

Gram Scale Synthesis of a β -Secretase 1 (BACE 1) Inhibitor

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Supporting Information

Table of Contents

Stereochemical proof of rac-12	S2
Copies of HPLC chromatograms, ¹ H and ¹³ C NMR spectra.....	S5

The relative stereochemistry of **rac-12** was established by observation of the illustrated nOe crosspeak in the 2D-NOESY spectrum.

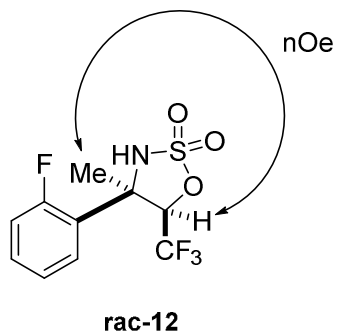


Figure S1. Illustration of observed nOe.

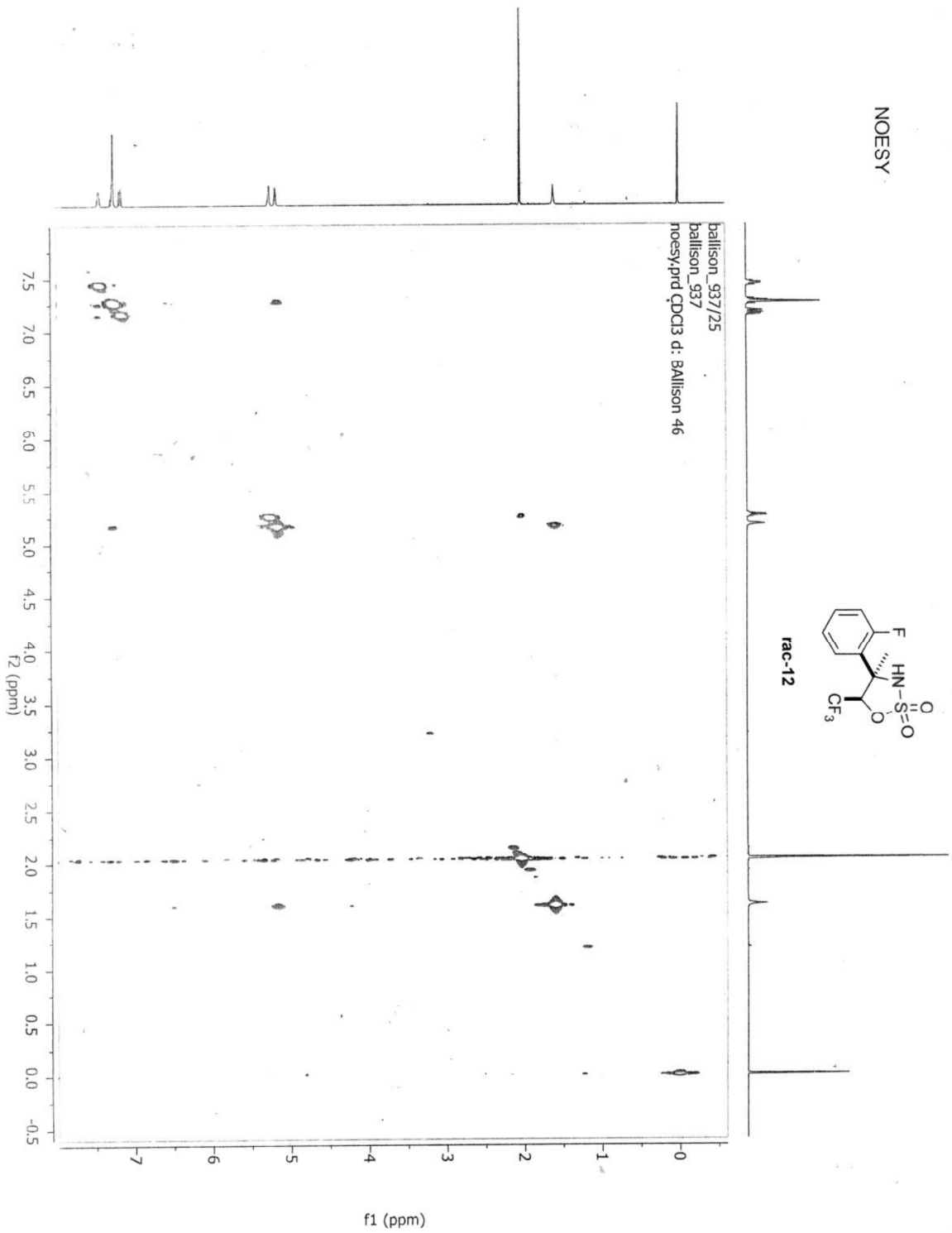


Figure S2. NOESY spectrum of **rac-12**.

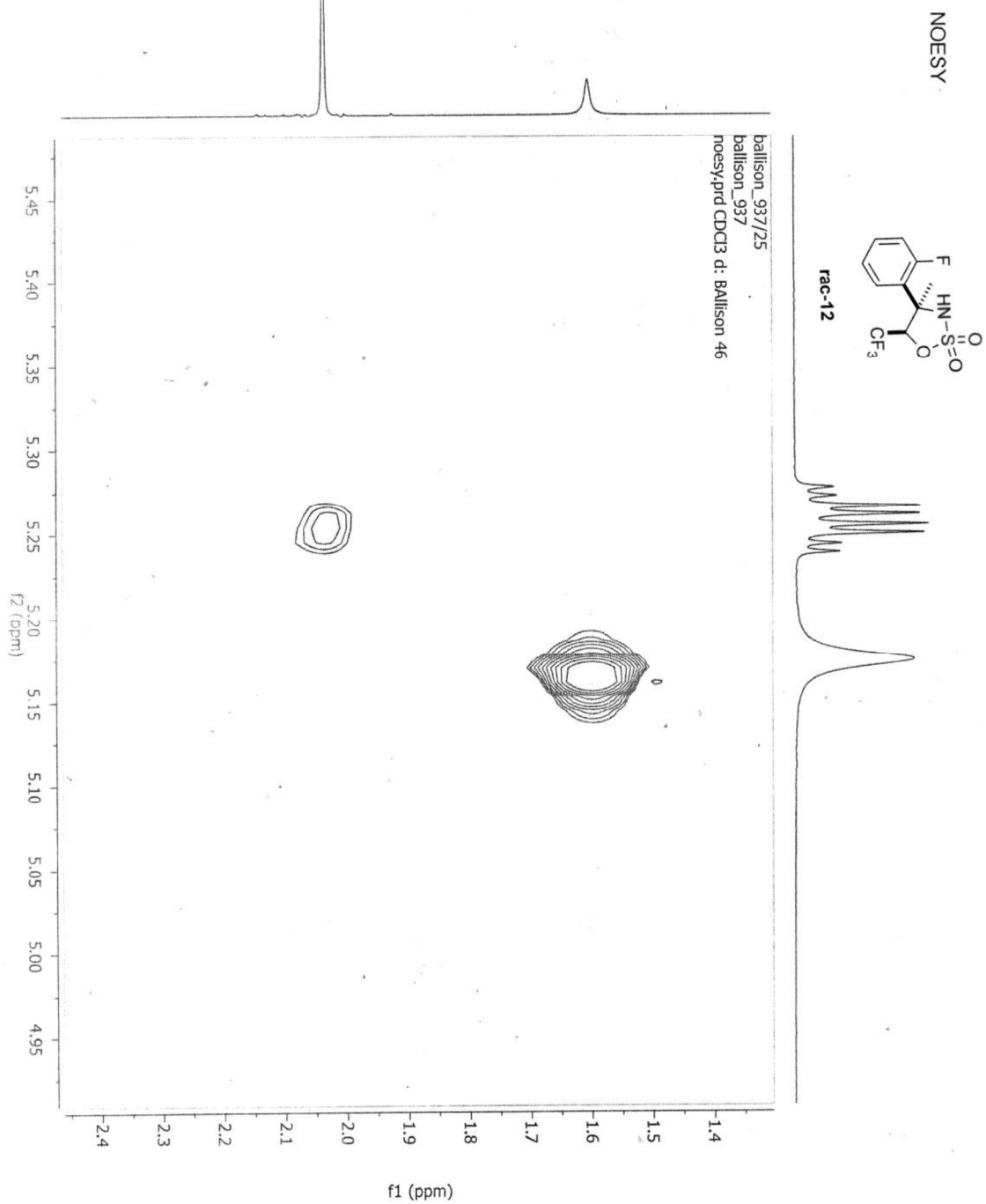
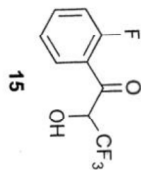
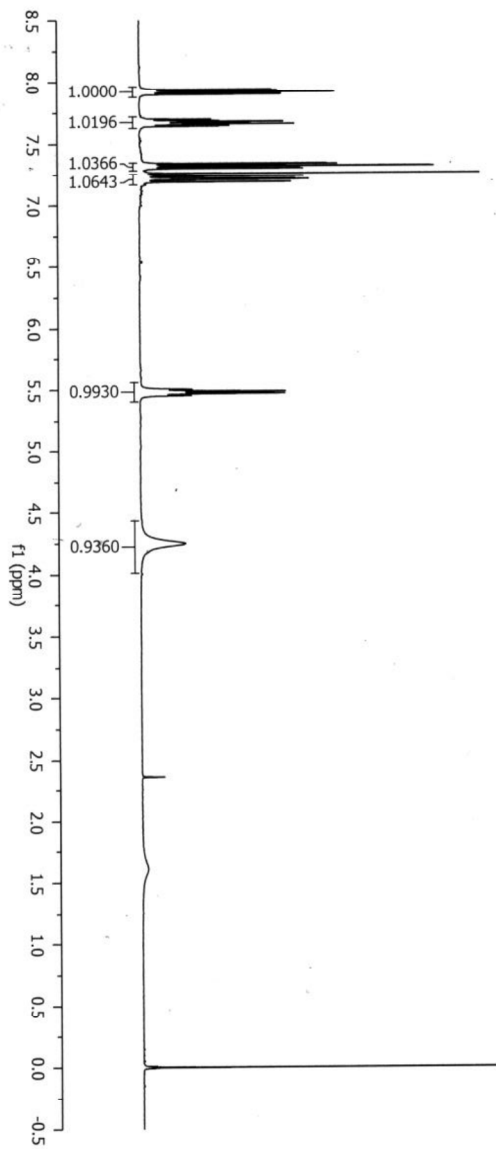


Figure S3. Expansion of NOESY spectrum of **rac-12** showing relevant crosspeak.



ballison_921
ballison_921 crude
proton.prd CDCl3 D:\Ballison 66

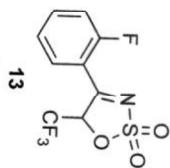
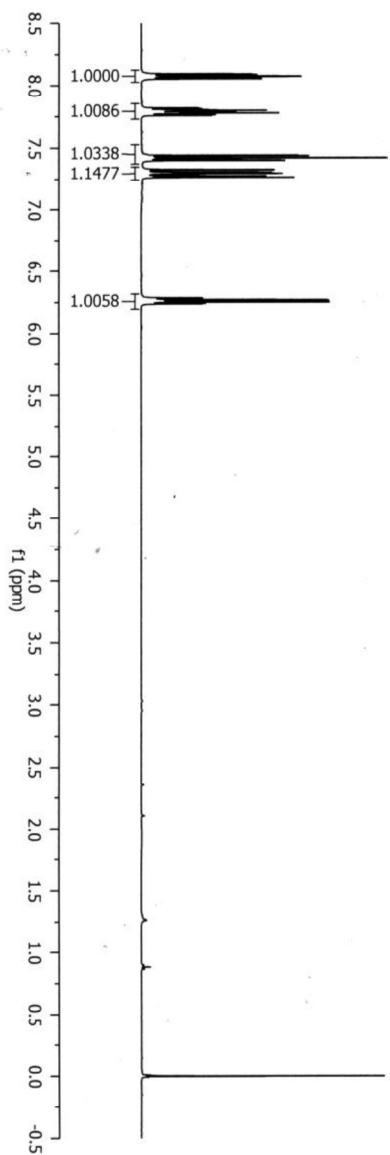
Current Data Parameters
NAME: ballison_921
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters
Date: 20111222
Time: 18.01
INSTRUM: nmr400-1
PROBHD: 5 mm QNP 1H/13
PULPROG: zg30
TD: 65536
Solvent: CDCl3
NS: 8
DS: 0
SWH: 8278.1 Hz
AQ: 3.9584243 sec
RG: 322.5
DM: 60.400 usec
DE: 6.00 usec
TE: 294.2 K
D1: 5.00000000 sec
TD0: 1 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 9.00 usec
P1L: 0.00 dB
SF01: 400.1324710 MHz

F2 - Processing Parameters
SI: 0
SF: 400.1300163 MHz
FT: Hyper
Phase: N0PC

Figure S4. ¹H NMR spectrum of 15.



ballison_930
ballison_930 bulk recrystallized material, darker colored sample
proton.prd CDC13 D:\Ballison 91

Current Data Parameters
NAME: ballison_930
EXPNO: 40
PROCNO: 1

F2 - Acquisition Parameters
Date: 20120130
Time: 10.32
INSTRUM: nmr400-1
PROBHD: 5 mm QNP 1H/13
PULPROG: zg30
TD: 65536
SOLVENT: CDCl3
NS: 8
DS: 0
SMH: 8278.1 Hz
AQ: 3.9584243 sec
RG: 181
DW: 60.400 usec
DE: 6.00 usec
TE: 294.2 K
D1: 5.00000000 sec
TD0: 1 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 9.00 usec
PL1: 0.00 dB
SFO1: 400.1324710 MHz

F2 - Processing Parameters
SI: 0
SF: 400.1300161 MHz
FT: Hyper
Phase: NoPC

Figure S5. ¹H NMR spectrum of 13.

ballison_937
ballison_937 c. 4 and 5 after charcoal
proton.prd CDCl3 D:\Ballison 81

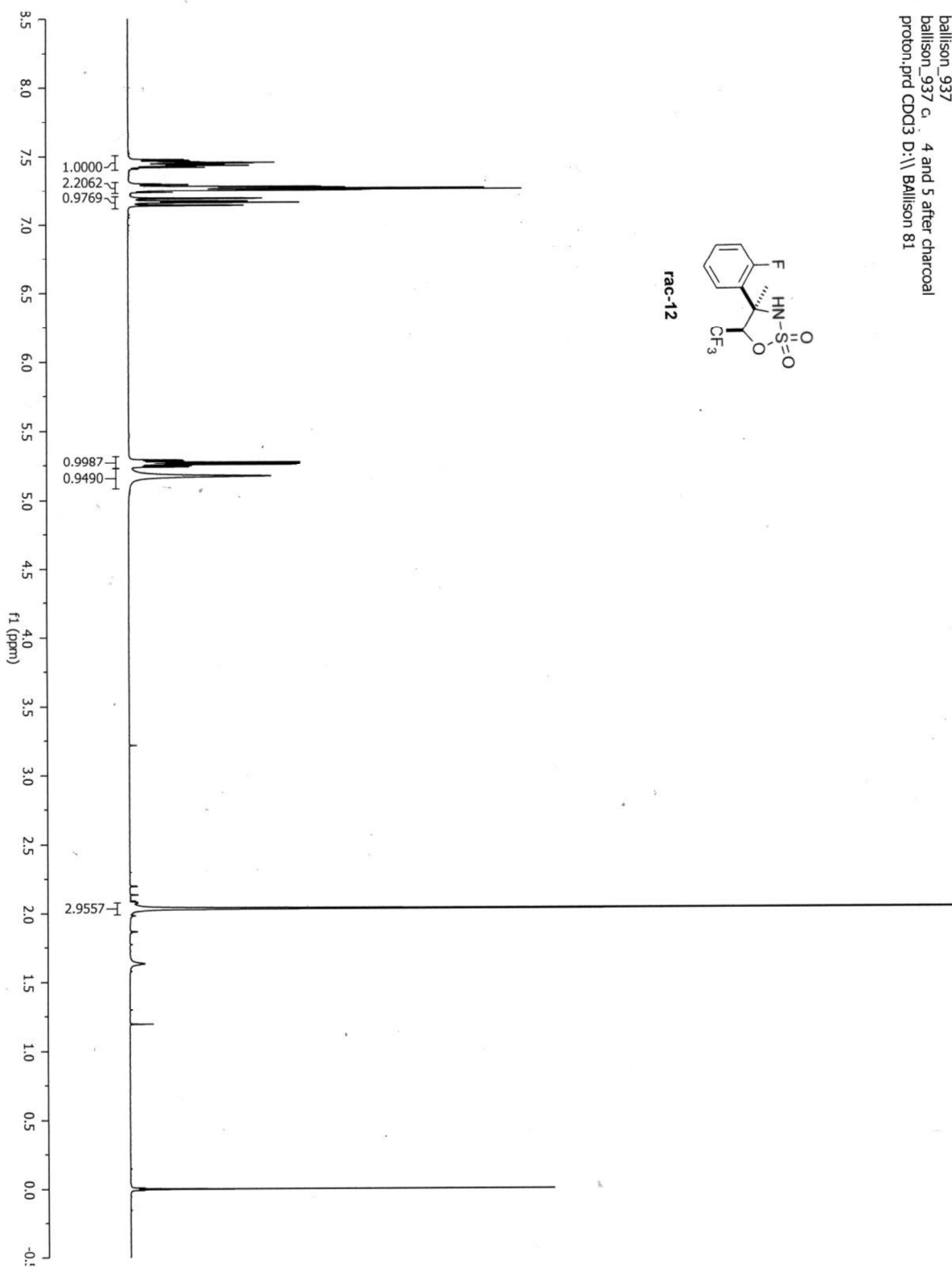
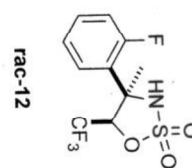


Figure S6. ¹H NMR spectrum of **rac-12**.

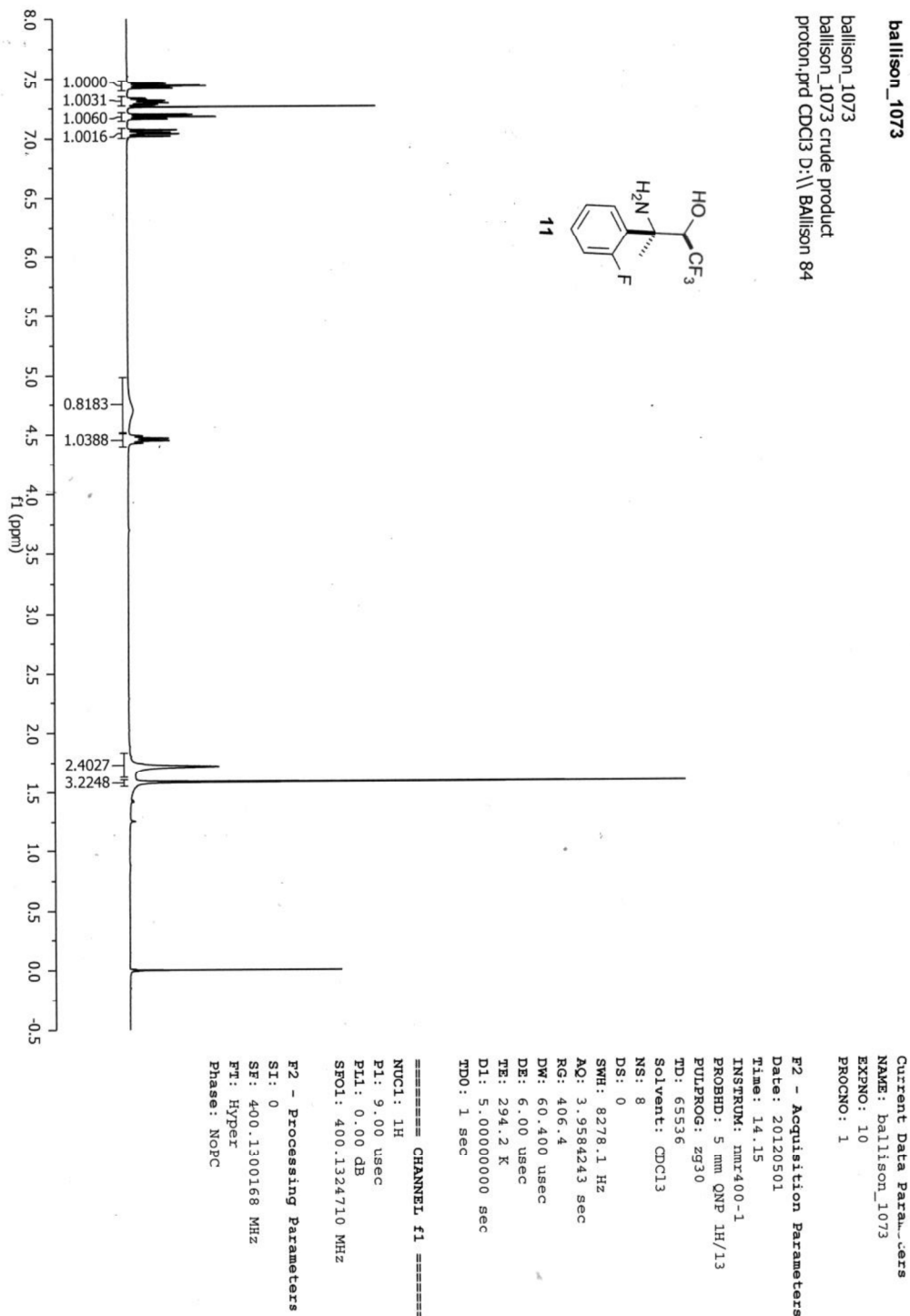


Figure S7. ¹H NMR spectrum of 11.

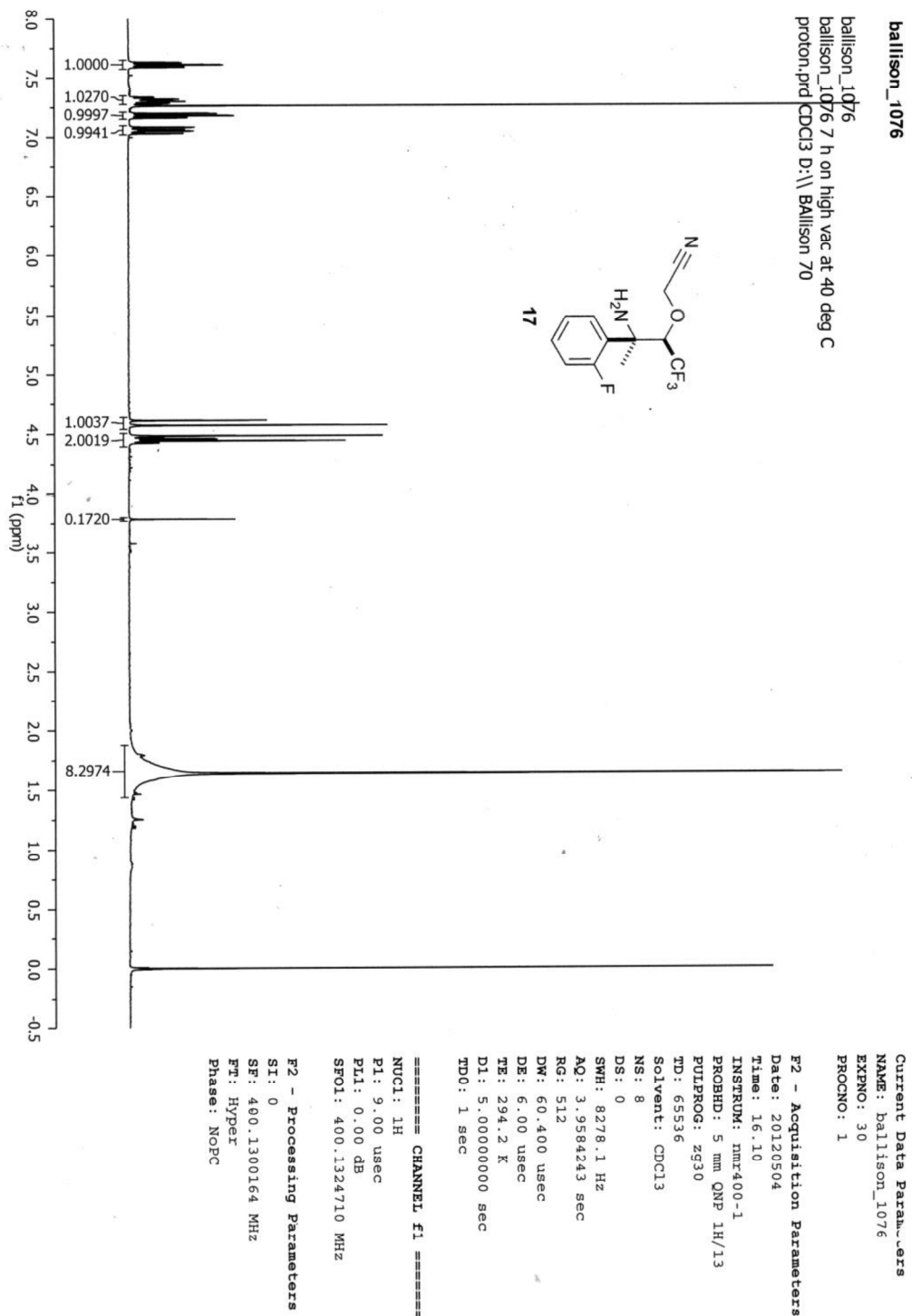
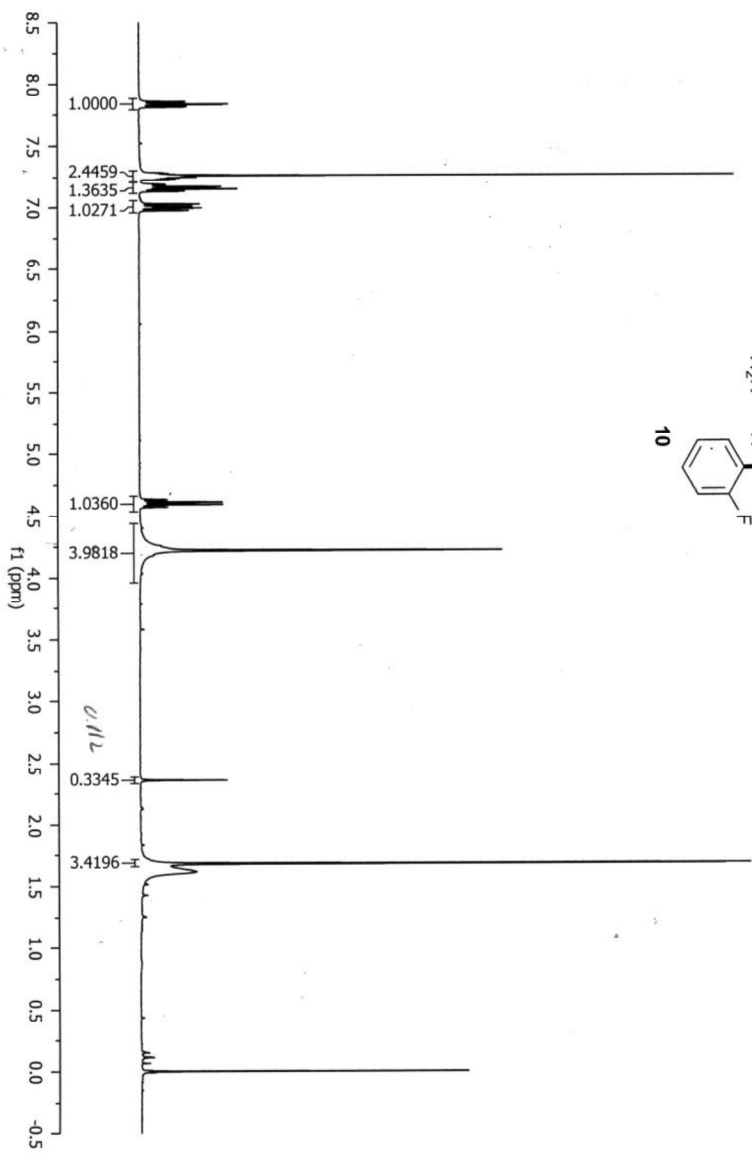
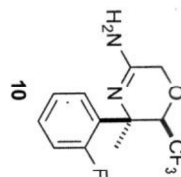


Figure S8. ¹H NMR spectrum of 17.

ballison_1078

ballison_1078
ballison_1078 crude immediately after conc. from toluene
proton.prd CDCl3 d: Ballison 9



Current Data Parameters
NAME: ballison_1078
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters
Date: 20120507
Time: 13.56
INSTRUM: nmr400-3
PROBHD: 5 mm QNP 1H/13
PULPROG: zg30
TD: 65536
Solvent: CDCl3
NS: 16
DS: 2
SWH: 8250.8 Hz
AQ: 3.9715922 sec
RG: 362
DM: 60.600 usec
DE: 6.50 usec
TE: 295 K
D1: 5.00000000 sec
TD0: 1 sec

==== CHANNEL f1 =====
NUC1: 1H
P1: 10.20 usec
PL1: -3.00 dB
SFO1: 400.1324710 MHz

F2 - Processing Parameters
SI: 0
SF: 400.1300087 MHz
FT: Hyper
Phase: NOFC

Figure S9. ¹H NMR spectrum of 10.

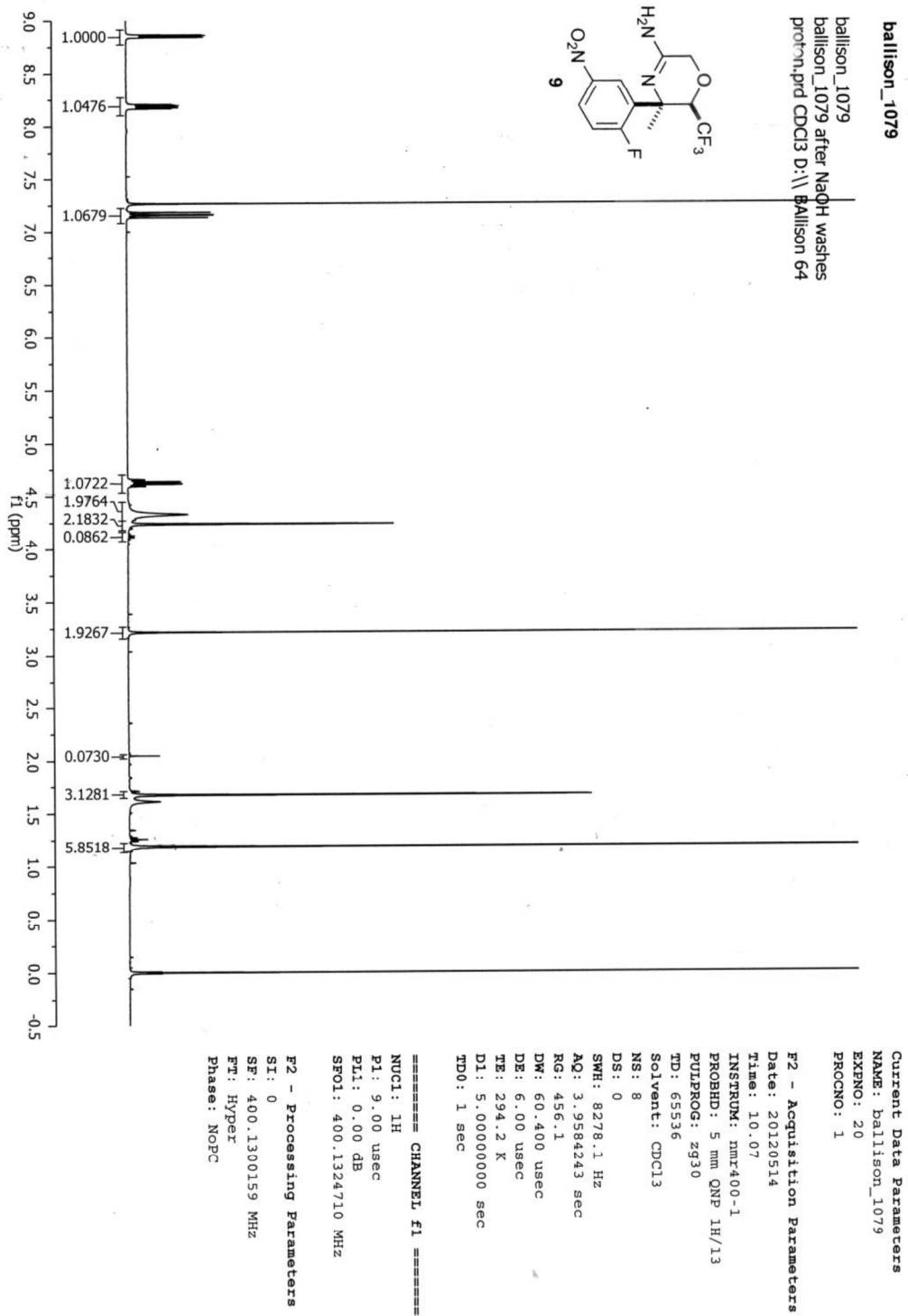
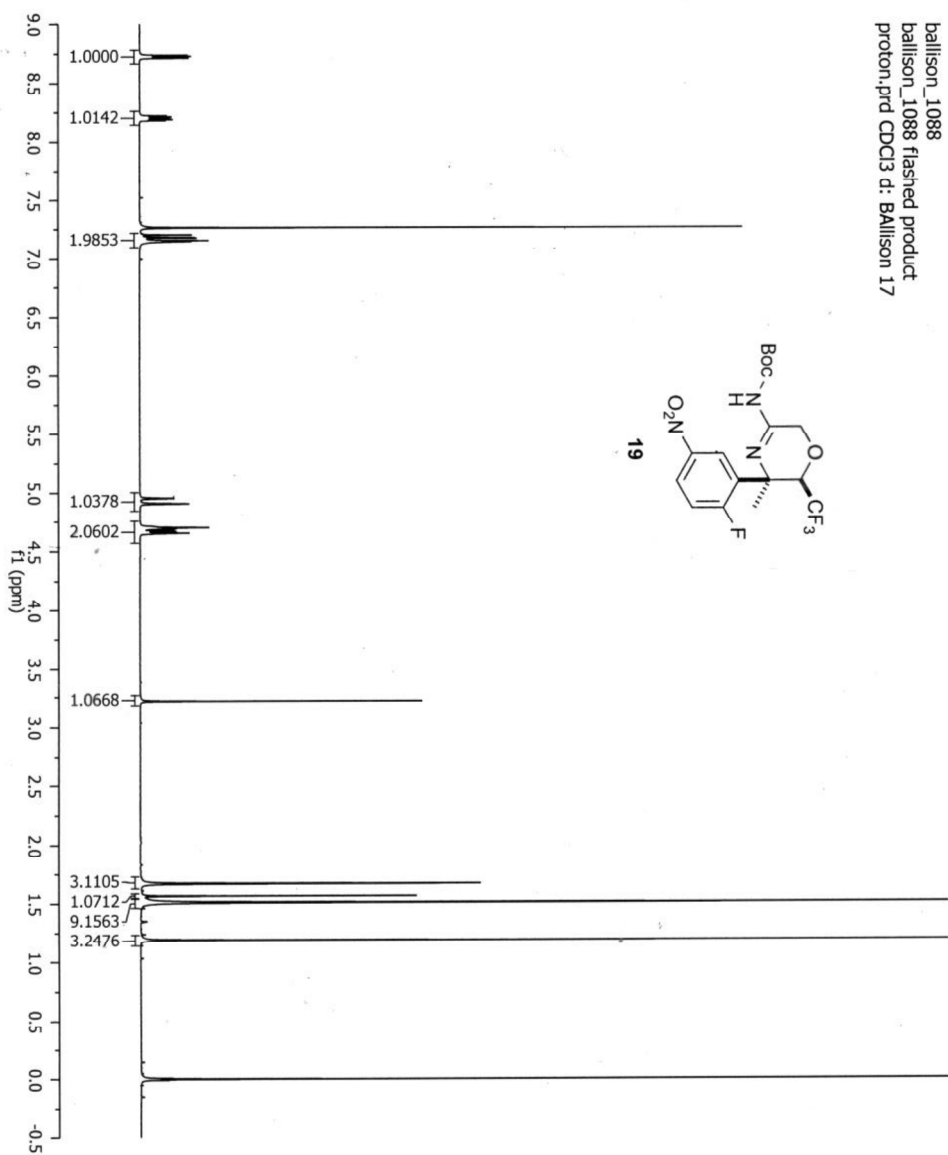


Figure S10. ¹H NMR spectrum of 9.

ballison_1088

ballison_1088
ballison_1088 flashed product
proton.prd CDCl3 d: Ballison 17



Current Data Parameters
NAME: ballison_1088
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters

Date: 20120515
Time: 22.17
INSTRUM: nmr400-3
PROBHD: 5 mm QNP 1H/13
PULPROG: zg30
TD: 65536
Solvent: CDCl3
NS: 16
DS: 2
SWH: 8250.8 Hz
AQ: 3.9715922 sec
RG: 322.5
DM: 60.600 usec
DE: 6.50 usec
TE: 294.7 K
D1: 5.00000000 sec
TD0: 1 sec

===== CHANNEL f1 =====

NUC1: 1H
PI: 10.20 usec
PL1: -3.00 dB
SF01: 400.1324710 MHz

F2 - Processing Parameters

SI: 0
SF: 400.1300084 MHz
FR: Hyper
Phase: NoPC

Figure S11. ¹H NMR spectrum of 19.

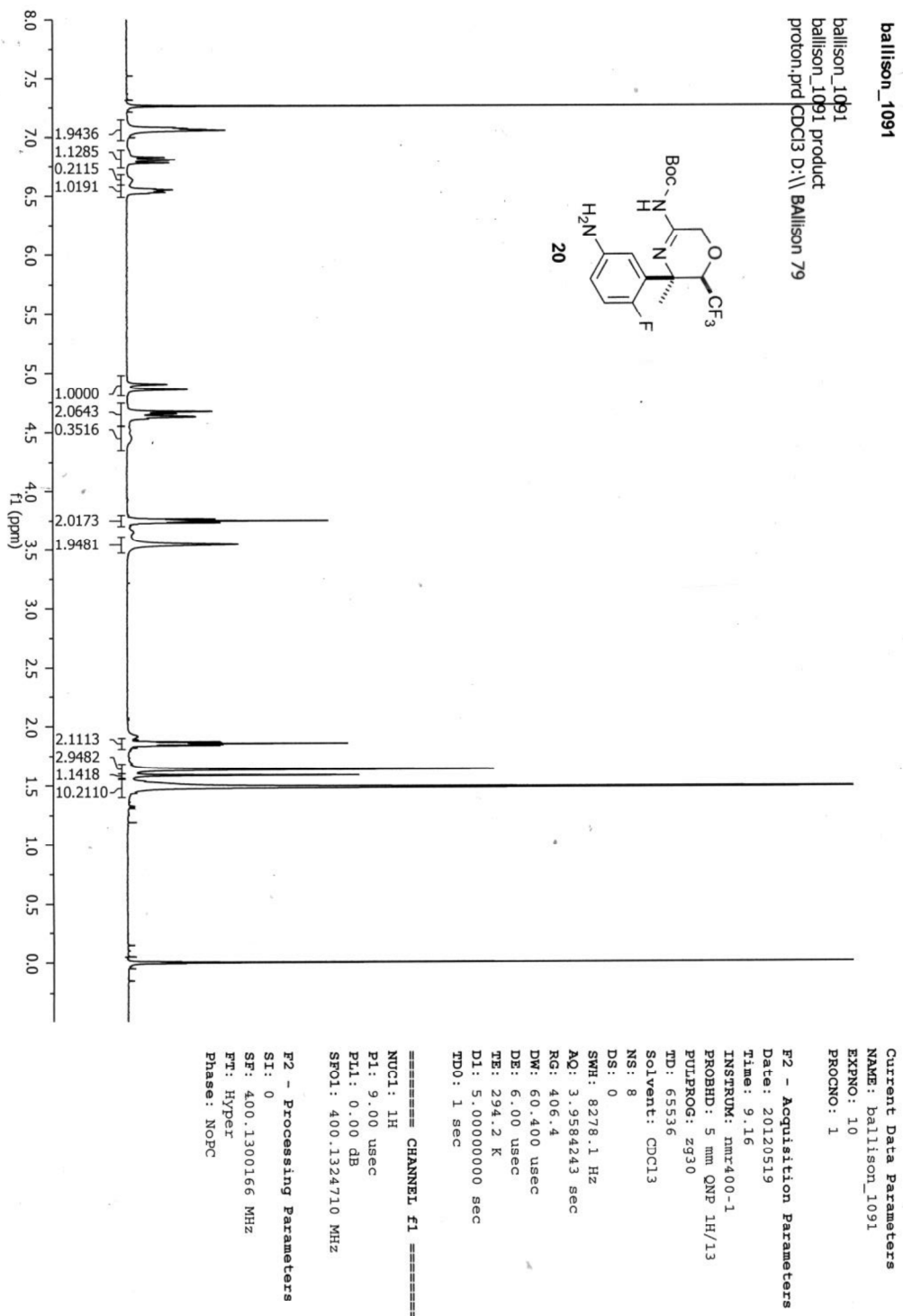
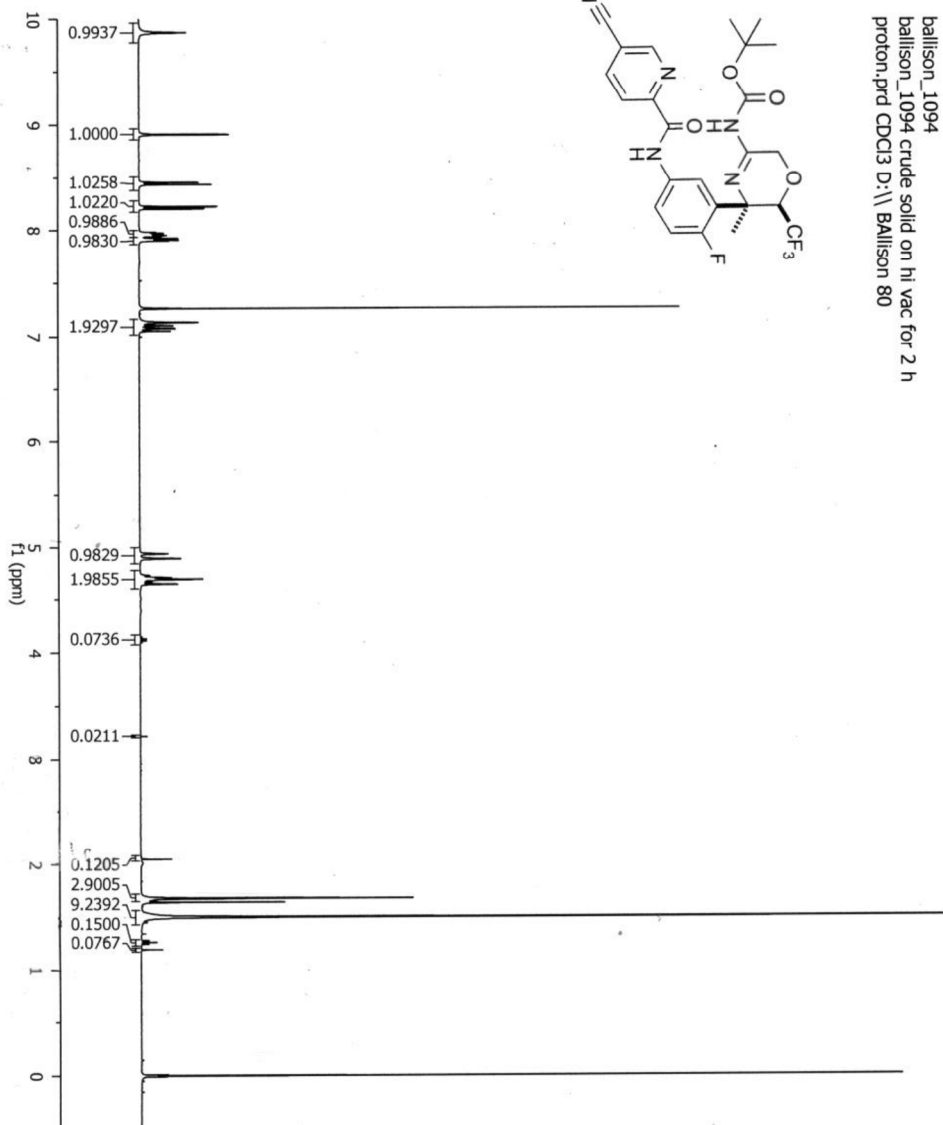
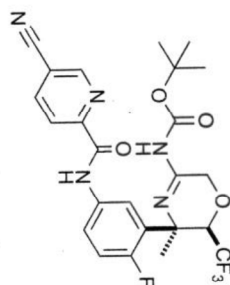


Figure S12. ¹H NMR spectrum of 20.

ballison_1094

ballison_1094
ballison_1094 crude solid on hi vac for 2 h
proton,prd CDCl3 D:\\Ballison 80



Current Data Parameters
NAME: ballison_1094
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters

Date: 20120520
Time: 3.35
INSTRUM: nmr400-1
PROBHD: 5 mm QNP 1H/13
PULPROG: zg30
TD: 65536
Solvent: CDCl3
NS: 8
DS: 0
SWH: 8278.1 Hz
AQ: 3.9584243 sec
RG: 406.4
DW: 60.400 usec
DE: 6.00 usec
TE: 294.2 K
D1: 5.00000000 sec
TD0: 1 sec

===== CHANNEL f1 =====

NUC1: 1H
P1: 9.00 usec
PL1: 0.00 dB
SF01: 400.1324710 MHz

F2 - Processing Parameters

SI: 0
SF: 400.1300161 MHz
FT: Hyper
Phase: NOBC

Figure S13. ¹H NMR spectrum of Boc-protected 1.

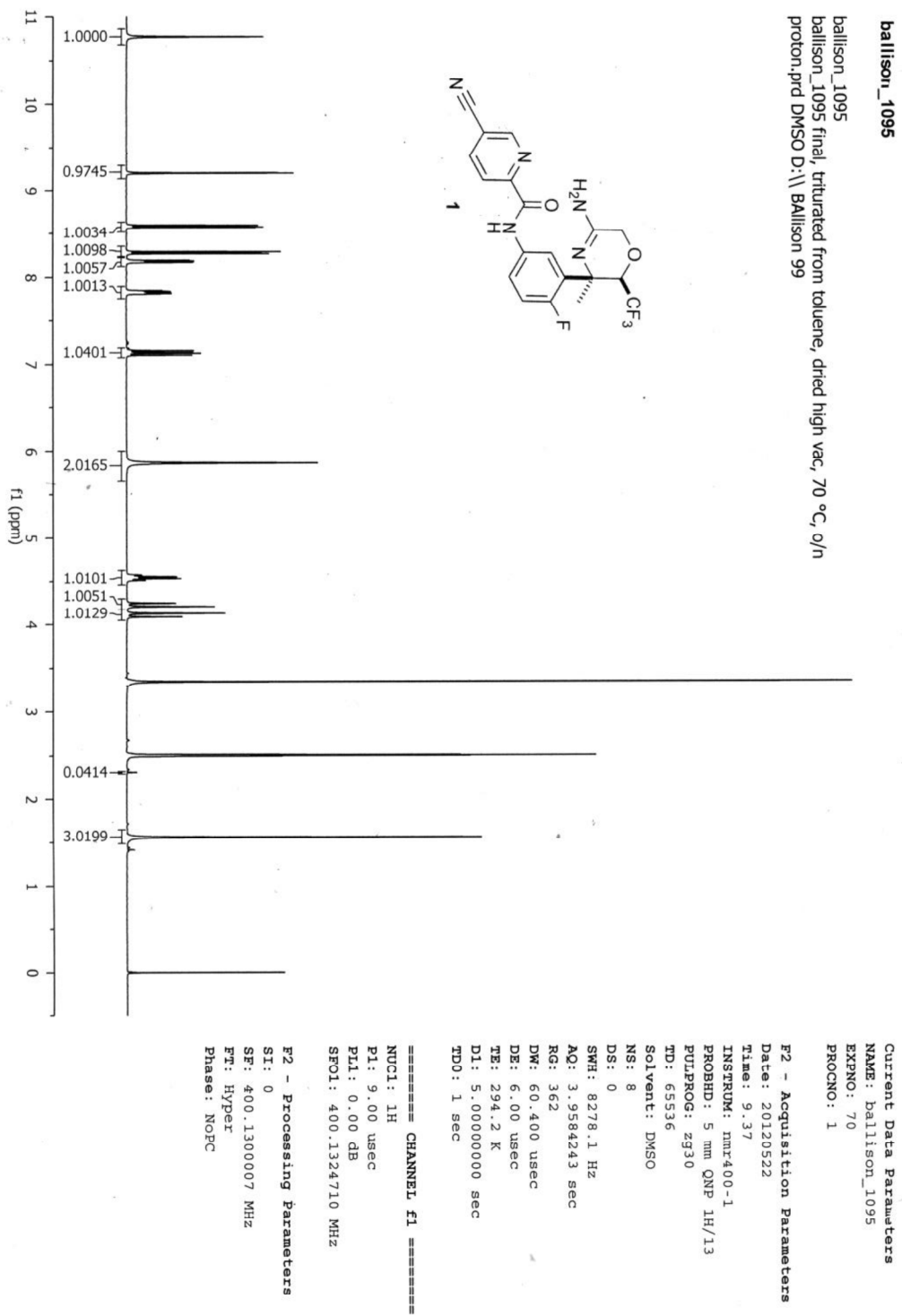


Figure S14. ¹H NMR spectrum of 1.

ballison_930.20.1.1r
ballison_930
c13cpd.prd CDCl3 d: BALLISON 12

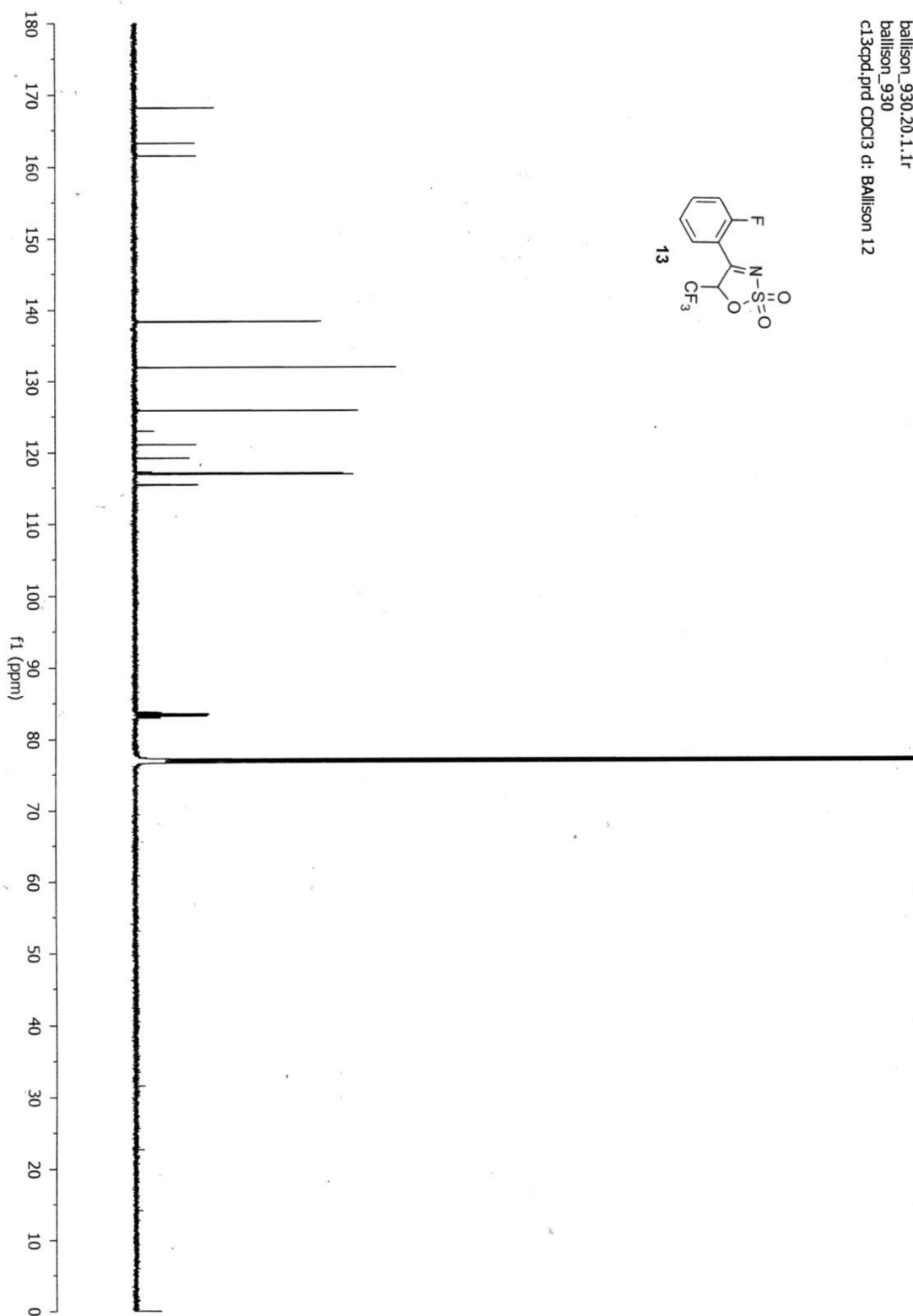
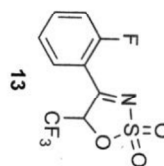


Figure S15. ^{13}C NMR spectrum of 13.

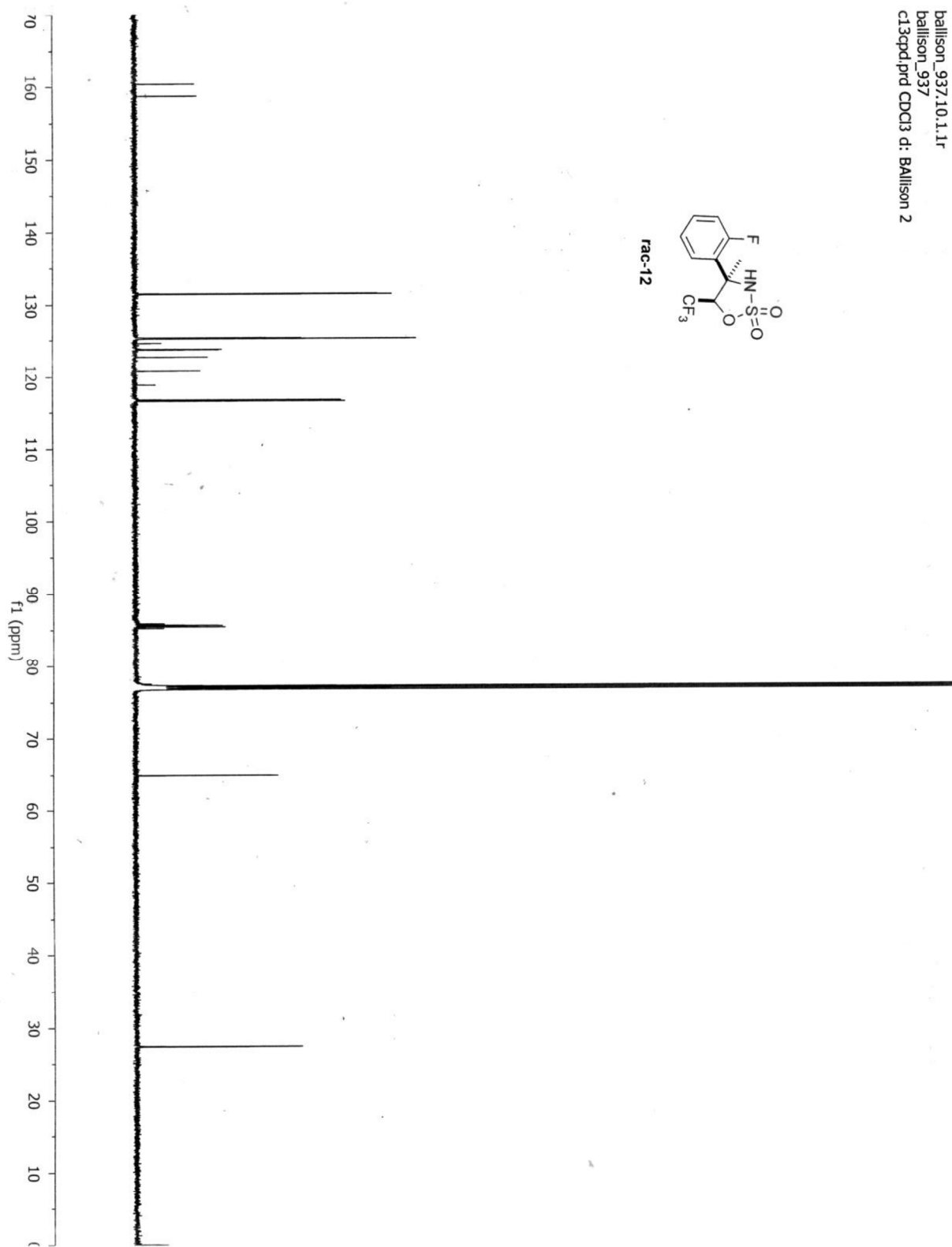


Figure S16. ¹³C NMR spectrum of **rac-12**.

ballison_1073.10.1.1f
ballison_1073
c13cpd.prd CDCl3 d: BALLISON 4

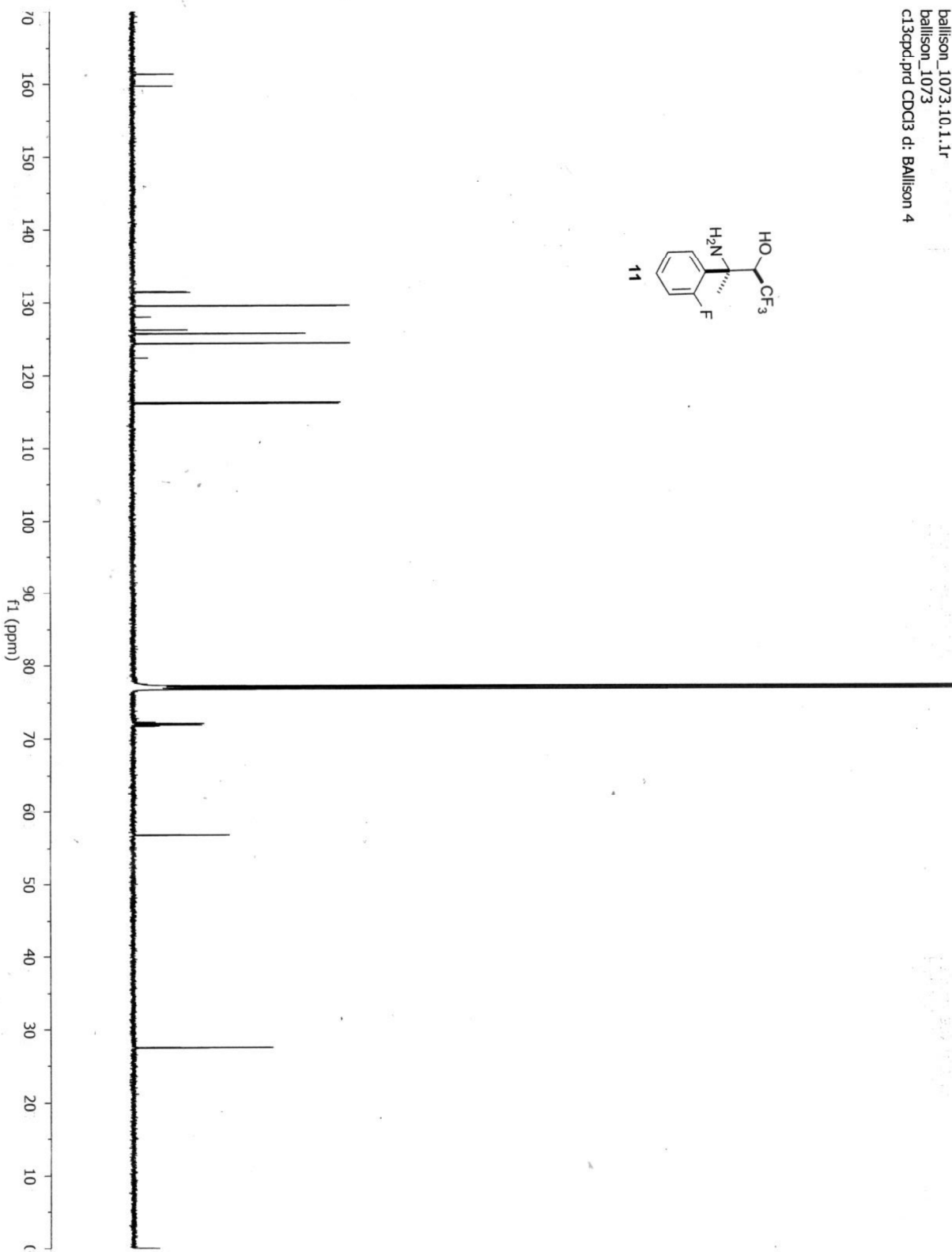
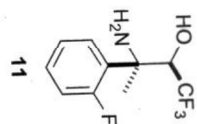


Figure S17. ¹³C NMR spectrum of 11.

ballison_1076.10.1.1f
ballison_1076
c13cpd.prd CDCl3 d: BALLISON 11

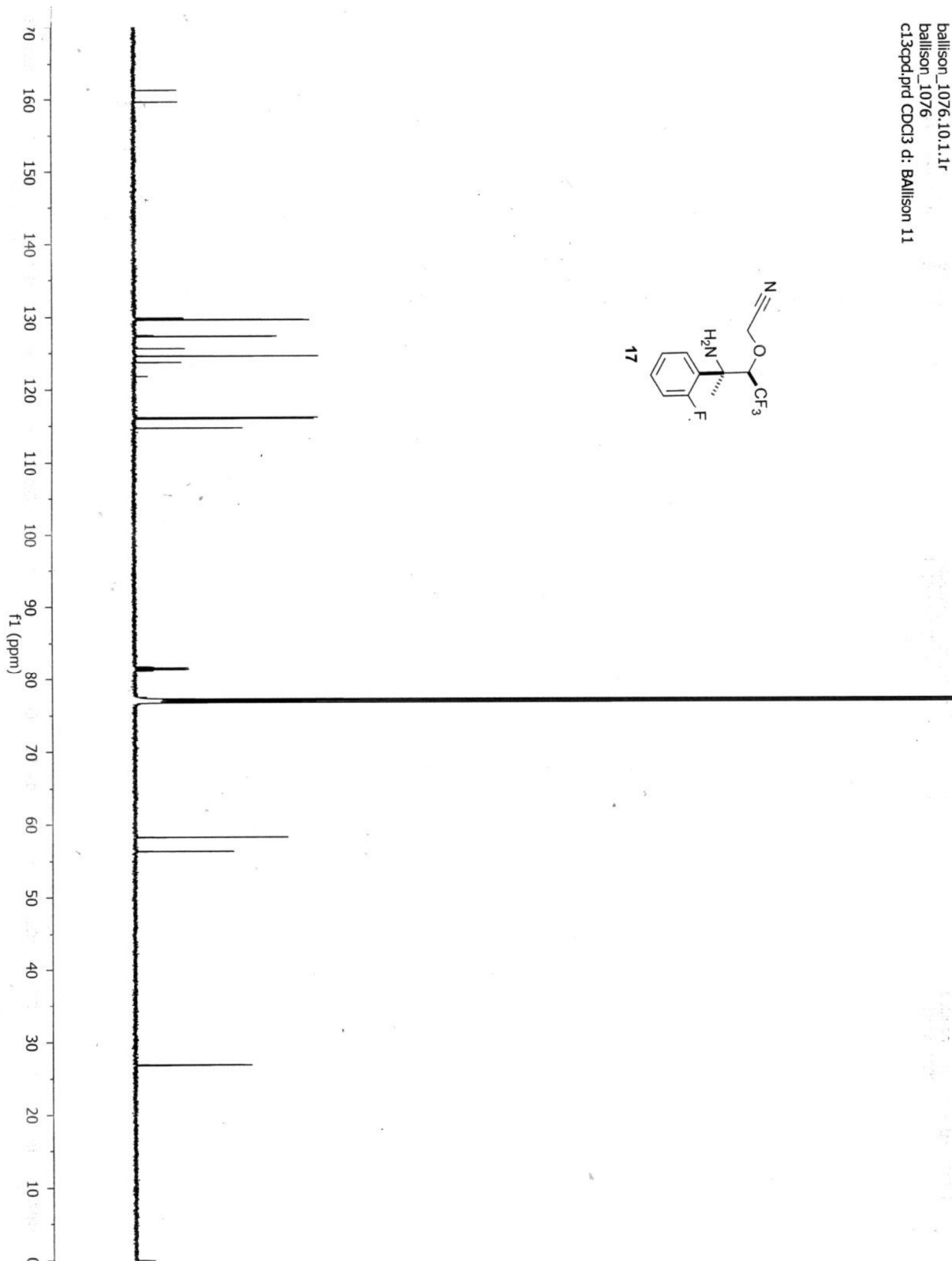
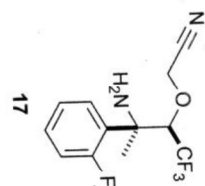


Figure S18. ¹³C NMR spectrum of 17.

ballison_1078.10.1.1f
ballison_1078
c13cpd.prd CDCl3 d: BALLISON 9

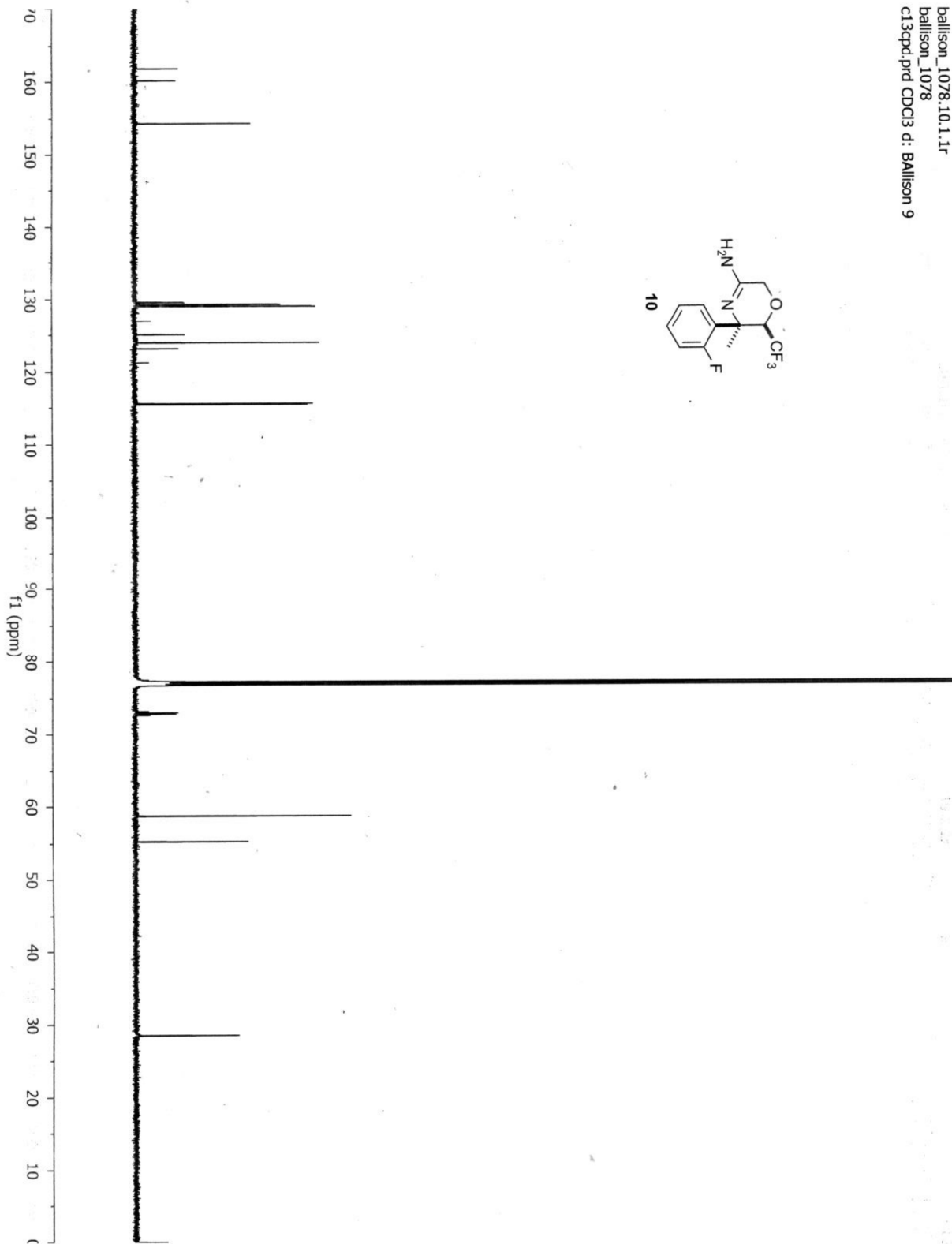
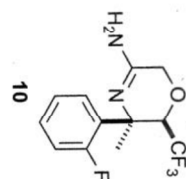


Figure S19. ¹³C NMR spectrum of 10.

ballison_1079.10.1.1r
ballison_1079
c13cpd.prd CDCl3 d: Ballison 6

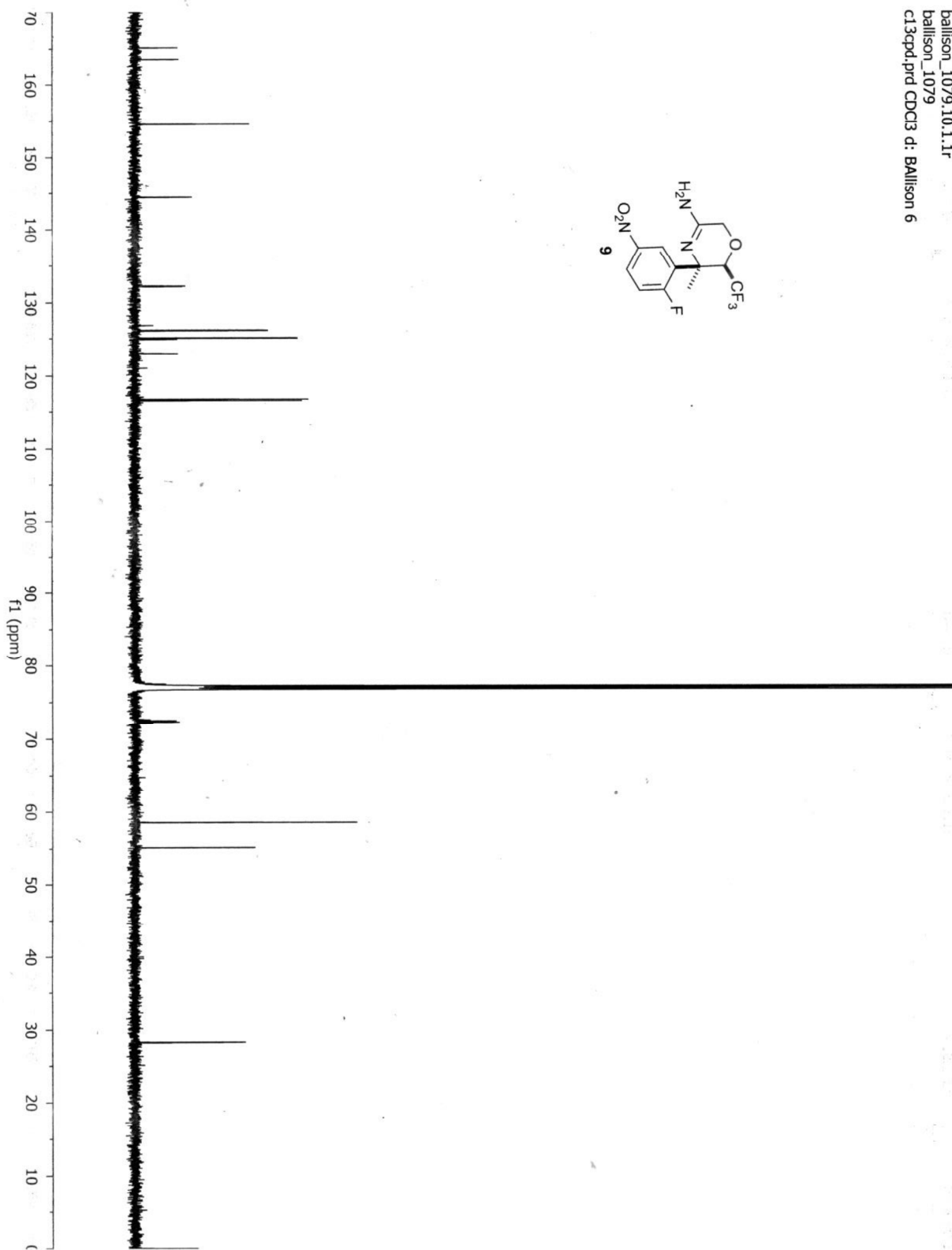
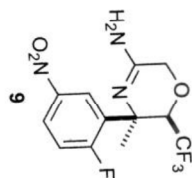


Figure S20. ¹³C NMR spectrum of 9.

ballison_1088.10.1.1r
ballison_1088
c13cpd.prd CDCl3 d: BALLISON 5

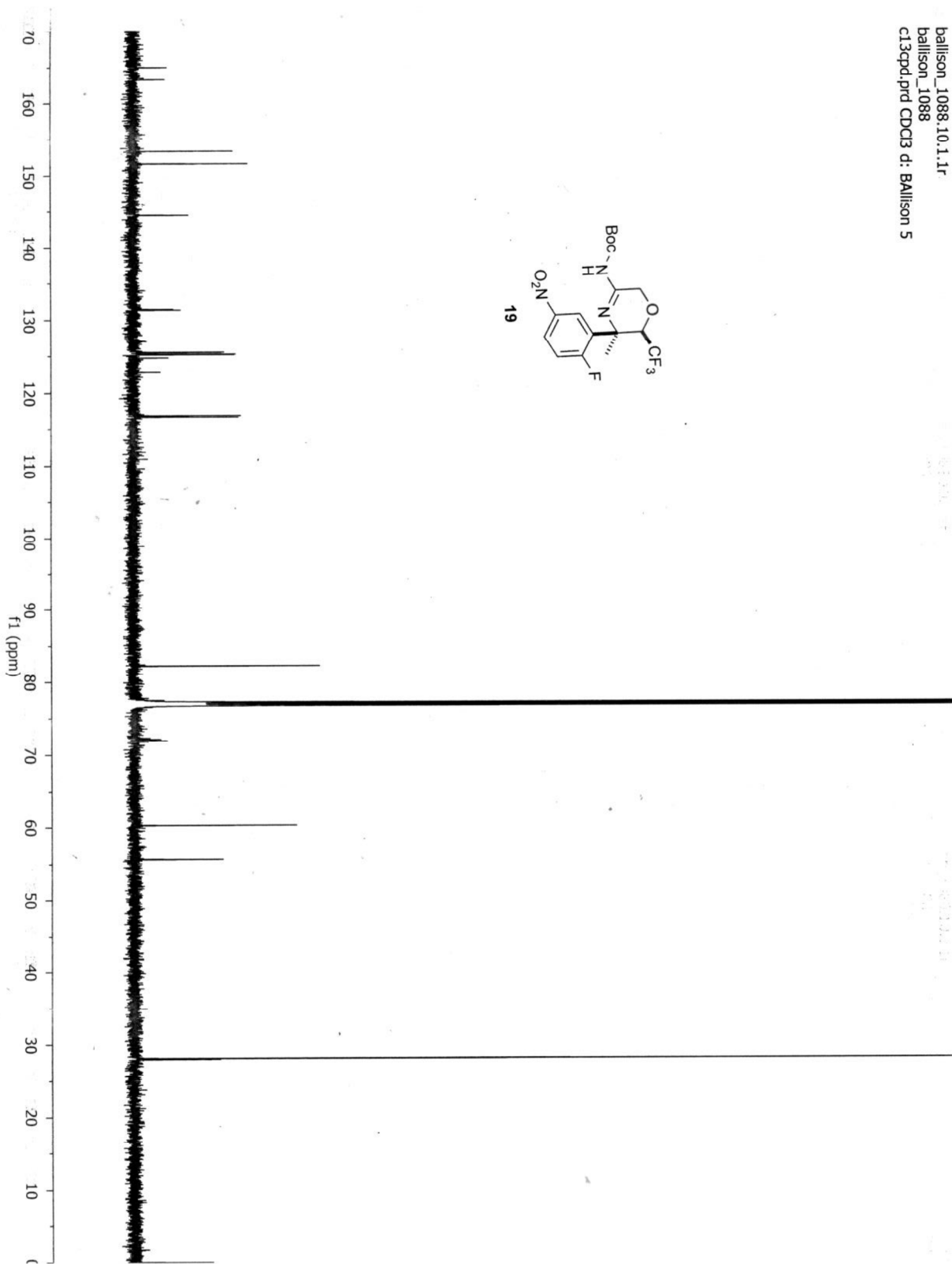
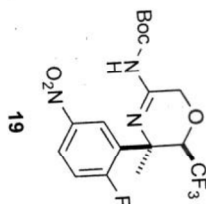


Figure S21. ^{13}C NMR spectrum of 19.

ballison_1090.20.1.1r
ballison_1090
c13cpd.prd CDCl3 d: BALLISON 13

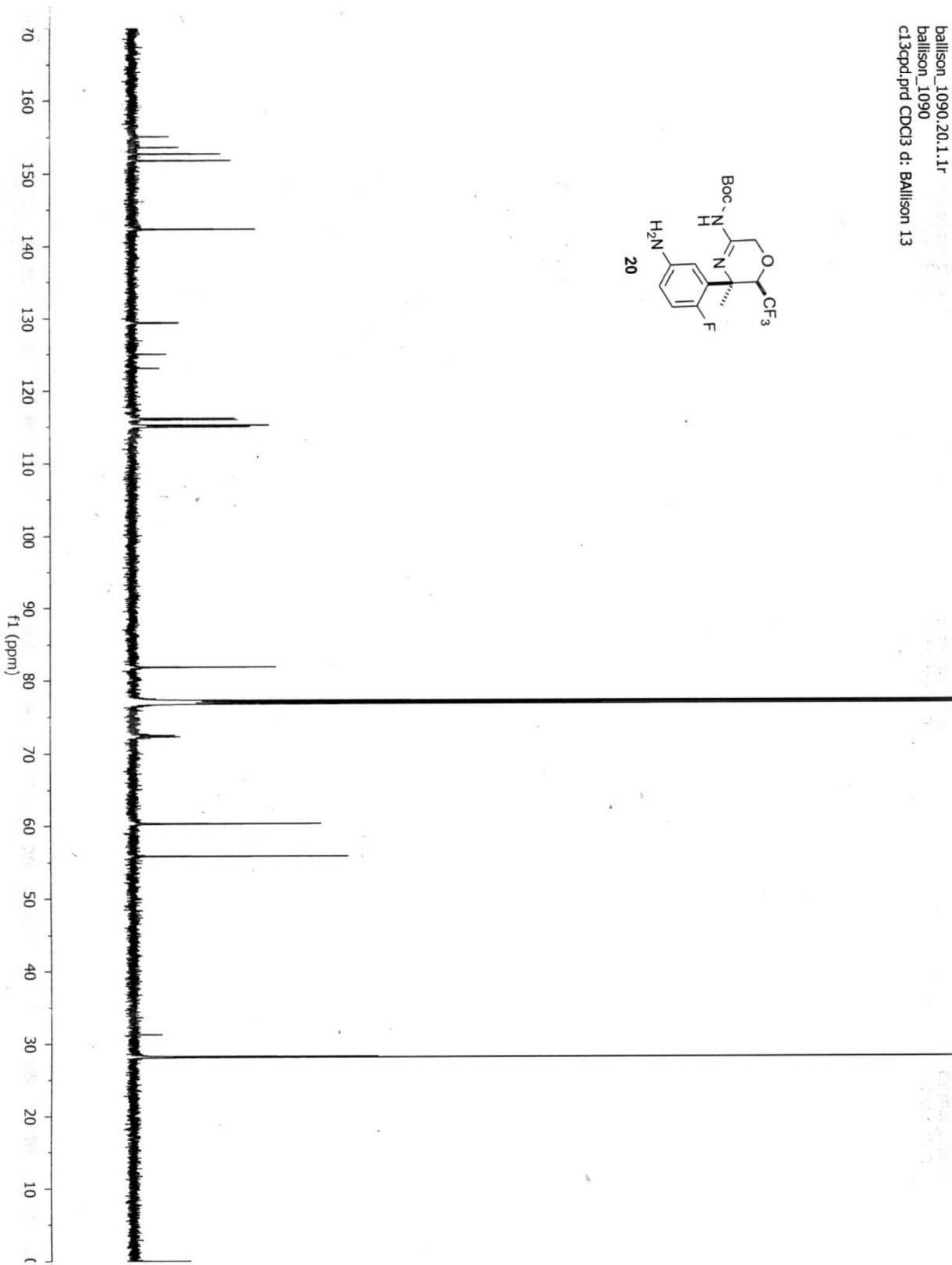
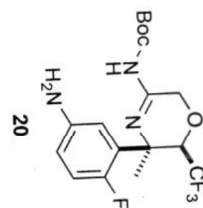


Figure S22. ^{13}C NMR spectrum of 20.

ballison_1094.10.1.1r
ballison_1094
C13cpd.prd CDC13 d: BALLISON 8

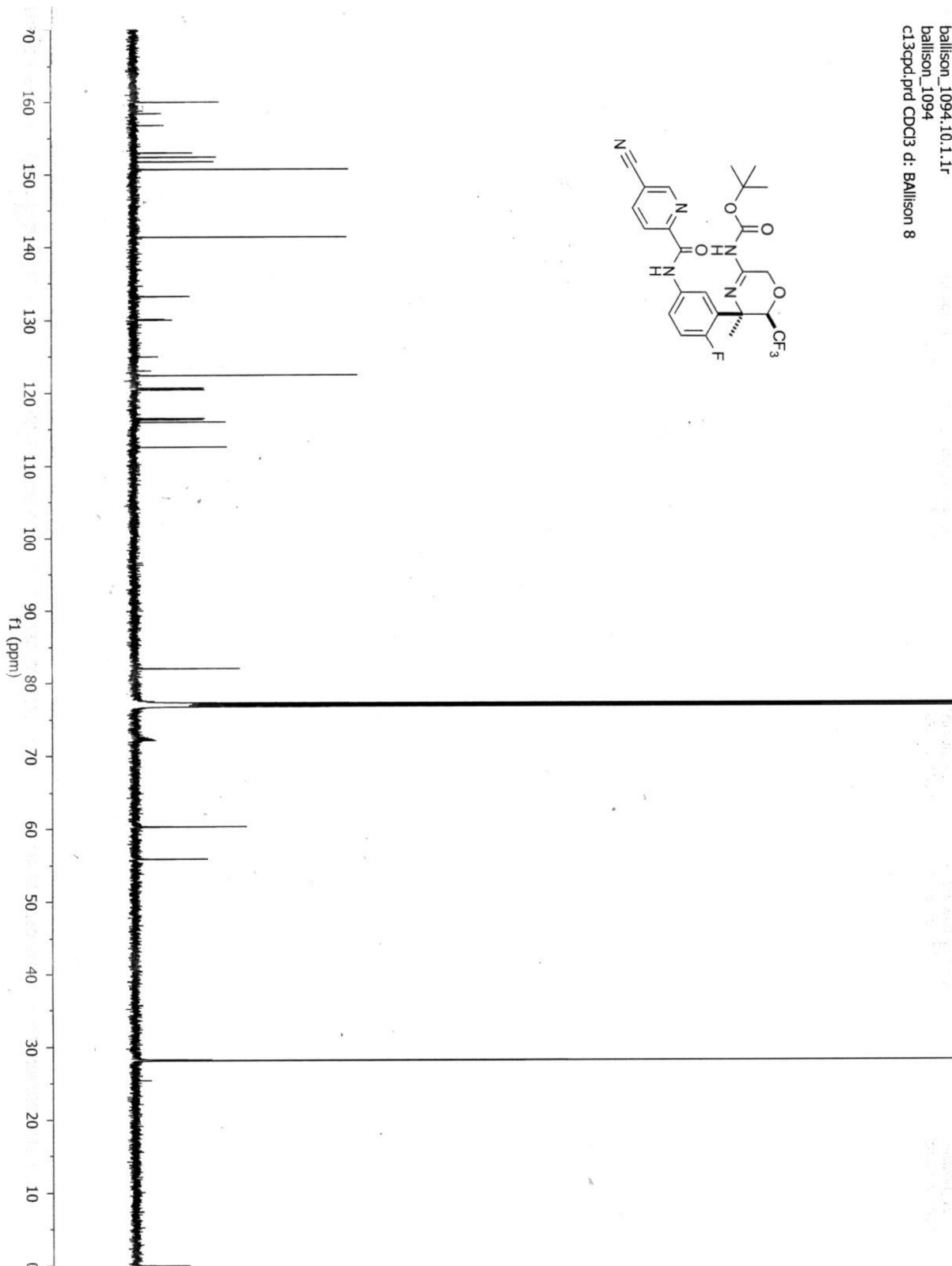
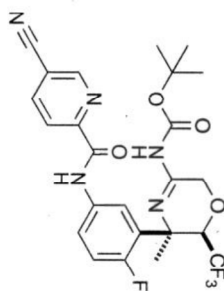


Figure S23. ^{13}C NMR spectrum of Boc-protected 1.

ballison_1095.10.1.1r
ballison_1095
c13cpd.prd CDCl3 d: Ballison 7

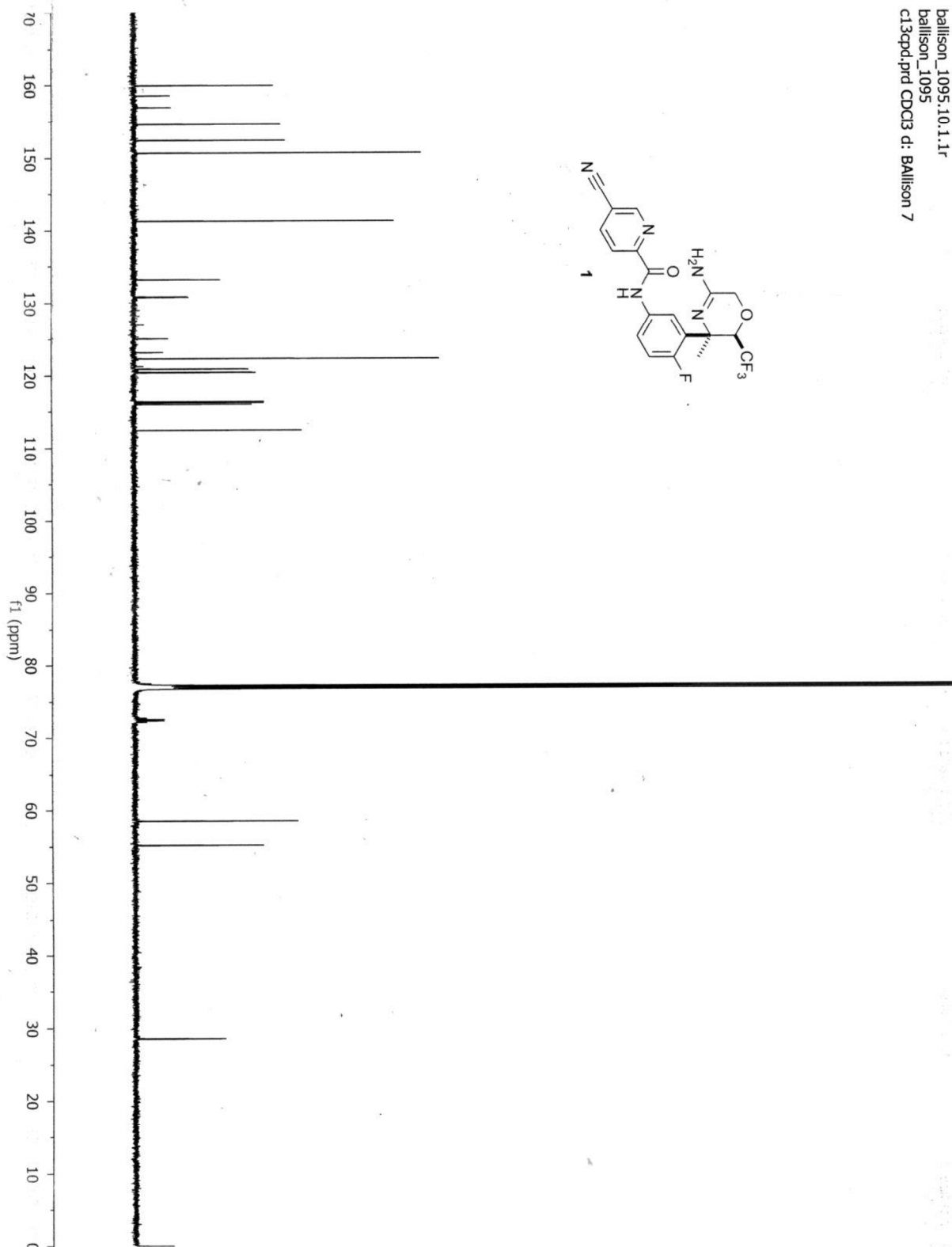
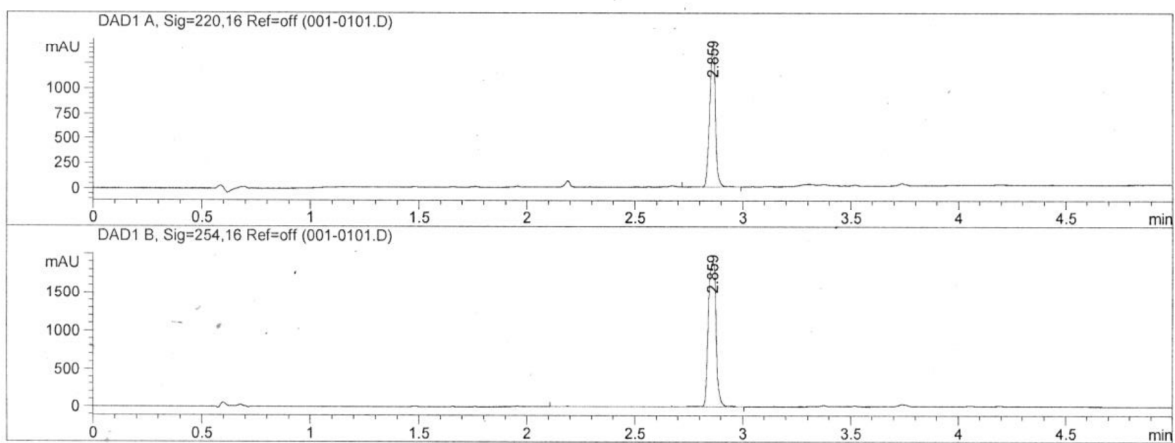


Figure S24. ^{13}C NMR spectrum of 1.

Data File C:\CHEM32\1\DATA\GENERAL\JGB1 2012-01-04 11-30-16\001-0101.D
Sample Name: ballison_921 crude dried

```
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Acq. Operator   :                               Seq. Line :    1
Acq. Instrument : Instrument 1                   Location  : Vial 1
Injection Date  : 04-Jan-2012 11:33:18          Inj       :    1
                                                Inj Volume: 3.0 µl
Sequence File   : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-01-04 11-30-16\JGB1.S
Method          : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-01-04 11-30-16\5TO99_35C.M (Sequence Method)
Last changed    : 27-Jul-2010 10:57:13
Method Info     : 5-99% ACN, Eclipse XDB C18, 5 µm, 150x4.6mm
=====
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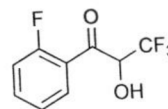
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Area Percent Report
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Sorted By : Retention Time
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=220,16 Ref=off
Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	2.859	2	BB	4829.85547	1881.63916	64.8125
2	2.859	1	VB	2622.19189	1338.22729	35.1875

Totals : 7452.04736 3219.86646



15

=====
*** End of Report ***

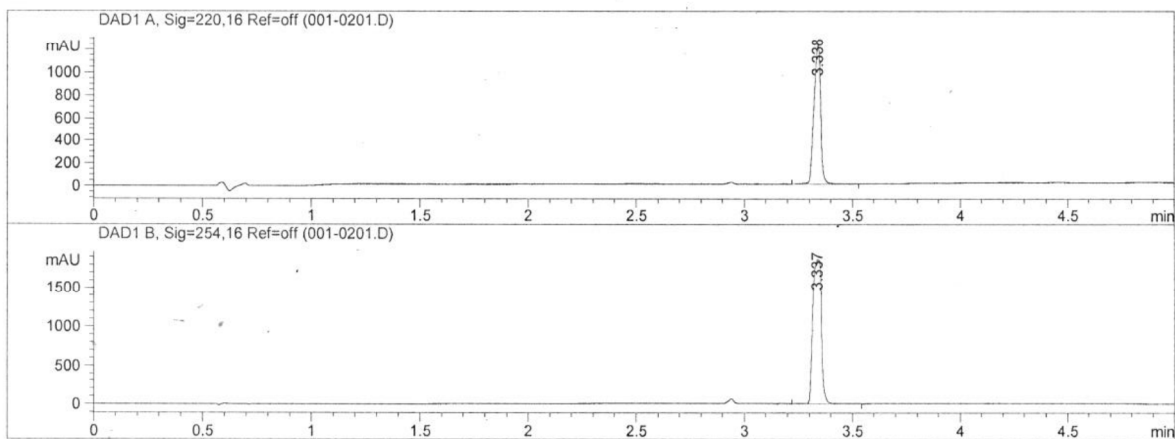
Figure S25. HPLC chromatogram of 15.

Data File C:\CHEM32\1\DATA\GENERAL\JGB1 2012-01-30 10-42-25\001-0201.D
Sample Name: ballison_930 bulk rex material

=====

Acq. Operator :		Seq. Line :	2
Acq. Instrument :	Instrument 1	Location :	Vial 1
Injection Date :	30-Jan-2012 10:54:49	Inj :	1
		Inj Volume :	3.0 µl

Sequence File : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-01-30 10-42-25\JGB1.S
Method : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-01-30 10-42-25\5TO99_35C.M (Sequence Method)
Last changed : 27-Jul-2010 10:57:13
Method Info : 5-99% ACN, Eclipse XDB C18, 5 µm, 150x4.6mm



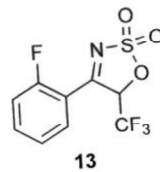
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Area Percent Report
=====

Sorted By : Retention Time
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=220,16 Ref=off
Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	3.337	2	BB	5111.39209	1867.87769	65.9035
2	3.338	1	BB	2644.47607	1182.93445	34.0965

Totals : 7755.86816 3050.81213



=====
*** End of Report ***
=====

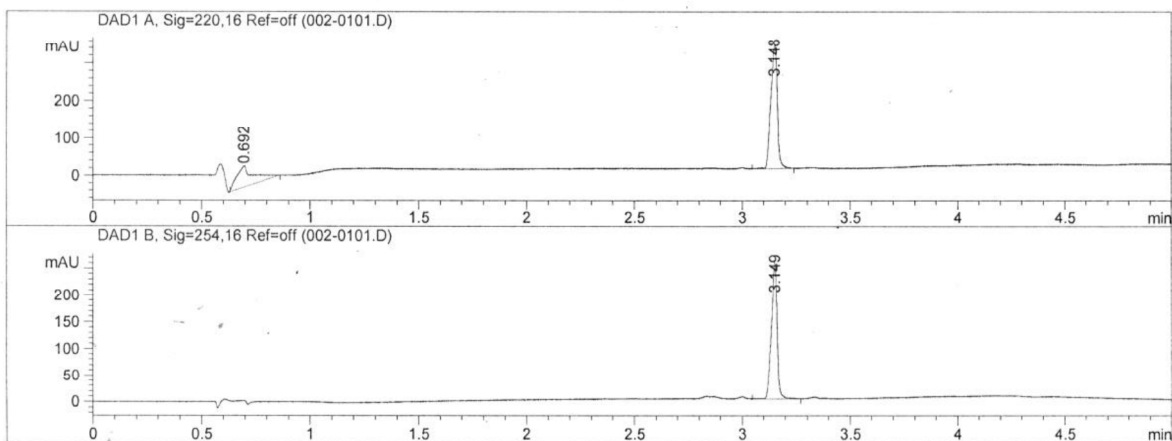
Figure S26. HPLC chromatogram of 13.

Data File C:\CHEM32\1\DATA\GENERAL\JGB1 2012-02-07 10-42-39\002-0101.D
 Sample Name: ballison_937 2nd crop

```

=====
Acq. Operator   :                               Seq. Line :    1
Acq. Instrument : Instrument 1                   Location  : Vial 2
Injection Date  : 07-Feb-2012 10:45:34         Inj       :    1
                                                Inj Volume: 3.0 µl

Sequence File   : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-02-07 10-42-39\JGB1.S
Method          : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-02-07 10-42-39\5TO99_35C.M (Sequence Method)
Last changed   : 27-Jul-2010 10:57:13
Method Info    : 5-99% ACN, Eclipse XDB C18, 5 µm, 150x4.6mm
=====
  
```



=====
 Area Percent Report
 =====

```

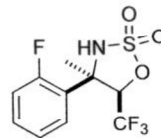
Sorted By      :      Retention Time
Multiplier:    :      1.0000
Dilution:      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
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```

Signal 1: DAD1 A, Sig=220,16 Ref=off
Signal 2: DAD1 B, Sig=254,16 Ref=off
  
```

Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	0.692	1	BB	298.16977	50.41683	20.2619
2	3.148	1	BB	700.86938	318.06860	47.6271
3	3.149	2	BB	472.53772	238.99857	32.1110

```
Totals :                1471.57687  607.48400
```



rac-12

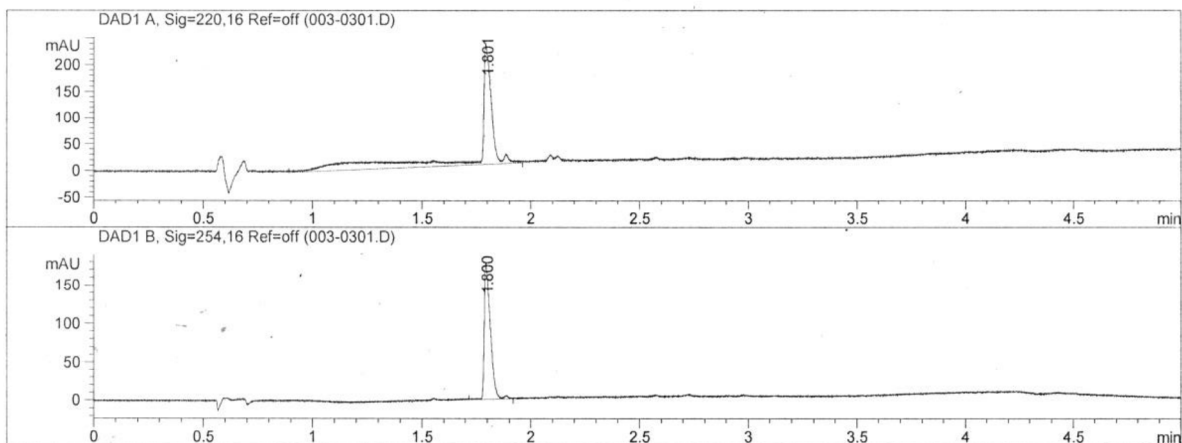
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 *** End of Report ***

Figure S27. HPLC chromatogram of rac-12.

Data File C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-01 13-53-48\003-0301.D
 Sample Name: ballison_1073 product

```

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Acq. Operator   :                               Seq. Line :    3
Acq. Instrument : Instrument 1                   Location  : Vial 3
Injection Date  : 01-May-2012 14:12:59         Inj       :    1
                                                Inj Volume: 3.0 µl
Sequence File   : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-01 13-53-48\JGB1.S
Method          : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-01 13-53-48\5TO99_35C.M (Sequence Method)
Last changed    : 27-Jul-2010 10:57:13
Method Info     : 5-99% ACN, Eclipse XDB C18, 5 µm, 150x4.6mm
=====
  
```



=====
 Area Percent Report
 =====

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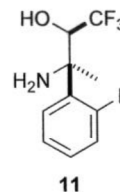
Sorted By      :      Retention Time
Multiplier:    :      1.0000
Dilution:      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

```

Signal 1: DAD1 A, Sig=220,16 Ref=off
Signal 2: DAD1 B, Sig=254,16 Ref=off
  
```

Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	1.800	2	BB	353.86276	136.43169	25.9080
2	1.801	1	BB	1011.98248	188.38135	74.0920

```
Totals :                1365.84525  324.81303
```



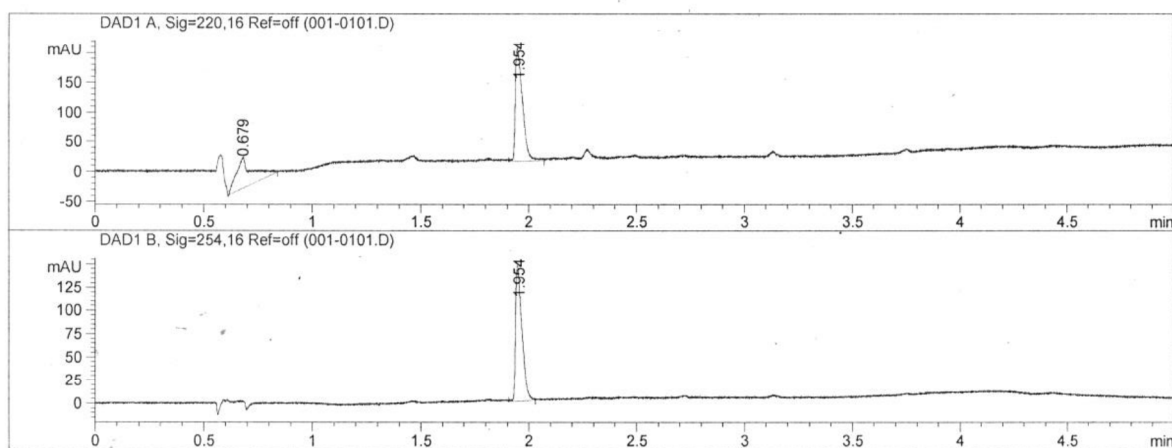
=====
 *** End of Report ***

Figure S28. HPLC chromatogram of 11.

Data File C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-03 15-01-42\001-0101.D
 Sample Name: ballison_1076 isolated product

```

=====
Acq. Operator   :                               Seq. Line :    1
Acq. Instrument : Instrument 1                   Location  : Vial 1
Injection Date  : 03-May-2012 15:04:27         Inj       :    1
                                                Inj Volume: 3.0 µl
Sequence File   : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-03 15-01-42\JGB1.S
Method          : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-03 15-01-42\5TO99_35C.M (Sequence Method)
Last changed    : 27-Jul-2010 10:57:13
Method Info     : 5-99% ACN, Eclipse XDB C18, 5 µm, 150x4.6mm
=====
  
```



Area Percent Report

```

=====
Sorted By      :      Retention Time
Multiplier:    :      1.0000
Dilution:      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

```

Signal 1: DAD1 A, Sig=220,16 Ref=off
Signal 2: DAD1 B, Sig=254,16 Ref=off
  
```

Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	0.679	1	BB	260.61084	45.55235	25.8199
2	1.954	2	BB	301.34943	131.94470	29.8560
3	1.954	1	BB	447.38214	177.02893	44.3241

Totals : 1009.34241 354.52598

*** End of Report ***

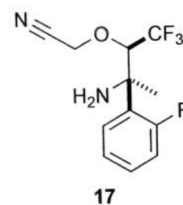


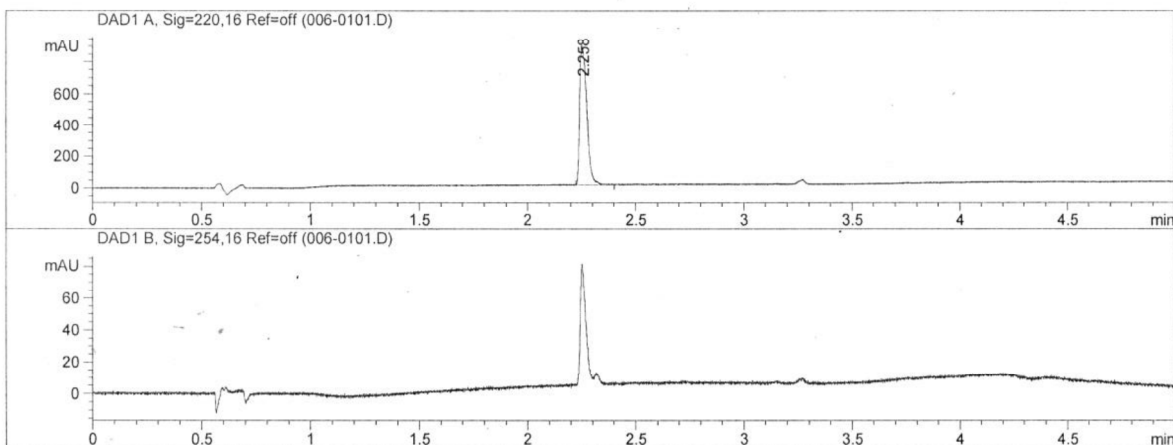
Figure S29. HPLC chromatogram of 17.

Data File C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-07 14-17-42\006-0101.D
Sample Name: ballison_1078 crude product

=====

Acq. Operator	:		Seq. Line	:	1
Acq. Instrument	:	Instrument 1	Location	:	Vial 6
Injection Date	:	07-May-2012 14:20:03	Inj	:	1
			Inj Volume	:	3.0 µl

Sequence File : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-07 14-17-42\JGB1.S
Method : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-07 14-17-42\5TO99_35C.M (Sequence Method)
Last changed : 27-Jul-2010 10:57:13
Method Info : 5-99% ACN, Eclipse XDB C18, 5 µm, 150x4.6mm



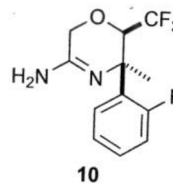
=====
Area Percent Report
=====

Sorted By : Retention Time
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=220,16 Ref=off

Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	2.258	1	BB	2040.04846	812.54700	100.0981

Totals : 2038.04846 810.54700



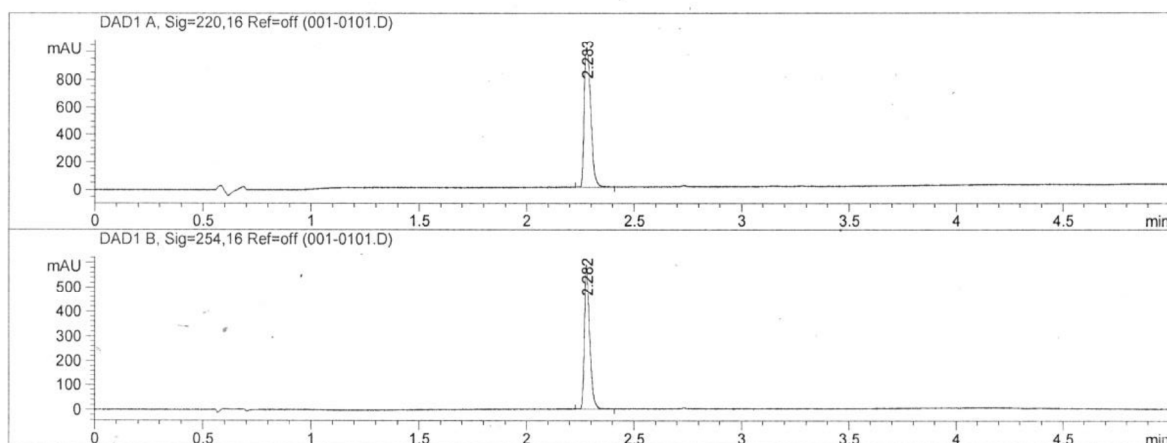
=====
*** End of Report ***

Figure S30. HPLC chromatogram of 10.

Data File C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-11 16-44-01\001-0101.D
 Sample Name: ballison_1079 TBME after NaOH wash

```

=====
Acq. Operator   :                               Seq. Line :    1
Acq. Instrument : Instrument 1                  Location  : Vial 1
Injection Date  : 11-May-2012 16:46:53         Inj       :    1
                                              Inj Volume: 3.0 µl
Sequence File   : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-11 16-44-01\JGB1.S
Method          : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-11 16-44-01\5TO99_35C.M (Sequence Method)
Last changed    : 27-Jul-2010 10:57:13
Method Info     : 5-99% ACN, Eclipse XDB C18, 5 µm, 150x4.6mm
=====
    
```



Area Percent Report

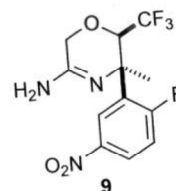
```

Sorted By      :          Retention Time
Multiplier:    :          1.0000
Dilution:      :          1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

Signal 1: DAD1 A, Sig=220,16 Ref=off
 Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	2.282	2	BB	1007.10522	468.54651	31.7918
2	2.283	1	BB	2160.70654	917.73279	68.2082

Totals : 3167.81177 1386.27930



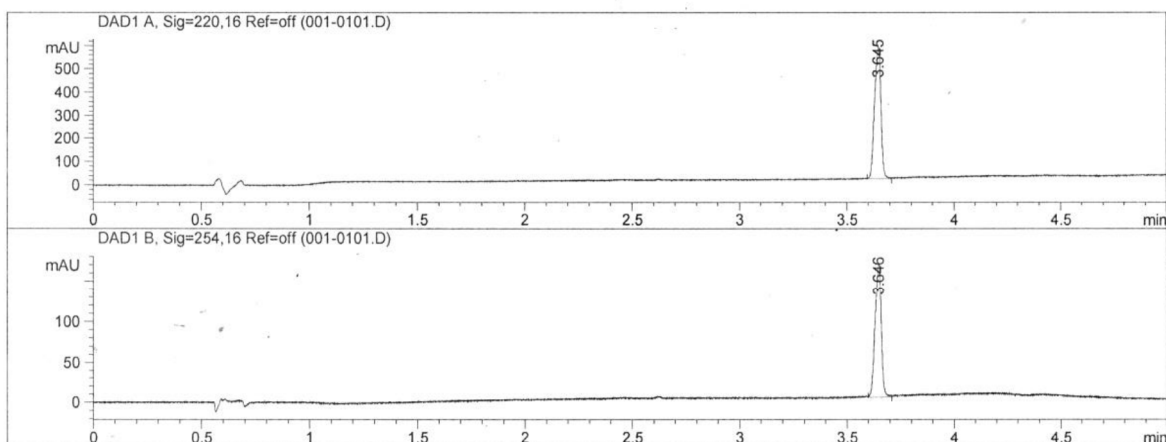
*** End of Report ***

Figure S31. HPLC chromatogram of 9.

Data File C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-15 22-04-26\001-0101.D
 Sample Name: ballison_1088 flashed product

```

=====
Acq. Operator   :                               Seq. Line :    1
Acq. Instrument : Instrument 1                   Location  : Vial 1
Injection Date  : 15-May-2012 22:07:19         Inj       :    1
                                                Inj Volume: 3.0 µl
Sequence File   : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-15 22-04-26\JGB1.S
Method          : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-15 22-04-26\5T099_35C.M (Sequence Method)
Last changed    : 27-Jul-2010 10:57:13
Method Info     : 5-99% ACN, Eclipse XDB C18, 5 µm, 150x4.6mm
=====
  
```



=====
 Area Percent Report
 =====

```

Sorted By      :      Retention Time
Multiplier:    :      1.0000
Dilution:      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

```

Signal 1: DAD1 A, Sig=220,16 Ref=off
Signal 2: DAD1 B, Sig=254,16 Ref=off
  
```

Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	3.645	1	BB	1182.91589	542.96851	77.9695
2	3.646	2	BB	334.23630	157.29256	22.0305

```
Totals :                1517.15219  700.26106
```

=====
 *** End of Report ***
 =====

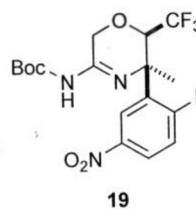
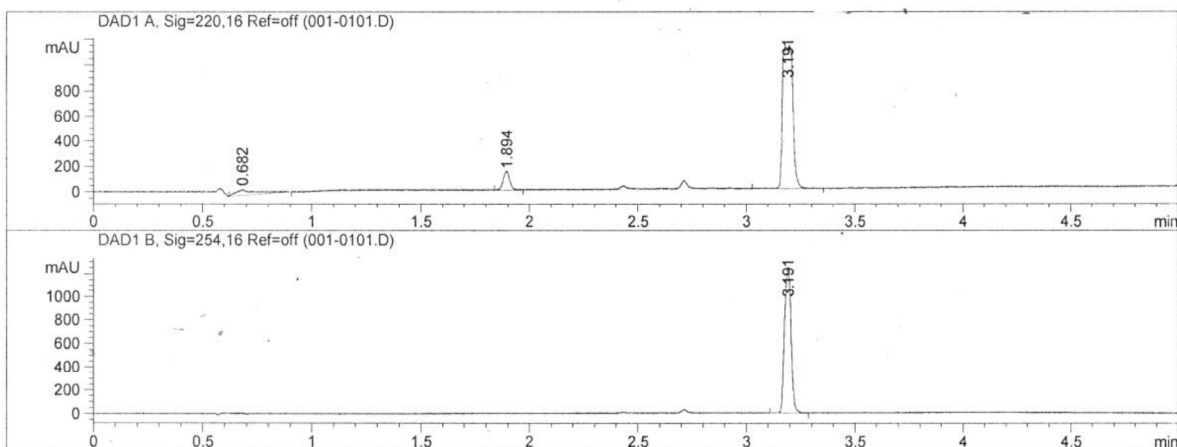


Figure S32. HPLC chromatogram of **19**.

Data File C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-19 23-11-53\001-0101.D
 Sample Name: ballison_1094 final org layer

```

=====
Acq. Operator   :                               Seq. Line :    1
Acq. Instrument : Instrument 1                   Location  : Vial 1
Injection Date  : 19-May-2012 23:14:39          Inj       :    1
                                                    Inj Volume: 3.0 µl
Sequence File   : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-19 23-11-53\JGB1.S
Method          : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-19 23-11-53\5TO99_35C.M (Sequ
Last changed    : 27-Jul-2010 10:57:13
Method Info     : 5-99% ACN, Eclipse XDB C18, 5 µm, 150x4.6mm
=====
  
```



=====
 Area Percent Report
 =====

```

Sorted By      :      Retention Time
Multiplier:    :      1.0000
Dilution:      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

```

Signal 1: DAD1 A, Sig=220,16 Ref=off
Signal 2: DAD1 B, Sig=254,16 Ref=off
  
```

Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	0.682	1	BB	304.38477	41.94170	4.3465
2	1.894	1	BB	320.65506	136.33331	4.5788
3	3.191	1	BB	3740.24951	1105.11914	53.4095
4	3.191	2	BB	2637.67920	1212.81763	37.6652

Totals : 7002.96854 2496.21178

=====
 *** End of Report ***

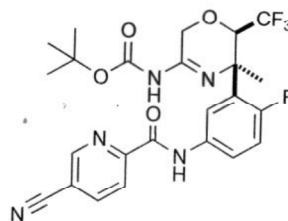


Figure S34. HPLC chromatogram of Boc-protected **1**.

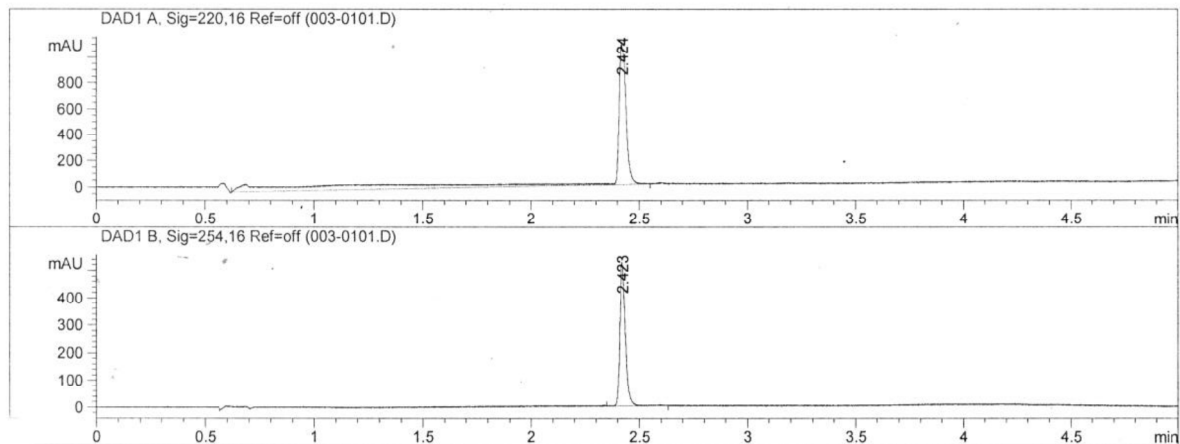
Data File C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-22 09-26-49\003-0101.D
Sample Name: ballison_1095 final

=====

Acq. Operator	:		Seq. Line	:	1
Acq. Instrument	:	Instrument 1	Location	:	Vial 3
Injection Date	:	22-May-2012 09:29:22	Inj	:	1
			Inj Volume	:	3.0 µl

Sequence File : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-22 09-26-49\JGB1.S
Method : C:\CHEM32\1\DATA\GENERAL\JGB1 2012-05-22 09-26-49\5TO99_35C.M (Sequence Method)
Last changed : 27-Jul-2010 10:57:13
Method Info : 5-99% ACN, Eclipse XDB C18, 5 µm, 150x4.6mm

Sample Info : triturated from toluene, dried high vac, 70 °C, o/n



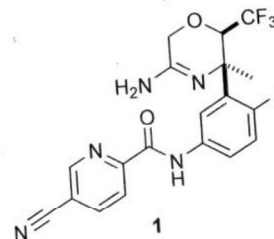
=====
Area Percent Report
=====

Sorted By : Retention Time
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=220,16 Ref=off
Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	2.423	2	BB	929.98712	489.57022	15.7597
2	2.424	1	BB	4971.06787	1060.04871	84.2403

Totals : 5901.05499 1549.61893



=====
*** End of Report ***
=====

Figure S35. HPLC chromatogram of 1.