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SUPPORTING INFORMATION

DOI: 10.1002/ejic.201300850
Title: Redox Reaction between Main-Group Elements (Te, Sn, Bi) and N-Heterocyclic-Carbene-Derived Selenium Halides: A Facile Method for the Preparation of Monomeric Halides
Author(s): Sudesh T. Manjare, Sangeeta Yadav, Harkesh B. Singh,* Ray J. Butcher

Contents

Figure S1. ^{1}H NMR spectrum of **4c** in $CDCl_3$.

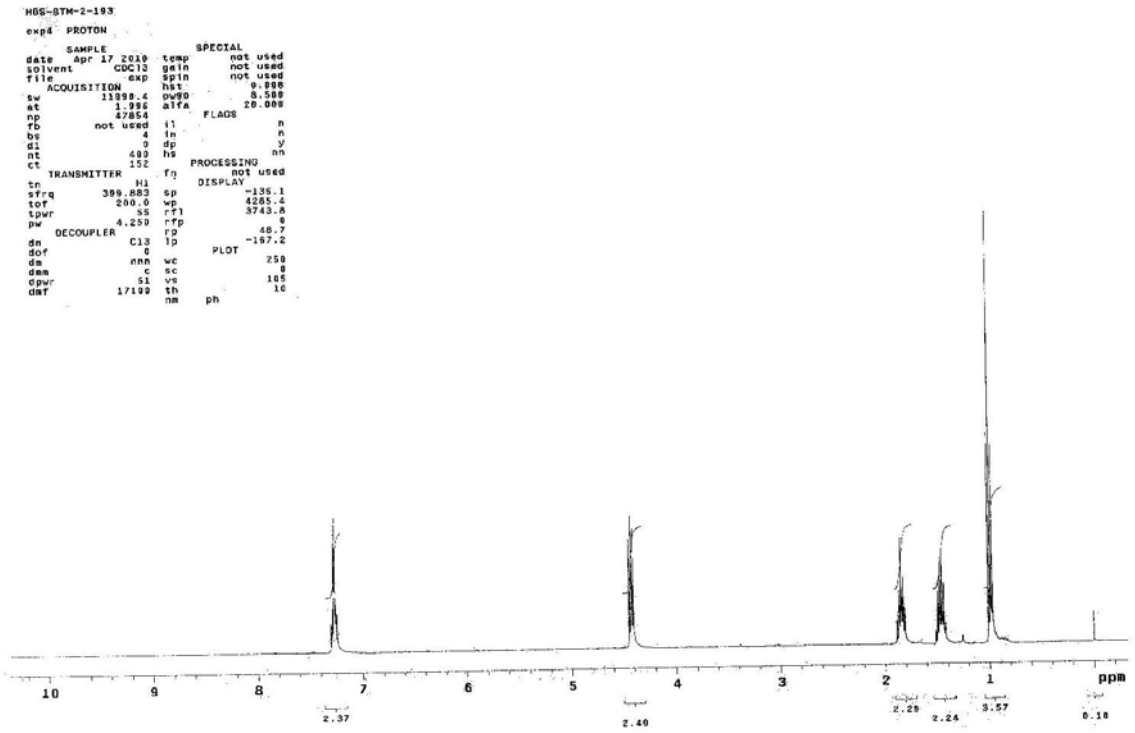


Figure S2. ^{13}C NMR spectrum of **4c** in $CDCl_3$.

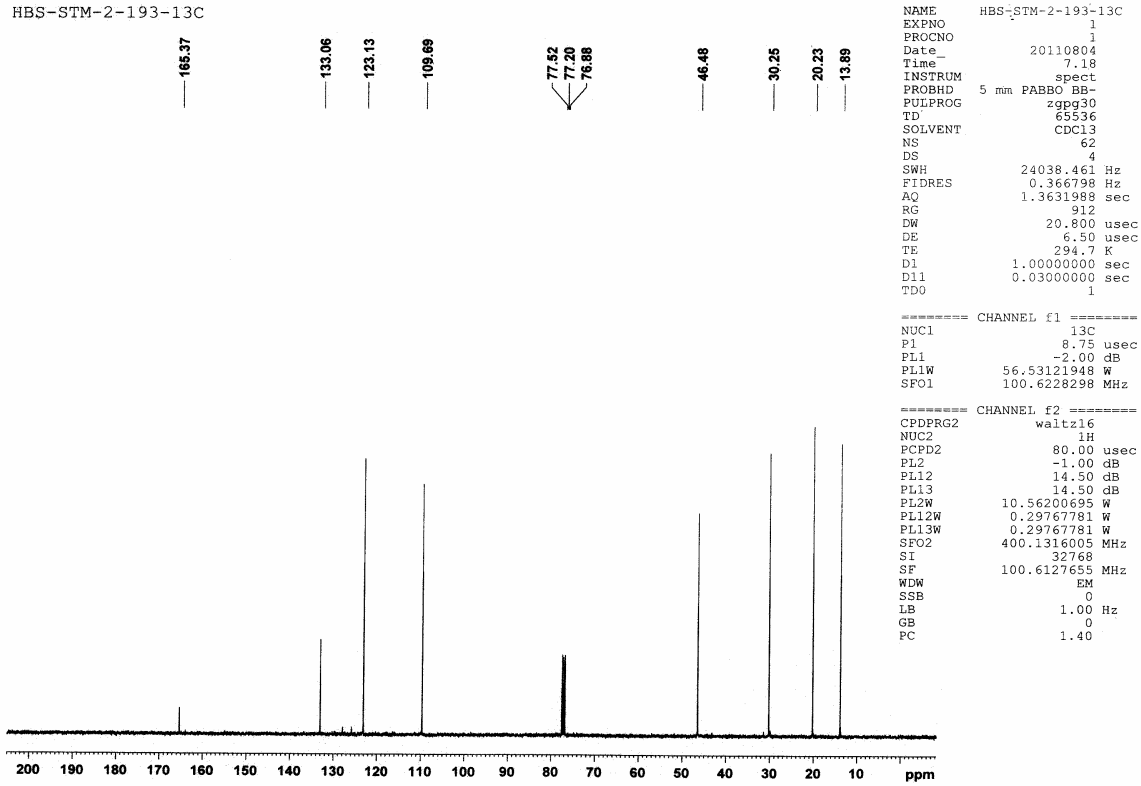


Figure S3. ^{77}Se NMR spectrum of **4c** in $CDCl_3$.

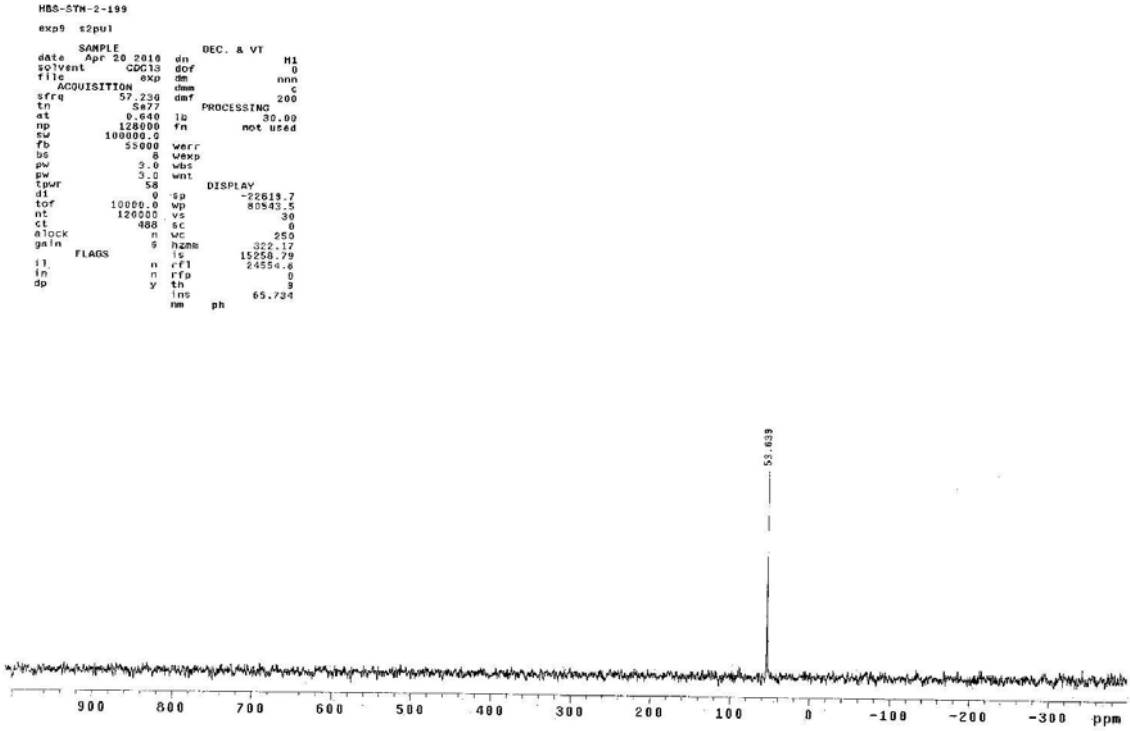


Figure S4. Mass spectrum of **4c**.

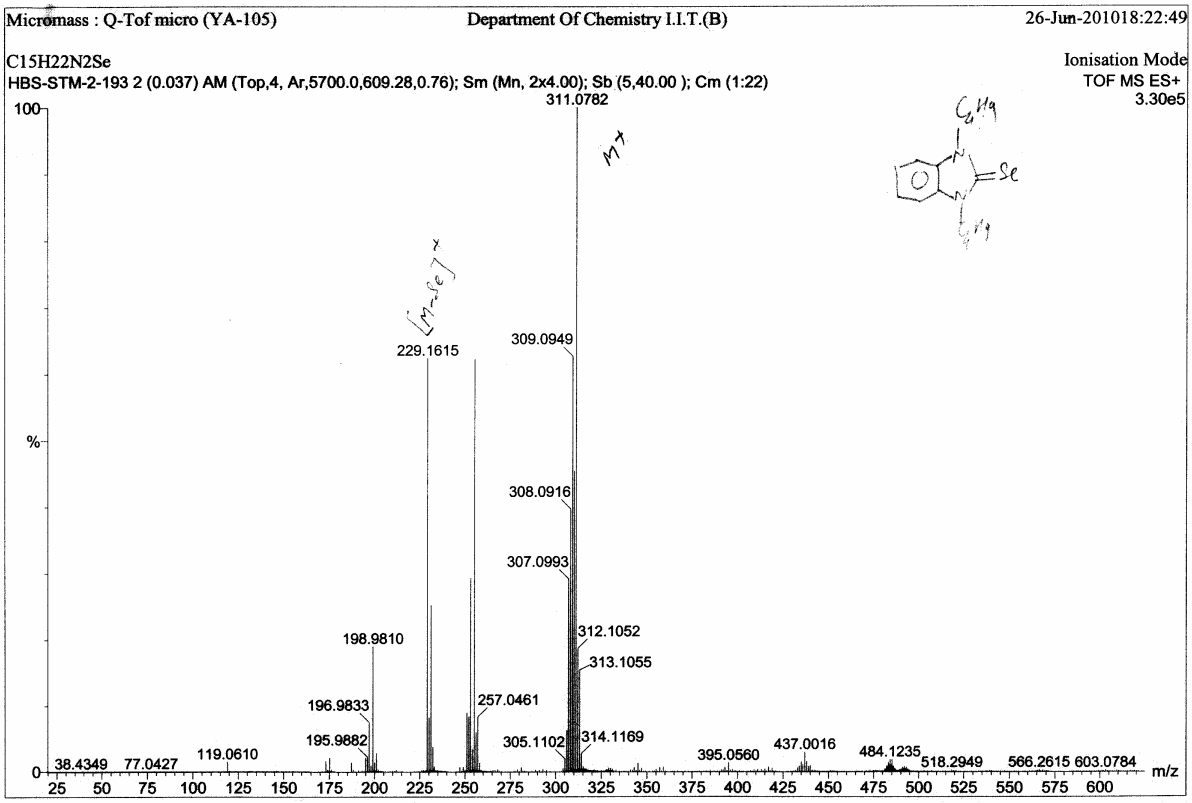


Figure S5. Elemental analysis of **4c**.

Eager 300 Report

Page: 1 Sample: STM2-193 (STM2-193)

Method Name : SP110510
Method File : D:\CHNS2008\SP110510.mth
Chromatogram : STM2-193
Operator ID : SP
Company Name : C.E. Instruments
Analysed : 07/20/2012 15:09
Printed : 7/20/2012 15:47
Sample ID : STM2-193 (# 23)
Instrument N. : Instrument #1
Analysis Type : UnkNown (Area)
Sample weight : 1.026

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	10.0126	44	125981	RS	12.196140	.122634E+07
Carbon	58.2835	67	1536476	RS	1.000000	.252191E+07
Hydrogen	7.4676	169	583840	RS	2.631672	.656520E+07
Totals	75.7637		2246296			

Figure S6. ^{1}H NMR spectrum of **4d** in $CDCl_3$.

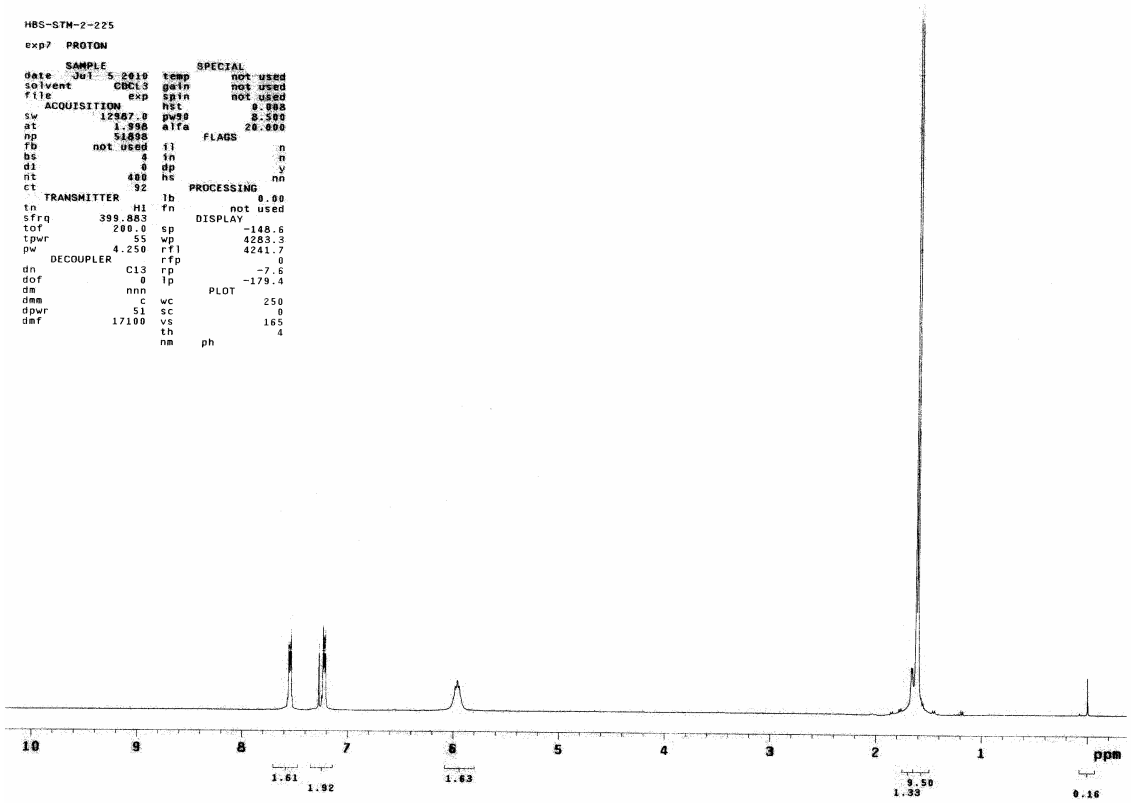
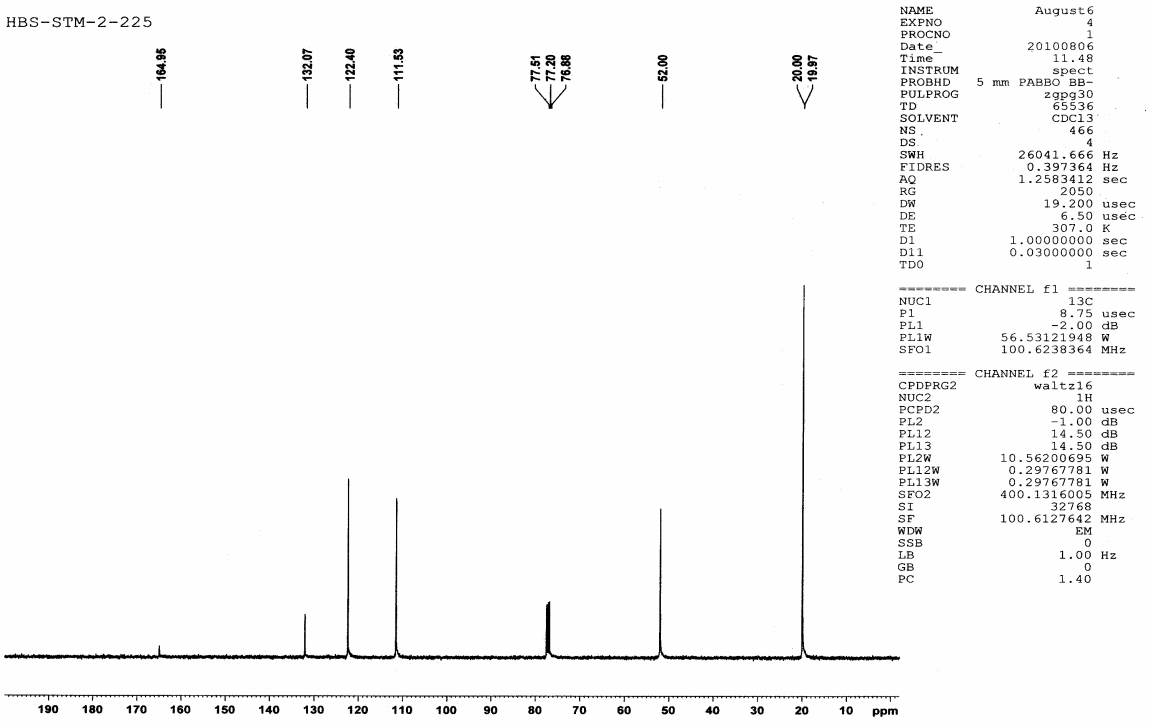


Figure S7. ^{13}C NMR spectrum of **4d** in $CDCl_3$.

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PROCNO                  1
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Time                11.48
INSTRUM             spect
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PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                    466
DS                      4
SWH             26041.666 Hz
FIDRES          0.397364 Hz
AQ              1.2583412 sec
RG                   2050
DW                 19.200 usec
DE                  6.50 usec
TE                 307.0 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.75 usec
PL1                 -2.00 dB
PL1W         56.53121948 W
SFO1        100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               14.50 dB
PL13               14.50 dB
PL2W         10.56200695 W
PL12W         0.29767781 W
PL13W         0.29767781 W
SFO2        400.1316005 MHz
SI                32768
SF          100.6127642 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
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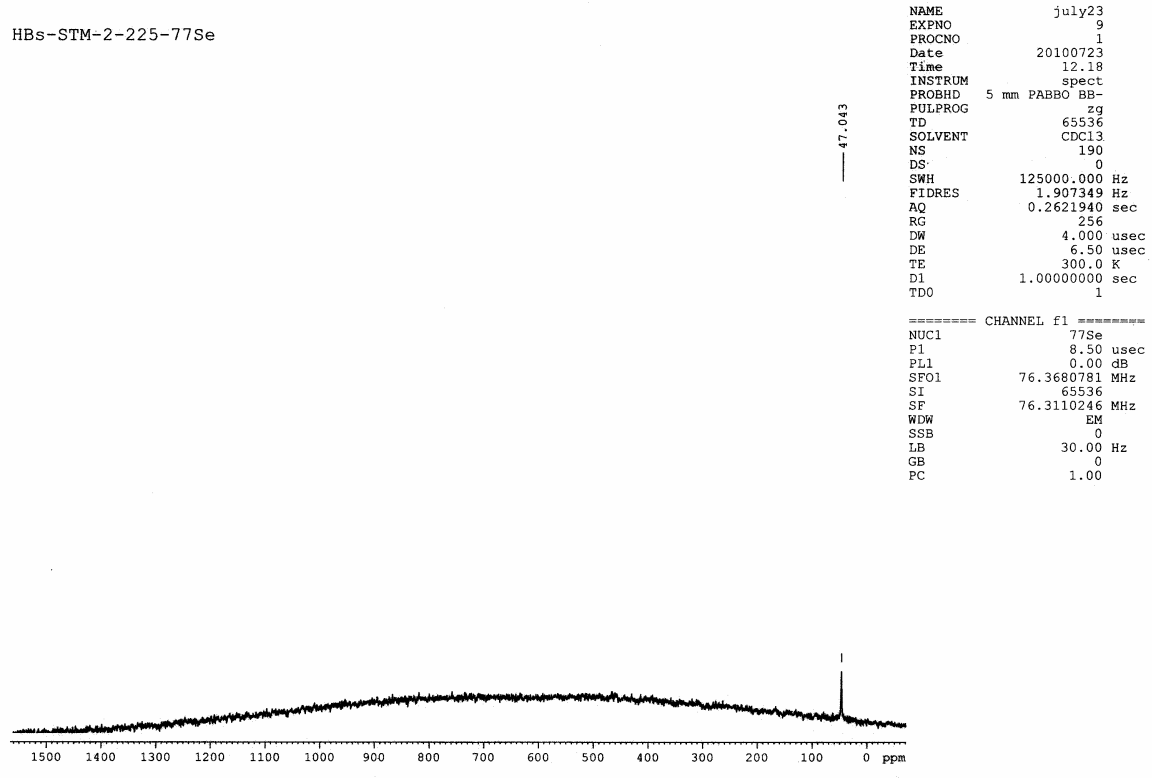
Figure S8. ^{77}Se NMR spectrum of **4d** in $CDCl_3$.

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EXPNO                  9
PROCNO                 1
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Time                12.18
INSTRUM             spect
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PULPROG                zg
TD                 65536
SOLVENT             CDCl3
NS                    190
DS                      0
SWH            125000.000 Hz
FIDRES          1.907349 Hz
AQ              0.2621940 sec
RG                   256
DW                 4.000 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                 77Se
P1                   8.50 usec
PL1                  0.00 dB
SFO1        76.3680781 MHz
SI                 65536
SF          76.3110246 MHz
WDW                  EM
SSB                   0
LB                30.00 Hz
GB                    0
PC                 1.00
```

Figure S9. HRMS of **4d**.

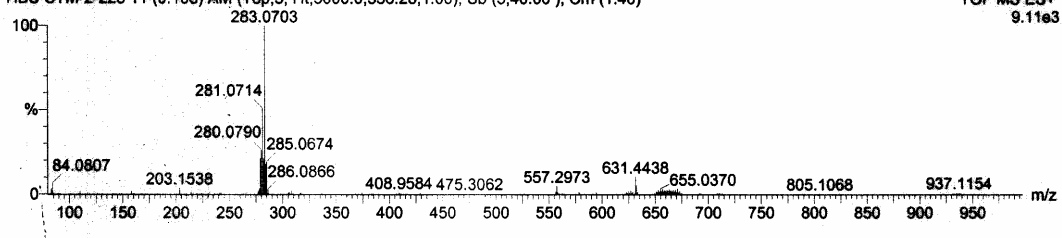
Elemental Composition Report **Page 1**

Single Mass Analysis (displaying only valid results)
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
113 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 18-May-201116:21:24

C13H18N2Se
HBS-STM-2-225 11 (0.108) AM (Top,5, Ht,5000.0,556.28,1.00); Sb (5,40.00); Cm (1:40) TOF MS ES+ 9.11e3



Minimum:				-1.5		
Maximum:		200.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
283.0703	283.0713	-1.0	-3.6	6.5	1	C13 H19 N2 Se

Figure S10. Elemental analysis of **4d**.

Eager 300 Report

Page: 1 Sample: STM-2-225 (STM-2-225)

Method Name : SP150910
Method File : D:\CHNS2008\SP150910.mth
Chromatogram : STM-2-225
Operator ID : SP **Company Name : C.E. Instruments**
Analysed : 09/15/2010 13:40 **Printed : 9/15/2010 15:41**
Sample ID : STM-2-225 (# 17) **Instrument N. : Instrument #1**
Analysis Type : UnkNown (Area) **Sample weight : .668**

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name		%	Ret.Time		Area	BC	Area ratio	K factor
1		0.0000		18	10507	RS		0.0000
Nitrogen	3.96	10.1106	0.15	43	73854	RS	13.312220	.109350E+07
Carbon	55.52	55.4093	0.12	67	983161	RS	1.000000	.265623E+07
Hydrogen	6.45	5.9657	0.48	175	238925	RS	4.114936	.567435E+07
Totals		71.4856			1306447			

Figure S11. ^{1}H NMR spectrum of **4i** in $CDCl_3$.

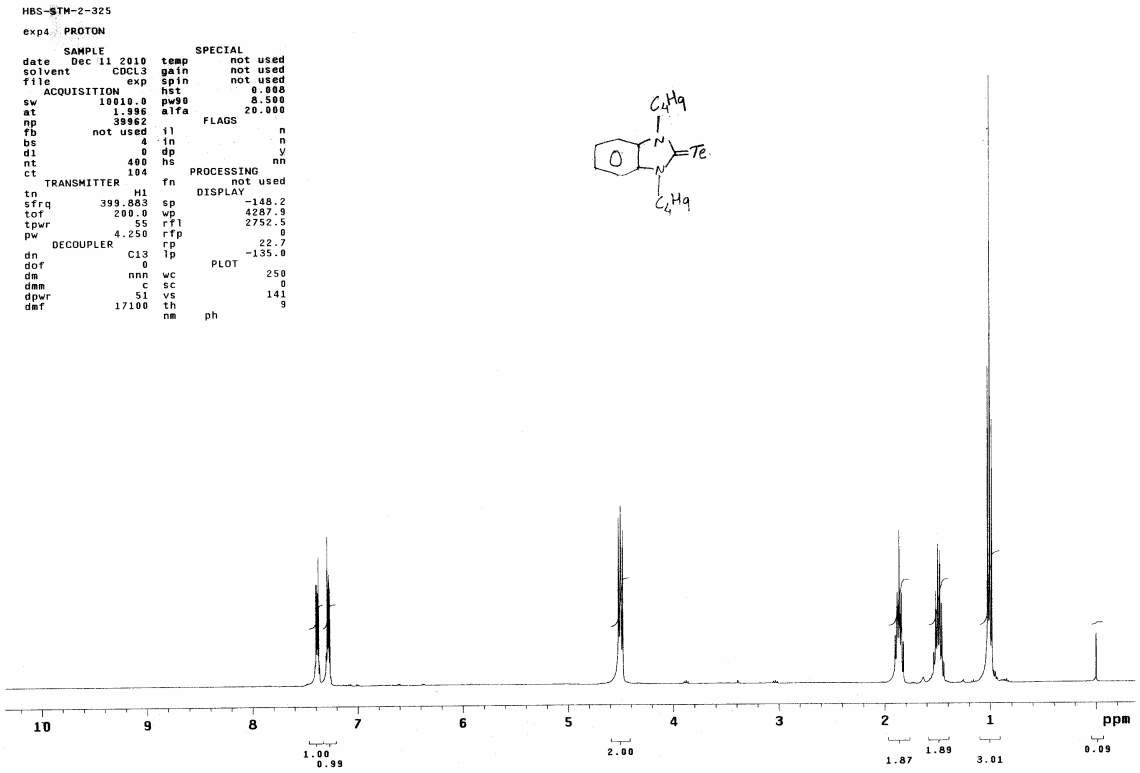


Figure S12. ^{13}C NMR spectrum of **4i** in $CDCl_3$.

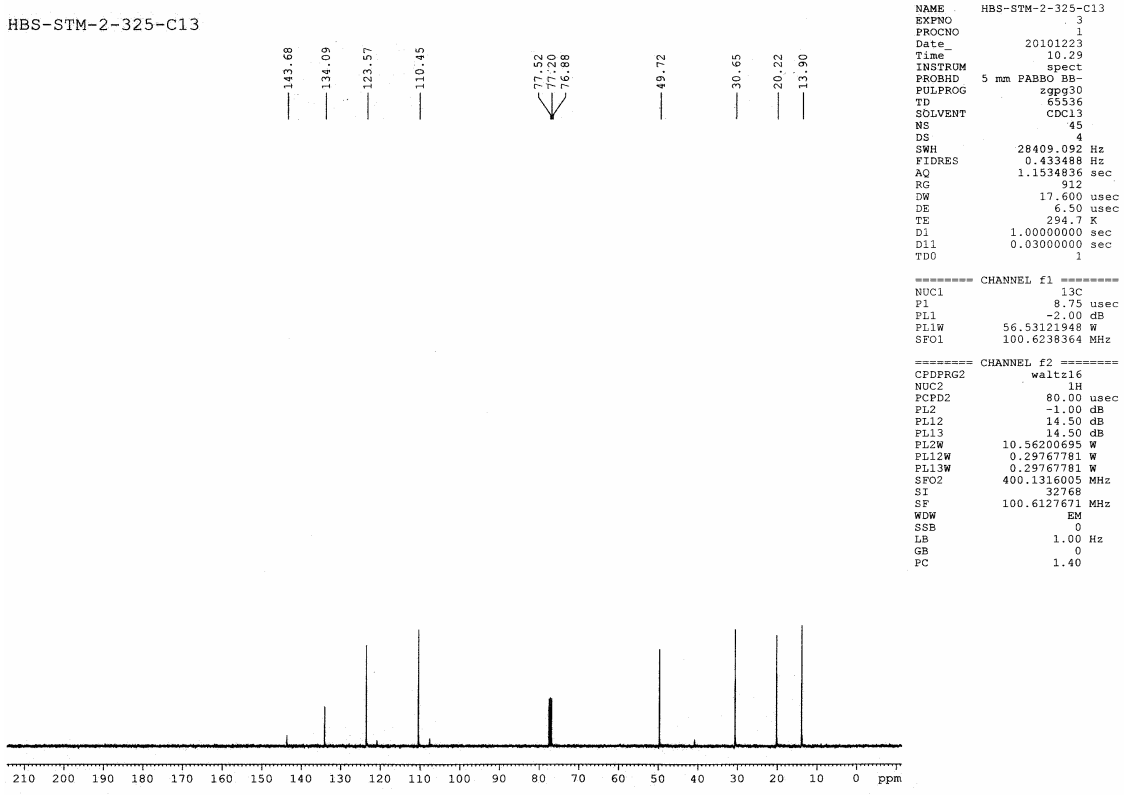
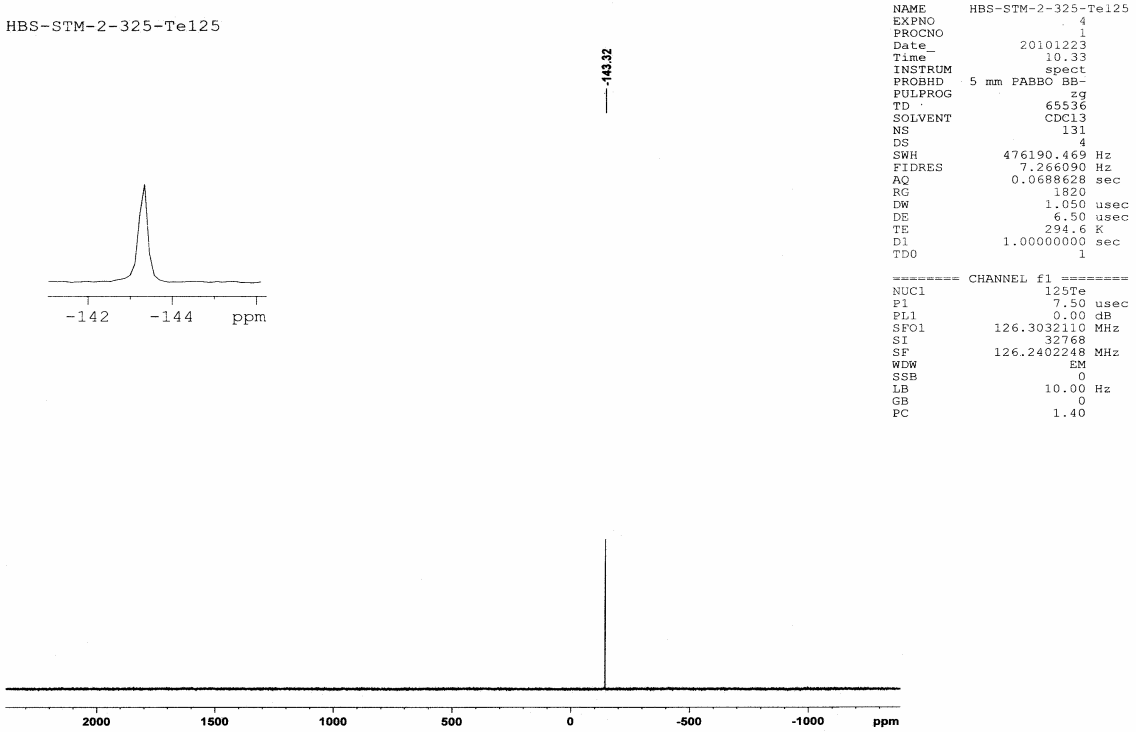


Figure S13. ^{125}Te NMR spectrum of **4i** in $CDCl_3$.

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PROCNO                            1
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Time                          10.33
INSTRUM                       spect
PROBHD       5 mm PABBO BB-
PULPROG                          zg
TD                            65536
SOLVENT                       CDCl3
NS                              131
DS                                4
SWH                      476190.469 Hz
FIDRES                     7.266090 Hz
AQ                         0.0688628 sec
RG                             1820
DW                            1.050 usec
DE                             6.50 usec
TE                            294.6 K
D1                      1.00000000 sec
TD0                               1

======== CHANNEL f1 ========
NUC1                          125Te
P1                             7.50 usec
PL1                            0.00 dB
SFO1                  126.3032110 MHz
SI                            32768
SF                    126.2402248 MHz
WDW                              EM
SSB                               0
LB                            10.00 Hz
GB                                0
PC                             1.40
```

Figure S14. HRMS spectrum of **4i**.

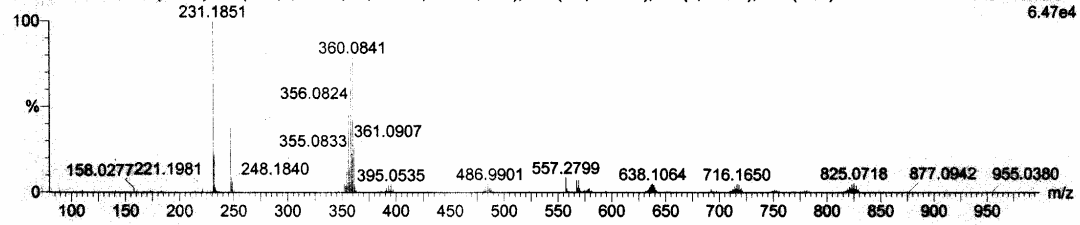
Elemental Composition Report **Page 1**

Single Mass Analysis (displaying only valid results)
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
131 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 18-May-201117:03:42

C15H22N2Te
HBS-STM-2-325 32 (0.321) AM (Cen,5, 80.00, Ar,5000.0,556.28,1.00); Sm (Mn, 3x6.00); Sb (5,40.00); Cm (1:36) TOF MS ES+ 6.47e4



Minimum:				-1.5		
Maximum:		200.0	10.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**Score**	**Formula**
360.0841	360.0845	-0.4	-1.2	6.0	1	C15 H22 N2 Te

Figure S15. Elemental analysis of **4i**.

Eager 300 Report

Page: 1 Sample: STM-2-325 (STM-2-325)

Method Name : SP131210
Method File : D:\CHNS2008\SP131210.mth
Chromatogram : STM-2-325
Operator ID : SD
Company Name : C.E. Instruments
Analysed : 12/13/2010 15:11
Printed : 12/13/2010 17:00
Sample ID : STM-2-325 (# 23)
Instrument N. : Instrument #1
Analysis Type : UnkNown (Area)
Sample weight : .866

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name		%	Ret.Time		Area	BC	Area ratio	K factor
Nitrogen	7.83	7.5839	0.25	43	103602	FU	11.107720	.157746E+07
Carbon	50.33	51.1088	0.77	66	1150778	FU	1.000000	.260003E+07
Hydrogen	6.19	5.7343	0.46	172	298356	RS	3.857063	.600812E+07
Totals		64.4269			1552736			

Figure S16. ^{1}H NMR spectrum of **5c** in $CDCl_3$.

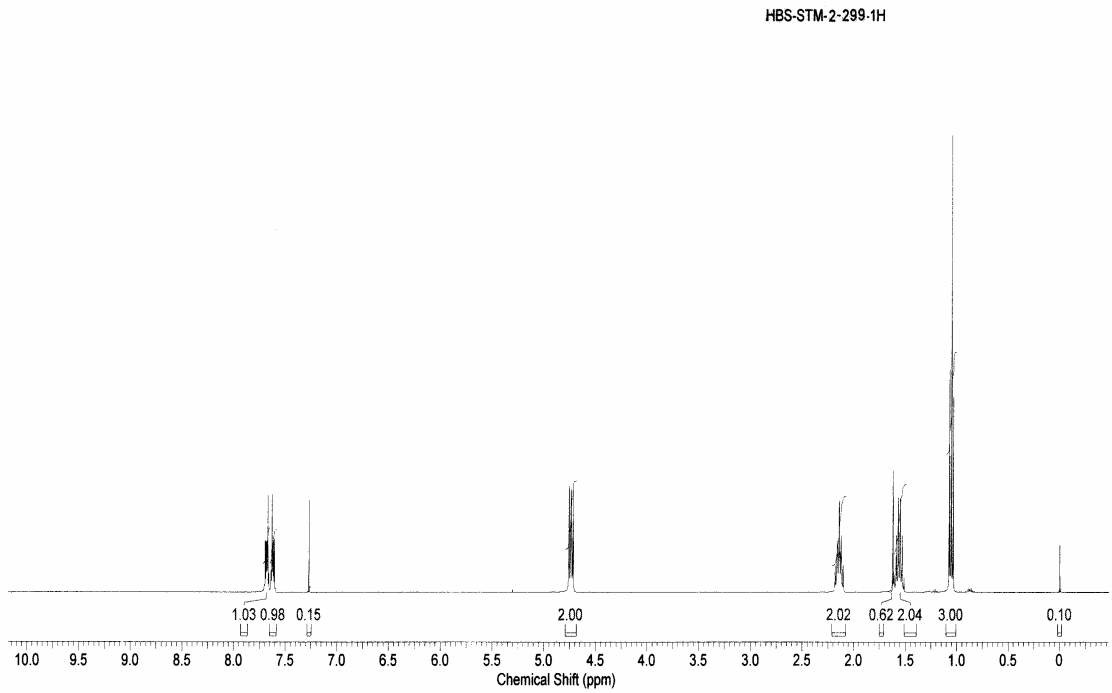


Figure S17. ^{13}C NMR spectrum of **5c** in $CDCl_3$.

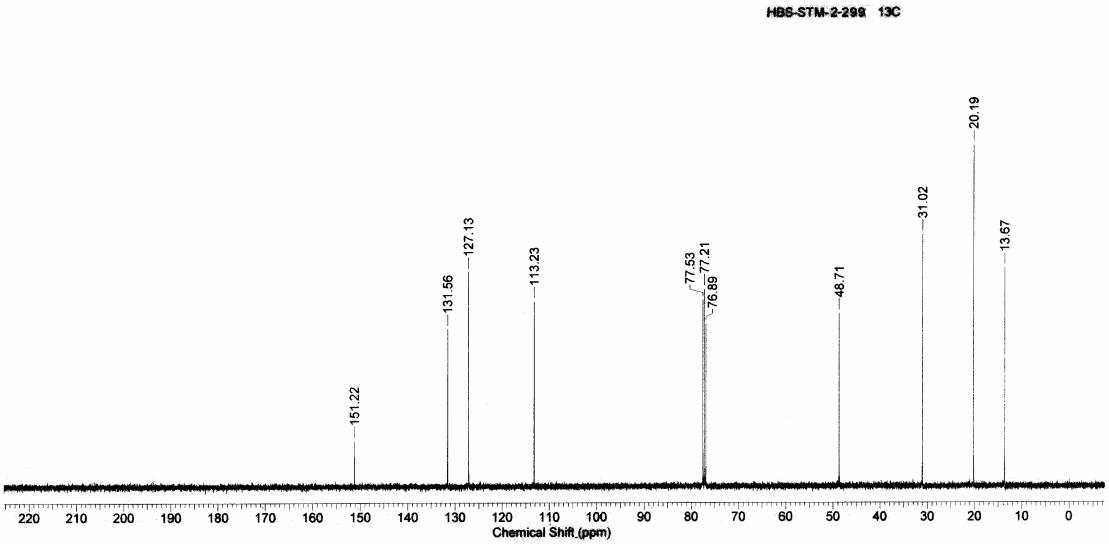


Figure S18. ^{77}Se NMR spectrum of **5c** in $CDCl_3$.

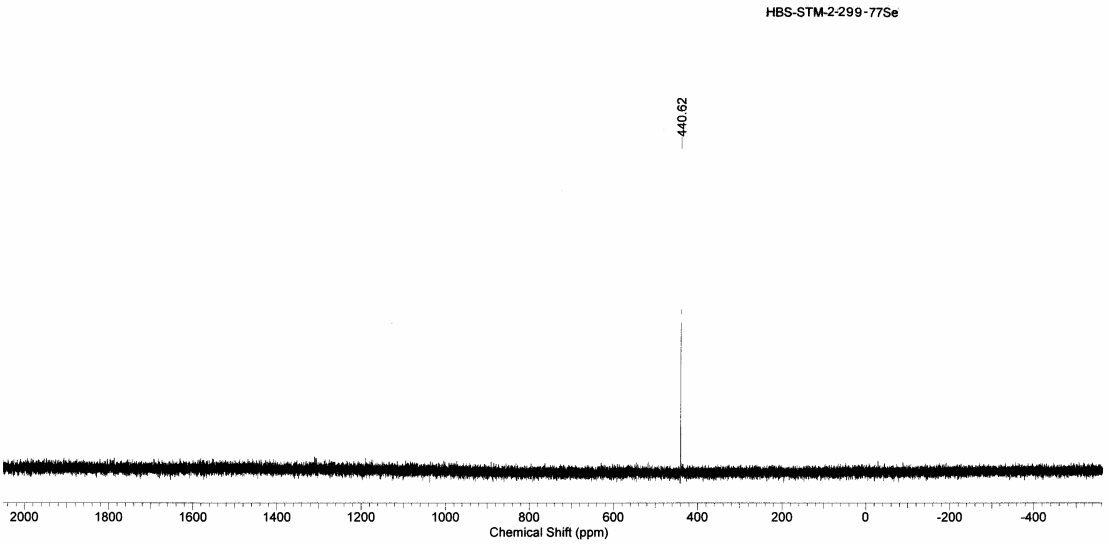


Figure S19. Elemental analysis of **5c**

.

Eager 300 Report

Page: 1 Sample: STM-2-SECL2 (STM-2-SECL2)

Method Name : SD-25-11-11
Method File : D:\CHNS2011\SD-25-11-11.mth
Chromatogram : STM-2-SECL2
Operator ID : SD
Analysed : 11/25/2011 14:44
Sample ID : STM-2-SECL2 (# 23)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 11/25/2011 16:18
Instrument N. : Instrument #1
Sample weight : 1.236

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%		Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	7.37	7.7176	0.34	43 127830	FU	11.438540	.134008E+07
Carbon	47.98	47.6178	0.23	66 1462184	FU	1.000000	.248436E+07
Hydrogen	5.83	6.5047	0.67	178 429982	RS	3.400569	.525488E+07
Totals		61.8401		2019995			

Figure S20. ^{1}H NMR spectrum of **5d** in $CDCl_3$.

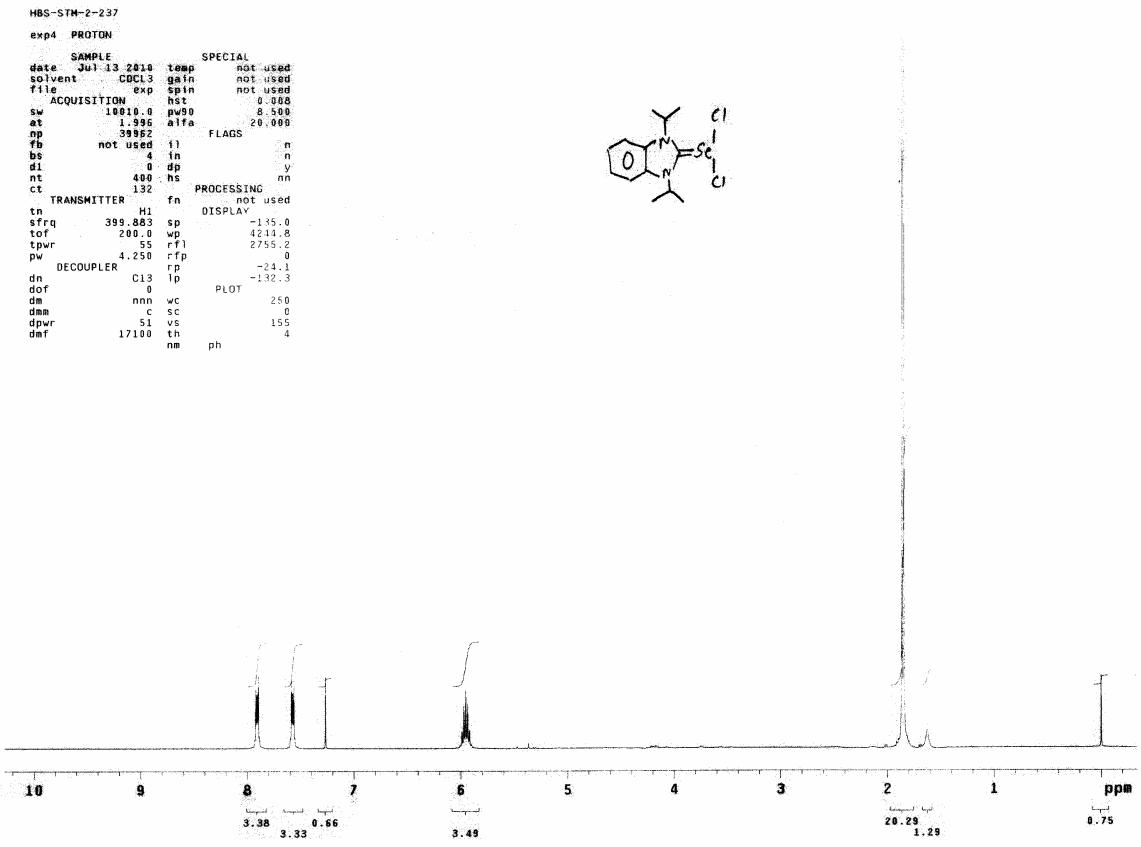


Figure S21. ^{13}C NMR spectrum of **5d** in $CDCl_3$.

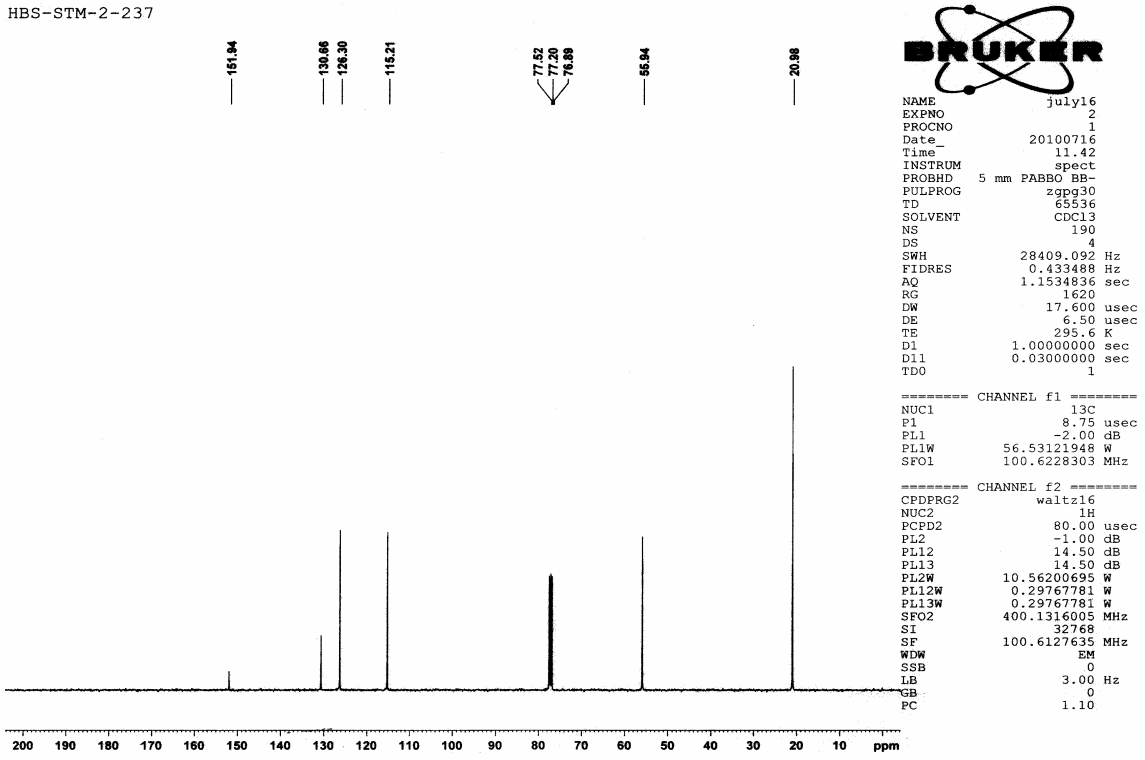


Figure S22. ^{77}Se NMR spectrum of **5d** in $CDCl_3$.

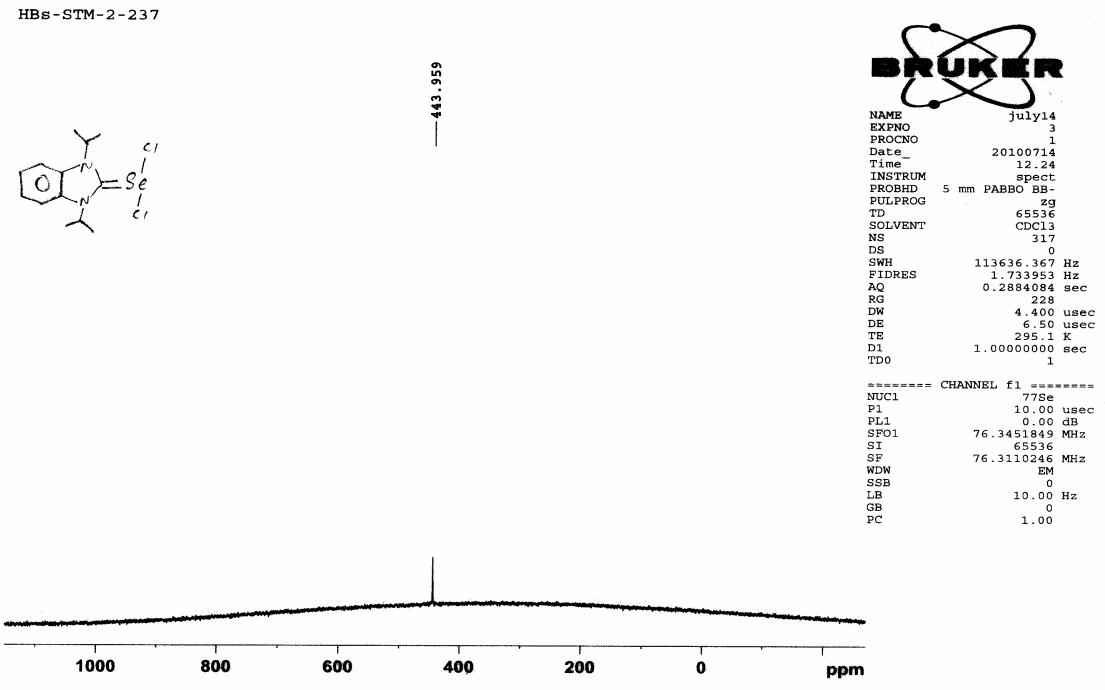


Figure S23. Mass spectrum of **5d**.

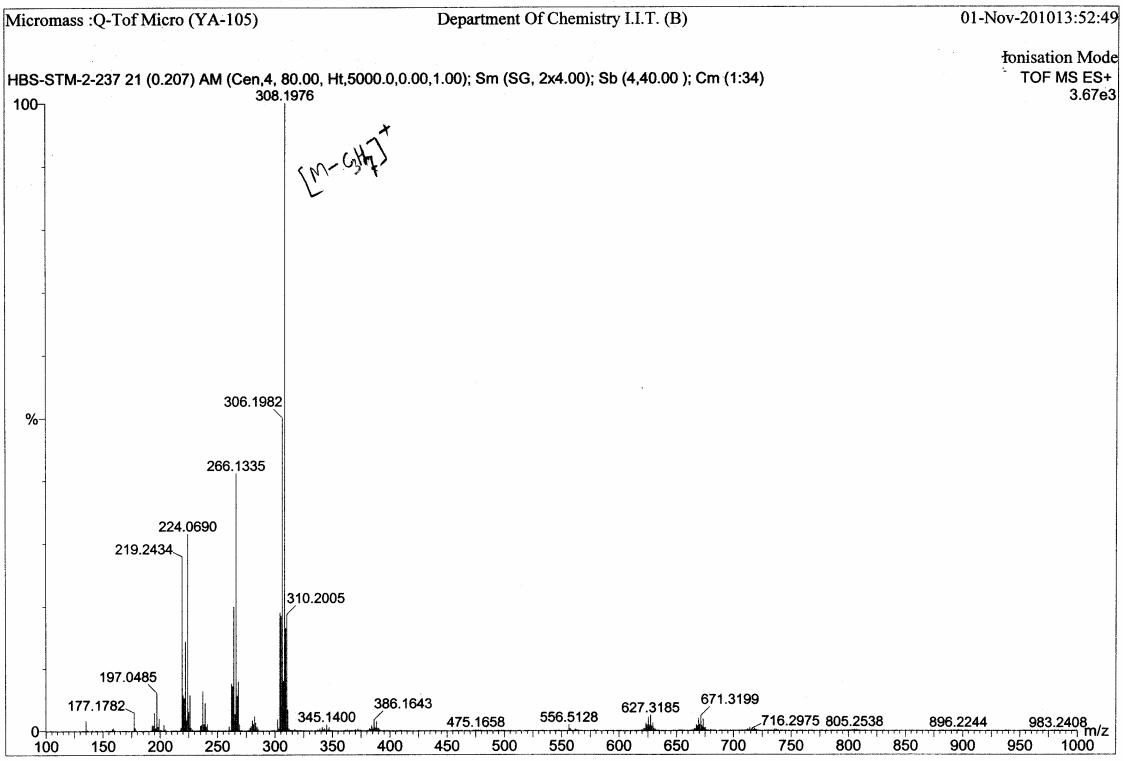


Figure S24. Elemental analysis of **5d**

Eager 300 Report

Page: 1 Sample: STM-2-237 (STM-2-237)

Method Name : SP150910
Method File : D:\CHNS2008\SP150910.mth
Chromatogram : STM-2-237
Operator ID : SP — **Company Name : C.E. Instruments**
Analysed : 09/15/2010 14:19 — **Printed : 9/15/2010 15:41**
Sample ID : STM-2-237 (# 21) — **Instrument N. : Instrument #1**
Analysis Type : UnkNown (Area) — **Sample weight : 1.126**

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name		%	Ret.Time		Area	BC	Area ratio	K factor
Nitrogen	7.95	7.9679	0.01	43	98108	RS	13.478960	.109350E+07
Carbon	44.34	44.2137	0.13	66	1322394	RS	1.000000	.265623E+07
Hydrogen	5.15	5.0596	0.09	175	336072	RS	3.934853	.567435E+07
Totals		57.2412			1756574			

Figure S25. ^{1}H NMR spectrum of **5e** in $CDCl_3$.

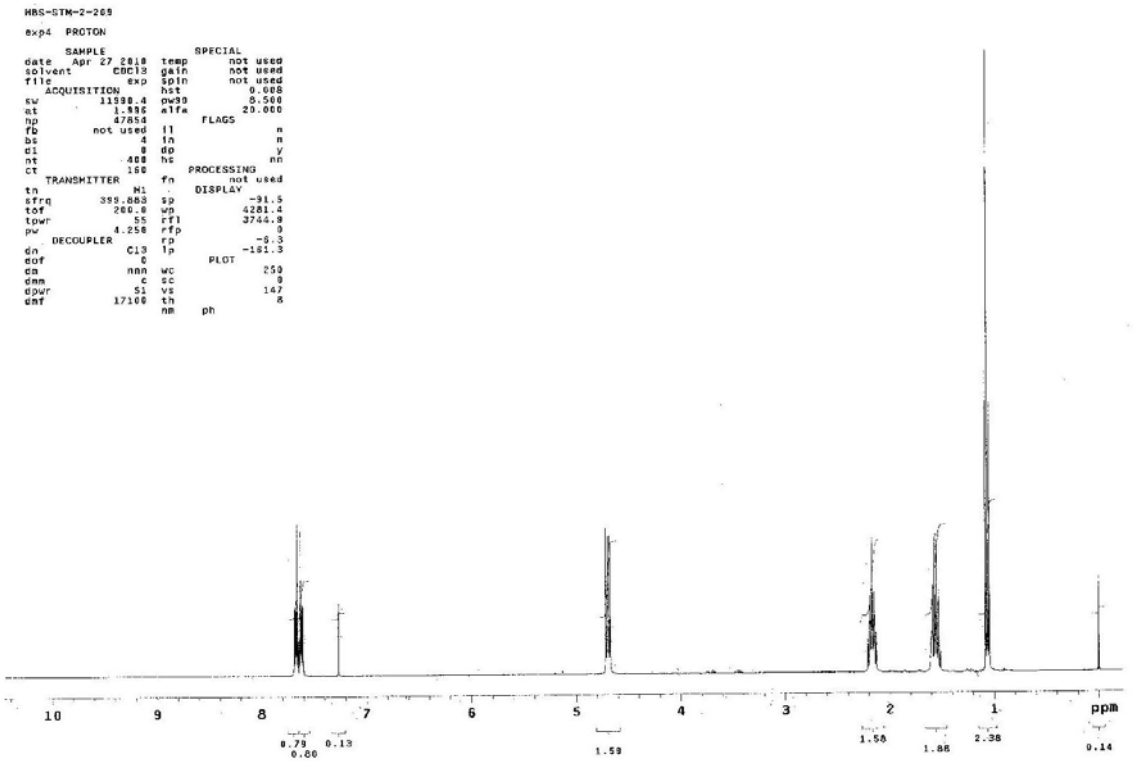


Figure S26. ^{13}C NMR spectrum of **5e** in $CDCl_3$.

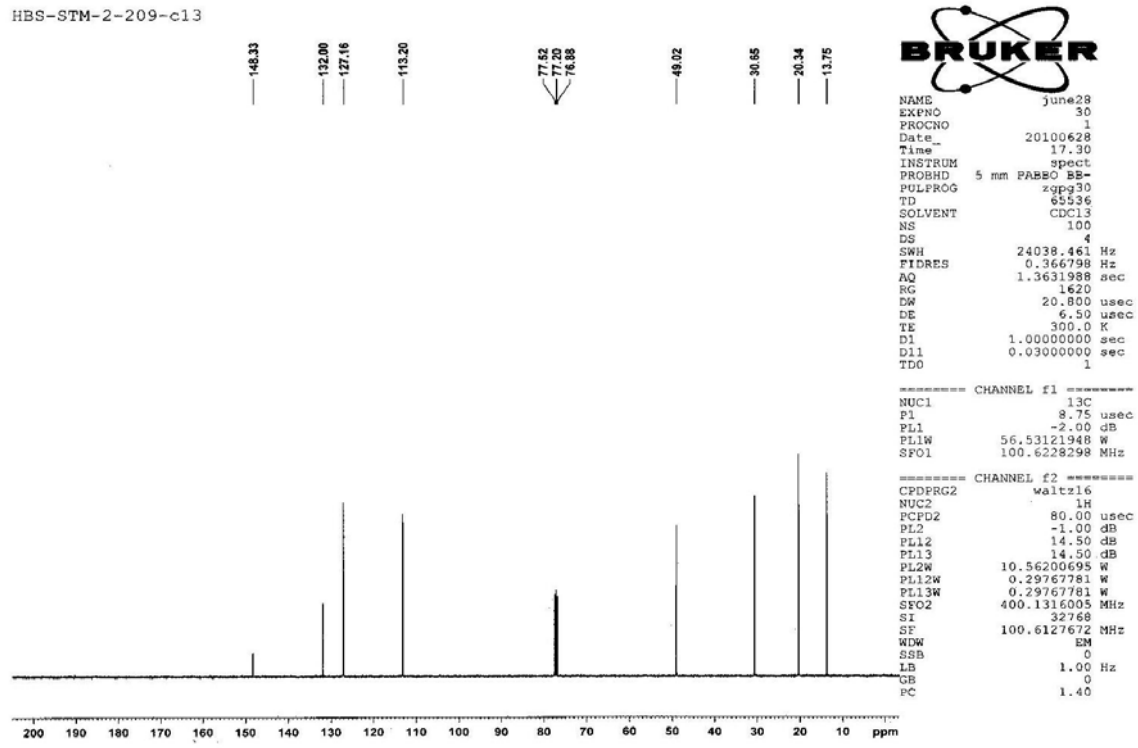


Figure S27. ^{77}Se NMR spectrum of **5e** in $CDCl_3$.

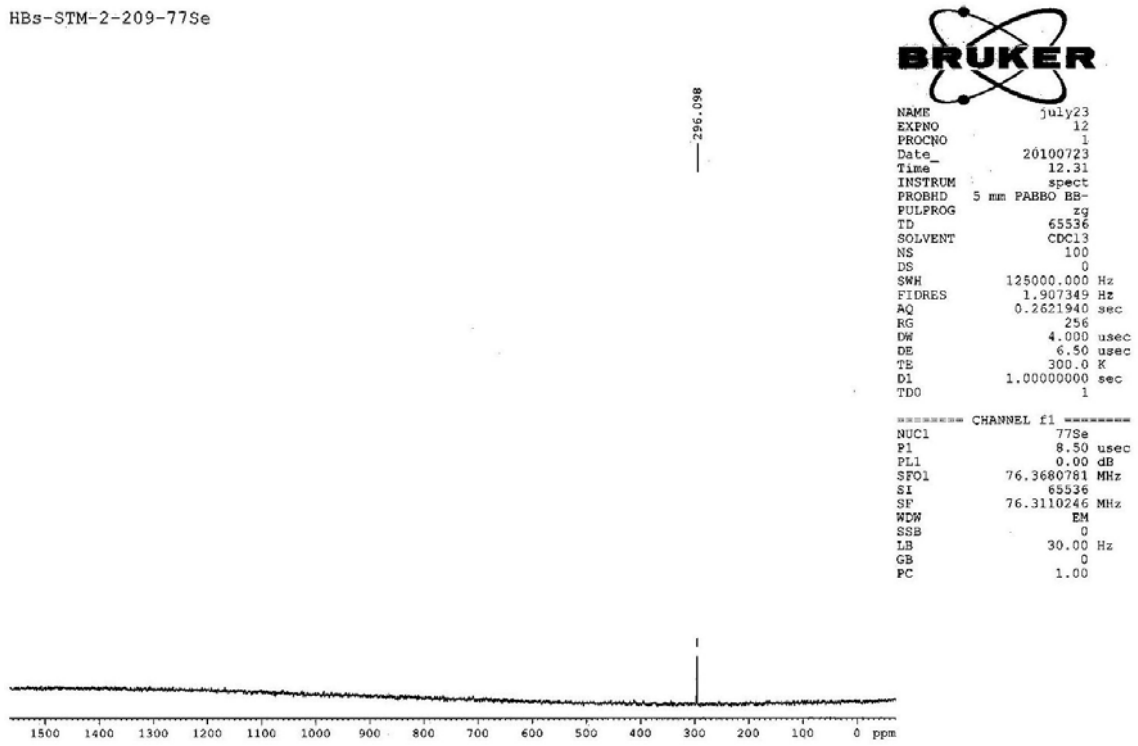


Figure S28. Mass spectrum of **5e**.

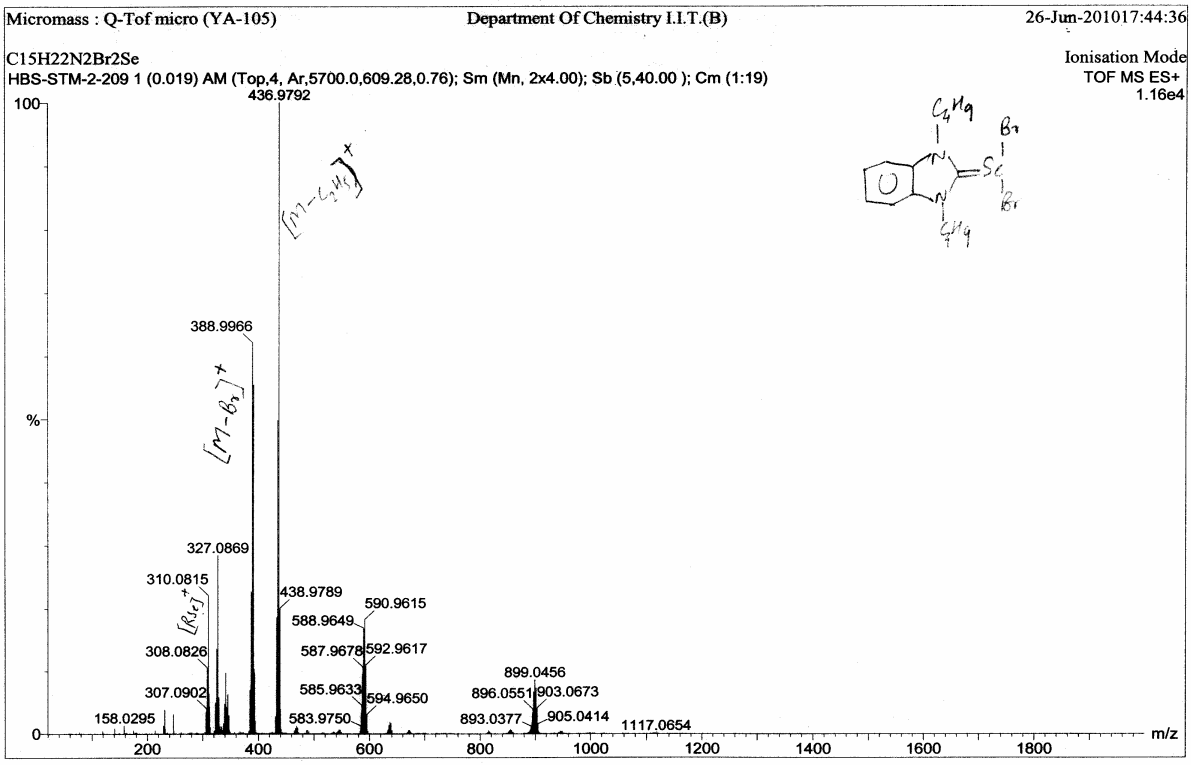


Figure S29. Elemental analysis of **5e**

Eager 300 Report

Page: 1 Sample: STM-2-209 (STM-2-209)

Method Name : SP150910
Method File : D:\CHNS2008\SP150910.mth
Chromatogram : STM-2-209
Operator ID : SP Company Name : C.E. Instruments
Analysed : 09/15/2010 14:01 Printed : 9/15/2010 15:41
Sample ID : STM-2-209 (# 19) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : .859

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
1	0.0000	18	11934	RS		0.0000
Nitrogen	6.2188	43	58415	RS	15.092350	.109350E+07
Carbon	38.6383	67	881612	RS	1.000000	.265623E+07
Hydrogen	4.4645	178	230412	RS	3.826242	.567435E+07
Totals	49.3217		1182373			

Figure S30. ^{1}H NMR spectrum of **5f** in $CDCl_3$.

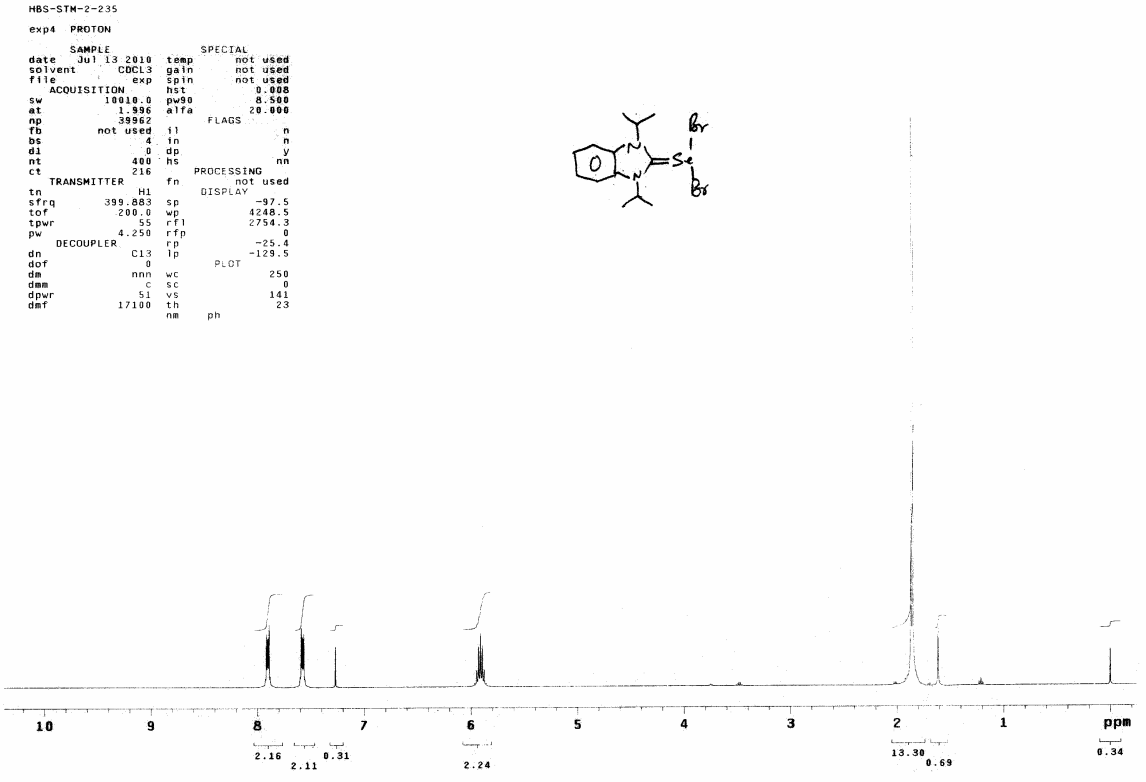


Figure S31. ^{13}C NMR spectrum of **5f** in $CDCl_3$.

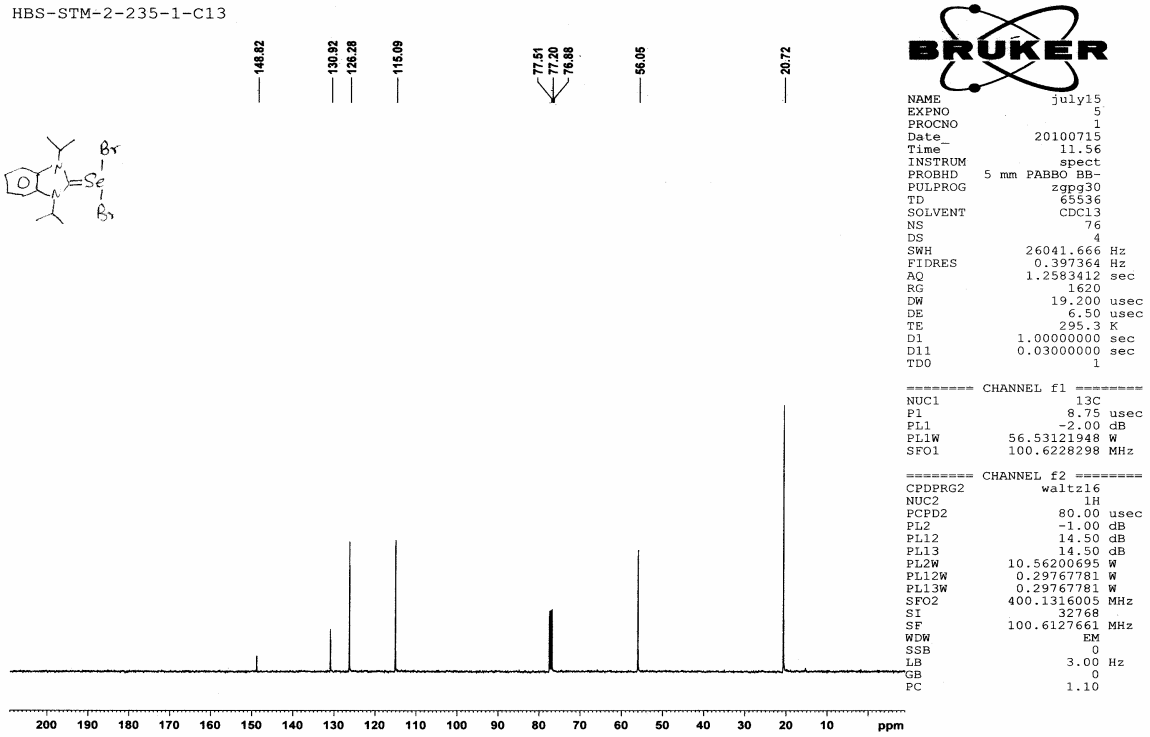


Figure S32. ^{77}Se NMR spectrum of **5f** in $CDCl_3$.

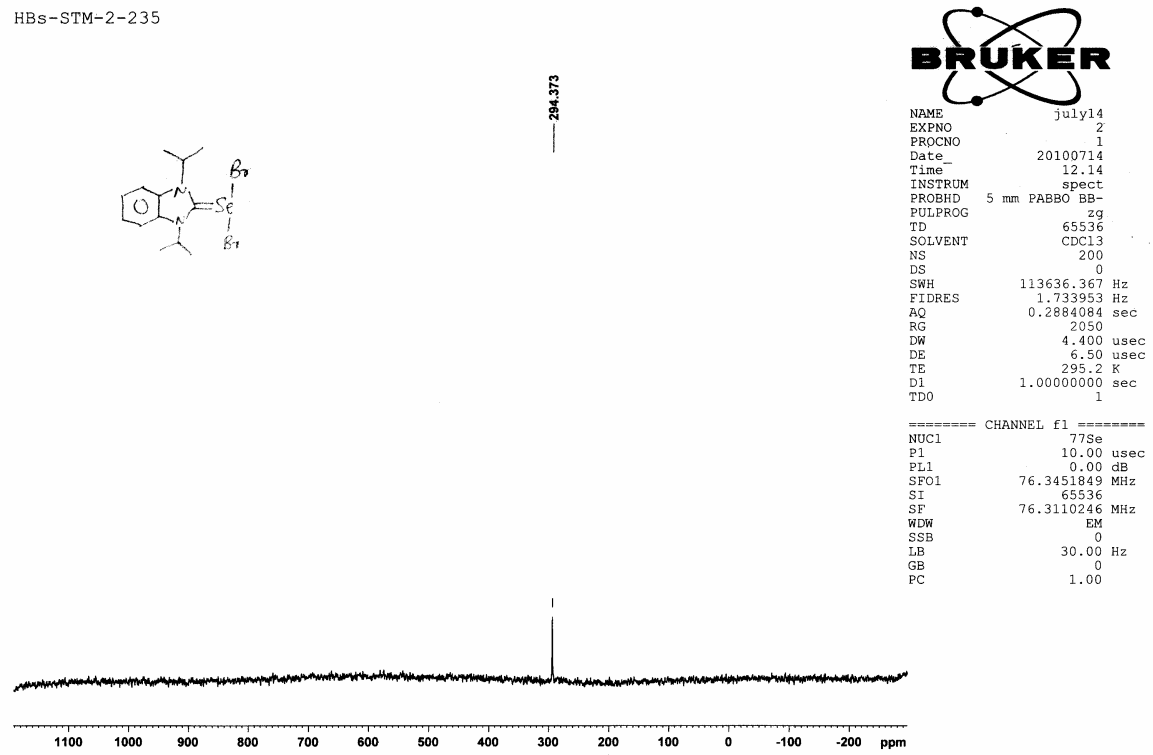


Figure S33. Mass spectrum of **5f**.

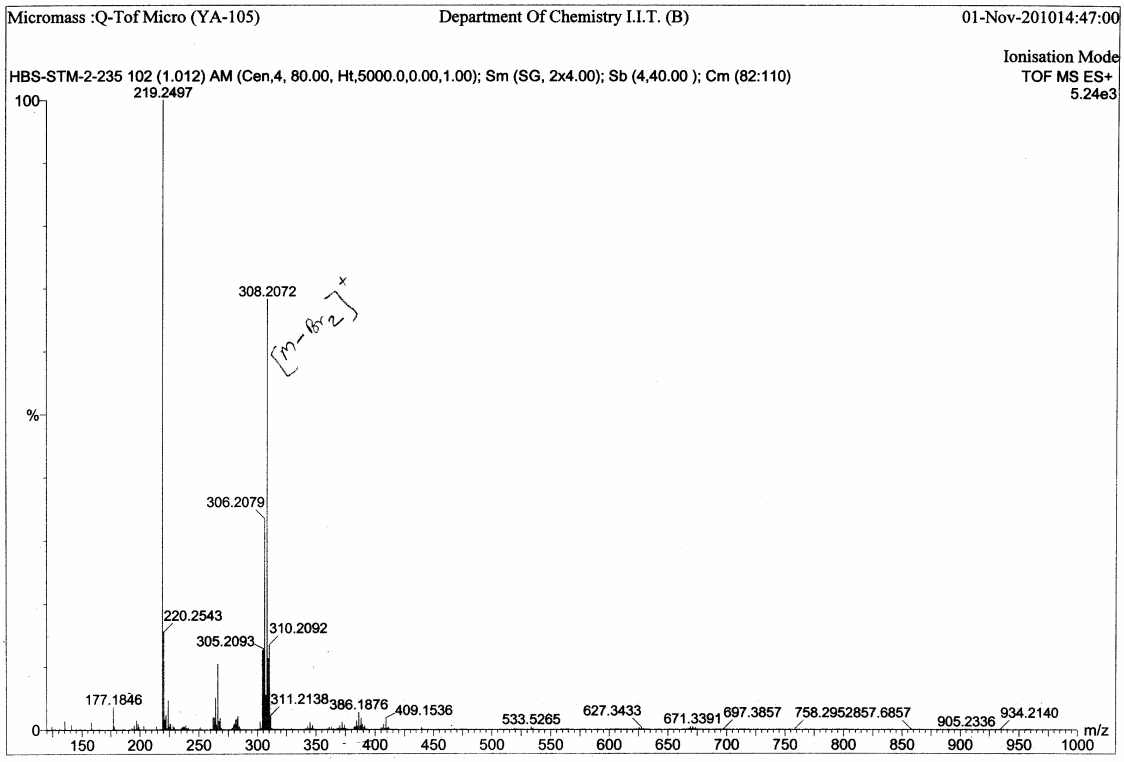
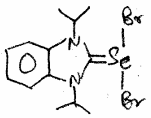


Figure S34. Elemental analysis of **5f**



Eager 300 Report

Page: 1 Sample: STM2235 (STM2235)

Method Name : SP100810
Method File : D:\CHNS2008\SD100810.mth
Chromatogram : STM2235
Operator ID : SD
Analysed : 08/10/2010 13:34
Sample ID : STM2235 (# 15)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 8/10/2010 15:31
Instrument N. : Instrument #1
Sample weight : .969

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name		%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	6.35	6.0967	0.26	43 69525	RS	13.057660	.117684E+07
Carbon	35.40	35.2921	0.11	66 907828	RS	1.000000	.265462E+07
Hydrogen	4.11	3.6624	0.26	175 218971	RS	4.145880	.593892E+07
Totals		45.0512		1196323			

Figure S35. ^{1}H NMR spectrum of **5g** in $CDCl_3$.

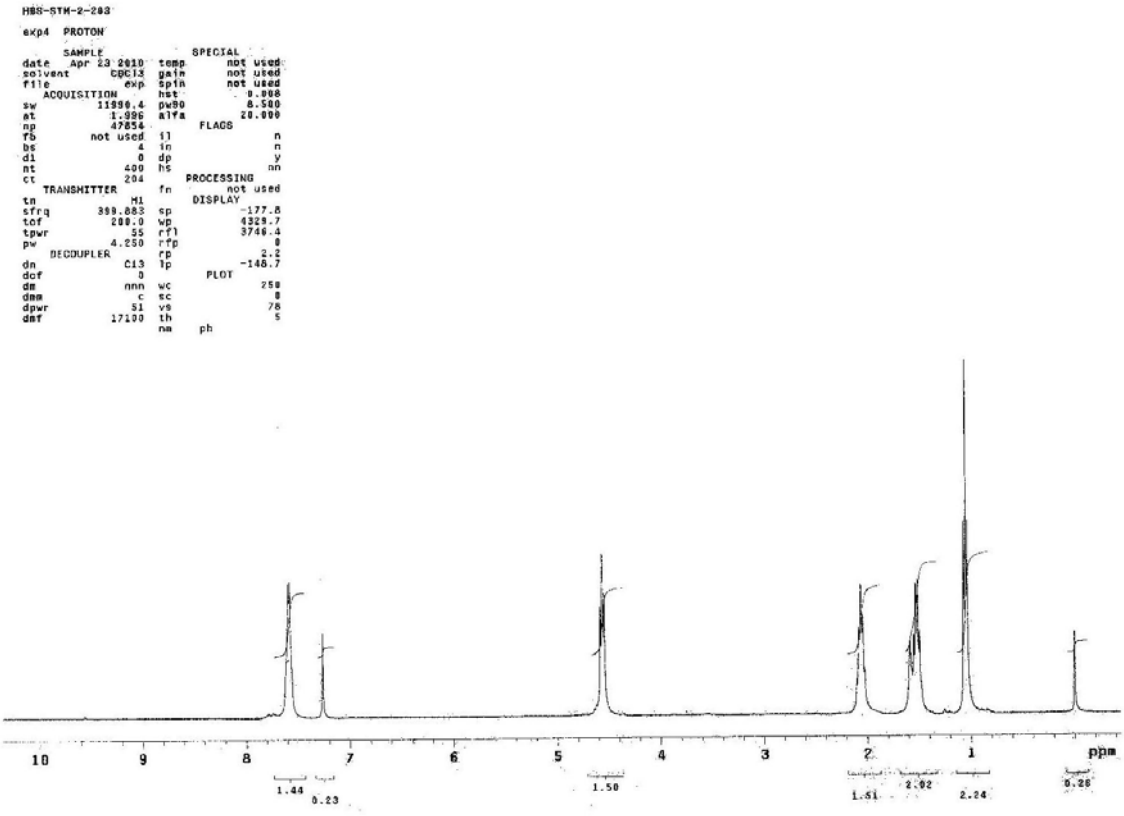


Figure S36. ^{13}C NMR spectrum of **5g** in $CDCl_3$.

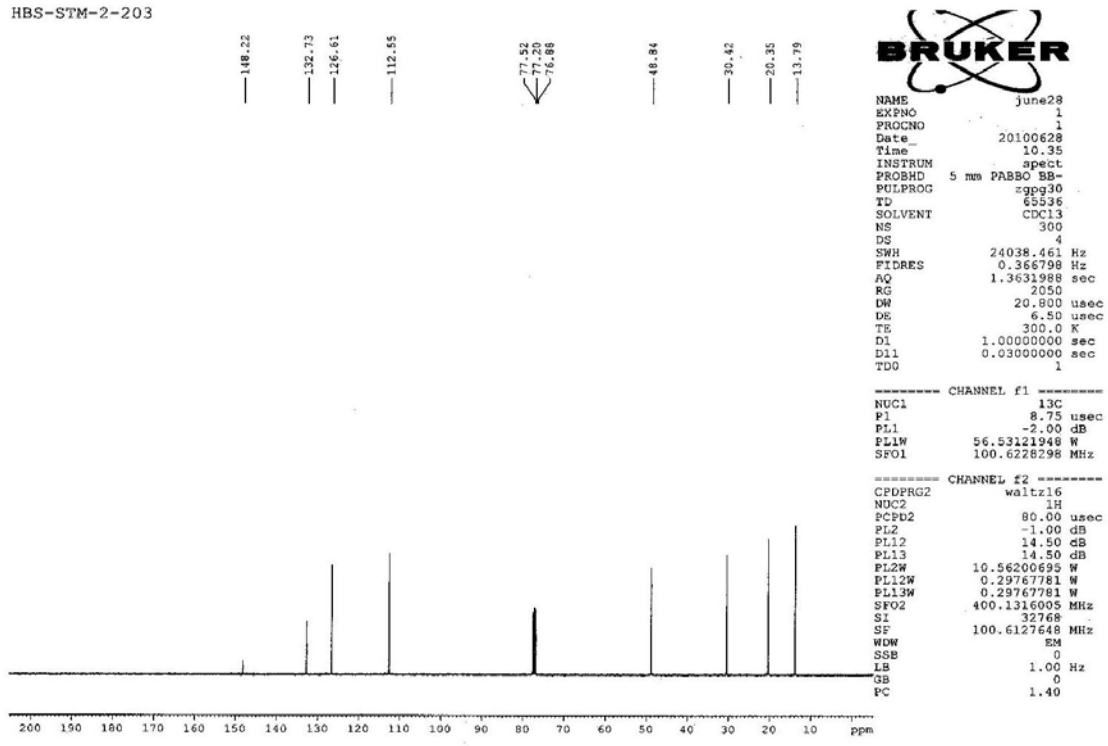


Figure S37. ^{77}Se NMR spectrum of **5g** in $CDCl_3$.

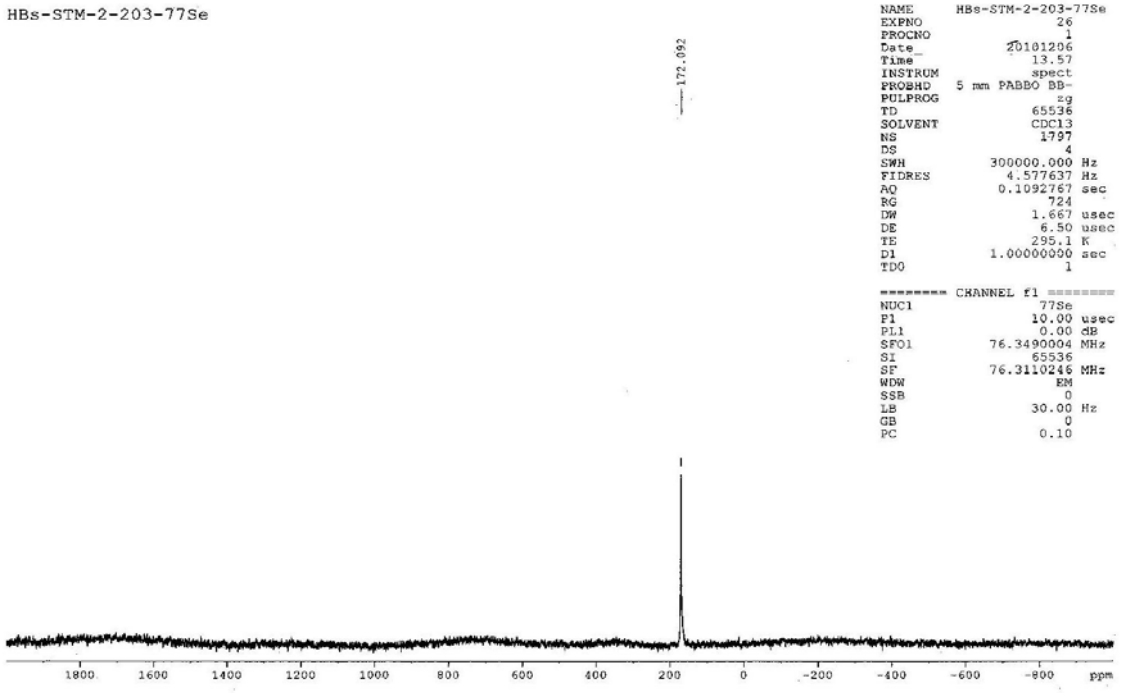


Figure S38. Mass spectrum of **5g**.

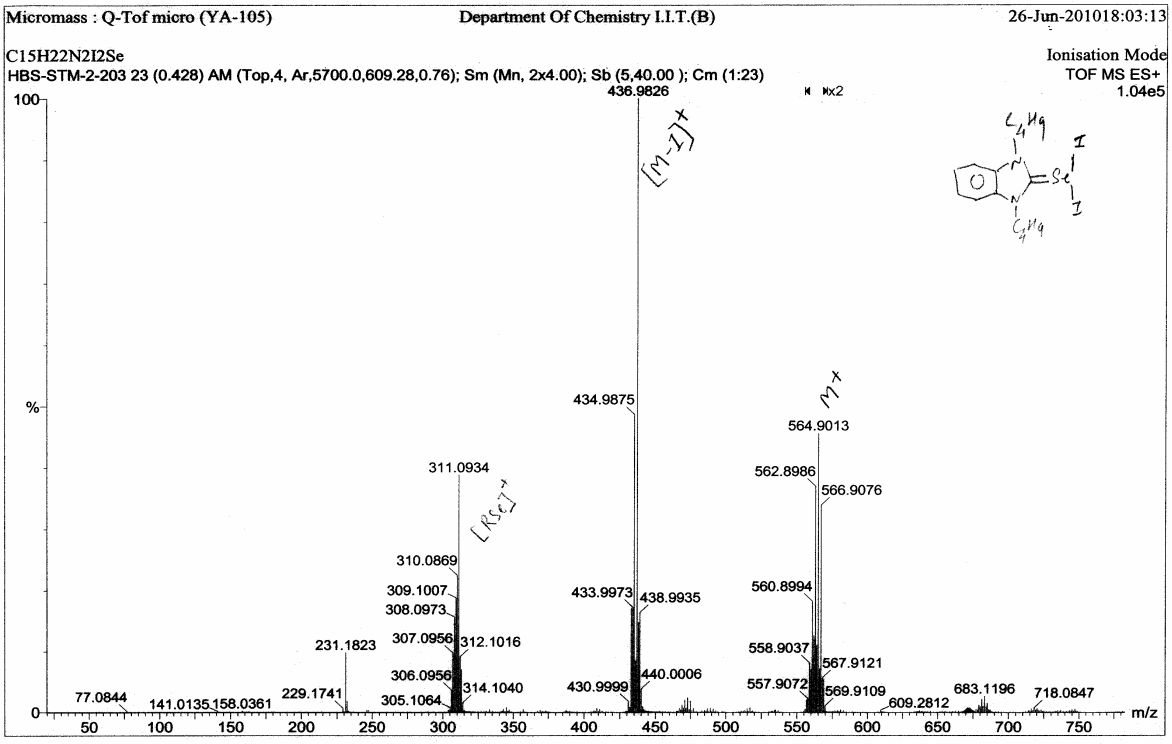


Figure S39. Elemental analysis of **5g**

Eager 300 Report

Page: 1 Sample: STM2-203 (STM2-203)

Method Name : SP110510
Method File : D:\CHNS2008\SP110510.mth
Chromatogram : STM2-203
Operator ID : SP **Company Name : C.E. Instruments**
Analysed : 07/20/2012 15:26 **Printed : 7/20/2012 15:47**
Sample ID : STM2-203 (# 25) **Instrument N. : Instrument #1**
Analysis Type : UnkNown (Area) **Sample weight : .827**

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	4.8866	44	69842	RS	9.727170	.122634E+07
Carbon	32.4527	69	679365	RS	1.000000	.252191E+07
Hydrogen	3.9353	169	294496	RS	2.306873	.656520E+07
Totals	41.2745		1043703			

Figure S40. ^{1}H NMR spectrum of **5h** in $CDCl_3$.

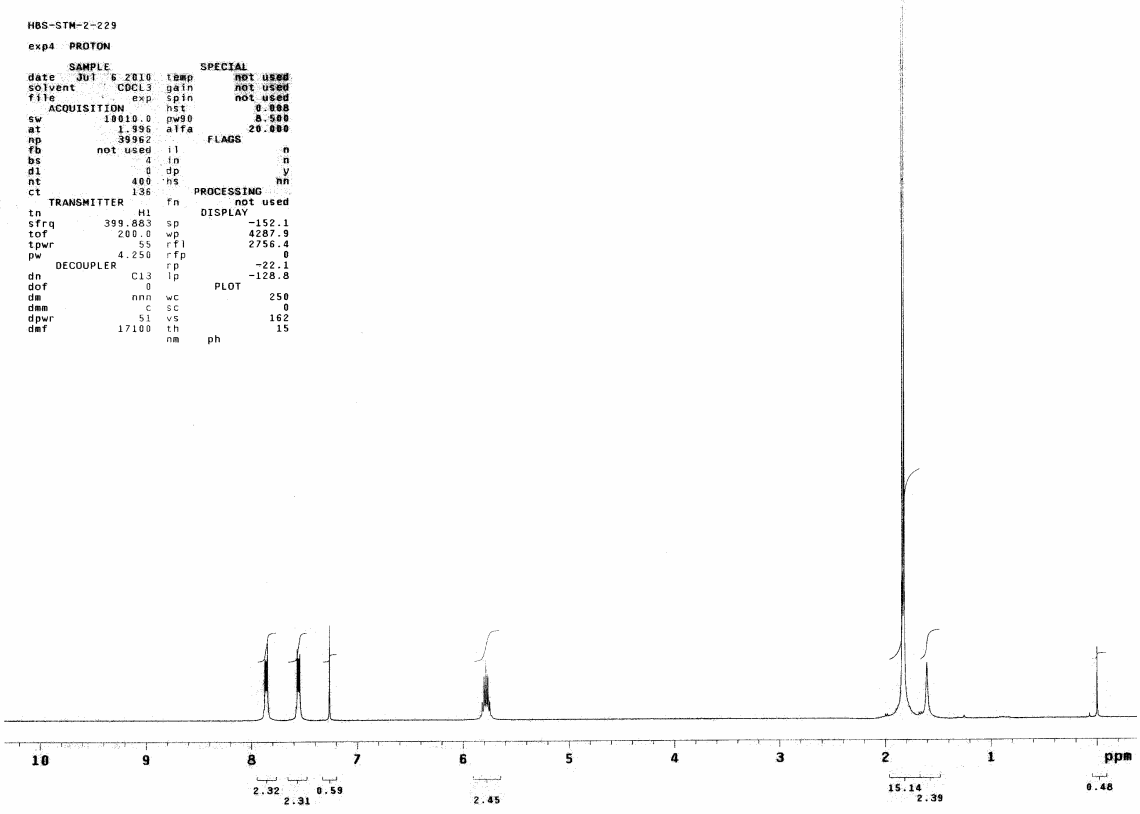


Figure S41. ^{13}C NMR spectrum of **5h** in $CDCl_3$.

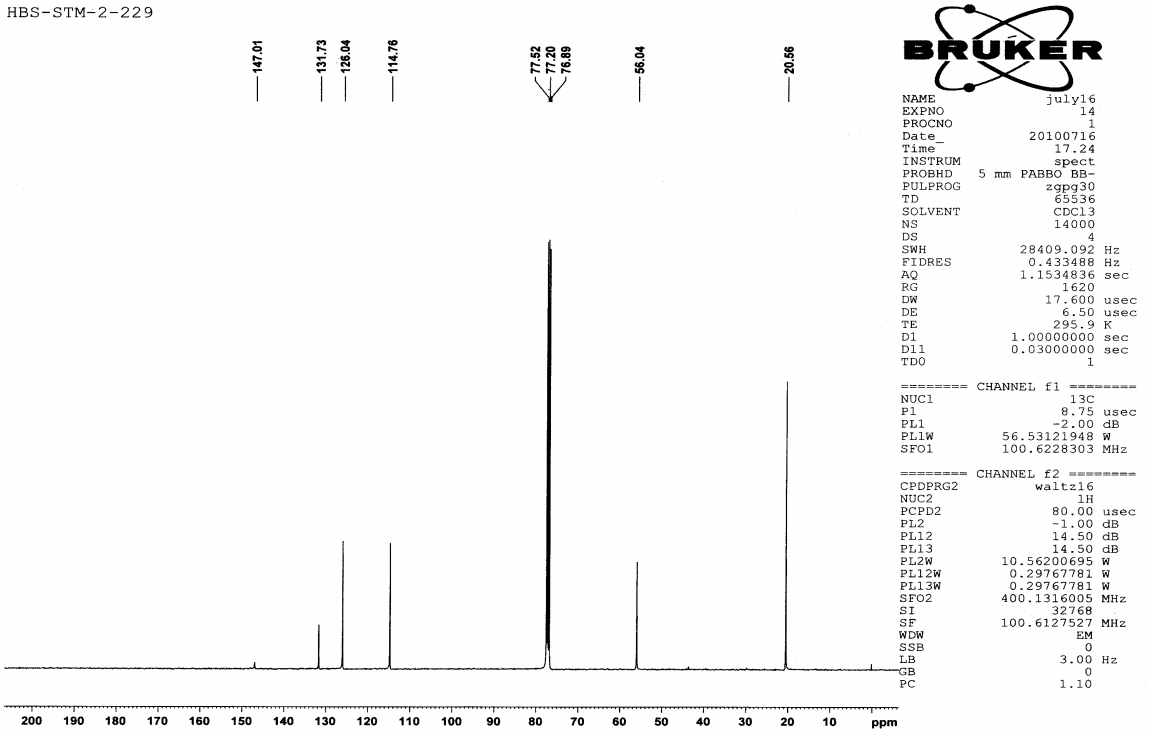


Figure S42. ^{77}Se NMR spectrum of **5h** in DMSO-d_6.

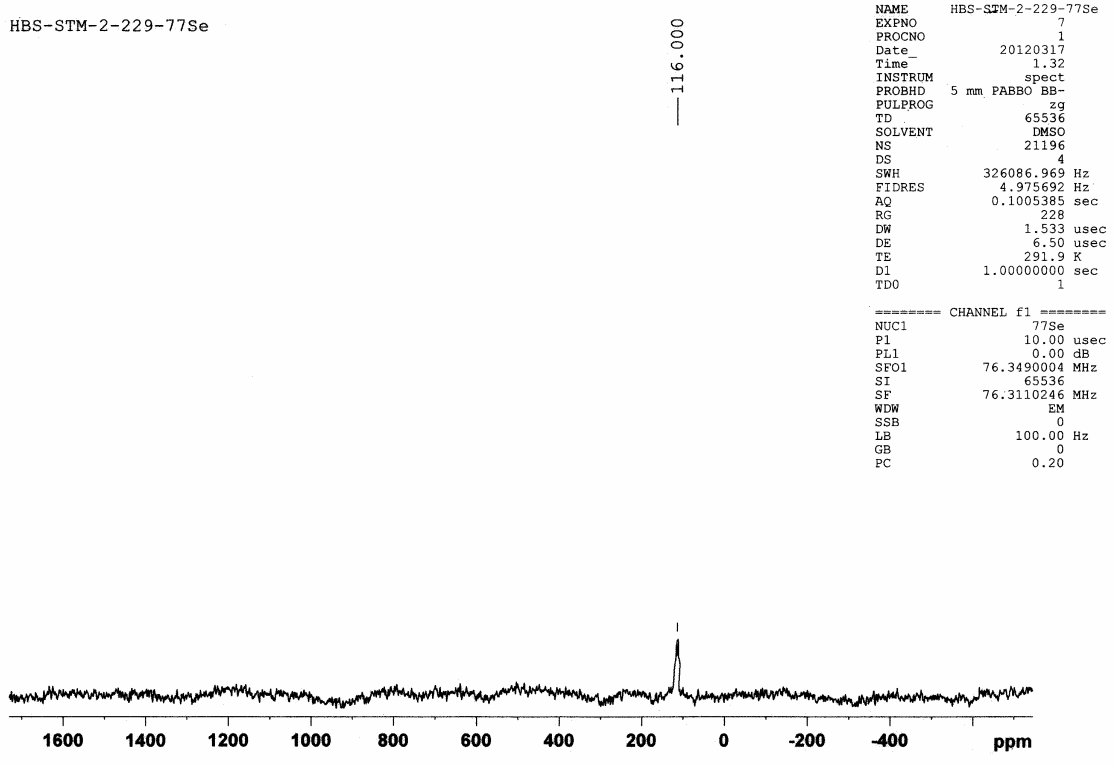


Figure S43. HRMS spectrum of **5h**.

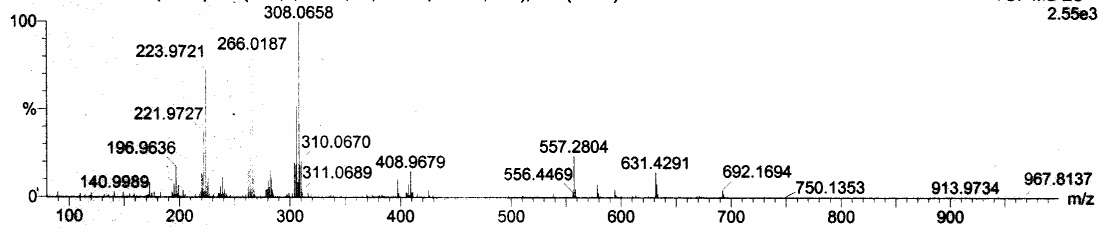
Elemental Composition Report **Page 1**

Single Mass Analysis (displaying only valid results)
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
101 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 18-May-201116:38:43

C13H18I2N2Se
HBS-STM-2-229 39 (0.389) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Cm (13:46) TOF MS ES+
2.55e3



Minimum:				-1.5		
Maximum:		200.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
408.9679	408.9680	-0.1	-0.3	6.5	1	C13 H18 N2 Se I

Figure S44. Elemental analysis of **5h**

Eager 300 Report

Page: 1 Sample: STM2233 (STM2233)

Method Name : SP100810
Method File : D:\CHNS2008\SD100810.mth
Chromatogram : STM2233
Operator ID : SD **Company Name : C.E. Instruments**
Analysed : 07/20/2012 13:45 **Printed : 7/20/2012 15:31**
Sample ID : STM2233 (# 16) **Instrument N. : Instrument #1**
Analysis Type : UnkNown (Area) **Sample weight : .889**

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	5.6447	43	48593	RS	13.187370	.117684E+07
Carbon	29.1536	67	640814	RS	1.000000	.265462E+07
Hydrogen	3.6405	178	147613	RS	4.341176	.593892E+07
Totals	38.4387		837020			

Figure S45. ^{1}H NMR spectrum of **5i** in $CDCl_3$.

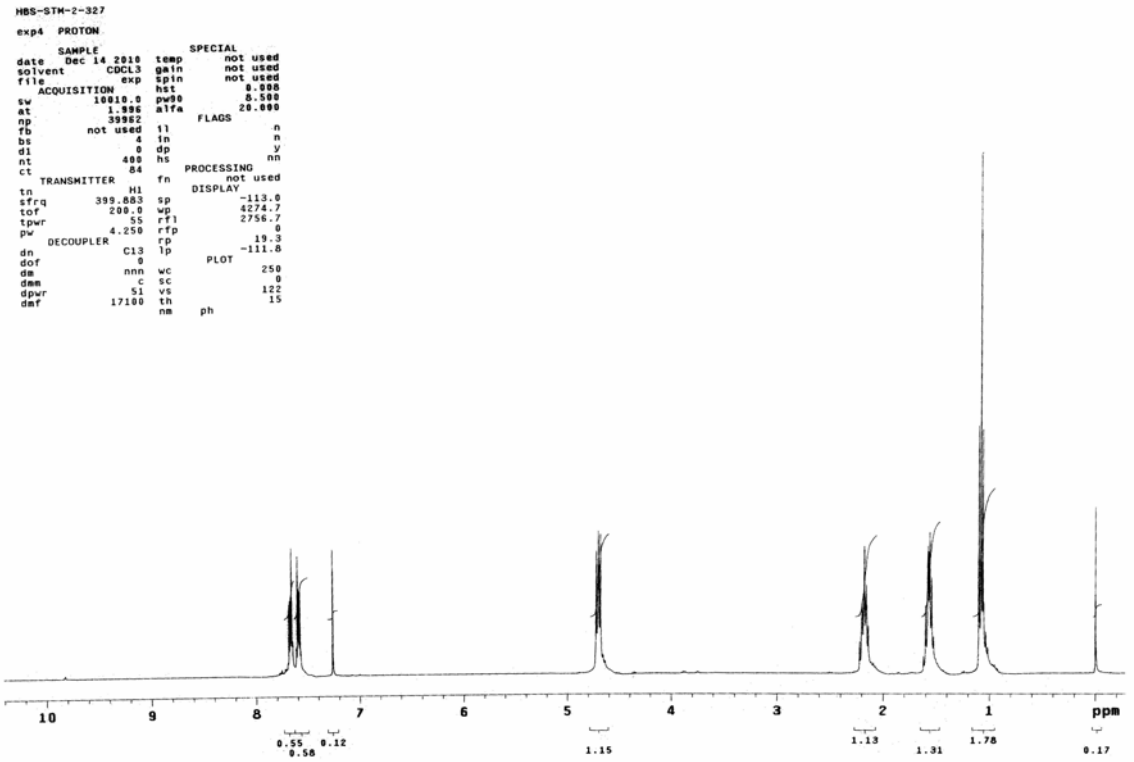


Figure S46. ^{13}C NMR spectrum of **5i** in $CDCl_3$.

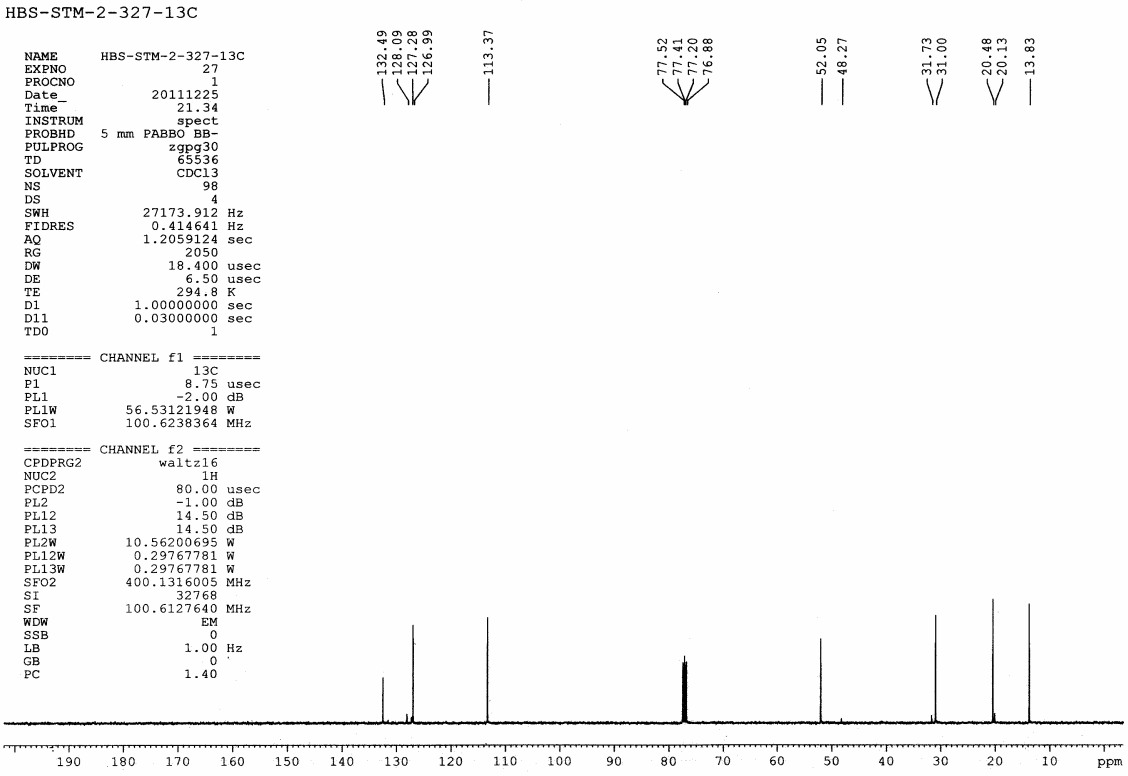


Figure S47. ^{125}Te NMR spectrum of **5i** in $CDCl_3$.

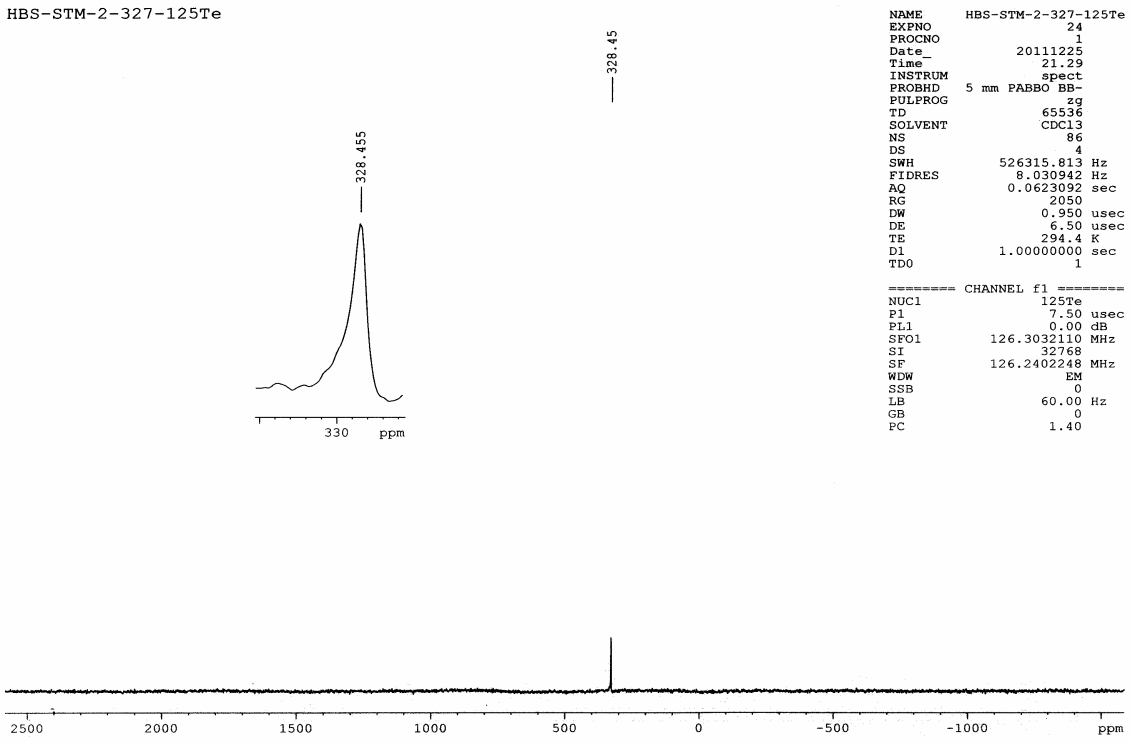


Figure S48. Mass spectrum of **5i**.

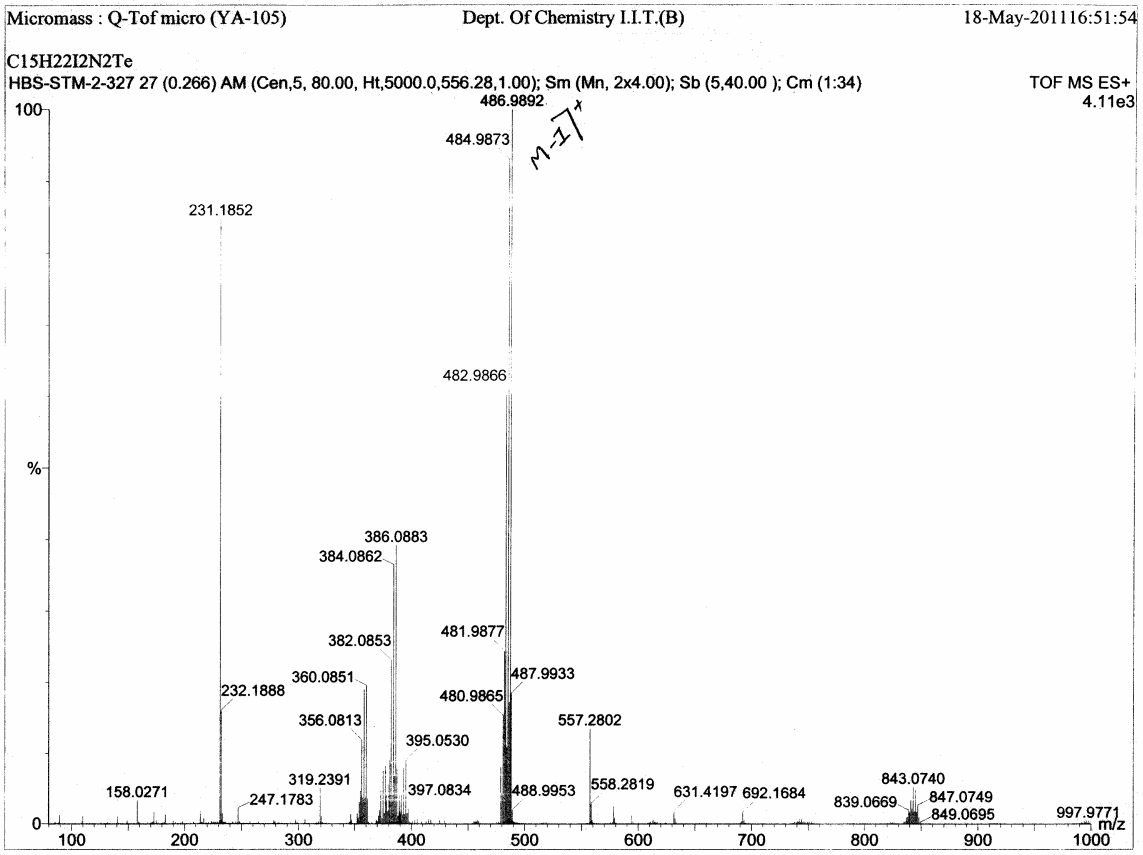


Figure S49. Elemental analysis of **5i**.

Eager 300 Report

Page: 1 Sample: STM-2-327 (STM-2-327)

Method Name : SD-25-11-11
Method File : D:\CHNS2011\SD-25-11-11.mth
Chromatogram : STM-2-327
Operator ID : SD
Analysed : 11/25/2011 13:53
Sample ID : STM-2-327 (# 18)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 11/25/2011 16:18
Instrument N. : Instrument #1
Sample weight : .664

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name		%	Ret.Time		Area	BC	Area ratio	K factor
Nitrogen	4.58	4.7451	0.16	43	60019	RS	8.056115	.134008E+07
Carbon	29.45	29.3111	0.14	67	483520	RS	1.000000	.248436E+07
Hydrogen	3.62	3.1382	0.49	184	117001	RS	4.132614	.525488E+07
Totals		37.1944			660540			

Figure S50. ^{1}H NMR spectrum of **7a** in $CDCl_3$.

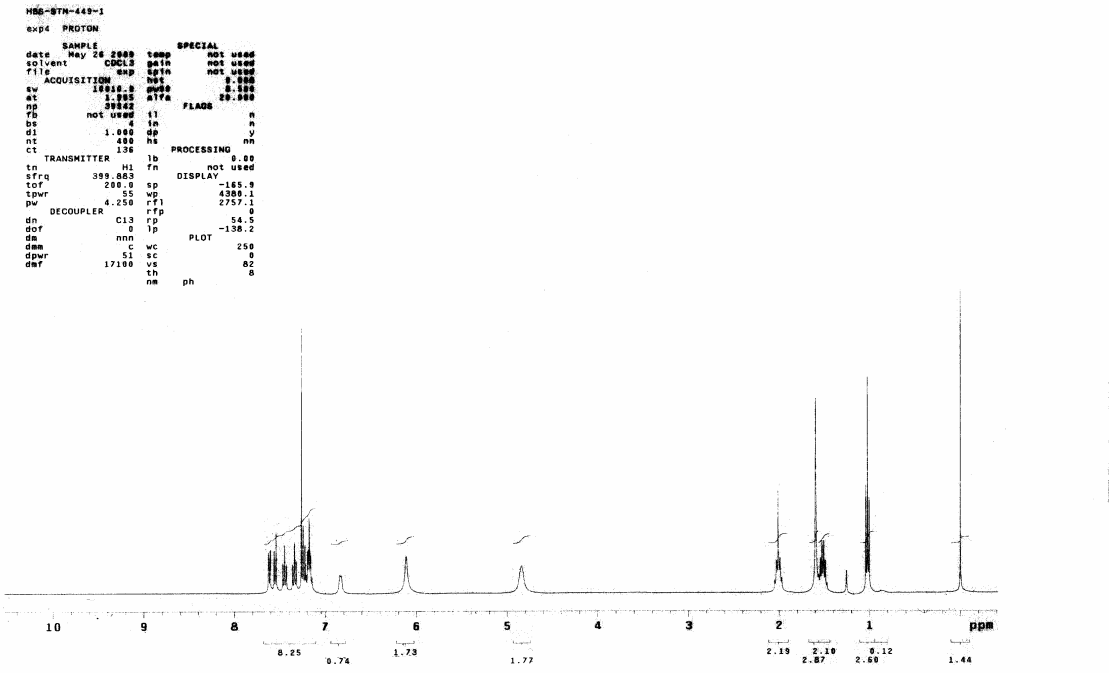


Figure S51. ^{13}C NMR spectrum of **7a** in $CDCl_3$.

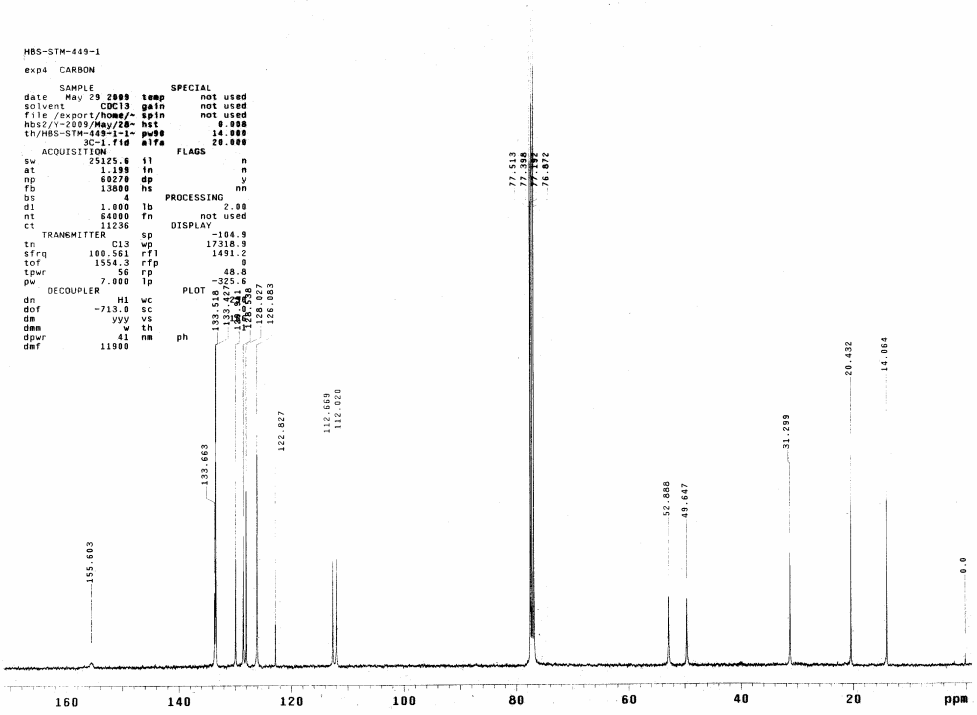


Figure S52. ^{77}Se NMR spectrum of **7a** in $CDCl_3$.

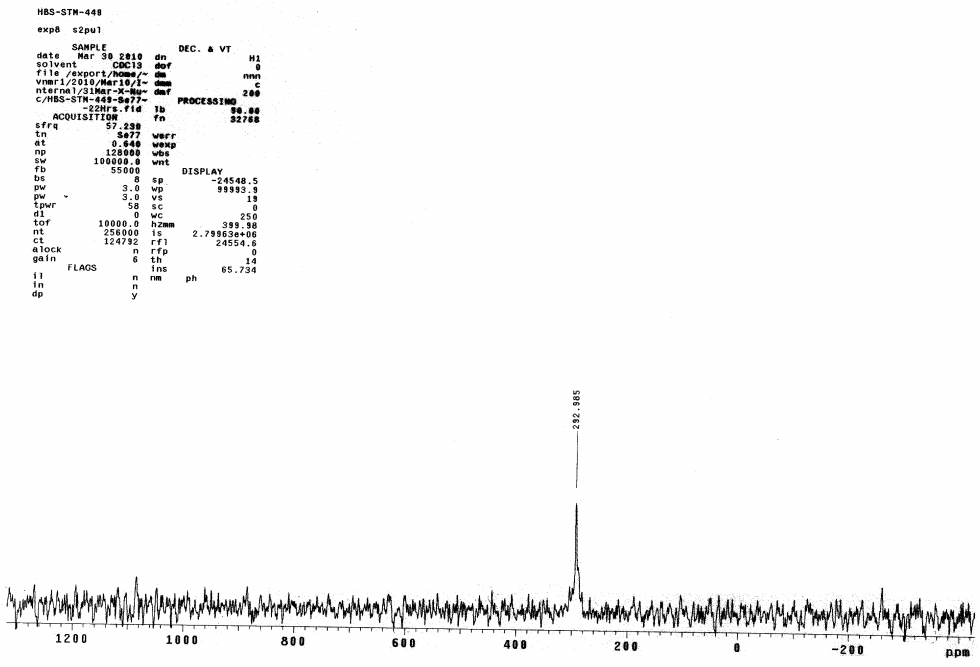


Figure S53. ^{125}Te NMR spectrum of **7a** in $CDCl_3$.

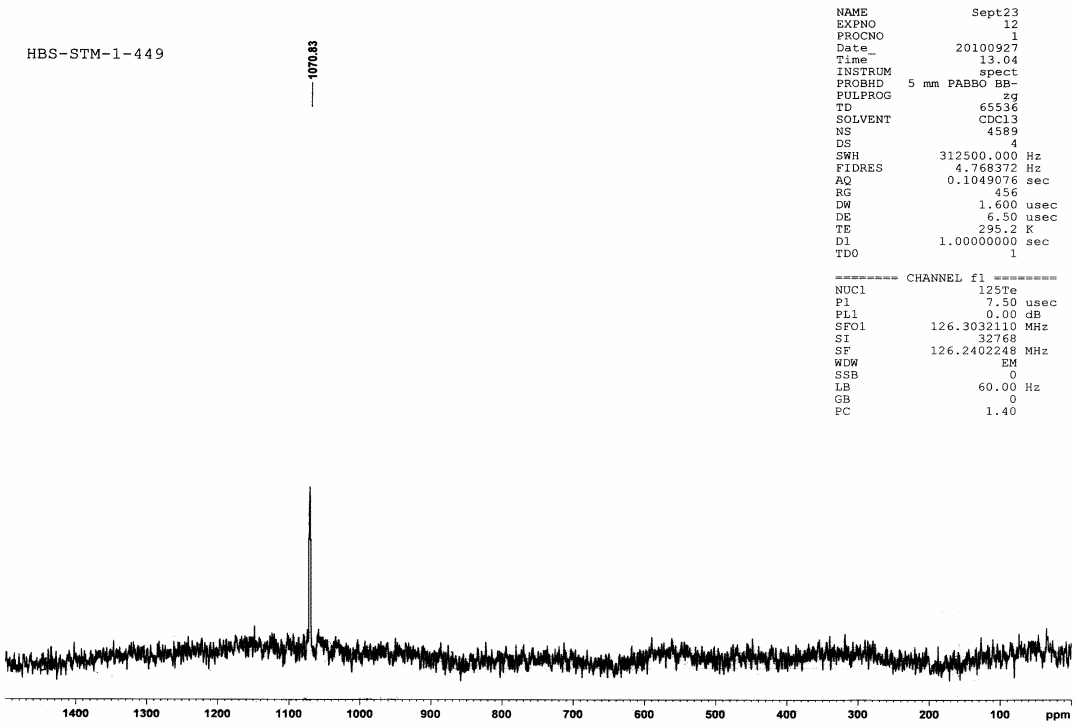


Figure S54. Mass spectrum of **7a**.

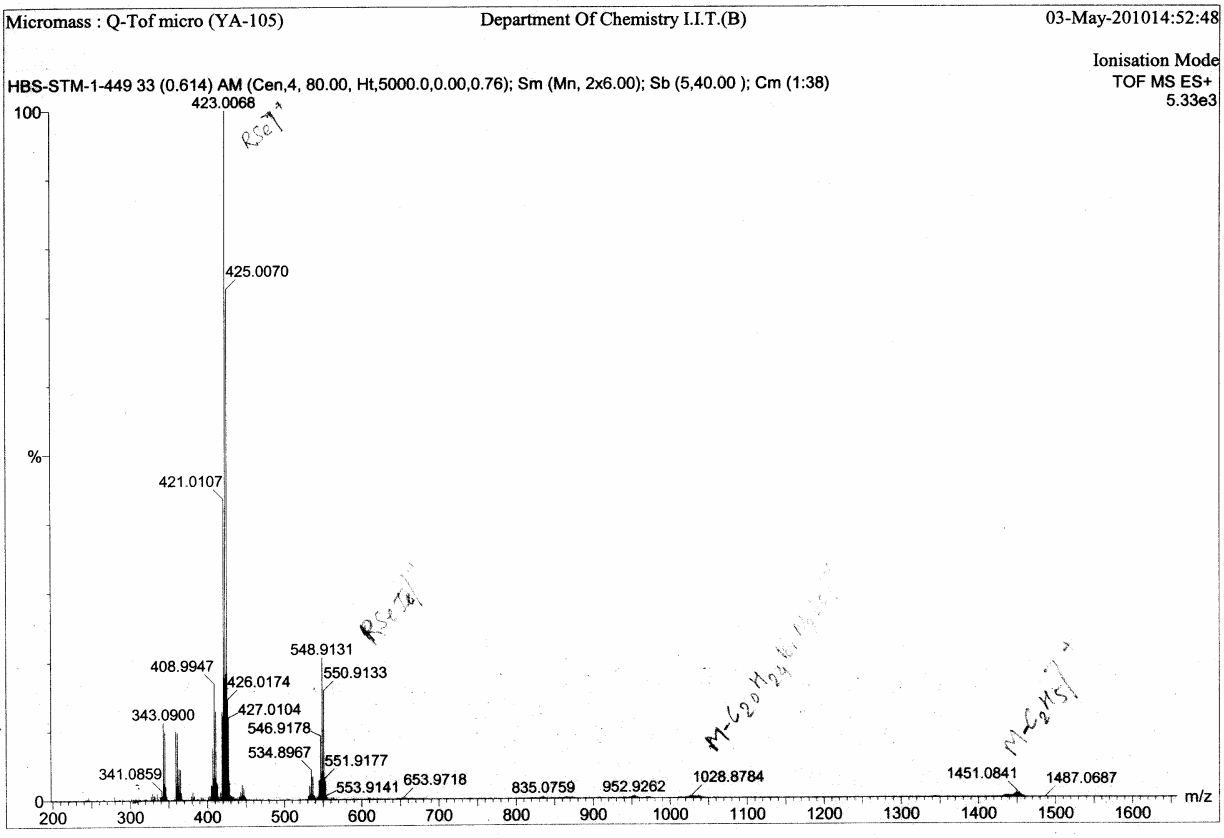


Figure S55. Elemental analysis of **7a**.

Eager 300 Report

Page: 1 Sample: STM449 (STM449)

Method Name : SP131109
Method File : D:\CHNS2008\SP131109.mth
Chromatogram : STM449
Operator ID : SP **Company Name : C.E. Instruments**
Analysed : 11/13/2009 13:37 **Printed : 11/13/2009 14:47**
Sample ID : STM449 (# 22) **Instrument N. : Instrument #1**
Analysis Type : UnkNown (Area) **Sample weight : .746**

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
1	0.0000	18	4100	RS		0.0000
Nitrogen 3.79	4.1871	0.39 43	34472	RS	17.046310	.110361E+07
Carbon 29.22	29.7995	0.57 67	587621	RS	1.000000	.263282E+07
Hydrogen 2.59	2.2635	0.33 178	107696	RS	5.456289	.577099E+07
Totals	36.2501		733888			

Figure S56. ^{1}H NMR spectrum of **7b** in $CDCl_3$.

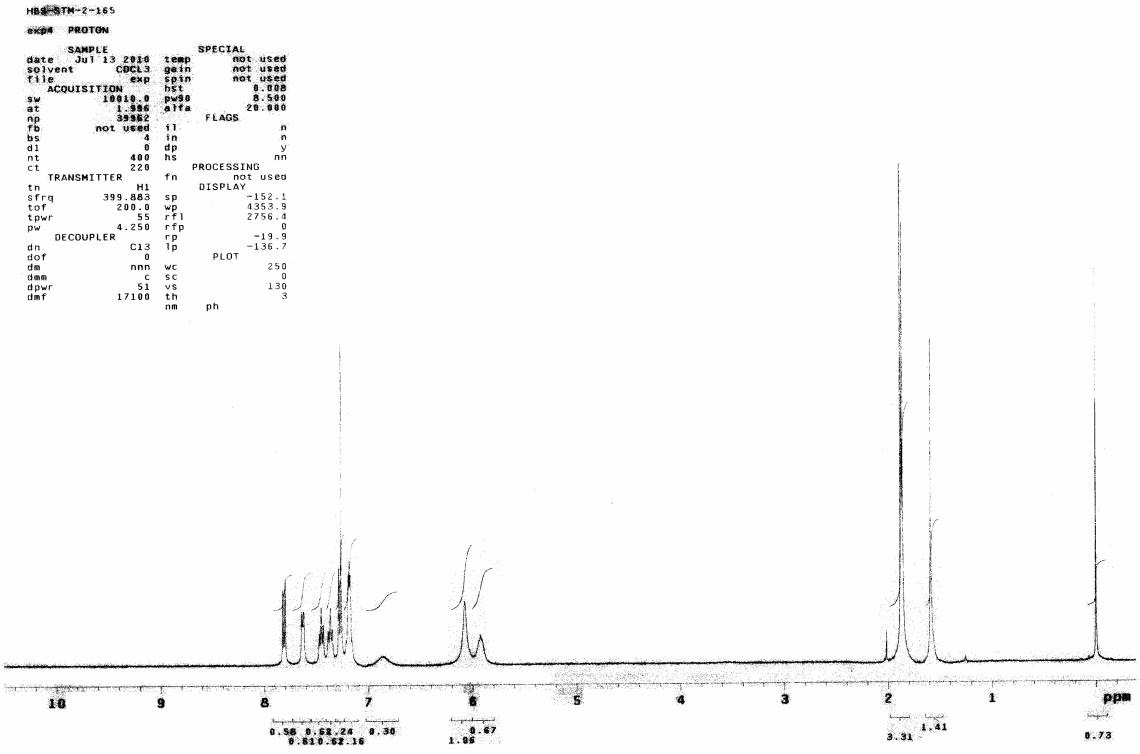
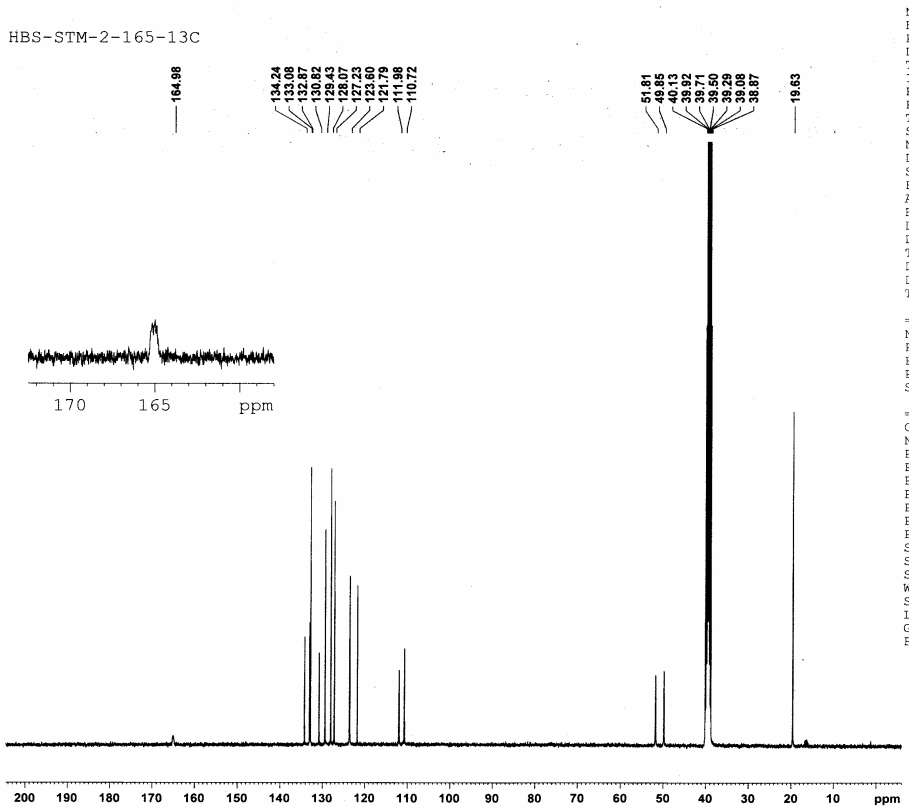
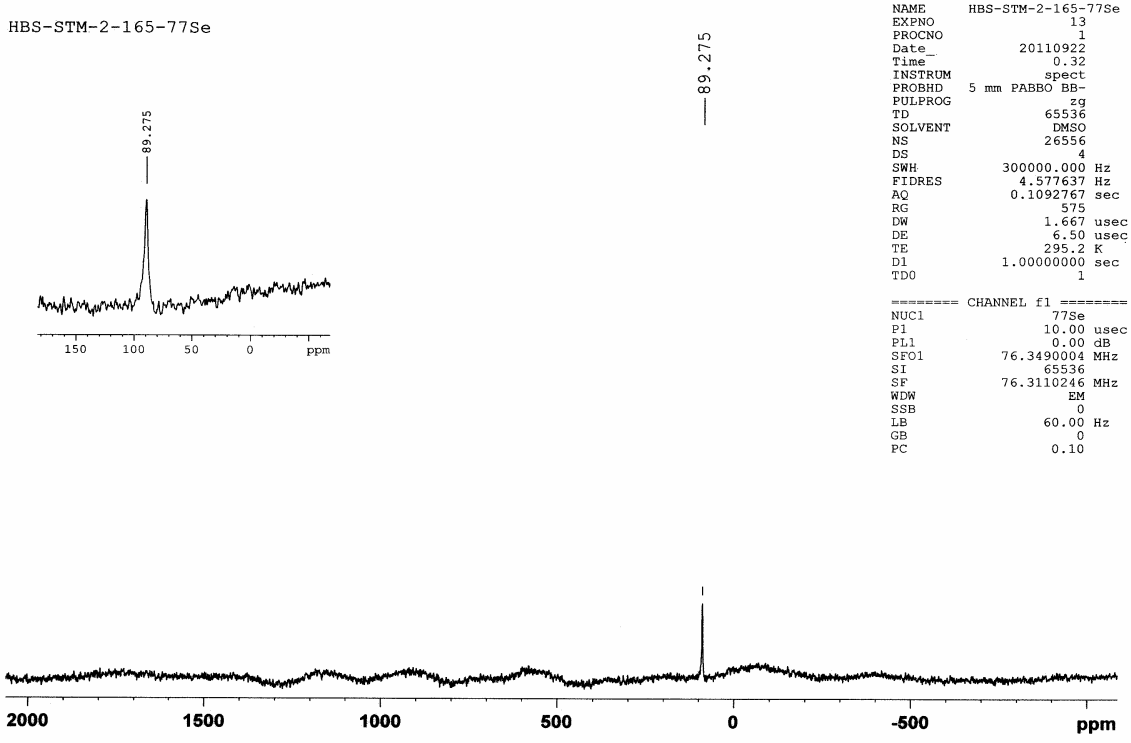


Figure S57. ^{13}C NMR spectrum of **7b** in DMSO-d_6.



NAME	HBS-STM-2-165-13C
EXPNO	16
PROCNO	1
Date_	20101012
Time	18.12
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	20000
DS	4
SWH	27173.912 Hz
FIDRES	0.414641 Hz
AQ	1.2059124 sec
RG	2050
DW	18.400 usec
DE	6.50 usec
TE	295.9 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.75 usec
PL1	-2.00 dB
PL1W	56.53121948 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	14.50 dB
PL13	14.50 dB
PL2W	10.56200695 W
PL12W	0.29767781 W
PL13W	0.29767781 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128119 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Figure S58. ^{77}Se NMR spectrum of **7b** in DMSO-d_6.



NAME	HBS-STM-2-165-77Se
EXPNO	13
PROCNO	1
Date_	20110922
Time	0.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	26556
DS	4
SWH	300000.000 Hz
FIDRES	4.577637 Hz
AQ	0.1092767 sec
RG	575
DW	1.667 usec
DE	6.50 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	77Se
P1	10.00 usec
PL1	0.00 dB
SFO1	76.3490004 MHz
SI	65536
SF	76.3110246 MHz
WDW	EM
SSB	0
LB	60.00 Hz
GB	0
PC	0.10

Figure S59. ^{125}Te NMR spectrum of **7b** in $CDCl_3$.

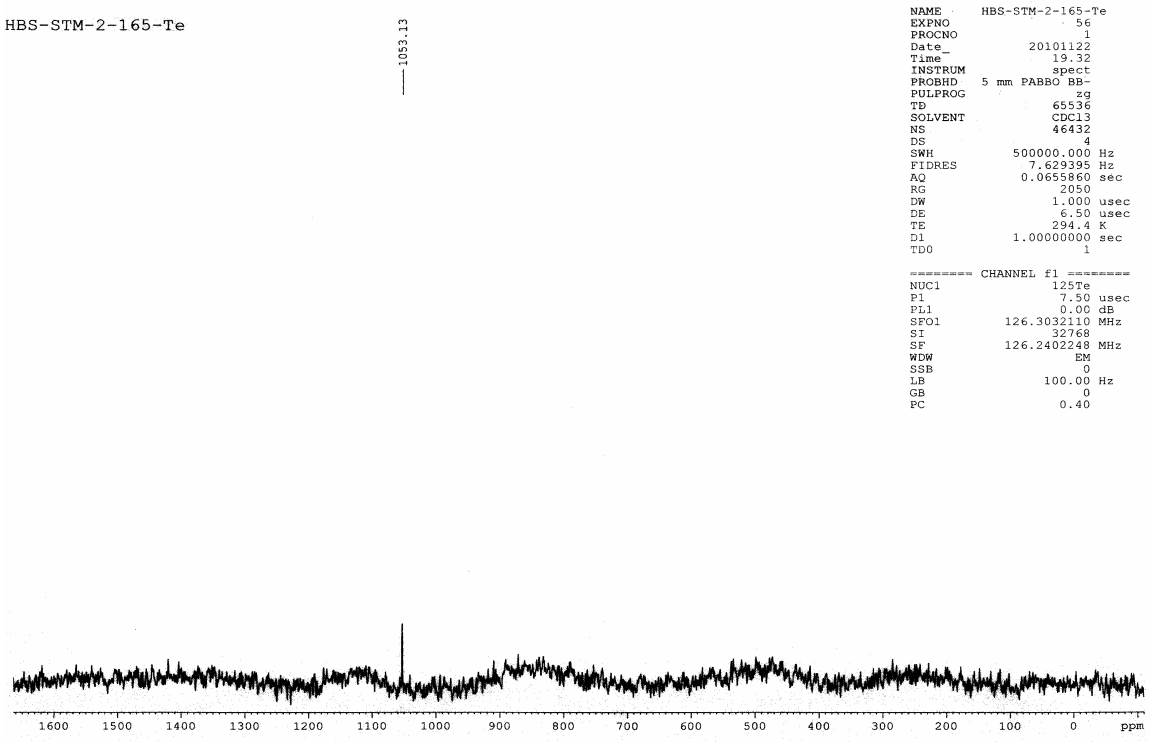


Figure S60. ^{125}Te NMR spectrum of **7b** in DMSO-d_6.

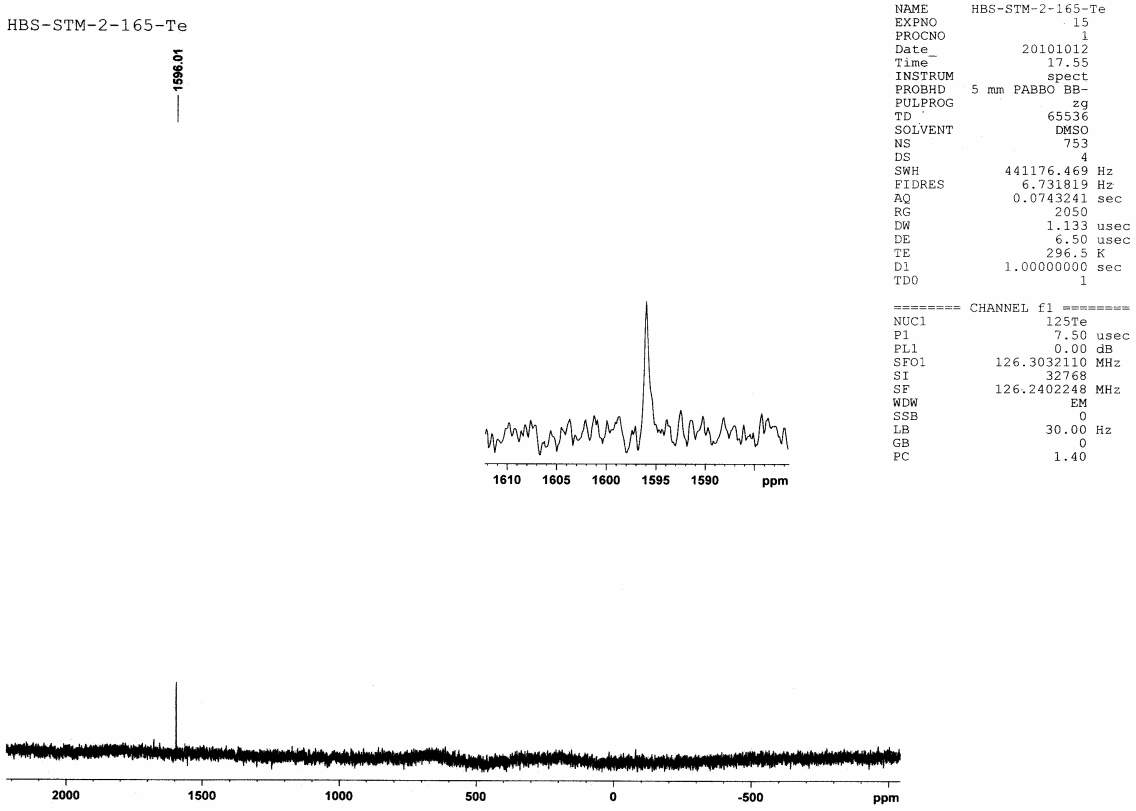


Figure S61. Mass spectrum of **7b**.

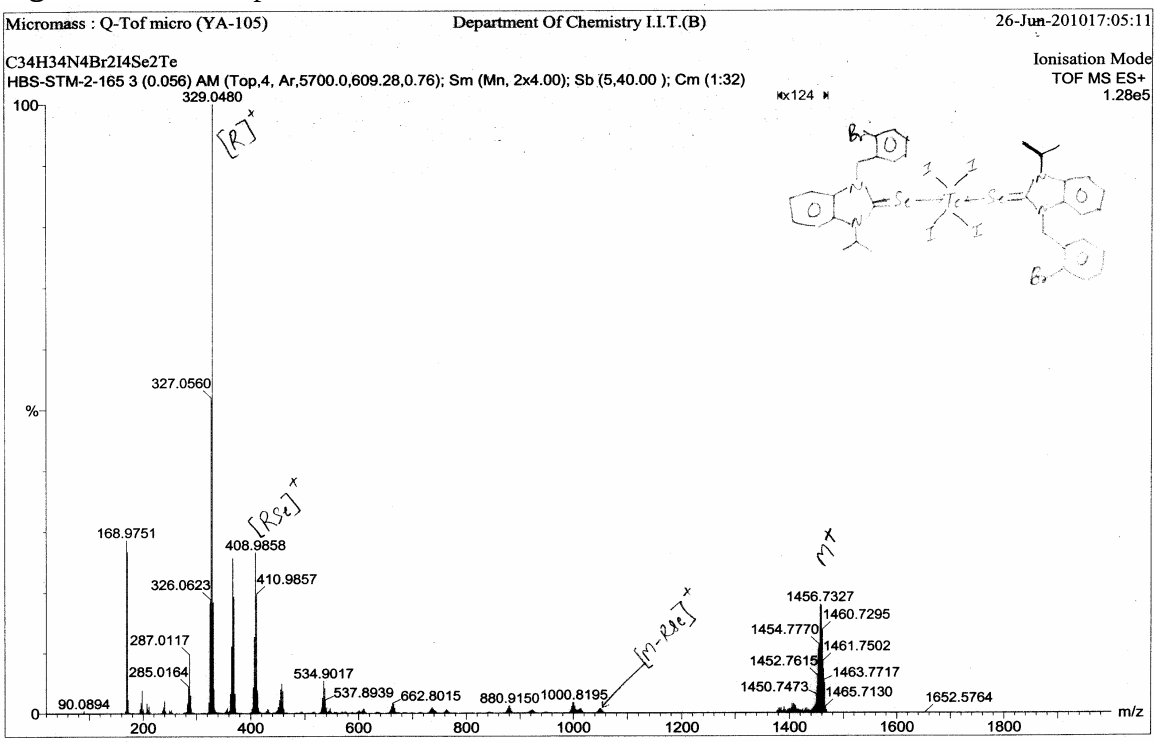


Figure S62. Elemental analysis of **7b**.

Eager 300 Report

Page: 1 Sample: STM165-1 (STM165-1)

Method Name : SP190310
Method File : D:\CHNS2008\SP190310.mth
Chromatogram : STM165-1
Operator ID : SP **Company Name : C.E. Instruments**
Analysed : 03/19/2010 14:44 **Printed : 3/19/2010 16:13**
Sample ID : STM165-1 (# 16) **Instrument N. : Instrument #1**
Analysis Type : UnkNown (Area) **Sample weight : .945**

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen 3.86	4.2519	0.39 43	46258	RS	15.390250	.115127E+07
Carbon 28.13	28.1167	0.01 68	711922	RS	1.000000	.266907E+07
Hydrogen 2.36	2.4318	0.07 175	207686	RS	3.427877	.667605E+07
Totals	34.8004		965866			

Figure S63. ^{1}H NMR spectrum of **7d** in $CDCl_3$.

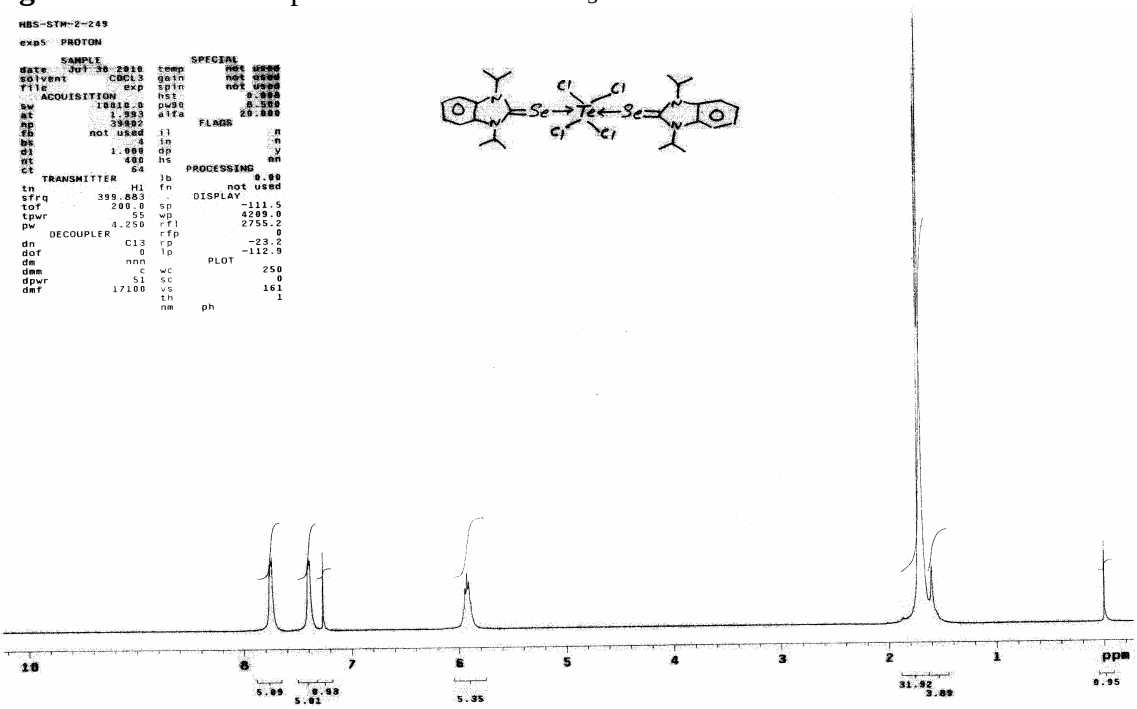


Figure S64. ^{13}C NMR spectrum of **7d** in $CDCl_3$.

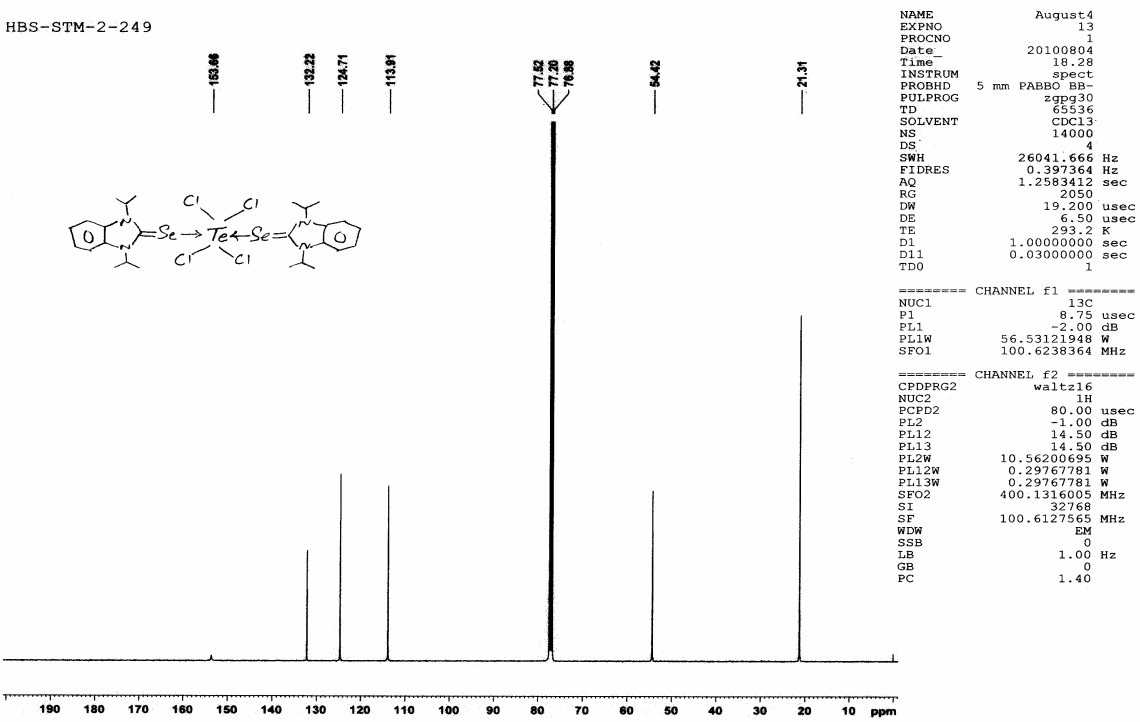


Figure S65. ^{77}Se NMR spectrum of **7d** in $CDCl_3$.

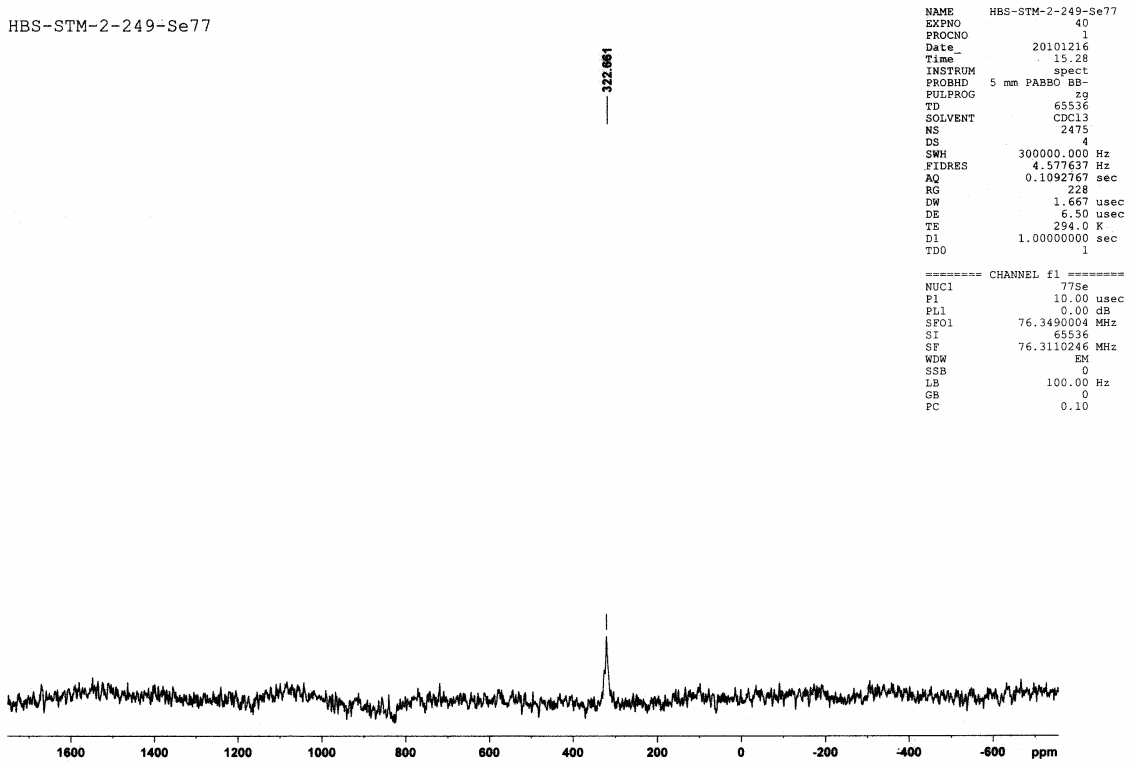


Figure S66. ^{125}Te NMR spectrum of **7d** in $CDCl_3$.

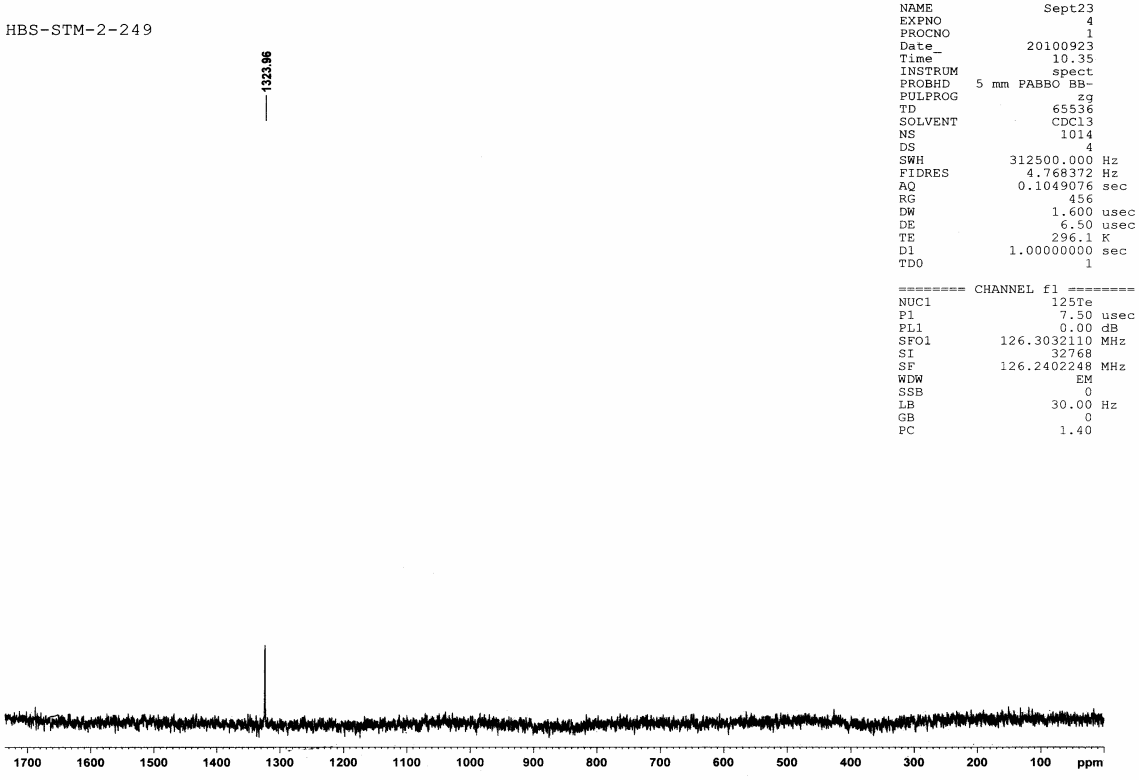


Figure S67. Mass spectrum of **7d**.

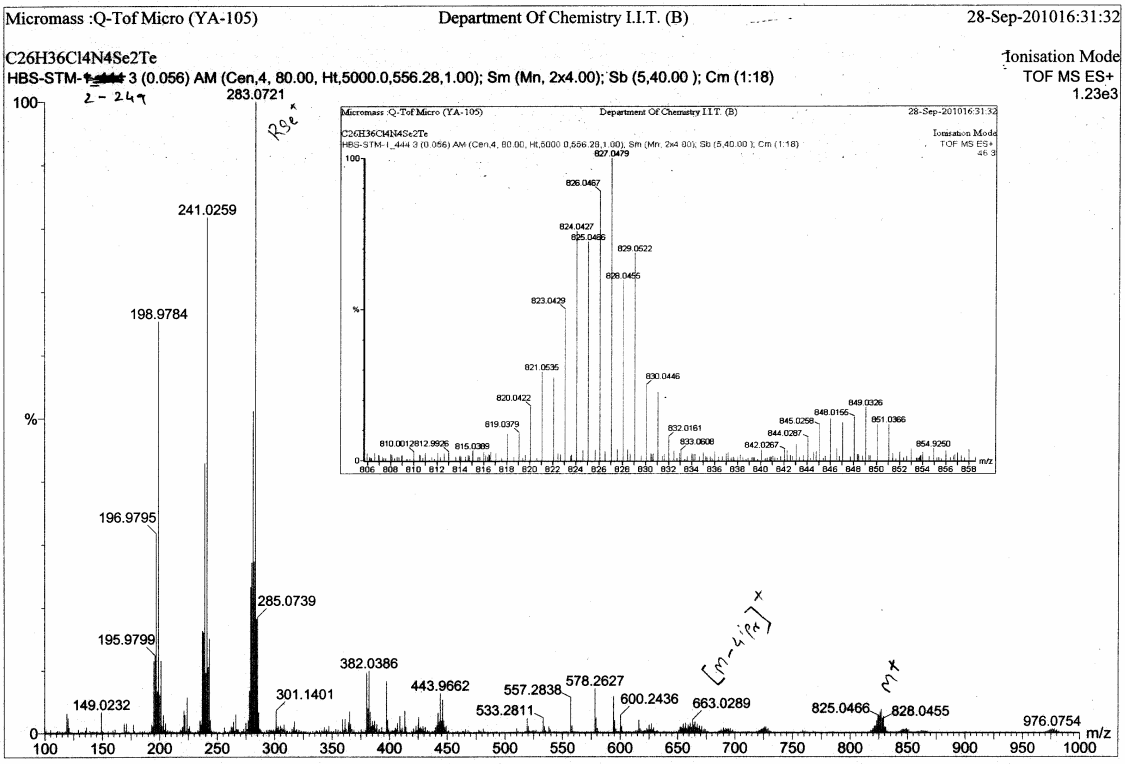


Figure S68. Elemental analysis of **7d**

Eager 300 Report

Page: 1 Sample: STM-2-249 (STM-2-249)

Method Name : SP150910
Method File : D:\CHNS2008\SP150910.mth
Chromatogram : STM-2-249
Operator ID : SP
Analysed : 09/15/2010 13:50
Sample ID : STM-2-249 (# 18)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 9/15/2010 15:41
Instrument N. : Instrument #1
Sample weight : 1.263

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name		%	Ret.Time	Area	BC	Area ratio	K factor
1		0.0000	18	12091	RS		0.0000
Nitrogen	6.73	7.0175	0.28 43	96918	RS	12.986460	.109350E+07
Carbon	37.54	37.5168	0.02 66	1258622	RS	1.000000	.265623E+07
Hydrogen	4.36	4.0493	0.38 175	302999	RS	4.153880	.567435E+07
Totals		48.5836		1670629			

Figure S69. ^{1}H NMR spectrum of **7e** in $CDCl_3$.

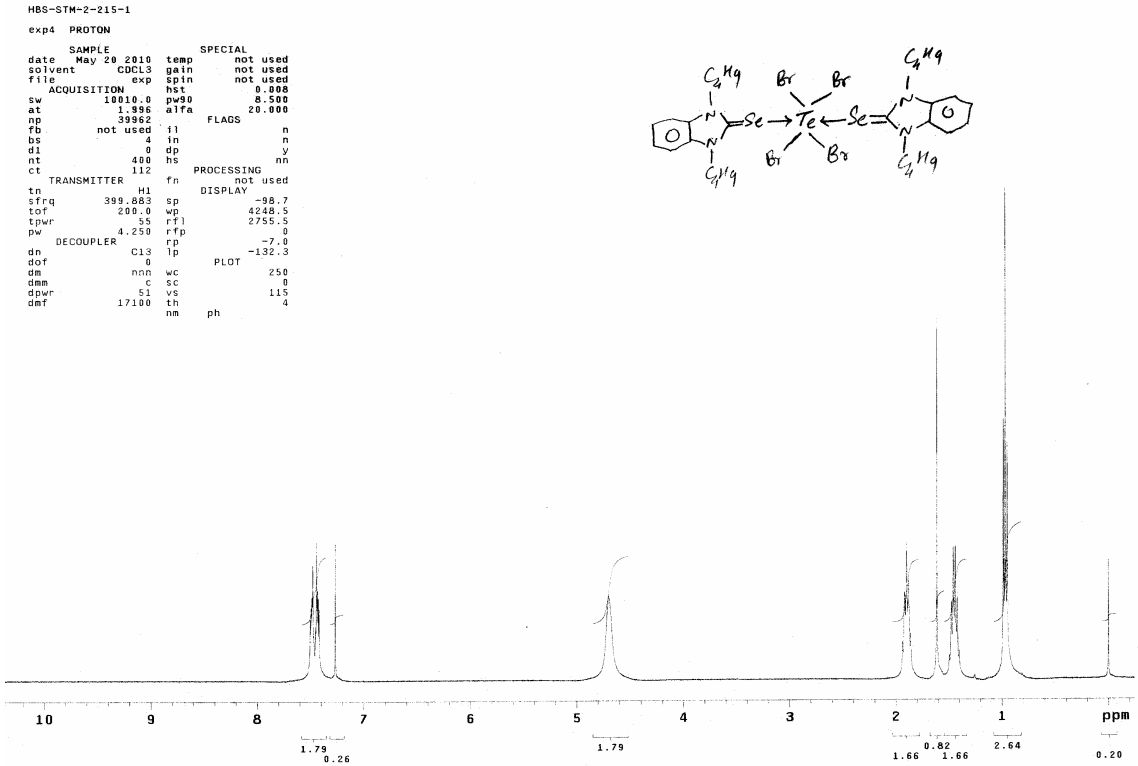


Figure S70. ^{13}C NMR spectrum of **7e** in $CDCl_3$.

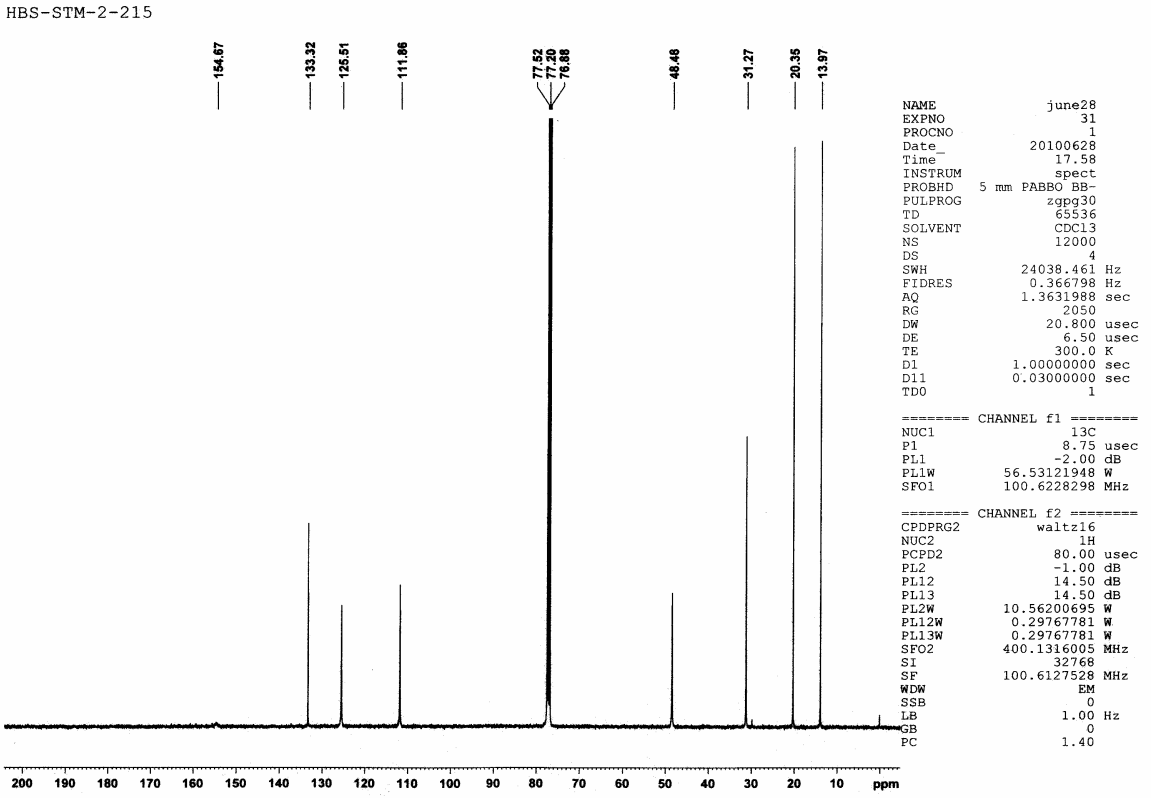


Figure S71. ^{77}Se NMR spectrum of **7e** in $CDCl_3$.

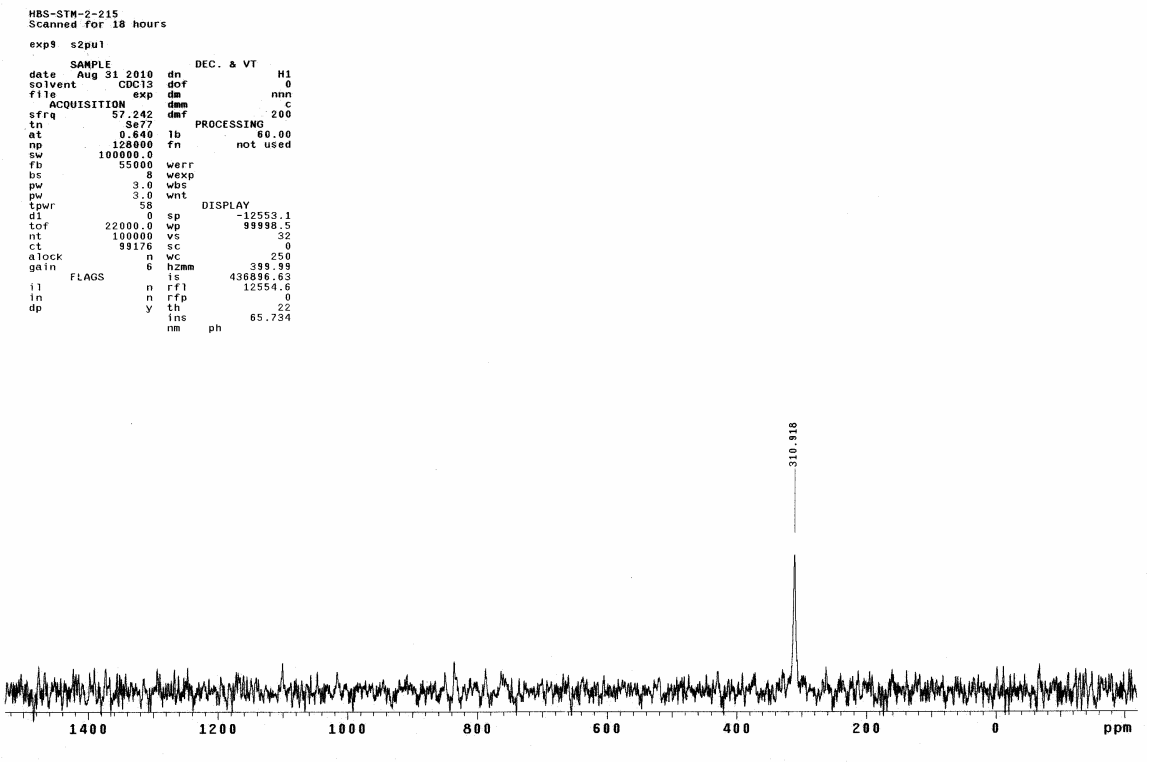


Figure S72. ^{125}Te NMR spectrum of **7e** in $CDCl_3$.

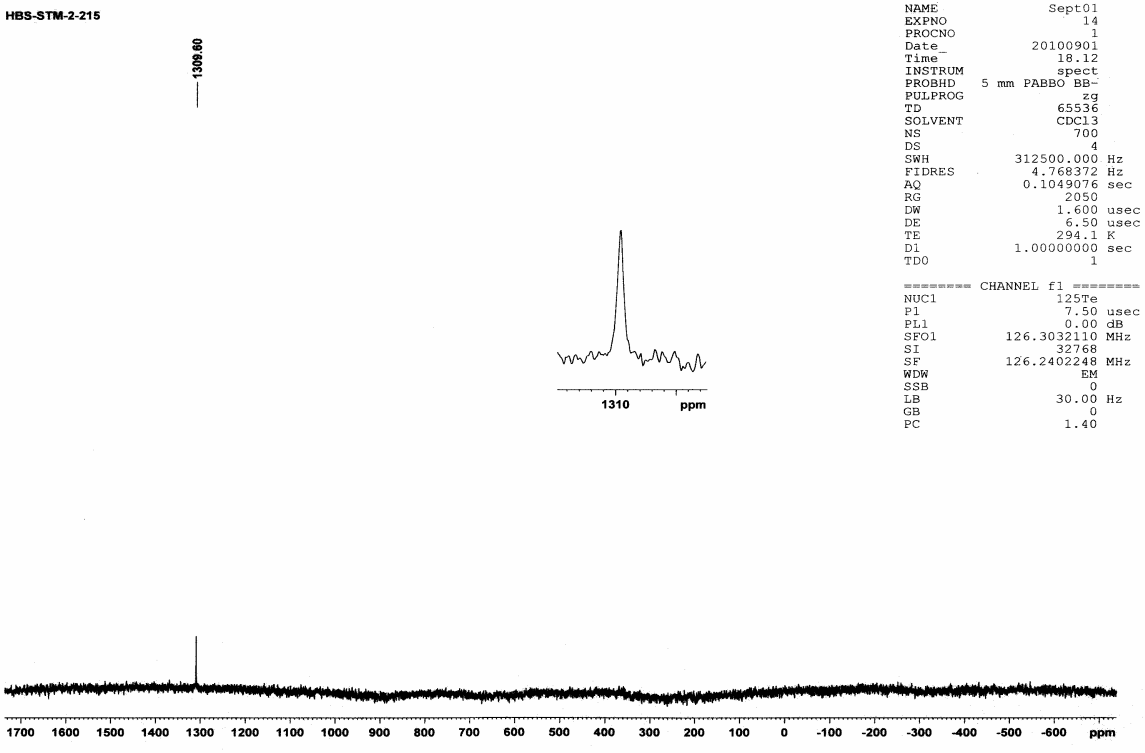


Figure S73. Mass spectrum of **7e**.

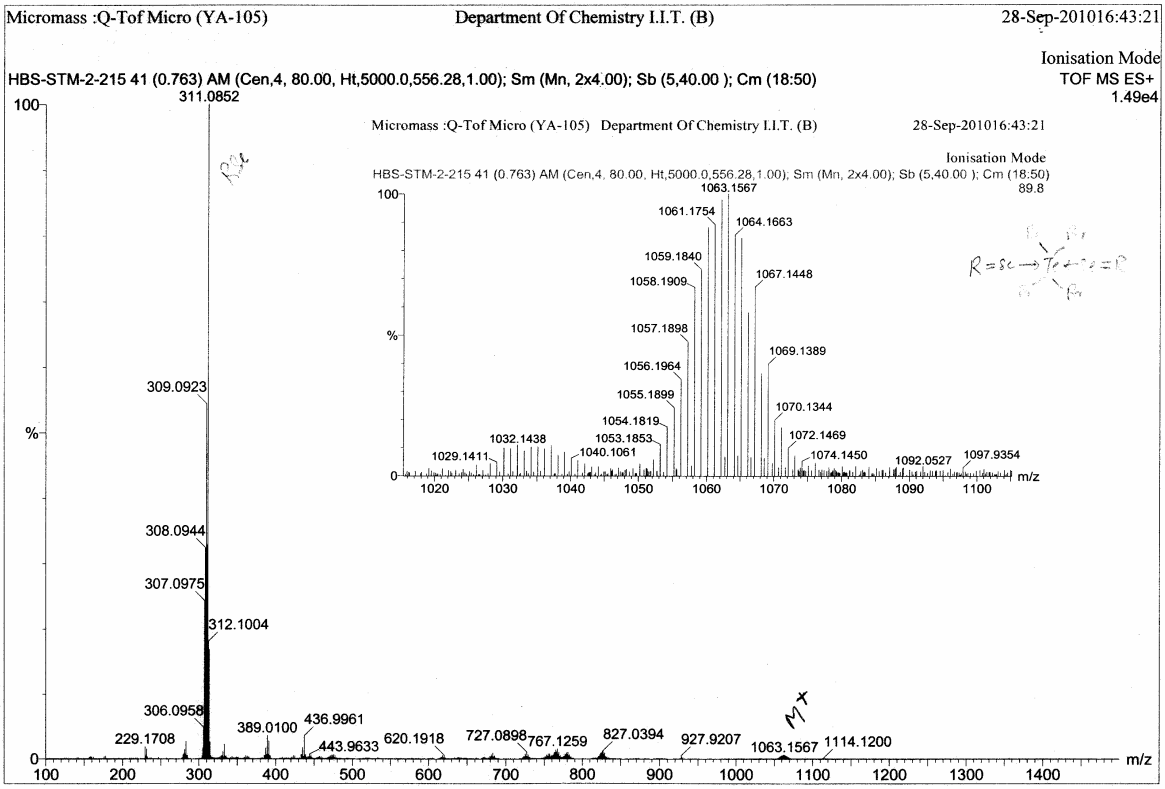


Figure S74. Elemental analysis of **7e**

Eager 300 Report

Page: 1 Sample: STM-2-281 (STM-2-281)

Method Name : SD290411
Method File : D:\CHNS2011\SD290411.mth
Chromatogram : STM-2-281
Operator ID : SD
Analysed : 04/29/2011 15:45
Sample ID : STM-2-281 (# 25)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 4/29/2011 16:43
Instrument N. : Instrument #1
Sample weight : .564

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	6.0649	44	73844	FU	6.769152	.185324E+07
Carbon	34.7273	69	499862	FU	1.000000	.255212E+07
Hydrogen	3.6561	184	129164	RS	3.869978	.575442E+07
Totals	44.4482		702870			

Figure S75. ^{1}H NMR spectrum of **8** in $CDCl_3$.

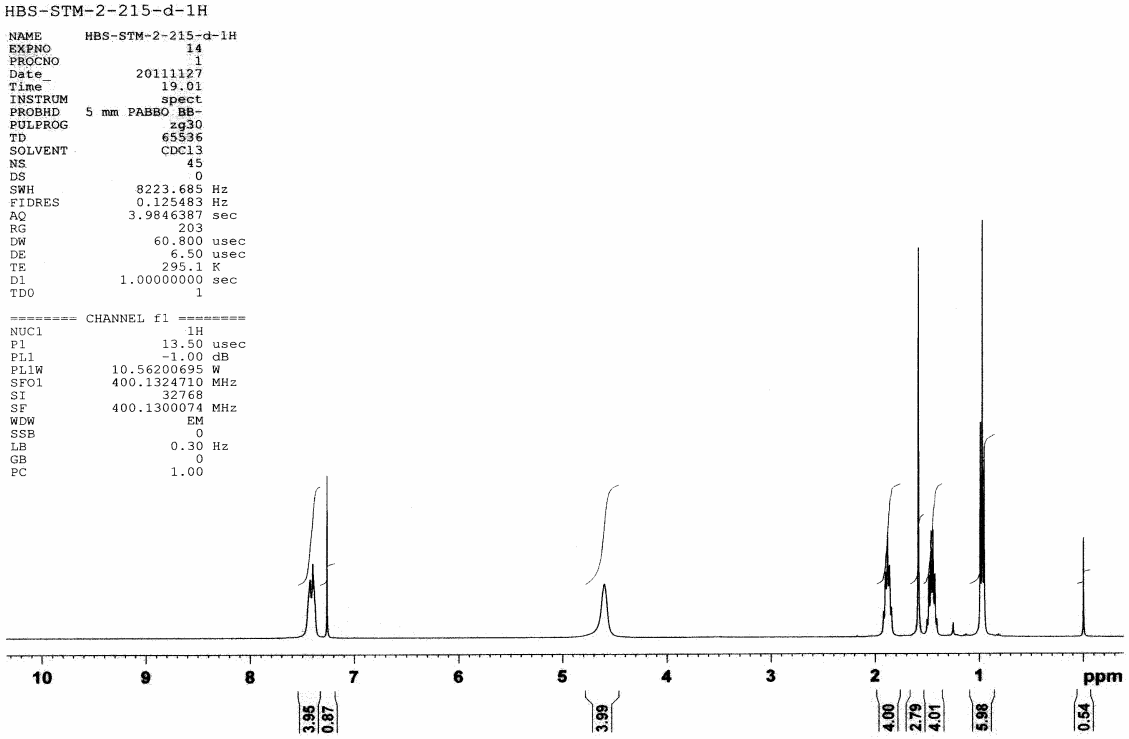


Figure S76.^{77}Se NMR spectrum of **8** in $CDCl_3$.

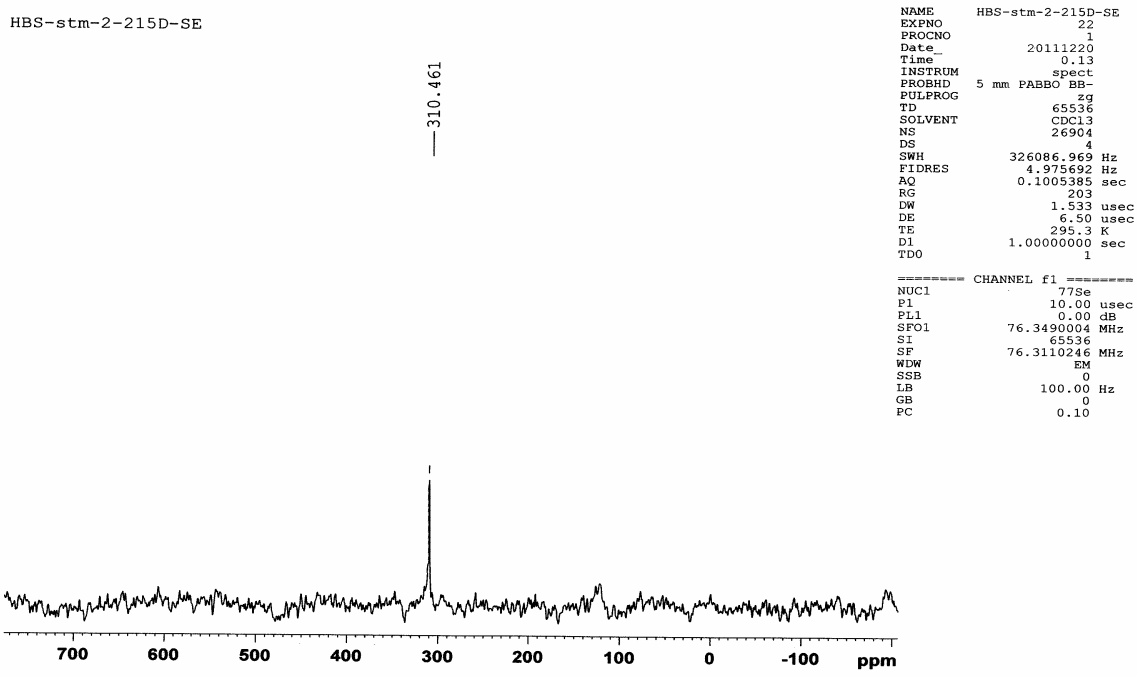


Figure S77. ^{125}Te NMR spectrum of **8** in $CDCl_3$.

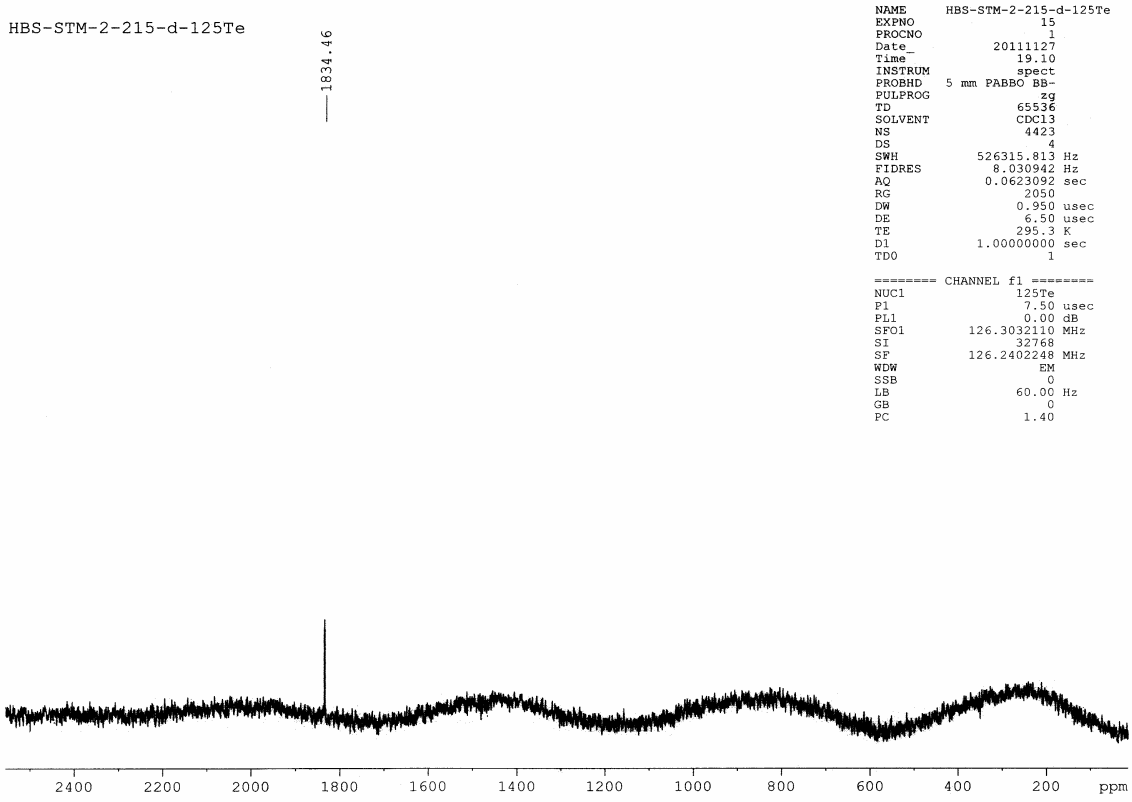


Figure S78. Elemental analysis of **8**

Eager 300 Report

Page: 1 Sample: STM-2-215 (STM-2-215)

Method Name : SD-25-11-11
Method File : D:\CHNS2011\SD-25-11-11.mth
Chromatogram : STM-2-215
Operator ID : SD
Analysed : 11/25/2011 12:30
Sample ID : STM-2-215 (# 10)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 11/25/2011 16:18
Instrument N. : Instrument #1
Sample weight : .713

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name		%	Ret.Time	Area	BC	Area ratio	K factor
1		0.0000	17	8853	RS		0.0000
Nitrogen	6.18	6.6904	0.51	63925	FU	11.015330	.134008E+07
Carbon	39.77	39.7526	0.02	704155	FU	1.000000	.248436E+07
Hydrogen	4.89	4.3118	0.55	169055	RS	4.165242	.525488E+07
Totals		50.7548		945988			

Br
RSeTe-SeR
Br

Figure S79. ^{1}H NMR spectrum of **7f** in $CDCl_3$.

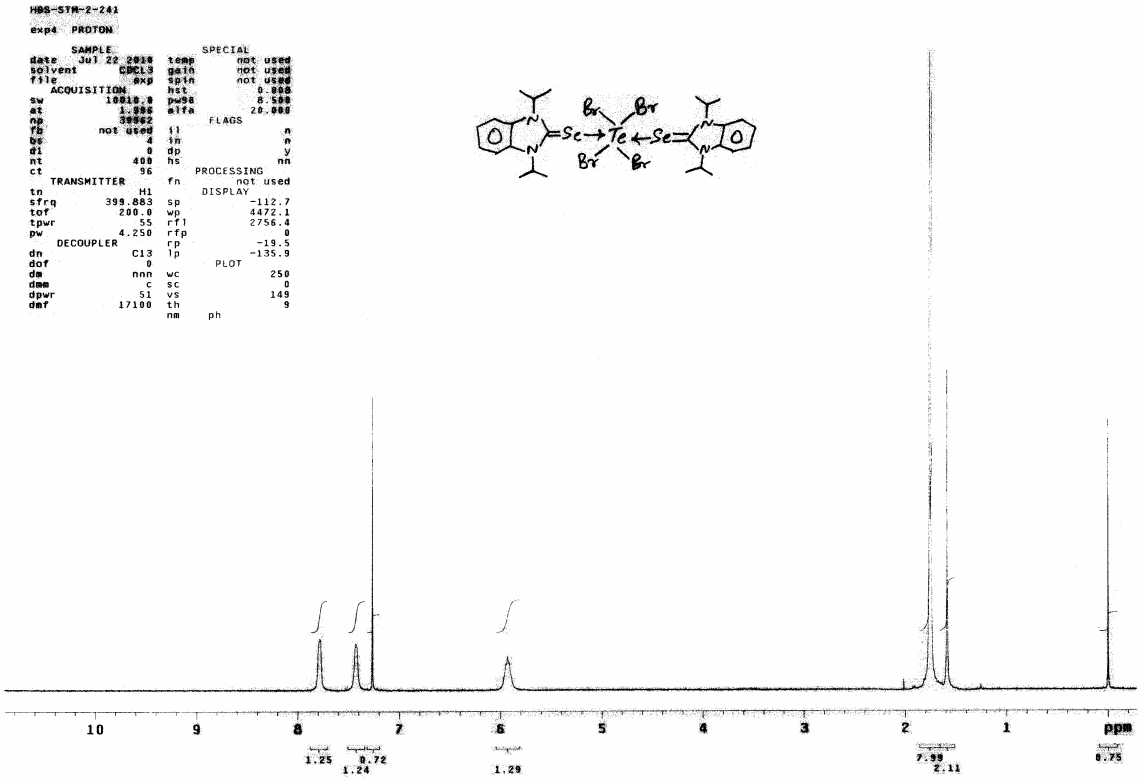


Figure S80. ^{13}C NMR spectrum of **7f** in $CDCl_3$.

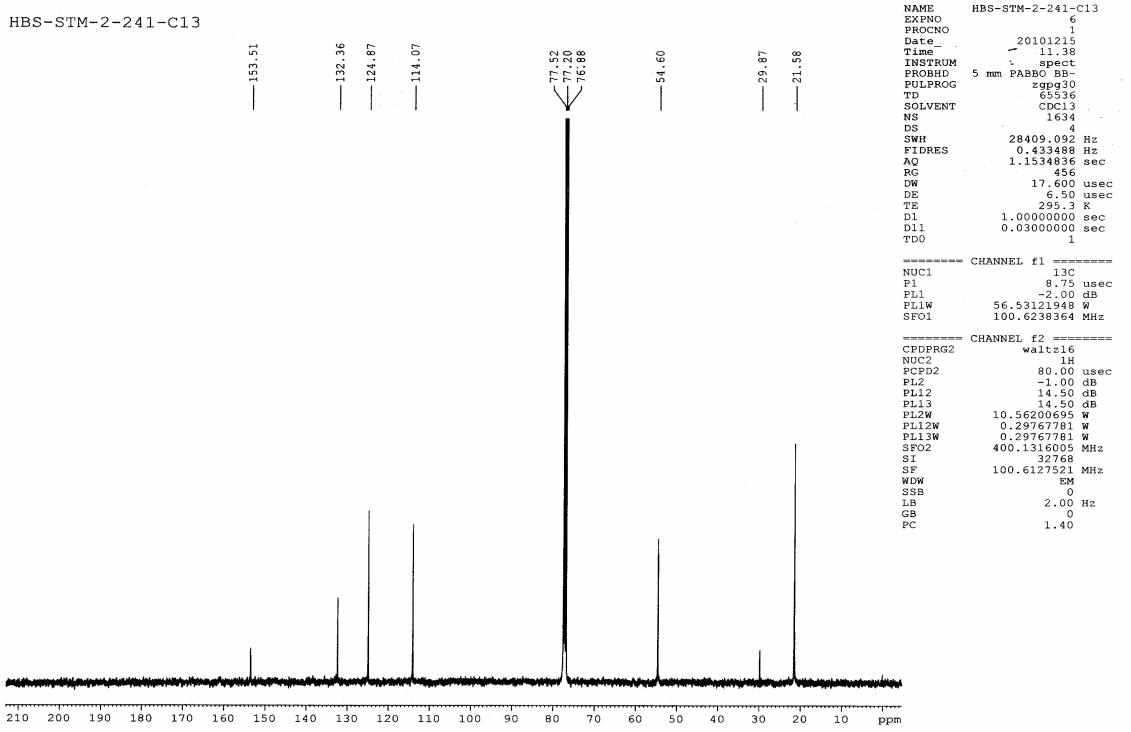


Figure S81. ^{77}Se NMR spectrum of **7f** in $CDCl_3$

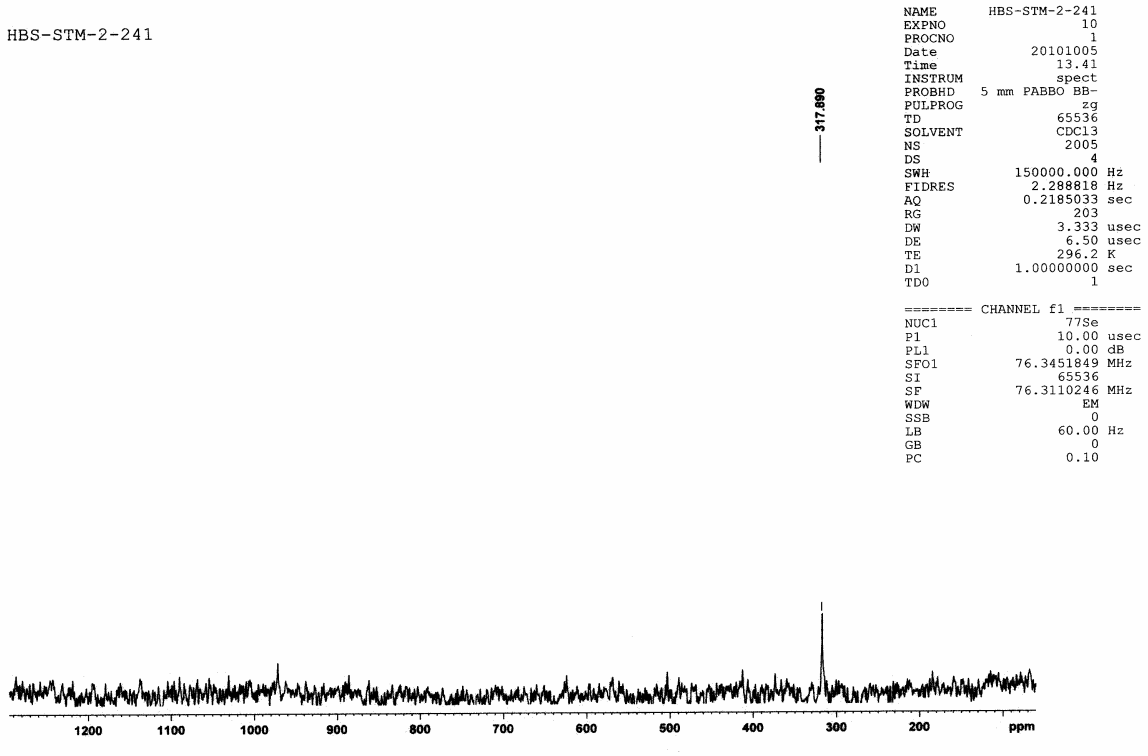


Figure S82. ^{125}Te NMR spectrum of **7f** in $CDCl_3$.

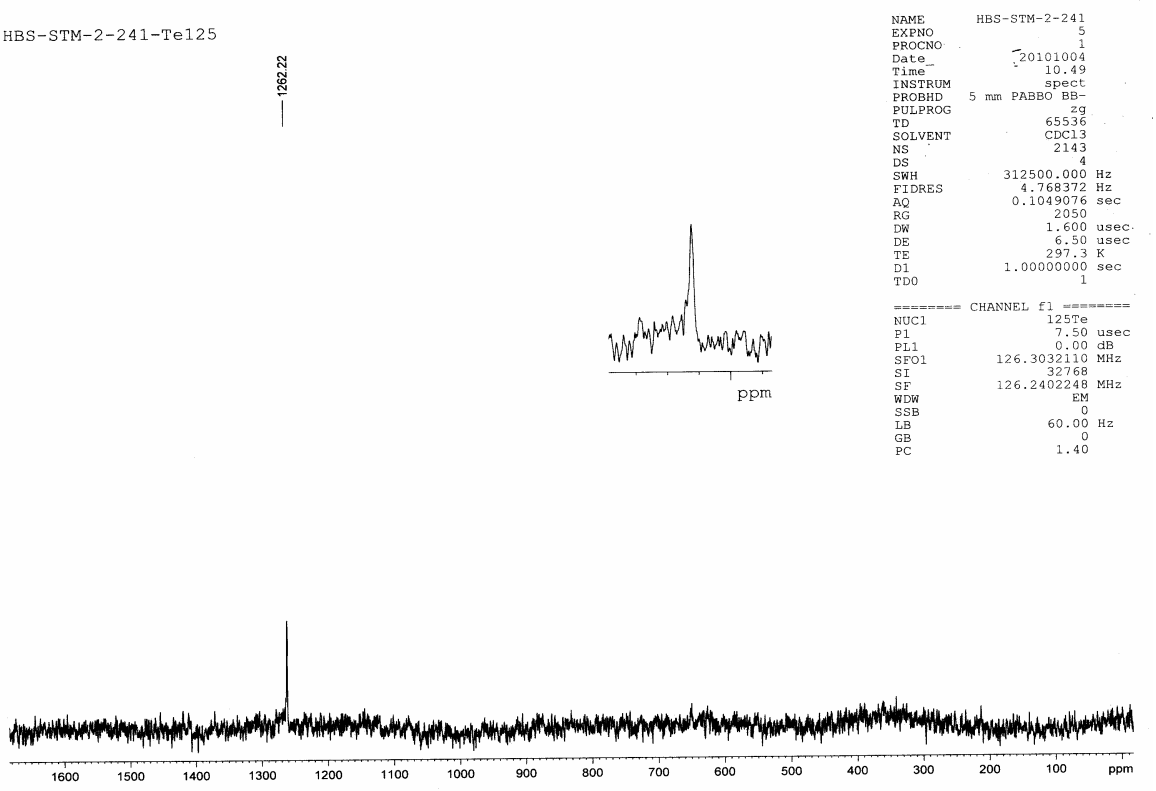


Figure S83. Mass spectrum of **7f**.

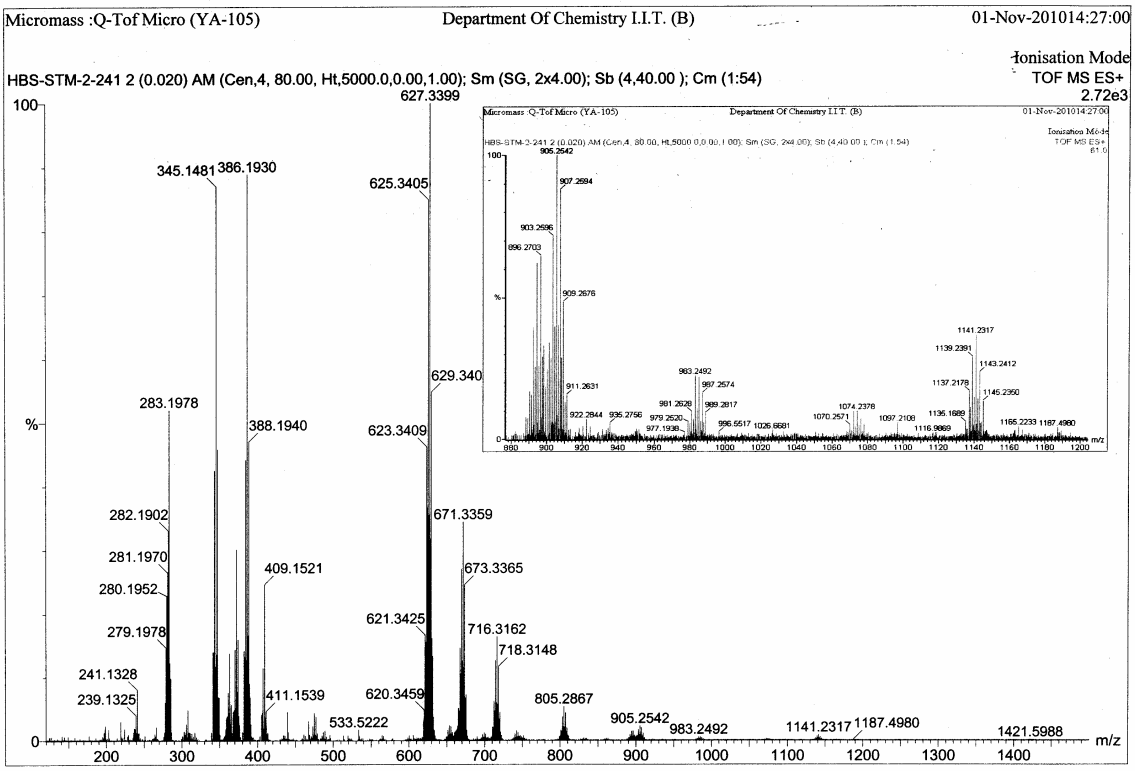


Figure S84. Elemental analysis of **7f**

Eager 300 Report

Page: 1 Sample: STM2-241 (STM2-241)

Method Name : SP100810
Method File : D:\CHNS2008\SD100810.mth
Chromatogram : STM2-241
Operator ID : SD
Analysed : 08/10/2010 14:41
Sample ID : STM2-241 (# 21)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 8/10/2010 15:31
Instrument N. : Instrument #1
Sample weight : .704

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name		%	Ret.Time	Area	BC	Area ratio	K factor
1		0.0000	18	5001	RS		0.0000
Nitrogen	5.55	5.8881	0.33	43	48783	RS	10.931820	.117684E+07
Carbon	30.93	30.5355	0.4	67	533287	RS	1.000000	.265462E+07
Hydrogen	3.59	2.7005	0.89	181	121111	RS	4.403291	.593892E+07
Totals		39.1241			708182			

Figure S85. ^{1}H NMR spectrum of **7g** in $CDCl_3$.

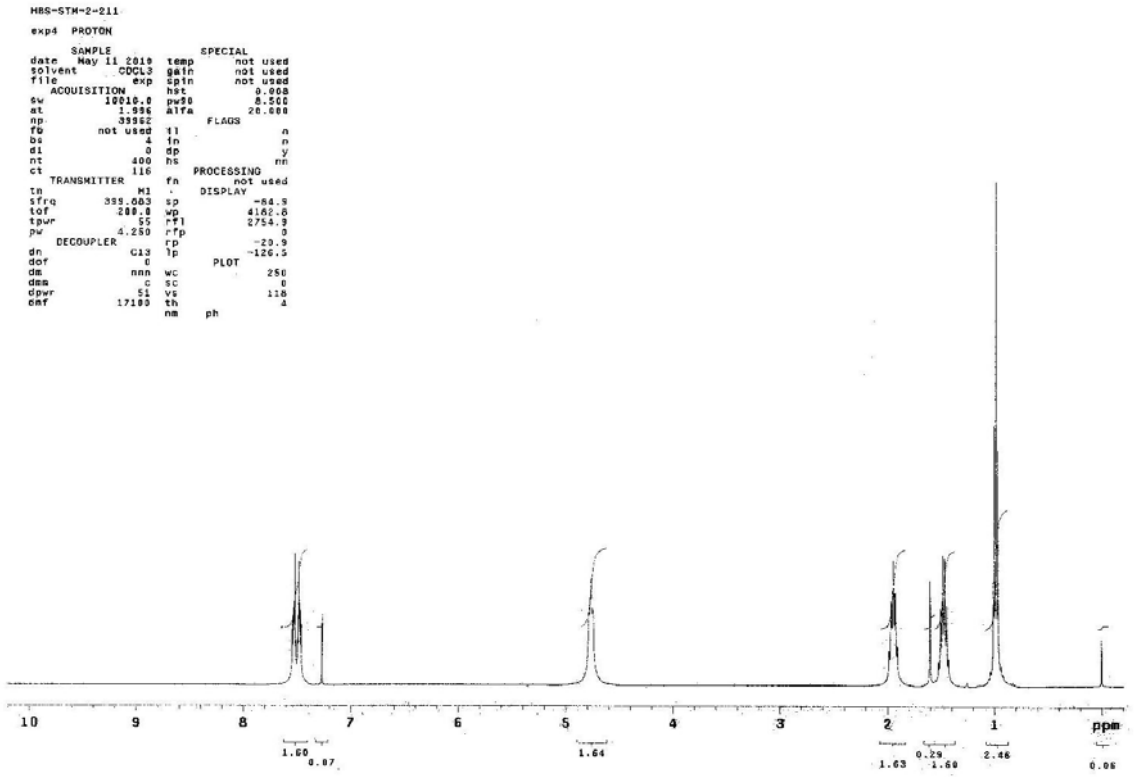


Figure S86. ^{13}C NMR spectrum of **7g** in $CDCl_3$.

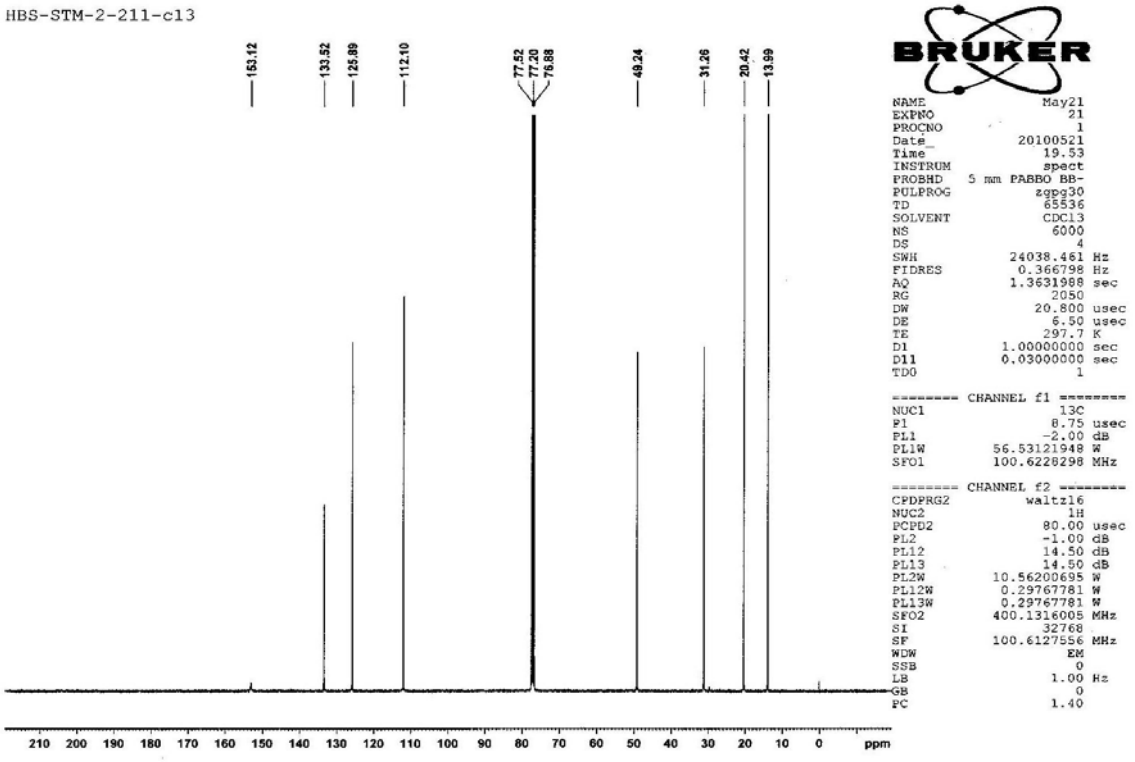


Figure S87. ^{77}Se NMR spectrum of **7g** in $CDCl_3$.

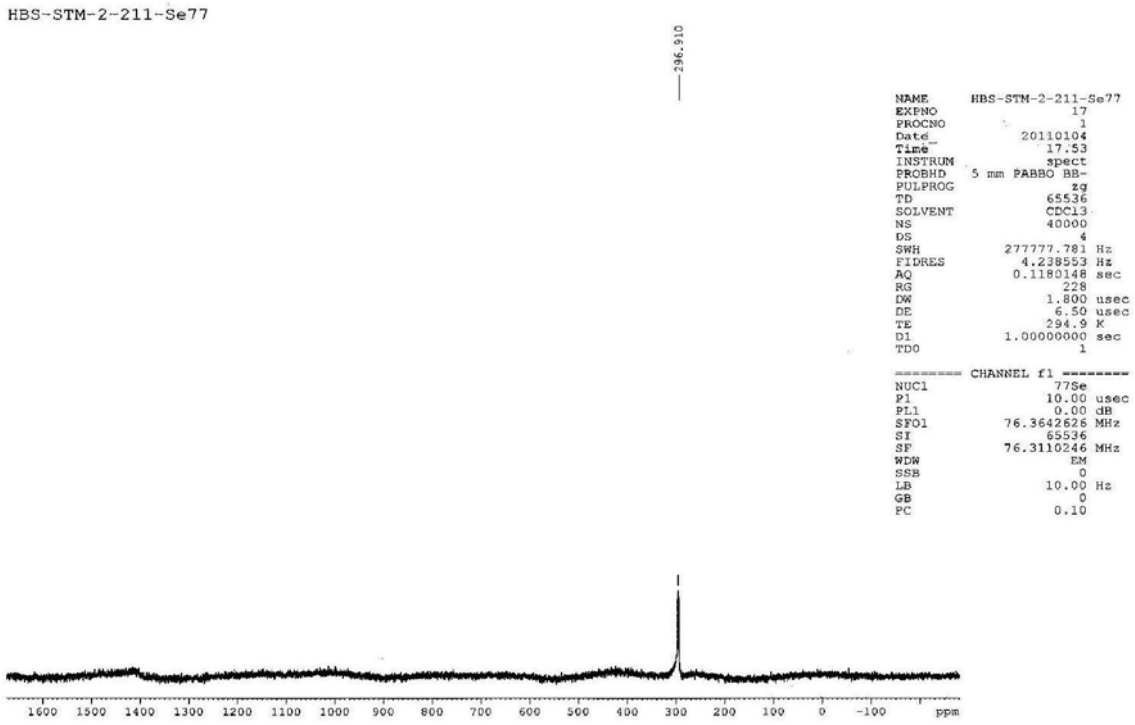


Figure S88. ^{77}Se NMR spectrum of **7g** in $CDCl_3$ at 233K.

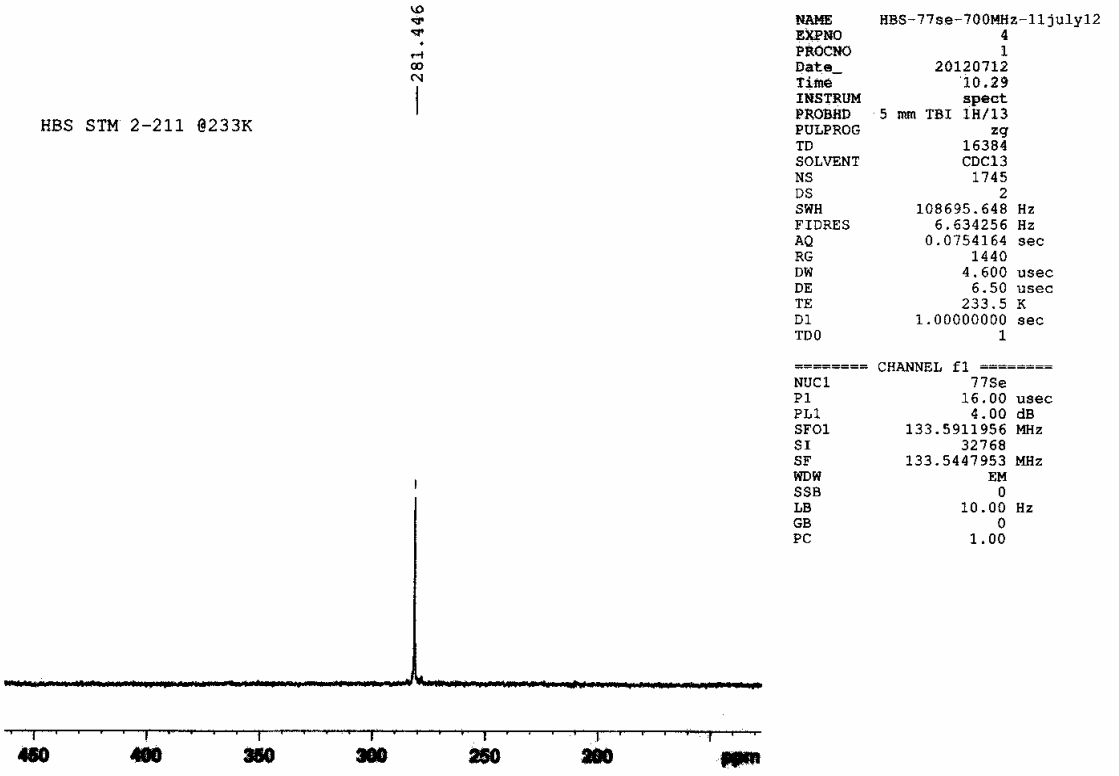


Figure S89. ^{125}Te NMR spectrum of **7g** in $CDCl_3$.

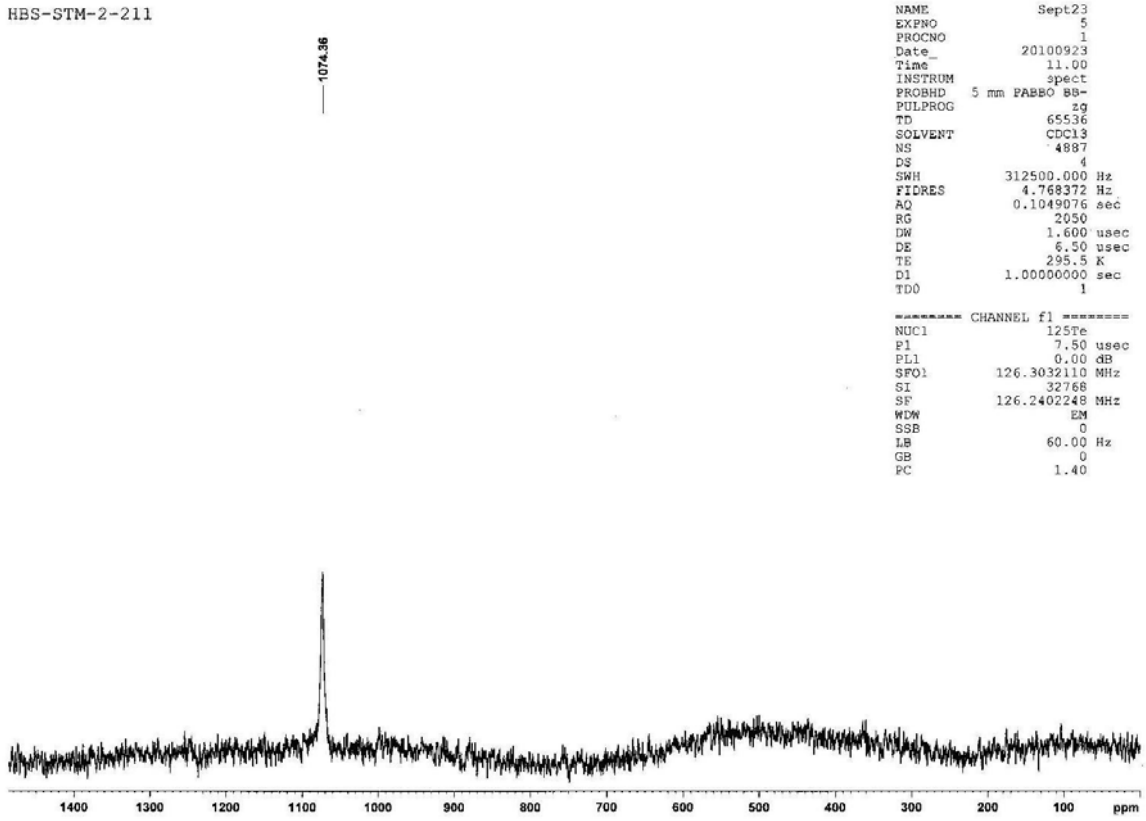


Figure S90. Mass spectrum of **7g**.

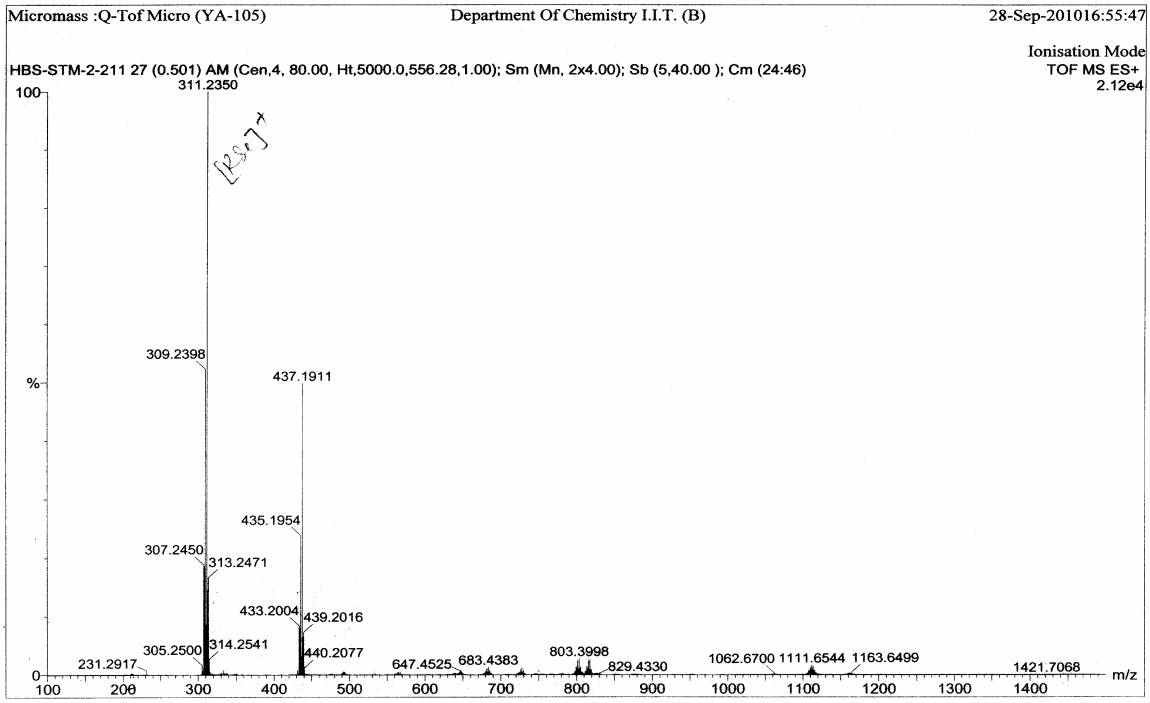


Figure S91. Elemental analysis of **7g.**

Eager 300 Report

Page: 1 Sample: STM2-211 (STM2-211)

Method Name : SP110510
Method File : D:\CHNS2008\SP110510.mth
Chromatogram : STM2-211
Operator ID : SP
Analysed : 05/11/2010 15:35
Sample ID : STM2-211 (# 26)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 5/11/2010 15:47
Instrument N. : Instrument #1
Sample weight : 1.089

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name		%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	4.47	5.0123	44	77622	RS	10.249610	.122634E+07
Carbon	28.74	28.8771	68	795595	RS	1.000000	.252191E+07
Hydrogen	3.54	3.5091	169	331715	RS	2.398429	.656520E+07
Totals		37.3985		1204932			

Figure S92. Molecular structure of **7g.** Hydrogen atoms are omitted for clarity.

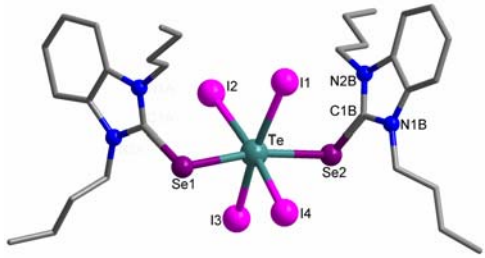


Figure S93. Crystal packing diagram of **7g.** Hydrogen atoms (except those are involved in interactions) are omitted for clarity.

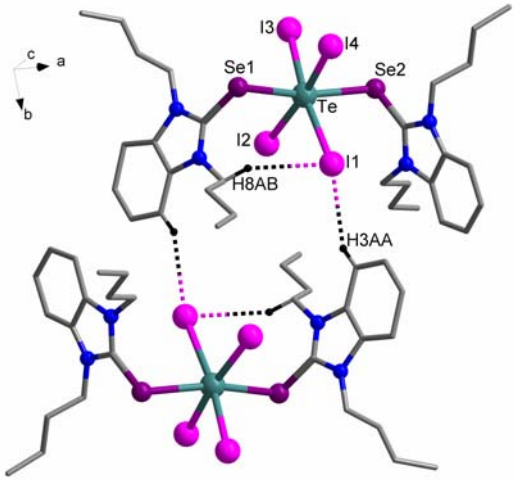


Figure S94. ^{77}Se NMR spectrum of **7g** in $CDCl_3$ at 27 ^{o}C.

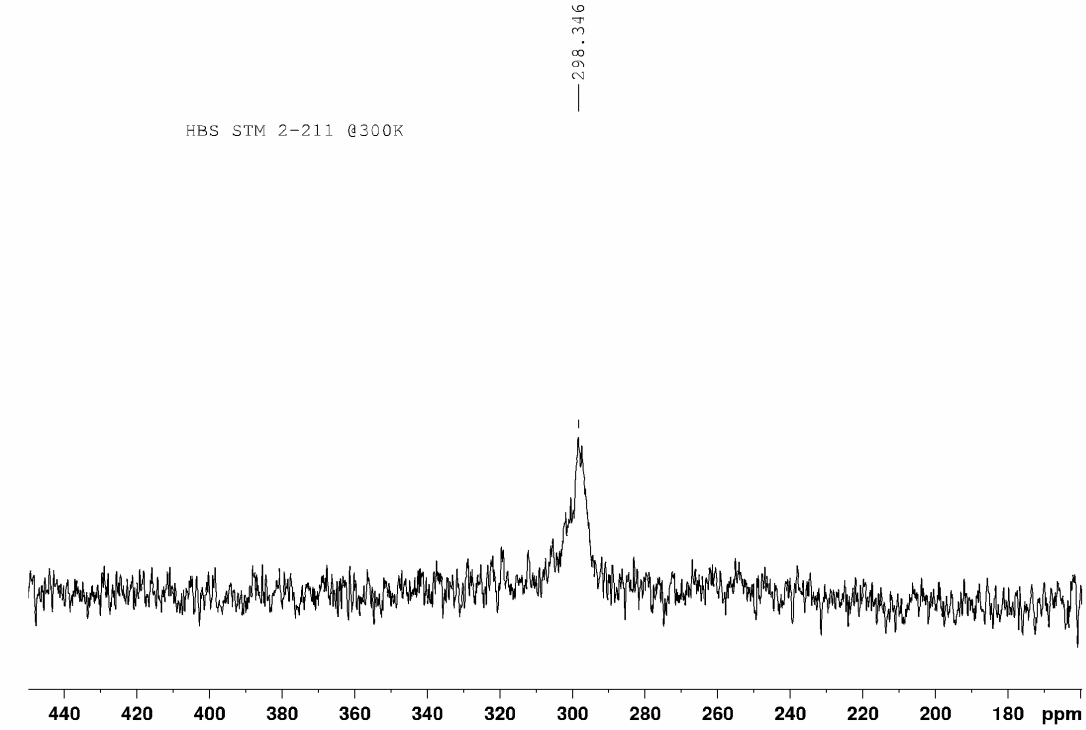
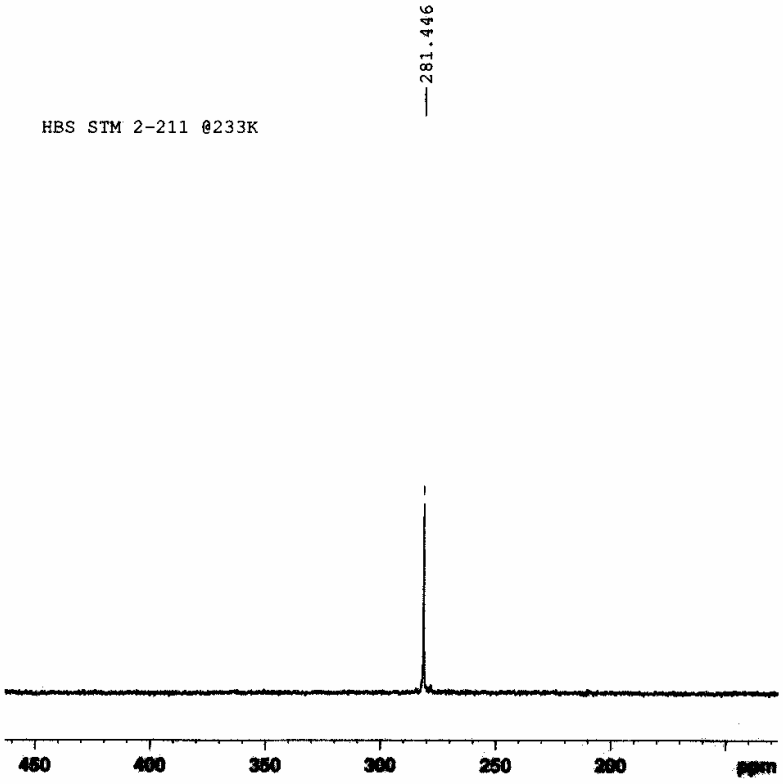


Figure S95. ^{77}Se NMR spectrum of **7g** in $CDCl_3$ at -40 ^{o}C.



NAME	HBS-77se-700MHz-11july12
EXPNO	4
PROCNO	1
Date_	20120712
Time	10.29
INSTRUM	spect
PROBHD	5 mm TBI 1H/13
PULPROG	zg
TD	16384
SOLVENT	CDCl3
NS	1745
DS	2
SWH	108695.648 Hz
FIDRES	6.634256 Hz
AQ	0.0754164 sec
RG	1440
DW	4.600 usec
DE	6.50 usec
TE	233.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	77Se
P1	16.00 usec
PL1	4.00 dB
SFO1	133.5911956 MHz
SI	32768
SF	133.5447953 MHz
WDW	EM
SSB	0
LB	10.00 Hz
GB	0
PC	1.00

Figure S96. ^{77}Se NMR spectra of **7g** in $CDCl_3$ at 27 ^{o}C (**a**) and -40 ^{o}C (**b**).

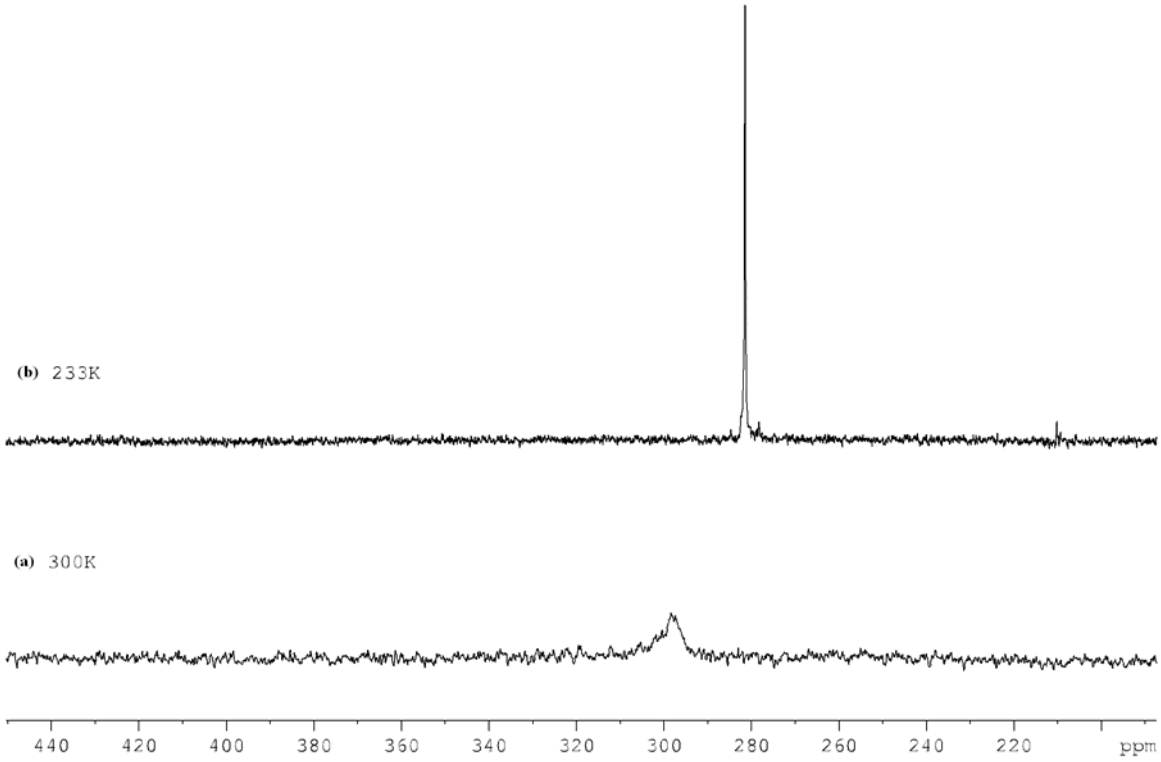


Figure S97. ^{1}H NMR spectrum of **7e** through the reaction between benzimidazolin-2-selenone (**4c**) and tellurium tetrabromide in $CDCl_3$.

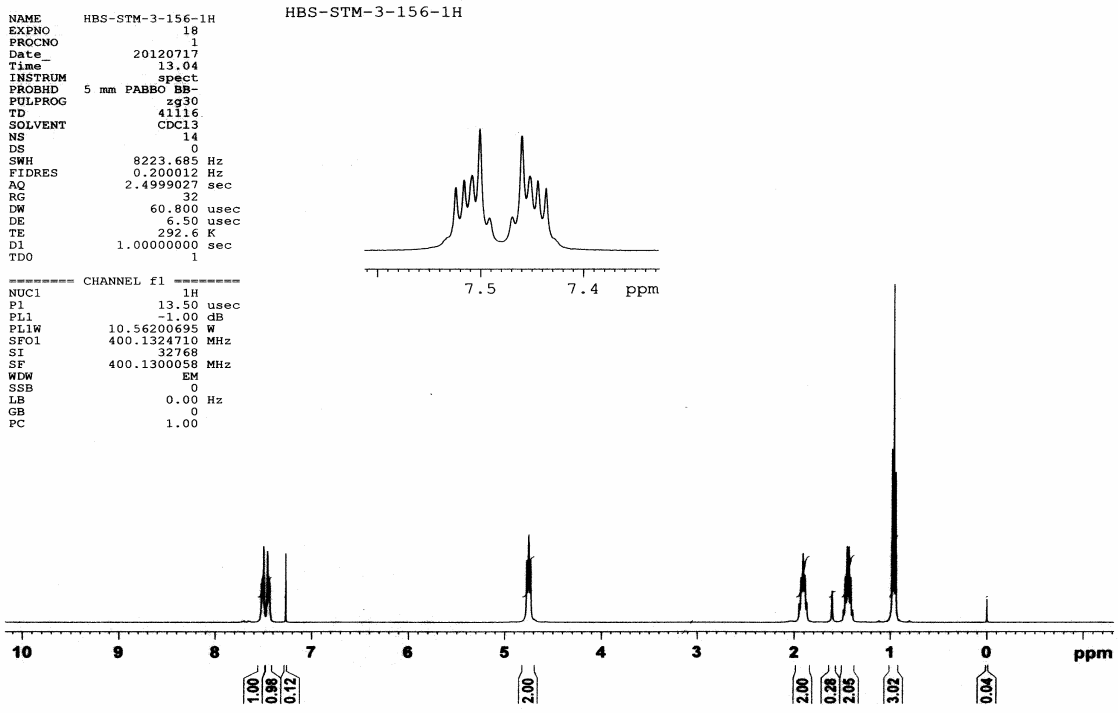


Figure S98. ^{13}C NMR spectrum of **7e** through the reaction between benzimidazolin-2-selenone (**4c**) and tellurium tetrabromide in $CDCl_3$.

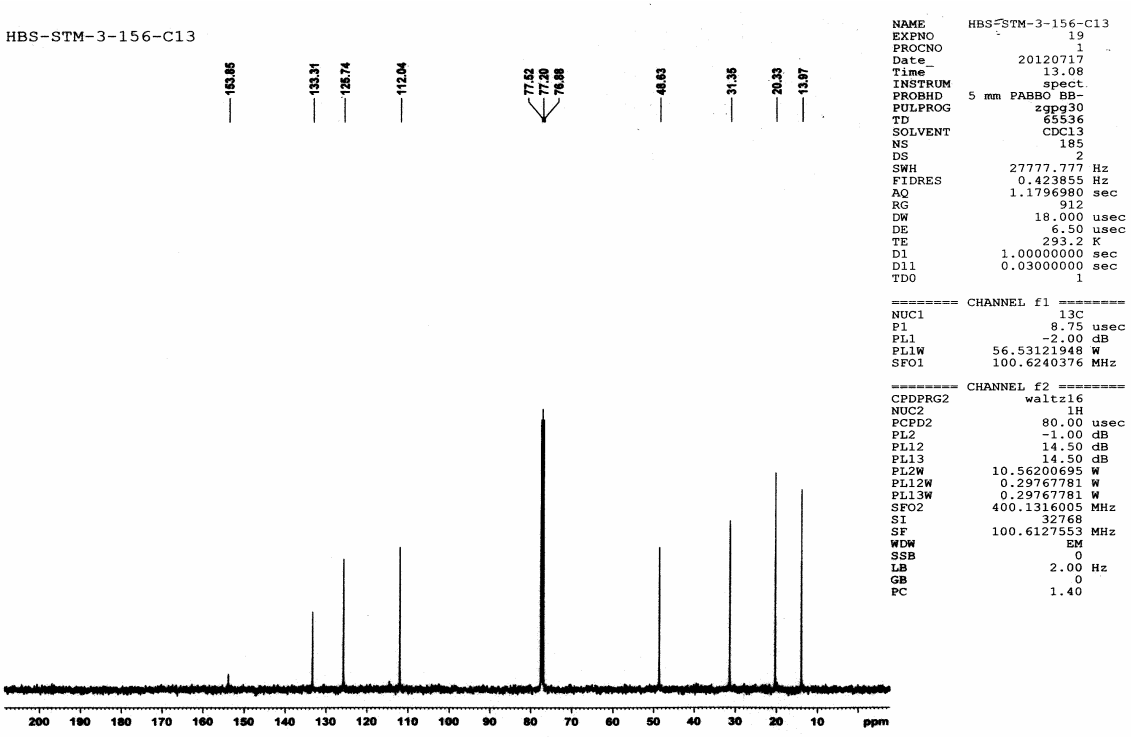


Figure S99. ^{77}Se NMR spectrum of **7e** through the reaction between benzimidazolin-2-selenone (**4c**) and tellurium tetrabromide in $CDCl_3$.

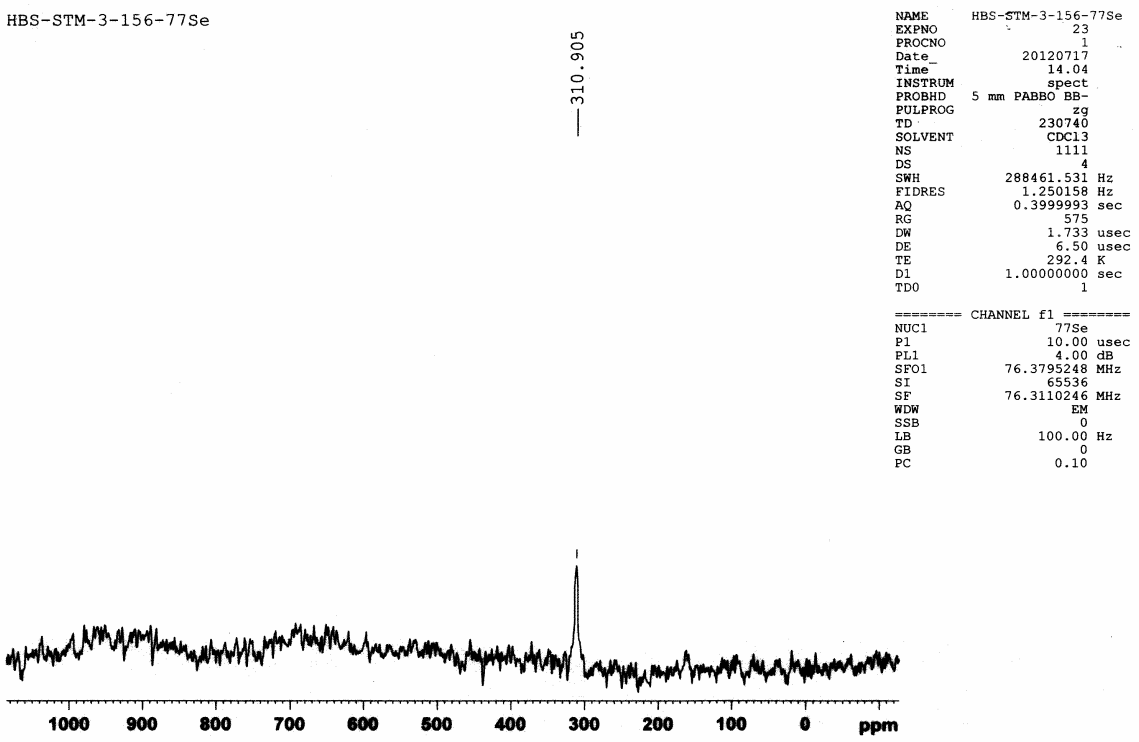


Figure S100. ^{125}Te NMR spectrum of **7e** through the reaction between benzimidazolin-2-selenone (**4c**) and tellurium tetrabromide in $CDCl_3$.

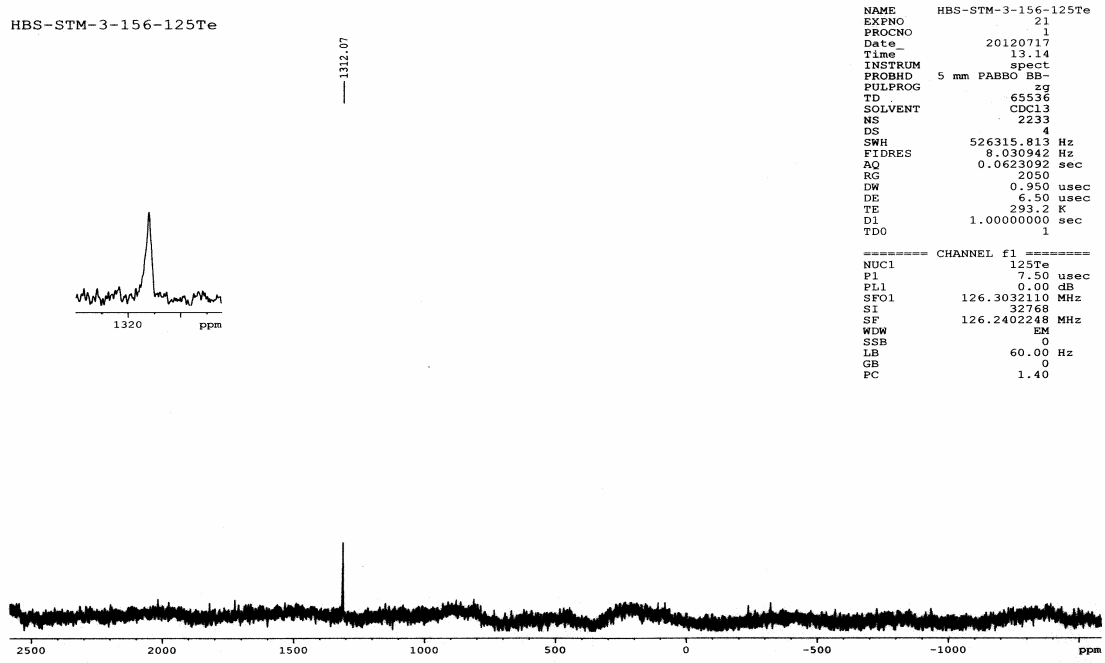


Figure S101. ^{1}H NMR spectrum of **9a** in $CDCl_3$.

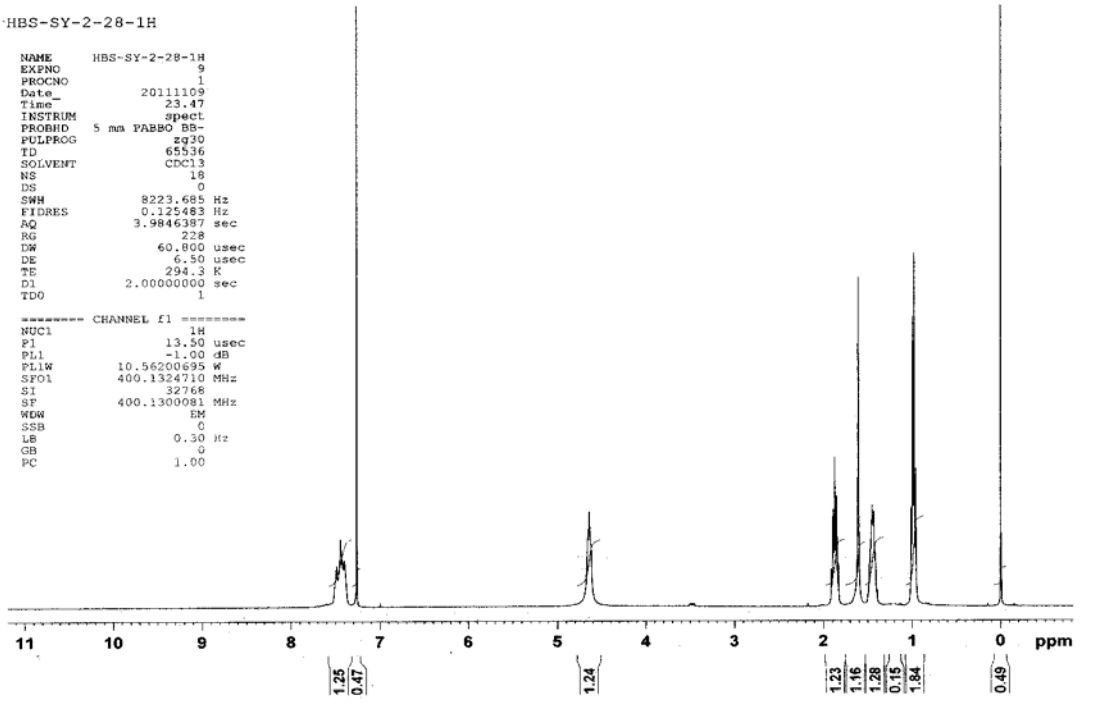


Figure S102. ^{13}C NMR spectrum of **9a** in $CDCl_3$.

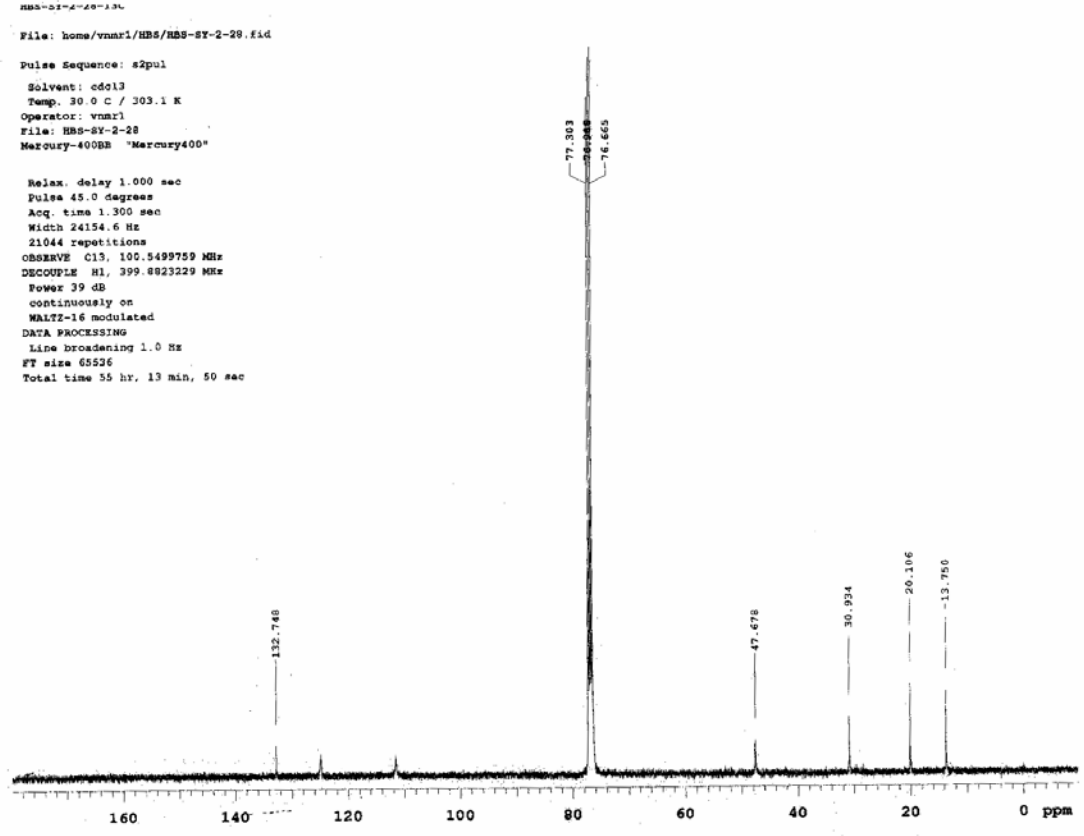


Figure S103. ^{77}Se NMR spectrum of **9a** in $CDCl_3$.

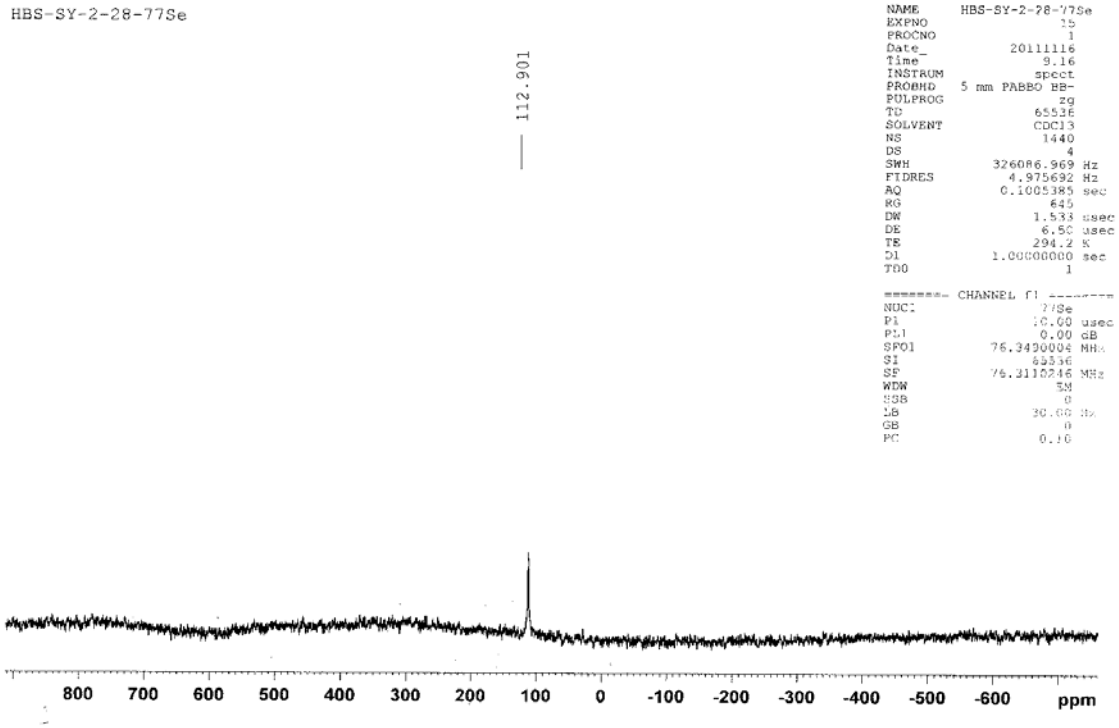


Figure S104. Mass spectrum of **9a**.

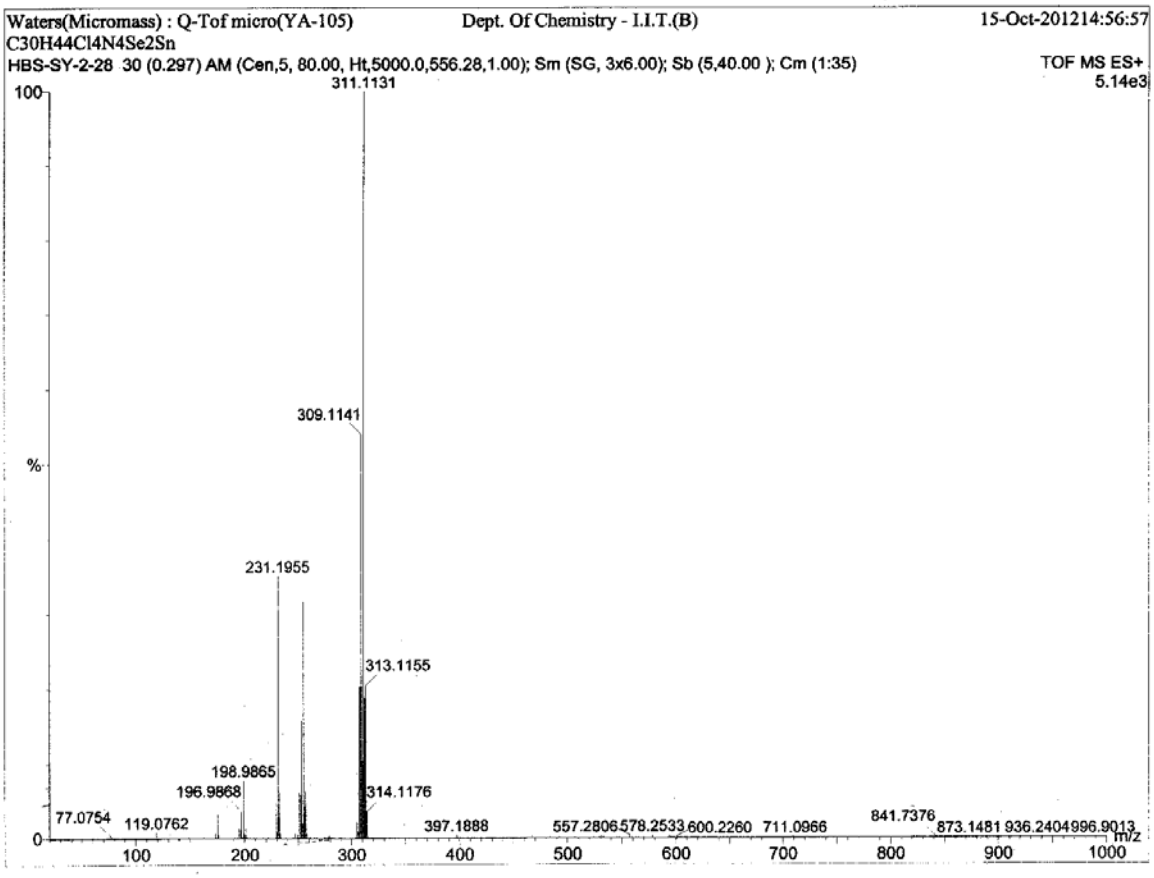


Figure S105. Elemental analysis of **9a**.

Eager 300 Report

Page: 1 Sample: SY-2-28 (SY-2-28)

Method Name : SP260912
Method File : D:\CHNS2012\SP260912.mth
Chromatogram : SY-2-28
Operator ID : SP
Analysed : 09/26/2012 12:49
Sample ID : SY-2-28 (# 13)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 9/26/2012 16:47
Instrument N. : Instrument #1
Sample weight : .926

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	6.1841	43	67876	RS	14.706950	.118530E+07
Carbon	40.4493	67	998249	RS	1.000000	.265764E+07
Hydrogen	4.7925	181	281074	RS	3.551552	.633357E+07
Totals	51.4259		1347199			

Figure S106. Molecular structure of **9a.** Hydrogen atoms are omitted for clarity.

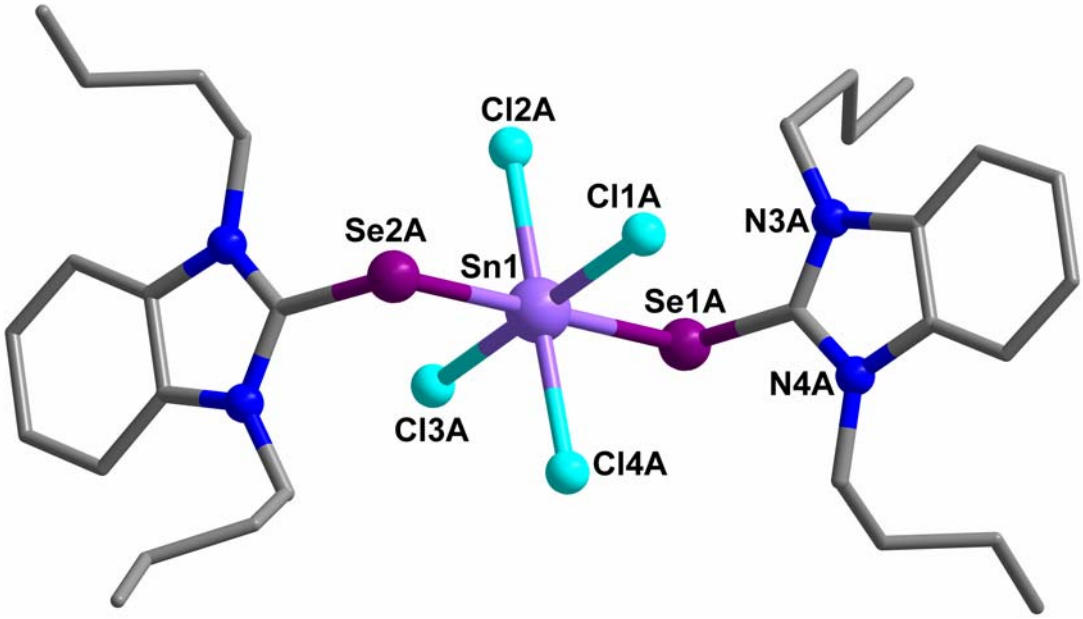


Figure S107. Crystal packing diagram of **9a.** Hydrogen atoms (except those are involved in interactions) are omitted for clarity.

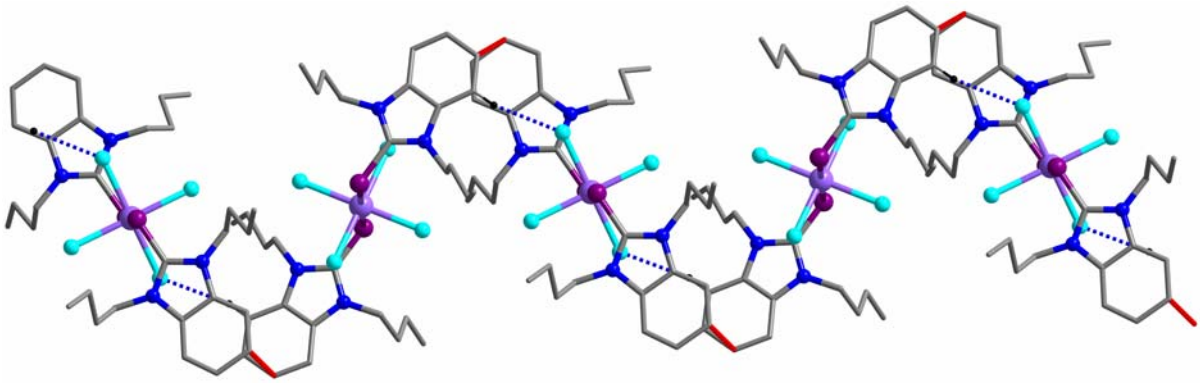


Figure S108. ^{1}H NMR spectrum of **9b** in $CDCl_3$.

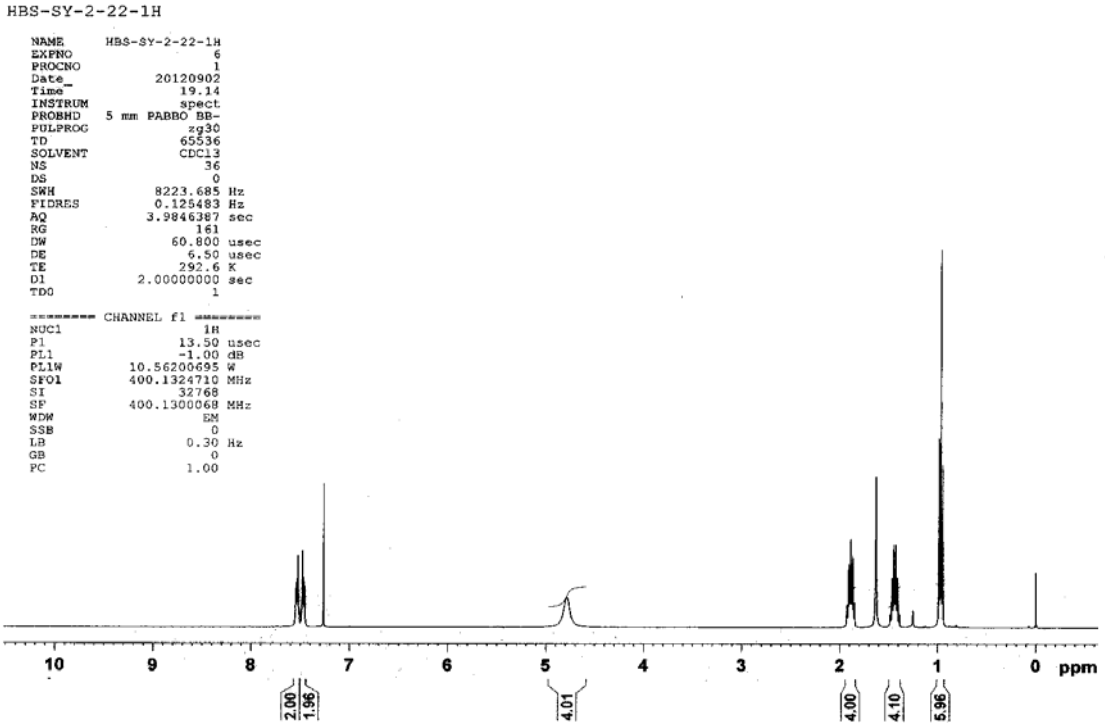


Figure S109. ^{13}C NMR spectrum of **9b** in $CDCl_3$.

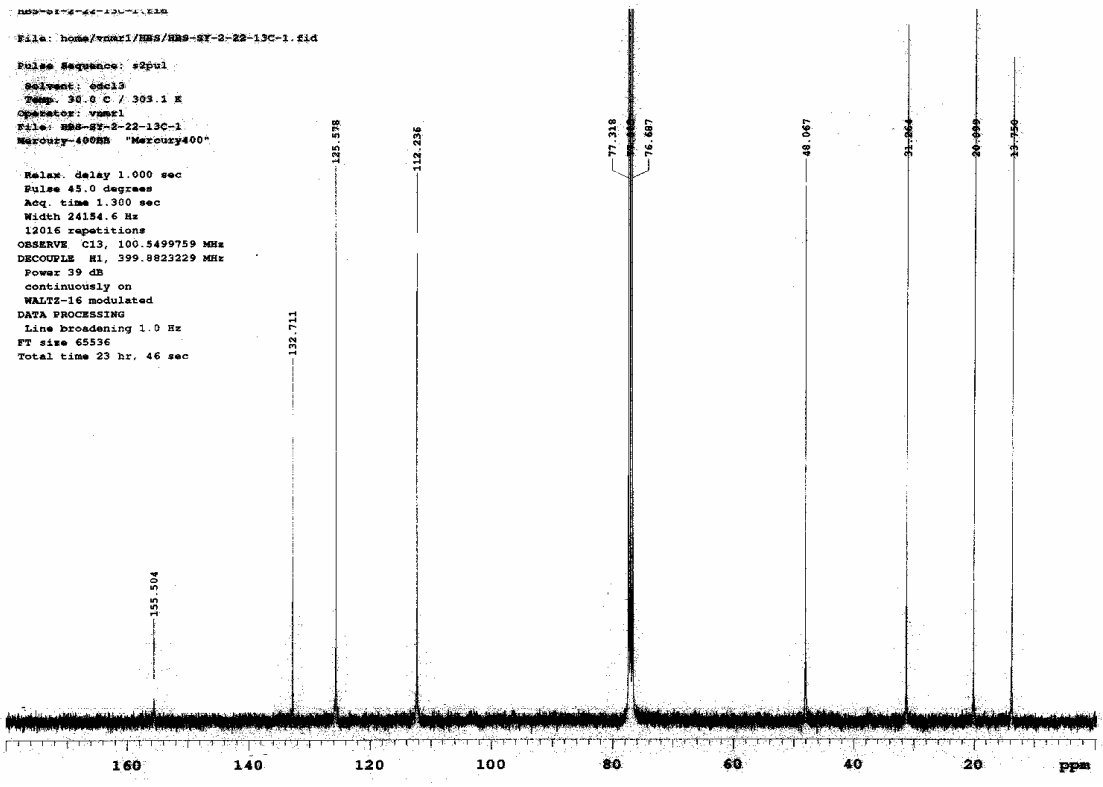


Figure S110. Mass spectrum of **9b**.

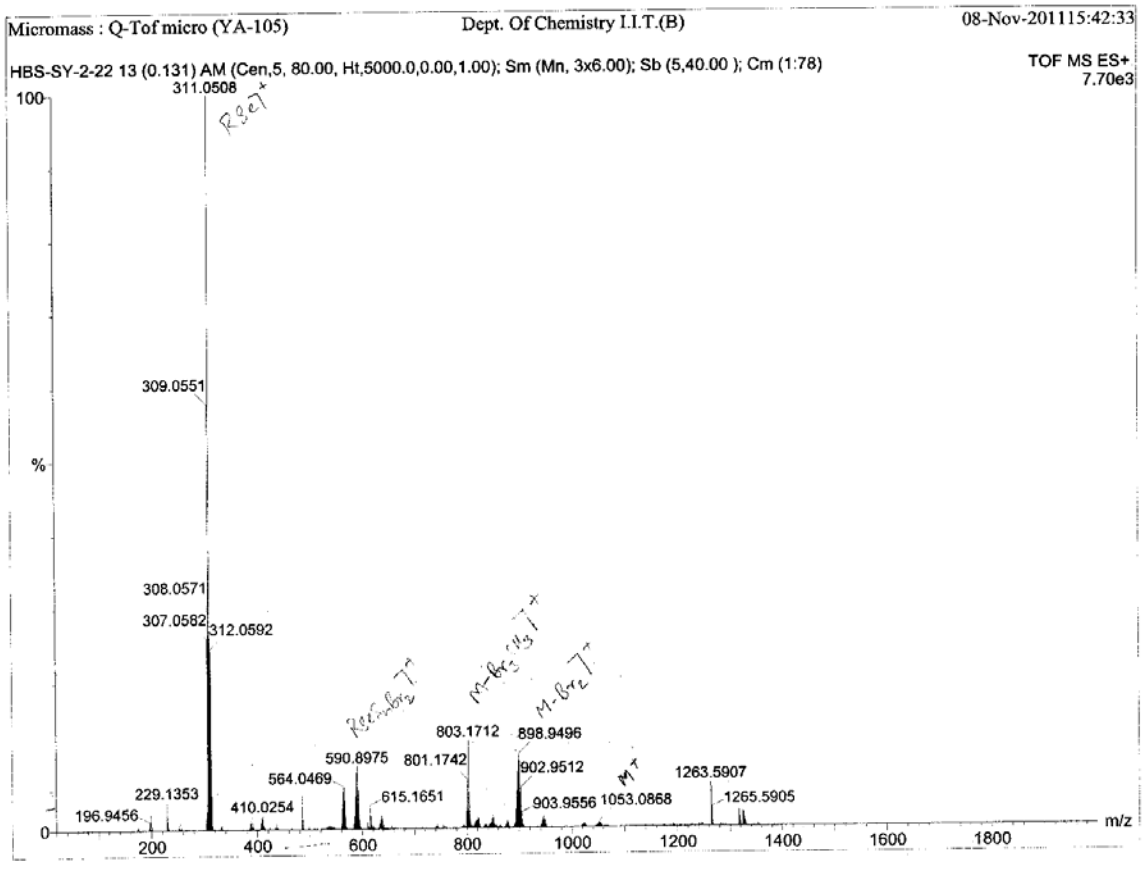


Figure S111. Elemental analysis of **9b**.

Eager 300 Report

Page: 1 Sample: SY-2-14 (SY-2-14)

Method Name : SD-25-11-11
Method File : D:\CHNS2011\SD-25-11-11.mth
Chromatogram : SY-2-14
Operator ID : SD
Analysed : 11/25/2011 15:12
Sample ID : SY-2-14 (# 25)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 11/25/2011 16:18
Instrument N. : Instrument #1
Sample weight : .953

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
1	0.0000	18	4327	RS		0.0000
Nitrogen	6.3605	43	81230	RS	9.874565	.134008E+07
Carbon	33.8786	67	802106	RS	1.000000	.248436E+07
Hydrogen	3.8633	181	200970	RS	3.991173	.525488E+07
Totals	44.1023		1088633			

Figure S112. ^{1}H NMR spectrum of **9c** in $CDCl_3$.

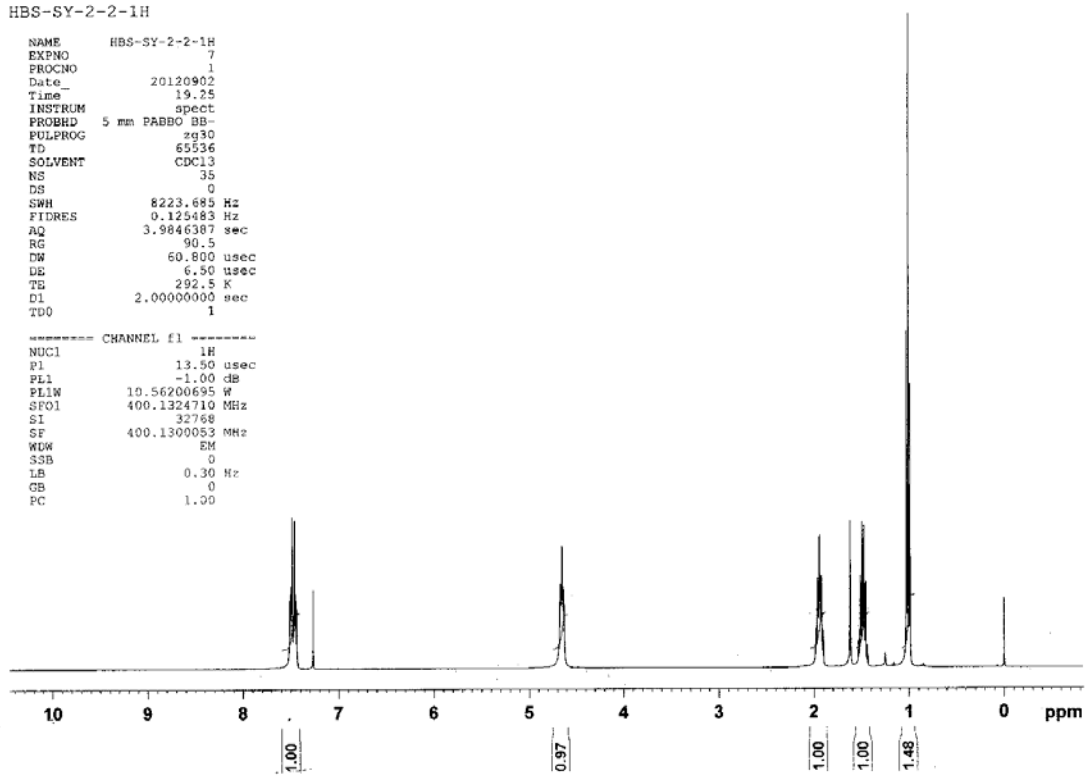


Figure S113. ^{13}C NMR spectrum of **9c** in $CDCl_3$.

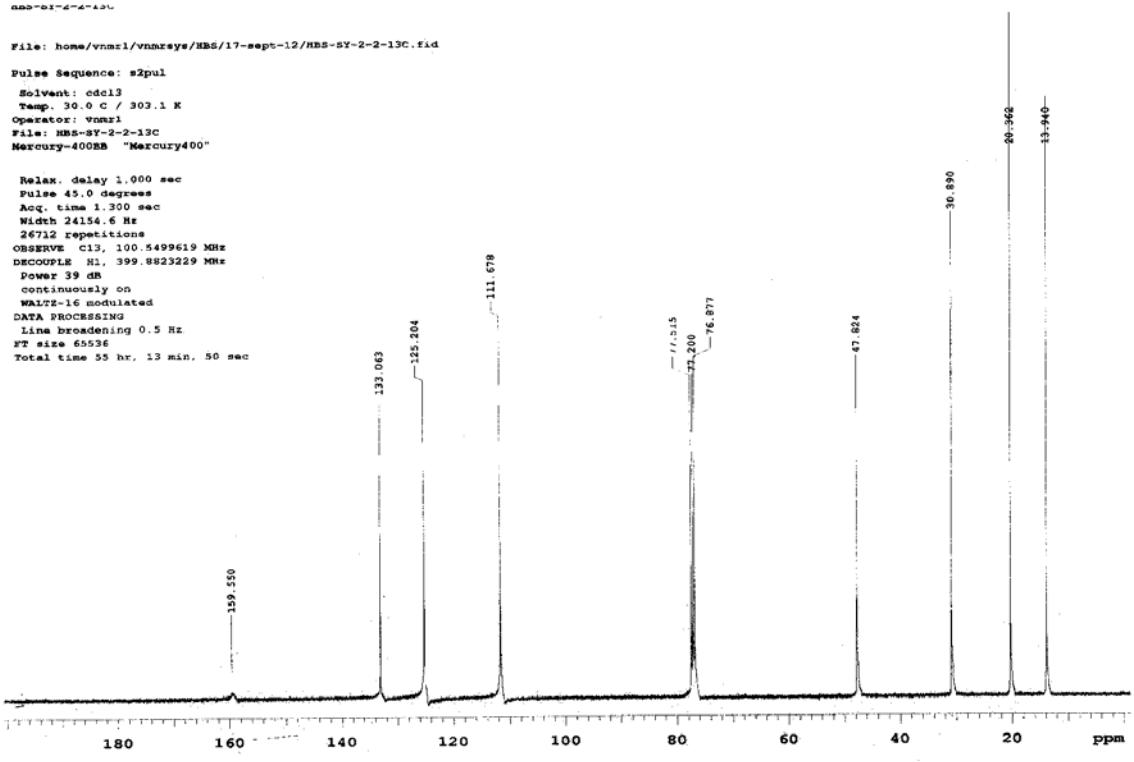


Figure S114. Mass spectrum of **9c**.

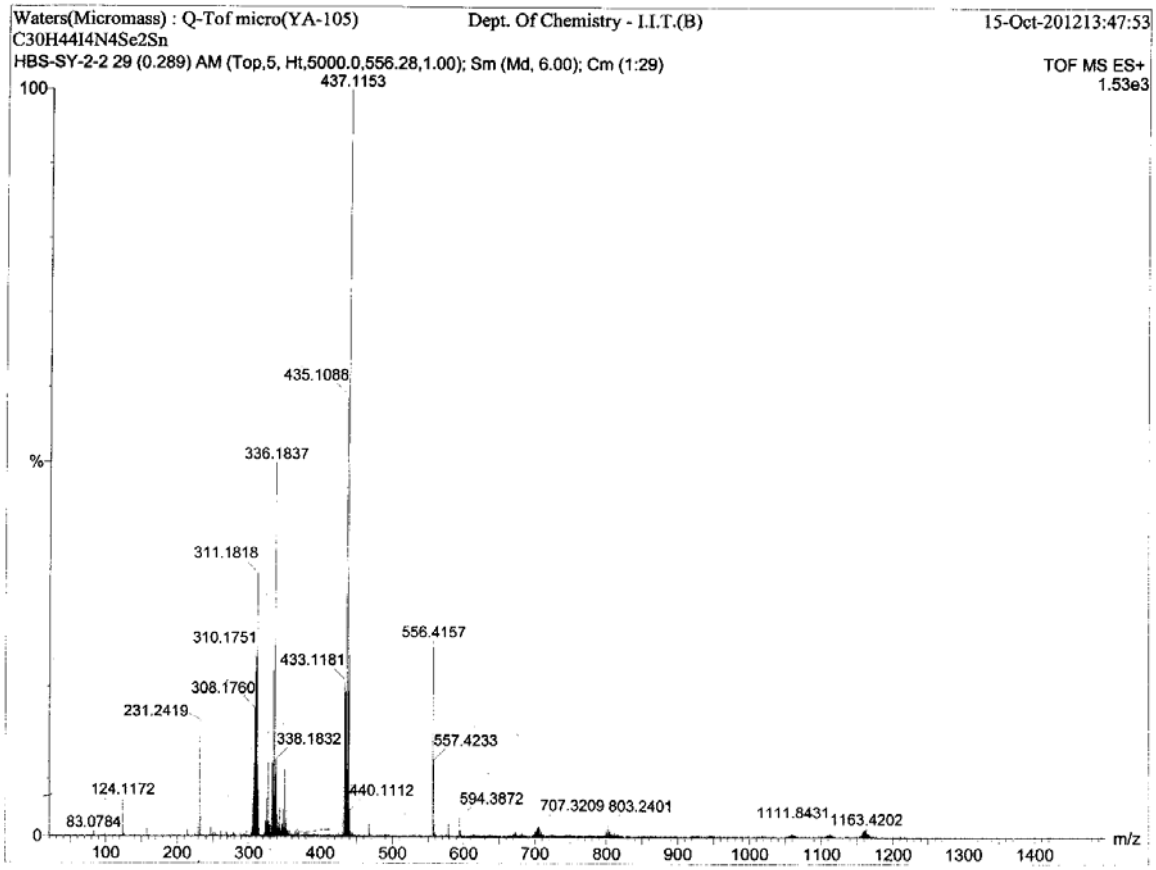


Figure S115. Elemental analysis of **9c**.

Eager 300 Report

Page: 1 Sample: HBS-SY-2-2 (HBS-SY-2-2)

Method Name : SP141211
Method File : D:\CHNS2011\SP141211.mth
Chromatogram : HBS-SY-2-2
Operator ID : SP
Company Name : C.E. Instruments
Analysed : 12/14/2011 14:26
Printed : 12/14/2011 15:54
Sample ID : HBS-SY-2-2 (# 21)
Instrument N. : Instrument #1
Analysis Type : UnkNown (Area)
Sample weight : 1.308

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
1	0.0000	18	4611	RS		0.0000
Nitrogen	5.1934	43	98505	FU	10.473860	.145011E+07
Carbon	29.4581	67	1031726	FU	1.000000	.267152E+07
Hydrogen	3.4900	181	268484	RS	3.842783	.562667E+07
Totals	38.1414		1403326			

Figure S116. ^{1}H NMR spectrum of **10** in THF-d_8.

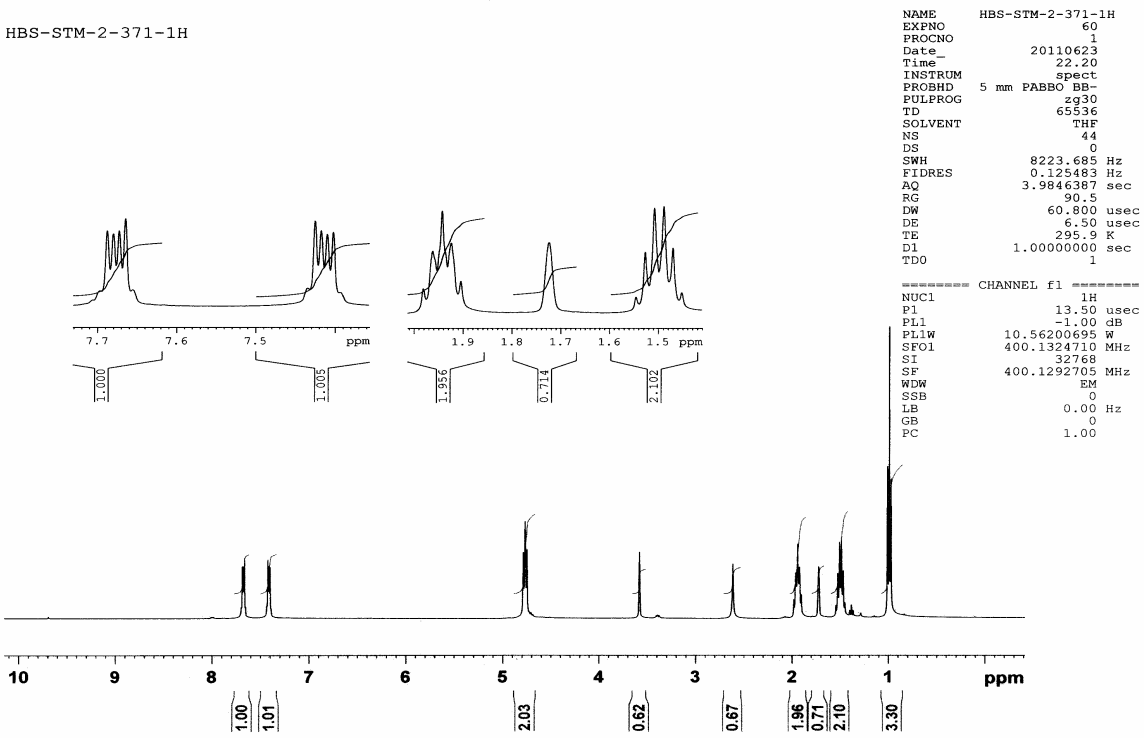


Figure S117. ^{13}C NMR spectrum of **10** in THF-d_8.

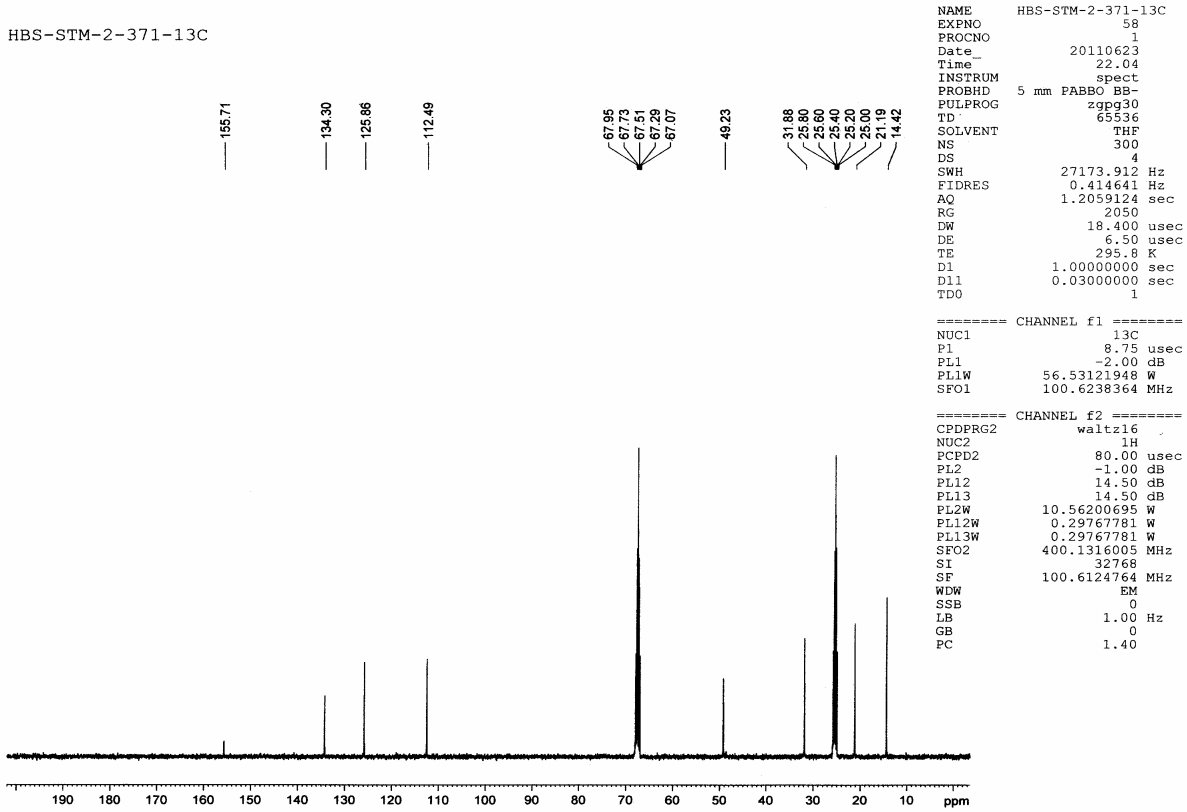
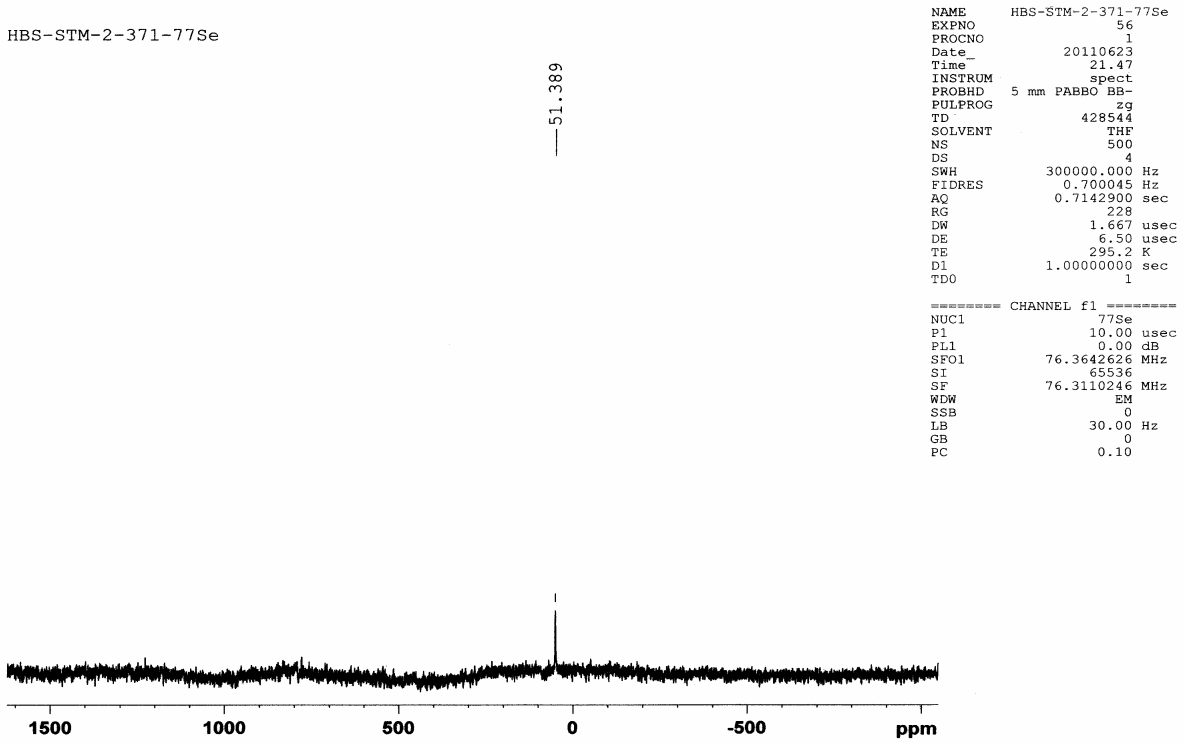


Figure S118. ^{77}Se NMR spectrum of **10** in THF-d_8.



NAME	HBS-STM-2-371-77Se
EXPNO	56
PROCNO	1
Date_	20110623
Time	21.47
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg
TD	428544
SOLVENT	THF
NS	500
DS	4
SWH	300000.000 Hz
FIDRES	0.700045 Hz
AQ	0.7142900 sec
RG	228
DW	1.667 usec
DE	6.50 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	77Se
P1	10.00 usec
PL1	0.00 dB
SFO1	76.3642626 MHz
SI	65536
SF	76.3110246 MHz
WDW	EM
SSB	0
LB	30.00 Hz
GB	0
PC	0.10

Figure S119. Mass spectrum of **10.**

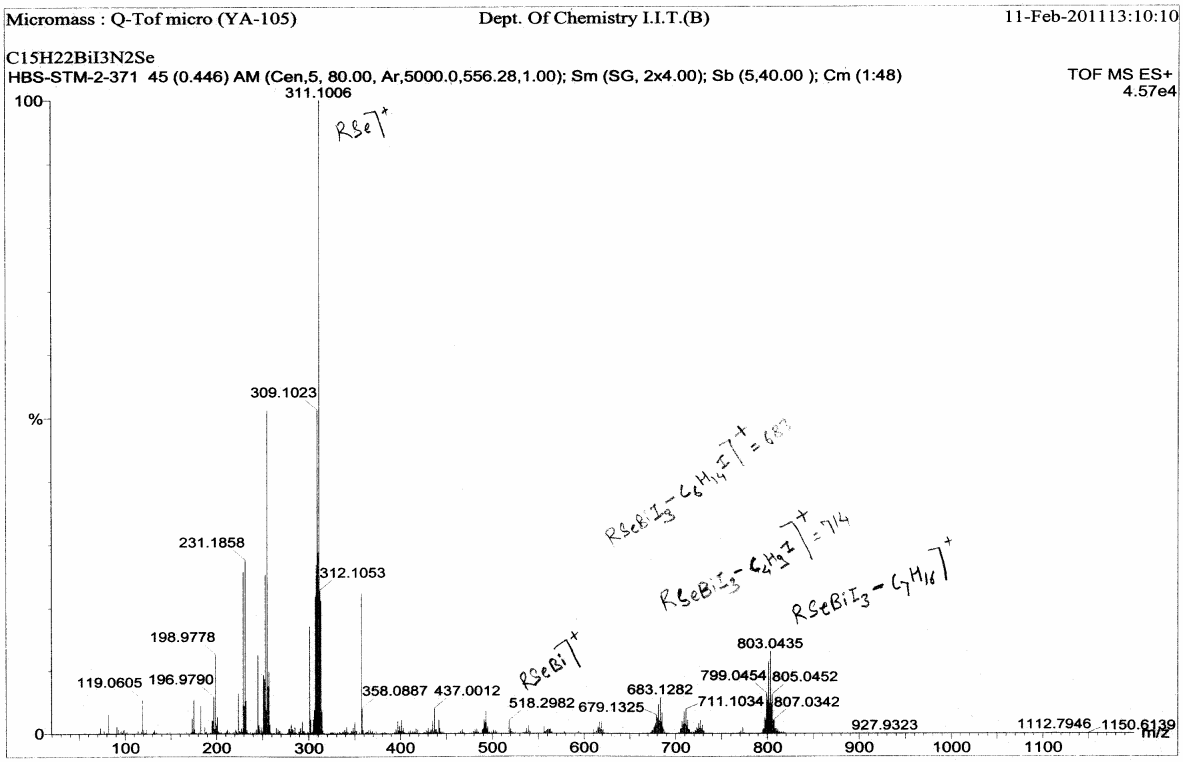


Figure S120. Elemental analysis of **10**.

Eager 300 Report

Page: 1 Sample: STM-2-371 (STM-2-371)

Method Name : SP21012011
Method File : D:\CHNS2011\SP21012011.mth
Chromatogram : STM-2-371
Operator ID : SD **Company Name : C.E. Instruments**
Analysed : 01/21/2011 12:49 **Printed : 1/21/2011 14:52**
Sample ID : STM-2-371 (# 13) **Instrument N. : Instrument #1**
Analysis Type : UnkNown (Area) **Sample weight : 1.025**

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name		%	Ret.Time		Area	BC	Area ratio	K factor
Nitrogen	N = 3.12	3.8363	0.71	44	72540	FU	7.601289	.184477E+07
Carbon	C = 20.04	20.2715	0.23	68	551400	FU	1.000000	.265374E+07
Hydrogen	H = 2.47	2.1505	0.32	178	129247	RS	4.266251	.586343E+07
Totals		26.2583			753188			

Figure S121. TG-DTA of **10**.

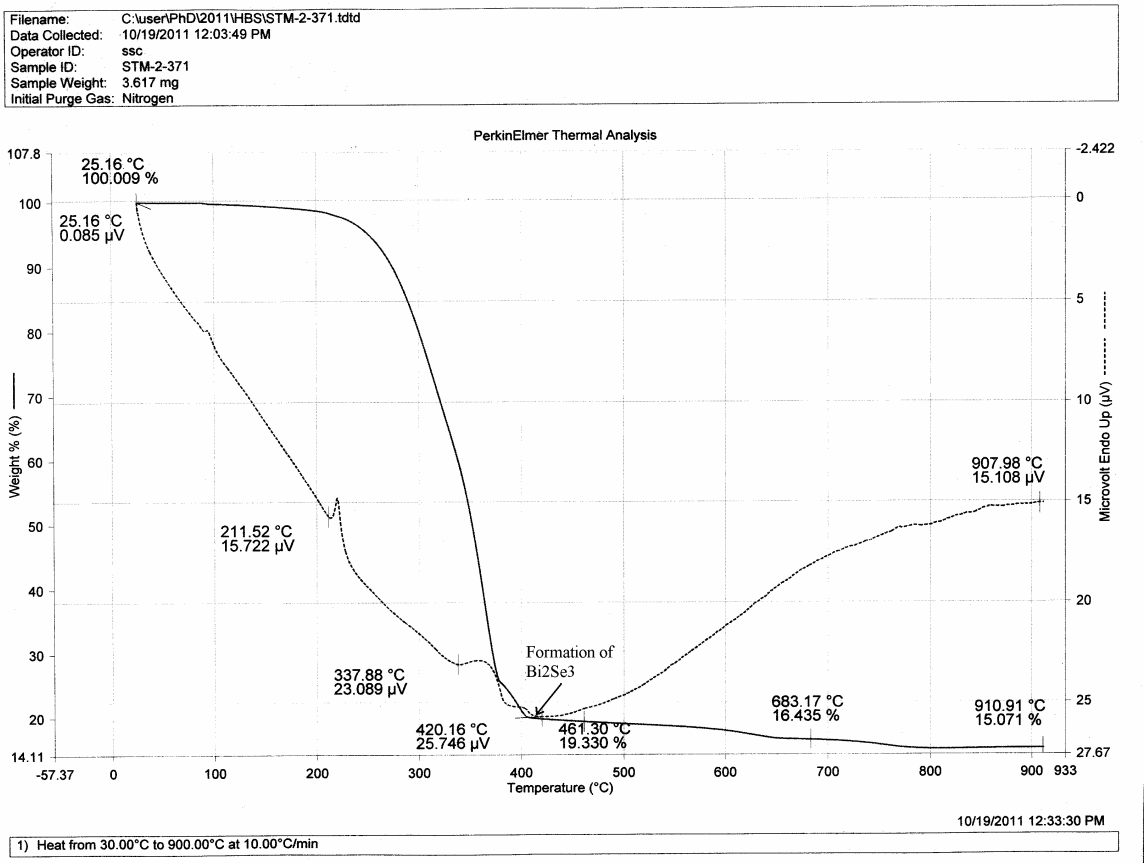


Table S1. Selected bond lengths and bond angles for compounds **7g** and **9a**

7g	**Se1-C1A**	**Te-Se1 2.799(2)**	**Te-I1**	**Se1-Te-Se2**	**I1-Te-I3**	**Se1-Te-I1**
	1.91(2)		**2.9619(18)**	**168.98(8)**	**170.21(6)**	**94.46(7)**
	Se2-C1B	**Te-Se(2)**	**Te-I3**	**C1A-Se1-Te**	**Se1-Te-I4**	**Se2-Te-I1**
	1.859(18)	**2.855(2)**	**2.8870(18)**	**102.5(5)**	**77.91(6)**	**91.33(6)**
9a	**Se1A-C16A**	**Sn1-Se1A**	**Sn1-Cl1A**	**Se2A-Sn1-Se1A**	**Cl1A-Sn1-Se2A**	**Cl3A-Sn1-Se2A**
	1.886(15)	**2.6625(17)**	**2.448(3)**	**179.3(6)**	**84.5(9)**	**95.8(9)**
	Se2A-C1A	**Sn1-Se2A**	**Sn1-Cl3A**	**C1A-Se2A-Sn1**	**Cl2A-Sn1-Cl4A**	**Cl2A-Sn1-Se2A**
	1.915(14)	**2.6543(19)**	**2.450(3)**	**100.9(4)**	**179.0(3)**	**90.61(8)**

Table S2. Details of the X-ray data collection parameters for **7g** and **9a**

Compound	**7g**	**9a**
formula	$C_{30}H_{44}I_4N_4Se_2Te$	$C_{30}H_{44}Cl_4N_4Se_2Sn$
Mr	1253.81	879.10
system	Monoclinic	Monoclinic
space group	*P*21/n	P 21
a[Å]	11.8041(5)	9.2286(2)
b[Å]	21.7135(7)	22.9106(4)
c[Å]	16.6329(6)	17.4761(4)
α[°]	90	90
β[°]	104.709(4)	90.172(2)
γ[°]	90	90
V[Å^3]	4123.4(3)	3695.00(13)
Z	4	4
Size [mm^3]	0.5555 x 0.3248 x 0.2047	0.5031 x 0.3602 x 0.2115
ρ_{calcd} [Mg/m^3]	2.020	1.580
μ [mm^{-1}]	5.505	10.607
Refls. collected	47478	10085
Observed reflns	8323	8219
R_1 [$I>2\sigma(I)$]	0.1103	0.0500
wR_2 [$I>2\sigma(I)$]	0.2170	0.1300