

Supporting information

Synthesis, characterization and properties of amino acid ionic liquids derived from the triaminocyclopropenium cation

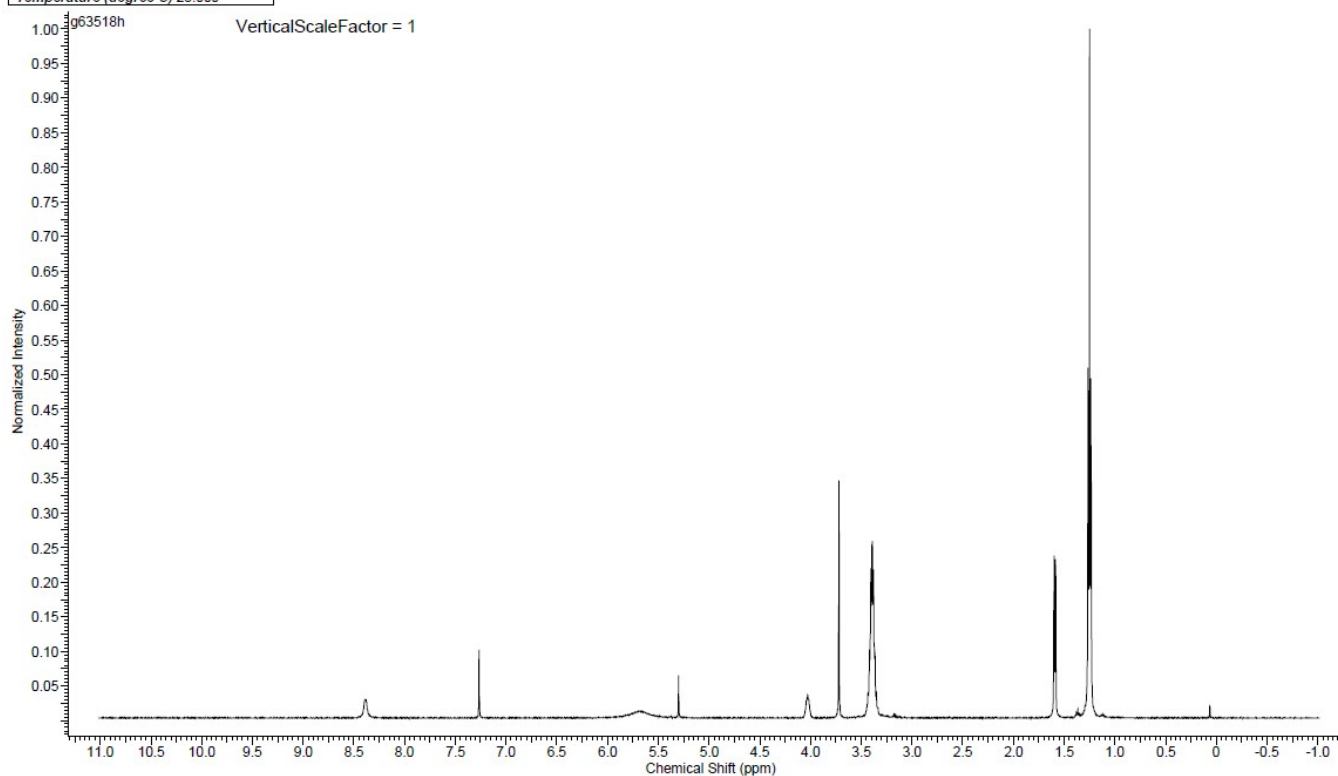
Owen J Curnow* and Ruhamah Yunis

Department of Chemistry, University of Canterbury, Private Bag 4800, Christchurch 8140, New Zealand

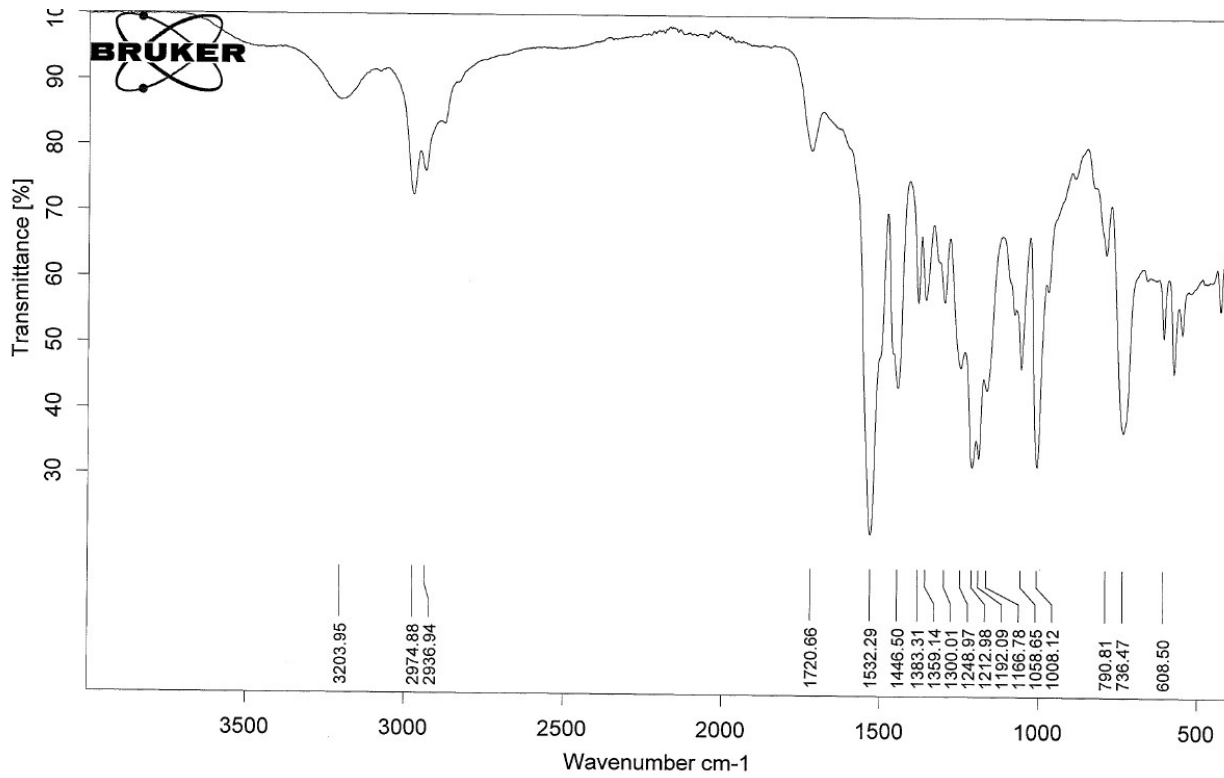
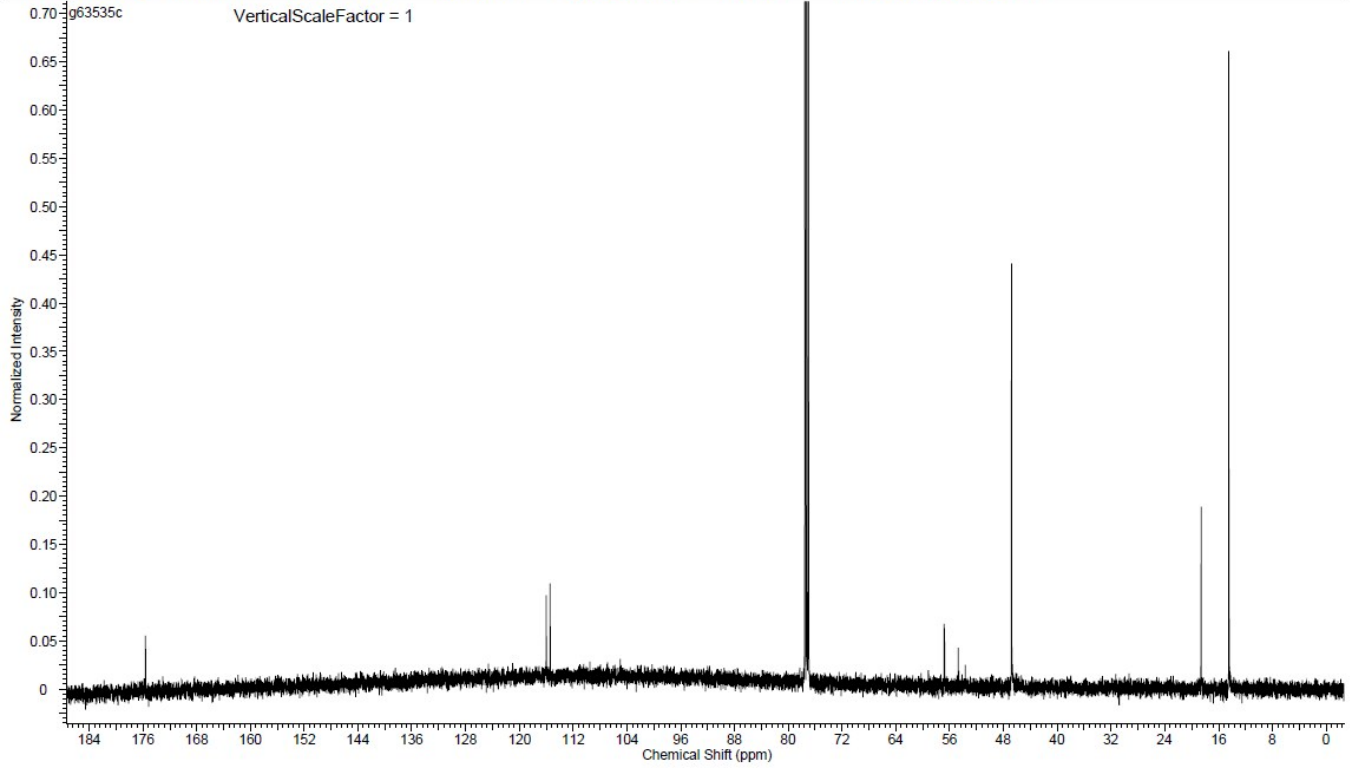
NMR and IR spectra are provided in numerical order.

Bis(diethylamino)-S-(1-carboxyethylamino)cyclopropenium methylsulfate, $[C_3(NEt_2)_2(NH(CHMeCOOH))][MeSO_4]$, $[E_4Ala]MeSO_4$ (1a)

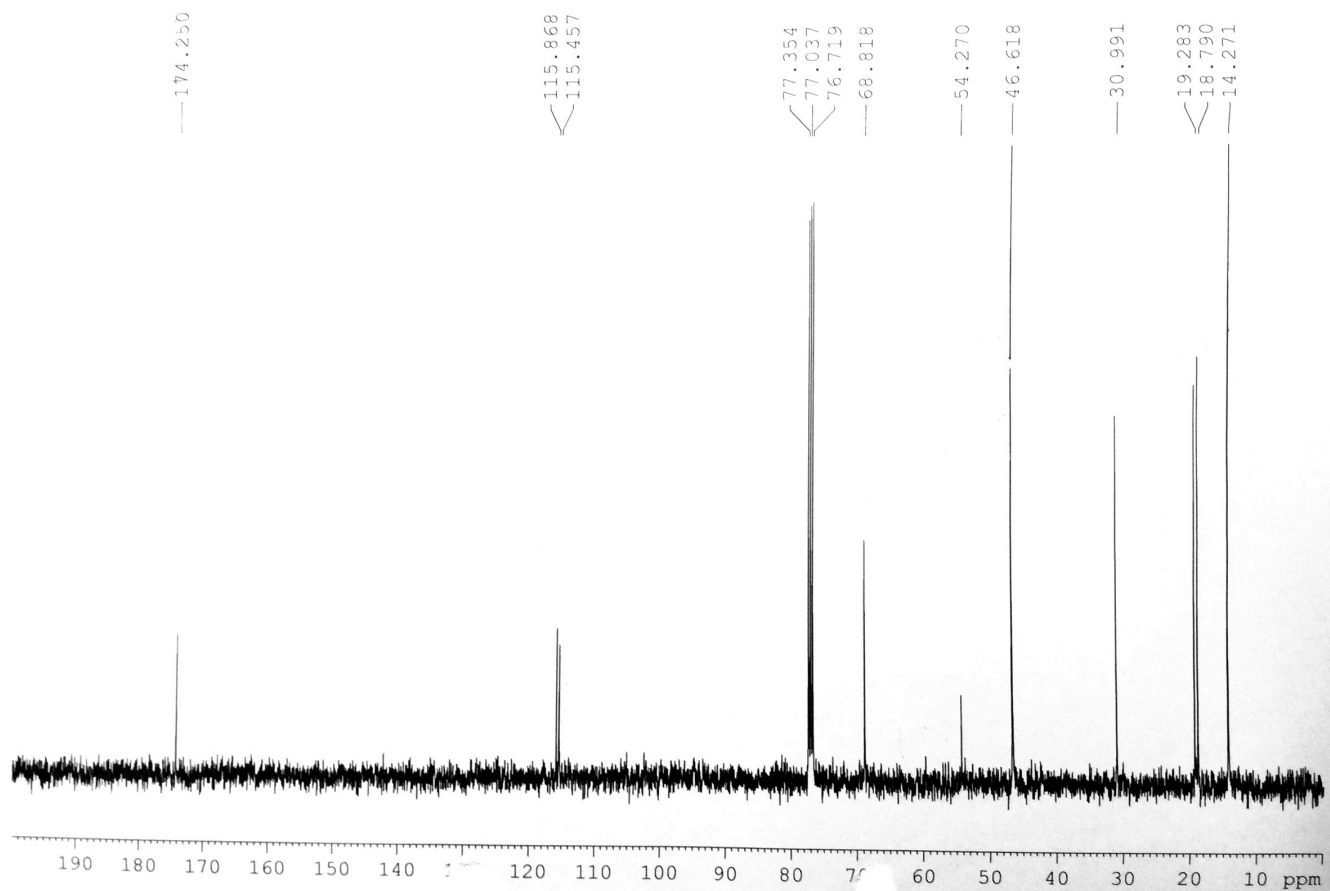
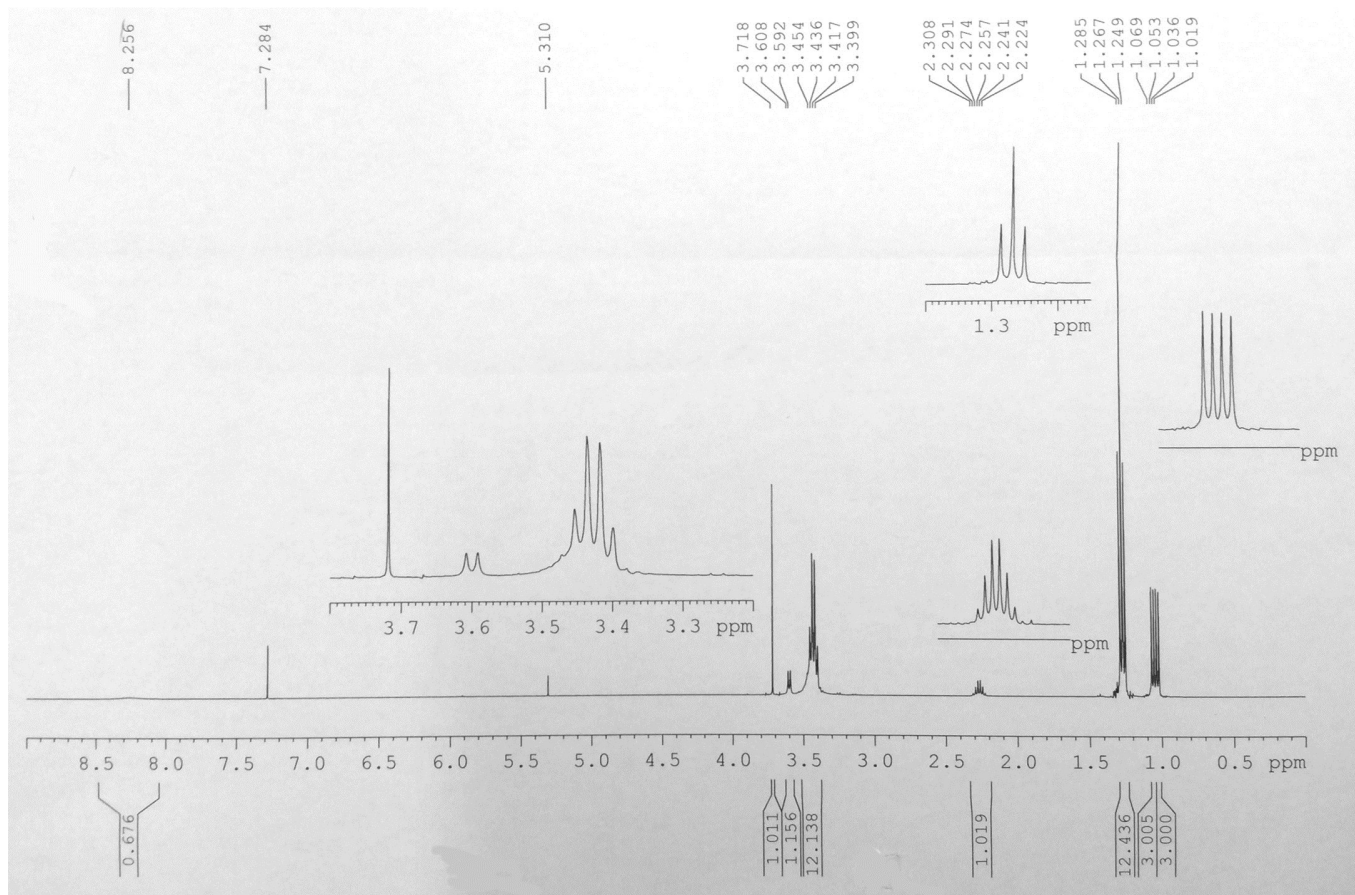
Acquisition Time (sec)	1.8920	Comment	rv-01-38-54c(DCM)	Date	Feb 11 2011	Date Stamp	Feb 11 2011
File Name	\\fileUsersO:\o\c10\Home\My Documents\AAIL paper\g63518h.fid\fid			Frequency (MHz)	499.68	Nucleus	1H
Number of Transients	8	Original Points Count	11370	Points Count	16384	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2498.4285	Spectrum Type	STANDARD	Receiver Gain	36.00
Temperature (degree C)	23.000					Sweep Width (Hz)	6009.62

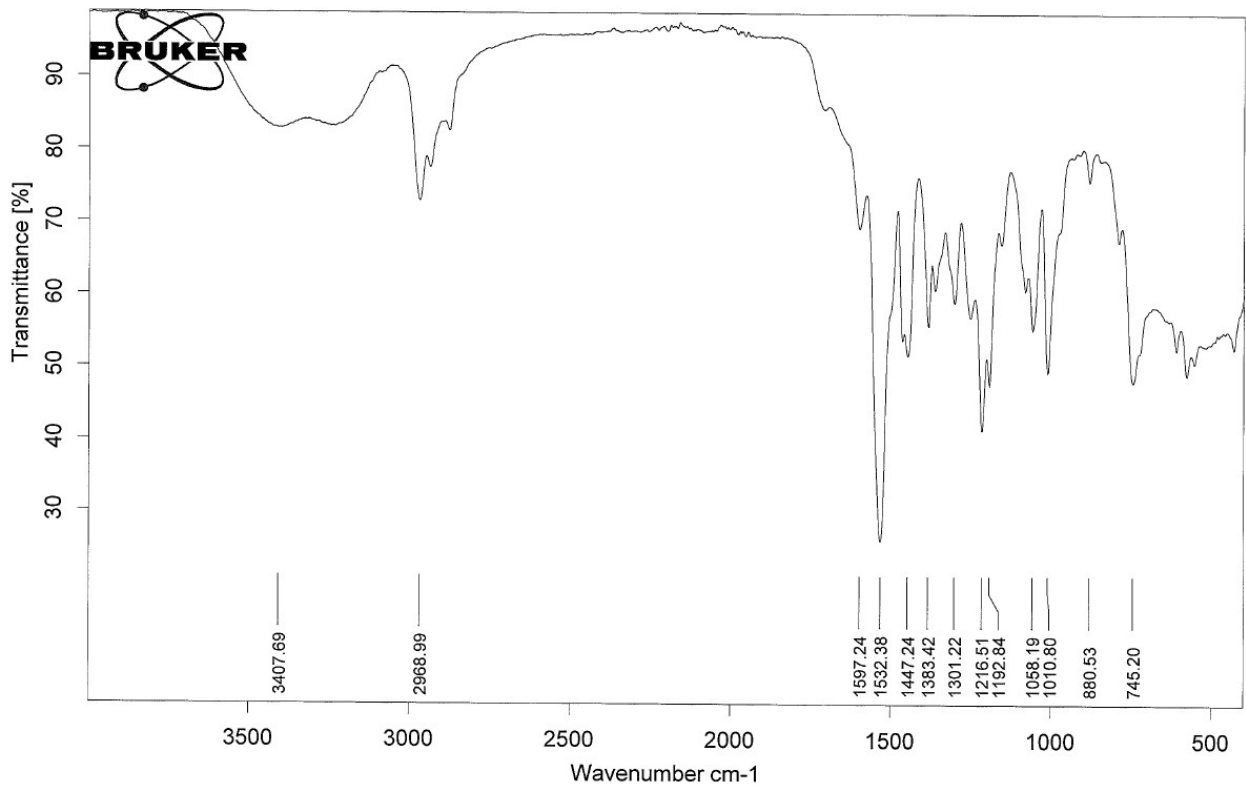


Acquisition Time (sec)	1.3005	Comment	ry-01-38-55a(DCM) IE4alaI MeSO4	Date	Feb 12 2011
Date Stamp	Feb 12 2011	File Name	\\file\Users\O:\cic10\Home\My Documents\AAIL paper\g63535c.fid.fid		
Frequency (MHz)	125.66	Nucleus	13C	Number of Transients	24940
Points Count	65536	Pulse Sequence	s2pul	Receiver Gain	30.00
Spectrum Offset (Hz)	13192.7188	Spectrum Type	STANDARD	Sweep Width (Hz)	30487.80
				Temperature (degree C)	23.000



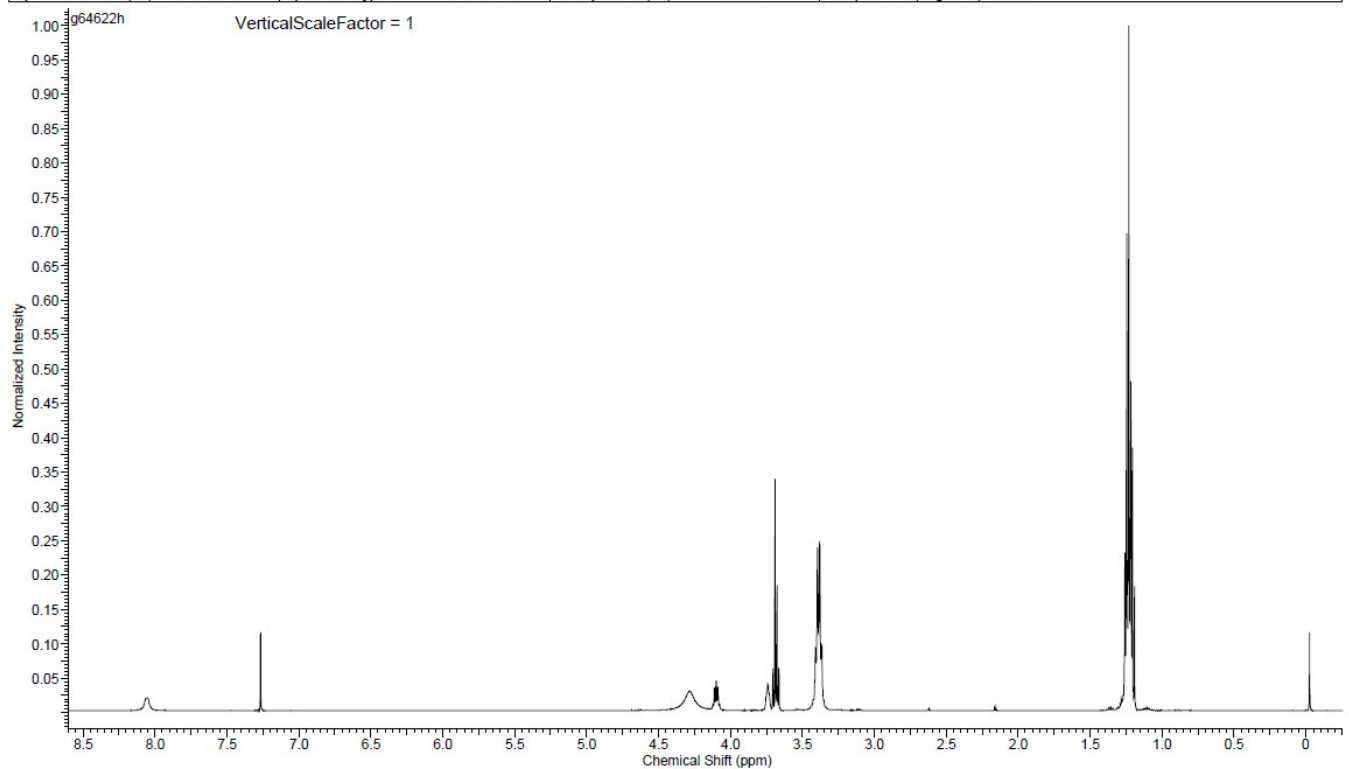
Bis(diethylamino)-S-(1-carboxy-2-methylpropylamino)cyclopropenium methylsulfate, [C₃(NEt₂)₂(NH(C₄H₈COOH))][MeSO₄], [E₄Val][MeSO₄] (1b)



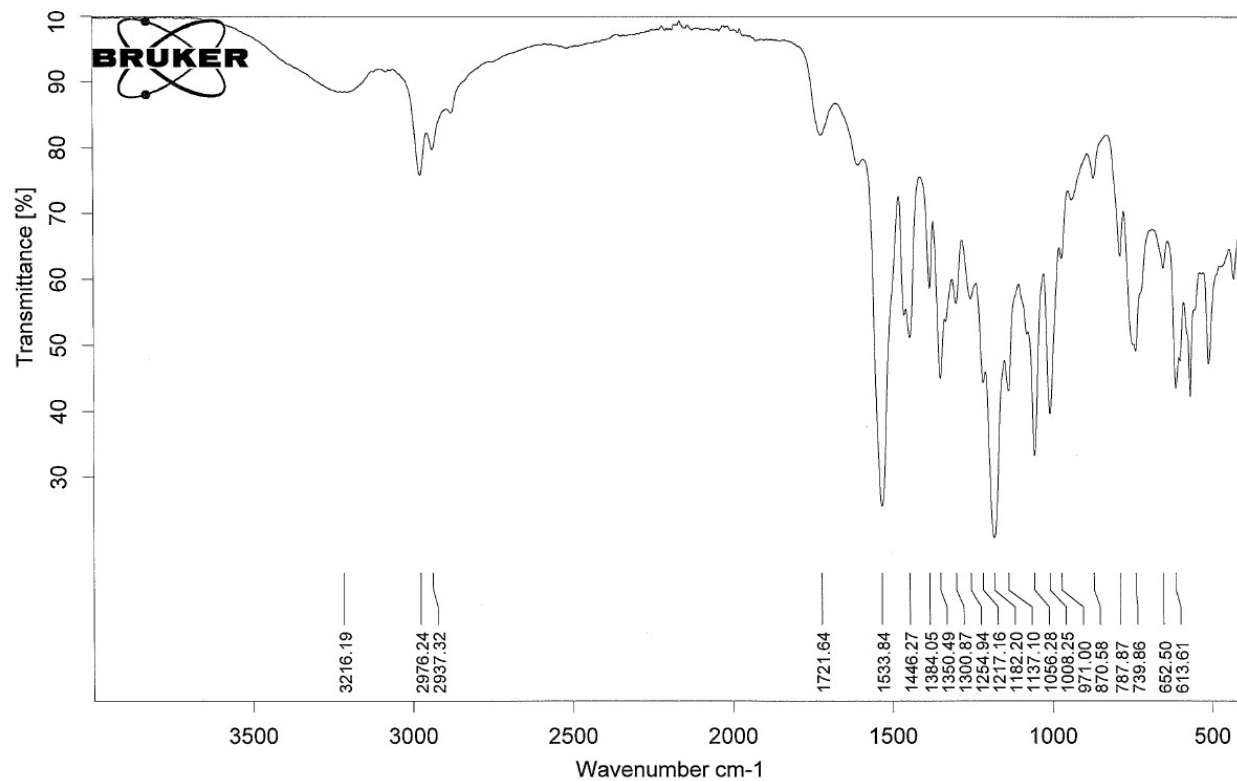
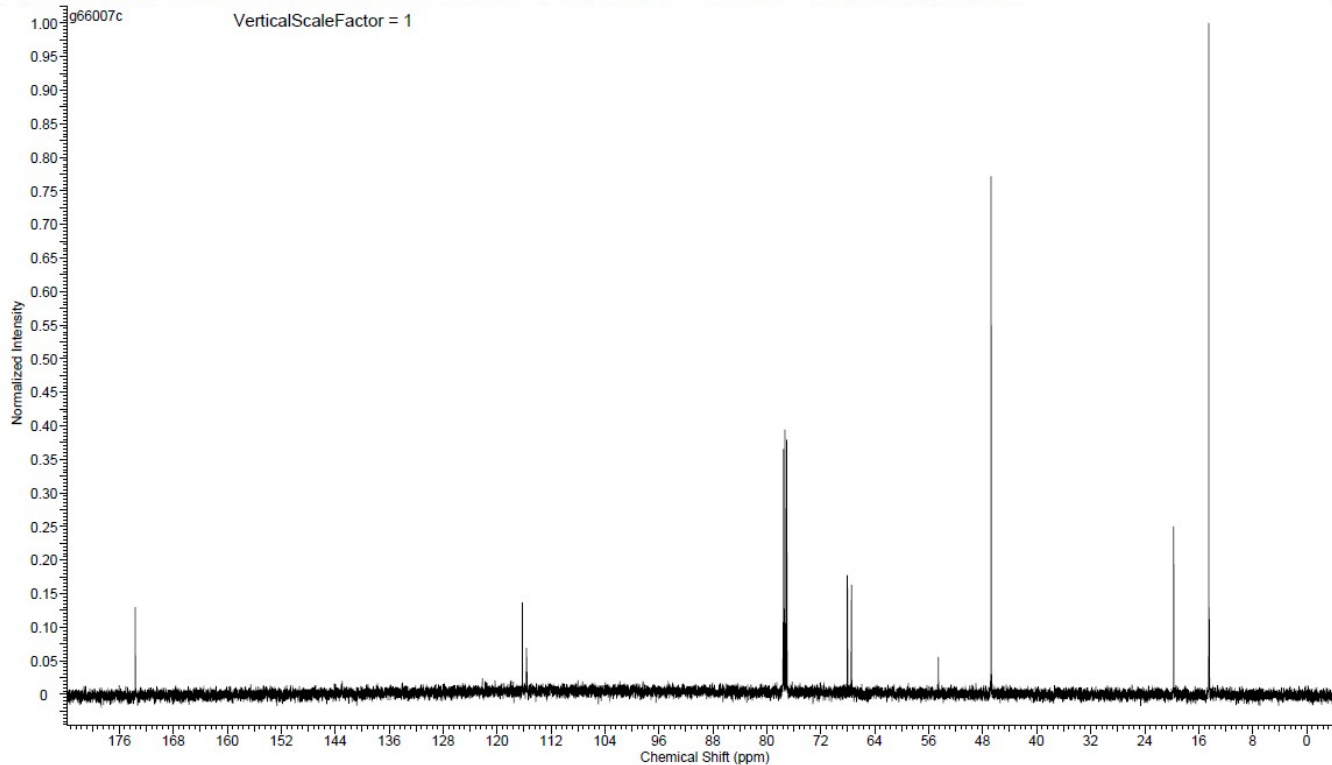


**Bis(diethylamino)-S-(1-carboxy-2-hydroxypropylamino)cyclopropenium methylsulfate,
[C₃(NEt₂)₂(NH(C₃H₆OCOOH))]⁺MeSO₄⁻, [E₄Thr]⁺MeSO₄⁻ (1j)**

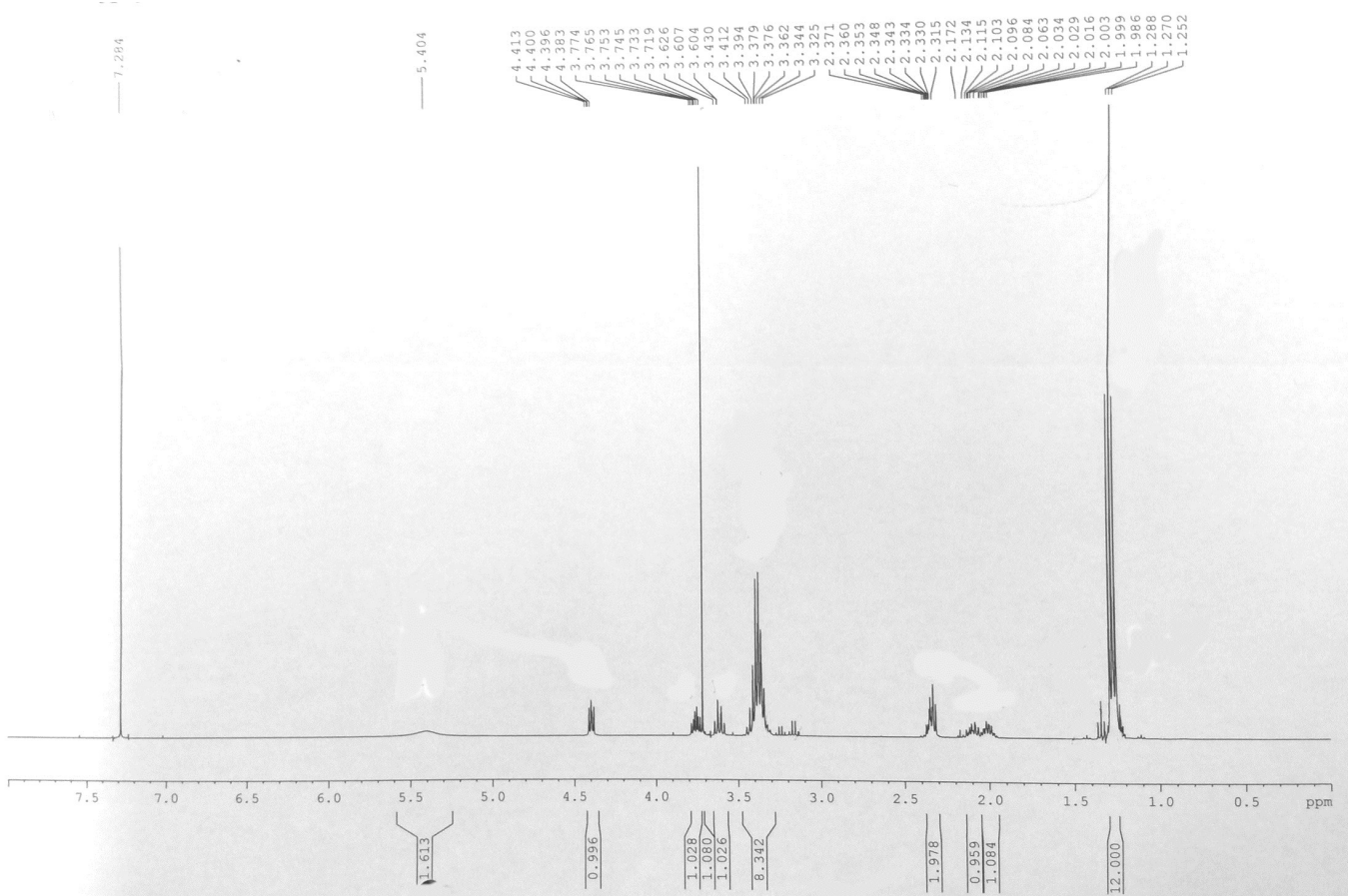
Acquisition Time (sec)	1.8920	Comment	ry-01-79-46q (CHCl ₃ + ethanol layer)	Date	Aug 3 2011
Date Stamp	Aug 3 2011	File Name	\file\Users\O...ojc10\Home\My Documents\AAIL paper\g64622h.fid\fid		
Frequency (MHz)	499.68	Nucleus	¹ H	Number of Transients	8
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	26.00
Spectrum Offset (Hz)	2498.3643	Spectrum Type	STANDARD	Sweep Width (Hz)	6009.62
				Temperature (degree C)	23.000



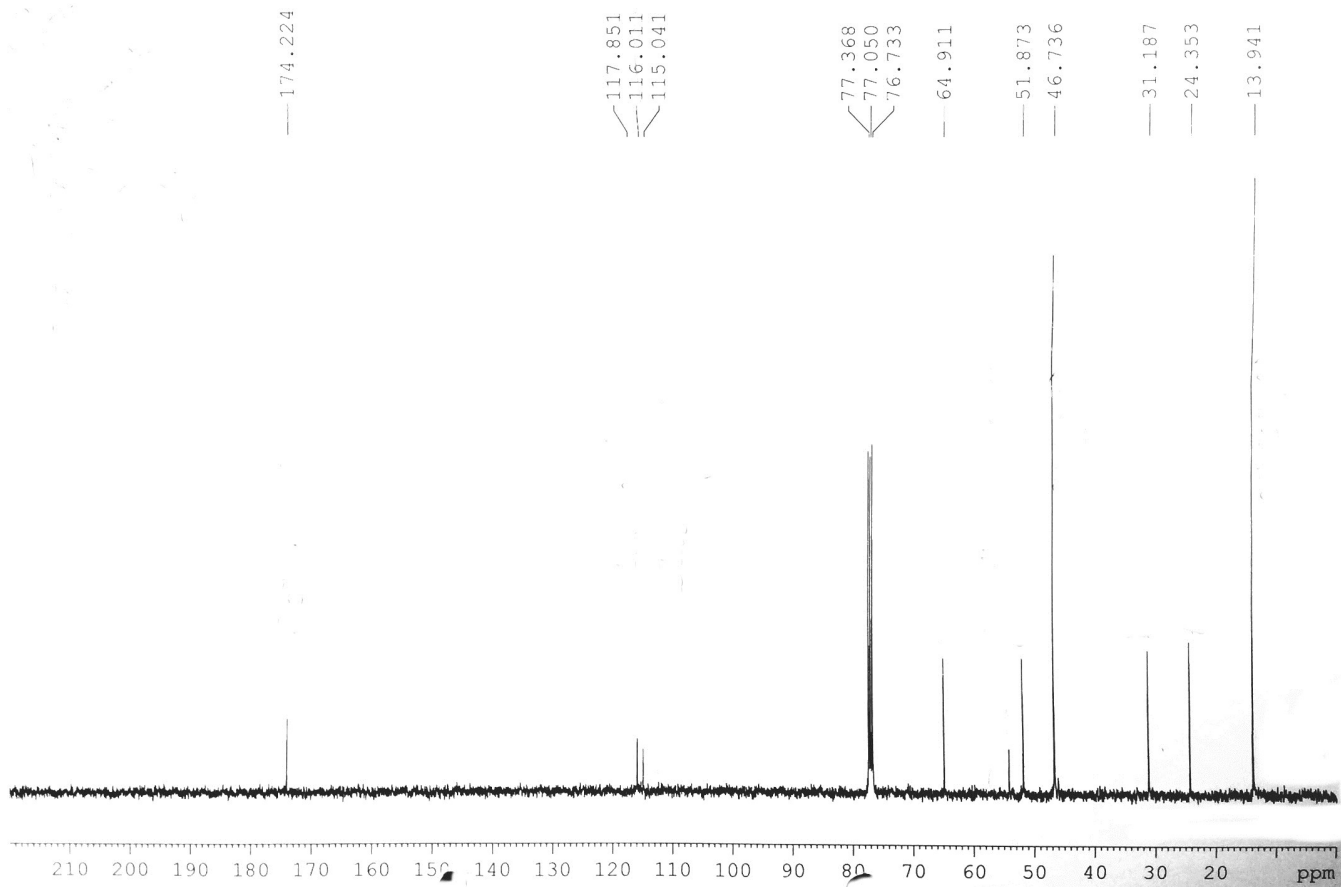
Acquisition Time (sec)	1.3005	Comment	ry-01-79-46q IETMeSO4	Date	Oct 5 2011
Date Stamp	Oct 5 2011	File Name	\file\Users\O...oic10\Home\My Documents\AAIL paper\g66007c.fid\fid		
Frequency (MHz)	125.66	Nucleus	13C	Number of Transients	2728
Points Count	65536	Pulse Sequence	s2pul	Receiver Gain	30.00
Spectrum Offset (Hz)	13192.7188	Spectrum Type	STANDARD	Sweep Width (Hz)	30487.80
				Temperature (degree C)	23.000



Bis(diethylamino)-S-(2-carboxypyrrolidino)cyclopropenium methylsulfate, [C₃(NEt₂)₂(N(C₄H₇COOH))][MeSO₄], [E₄Pro]MeSO₄ (1k)

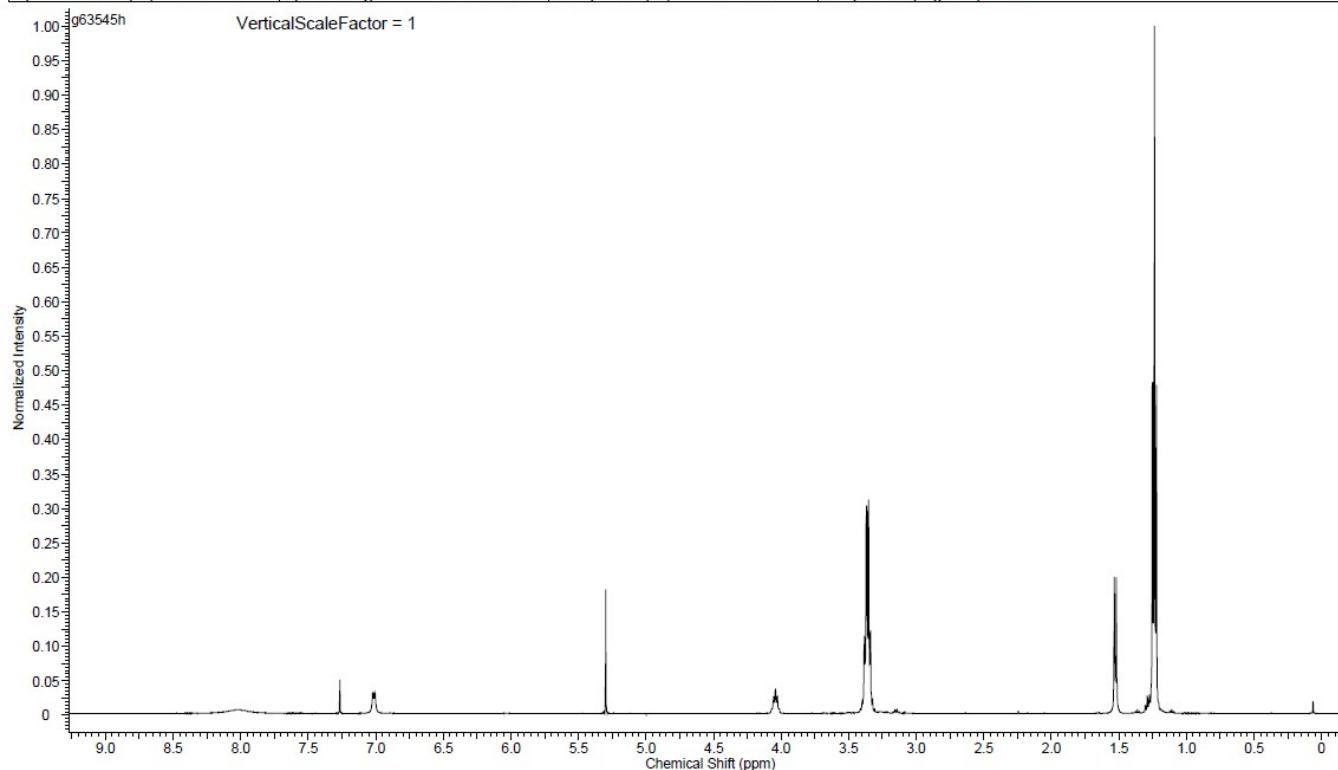


13C of ry-01-54-85b

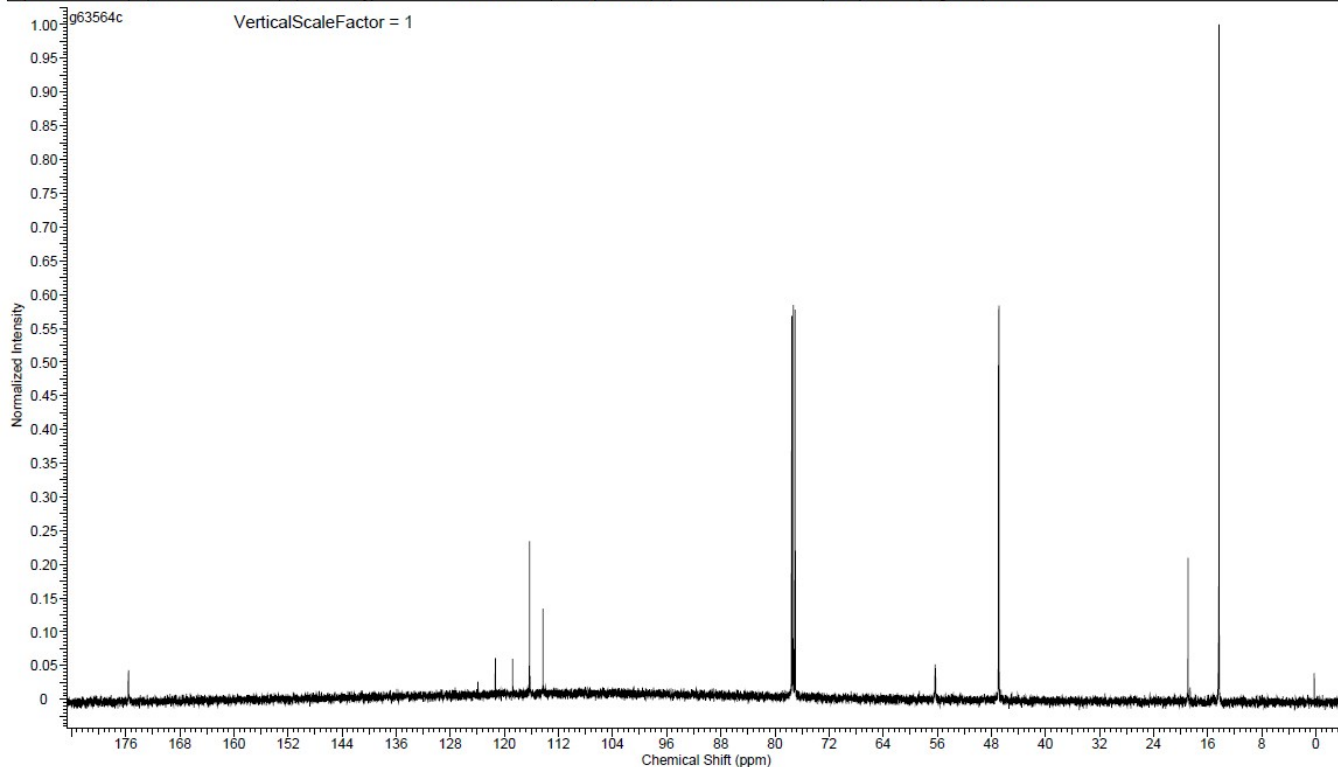


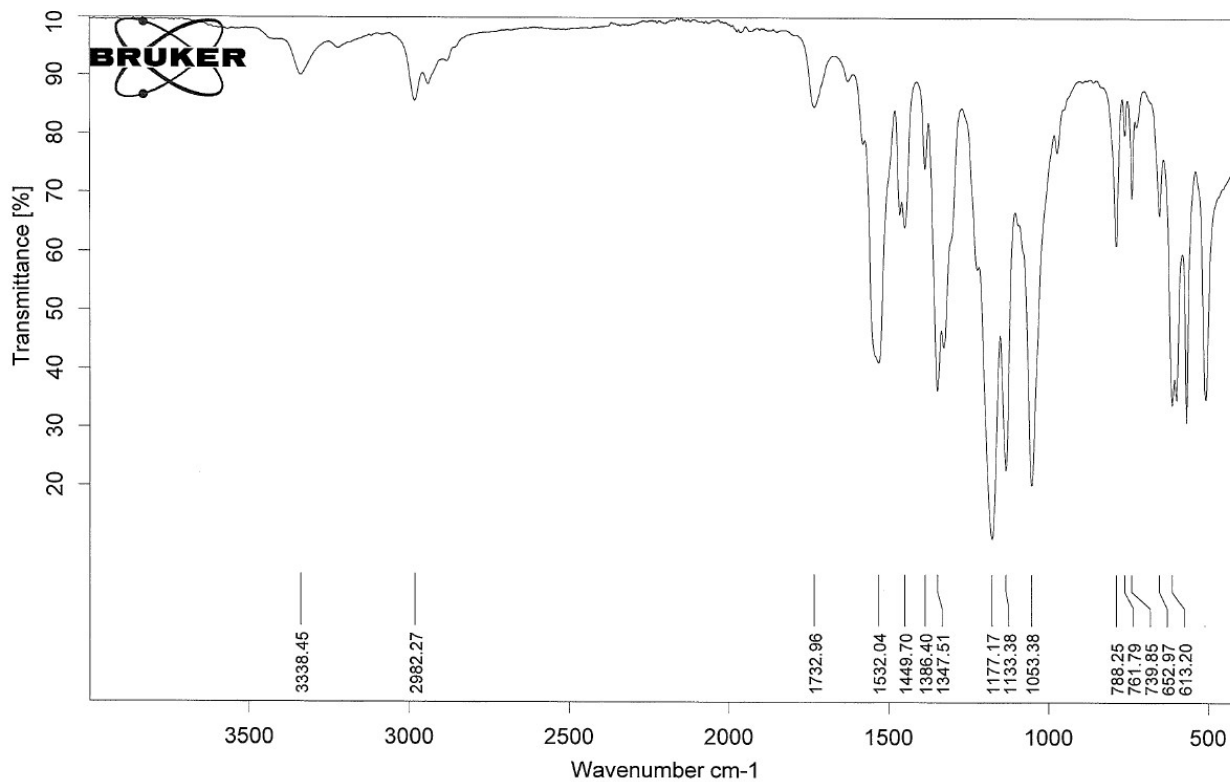
Bis(diethylamino)-S-(1-carboxyethylamino)cyclopropenium bistriflamide, [C₃(NEt₂)₂(NH(CHMeCOOH))]NTf₂, [E₄Ala]NTf₂ (2a)

Acquisition Time (sec)	1.8920	Comment	ry-01-41-59b[E4 alanine]TFSA	Date	Feb 14 2011
Date Stamp	Feb 14 2011	File Name	\\file\Users\O...oic10\Home\My Documents\AAIL_paper\g63545h.fid\fid		
Frequency (MHz)	499.68	Nucleus	¹ H	Number of Transients	8
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	30.00
Spectrum Offset (Hz)	2498.3643	Spectrum Type	STANDARD	Sweep Width (Hz)	6009.62
				Temperature (degree C)	23.000



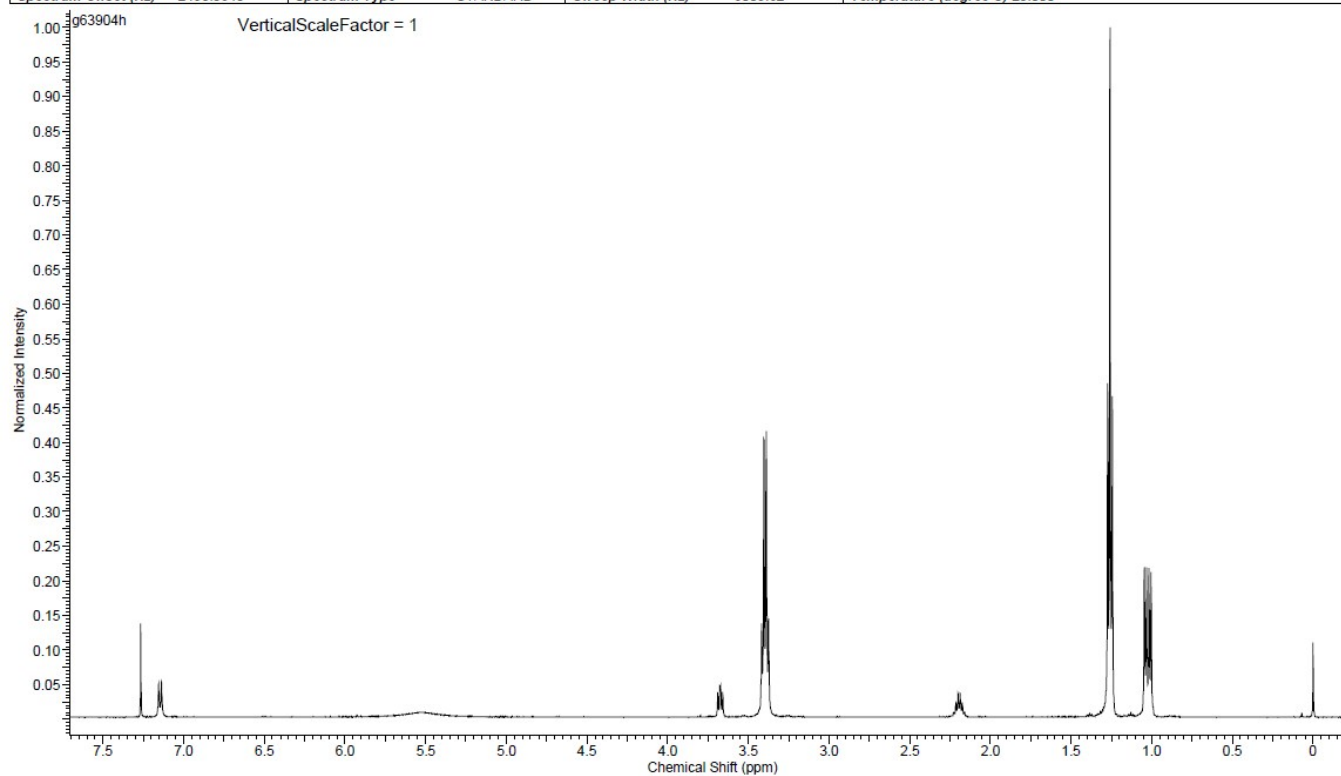
Acquisition Time (sec)	1.3005	Comment	ry-01-41-59a[E4alanine]TFSA	Date	Feb 15 2011
Date Stamp	Feb 15 2011	File Name	\\file\Users\O...oic10\Home\My Documents\AAIL_paper\g63564c.fid\fid		
Frequency (MHz)	125.66	Nucleus	¹³ C	Number of Transients	23380
Points Count	65536	Pulse Sequence	s2pul	Receiver Gain	30.00
Spectrum Offset (Hz)	13192.7188	Spectrum Type	STANDARD	Sweep Width (Hz)	30487.80
				Temperature (degree C)	23.000





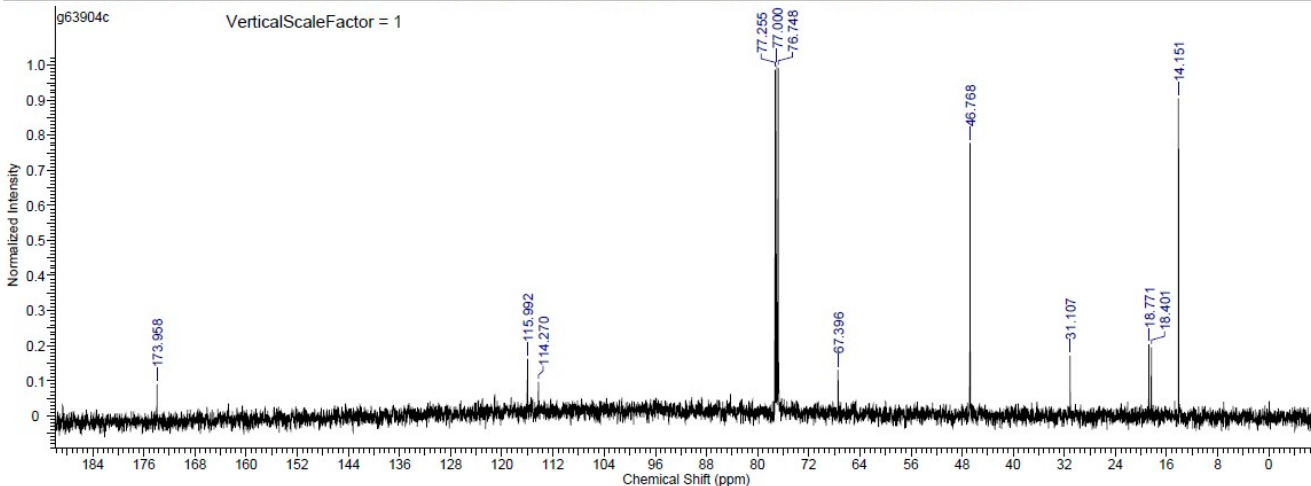
**Bis(diethylamino)-S-(1-carboxy-2-methylpropylamino)cyclopropenium bistriflamide,
[C₃(NEt₂)₂(NH(C₄H₈COOH))]NTf₂, [E₄Val]NTf₂ (2b)**

Acquisition Time (sec)	1.8920	Comment	ny-01-62-05c [E4val]TfSA three times water wash	Date	Jun 3 2011
Date Stamp	Jun 3 2011	File Name	\\file\Users\O...jc10\Home\My Documents\AAIL paper\g63904h.fid\fid		
Frequency (MHz)	499.68	Nucleus	1H	Number of Transients	8
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	32.00
Spectrum Offset (Hz)	2498.3643	Spectrum Type	STANDARD	Sweep Width (Hz)	6009.62
				Solvent	CHLOROFORM-d
				Temperature (degree C)	23.000

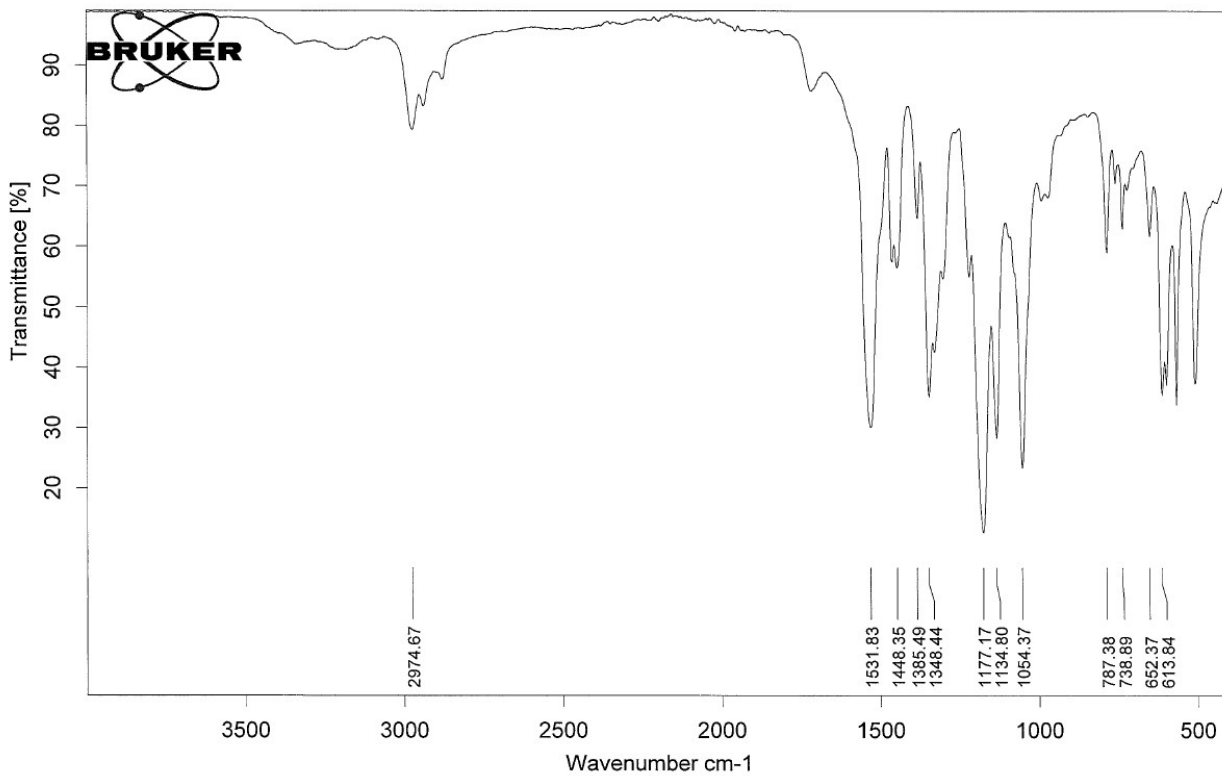


RMS of Noise 13335.6494

Acquisition Time (sec)	1.3005	Comment	ry-01-62-05c [E4va]TFSA three times water wash	Date	Jun 3 2011
Date Stamp	Jun 3 2011	File Name	\\fileUsersO...ojc10\Home\My Documents\AAIL paper\g63904c.fid.fid		
Frequency (MHz)	125.66	Nucleus	¹³ C	Number of Transients	3008
Points Count	65536	Pulse Sequence	s2pul	Receiver Gain	30.00
Spectrum Offset (Hz)	13161.7480	Spectrum Type	STANDARD	Sweep Width (Hz)	30487.80
				Temperature (degree C)	23.000



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.15	1778.2	0.9057	4	31.11	3908.9	0.1725	7	76.75	9644.0	0.9916	10	114.27	14359.0	0.0965
2	18.40	2312.3	0.1950	5	46.77	5876.7	0.7780	8	77.00	9675.7	1.0000	11	115.99	14575.3	0.1621
3	18.77	2358.8	0.2038	6	67.40	8468.9	0.1308	9	77.26	9707.8	0.9870	12	173.96	21859.2	0.0903



2974.67

1531.83
1448.35
1385.49
1348.44

1177.17
1134.80
1054.37

767.38
738.89
652.37
613.84

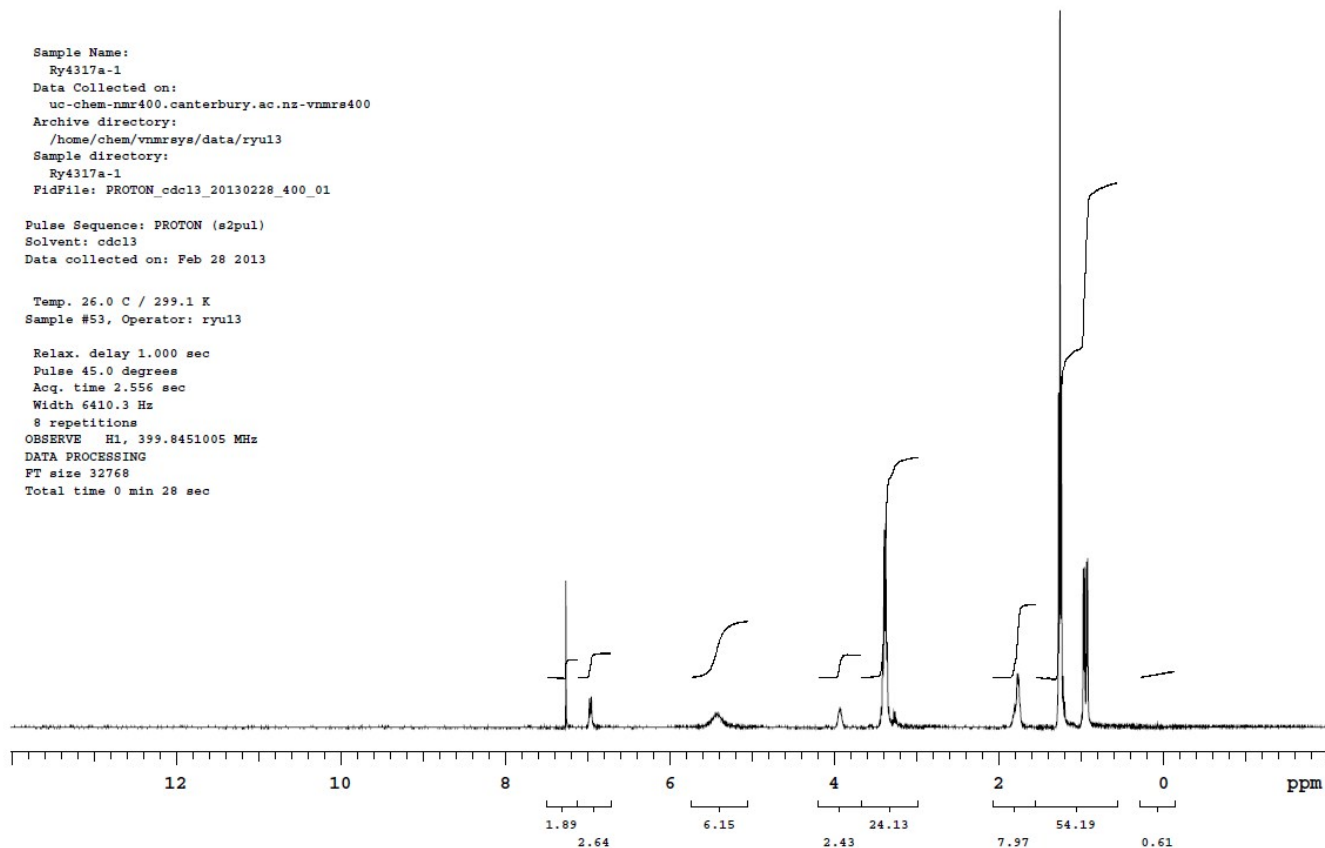
Bis(diethylamino)-S-(1-carboxy-3,3-dimethylethylamino)cyclopropenium bistriflamide, [C₃(NEt₂)₂(NHCOOHCH₃H₄(CH₃)₂)]NTf₂, [E₄Leu]NTf₂ (2c)

Sample Name:
Ry4317a-1
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmr400
Archive directory:
/home/chem/vmr400/data/ryul3
Sample directory:
Ry4317a-1
FidFile: PROTON_cdc13_20130228_400_01

Pulse Sequence: PROTON (s2pul)
Solvent: cdc13
Data collected on: Feb 28 2013

Temp. 26.0 C / 299.1 K
Sample #53, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8451005 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



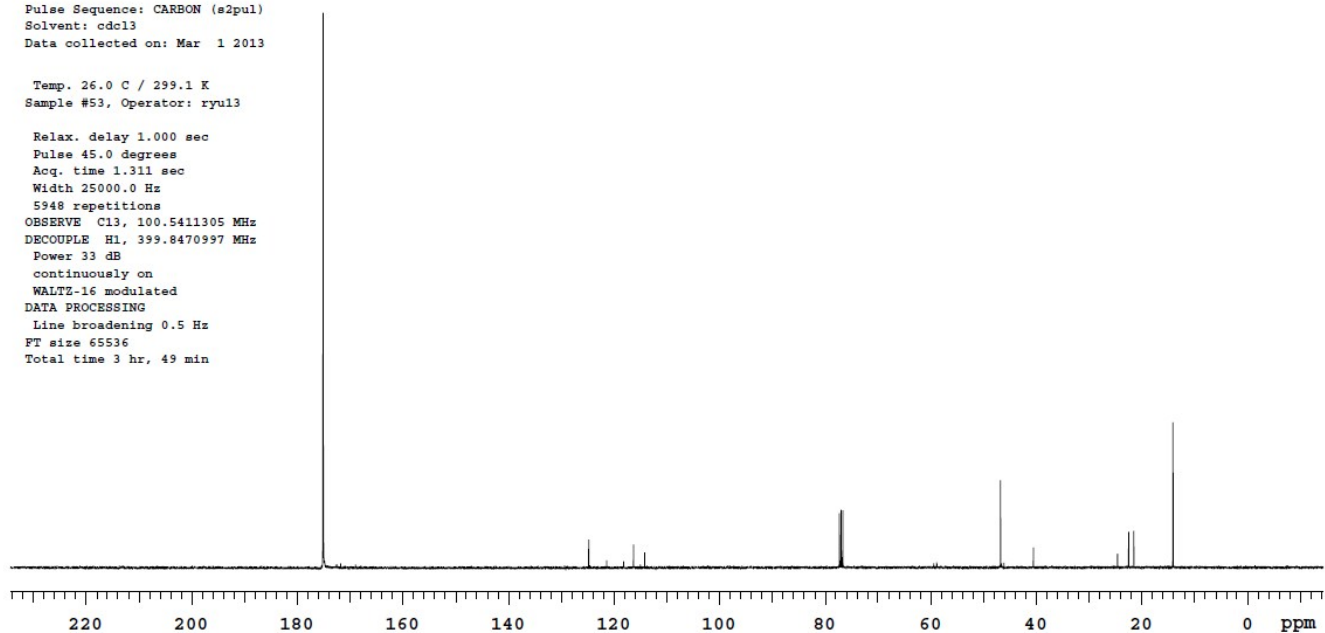
Plotname: PROTON_cdc13_20130228_400_01_plot01

Sample Name:
Ry4317a-1
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmr400
Archive directory:
/home/chem/vmr400/data/ryul3
Sample directory:
Ry4317a-1
FidFile: CARBON_cdc13_20130301_400_01

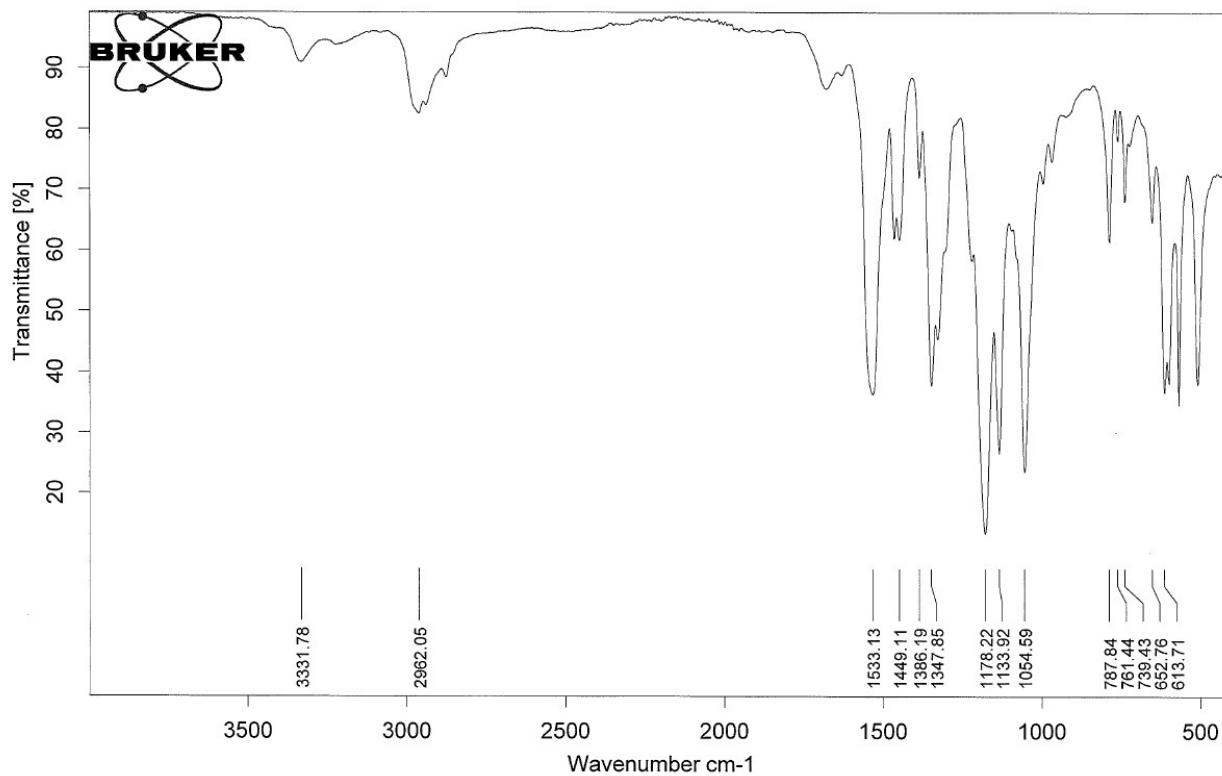
Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Mar 1 2013

Temp. 26.0 C / 299.1 K
Sample #53, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
5948 repetitions
OBSERVE C13, 100.5411305 MHz
DECOUPLE H1, 399.8470997 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 hr, 49 min



Plotname: CARBON_cdc13_20130301_400_01_plot01



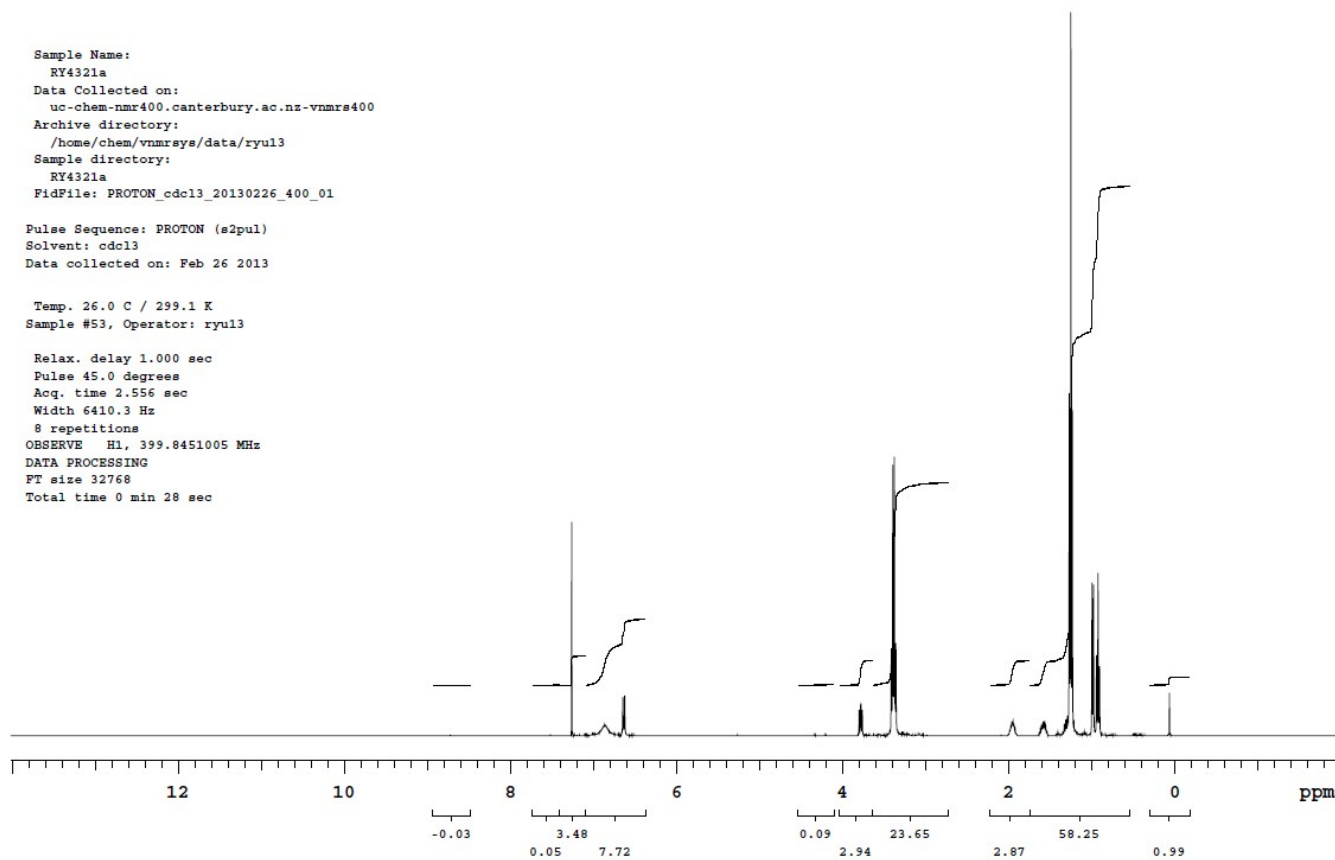
Bis(diethylamino)-S-(1-carboxy-2-methylbutylamino)cyclopropenium bistriflamide, [C₃(NEt₂)₂(NHCOOHC₂H₂(CH₃)CH₂CH₃COOH)]NTf₂, [E₄Ile]NTf₂ (2d)

Sample Name:
RY4321a
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmr400
Archive directory:
/home/chem/vmr400/data/ryul3
Sample directory:
RY4321a
FidFile: PROTON_cdcl3_20130226_400_01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 26 2013

Temp. 26.0 C / 299.1 K
Sample #53, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8451005 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



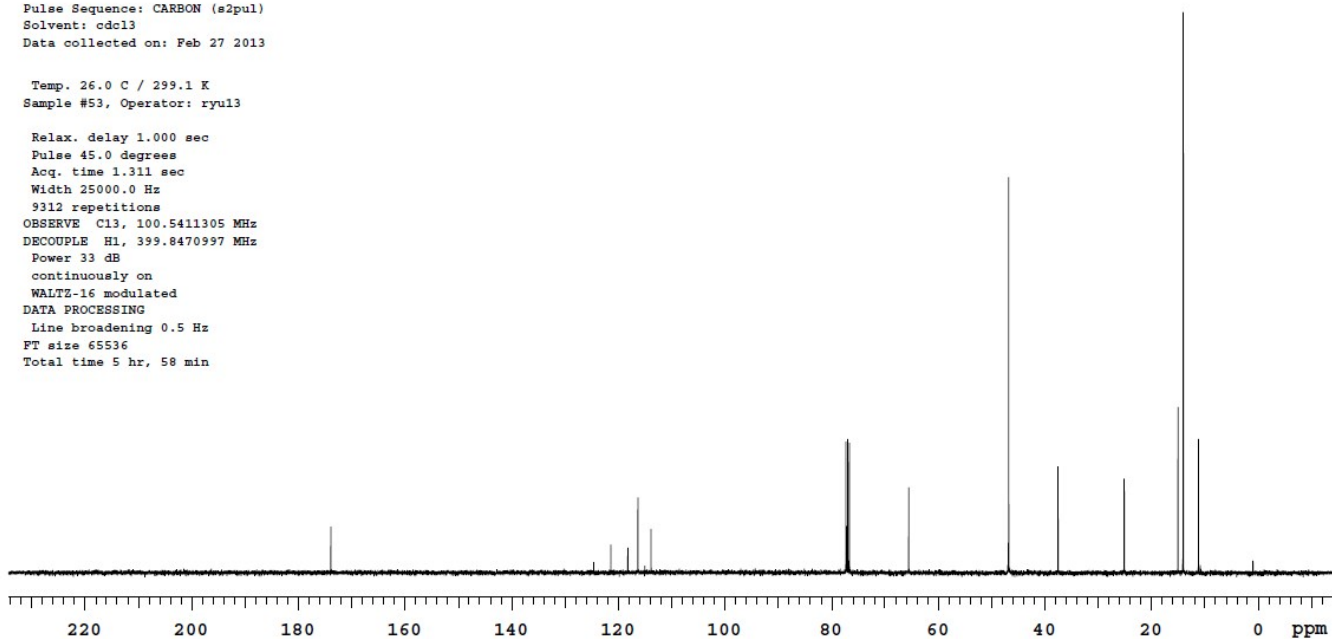
Plotname: PROTON_cdcl3_20130226_400_01_plot01

Sample Name:
RY4321a
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmnrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RY4321a
FidFile: CARBON_cdcl3_20130228_400_01

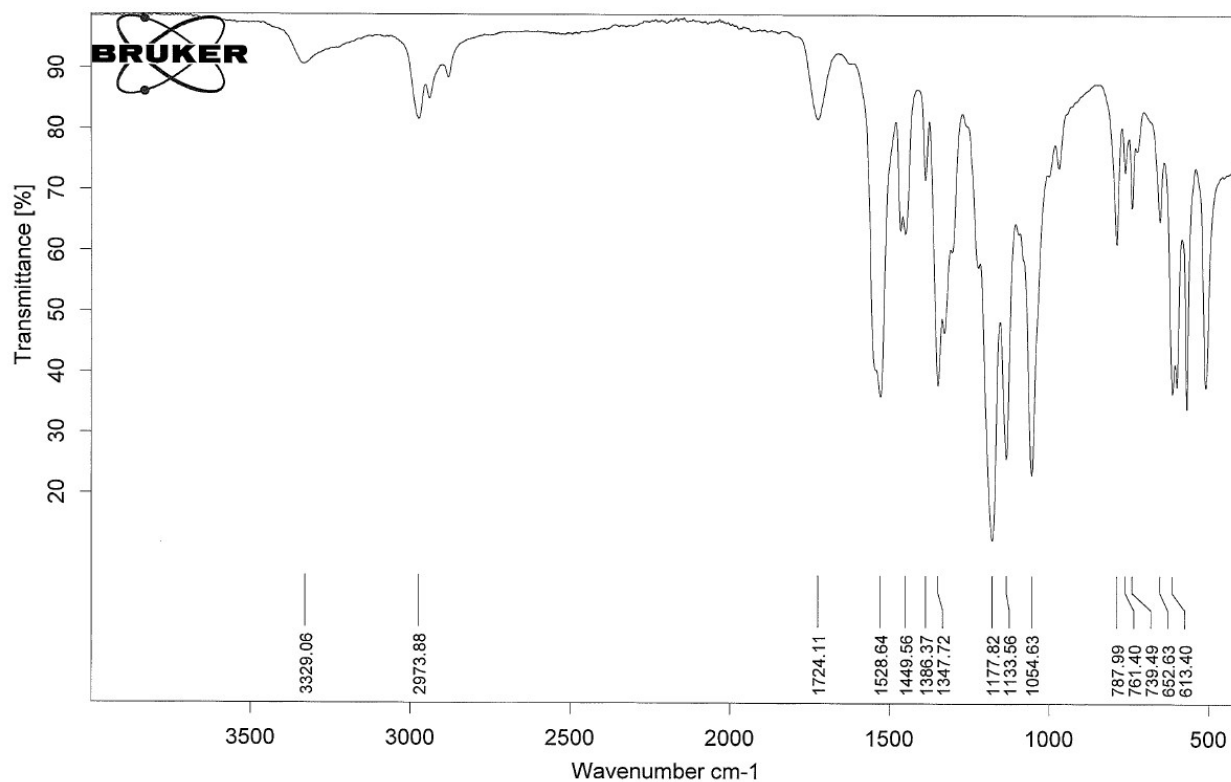
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 27 2013

Temp. 26.0 C / 299.1 K
Sample #53, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
9312 repetitions
OBSERVE C13, 100.5411305 MHz
DECOUPLE H1, 399.8470997 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 58 min



Plotname: CARBON_cdcl3_20130228_400_01_plot01



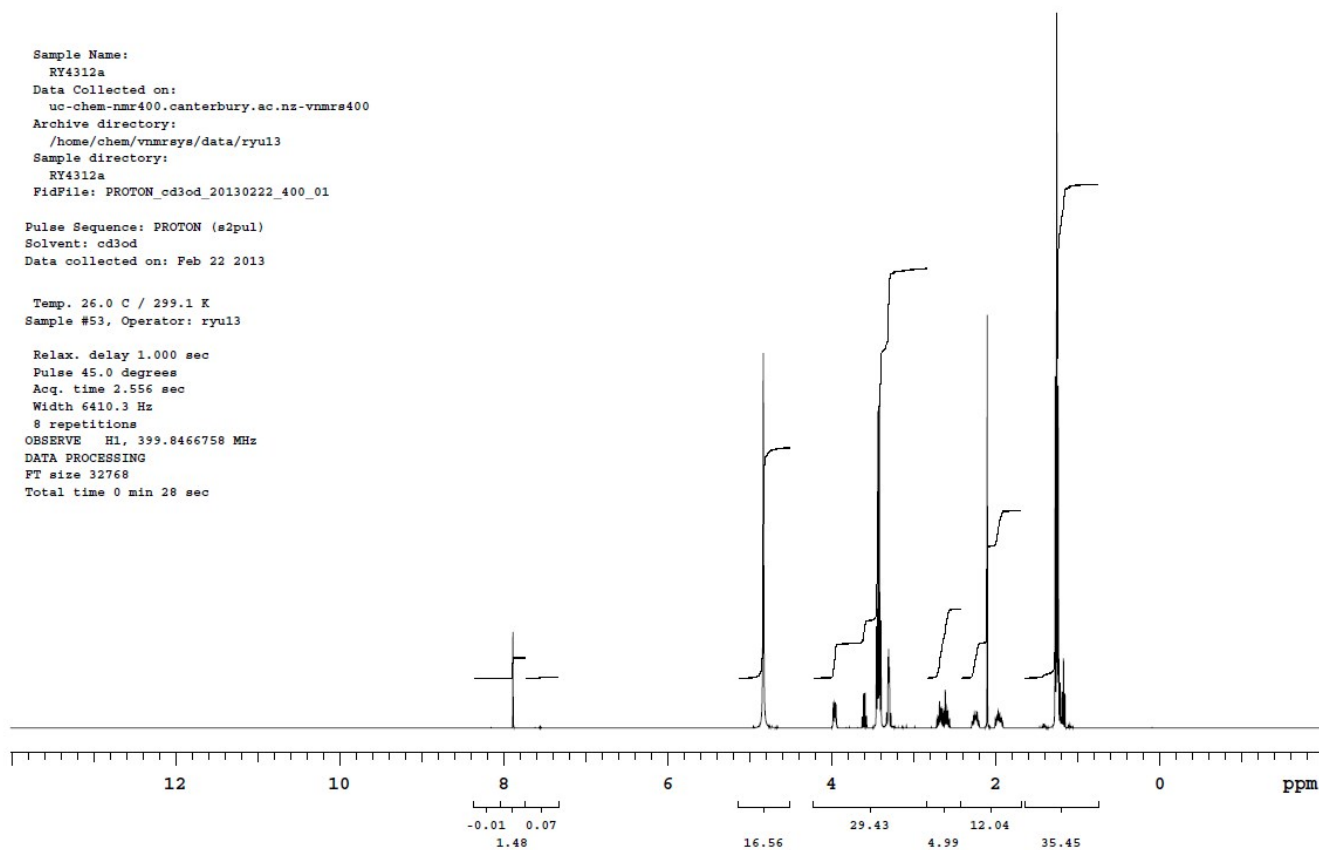
Bis(diethylamino)-S-(1-carboxy-3-methylthiopropylamino)cyclopropenium bistriflamide, [C₃(NEt₂)₂(NHCOOHC₃H₅SCH₃)]NTf₂, [E₄Met]NTf₂ (2e)

Sample Name:
RY4312a
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmrs400
Archive directory:
/home/chem/vmrsys/data/ryul3
Sample directory:
RY4312a
FidFile: PROTON_cd3od_20130222_400_01

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Feb 22 2013

Temp. 26.0 C / 299.1 K
Sample #53, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8466758 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



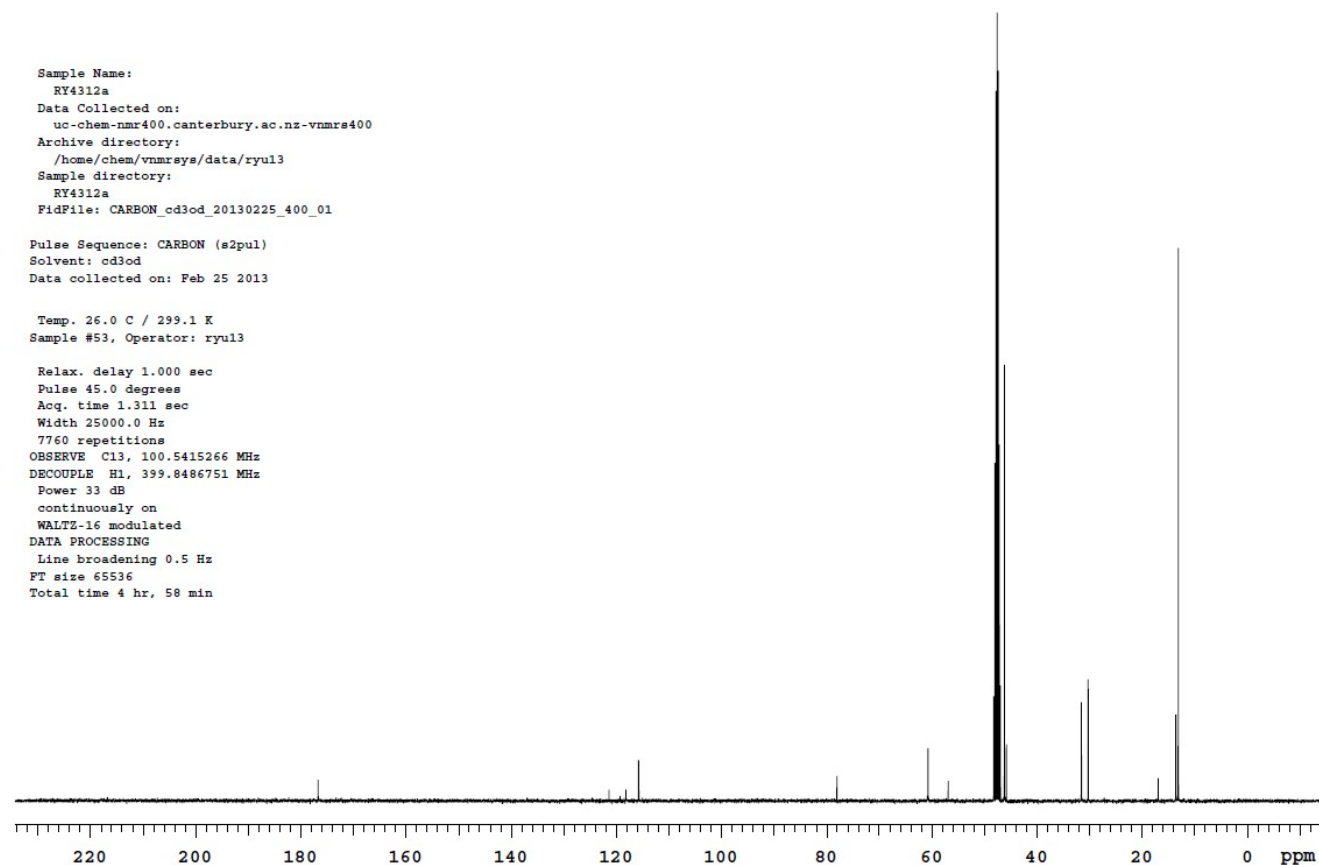
Plotname: PROTON_cd3od_20130222_400_01_plot01

Sample Name:
RY4312a
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmrs400
Archive directory:
/home/chem/vmrsys/data/ryul3
Sample directory:
RY4312a
FidFile: CARBON_cd3od_20130225_400_01

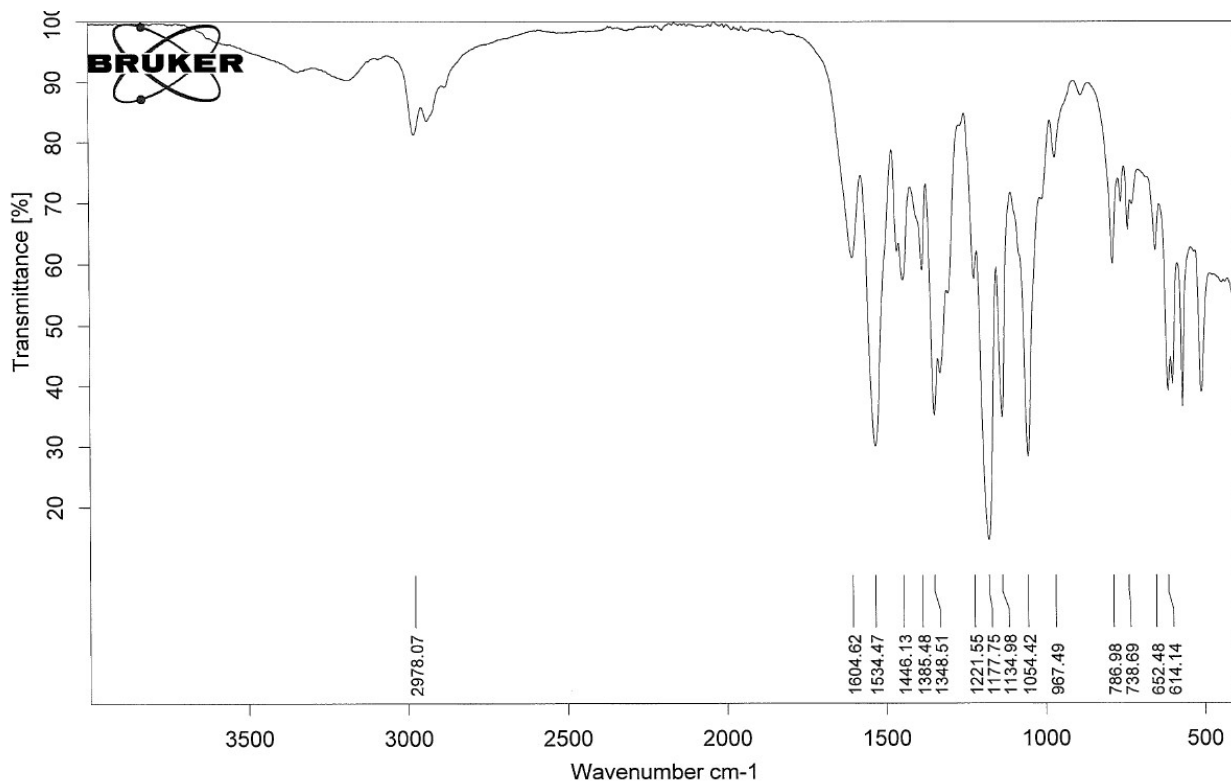
Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Feb 25 2013

Temp. 26.0 C / 299.1 K
Sample #53, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
7760 repetitions
OBSERVE C13, 100.5415266 MHz
DECOUPLE H1, 399.8486751 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 4 hr, 58 min



Plotname: CARBON_cd3od_20130225_400_01_plot01



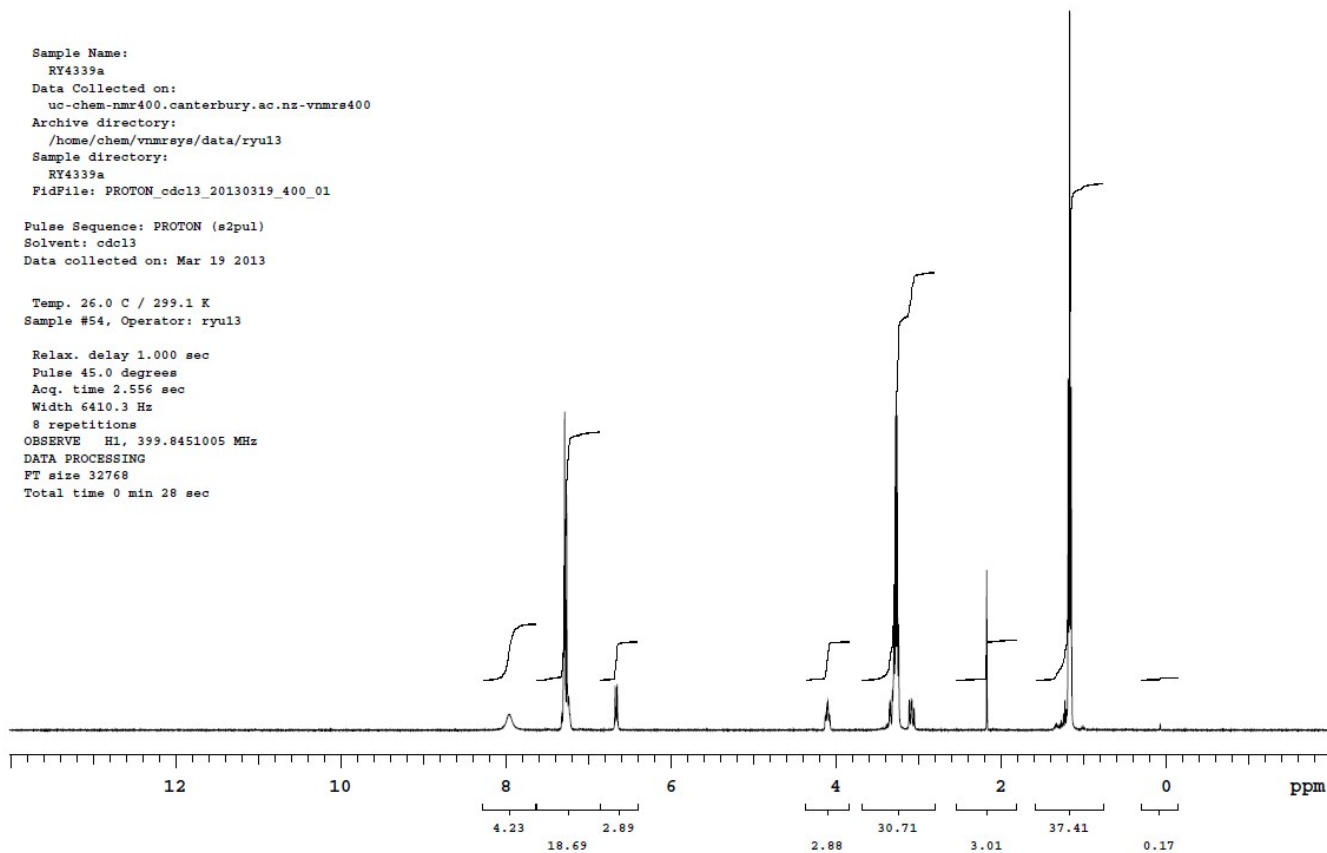
**Bis(diethylamino)-S-(1-carboxy-2-phenylethylamino)cyclopropenium bistriflamide,
[C₃(NEt₂)₂(NHCOHC₂H₃C₆H₅)]NTf₂, [E₄Phe]NTf₂ (2f)**

Sample Name:
RY4339a
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmr400
Archive directory:
/home/chem/vmr400/data/ryul3
Sample directory:
RY4339a
FidFile: PROTON_cdc13_20130319_400_01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 19 2013

Temp. 26.0 C / 299.1 K
Sample #54, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8451005 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



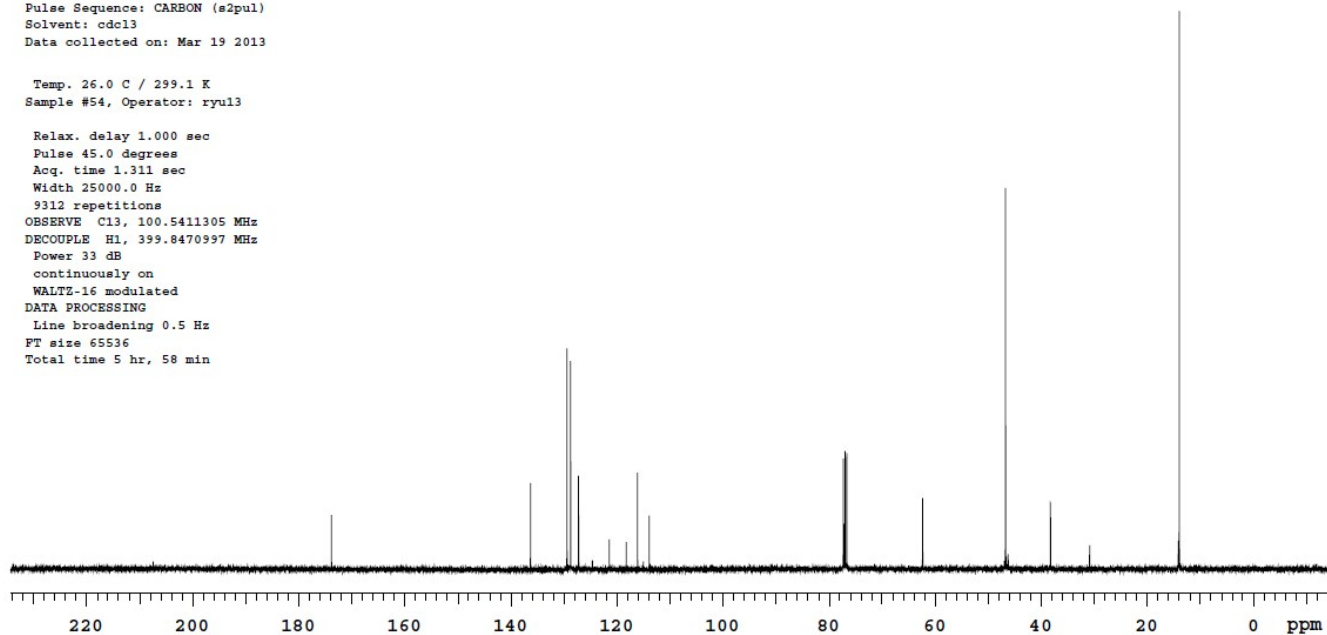
Plotname: PROTON_cdc13_20130319_400_01_plot01

Sample Name:
RY4339a
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmnrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RY4339a
FidFile: CARBON_cdc13_20130320_400_01

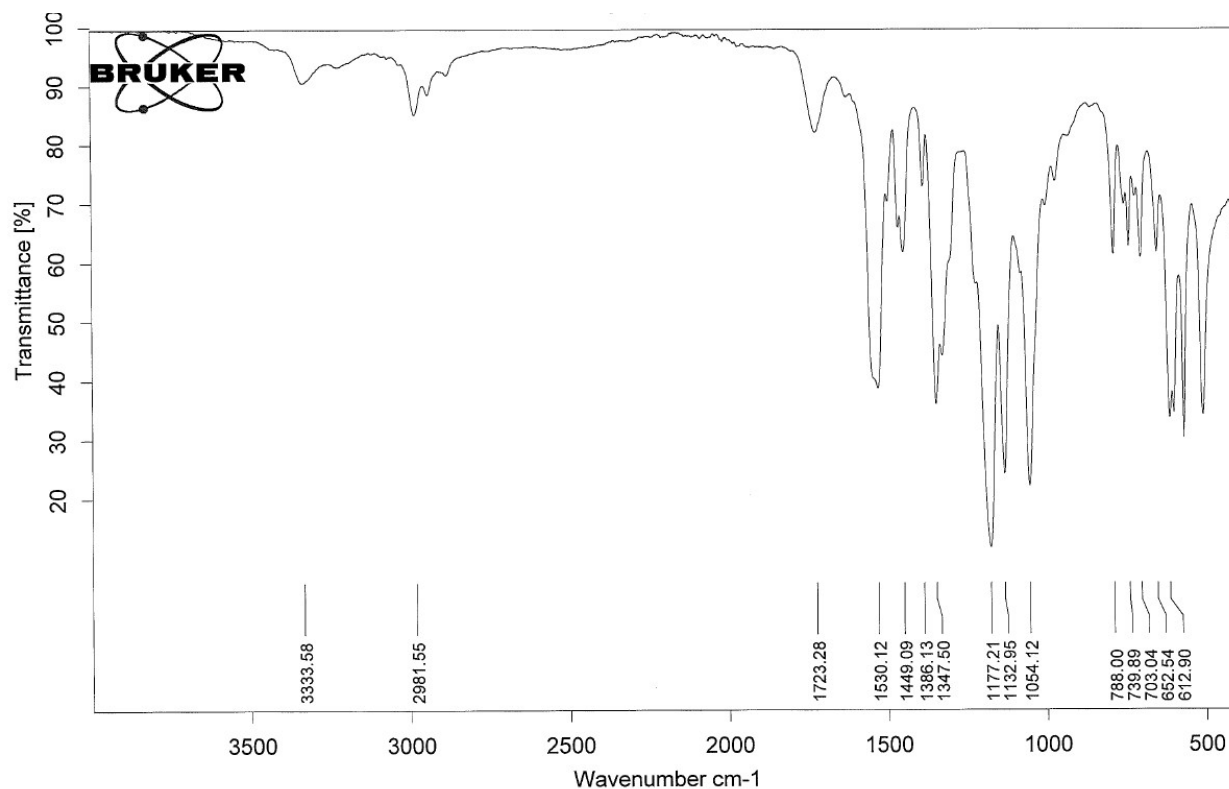
Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Mar 19 2013

Temp. 26.0 C / 299.1 K
Sample #54, Operator: ryul3

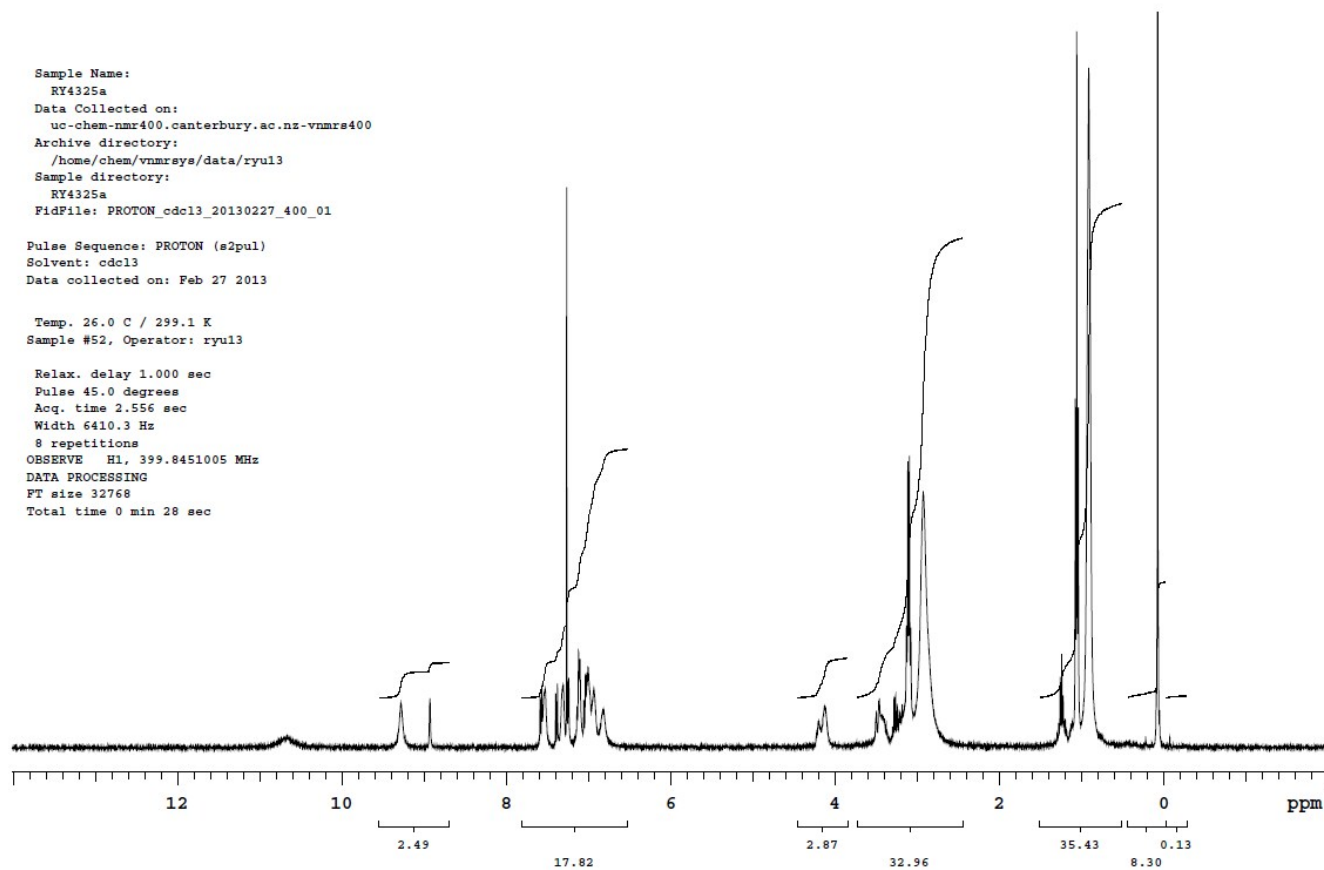
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
9312 repetitions
OBSERVE C13, 100.5411305 MHz
DECOUPLE H1, 399.8470997 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 58 min



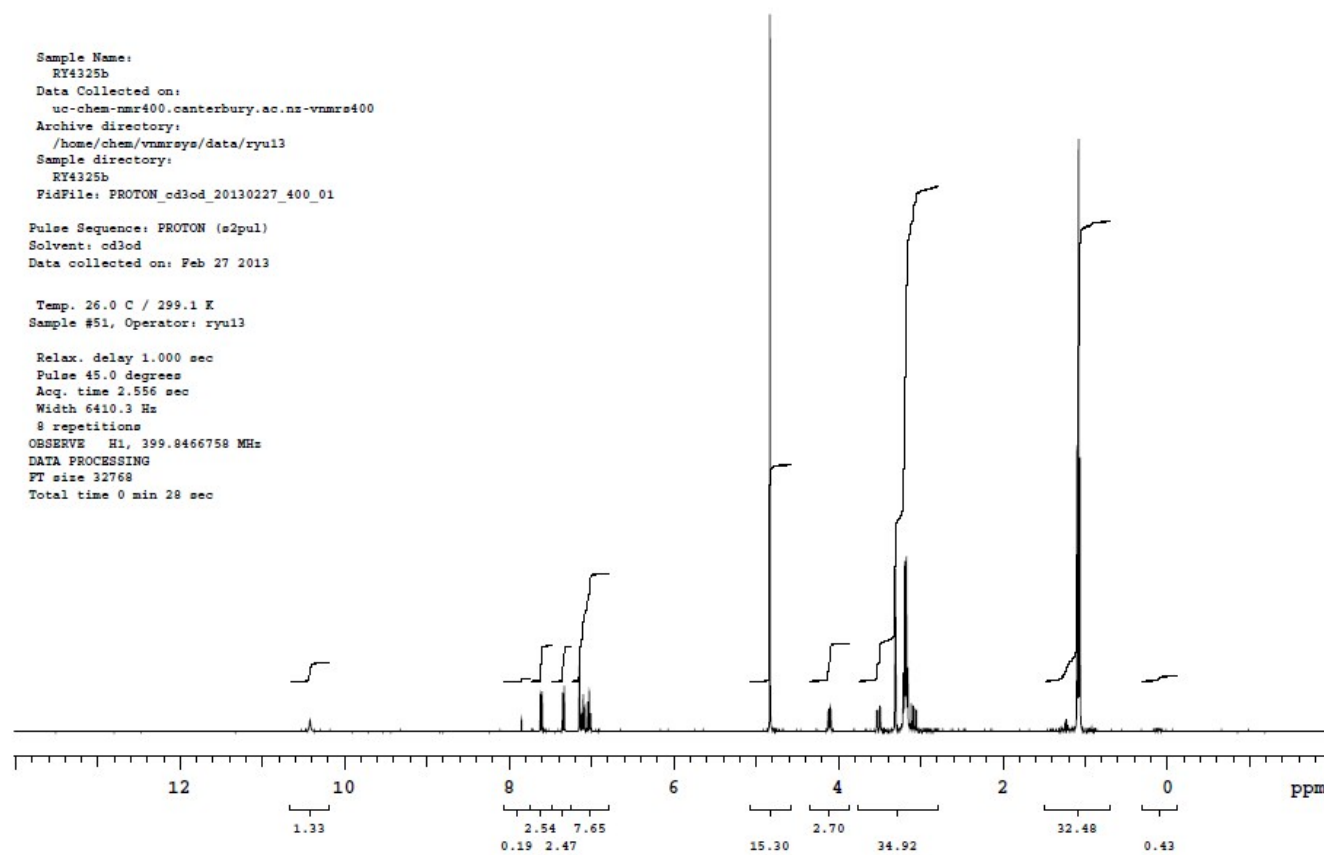
Plotname: CARBON_cdc13_20130320_400_01_plot01



Bis(diethylamino)-S-(1-carboxy-2-(1H-indol-3-yl)ethylamino)cyclopropenium bistriflamide, [C₃(NEt₂)₂(NHCOOHC₂H₃C₈H₆N)]NTf₂, [E₄Try]NTf₂ (2g)



Plotname: PROTON_cdcl3_20130227_400_01_plot01



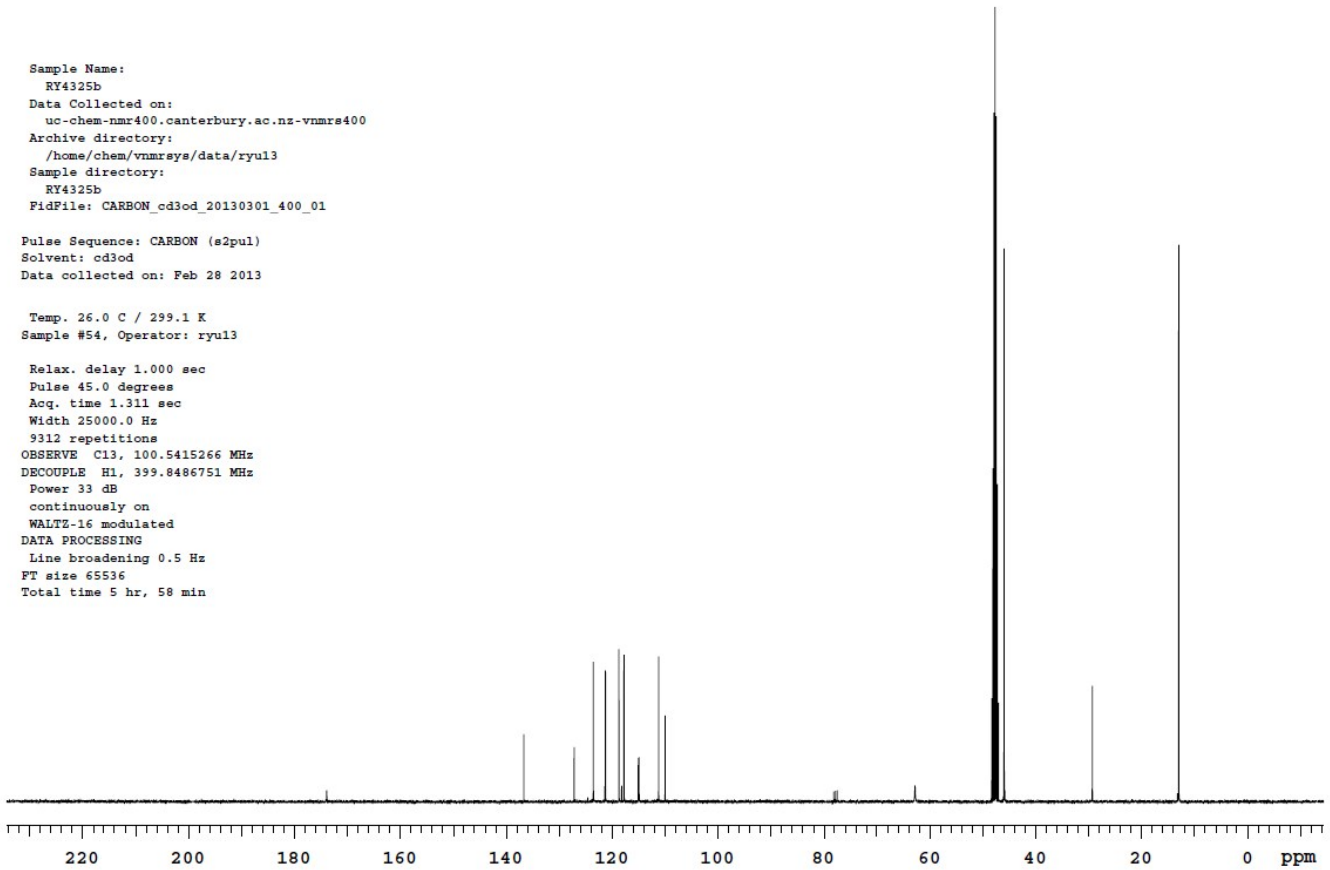
Plotname: PROTON_cd3od_20130227_400_01_plot01

Sample Name:
RY4325b
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmrs400
Archive directory:
/home/chem/vmrsys/data/ryu13
Sample directory:
RY4325b
FidFile: CARBON_cd3od_20130301_400_01

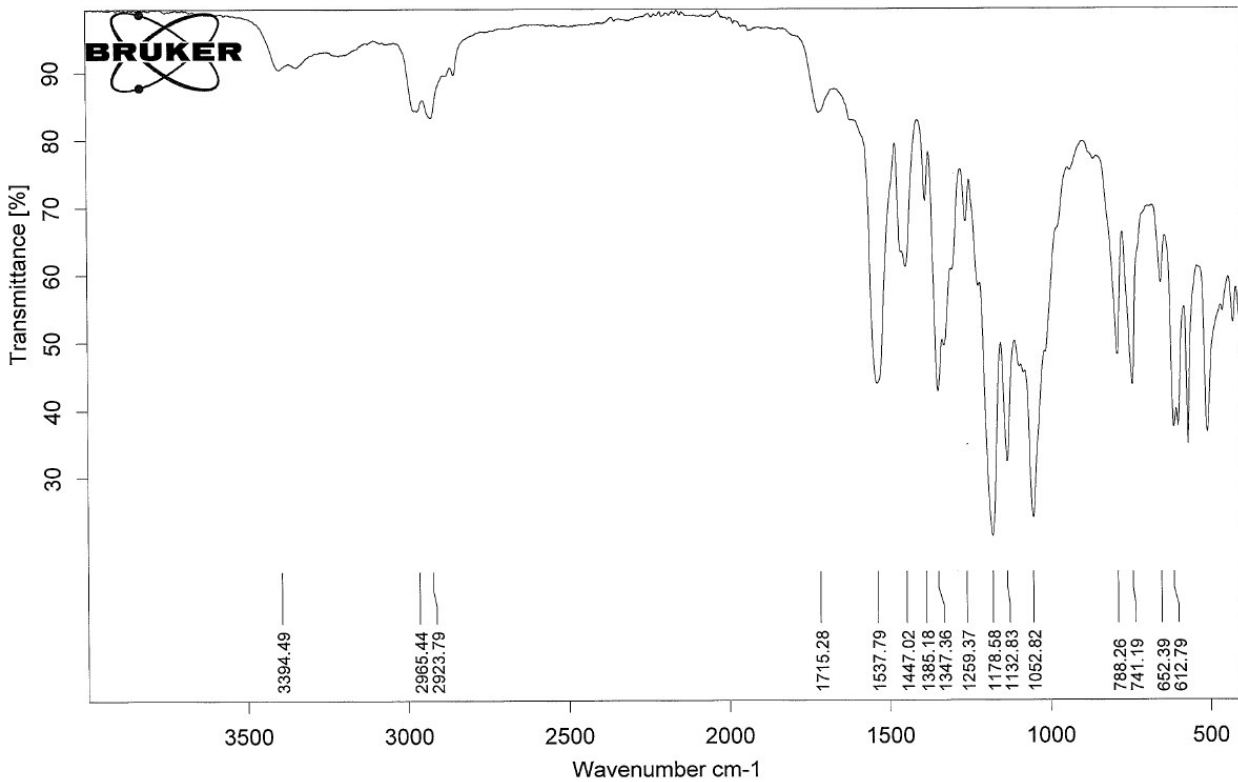
Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Feb 28 2013

Temp. 26.0 C / 299.1 K
Sample #54, Operator: ryu13

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
9312 repetitions
OBSERVE C13, 100.5415266 MHz
DECOUPLE H1, 399.8486751 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 58 min



Plotname: CARBON_cd3od_20130301_400_01_plot01



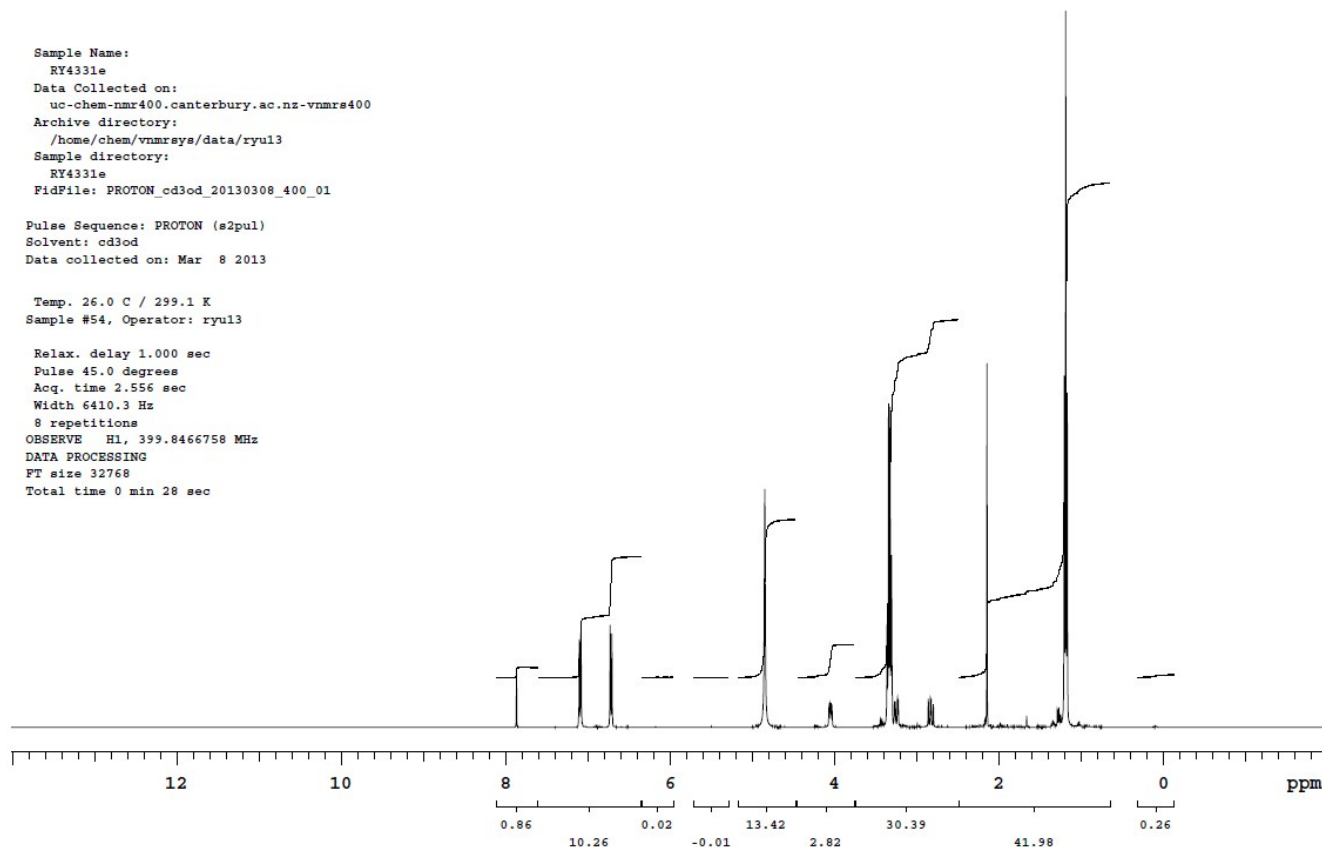
Bis(diethylamino)-S-(1-carboxy-2-hydroxyphenylethylamino)cyclopropenium bistriflamide, [C₃(NEt₂)₂(NHCOOHC₂H₃C₆H₅O)]NTf₂, [E₄Tyr]NTf₂ (2h)

Sample Name:
RY4331e
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmr400
Archive directory:
/home/chem/vmr400/data/ryul3
Sample directory:
RY4331e
FidFile: PROTON_cd3od_20130308_400_01

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Mar 8 2013

Temp. 26.0 C / 299.1 K
Sample #54, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8466758 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



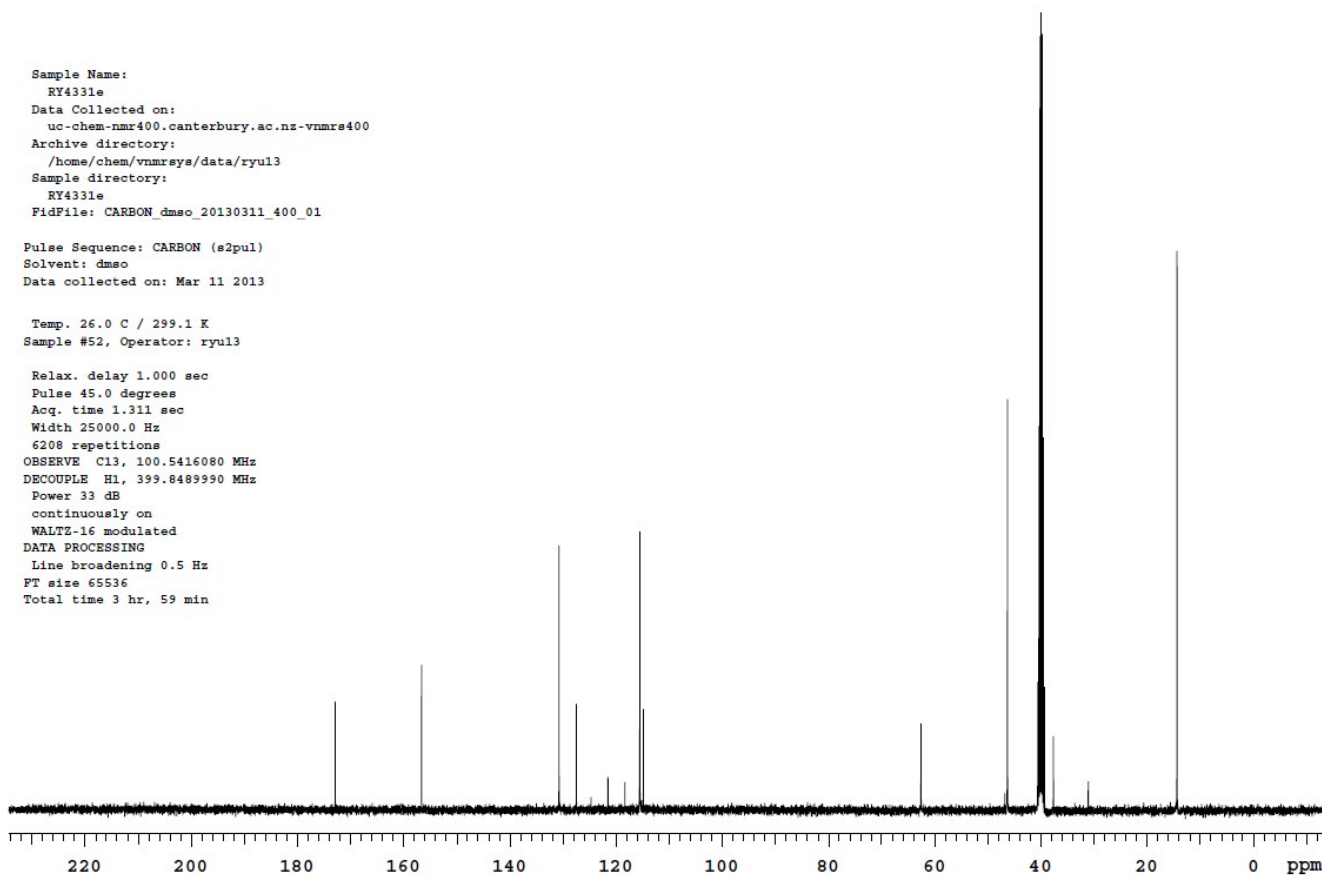
Plotname: PROTON_cd3od_20130308_400_01_plot01

Sample Name:
RY4331e
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmr400
Archive directory:
/home/chem/vmr400/data/ryul3
Sample directory:
RY4331e
FidFile: CARBON_dms0_20130311_400_01

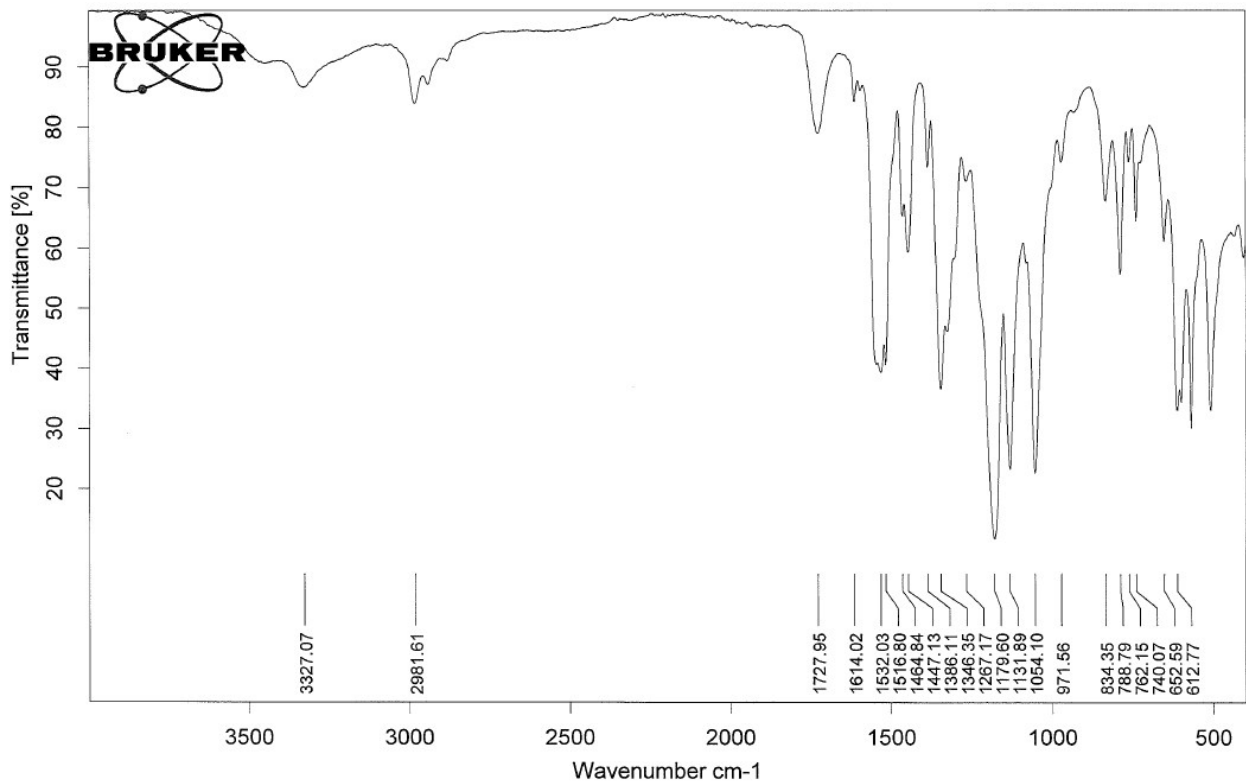
Pulse Sequence: CARBON (s2pul)
Solvent: dms0
Data collected on: Mar 11 2013

Temp. 26.0 C / 299.1 K
Sample #52, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
6208 repetitions
OBSERVE C13, 100.5416080 MHz
DECOUPLE H1, 399.8489990 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 hr, 59 min



Plotname: CARBON_dms0_20130311_400_01_plot01



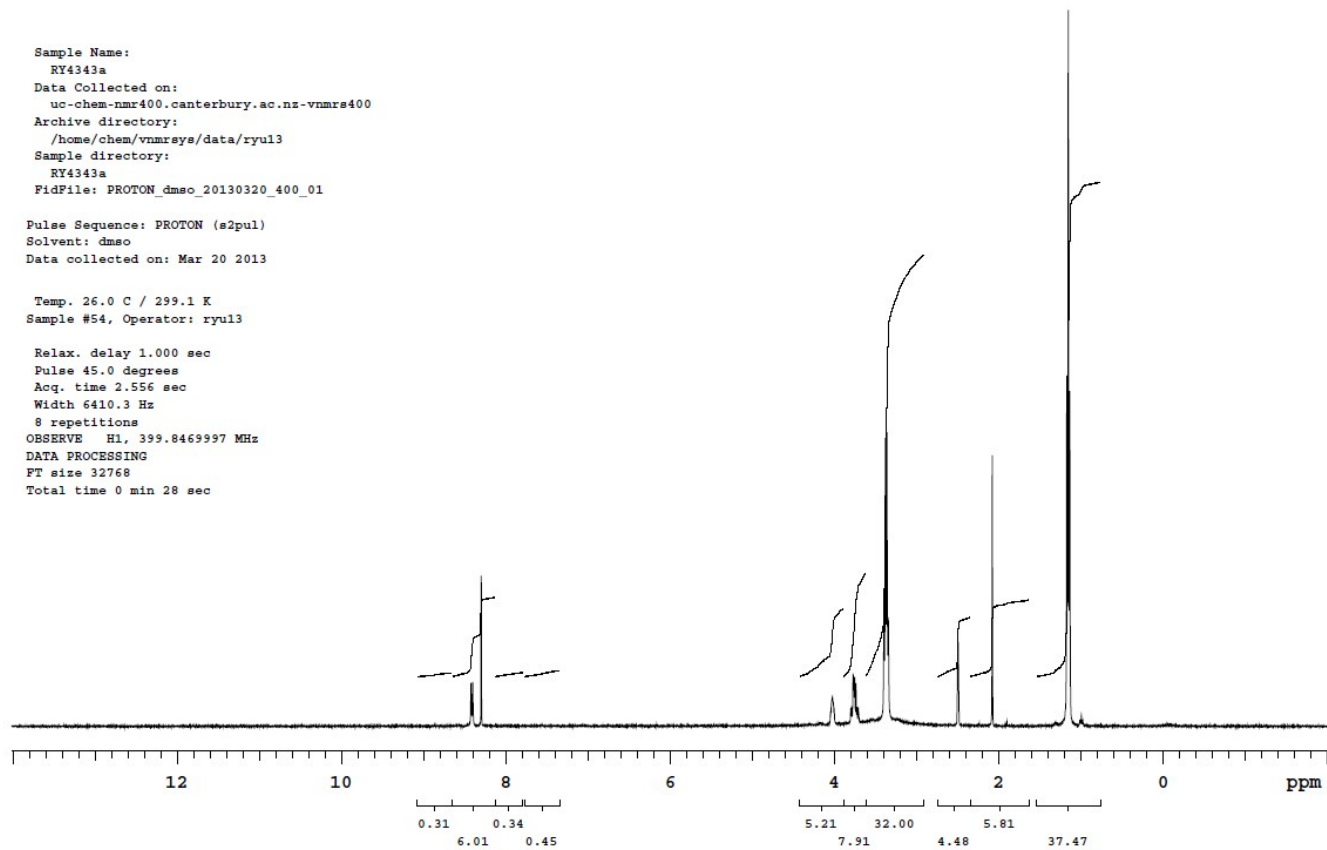
**Bis(diethylamino)-S-(1-carboxy-2-hydroxyethylamino)cyclopropenium bistriflamide,
[C₃(NEt₂)₂(NHCOHC₂H₃CH₂OH)]NTf₂, [E₄Ser]NTf₂ (2i)**

Sample Name:
RY4343a
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vnmrs400
Archive directory:
/home/chem/vnmrsys/data/ryu13
Sample directory:
RY4343a
FidFile: PROTON_dmsc_20130320_400_01

Pulse Sequence: PROTON (s2pul)
Solvent: dmsc
Data collected on: Mar 20 2013

Temp. 26.0 C / 299.1 K
Sample #54, Operator: ryu13

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8469997 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



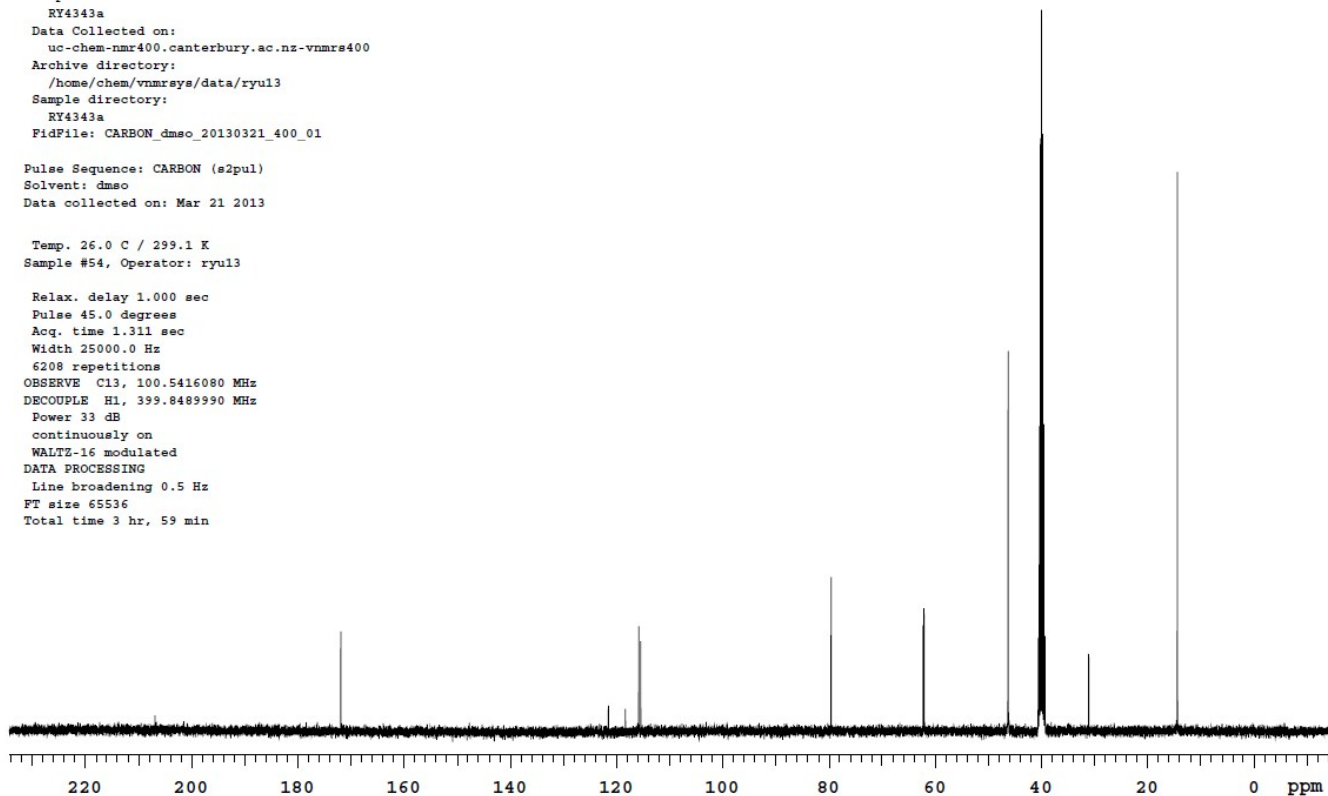
Plotname: PROTON_dmsc_20130320_400_01_plot01

Sample Name:
RY4343a
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmr400
Archive directory:
/home/chem/vmr400/data/ryul3
Sample directory:
RY4343a
FidFile: CARBON_dms0_20130321_400_01

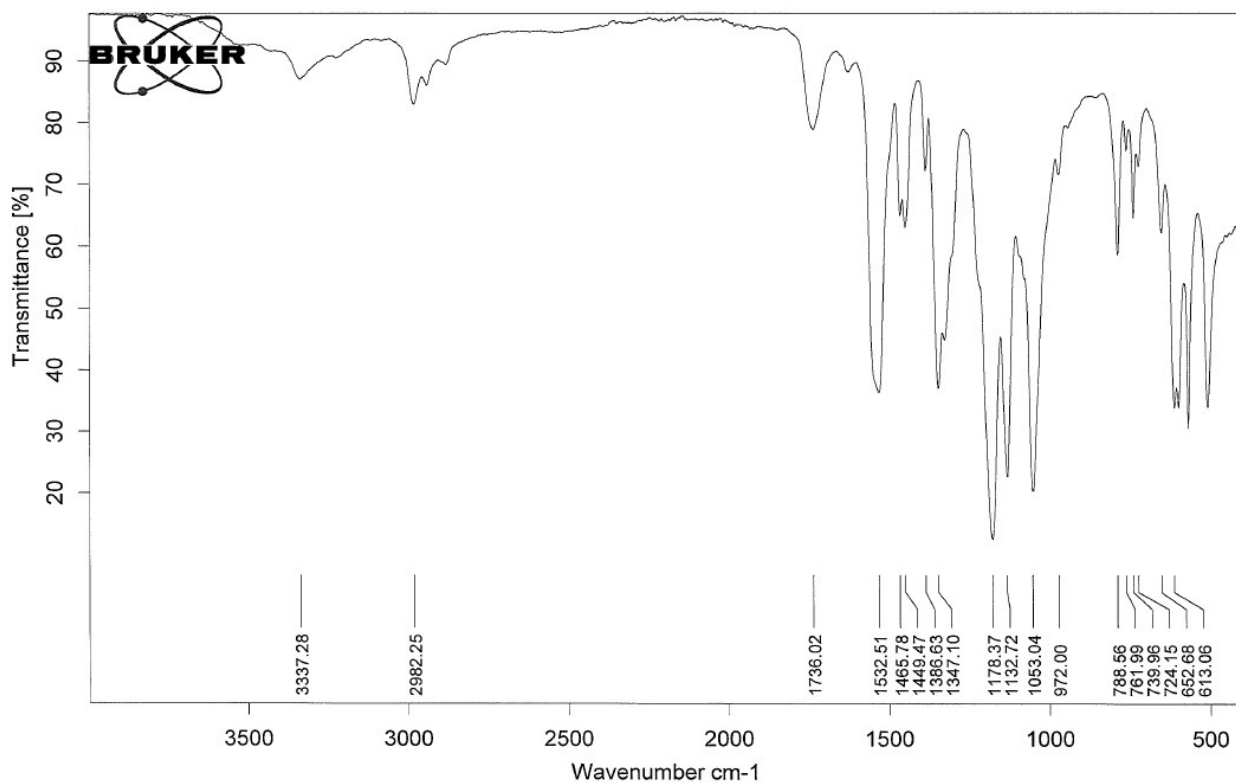
Pulse Sequence: CARBON (s2pul)
Solvent: dms0
Data collected on: Mar 21 2013

Temp. 26.0 C / 299.1 K
Sample #54, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
6208 repetitions
OBSERVE C13, 100.5416080 MHz
DECOUPLE H1, 399.8489990 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 hr, 59 min

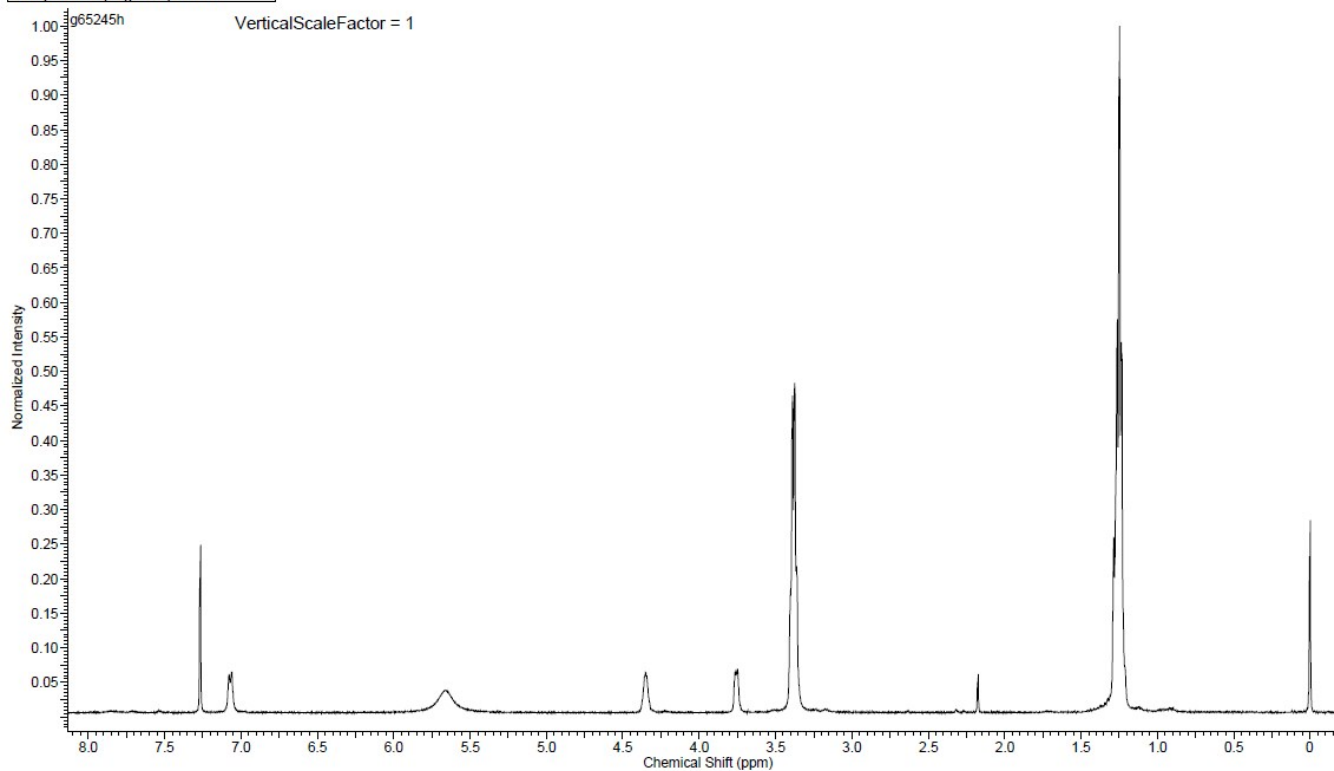


Plotname: CARBON_dms0_20130321_400_01_plot01

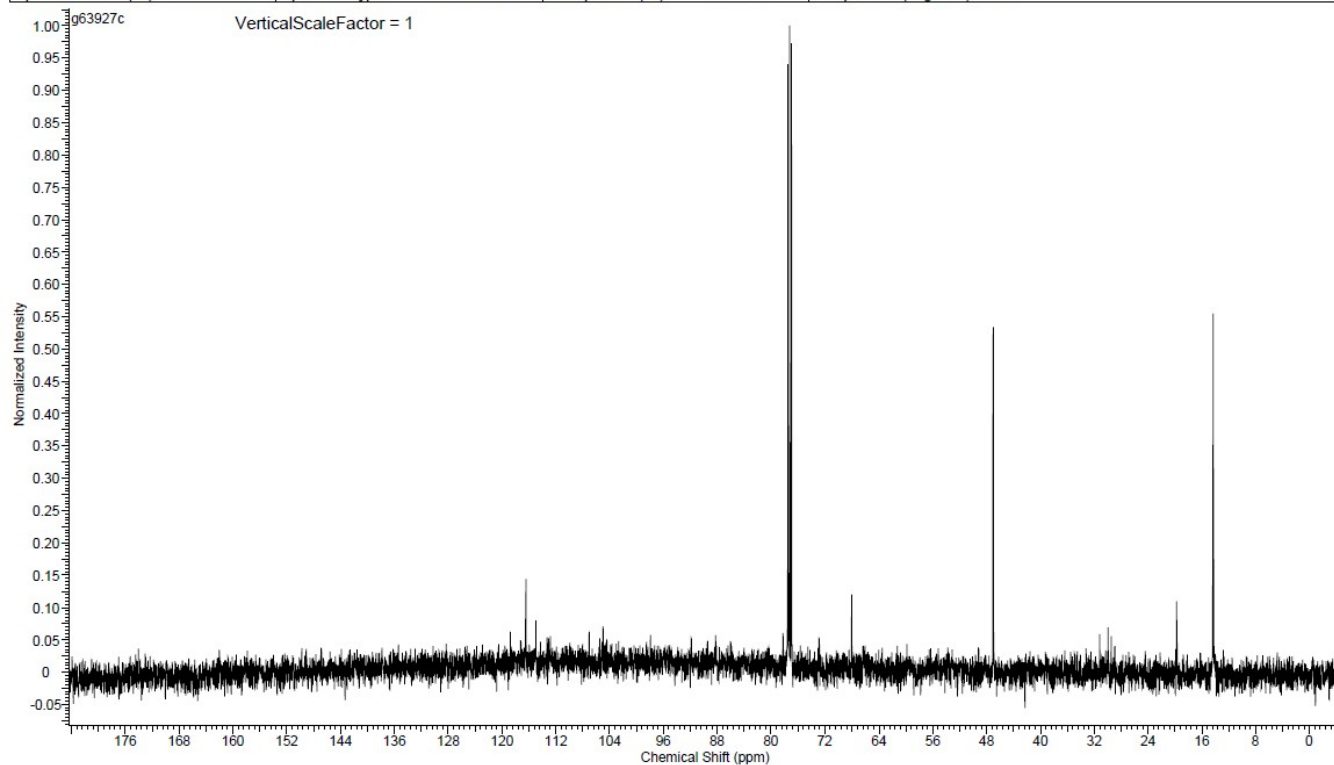


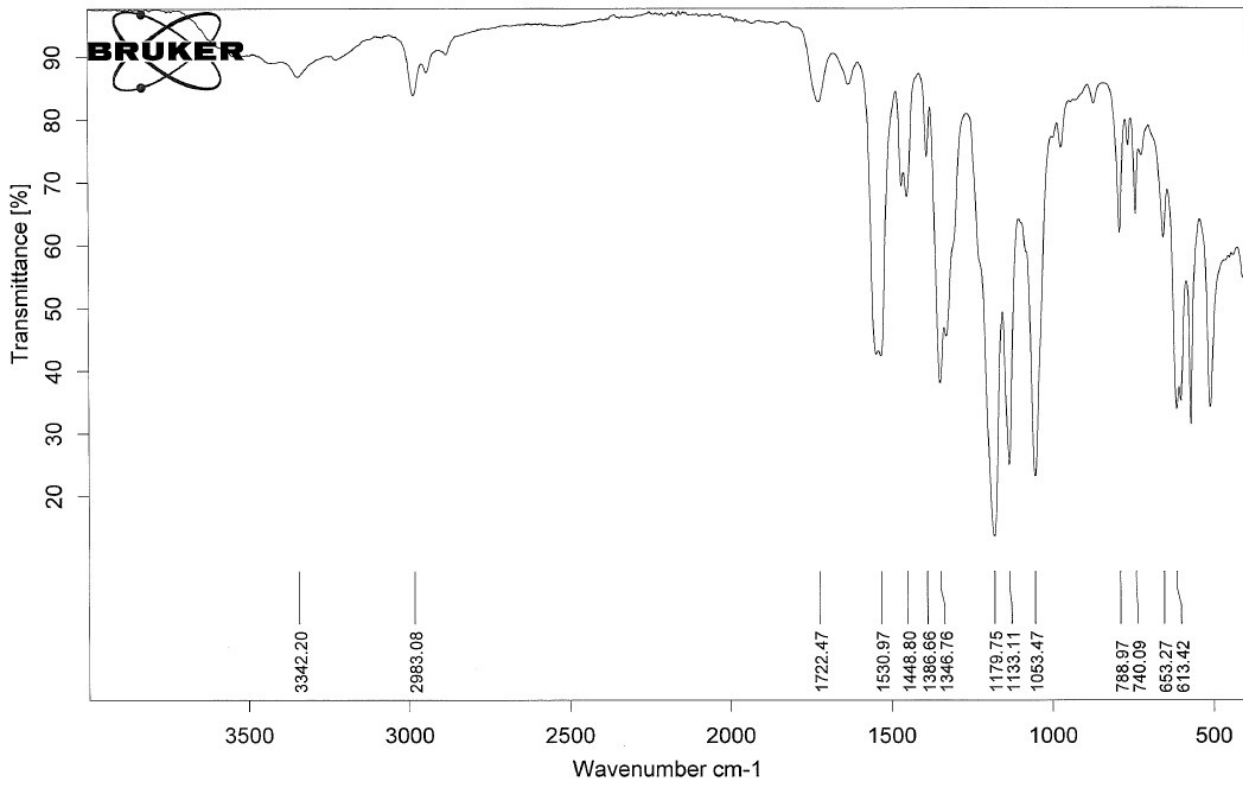
Bis(diethylamino)-S-(1-carboxy-2-hydroxypropylamino)cyclopropenium bistriflamide, [C₃(NEt₂)₂(NH(C₃H₆COOH))]NTf₂, [E₄Thr]NTf₂ (2j)

Acquisition Time (sec)	1.8920	Comment	ry-01-87-69a [E4th]TFSA	Date	Sep 1 2011	Date Stamp	Sep 1 2011
File Name	\file\UsersO:\ojc10\Home\My Documents\AAIL_paper\g65245h.fid\fid			Frequency (MHz)	499.68	Nucleus	1H
Number of Transients	8	Original Points Count	11370	Points Count	16384	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2498.3643	Spectrum Type	STANDARD	Receiver Gain	34.00
Temperature (degree C)	23.000					Sweep Width (Hz)	6009.62



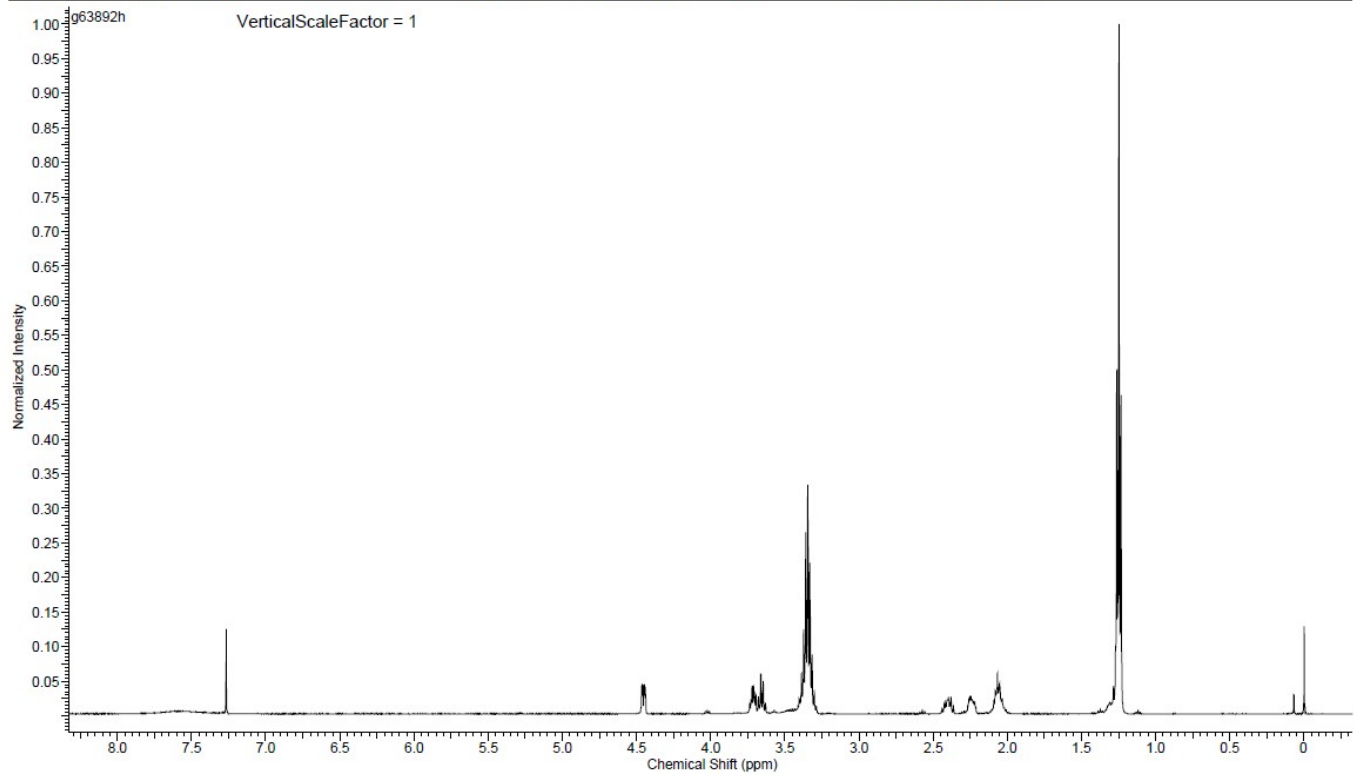
Acquisition Time (sec)	1.3005	Comment	ry-01-63-08 [E]TFSA	Date	Oct 6 2011
Date Stamp	Oct 6 2011	File Name	\file\UsersO:\ojc10\Home\My Documents\AAIL_paper\g63927c.fid\fid		
Frequency (MHz)	125.66	Nucleus	13C	Number of Transients	2984
Points Count	65536	Pulse Sequence	s2pul	Receiver Gain	30.00
Spectrum Offset (Hz)	13192.7188	Spectrum Type	STANDARD	Sweep Width (Hz)	30487.80
		Temperature (degree C)	23.000		



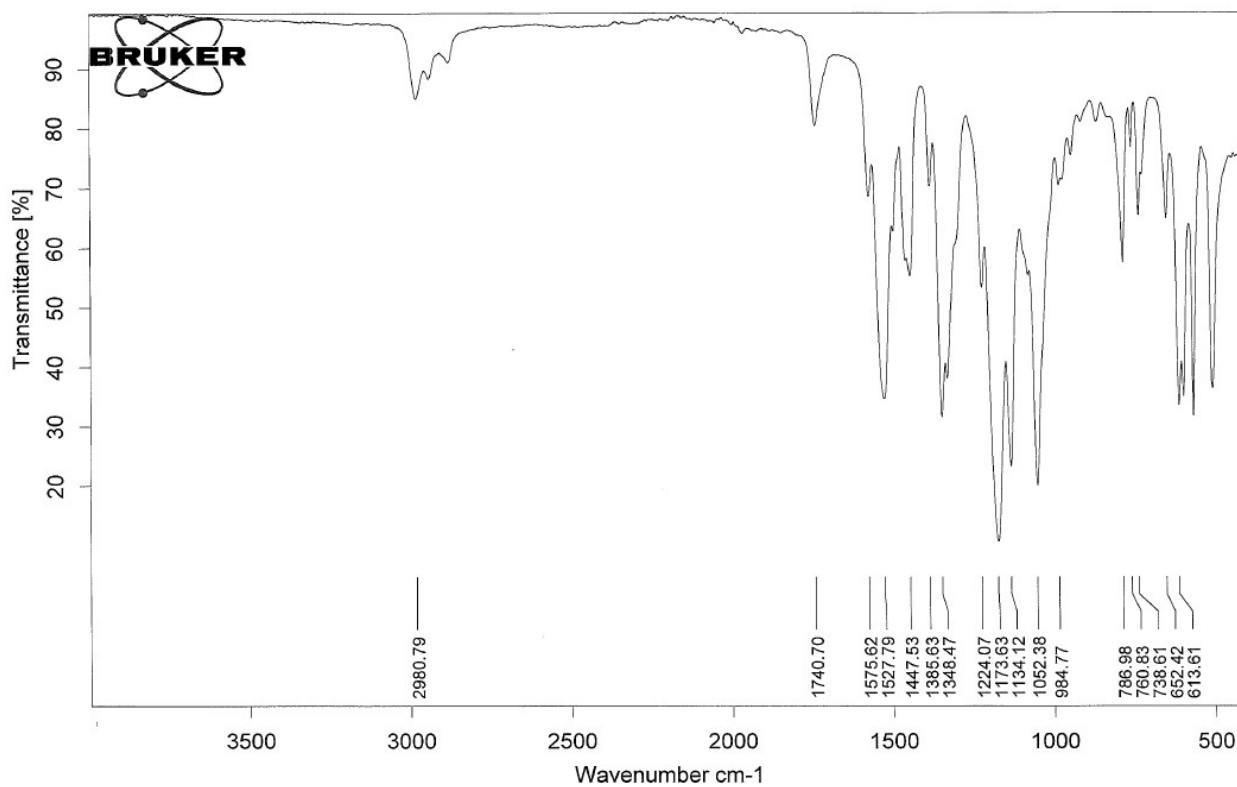
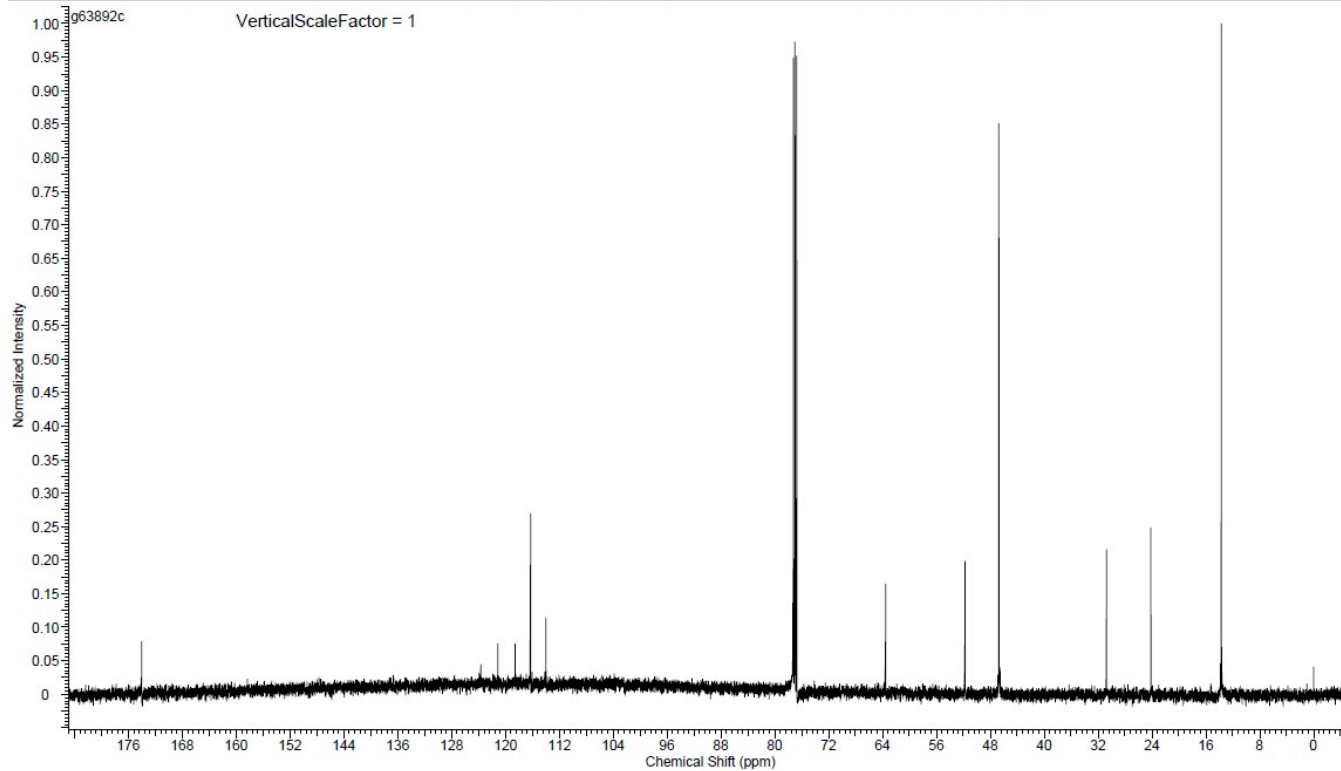


Bis(diethylamino)-S-(2-carboxypyrrolidino)cyclopropenium bistriflamide, $[C_3(NEt_2)_2(N(C_4H_7COOH))]NTf_2$, $[E_4Pro]NTf_2$ (2k)

Acquisition Time (sec)	1.8920	Comment	ry-01-61-02b [E4pro]TFSA two water wash	Date	Jun 2 2011
Date Stamp	Jun 2 2011	File Name	\\file\Users\O...o\c10\Home\My Documents\AAIL paper\g63892h.fid\fid		
Frequency (MHz)	499.68	Nucleus	1H	Number of Transients	8
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	30.00
Spectrum Offset (Hz)	2498.3643	Spectrum Type	STANDARD	Sweep Width (Hz)	6009.62
				Solvent	CHLOROFORM-d
				Temperature (degree C)	23.000



Acquisition Time (sec)	1.3005	Comment	rv-01-61-02b [E4pro]ITFSA	Date	Jun 2 2011
Date Stamp	Jun 2 2011	File Name	\\file\Users\O...ojc10\Home\My Documents\AAIL paper\g63892c.fid\fid		
Frequency (MHz)	125.66	Nucleus	13C	Number of Transients	23772
Points Count	65536	Pulse Sequence	s2pul	Receiver Gain	30.00
Spectrum Offset (Hz)	13160.3525	Spectrum Type	STANDARD	Sweep Width (Hz)	30487.80
				Temperature (degree C)	23.000



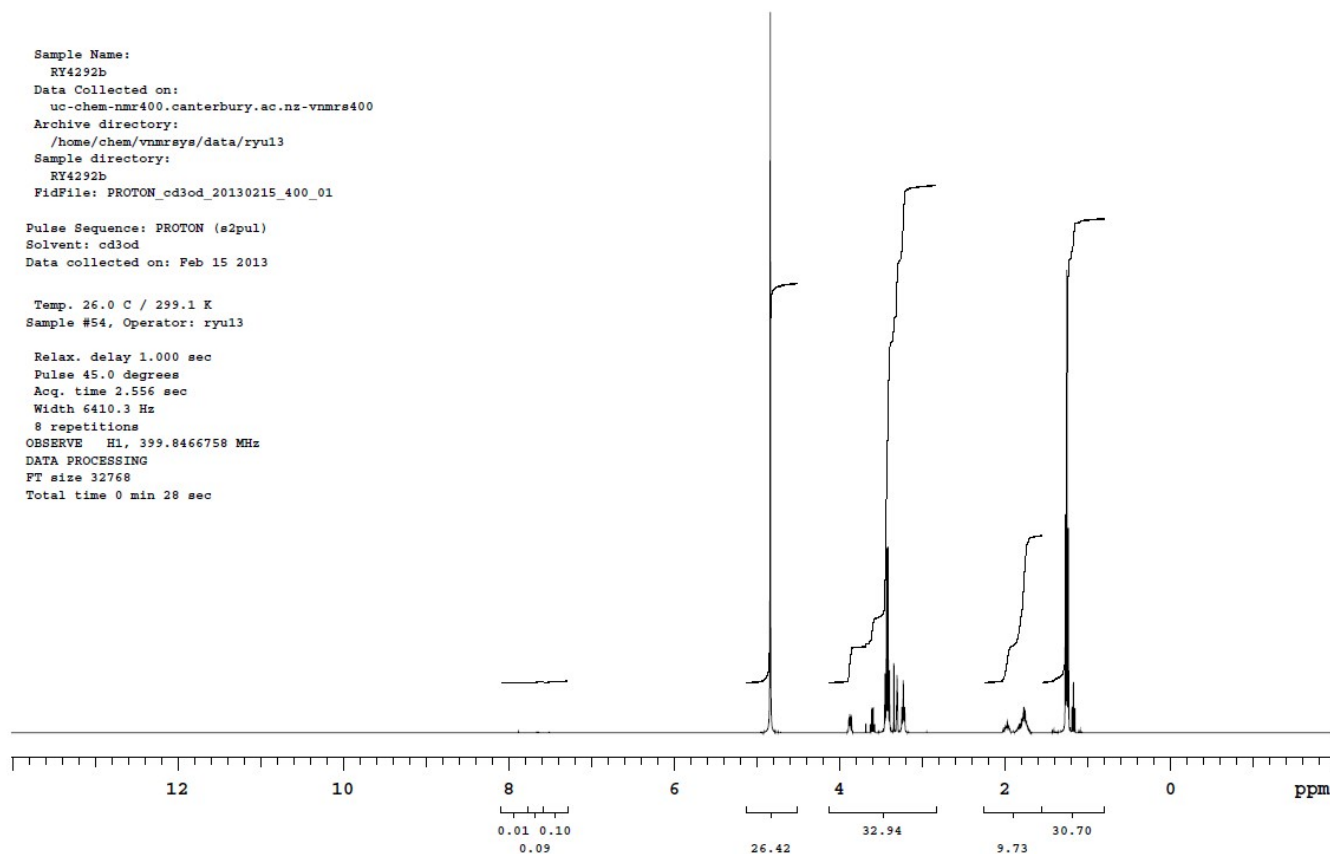
Bis(diethylamino)-S-(1-carboxy-4-guanidiniumbutylamino)cyclopropenium bistriflamide, [C₃(NEt₂)₂(NH(COOH)(C₅H₁₂N₃))][NTf₂]₂ [E₄ArgH][NTf₂]₂ (2l)

Sample Name:
RY4292b
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vnmrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RY4292b
FidFile: PROTON_cd3od_20130215_400_01

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Feb 15 2013

Temp. 26.0 C / 299.1 K
Sample #54, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8466758 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



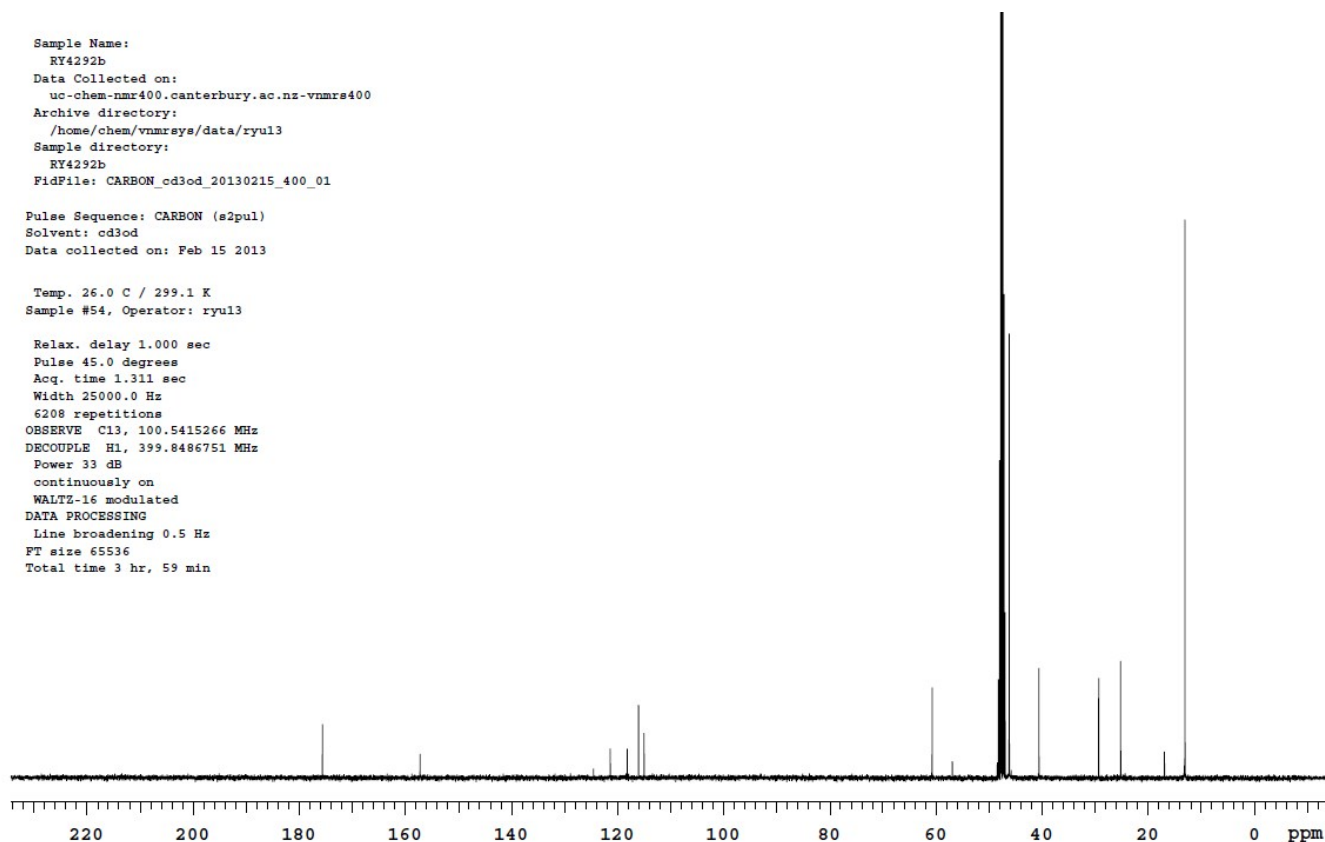
Plotname: PROTON_cd3od_20130215_400_01_plot01

Sample Name:
RY4292b
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vnmrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RY4292b
FidFile: CARBON_cd3od_20130215_400_01

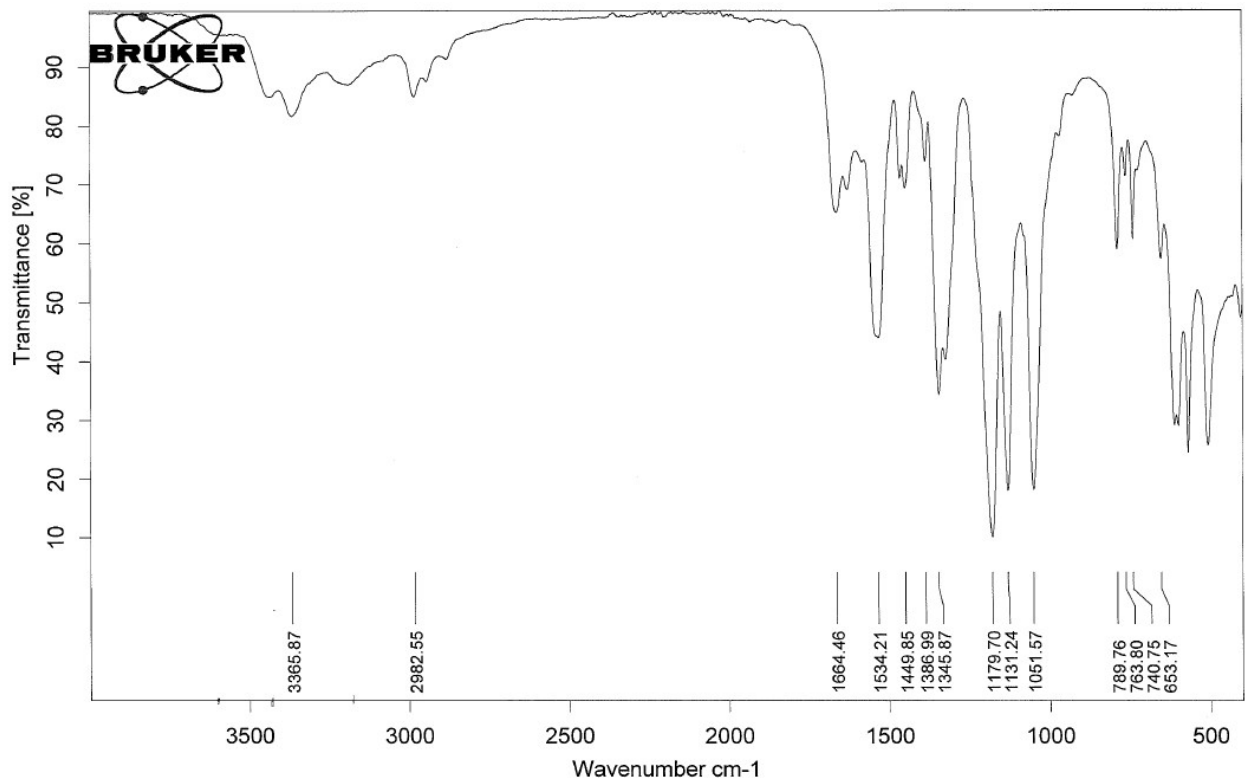
Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Feb 15 2013

Temp. 26.0 C / 299.1 K
Sample #54, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
6208 repetitions
OBSERVE C13, 100.5415266 MHz
DECOUPLE H1, 399.8486751 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 hr, 59 min



Plotname: CARBON_cd3od_20130215_400_01_plot01



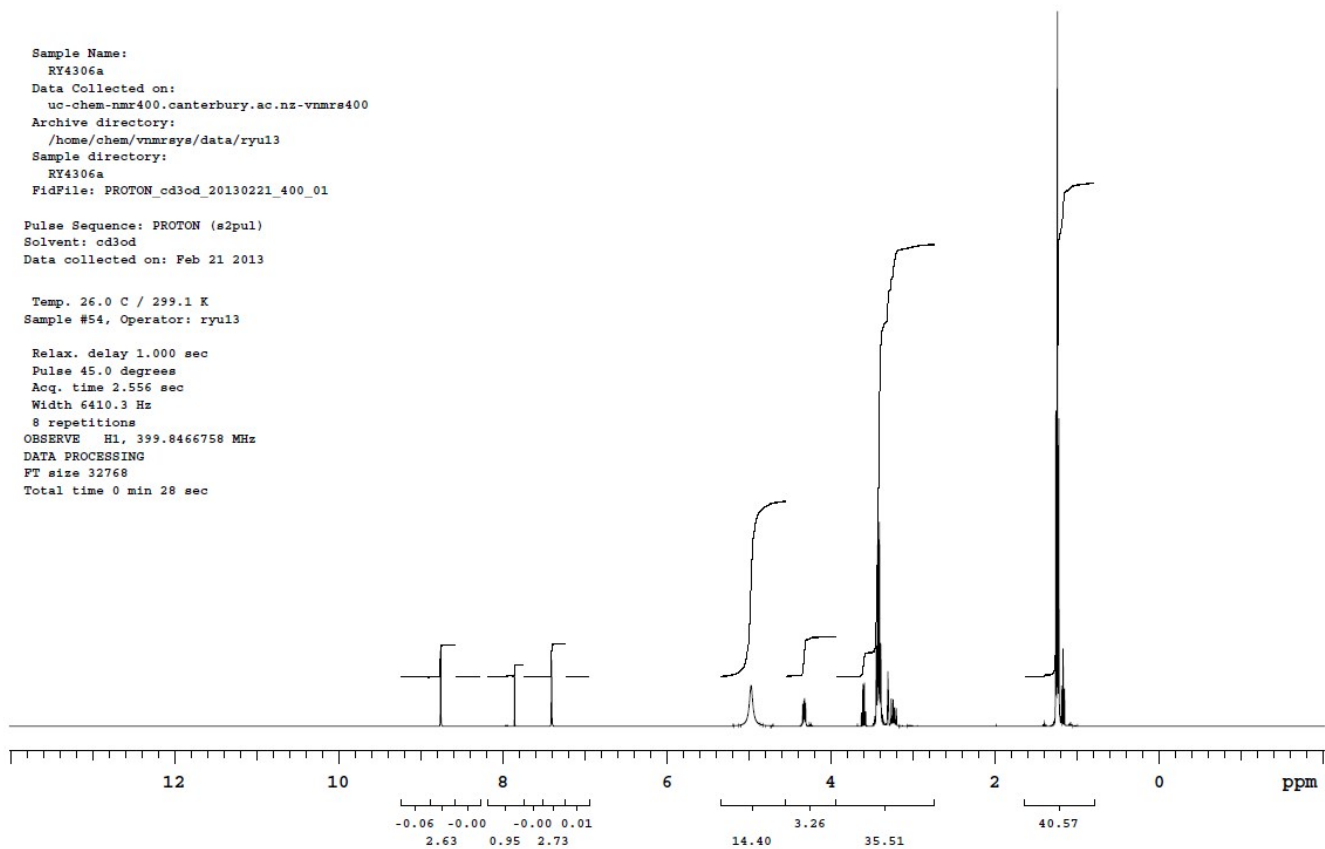
Bis(diethylamino)-S-(1-carboxy-2-imidazoliummethylamino)cyclopropenium bistriflamide, [C₃(NEt₂)₂(NH(COOH)C₂H₃C₃N₂H₄)]⁺[NTf₂]₂⁻, [E₄HisH]⁺[NTf₂]₂⁻ (2m)

Sample Name:
RY4306a
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vnmrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RY4306a
FidFile: PROTON_cd3od_20130221_400_01

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Feb 21 2013

Temp. 26.0 C / 299.1 K
Sample #54, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8466758 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



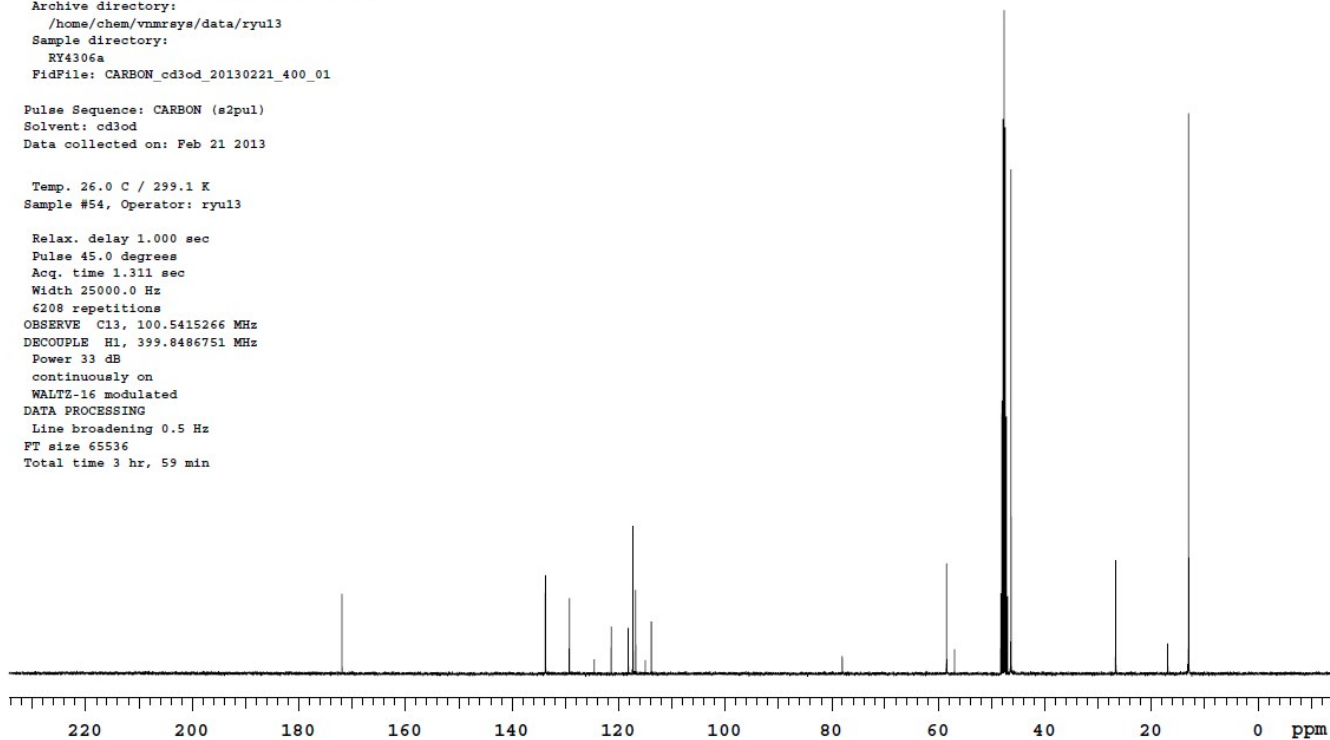
Plotname: PROTON_cd3od_20130221_400_01_plot01

Sample Name:
RY4306a
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmrs400
Archive directory:
/home/chem/vmrsys/data/ryul3
Sample directory:
RY4306a
FidFile: CARBON_cd3od_20130221_400_01

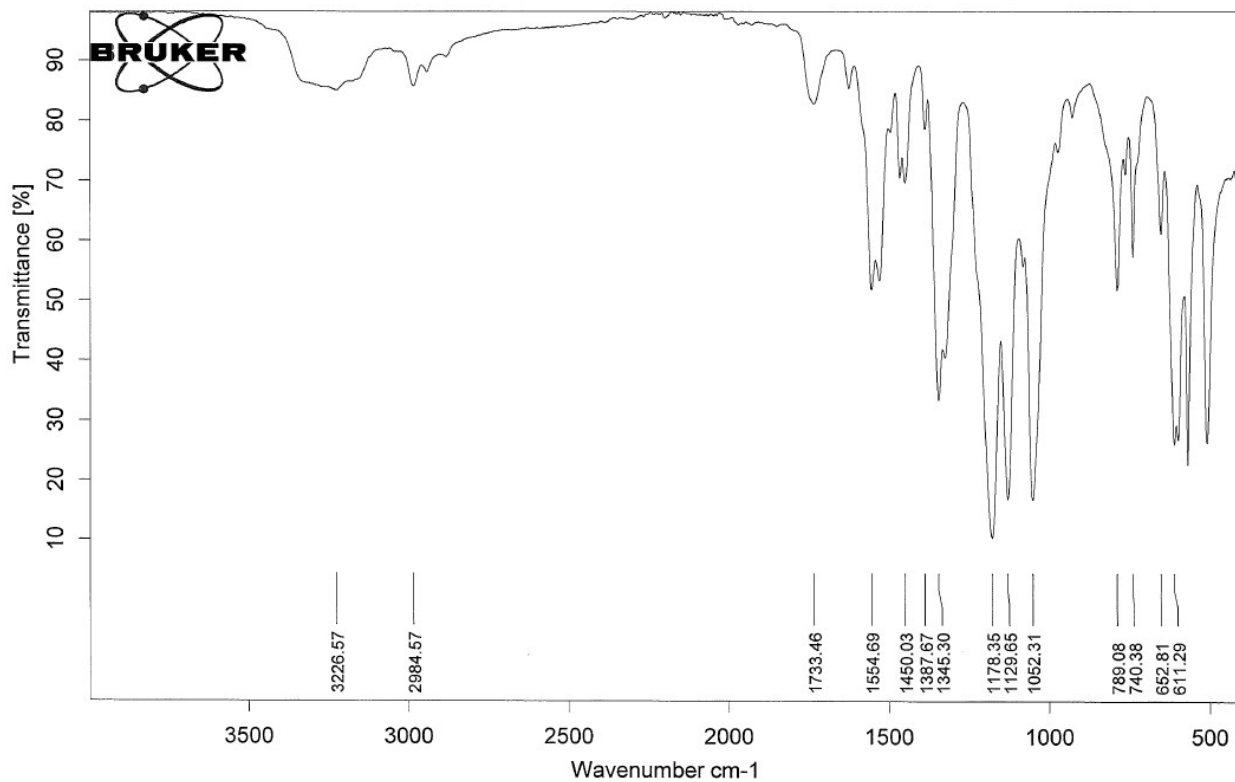
Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Feb 21 2013

Temp. 26.0 C / 299.1 K
Sample #54, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
6208 repetitions
OBSERVE C13, 100.5415266 MHz
DECOUPLE H1, 399.8486751 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 hr, 59 min



Plotname: CARBON_cd3od_20130221_400_01_plot01



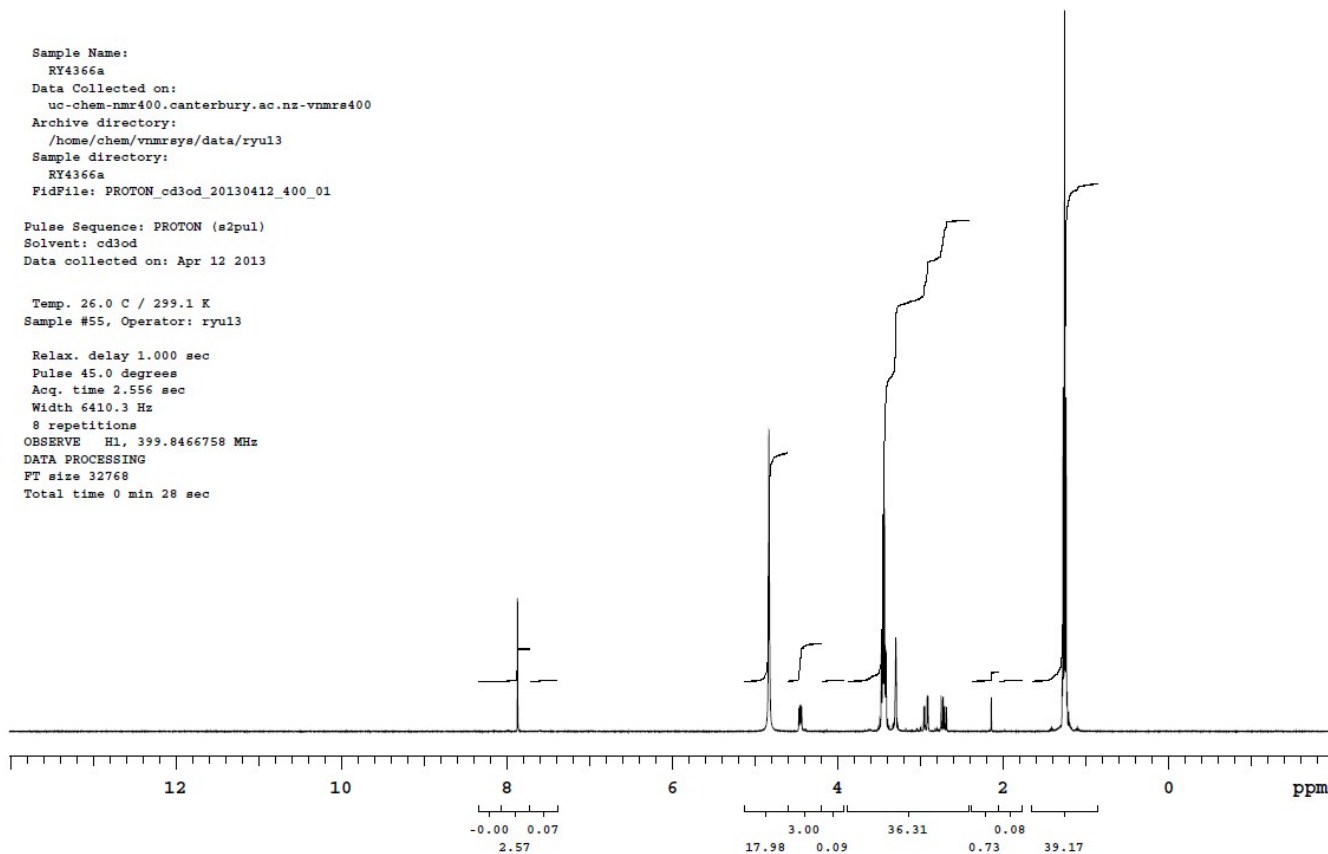
Bis(diethylamino)-S-(1-carboxy-3-carbamoylpropylamino)cyclopropenium bistriflamide, [C₃(NEt₂)₂(NHCH(COOH)(CH₂CONH₂)]NTf₂, [E₄Asn]NTf₂ (2p)

Sample Name:
RY4366a
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vnmrs400
Archive directory:
/home/chem/vnmrsys/data/ryu13
Sample directory:
RY4366a
FidFile: PROTON_cd3od_20130412_400_01

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Apr 12 2013

Temp. 26.0 C / 299.1 K
Sample #55, Operator: ryu13

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8466758 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



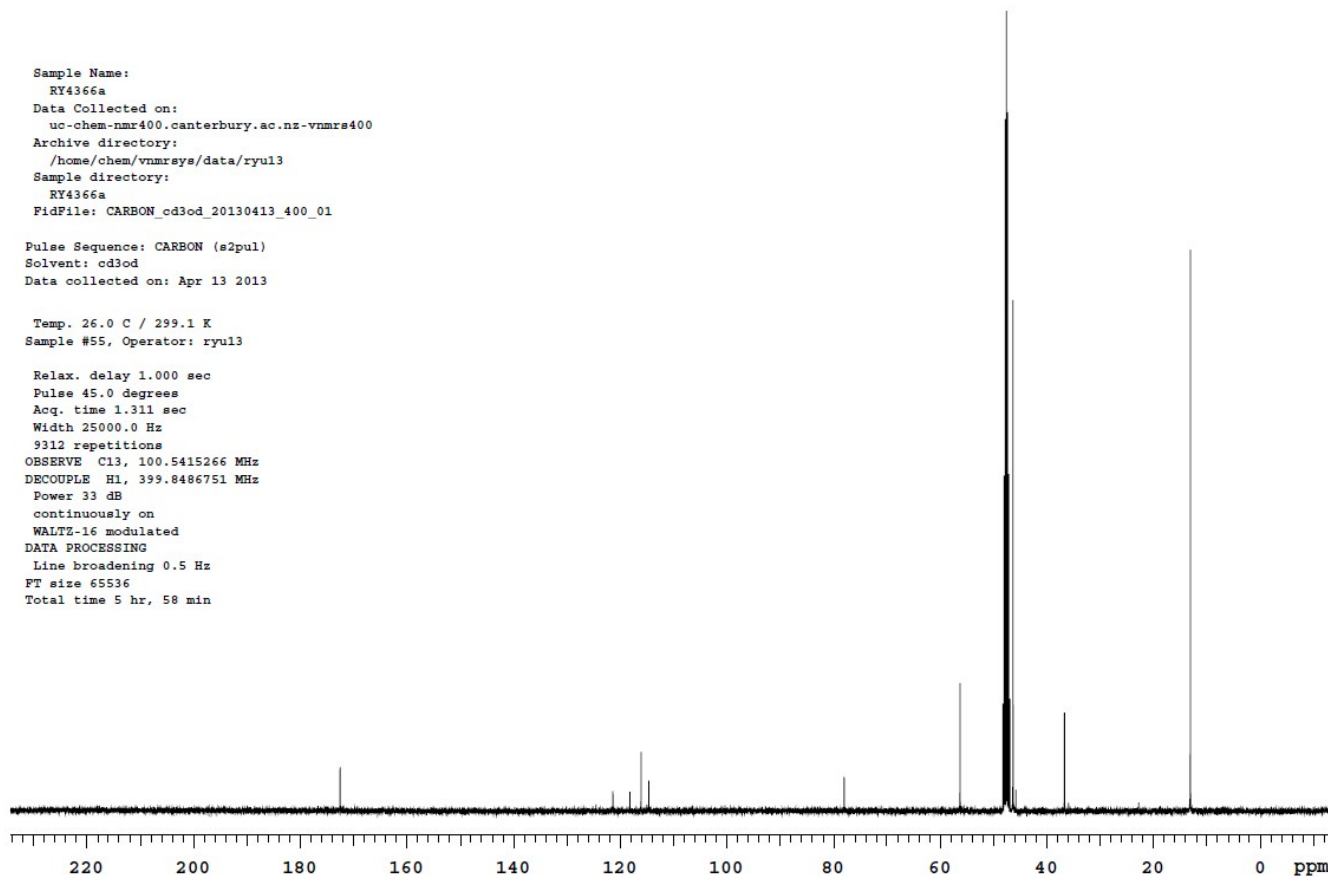
Plotname: PROTON_cd3od_20130412_400_01_plot01

Sample Name:
RY4366a
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vnmrs400
Archive directory:
/home/chem/vnmrsys/data/ryu13
Sample directory:
RY4366a
FidFile: CARBON_cd3od_20130413_400_01

Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Apr 13 2013

Temp. 26.0 C / 299.1 K
Sample #55, Operator: ryu13

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
9312 repetitions
OBSERVE C13, 100.5415266 MHz
DECOUPLE H1, 399.8486751 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 58 min



Plotname: CARBON_cd3od_20130413_400_01_plot01

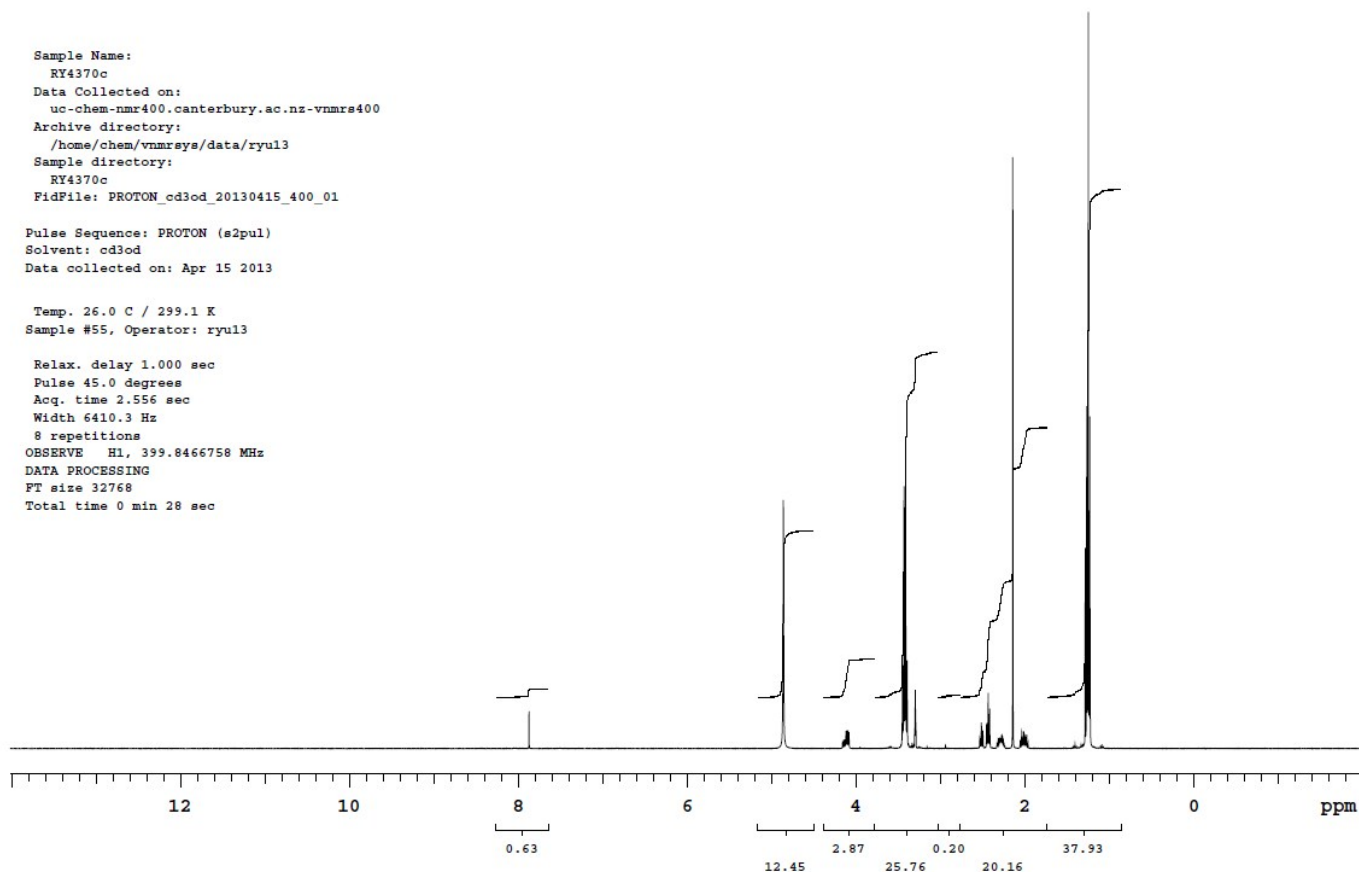
Bis(diethylamino)-S-(1-carboxy-4-carbamoylbutylamino)cyclopropenium bistriflamide,
[C₃(NEt₂)₂(NHCH(COOH)(CH₂CH₂CONH₂)]NTf₂, [E₄Gln]NTf₂ (2q)

Sample Name:
RY4370c
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vnmrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RY4370c
FidFile: PROTON_cd3od_20130415_400_01

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Apr 15 2013

Temp. 26.0 C / 299.1 K
Sample #55, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8466758 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



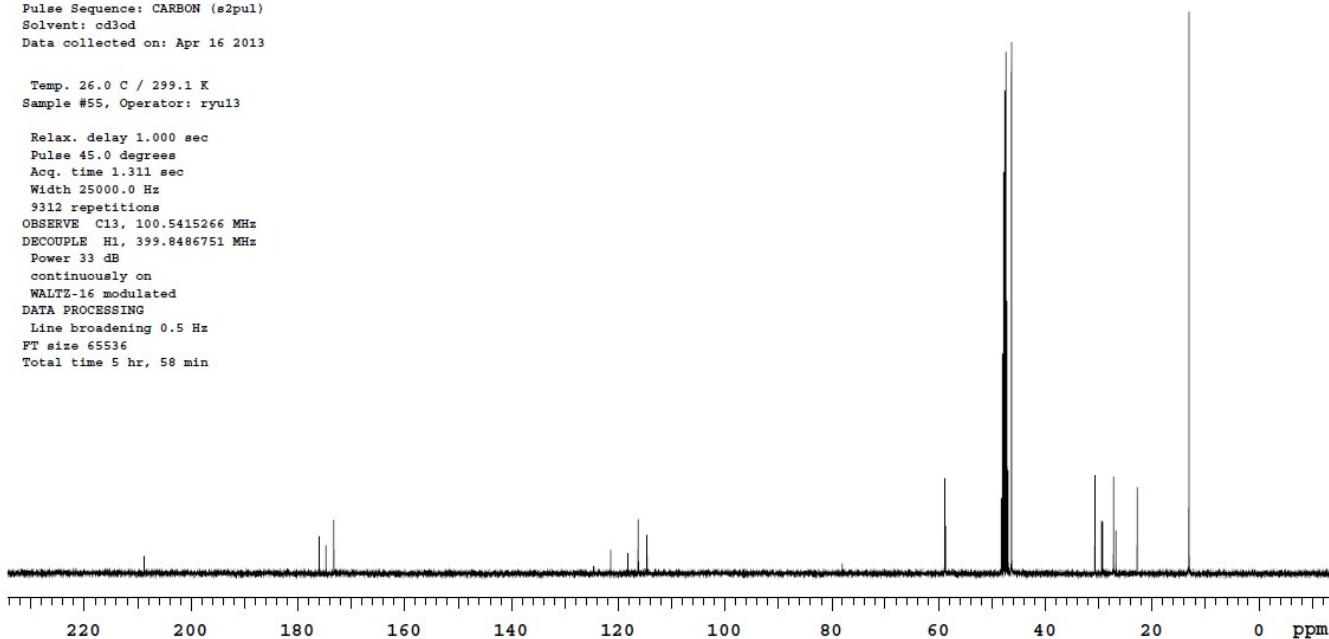
Plotname: PROTON_cd3od_20130415_400_01_plot01

Sample Name:
RY4370c
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vnmrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RY4370c
FidFile: CARBON_cd3od_20130417_400_01

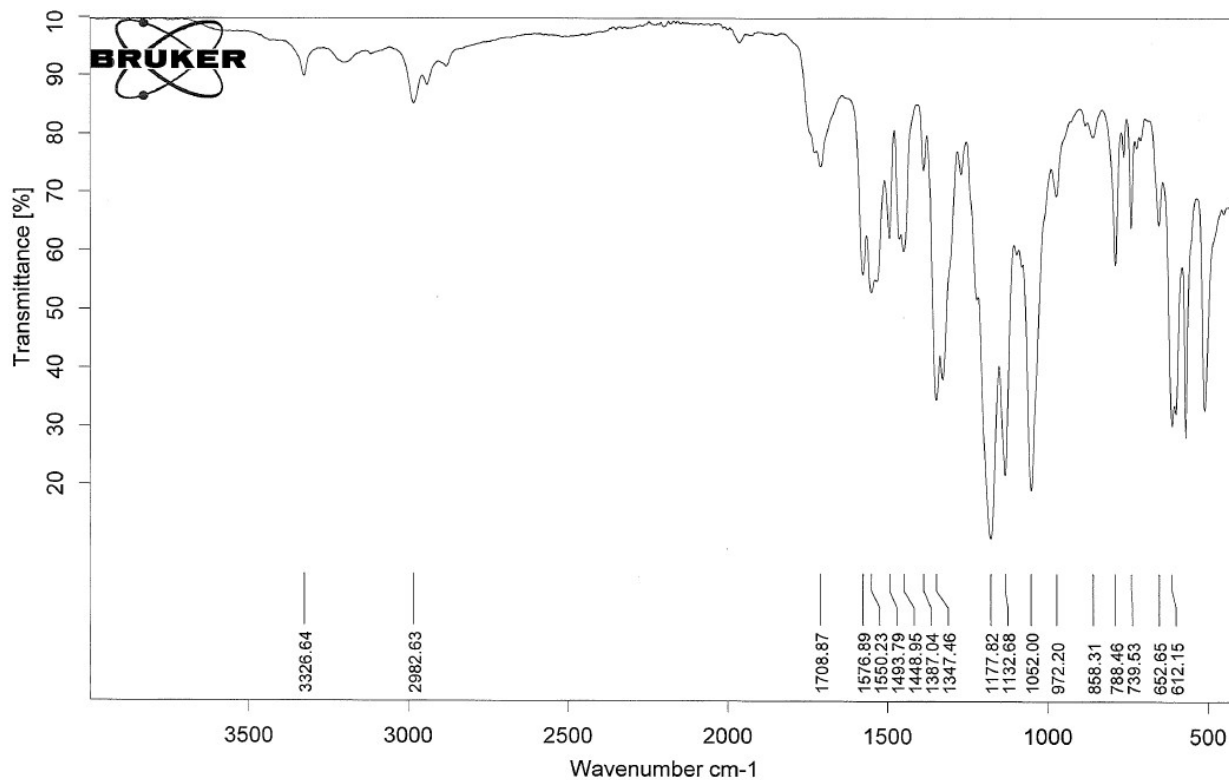
Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Apr 16 2013

Temp. 26.0 C / 299.1 K
Sample #55, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
9312 repetitions
OBSERVE C13, 100.5415266 MHz
DECOUPLE H1, 399.8486751 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 58 min



Plotname: CARBON_cd3od_20130417_400_01_plot01



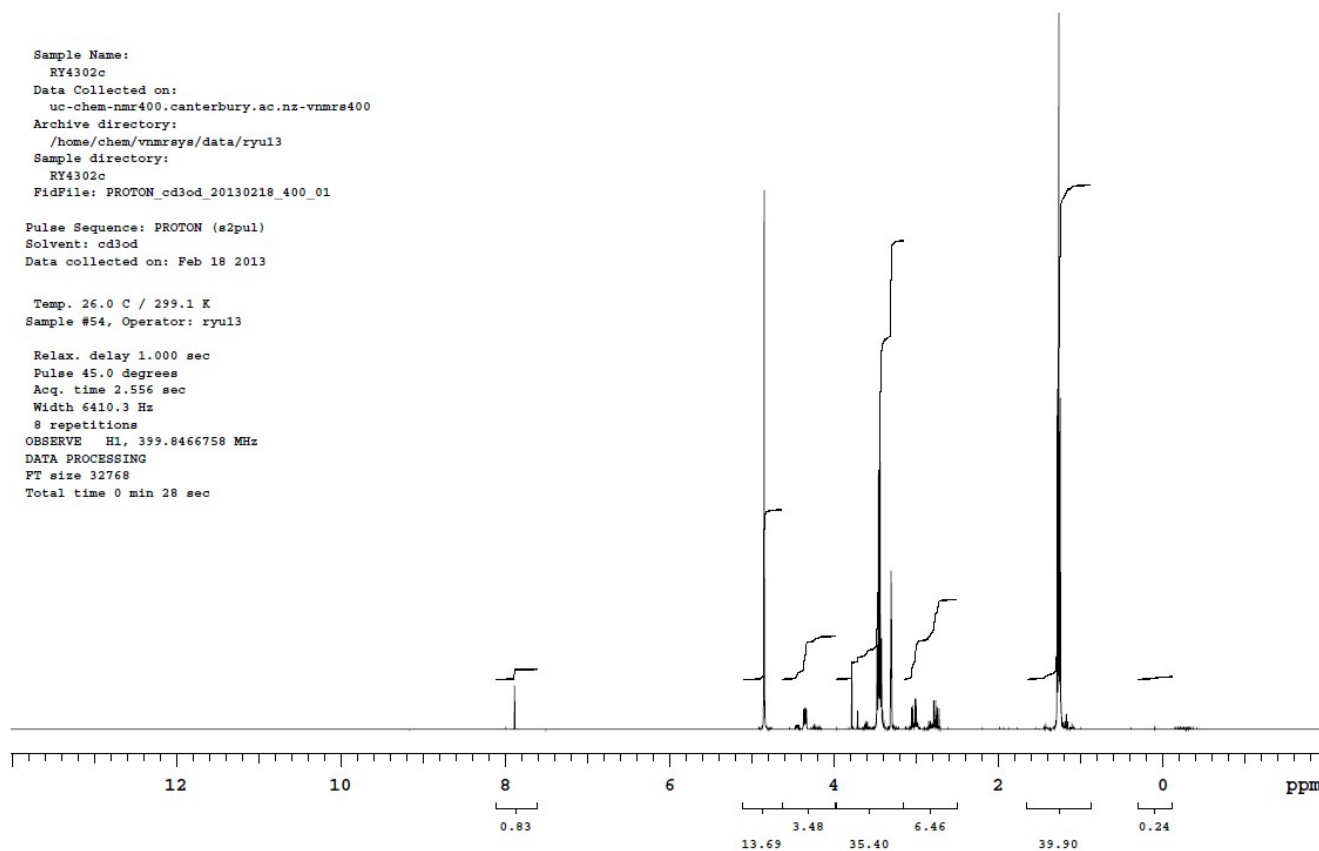
**Bis(diethylamino)-S-(1,2-dicarboxyethylamino)cyclopropenium bistriflate,
[C₃(NET₂)₂(NHCH(COOH)CH₂COOH)]NTf₂, [E₄Asp]NTf₂ (2r)**

Sample Name:
RY4302c
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vnmrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RY4302c
FidFile: PROTON_cd3od_20130218_400_01

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Feb 18 2013

Temp. 26.0 C / 299.1 K
Sample #54, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE HL 399.8466758 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



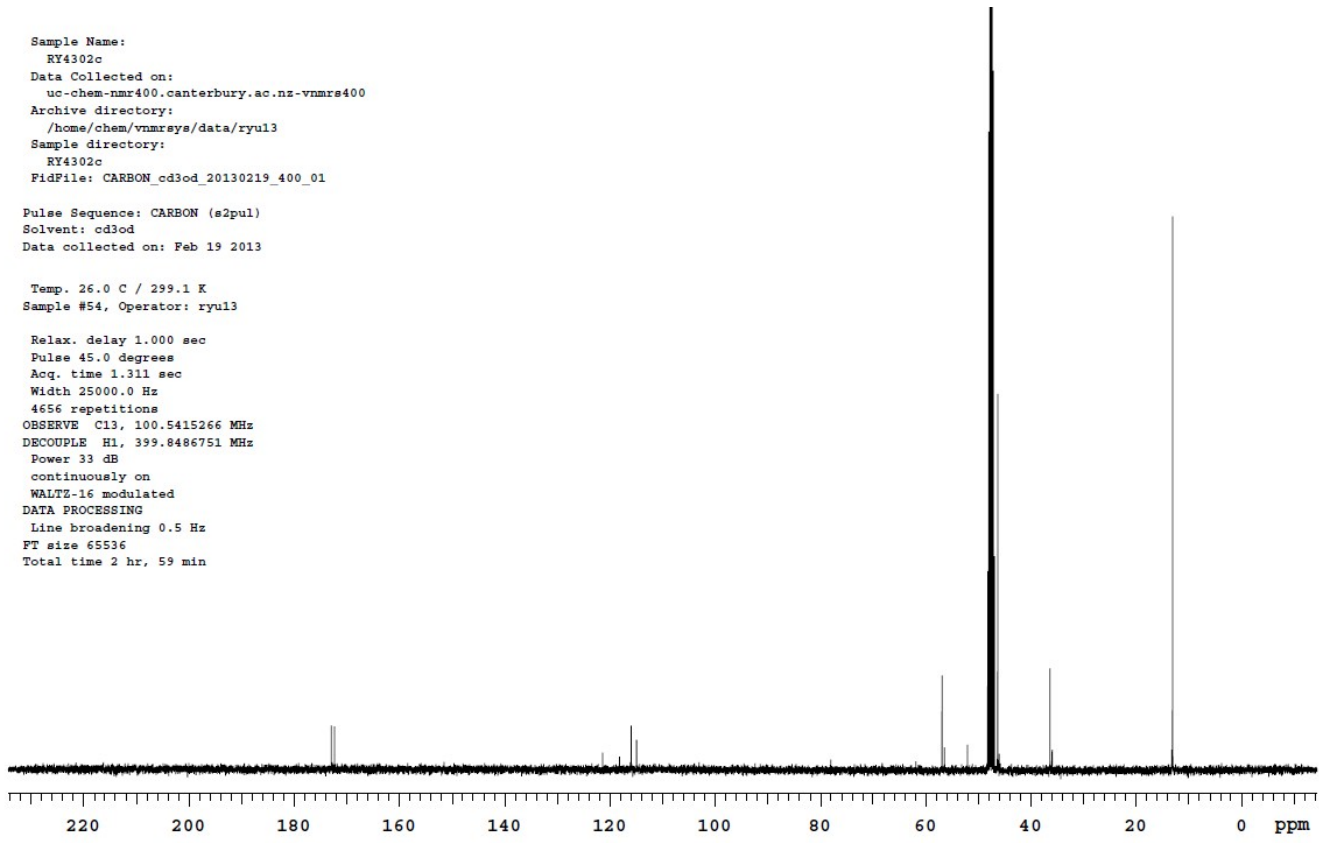
Plotname: PROTON_cd3od_20130218_400_01_plot01

Sample Name:
RY4302c
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vnmrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RY4302c
FidFile: CARBON_cd3od_20130219_400_01

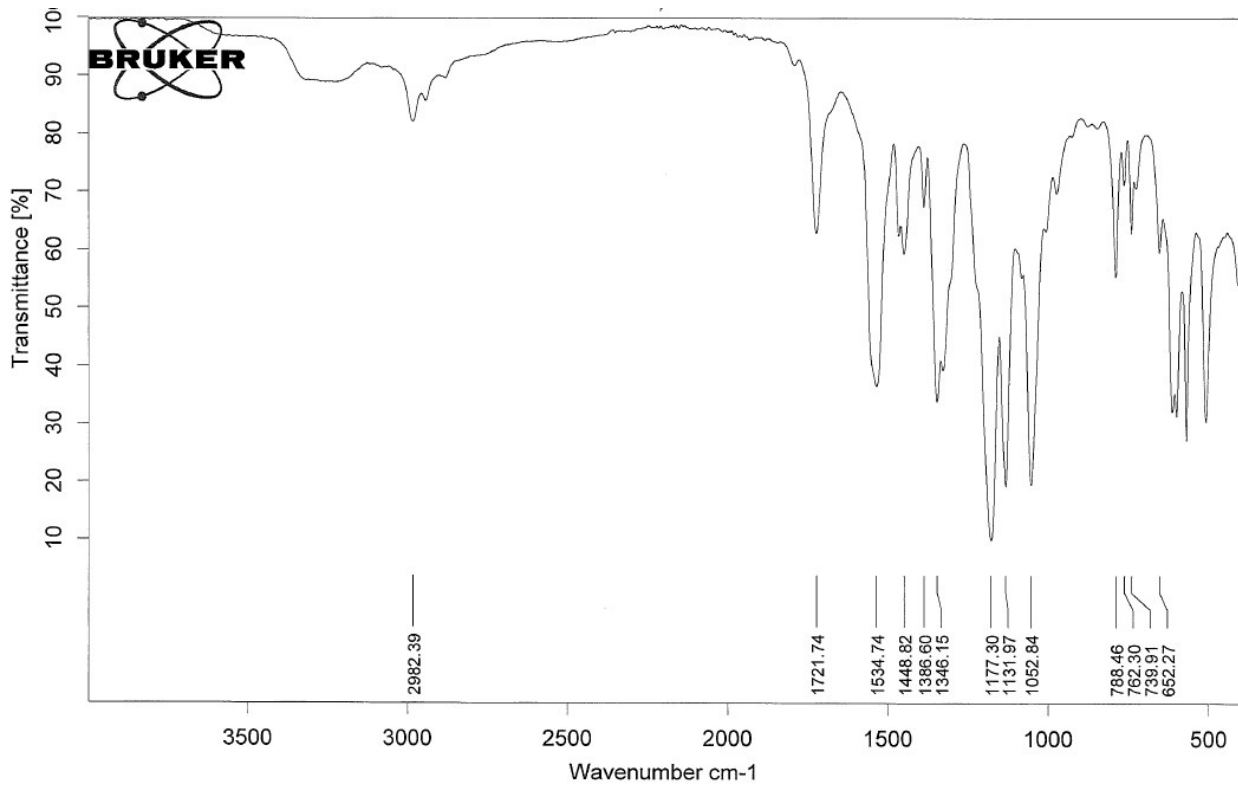
Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Feb 19 2013

Temp. 26.0 C / 299.1 K
Sample #54, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
4656 repetitions
OBSERVE C13, 100.5415266 MHz
DECOUPLE H1, 399.8486751 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 2 hr, 59 min



Plotname: CARBON_cd3od_20130219_400_01_plot01



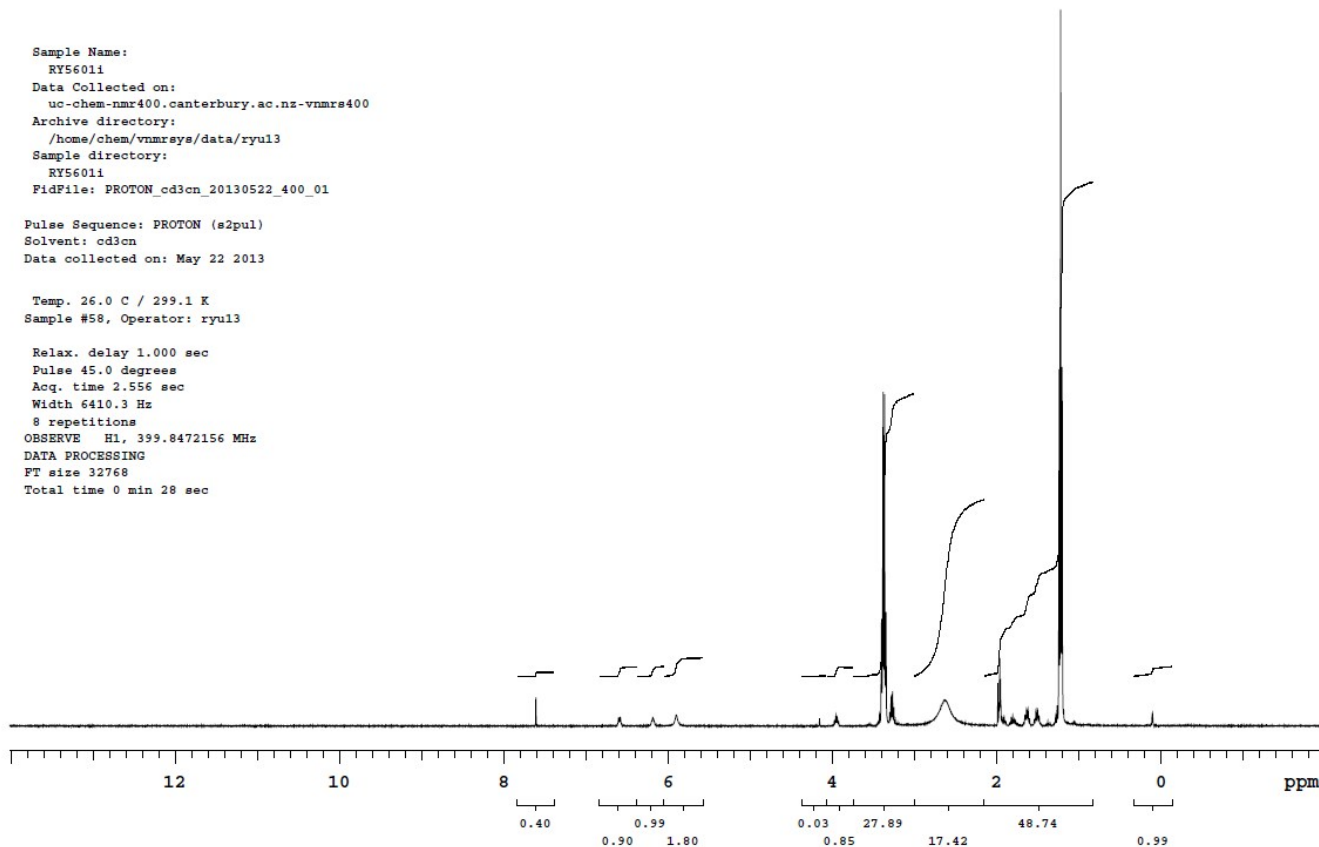
Tetrakis(diethylamino)-bis(bis(diethylamino)cyclopropenium)-S-(1-carboxy-5-aminopentylamine)cyclopropenium bistriflamide, [C₃(NEt₂)₂(NHCOOHCH₂CH₂CH₂CH₂NH)C₃(NEt₂)₂][NTf₂]₂, [E₈Lys][NTf₂]₂ (4)

Sample Name:
RYS6011
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vnmrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RYS6011
FidFile: PROTON_cd3cn_20130522_400_01

Pulse Sequence: PROTON (s2pul)
Solvent: cd3cn
Data collected on: May 22 2013

Temp. 26.0 C / 299.1 K
Sample #58, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8472156 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



Plotname: PROTON_cd3cn_20130522_400_01_plot01

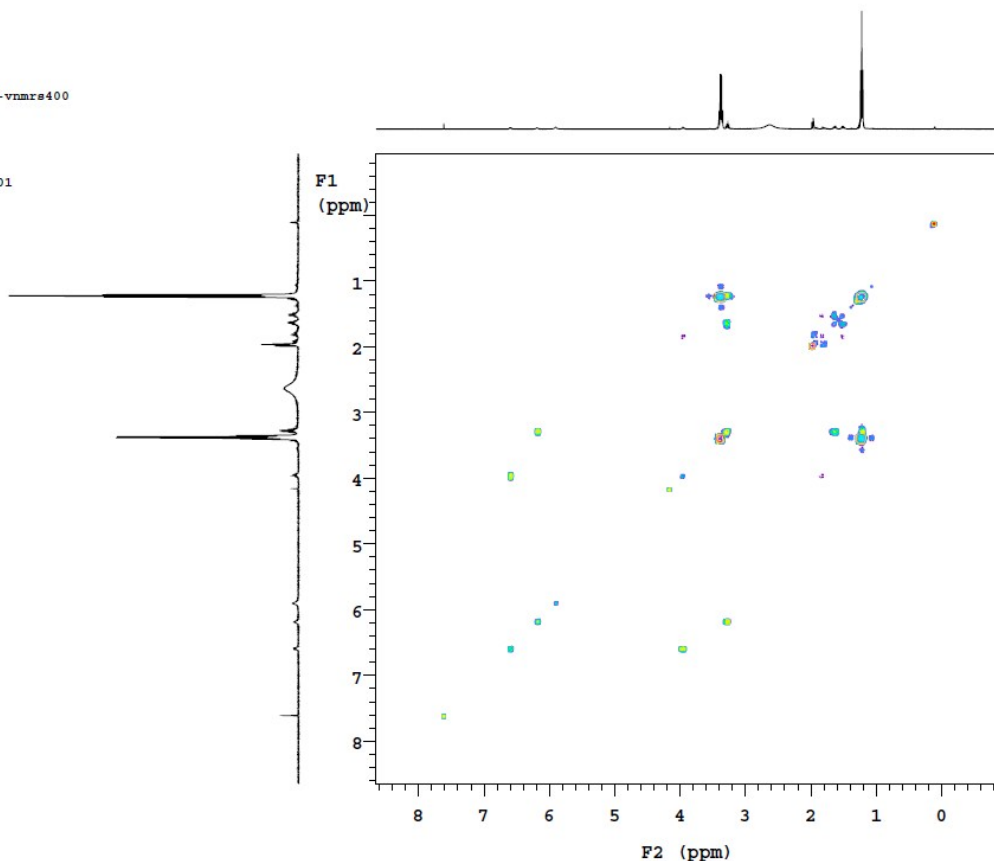
COSY

Sample Name:
RYS6011
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vnmrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RYS6011
FidFile: COSY_cd3cn_20130528_400_01

Pulse Sequence: COSY
Solvent: cd3cn
Data collected on: May 28 2013

Temp. 26.0 C / 299.1 K
Sample #58, Operator: ryul3

Relax. delay 1.000 sec
Mixing 0.080 sec
Acq. time 0.150 sec
Width 3834.4 Hz
2D Width 3834.4 Hz
4 repetitions
128 increments
OBSERVE H1, 399.8472156 MHz
DATA PROCESSING
Sq. sine bell 0.075 sec
F1 DATA PROCESSING
Sq. sine bell 0.033 sec
FT size 2048 x 2048
Total time 10 min



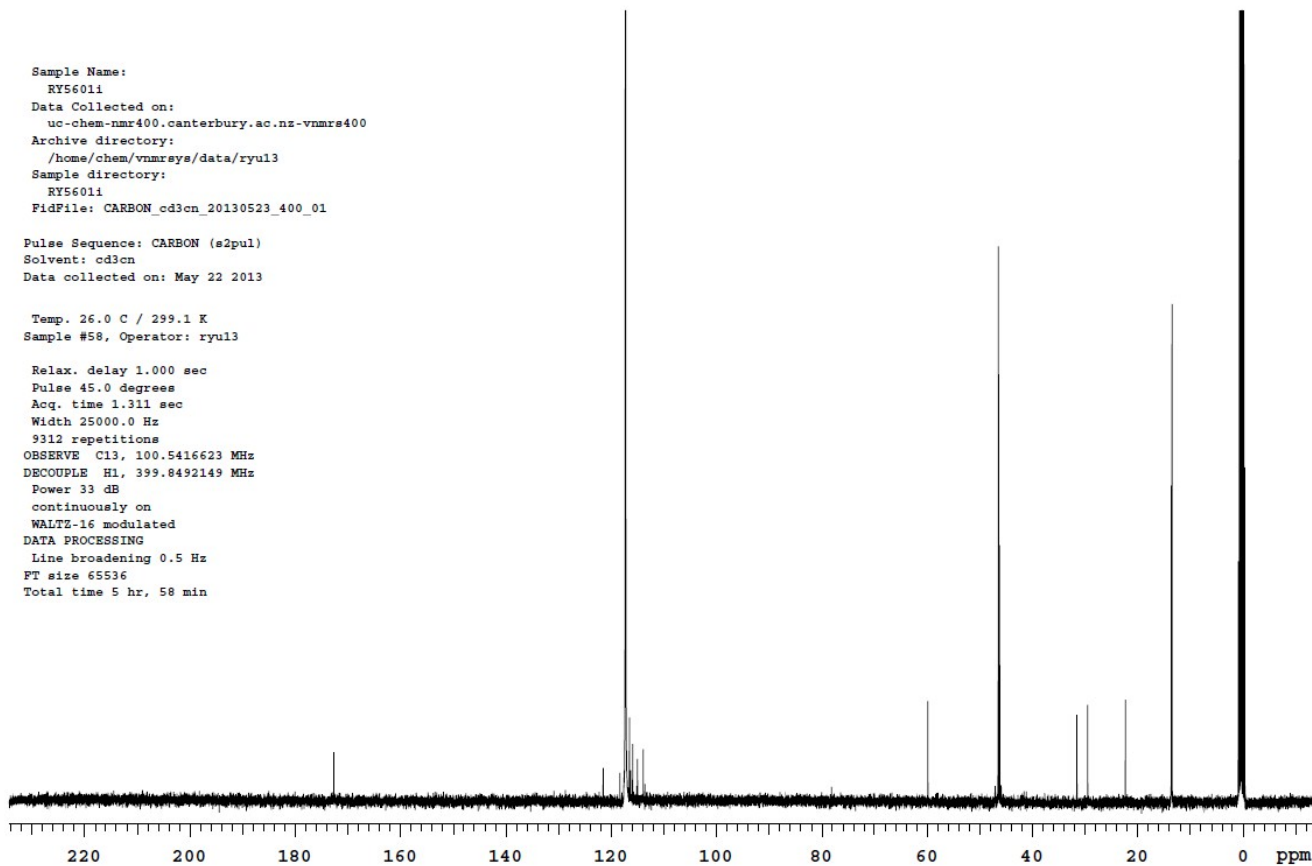
Plotname: COSY_cd3cn_20130528_400_01_plot01

Sample Name:
RYS6011
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmnrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RYS6011
FidFile: CARBON_cd3cn_20130523_400_01

Pulse Sequence: CARBON (s2pul)
Solvent: cd3cn
Data collected on: May 22 2013

Temp. 26.0 C / 299.1 K
Sample #58, Operator: ryul3

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
9312 repetitions
OBSERVE C13, 100.5416623 MHz
DECOUPLE H1, 399.8492149 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 58 min



Plotname: CARBON_cd3cn_20130523_400_01_plot01

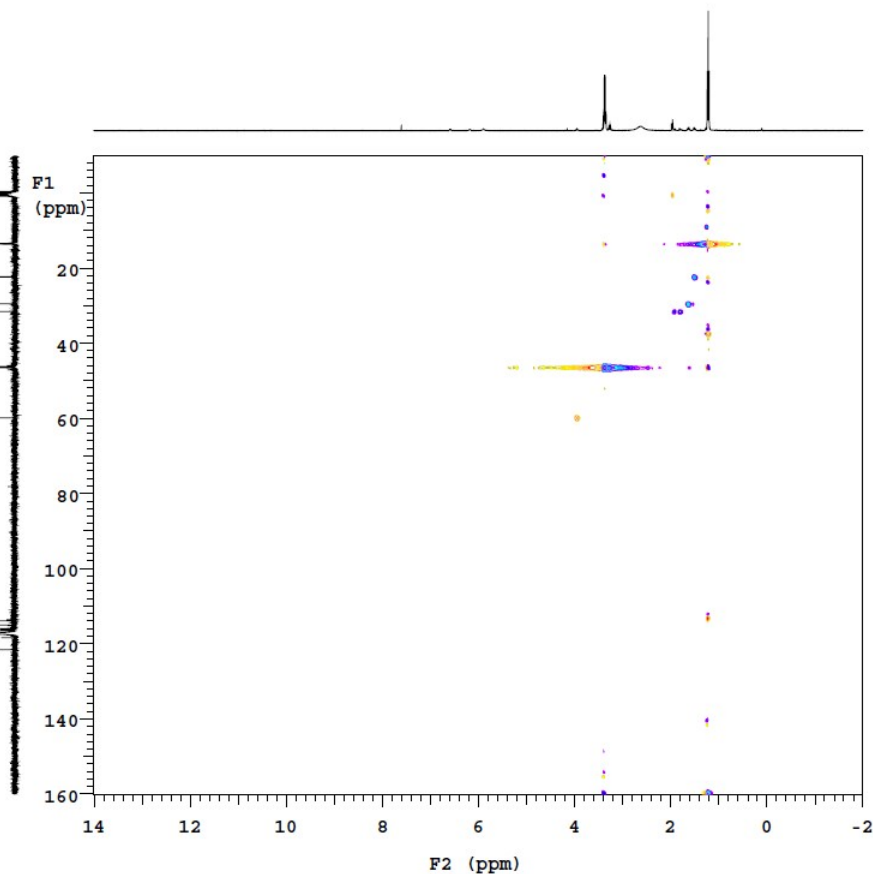
HSQC

Sample Name:
RYS6011
Data Collected on:
uc-chem-nmr400.canterbury.ac.nz-vmnrs400
Archive directory:
/home/chem/vnmrsys/data/ryul3
Sample directory:
RYS6011
FidFile: HSQC_cd3cn_20130528_400_01

Pulse Sequence: HSQC
Solvent: cd3cn
Data collected on: May 28 2013

Temp. 26.0 C / 299.1 K
Sample #58, Operator: ryul3

Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 6410.3 Hz
2D Width 17090.4 Hz
4 repetitions
2 x 128 increments
OBSERVE H1, 399.8472156 MHz
DECOUPLE C13, 100.5492030 MHz
Power 35 dB
on during acquisition
off during delay
W40_oneprobe modulated
DATA PROCESSING
Gauss apodization 0.069 sec
F1 DATA PROCESSING
Gauss apodization 0.007 sec
FT size 2048 x 2048
Total time 20 min



Plotname: HSQC_cd3cn_20130528_400_01_plot01

