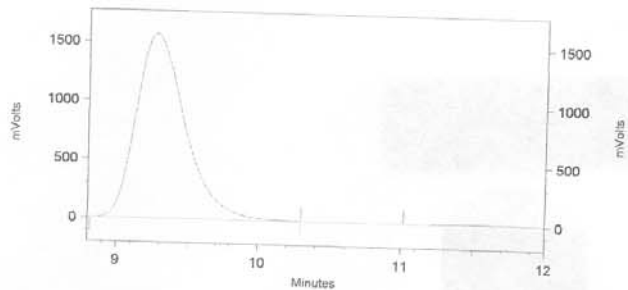
Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
9.375	5279371	52.511
10.617	4774524	47.489
Totals	10053895	100.000



OD-H
1% IPA/Hex
0.5 mL/min

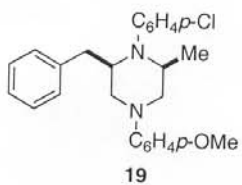
Data: C:\CLASS-VP\Enterprise\Projects\Default\Data\Nakhla Data\New Folder\JSNVIII-146-2.dat



OD-H
1% IPA/Hex
0.5 mL/min

Detector 1 Ch2-254nm
Results

Retention Time	Area	Area Percent
9.267	37419978	99.808
10.300	71949	0.192
Totals	37491927	100.000



OD-H
1% IPA/Hex
0.5 mL/min

Std proton

File: JSNVIII-152-2-sp2-2H1

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jpakhla

File: JSNVIII-152-2-sp2-2H1

INOVA-400 "Dy.Chem.LSA.DMach.Edu"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6399.5 Hz

4 repetitions

OBSERVE H1, 399.9649482 MHz

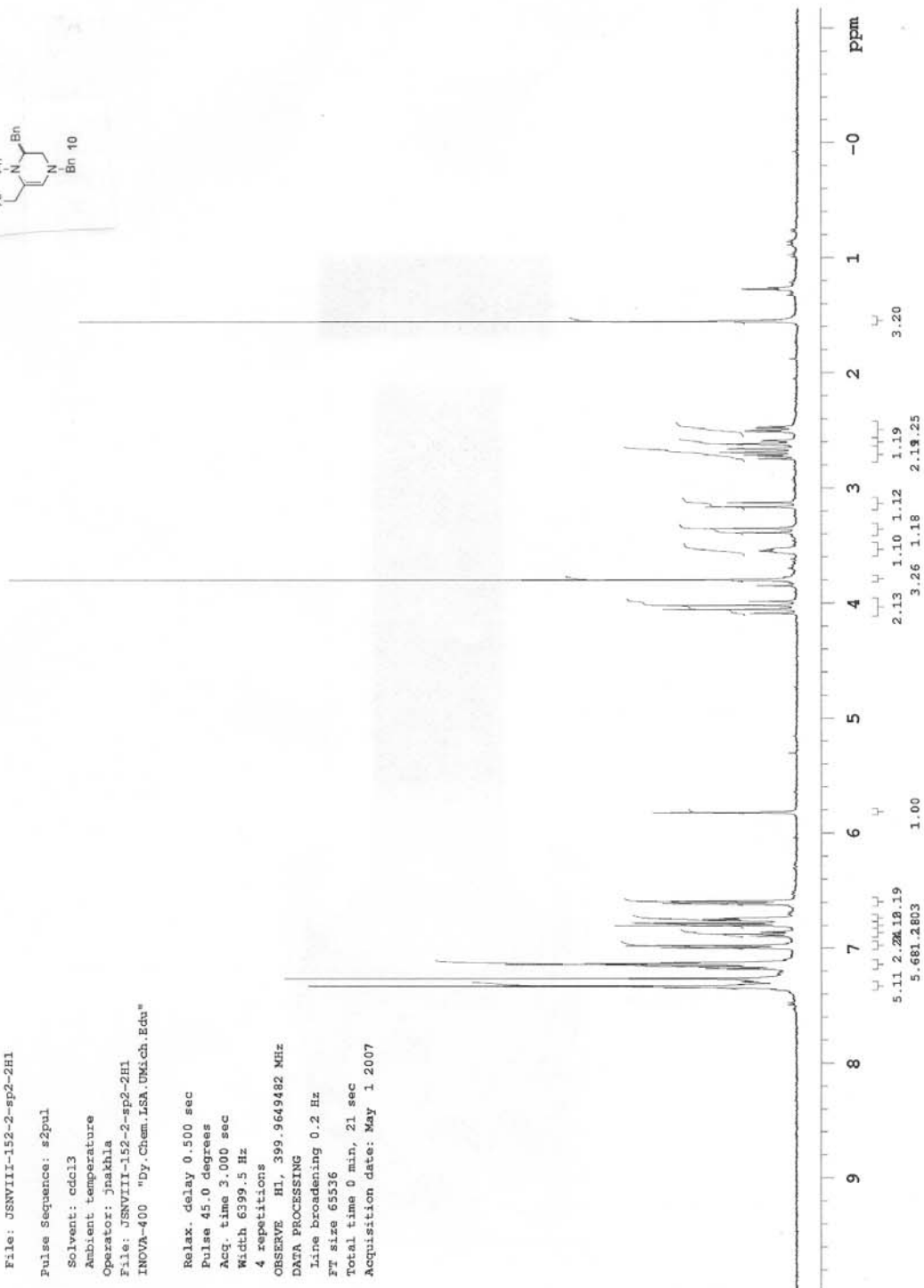
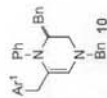
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min, 21 sec

Acquisition date: May 1 2007



Std proton

File: JSNVIII-152-2-sp2-COSY

Pulse Sequence: gCOSY

Solvent: cdcl3

Ambient temperature

Operator: jhakkla

File: JSNVIII-152-2-sp2-COSY

INOVA-400 "Md.Chem.LSA.UMich.Edu"

Relax. delay 1.301 sec

Acq. time 0.160 sec

Width 6399.5 Hz

2D Width 6399.5 Hz

2 repetitions

200 increments

OBSERVE F1, 399.9649496 MHz

DATA PROCESSING

Sq. sine bell 0.080 sec

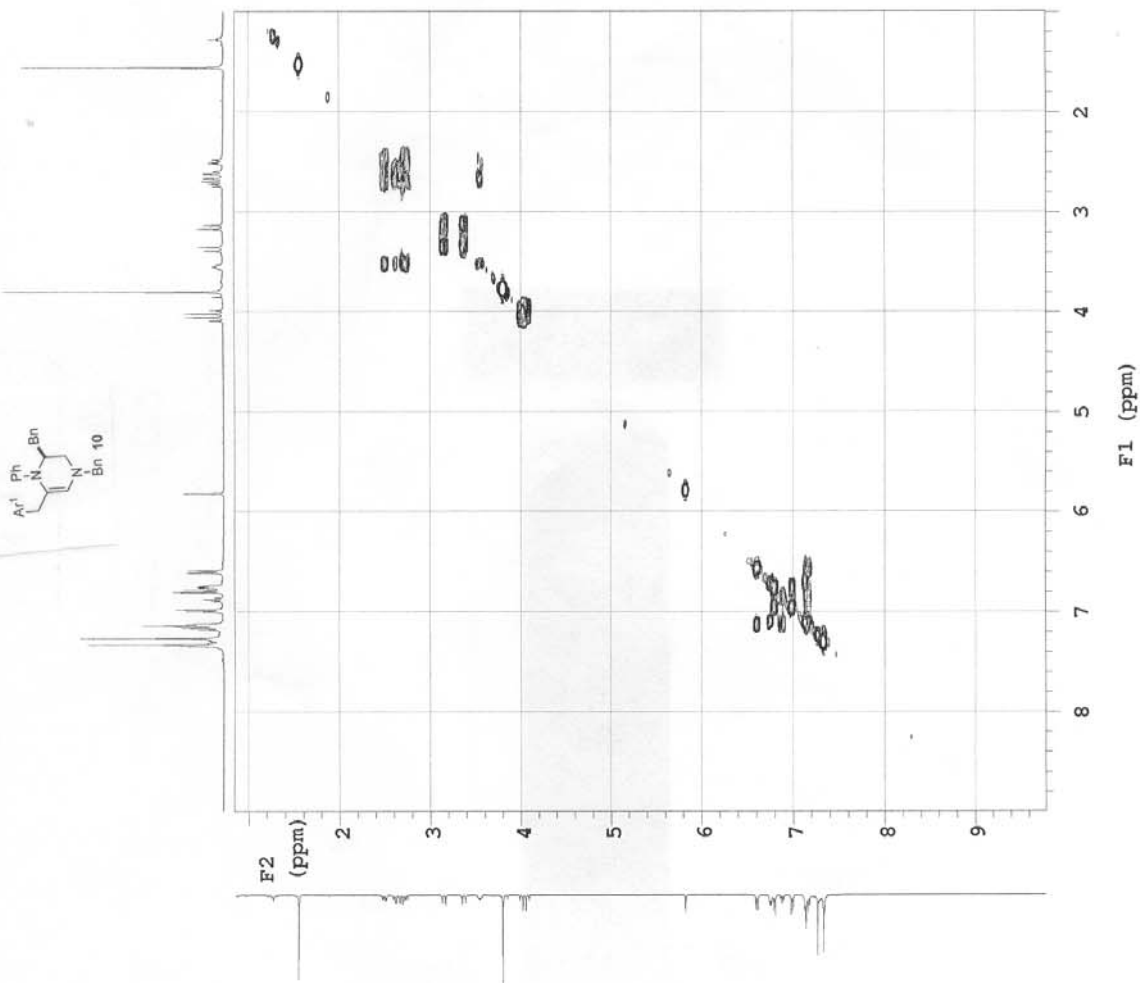
F1 DATA PROCESSING

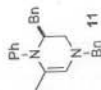
Sq. sine bell 0.031 sec

FT size 2048 x 2048

Total time 10 min, 19 sec

Acquisition date: May 1 2007





File: J5NVIII-151-2-spl-H1

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: jnakhla

File: J5NVIII-151-2-spl-H1

INOVA-500 "Dy. Chem. LSA, UMich. Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

4 repetitions

OBSERVE H1, 499.9042669 MHz

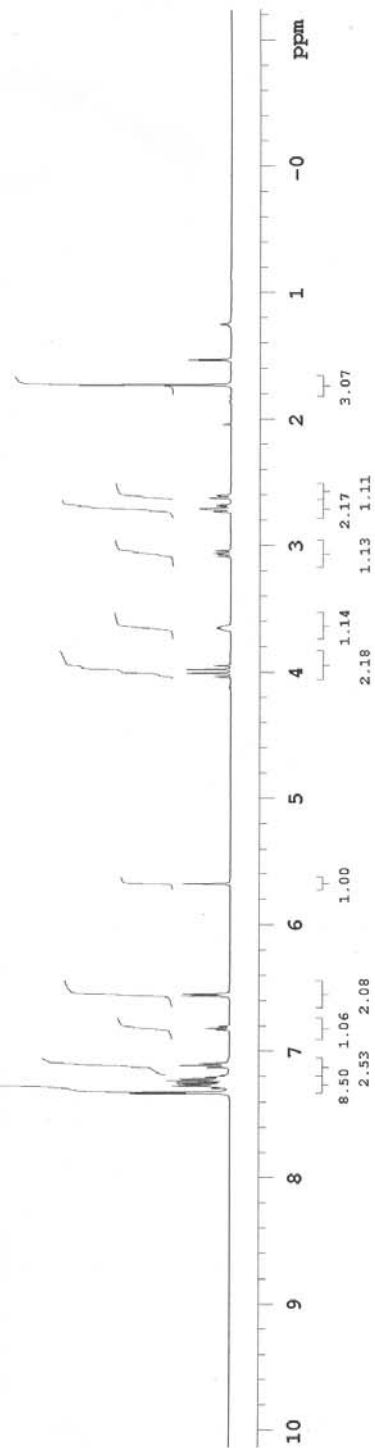
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min, 18 sec

Acquisition date: May 1 2007



Standard Proton

File: Gcoosy

Pulse Sequence: gCOSY

Solvent: cdcl3

Ambient temperature

Operator: jprakhla

INOVA-500 "Sn.Chem.LSA.UMich.Edu"

Relax. delay 1.301 sec

Acq. time 0.206 sec

Width 4970.2 Hz

2D Width 4970.2 Hz

4 repetitions

256 increments

OBSERVE H1, 499.9042683 MHz

DATA PROCESSING

Sq. sine bell 0.103 sec

F1 DATA PROCESSING

Sq. sine bell 0.052 sec

FT size 2048 x 2048

Total time 26 min, 46 sec

Acquisition date: May 1 2007

