

## Supporting Information

### Selone-stabilized aryltellurenyl cations

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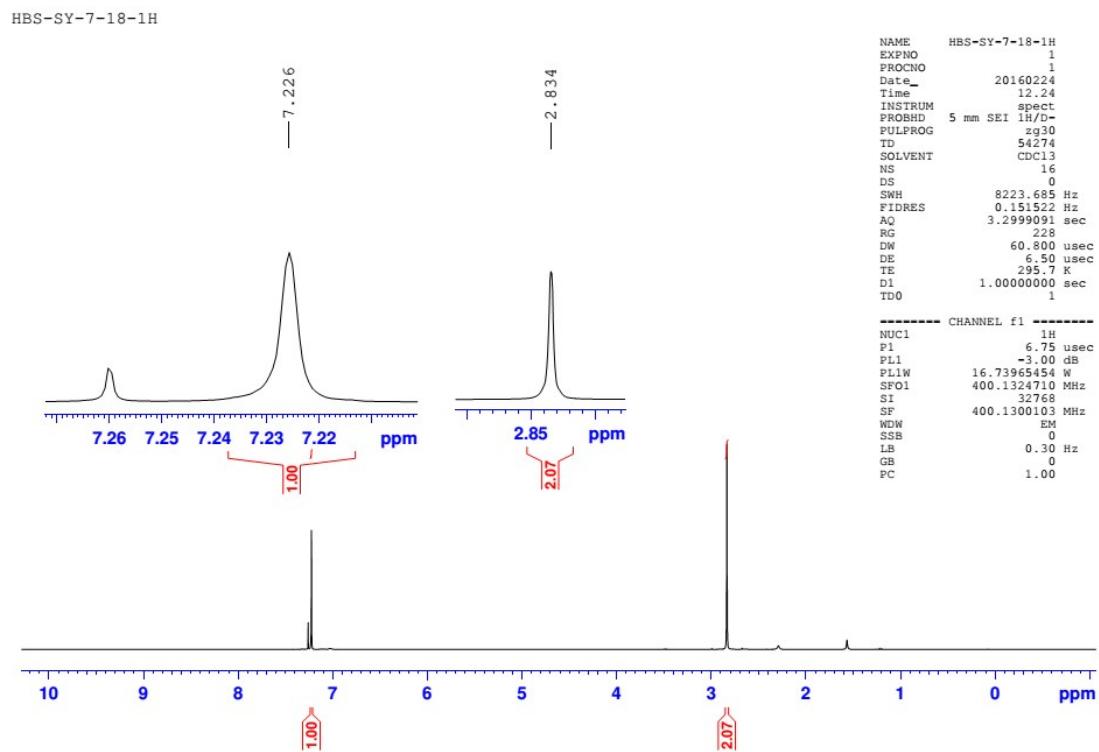
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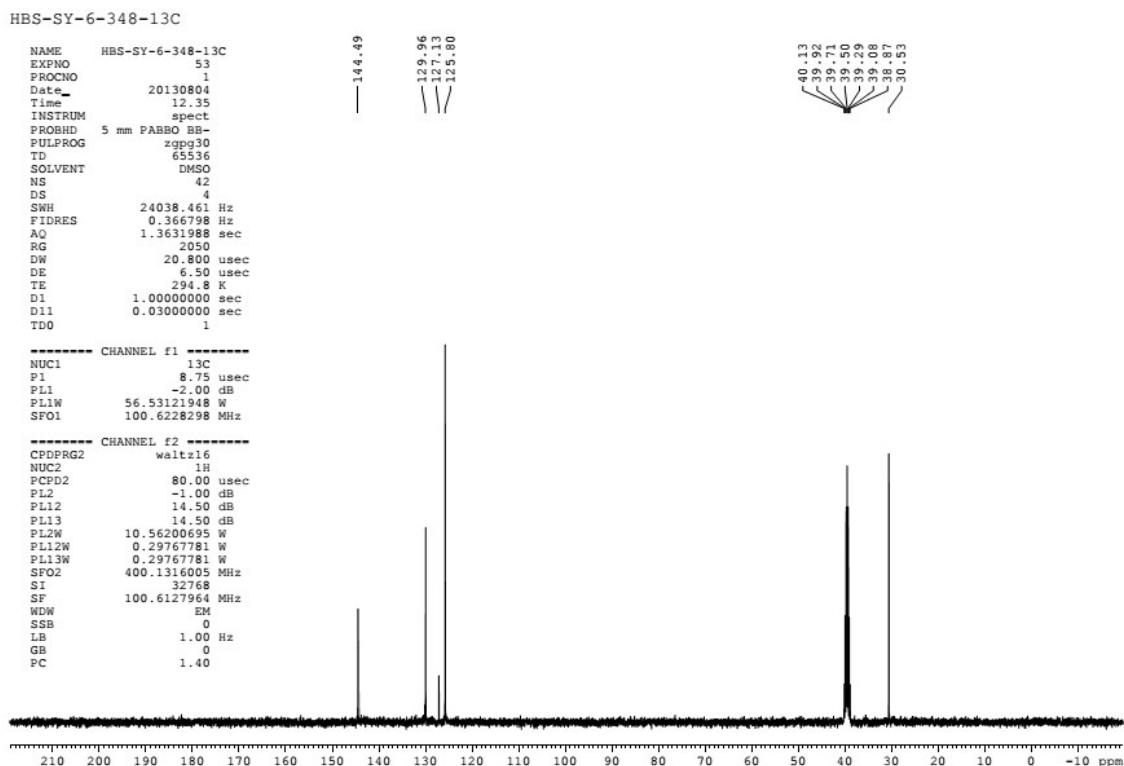
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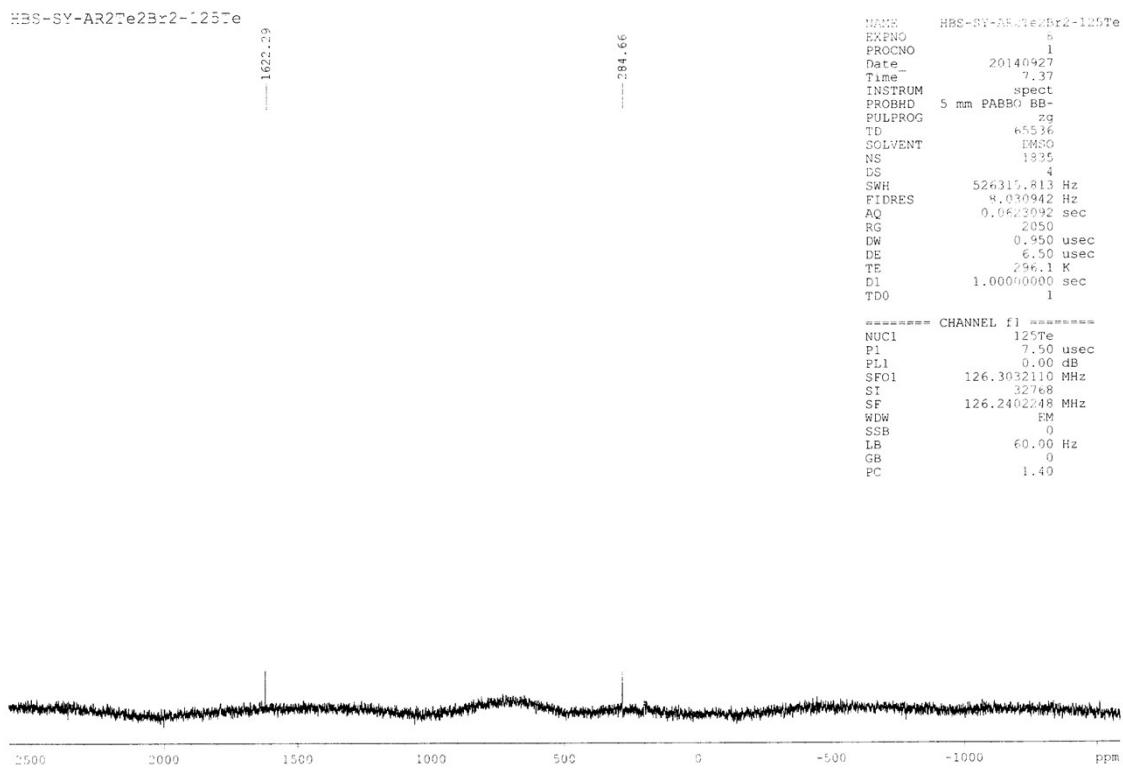
## Spectral data



**Figure S1.**  $^1\text{H}$  NMR spectrum of compound 7.



**Figure S2.**  $^{13}\text{C}$  NMR spectrum of compound 7.



**Figure S3.** <sup>125</sup>Te NMR spectrum of compound 7.

### Eager 300 Report

Page: 1 Sample: SY-7-18 (SY-7-18)

```

Method Name   : HBS-VT-18-07-2014
Method File   : D:\CHNS-2014\HBS-VT-18-07-2014.mth
Chromatogram  : SY-7-18
Operator ID   : VARSHA
Analysed      : 07/18/2014 14:09
Sample ID     : SY-7-18 (# 17)
Analysis Type : UnkNowN (Area)           Company Name : C.E. Instruments
                                                Printed    : 7/18/2014 18:41
                                                Instrument N. : Instrument #1
                                                Sample weight : .736

```

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Carbon	30.7874	66	613947	RS	1.000000	.270944E+0
Hydrogen	2.4733	181	135581	RS	4.528267	.679637E+0
Totals	33.2608		749528			

**Figure S4.** Elemental analysis of compound 7.

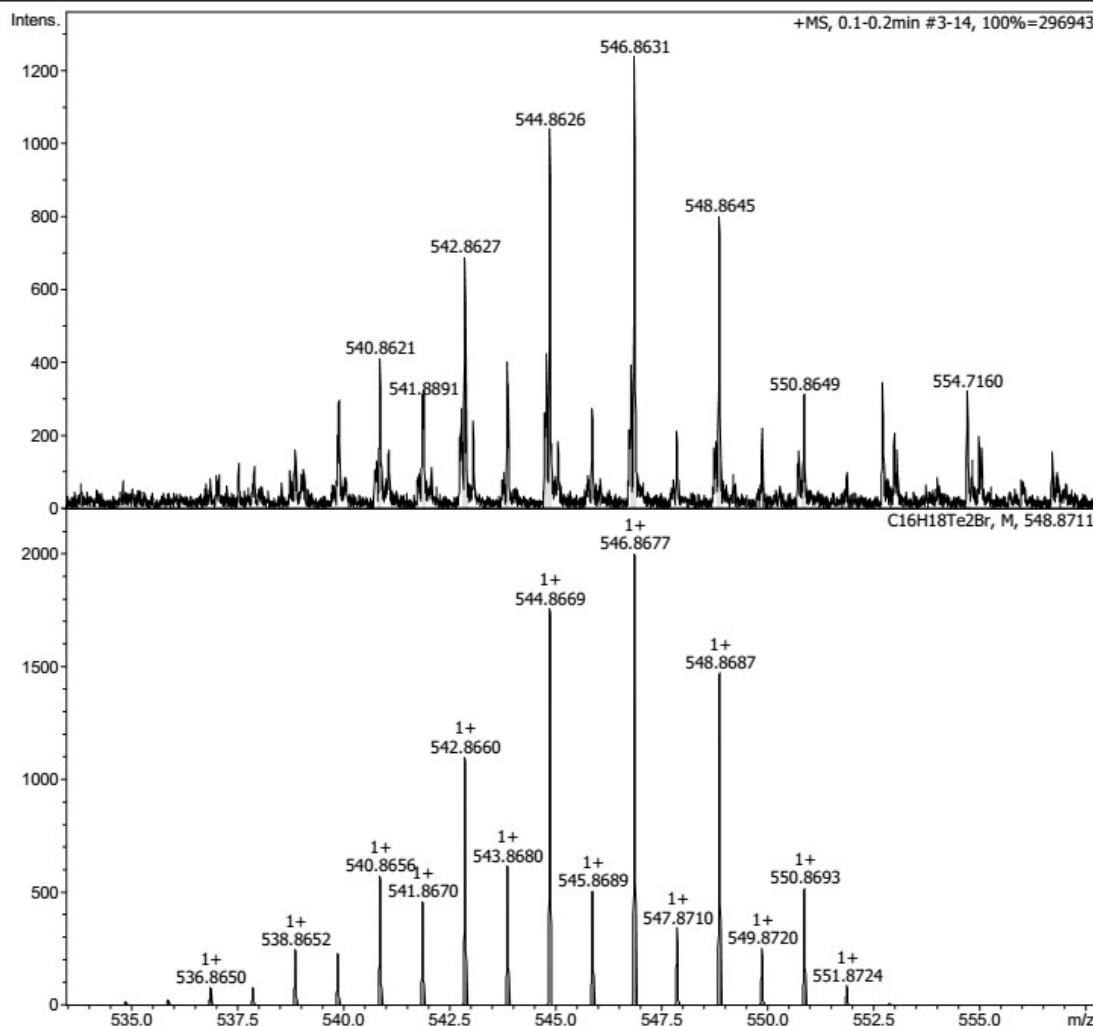
## Display Report

**Analysis Info**

Analysis Name	D:\Data\JULY-2014\HBS-SY-AR2TE2BR2.d	Acquisition Date	7/9/2014 5:17:57 PM
Method	Tune_pos_Standard_NAI_1000 MAY 2014.m	Operator	HBS-SY
Sample Name	HBS-SY-AR2TE2BR2	Instrument	maXis impact
Comment			282001.00081

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



HBS-SY-AR2TE2BR2.d

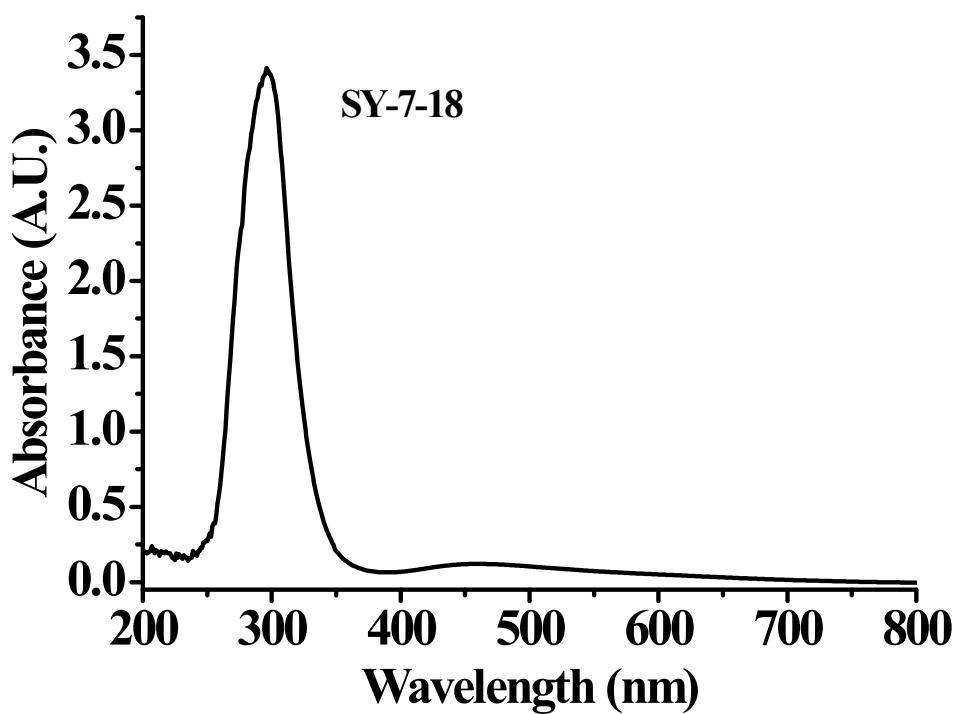
Bruker Compass DataAnalysis 4.1

printed: 2/24/2016 2:35:26 PM

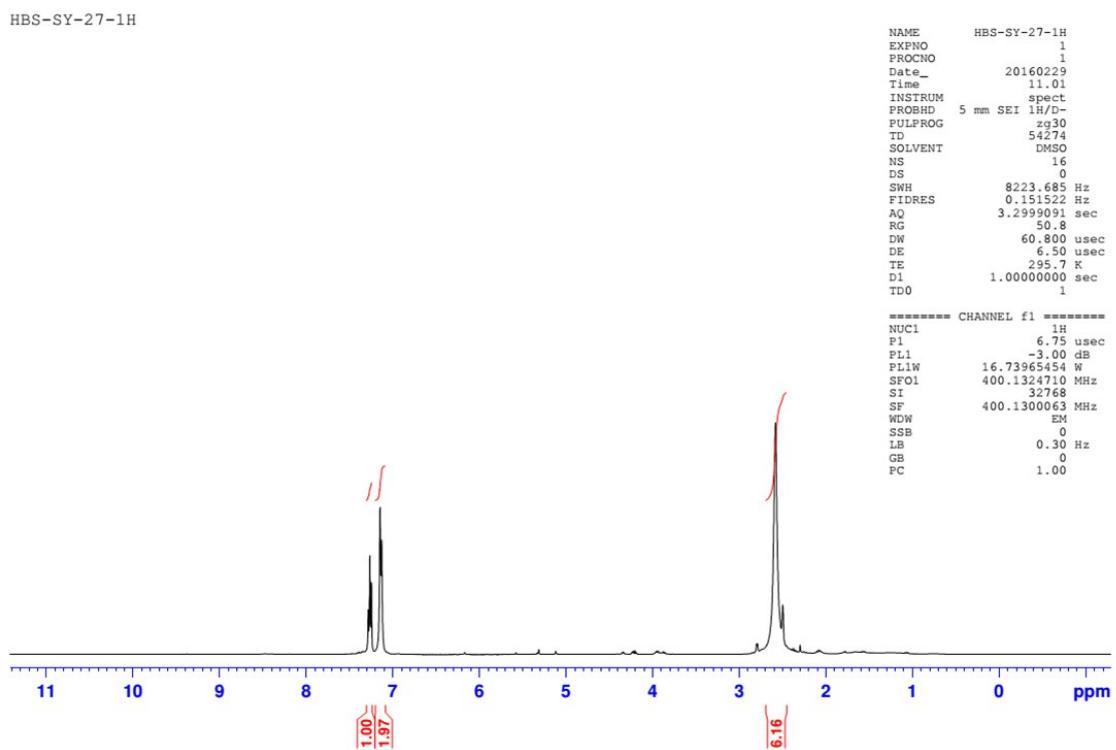
by: RAJ

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**Figure S5.** ESI-MS spectrum of compound 7.



**Figure S6.** UV-Visible spectrum of compound 7.



**Figure S7.**  $^1\text{H}$  NMR spectrum of compound 8.

HBS-SY-27-13C

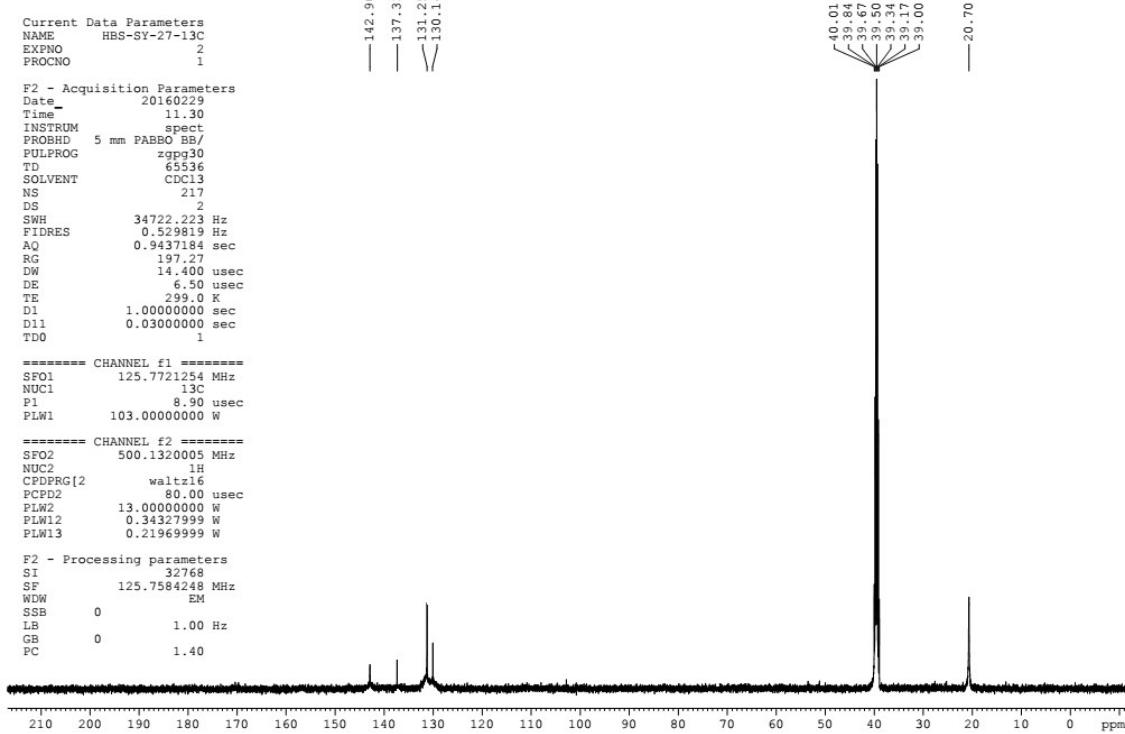


Figure S8. <sup>13</sup>C NMR spectrum of compound 8.

HBS-SY-27-125Te

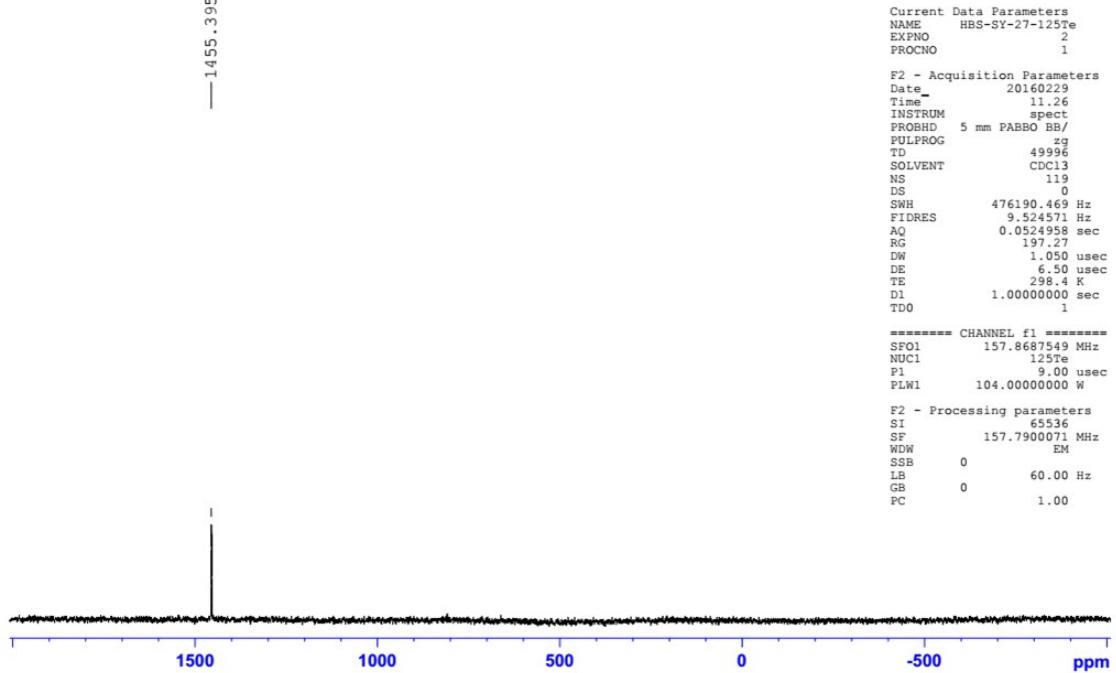


Figure S9. <sup>125</sup>Te NMR spectrum of compound 8.

**Eager 300 Report**  
 Page: 1 Sample: SY-6-348 (SY-6-348)

```

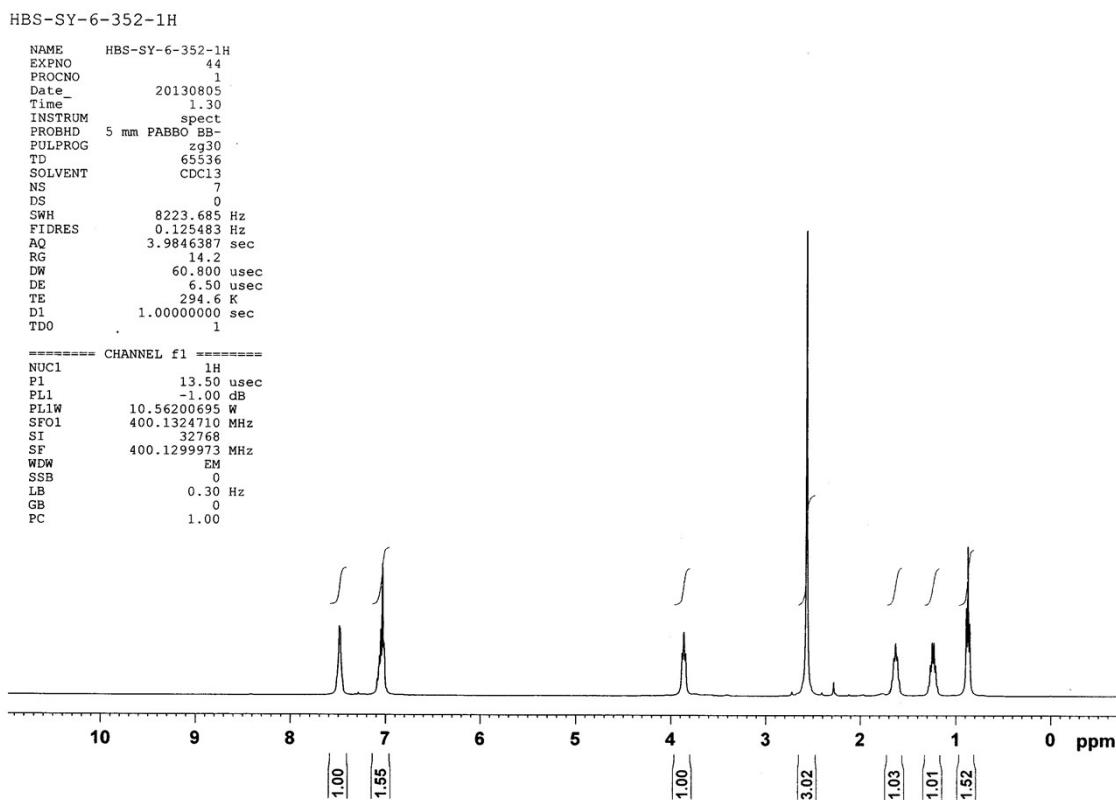
Method Name : sd041013
Method File : D:\CHNS2012-13\sd041013.mth
Chromatogram : SY-6-348
Operator ID : SD
Analysed : 10/04/2013 15:09
Sample ID : SY-6-348 (# 25)
Analysis Type : Unknown (Area)          Company Name : C.E. Instruments
                                                Printed : 10/4/2013 16:44
                                                Instrument N. : Instrument #1
                                                Sample weight : .952

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 9821 RS 0.0000
Carbon 20.4086 67 528134 RS 1.000000 .270372E+07
Hydrogen 1.4529 184 105377 RS 5.011853 .632918E+07
Totals 21.8615 643332
    
```

**Figure S10.** ESI-MS spectrum of compound 8.



**Figure S11.**  $^1\text{H}$  NMR spectrum of compound 10.

HBS-SY-6-352-13C

```

NAME      HBS-SY-6-352-13C
EXPNO        45
PROCNO       1
Date       20130805
Time       1.34
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT    CDCl3
NS         66
DS          4
SWH       24038.461 Hz
FIDRES     0.366798 Hz
AQ        1.3631988 sec
RG        2050
DW        20.800 usec
DE        6.50 usec
TE        295.1 K
D1        1.0000000 sec
D11       0.03000000 sec
TDO        1

```

```

===== CHANNEL f1 =====
NUC1        13C
P1        8.75 usec
PL1       -2.00 dB
PL1W      56.53121948 W
SF01      100.6228298 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2      80.00 usec
PL2       -1.00 dB
PL12      14.00 dB
PL13      14.50 dB
PL2W      10.56200695 W
PL12W     0.29767781 W
PL13W     0.29767781 W
SF02      400.1316005 MHz
SI        32768
SF      100.6128016 MHz
WDW        EM
SSB        0
LB        1.00 Hz
GB        0
PC        1.40

```



**Figure S12.**  $^{13}\text{C}$  NMR spectrum of compound **10**.

HBS-SY-6-352-77Se

```

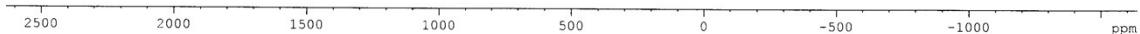
NAME      HBS-SY-6-352-77Se
EXPNO        46
PROCNO       1
Date       20130805
Time       1.36
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG  zg
TD        65536
SOLVENT    CDCl3
NS         69
DS          4
SWH       326086.969 Hz
FIDRES     4.975692 Hz
AQ        0.1005385 sec
RG        2050
DW        1.533 usec
DE        6.50 usec
TE        294.7 K
D1        1.0000000 sec
TDO        1

```

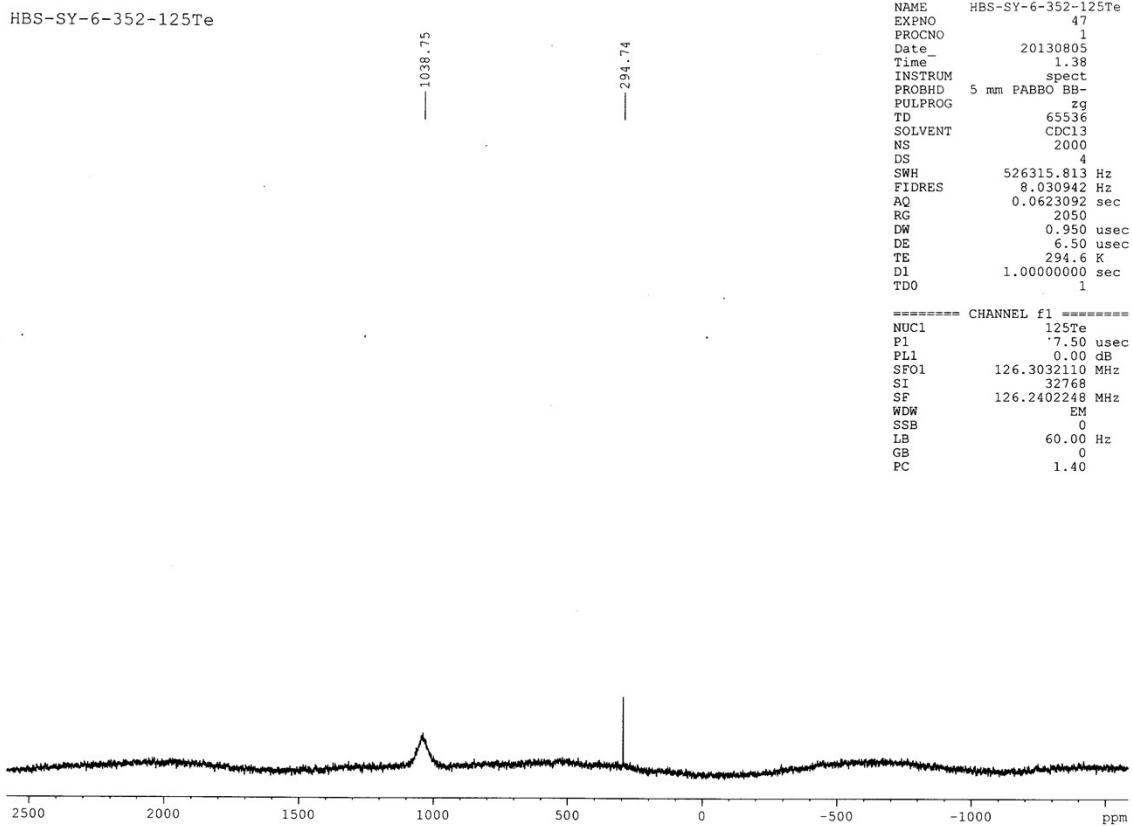
```

===== CHANNEL f1 =====
NUC1        77Se
P1        10.00 usec
PL1       0.00 dB
SF01      76.3490004 MHz
SI        65536
SF      76.3110246 MHz
WDW        EM
SSB        0
LB        60.00 Hz
GB        0
PC        0.00

```



**Figure S13.**  $^{77}\text{Se}$  NMR spectrum of compound **10**.



**Figure S14.**  $^{125}\text{Te}$  NMR spectrum of compound **10**.

### Eager 300 Report

Page: 1 Sample: SY-6-350 (SY-6-350)

Method Name : sd041013	Company Name : C.E. Instruments
Method File : D:\CHNS2012-13\sd041013.mth	Printed : 10/4/2013 16:44
Chromatogram : SY-6-350	Instrument N. : Instrument #1
Operator ID : SD	Sample weight : .882
Analysed : 10/04/2013 14:58	
Sample ID : SY-6-350 (# 24)	
Analysis Type : UnkNowN (Area)	

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	9672	RS		0.0000
Nitrogen	5.2019	43	59371	RS	16.148810	.129404E+07
Carbon	40.0868	66	958771	RS	1.000000	.270372E+07
Hydrogen	4.0634	178	244669	RS	3.918645	.632918E+07
Totals	49.3521		1272483			

**Figure S15.** Elemental analysis of compound **10**.

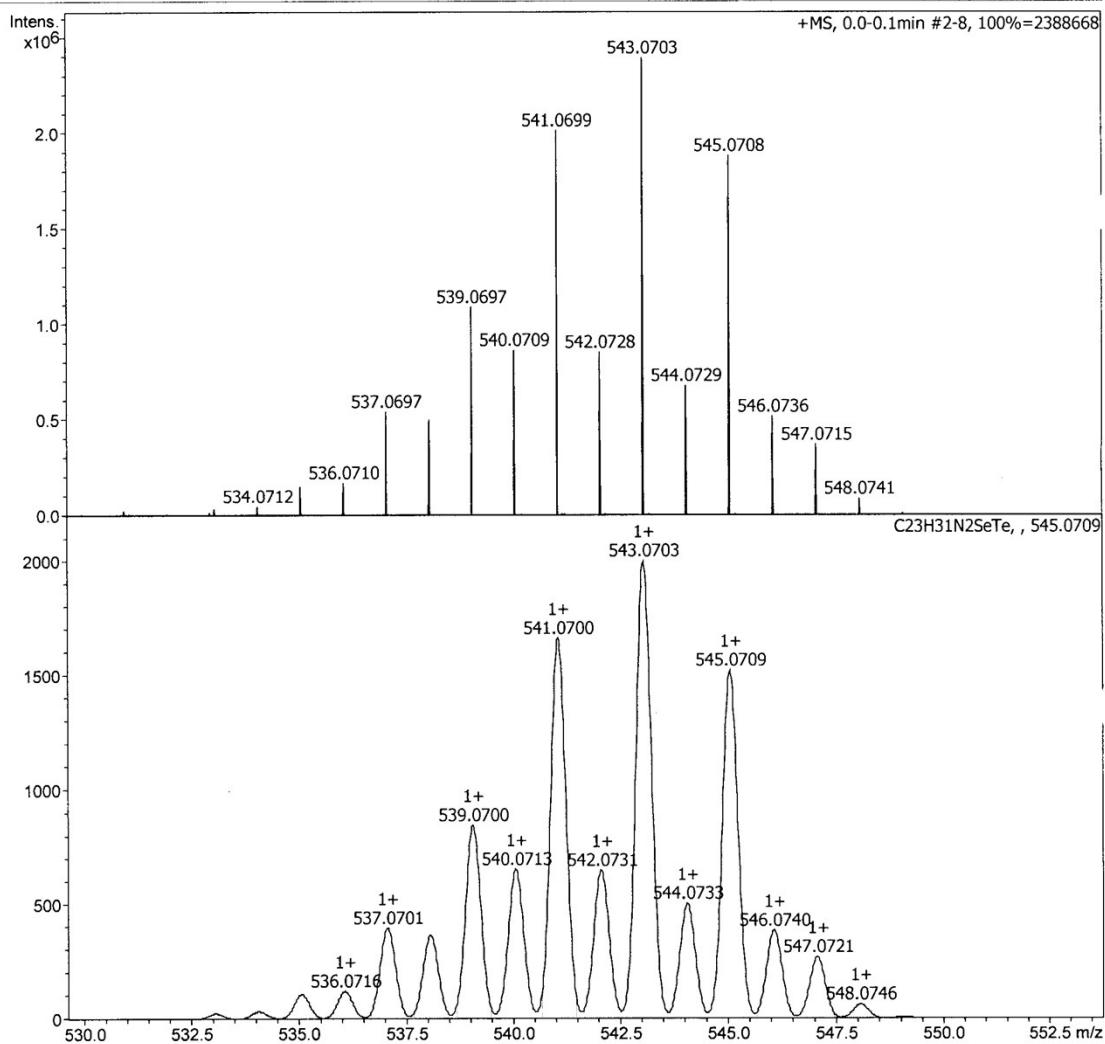
## Display Report

**Analysis Info**

Analysis Name	D:\Data\AUG_13\HBS-SY-6-352.d	Acquisition Date	8/7/2013 11:44:42 PM
Method	Tune_pos_Standard_NAI-1000.m	Operator	IIT-B
Sample Name	HBS-SY-6-352	Instrument	maXis impact 282001.00081
Comment	C8H9TeBr2		

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



HBS-SY-6-352.d

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by: IIT-B

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**Figure S16.** ESI-MS spectrum of compound **10** (positive mode of detection).

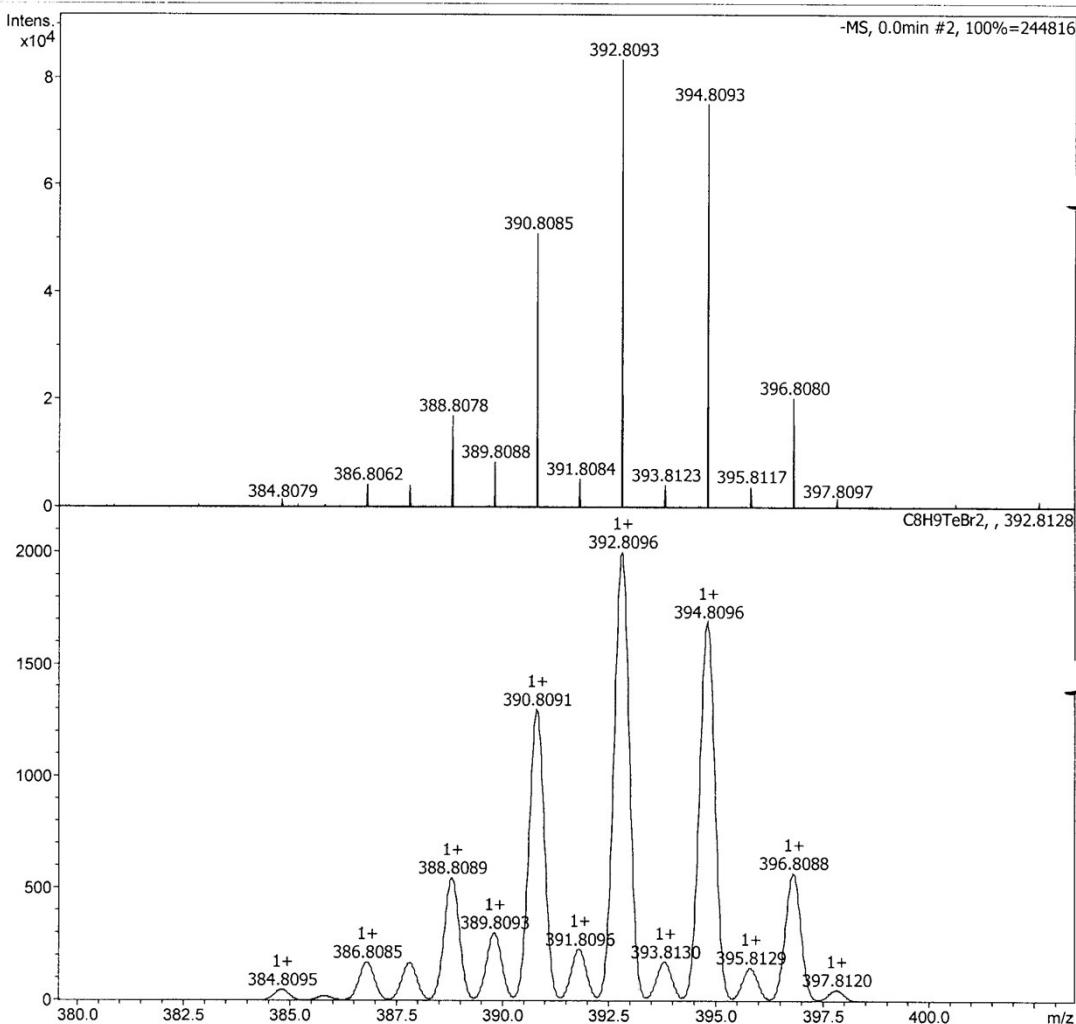
## Display Report

**Analysis Info**

Analysis Name D:\Data\AUG\_13\HBS-SY-6-350-VE.d      Acquisition Date 8/7/2013 11:24:15 PM  
 Method Tune\_neg\_Standard\_NAF-1000.m      Operator IIT-B  
 Sample Name HBS-SY-6-350-VE      Instrument maXis impact 282001.00081  
 Comment C8H9TeBr2

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



HBS-SY-6-350-VE.d

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by: IIT-B

Page 1 of 1

**Figure S17.** ESI-MS spectrum of compound **10** (negative mode of detection).

HBS-SY-7-22-1H

```

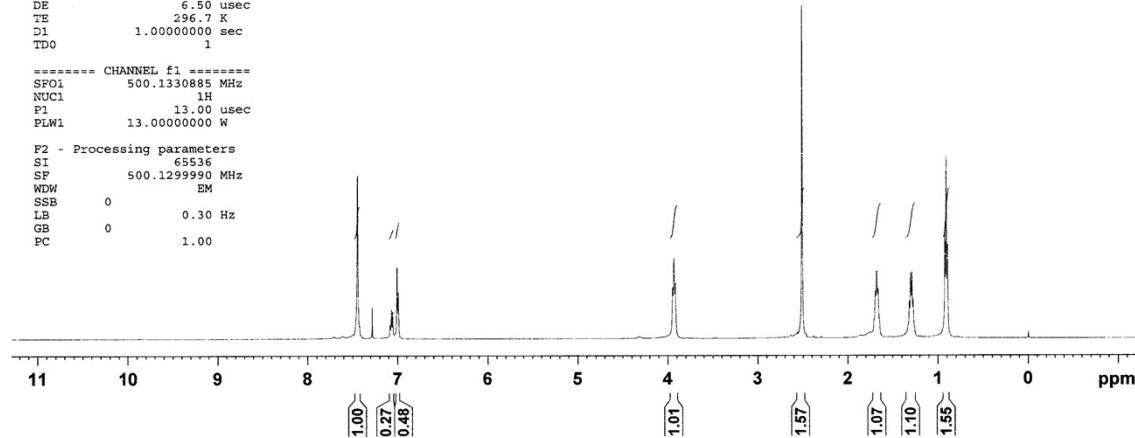
Current Data Parameters
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EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_   20131005
Time_   12.56
INSTRUM spect
PROBHD  5 mm PABBO BB/
PULPROG zpg30
TD      65536
SOLVENT  CDCl3
NS      9
DS      2
SWH     10000.000 Hz
FIDRES  0.152588 Hz
AQ      3.2767999 sec
RG      16.74
DW      50.000 usec
DE      6.50 usec
TE      296.7 K
D1      1.0000000 sec
TD0     1

===== CHANNEL f1 =====
SF01   500.1330885 MHz
NUC1    1H
P1      13.00 usec
PLW1   13.0000000 W

F2 - Processing parameters
SI      65536
SF      500.1299990 MHz
WDW    EM
SSB    0
LB     0.30 Hz
GB     0
PC     1.00

```



**Figure S18.**  $^1\text{H}$  NMR spectrum of compound **11a**.

HBS-SY-7-22-13C

```

Current Data Parameters
NAME      HBS-SY-7-22-13C
EXPNO    11
PROCNO    1

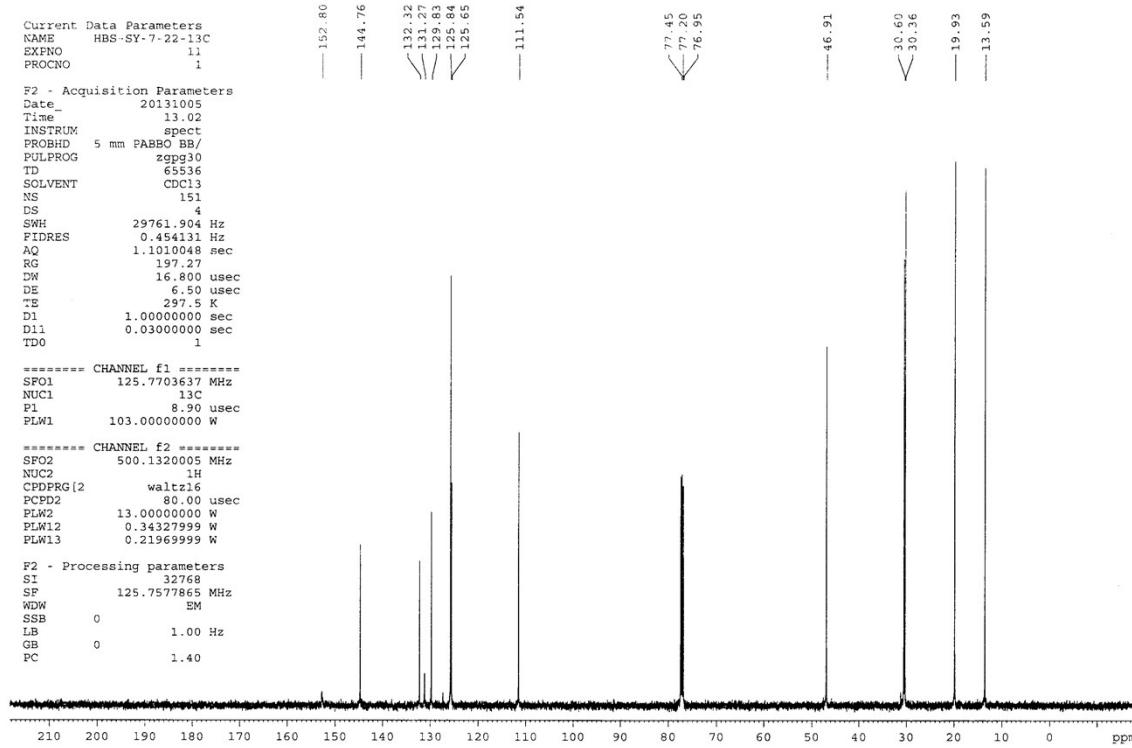
F2 - Acquisition Parameters
Date_   20131005
Time_   13.02
INSTRUM spect
PROBHD  5 mm PABBO BB/
PULPROG zpg30
TD      65536
SOLVENT  CDCl3
NS      151
DS      4
SWH     29761.904 Hz
FIDRES  0.454131 Hz
AQ      1.1010048 sec
RG      197.27
DW      16.800 usec
DE      6.50 usec
TE      297.5 K
D1      1.0000000 sec
D11     0.03000000 sec
TD0     1

===== CHANNEL f1 =====
SF01   125.7703637 MHz
NUC1    13C
P1      8.90 usec
PLW1   103.0000000 W

===== CHANNEL f2 =====
SF02   500.1320005 MHz
NUC2    1H
CPDPRG[2] waltz16
PCPD2   80.00 usec
PLW2   13.00000000 W
PLW12   0.34327999 W
PLW13   0.21969999 W

F2 - Processing parameters
SI      32768
SF      125.7577865 MHz
WDW    EM
SSB    0
LB     1.00 Hz
GB     0
PC     1.40

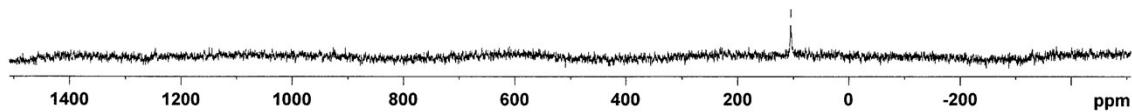
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**Figure S19.**  $^{13}\text{C}$  NMR spectrum of compound **11a**.

HBS-SY-7-22-77Se

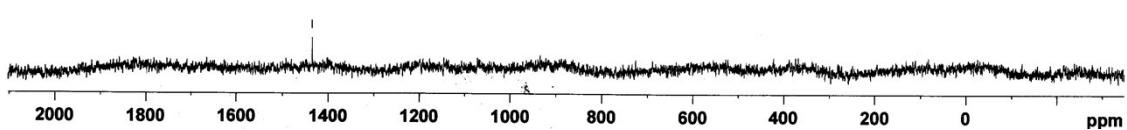
Current Data Parameters  
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 EXPNO 12  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20131005  
 Time 13.08  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 48074  
 SOLVENT CDCl<sub>3</sub>  
 NS 501  
 DS 0  
 SWH 192307.688 Hz  
 FIDRES 4.000243 Hz  
 AQ 0.1249924 sec  
 RG 197.27  
 DW 2.600 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D1 1.0000000 sec  
 TDO 1  
 ===== CHANNEL f1 ======  
 SFO1 95.4300492 MHz  
 NUC1 77Se  
 P1 9.00 usec  
 PLWI 104.00000000 W  
 F2 - Processing parameters  
 SI 65536  
 SF 95.3822928 MHz  
 WDW EM  
 SSB 0  
 LB 30.00 Hz  
 GB 0  
 PC 1.00



**Figure S20.** <sup>77</sup>Se NMR spectrum of compound 11a.

HBS-SY-7-22-125Te

Current Data Parameters  
 NAME HBS-SY-7-22-125Te  
 EXPNO 18  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20131008  
 Time 8.21  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 49996  
 SOLVENT CDCl<sub>3</sub>  
 NS 4499  
 DS 0  
 SWH 625000.000 Hz  
 FIDRES 12.501000 Hz  
 AQ 0.0399965 sec  
 RG 197.27  
 DW 0.00 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 1.0000000 sec  
 TDO 1  
 ===== CHANNEL f1 ======  
 SFO1 157.8687549 MHz  
 NUC1 125Te  
 P1 9.00 usec  
 PLWI 104.00000000 W  
 F2 - Processing parameters  
 SI 65536  
 SF 157.7900071 MHz  
 WDW EM  
 SSB 0  
 LB 60.00 Hz  
 GB 0  
 PC 1.00



**Figure S21.** <sup>125</sup>Te NMR spectrum of compound 11a.

### Eager 300 Report

Page: 1 Sample: SY-5-4 (SY-5-4)

Method Name : SD12102012  
Method File : D:\CHNS2012\SD12102012.mth  
Chromatogram : SY-5-4  
Operator ID : VARSHA Company Name : C.E. Instruments  
Analysed : 10/12/2012 14:30 Printed : 10/12/2012 16:55  
Sample ID : SY-5-4 (# 20) Instrument N. : Instrument #1  
Analysis Type : UnkNowN (Area) Sample weight : .869

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	50858	FU		0.0000
Nitrogen	7.1856	43	77982	FU	13.220220	.124886E+07
3	0.0000	60	50080	FU		0.0000
Carbon	48.1121	66	1030937	FU	1.000000	.246000E+07
Hydrogen	5.4349	184	257769	RS	3.999461	.545778E+07
Totals	60.7327		1467626			

Figure S22. Elemental analysis of compound 11a.

## Display Report

**Analysis Info**

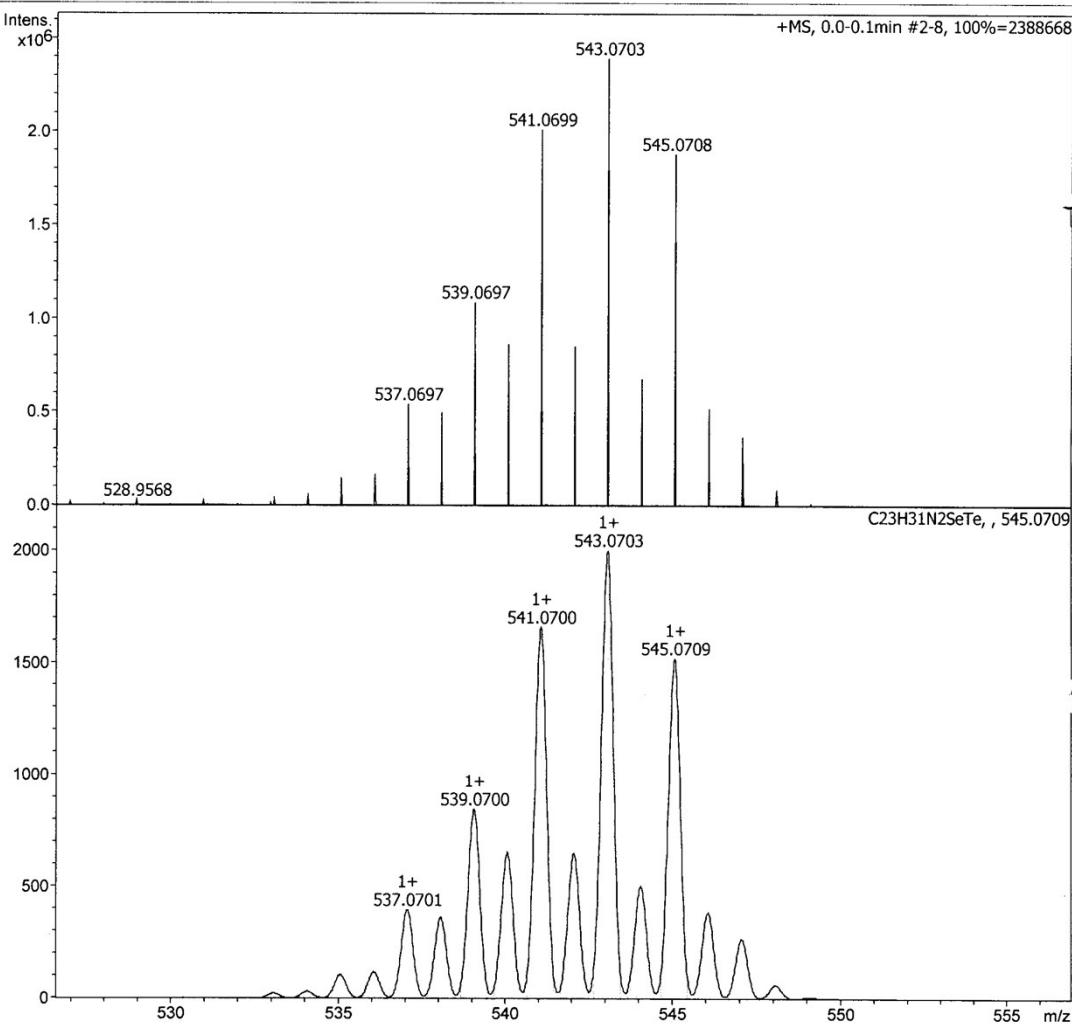
Analysis Name D:\Data\AUG\_13\HBS-SY-6-360.d  
 Method Tune\_pos\_Standard\_NAI-1000.m  
 Sample Name HBS-SY-6-360  
 Comment

Acquisition Date 8/8/2013 12:50:33 AM

 Operator IIT-B  
 Instrument maXis impact 282001.00081

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



HBS-SY-6-360.d

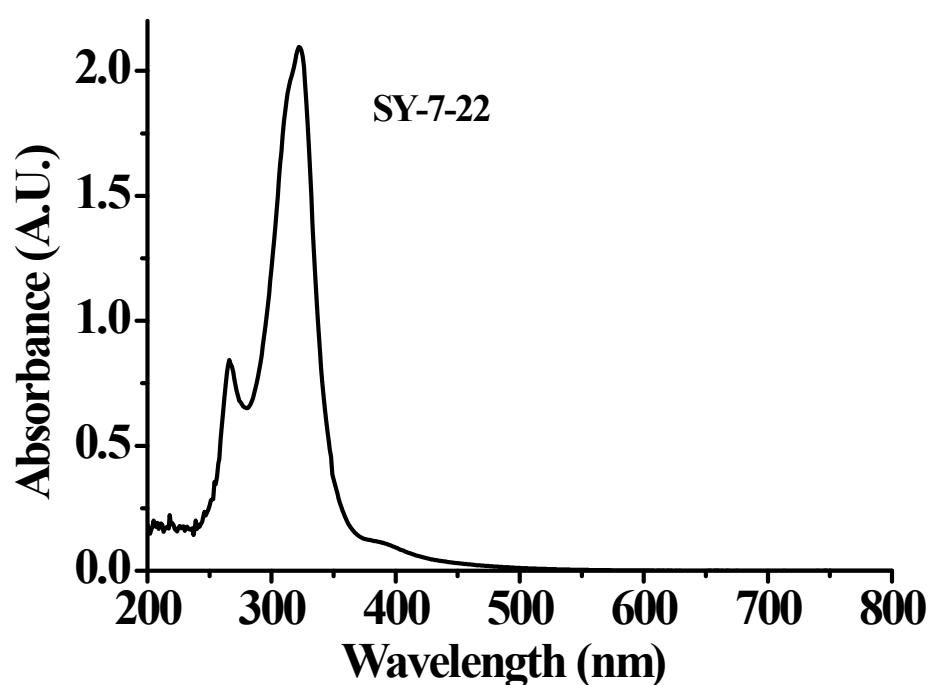
Bruker Compass DataAnalysis 4.1

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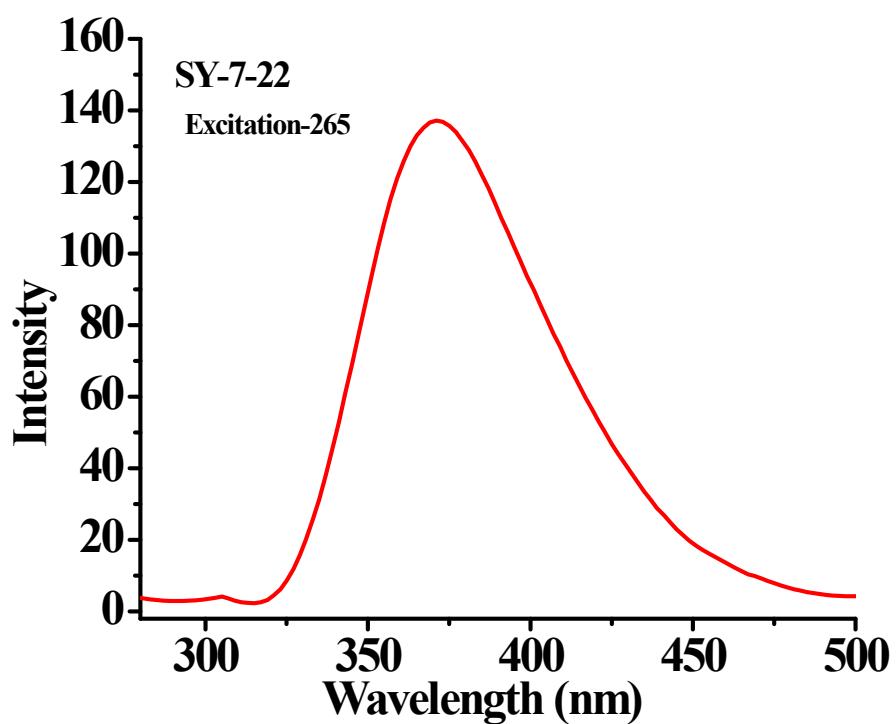
by: IIT-B

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**Figure S23.** ESI-MS spectrum of compound **11a**.



**Figure S24.** UV-Visible spectrum of compound **11a**.



**Figure S25.** Emission spectrum of compound **11a**.

HBS-SY-7-14-1H

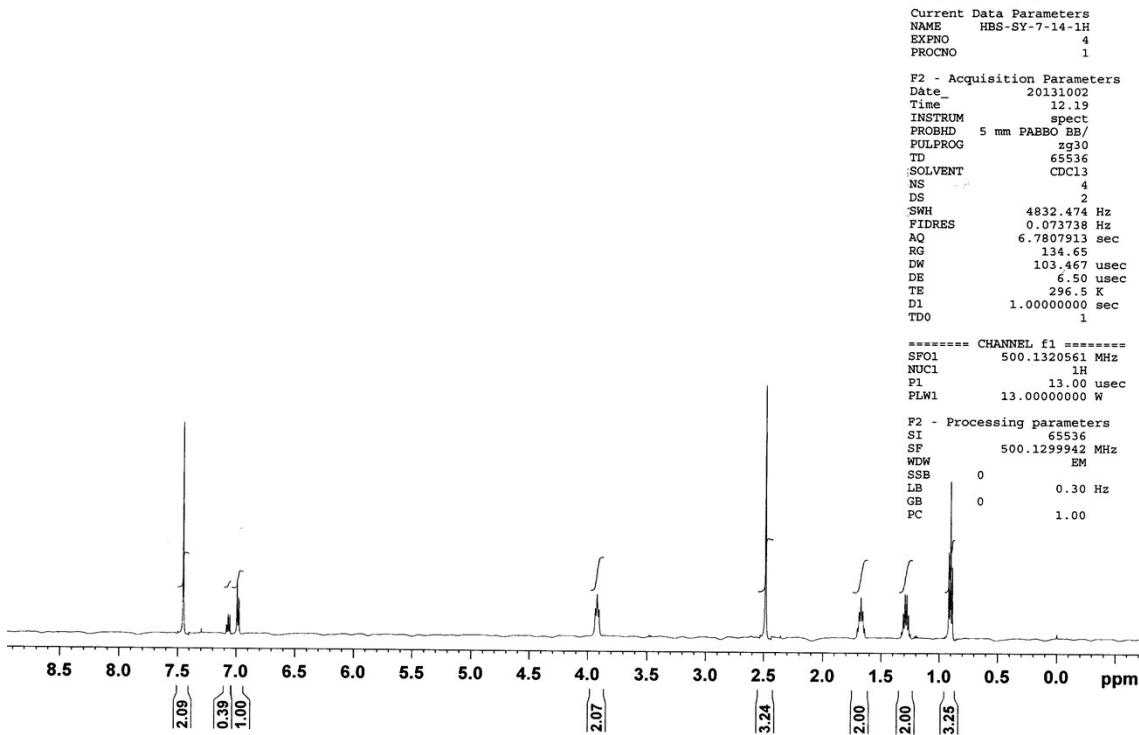


Figure S26. <sup>1</sup>H NMR spectrum of compound 11b.

HBS-SY-7-14-13C

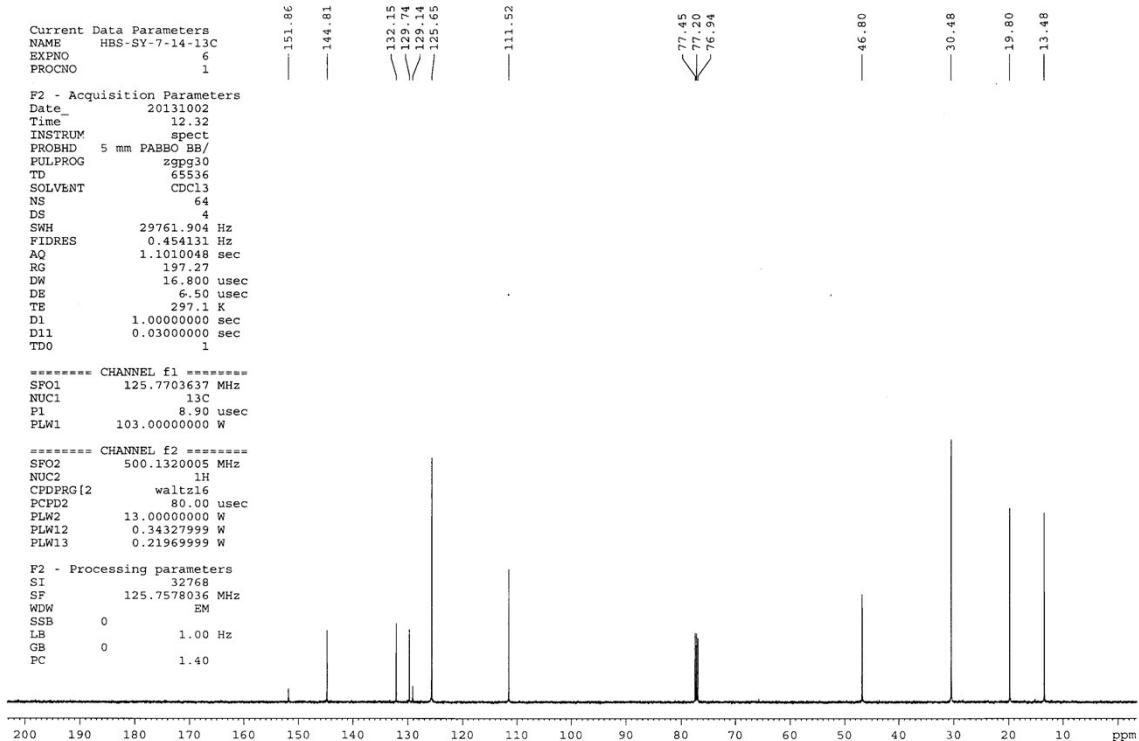
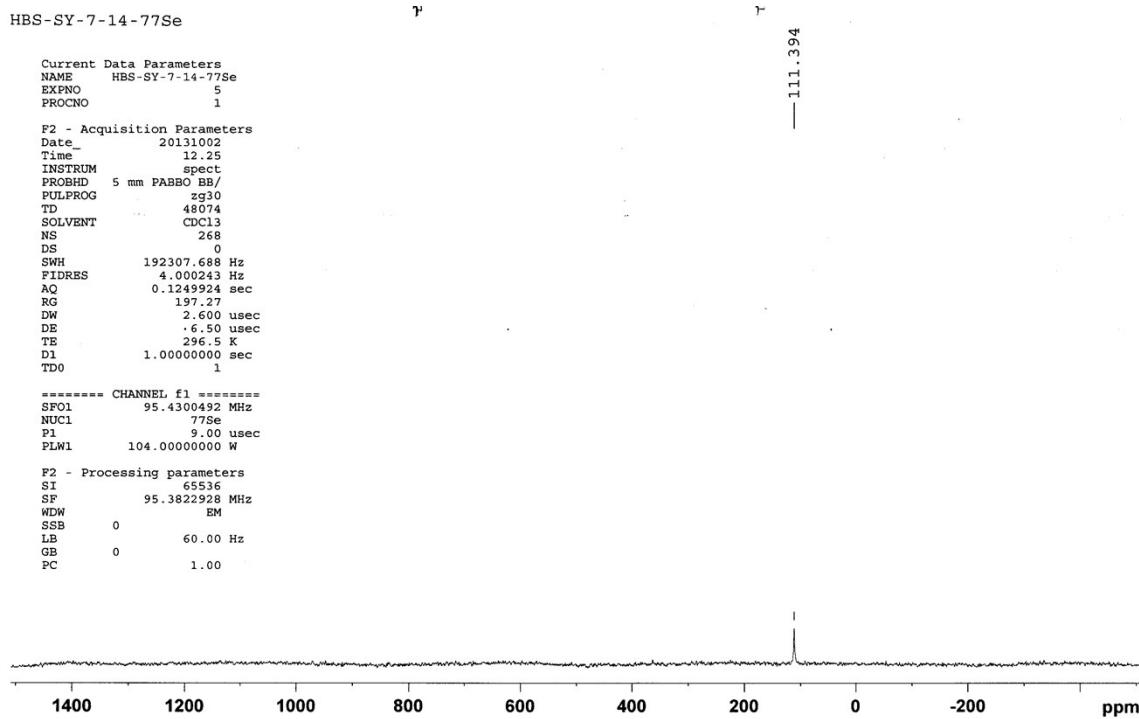
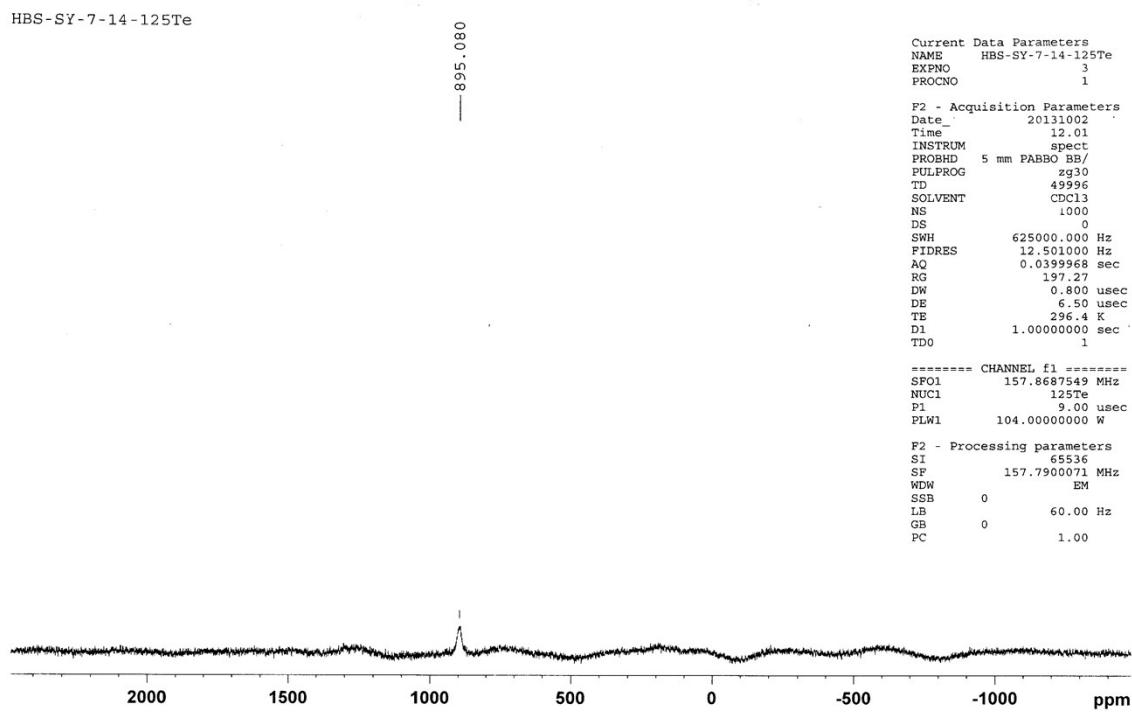


Figure S27. <sup>13</sup>C NMR spectrum of compound 11b.



**Figure S28.** <sup>77</sup>Se NMR spectrum of compound **11b**.



**Figure S29.** <sup>125</sup>Te NMR spectrum of compound **11b**.

### Eager 300 Report

Page: 1 Sample: SY-5-4 (SY-5-4)

Method Name : SD030812  
Method File : D:\CHNS2012\SD030812.mth  
Chromatogram : SY-5-4  
Operator ID : SD Company Name : C.E. Instruments  
Analysed : 08/03/2012 14:17 Printed : 8/3/2012 16:59  
Sample ID : SY-5-4 (# 21) Instrument N. : Instrument #1  
Analysis Type : UnkNowN (Area) Sample weight : .652

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	5.6452	42	49769 RS	14.200830	937896.0000
Carbon	44.4240	66	706761 RS	1.000000	.244010E+07
Hydrogen	4.8447	179	211565 RS	3.340641	.593761E+07
Totals	54.9139		968095		

**Figure S30.** Elemental analysis of compound **11b**.

## Display Report

**Analysis Info**

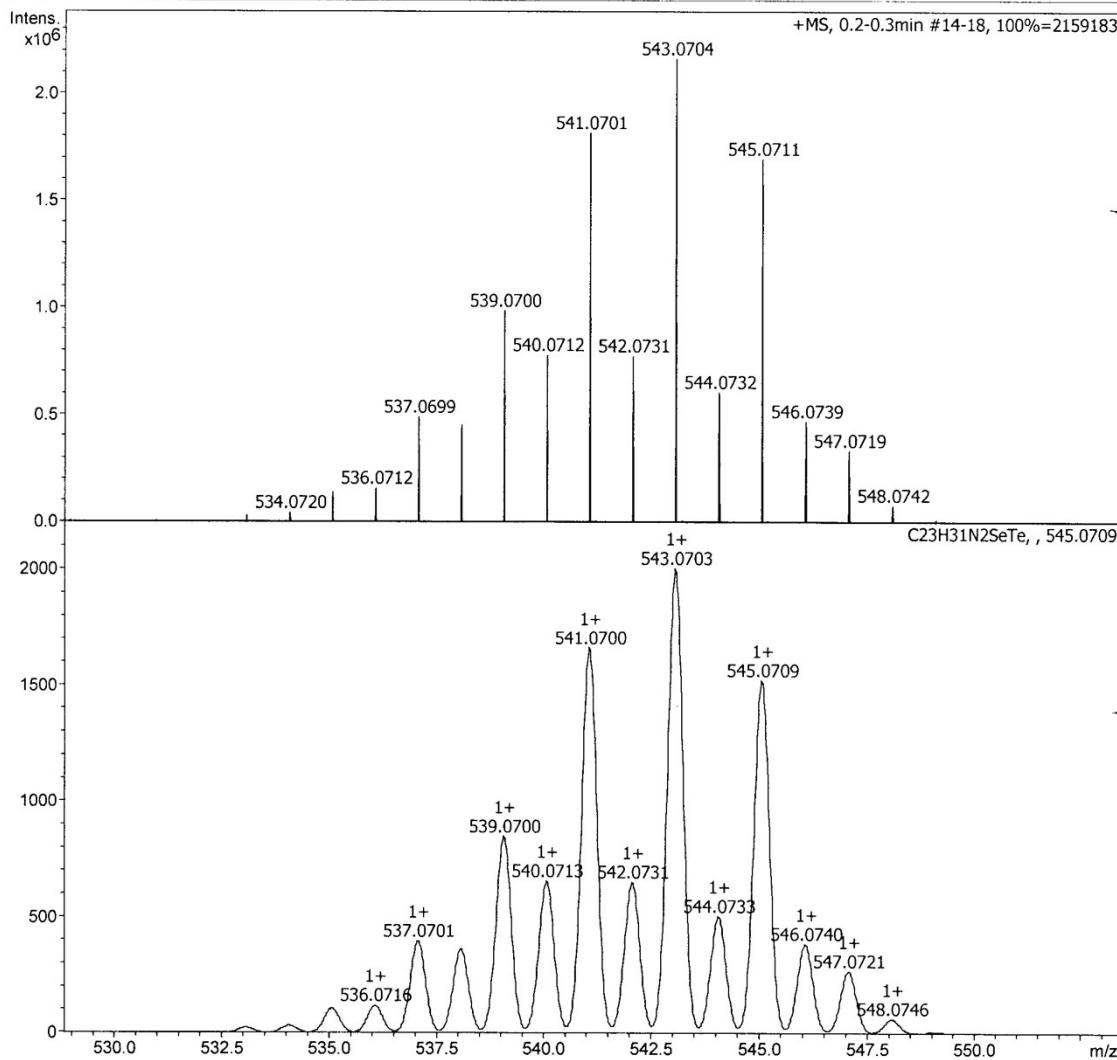
Analysis Name D:\Data\AUG\_13\HBS-SY-6-350.d  
 Method Tune\_pos\_Standard\_NAI-1000.m  
 Sample Name HBS-SY-6-350  
 Comment C23H31N2SeTe

Acquisition Date 8/7/2013 11:20:09 PM

 Operator IIT-B  
 Instrument maXis impact 282001.00081

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



HBS-SY-6-350.d

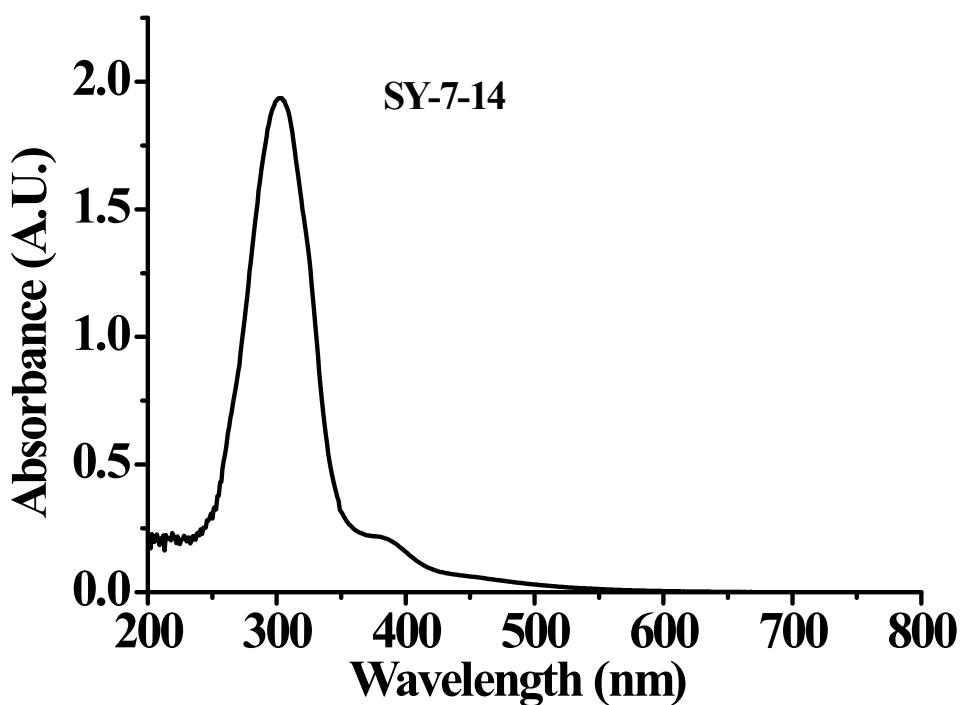
Bruker Compass DataAnalysis 4.1

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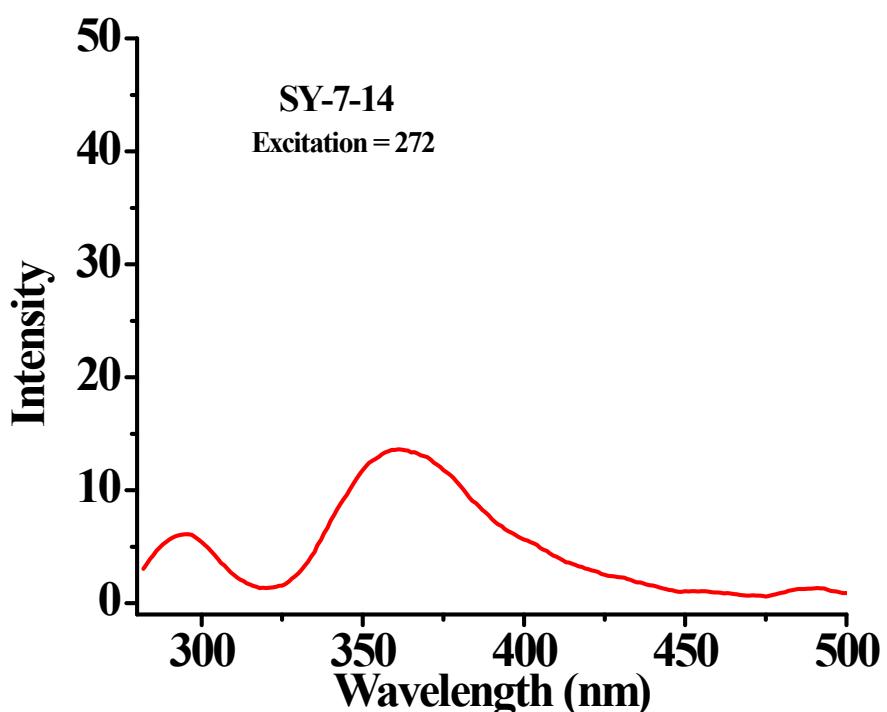
by: IIT-B

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**Figure S31.** ESI-MS spectrum of compound **11b**.



**Figure S32.** UV-Visible spectrum of compound **11b**.



**Figure S33.** Emission spectrum of compound **11b**.

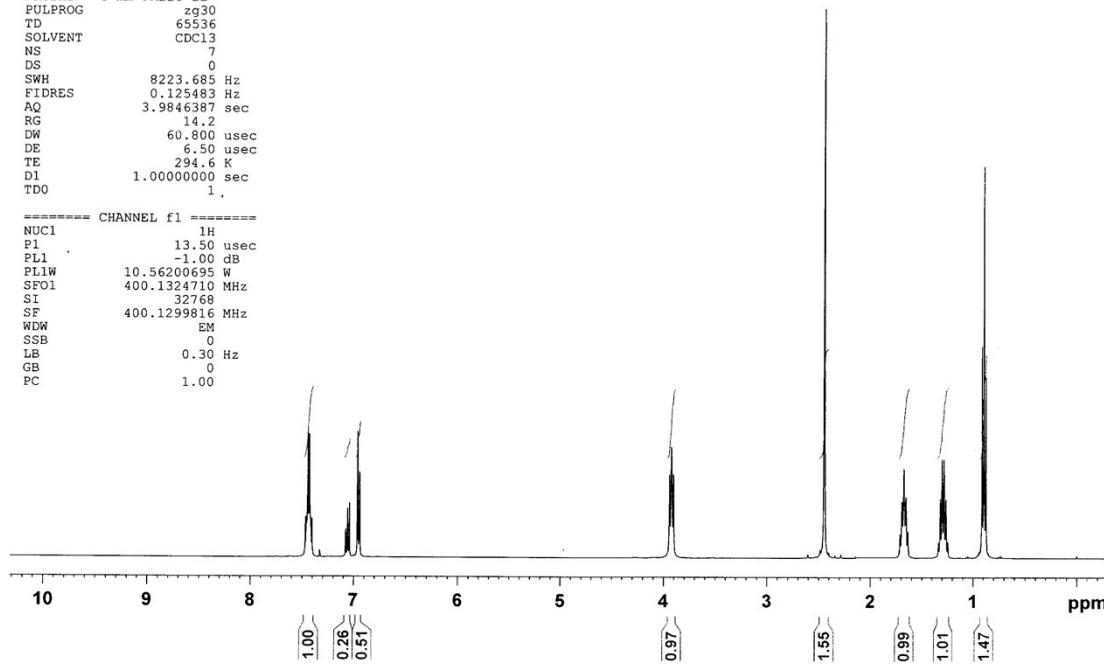
HBS-SY-6-354-1H

```

NAME      HBS-SY-6-354-1H
EXPNO        40
PROCNO        1
Date       20130805
Time       1.20
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT    CDCl3
NS         7
DS          0
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ        3.9846387 sec
RG        14.2
DW        60.800 usec
DE        6.50 usec
TE        294.6 K
D1      1.0000000 sec
TDO        1.

===== CHANNEL f1 =====
NUC1        1H
P1        13.50 usec
PL1       -1.00 dB
PL1W   10.56200695 W
SF01    400.1324710 MHz
SI        32768
SF      400.1299816 MHz
WDW
SSB
LB        0.50 Hz
GB
PC        1.00

```



**Figure S34.**  $^1\text{H}$  NMR spectrum of compound **11c**.

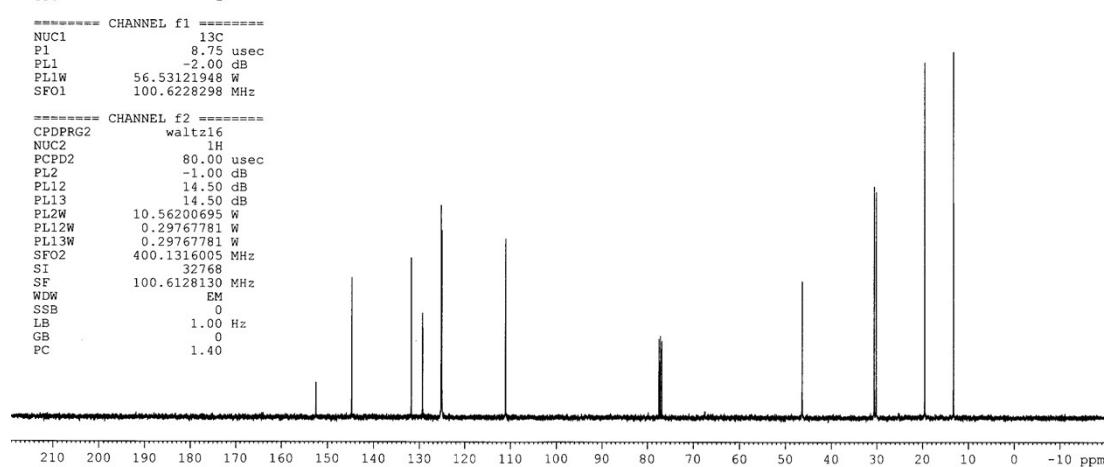
HBS-SY-6-354-13C

```

NAME      HBS-SY-6-354-13C
EXPNO        43
PROCNO        1
Date       20130805
Time       1.27
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG  zgppg30
TD        65536
SOLVENT    CDCl3
NS         18
DS          4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        2050
DW        20.800 usec
DE        6.50 usec
TE        294.7 K
D1      1.0000000 sec
D11     0.0300000 sec
TDO        1.

===== CHANNEL f1 =====
NUC1        13C
P1        8.75 usec
PL1       -2.00 dB
PL1W   56.53121948 W
SF01    100.6228298 MHz

```



**Figure S35.**  $^{13}\text{C}$  NMR spectrum of compound **11c**.

HBS-SY-6-354-77Se

```

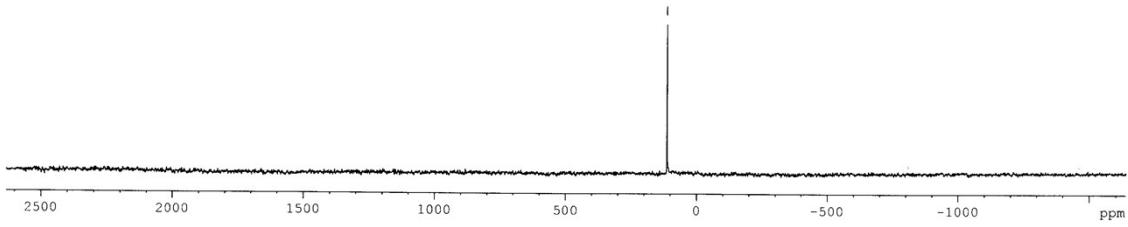
NAME      HBS-SY-6-354-77Se
EXPNO        41
PROCNO       1
Date_   20130805
Time_   1.22
INSTRUM spect
PROBHD  5 mm PABBO BB-
PULPROG zg
TD      65536
SOLVENT   CDCl3
NS       100
DS        4
SWH     326086.969 Hz
FIDRES   4.975692 Hz
AQ      0.1005385 sec
RG      2050
DW      1.533 usec
DE      6.50 usec
TE      294.6 K
D1      1.0000000 sec
TDO      1

```

```

===== CHANNEL f1 =====
NUC1      77Se
P1      10.00 usec
PL1      0.00 dB
SF01    76.3490004 MHz
SI      65536
SF      76.3110246 MHz
WDW      EM
SSB      0
LB      60.00 Hz
GB      0
PC      0.00

```

**Figure S36.**  $^{77}\text{Se}$  NMR spectrum of compound **11c**.

HBS-SY-6-354-125Te

```

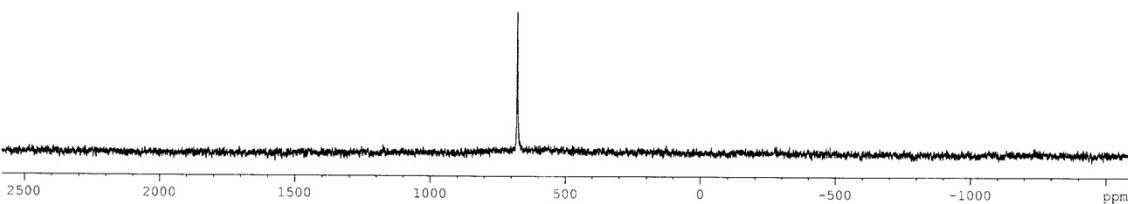
NAME      HBS-SY-6-354-125Te
EXPNO        42
PROCNO       1
Date_   20130805
Time_   1.24
INSTRUM spect
PROBHD  5 mm PABBO BB-
PULPROG zg
TD      65536
SOLVENT   CDCl3
NS       71
DS        4
SWH     526315.813 Hz
FIDRES   8.030942 Hz
AQ      0.0623092 sec
RG      2050
LM      0.950 usec
DE      6.50 usec
TE      294.5 K
D1      1.0000000 sec
TDO      1

```

```

===== CHANNEL f1 =====
NUC1      125Te
P1      7.50 usec
PL1      0.00 dB
SF01    126.3032110 MHz
SI      32768
SF      126.2402248 MHz
WDW      EM
SSB      0
LB      60.00 Hz
GB      0
PC      1.40

```

**Figure S37.**  $^{125}\text{Te}$  NMR spectrum of compound **11c**.

### Eager 300 Report

Page: 1 Sample: SY-7-30 (SY-7-30)

Method Name : HBS-VT-13-03-2015  
Method File : D:\CHNS-2015\HBS-VT-13-03-2015.mth  
Chromatogram : SY-7-30  
Operator ID : VARSHA Company Name : C.E. Instruments  
Analysed : 03/13/2015 14:50 Printed : 3/13/2015 18:44  
Sample ID : SY-7-30 (# 21) Instrument N. : Instrument #1  
Analysis Type : UnkNown (Area) Sample weight : 1.087

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	4.9131	41	59726	RS	19.800840	.111835E+07
Carbon	41.2643	64	1182625	RS	1.000000	.260916E+07
Hydrogen	4.4899	175	327814	RS	3.607610	.633286E+07
Totals	50.6674		1570165			

**Figure S38.** Elemental analysis of compound **11c**.

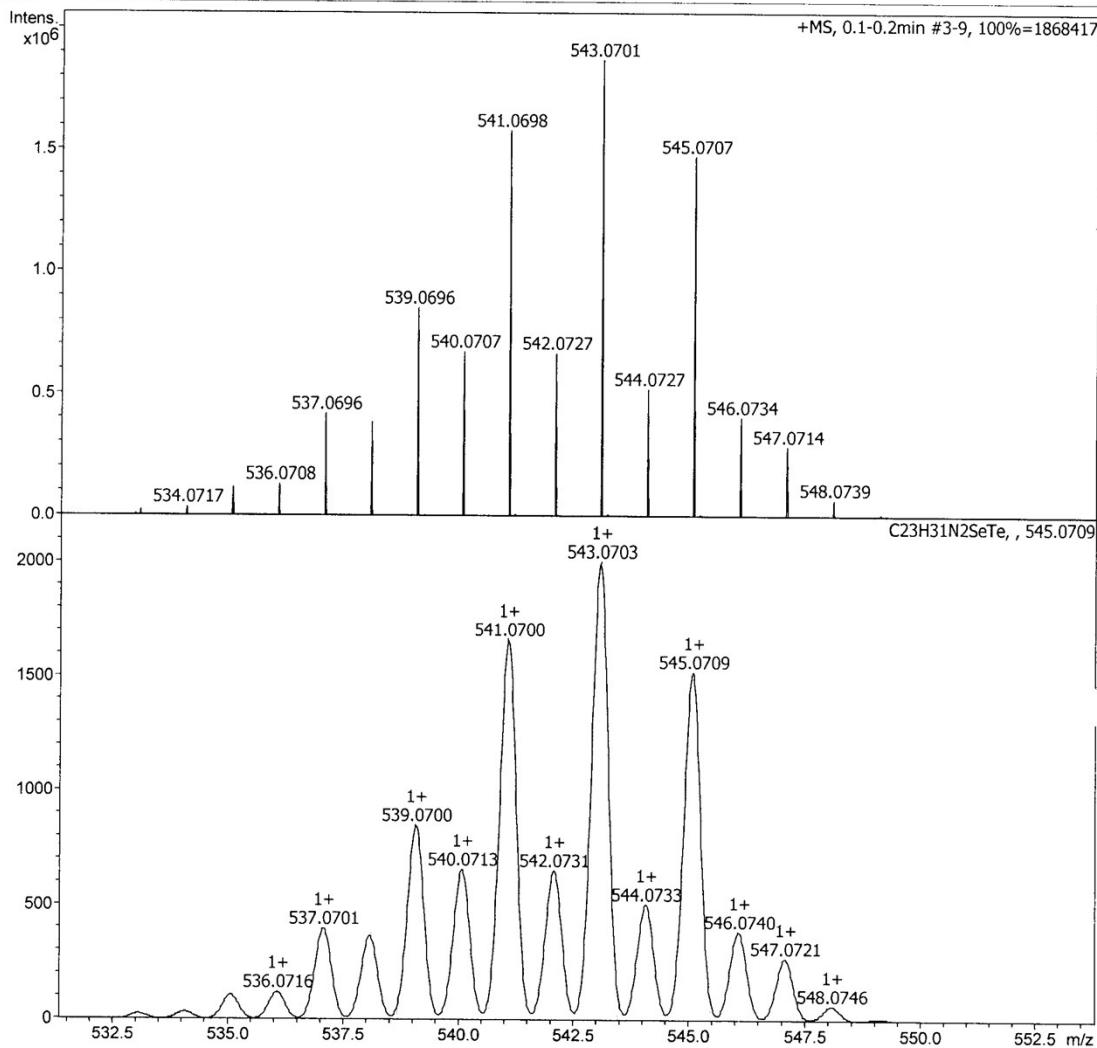
## Display Report

**Analysis Info**

Analysis Name	D:\Data\AUG_13\HBS-SY-6-354.d	Acquisition Date	8/7/2013 11:54:44 PM
Method	Tune_pos_Standard_NAI-1000.m	Operator	IIT-B
Sample Name	HBS-SY-6-354	Instrument	maXis impact 282001.00081
Comment	C23H31N2SeTe		

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



HBS-SY-6-354.d

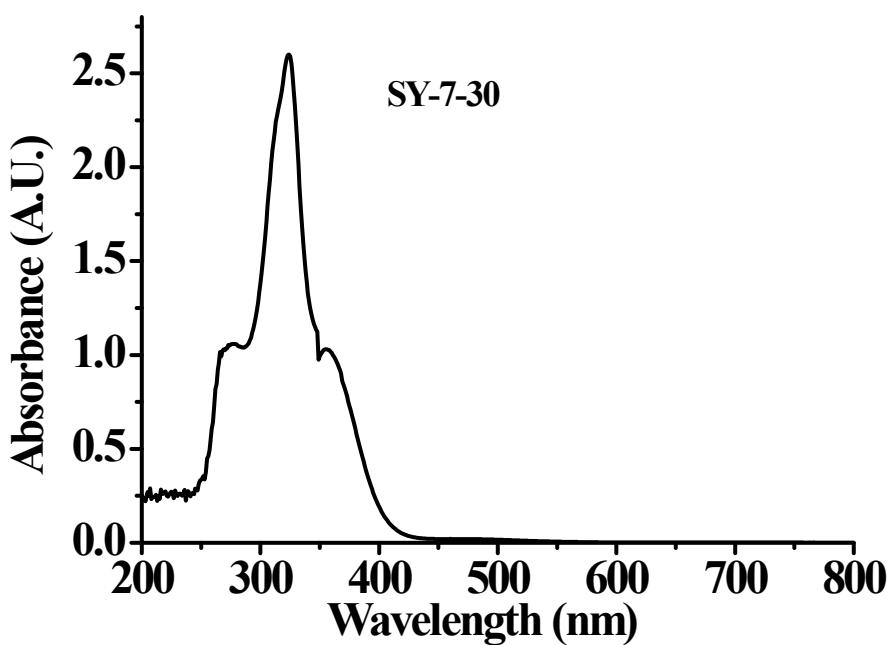
Bruker Compass DataAnalysis 4.1

printed: 8/8/2013 12:04:19 AM

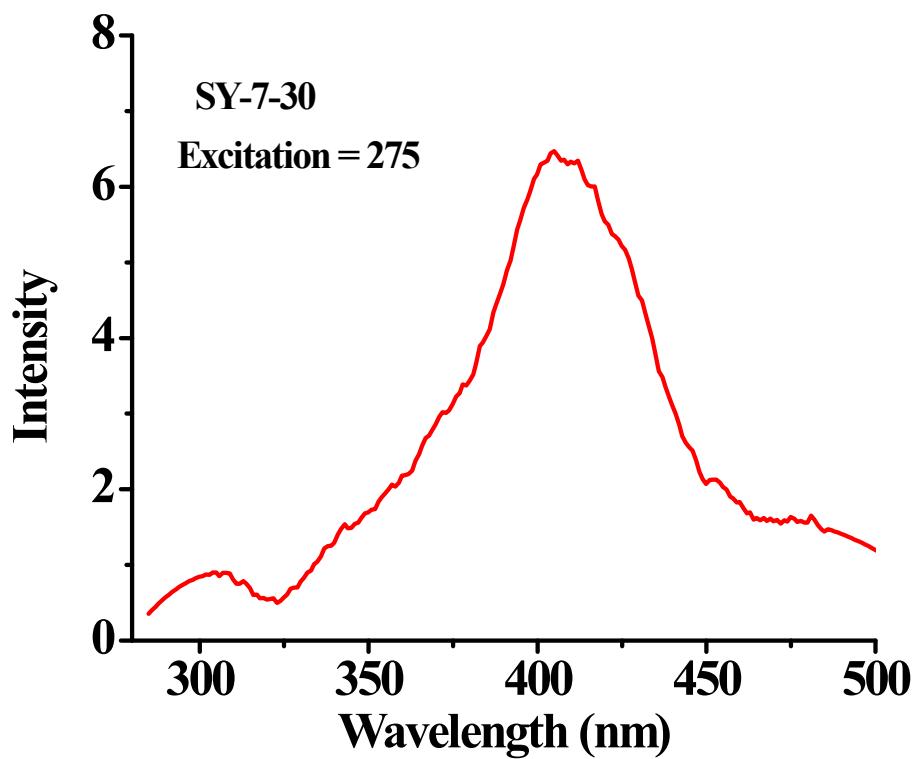
by: IIT-B

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**Figure S39.** ESI-MS spectrum of compound **11c**.



**Figure S40.** UV-Visible spectrum of compound **11c**.



**Figure S41.** Emission spectrum of compound **11c**.

HBS-SY-8-182-1H

```

NAME      HBS-SY-8-182-1H
EXPNO        1
PROCNO       1
Date        20150102
Time        11.47
INSTRUM    spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        54274
SOLVENT    CDC13
NS           13
DS            0
SWH        8223.685 Hz
FIDRES     0.151522 Hz
AQ        3.2999091 sec
RG          90.5
DW        60.800 usec
DE         6.50 usec
TE        296.8 K
D1      1.0000000 sec
TDO         1

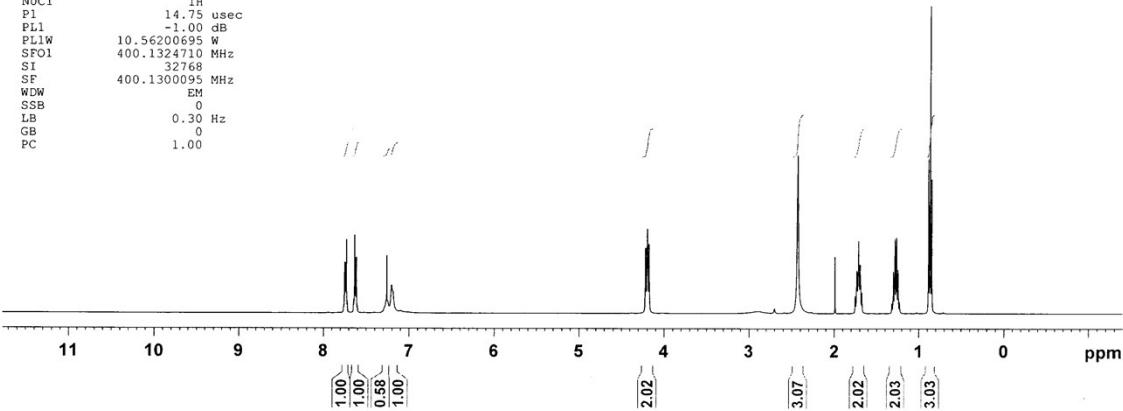
```

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

```

NUC1        1H
P1        14.75 usec
PL1       -1.00 dB
PL1W    10.56200695 W
SF01     400.1324710 MHz
SI          32768
SF      400.1300095 MHz
WDW        EM
SSB         0
LB        0.30 Hz
GB         0
PC        1.00

```



**Figure S42.**  $^1\text{H}$  NMR spectrum of compound **15**.

HBS-SY-8-182-13C

```

NAME      HBS-SY-8-182-13C
EXPNO        1
PROCNO       1
Date        20150122
Time        23.24
INSTRUM    spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT    CDC13
NS           108
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        297.6 K
D1      1.0000000 sec
D11      0.03000000 sec
TDO         1

```

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

```

NUC1        13C
P1        8.50 usec
PL1       -2.00 dB
PL1W    56.53121948 W
SF01     100.6238364 MHz

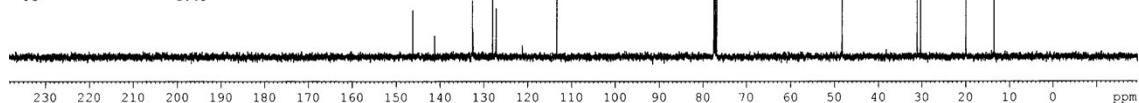
```

===== CHANNEL f2 =====

```

CPDPRG2   waltz16
NUC2        1H
PCPD2      80.00 usec
PL2       -1.00 dB
PL12      13.69 dB
PL13      14.50 dB
PL2W    10.56200695 W
PL12W    0.35871249 W
PL13W    0.29761781 W
SF02     400.1316005 MHz
SI          32768
SF      100.6127558 MHz
WDW        EM
SSB         0
LB        1.00 Hz
GB         0
PC        1.40

```

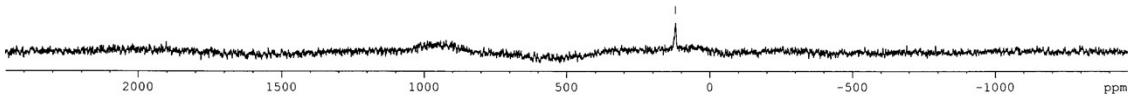


**Figure S43.**  $^{13}\text{C}$  NMR spectrum of compound **15**.

HBS-SY-8-182-77Se

```
NAME      HBS-SY-8-182-77Se
EXPNO          3
PROCNO         1
Date_   20150102
Time_    11.56
INSTRUM   spect
PROBHD  5 mm PABBO BB-
PULPROG  zg
TD        65536
SOLVENT    CDCl3
NS           1784
DS            4
SWH       326086.969 Hz
FIDRES     4.975692 Hz
AQ        0.1005385 sec
RG          2050
DW        1.533 usec
DE        6.50 usec
TE        296.6 K
D1      1.0000000 sec
TDO          1

===== CHANNEL f1 =====
NUC1      77Se
P1        10.00 usec
PL1        0.00 dB
SF01    76.3490004 MHz
SI        65536
SF       76.3110246 MHz
WDW        EM
SSB        0
LB        60.00 Hz
GB        0
PC        0.00
```

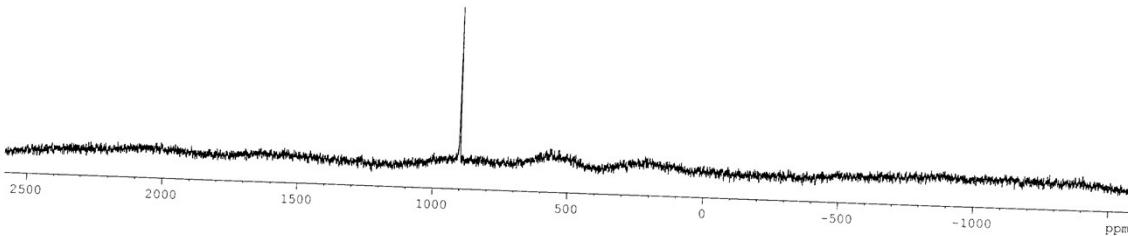


**Figure S44.** <sup>77</sup>Se NMR spectrum of compound **15**.

HBS-SY-8-182-125Te

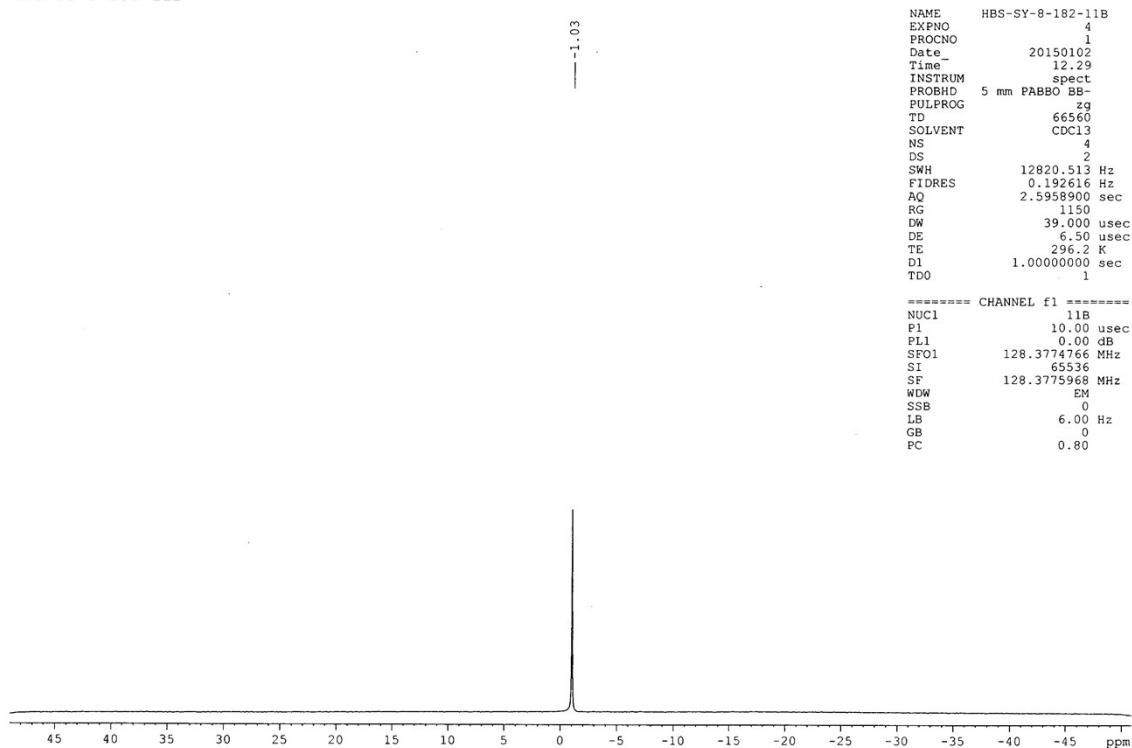
```
NAME      HBS-SY-8-182-125Te
EXPNO          16
PROCNO         1
Date_   20150106
Time_    0.39
INSTRUM   spect
PROBHD  5 mm PABBO BB-
PULPROG  zg
TD        65536
SOLVENT    CDCl3
NS           1000
DS            4
SWH       526315.813 Hz
FIDRES     8.030942 Hz
AQ        0.0623092 sec
RG          2050
DW        0.950 usec
DE        6.50 usec
TE        297.4 K
D1      1.0000000 sec
TDO          1

===== CHANNEL f1 =====
NUC1      125Te
P1        7.50 usec
PL1        0.00 dB
SF01    126.3032110 MHz
SI        32768
SF       126.2402248 MHz
WDW        EM
SSB        0
LB        60.00 Hz
GB        0
PC        1.40
```



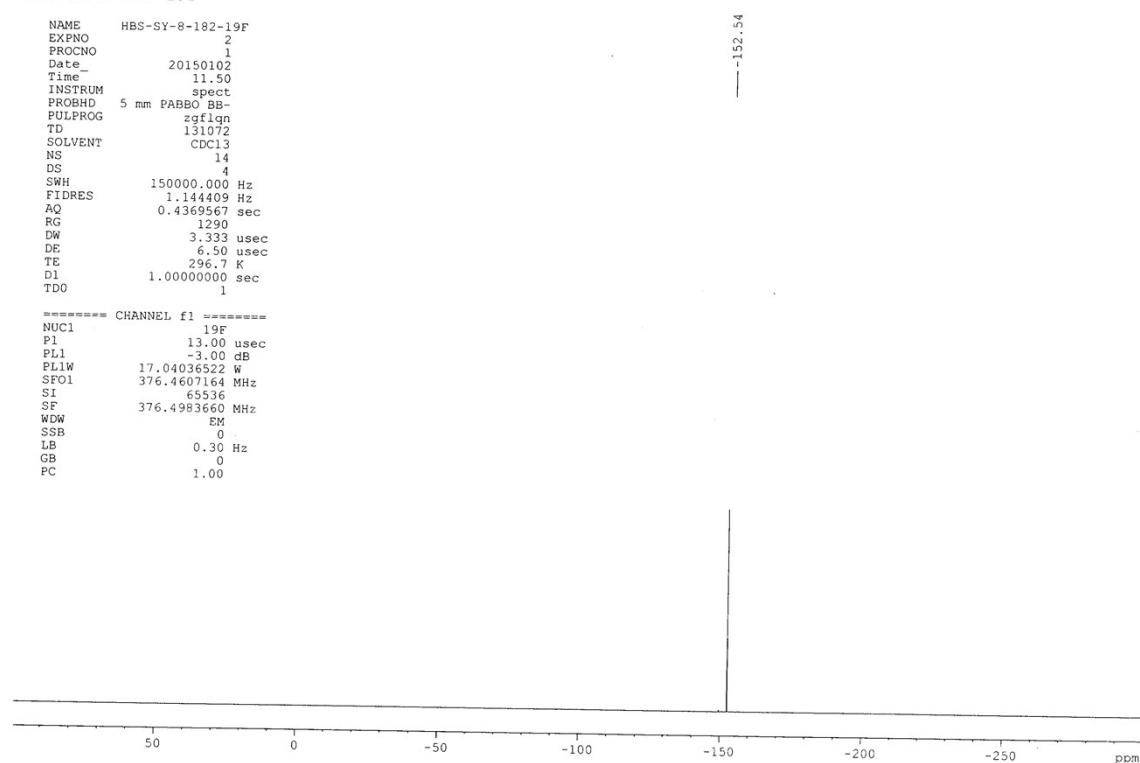
**Figure S45.** <sup>125</sup>Te NMR spectrum of compound **15**.

HBS-SY-8-182-11B



**Figure S46.**  $^{15}\text{B}$  NMR spectrum of compound **15**.

HBS-SY-8-182-19F



**Figure S47.**  $^{19}\text{F}$  NMR spectrum of compound **15**.

### Eager 300 Report

Page: 1 Sample: SY-5-18 (SY-5-18)

Method Name : SD030812  
Method File : D:\CHNS2012\SD030812.mth  
Chromatogram : SY-5-18  
Operator ID : SD Company Name : C.E. Instruments  
Analysed : 08/03/2012 15:49 Printed : 8/3/2012 16:59  
Sample ID : SY-5-18 (# 30) Instrument N. : Instrument #1  
Analysis Type : UnkNowN (Area) Sample weight : .803

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	5.6914	43	58112 RS	14.827250	937896.0000
Carbon	43.9748	66	861641 RS	1.000000	.244010E+07
Hydrogen	4.8655	178	255992 RS	3.365890	.593761E+07
Totals	54.5317		1175745		

Figure S48. Elemental analysis of compound 15.

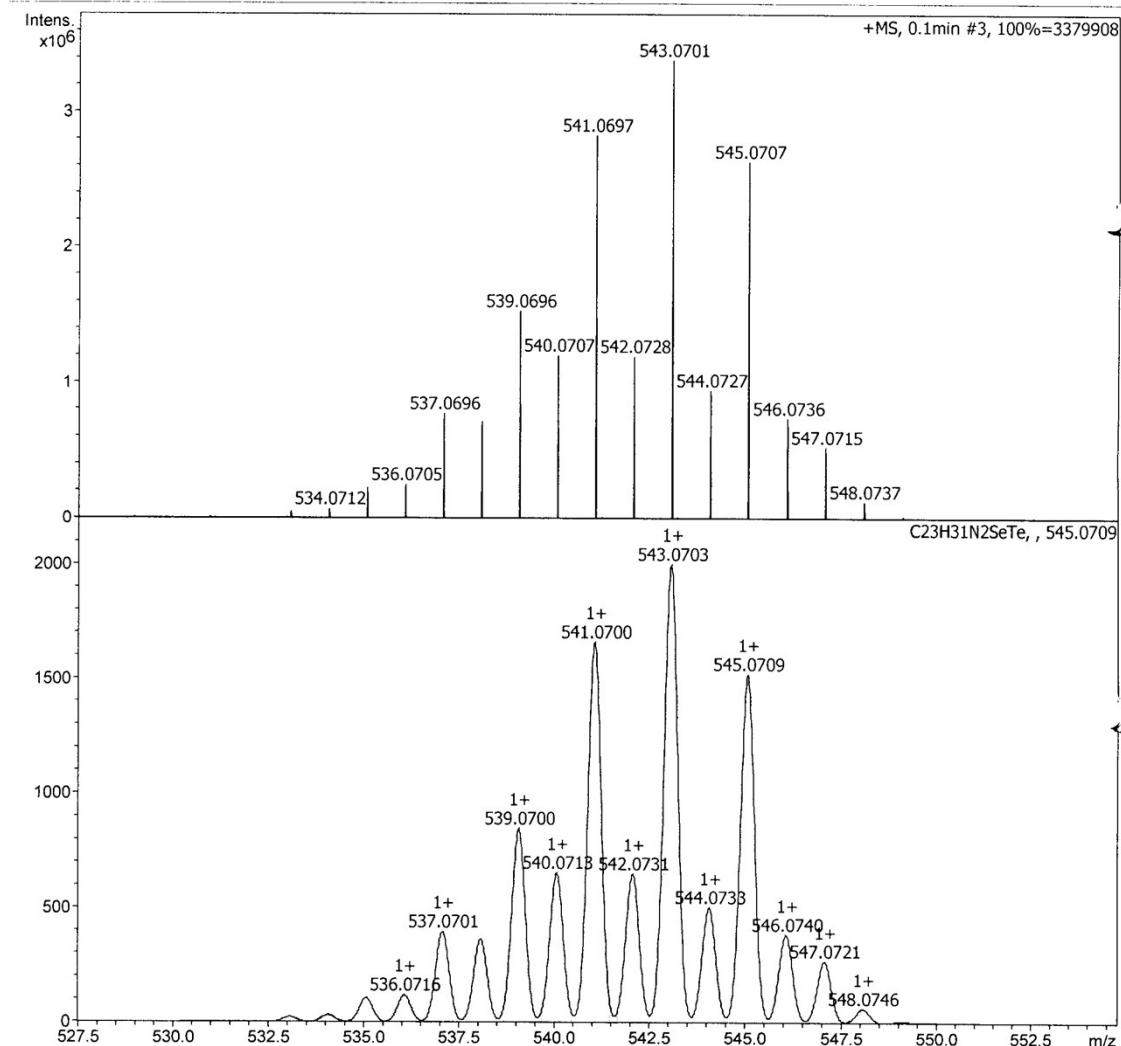
## Display Report

**Analysis Info**

Analysis Name	D:\Data\AUG_13\HBS-SY-6-356.d	Acquisition Date	8/8/2013 12:13:53 AM
Method	Tune_pos_Standard_NAI-1000.m	Operator	IIT-B
Sample Name	HBS-SY-6-356	Instrument	maXis impact 282001.00081
Comment	C23H31N2SeTe		

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



HBS-SY-6-356.d

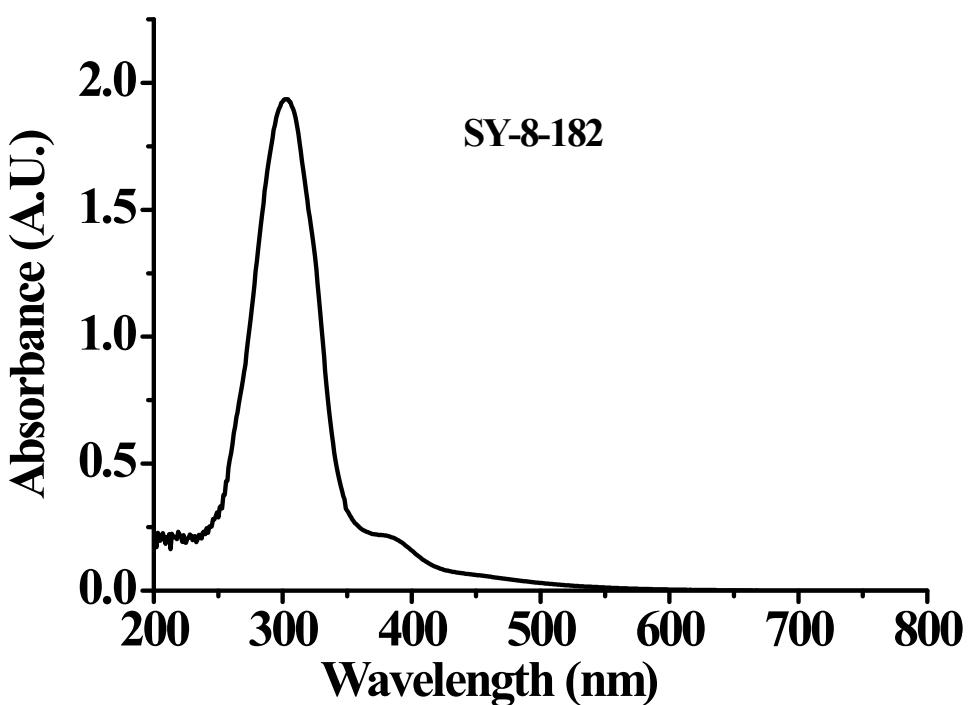
Bruker Compass DataAnalysis 4.1

printed: 8/8/2013 12:17:36 AM

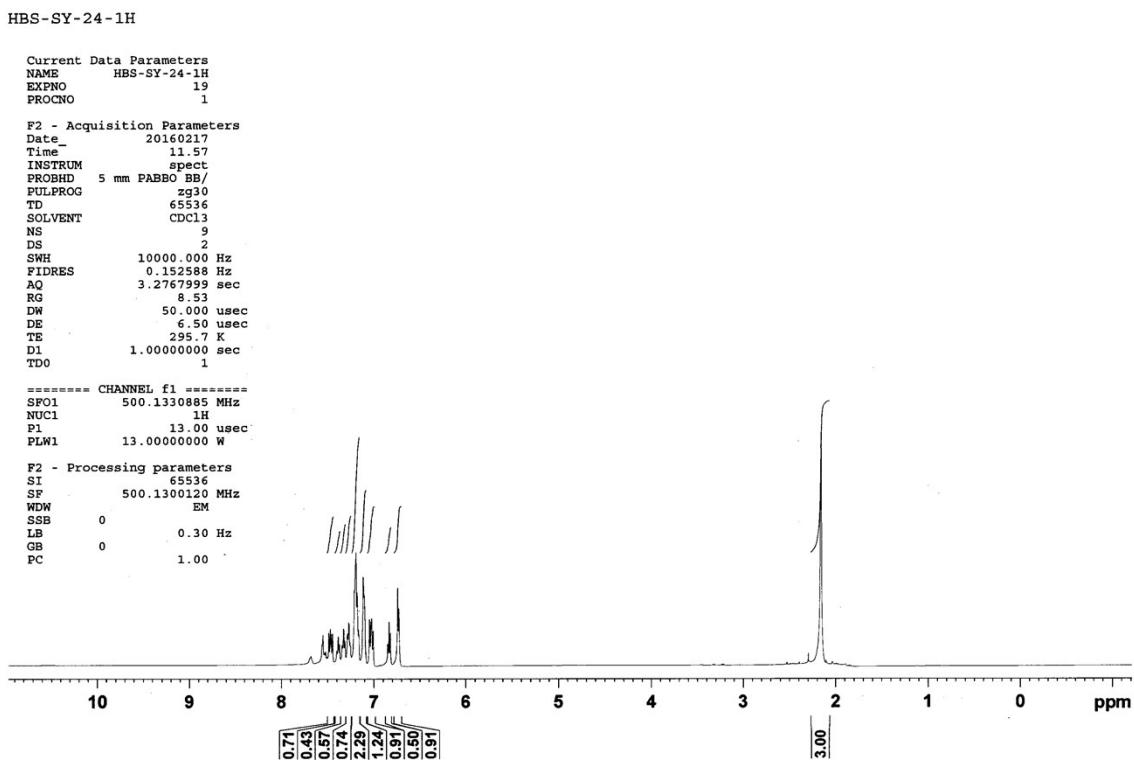
by: IIT-B

Page 1 of 1

**Figure S49.** ESI-MS spectrum of compound **15**.



**Figure S50.** UV-Visible spectrum of compound 15.



**Figure S51.**  $^1\text{H}$  NMR spectrum of compound 16a.

HBS-SY-24-13C

```

Current Data Parameters
NAME      HBS-SY-24-13C
EXPNO     8
PROCNO    1

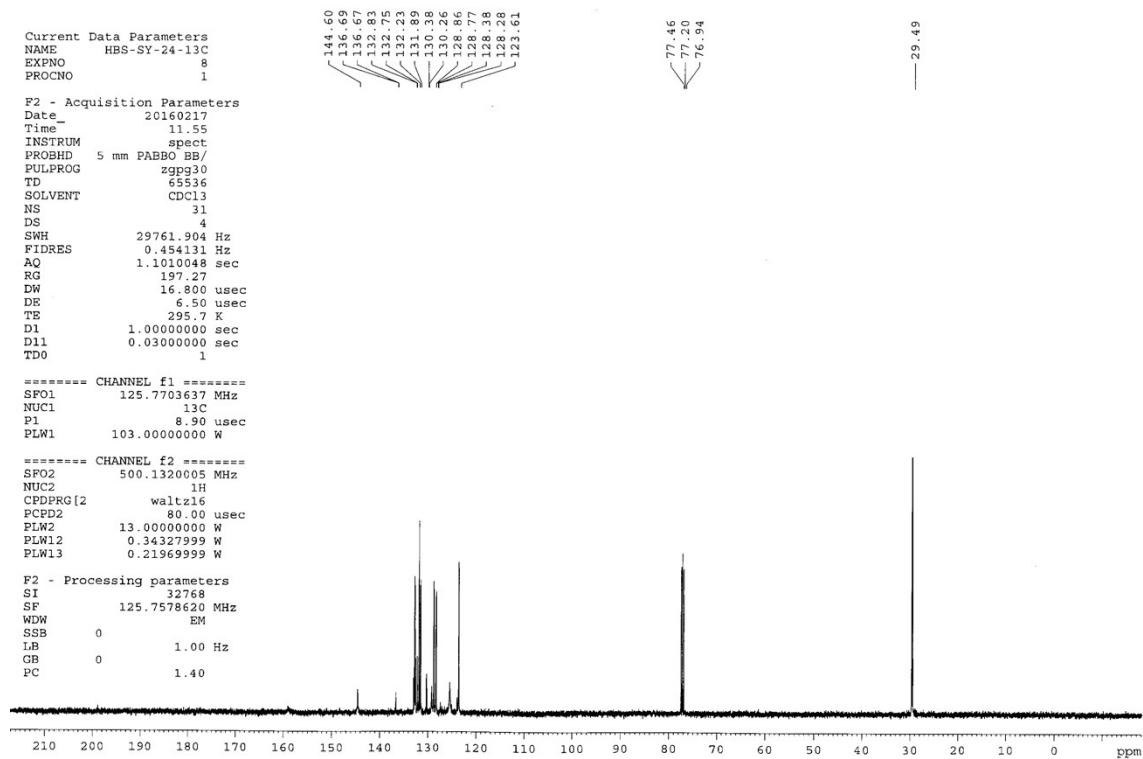
F2 - Acquisition Parameters
Date_   20160217
Time_   11.55
INSTRUM spect
PROBHD  5 mm PABBO BB/
PULPROG zpgpg30
TD      65536
SOLVENT  CDCl3
NS      31
DS      4
SWH     29761.904 Hz
FIDRES  0.454131 Hz
AQ      1.1010048 sec
RG      197.27
DW      16.800 usec
DE      6.50 usec
TE      295.7 K
D1      1.0000000 sec
D11     0.03000000 sec
TD0     1

===== CHANNEL f1 =====
SF01    125.7703637 MHz
NUC1    13C
P1      8.90 usec
PLW1    103.00000000 W

===== CHANNEL f2 =====
SF02    500.1320005 MHz
NUC2    1H
CPDPGR[2] waltz16
PCPD2   80.00 usec
PLW2    13.00000000 W
PLW12   0.34327999 W
PLW13   0.21969999 W

F2 - Processing parameters
SI      32768
SF      125.7578620 MHz
WDW    EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40

```



**Figure S52.**  $^{13}\text{C}$  NMR spectrum of compound **16a**.

HBS-SY-24-31P

```

Current Data Parameters
NAME      HBS-SY-24-31P
EXPNO     10
PROCNO    1

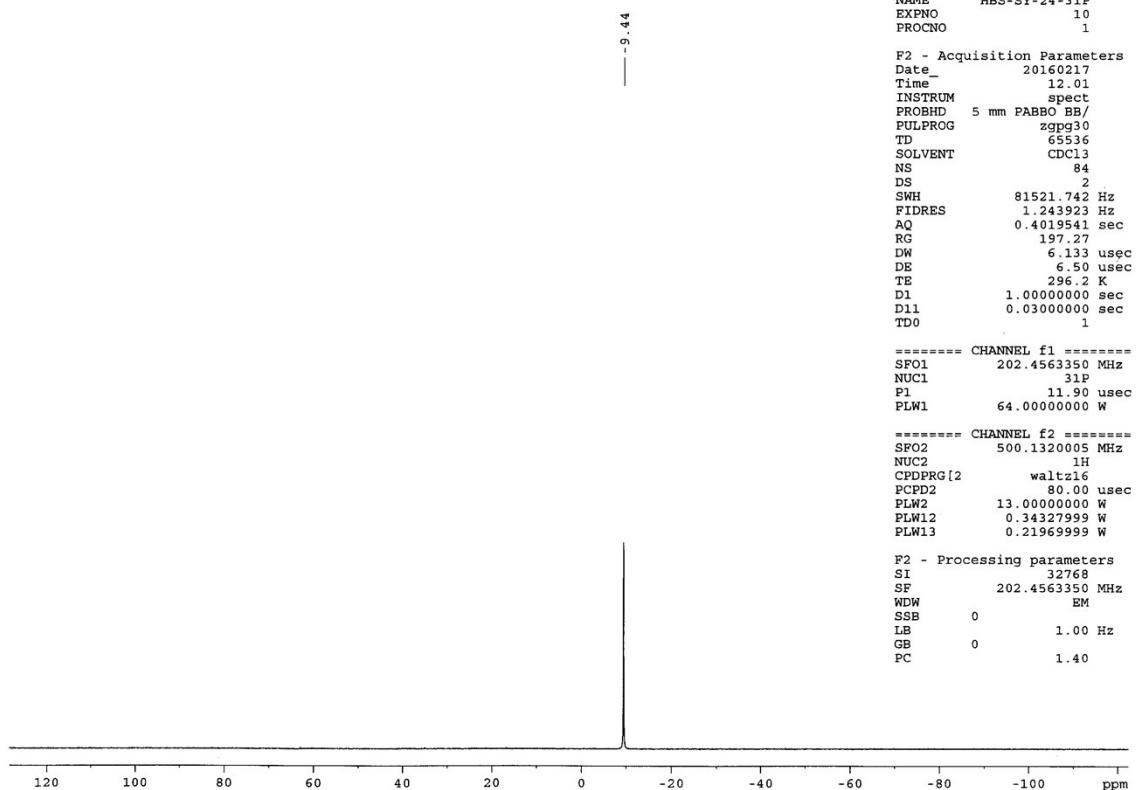
F2 - Acquisition Parameters
Date_   20160217
Time_   12.01
INSTRUM spect
PROBHD  5 mm PABBO BB/
PULPROG zpgpg30
TD      65536
SOLVENT  CDCl3
NS      84
DS      2
SWH     81521.742 Hz
FIDRES  1.243923 Hz
AQ      0.4019841 sec
RG      197.27
DW      6.133 usec
DE      6.50 usec
TE      296.2 K
D1      1.0000000 sec
D11     0.03000000 sec
TD0     1

===== CHANNEL f1 =====
SF01    202.4563350 MHz
NUC1    31P
P1      11.90 usec
PLW1    64.00000000 W

===== CHANNEL f2 =====
SF02    500.1320005 MHz
NUC2    1H
CPDPGR[2] waltz16
PCPD2   80.00 usec
PLW2    13.00000000 W
PLW12   0.34327999 W
PLW13   0.21969999 W

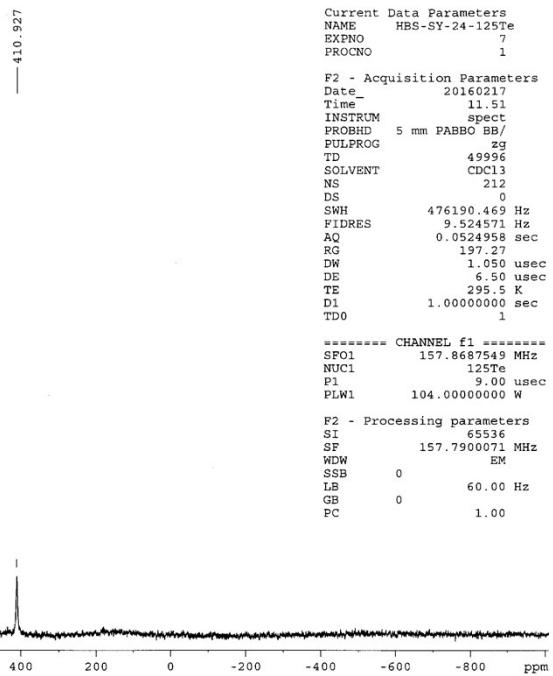
F2 - Processing parameters
SI      32768
SF      202.4563350 MHz
WDW    EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40

```



**Figure S53.**  $^{31}\text{P}$  NMR spectrum of compound **16a**.

HBS-SY-24-125Te



**Figure S54.** <sup>125</sup>Te NMR spectrum of compound **16a**.

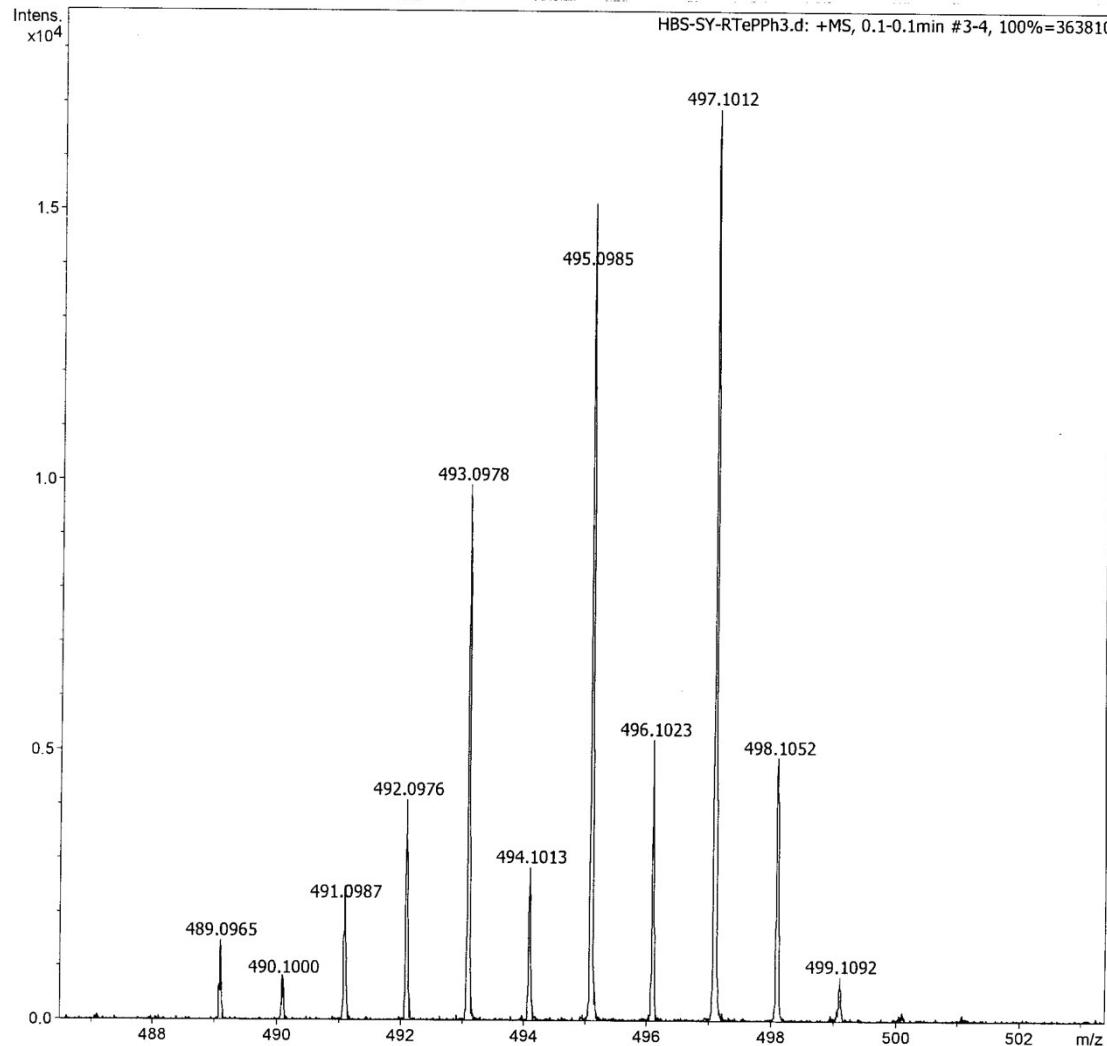
## Display Report

**Analysis Info**

Analysis Name	D:\Data\DEC-2014\HBS-SY-RTePPh3.d	Acquisition Date	2/18/2016 10:19:45 PM
Method	Tune_pos_NAICSI-1000.m	Operator	HBS-SY
Sample Name	HBS-SY-RTePPh3	Instrument	maXis impact 282001.00081
Comment			

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



HBS-SY-RTePPh3.d

Bruker Compass DataAnalysis 4.1

printed: 2/19/2016 2:57:03 PM

by: mMSB IN

Page 1 of 1

**Figure S55.** ESI-MS spectrum of compound 16a.

HBS-SY-25-1H

Current Data Parameters  
 NAME HBS-SY-25-1H  
 EXPNO 12  
 PROCNO 1

F2 - Acquisition Parameters

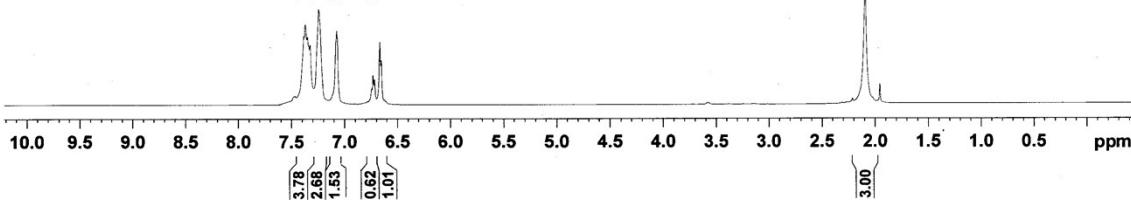
Date\_ 20160217  
 Time 12.07  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 17  
 DS 2  
 SWH 10000.000 Hz  
 FIDRES 0.152588 Hz  
 AQ 3.276719 sec  
 RG 8.53  
 DW 50.000 usec  
 DE 6.50 usec  
 TE 295.7 K  
 D1 1.0000000 sec  
 TDO 1

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

SF01 500.1330885 MHz  
 NUC1 1H  
 P1 13.00 usec  
 PLW1 13.0000000 W

F2 - Processing parameters

SI 65536  
 SF 500.1300120 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



**Figure S56.** <sup>1</sup>H NMR spectrum of compound 16b.

HBS-SY-25-13C

Current Data Parameters  
 NAME HBS-SY-25-13C  
 EXPNO 14  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20160217  
 Time 12.16  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 40  
 DS 4  
 SWH 29761.904 Hz  
 FIDRES 0.454131 Hz  
 AQ 1.101048 sec  
 RG 197.32  
 DW 16.800 usec  
 DE 6.50 usec  
 TE 296.2 K  
 D1 1.0000000 sec  
 D11 0.03000000 sec  
 TDO 1

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

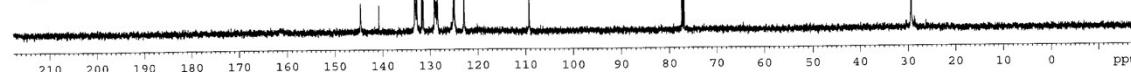
SF01 125.7703637 MHz  
 NUC1 13C  
 P1 8.90 usec  
 PLW1 103.0000000 W

===== CHANNEL f2 =====

SF02 500.1320005 MHz  
 NUC2 1H  
 CPDPG[2] waltz16  
 PCPD2 80.00 usec  
 PLW2 13.0000000 W  
 PLW12 0.34327999 W  
 PLW13 0.21969999 W

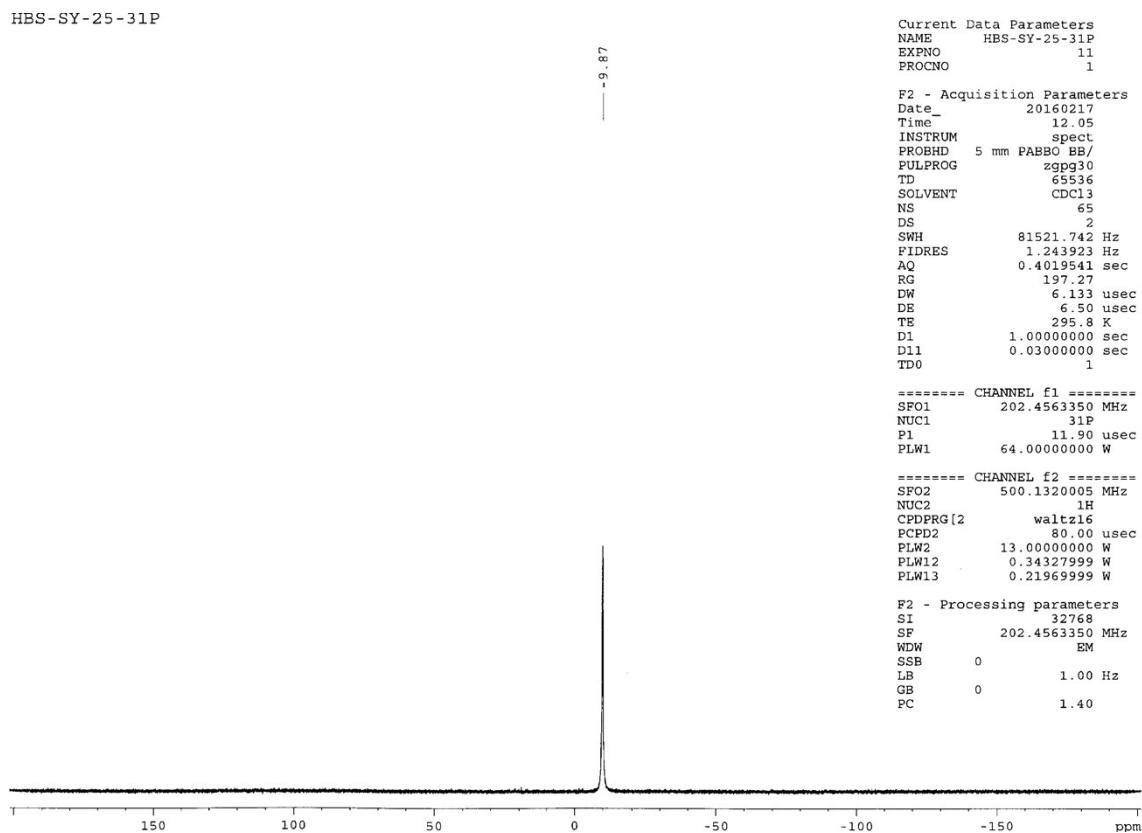
F2 - Processing parameters

SI 32768  
 SF 125.7578766 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

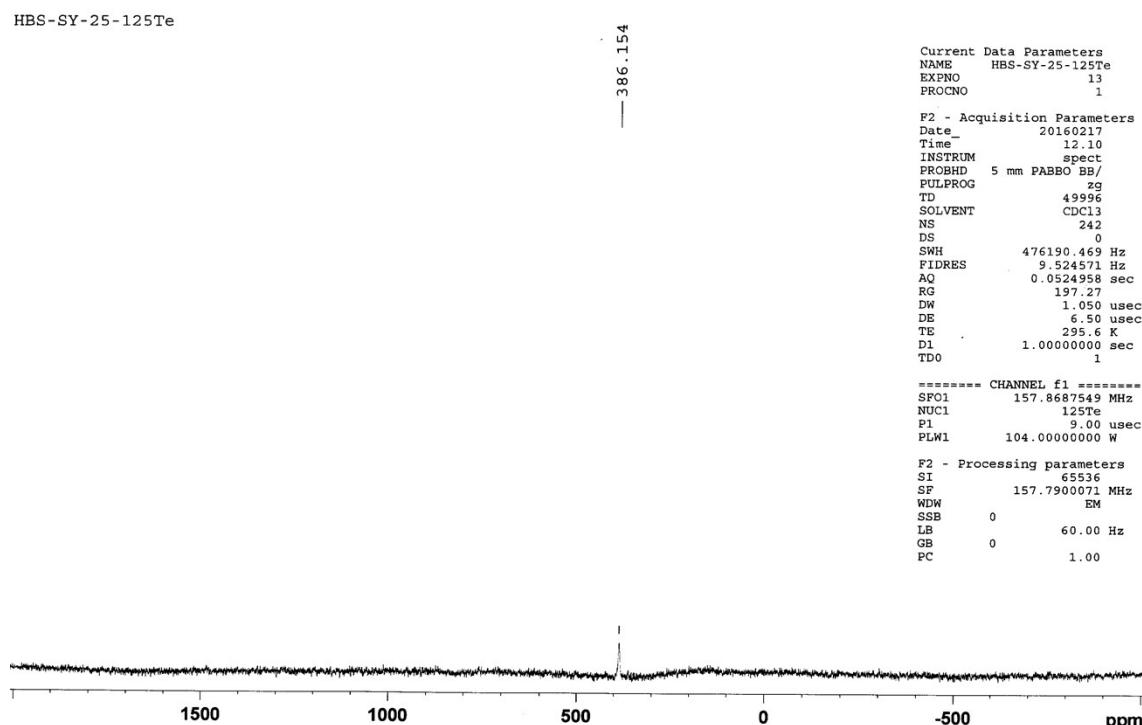


**Figure S57.** <sup>13</sup>C NMR spectrum of compound 16b.

HBS-SY-25-31P

**Figure S58.** <sup>31</sup>P NMR spectrum of compound **16b**.

HBS-SY-25-125Te

**Figure S59.** <sup>125</sup>Te NMR spectrum of compound **16b**.

## Display Report

**Analysis Info**

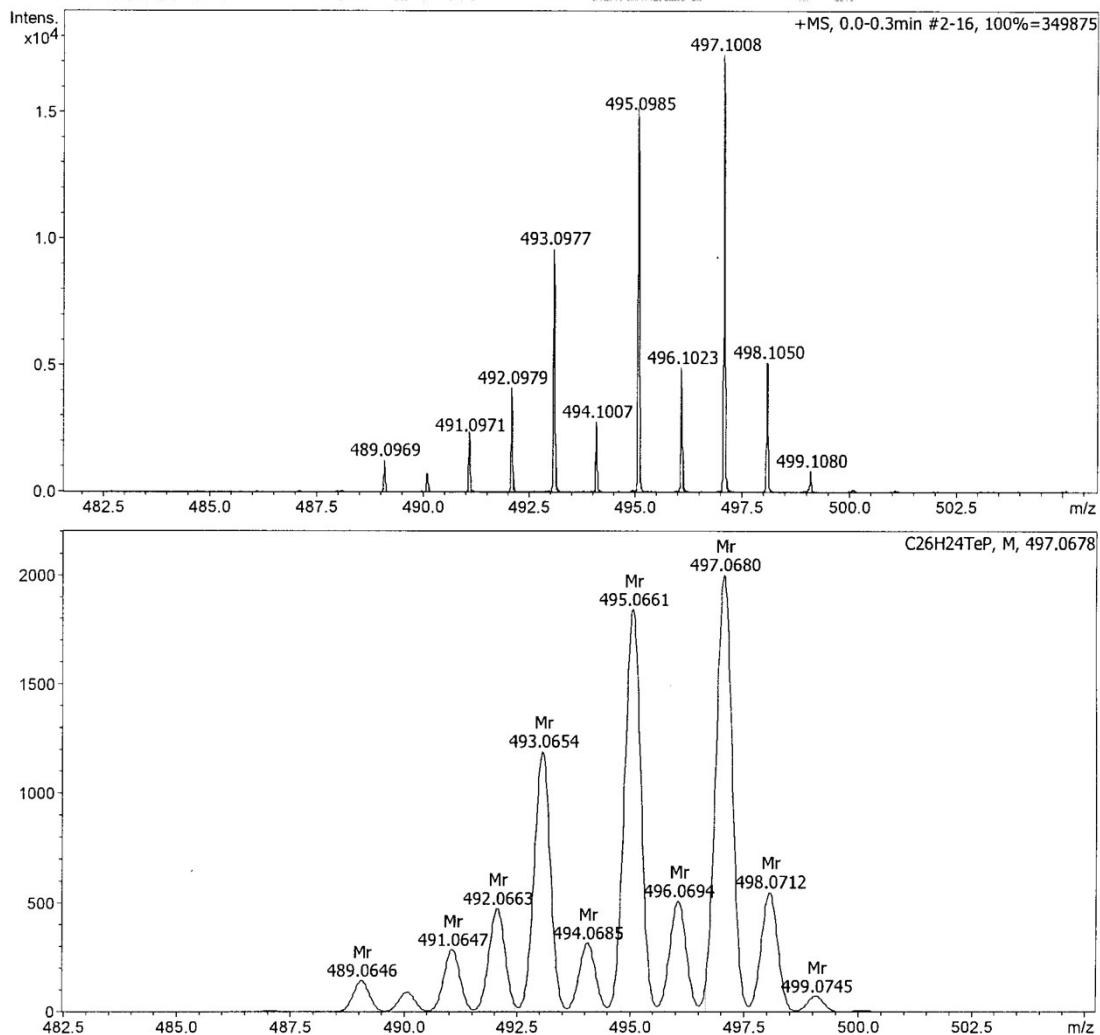
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 Sample Name HBS-SY-RTePPh3  
 Comment

Acquisition Date 12/24/2014 10:50:32 AM

 Operator HBS-SY  
 Instrument maXis impact 282001.00081

**Acquisition Parameter**

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Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



HBS-SY-RTePPh3.d

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by: mMSB IN

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**Figure S60.** ESI-MS spectrum of compound **16b**.

HBS-SY-8-184-1H

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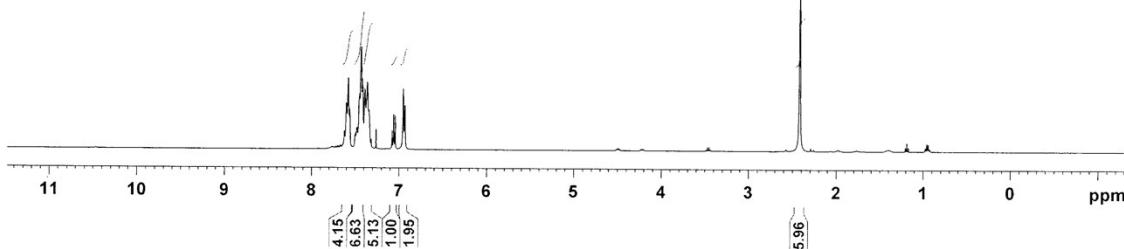
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PROCNO        1
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PULPROG  zg30
TD        54274
SOLVENT    CDCl3
NS         12
DS          0
SWH       8223.685 Hz
FIDRES     0.151522 Hz
AQ        3.299909 sec
RG        90.5
DW       60.800 usec
DE        6.50 usec
TE       297.1 K
D1      1.0000000 sec
TD0           1

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===== CHANNEL f1 =====
NUC1           1H
P1            14.75 usec
PL1          -1.00 dB
PL1W      10.56200695 W
SF01      400.1324710 MHz
SI            32768
SF      400.1300095 MHz
WDW           EM
SSB            0
LB            0.30 Hz
GB            0
PC            1.00

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**Figure S61.**  $^1\text{H}$  NMR spectrum of compound **16c**.

HBS-SY-8-184-13C

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EXPNO         2
PROCNO        1
Date       20150103
Time       11.56
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT    CDCl3
NS         142
DS          4
SWH       26041.666 Hz
FIDRES     0.397364 Hz
AQ        1.2583412 sec
RG        208
DW       19.200 usec
DPZ       6.00 usec
TE       297.8 K
D1      1.0000000 sec
D11      0.03000000 sec
TD0           1

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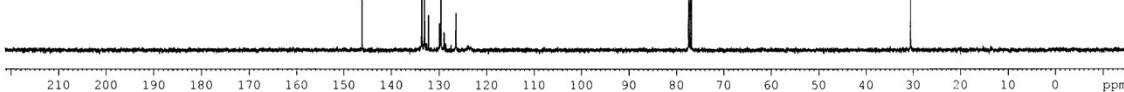
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P1            8.50 usec
PL1          -2.00 dB
PL1W      56.53121948 W
SF01      100.6238364 MHz

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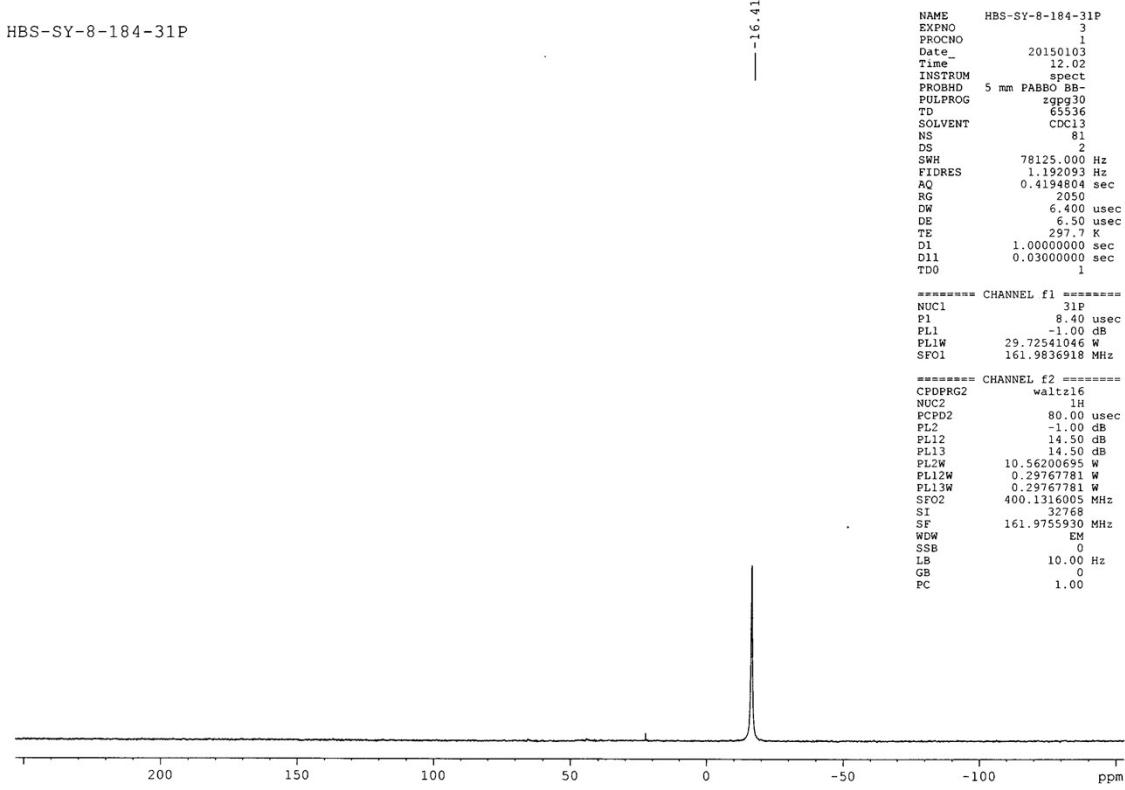
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===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2           1H
PCPD2        80.00 usec
PL2          -1.00 dB
PL12        13.69 dB
PL13        14.50 dB
PL2W      10.56200695 W
PL12W     0.35871249 W
PL13W     0.29767781 W
SF02      400.1316005 MHz
SI            32768
SF      100.6127656 MHz
WDW           EM
SSB            0
LB            1.00 Hz
GB            0
PC            1.40

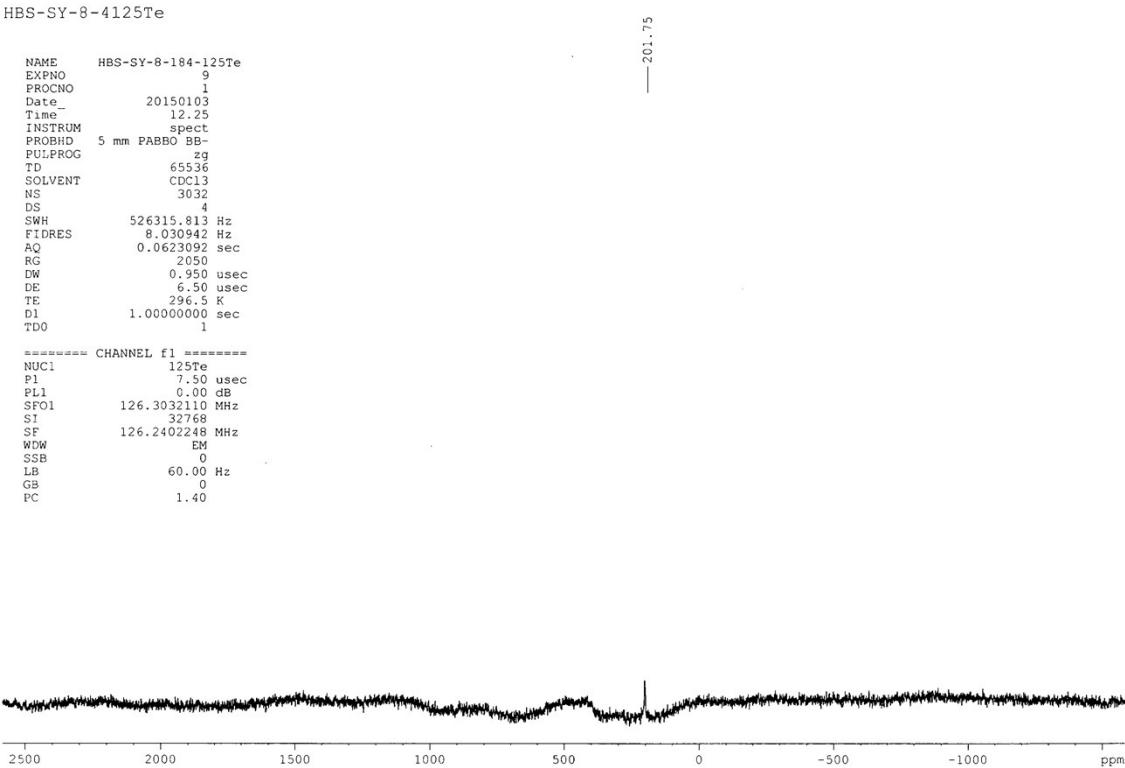
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**Figure S62.**  $^{13}\text{C}$  NMR spectrum of compound **16c**.



**Figure S63.**  $^{31}\text{P}$  NMR spectrum of compound **16c**.



**Figure S64.**  $^{125}\text{Te}$  NMR spectrum of compound **16c**.

## Display Report

**Analysis Info**

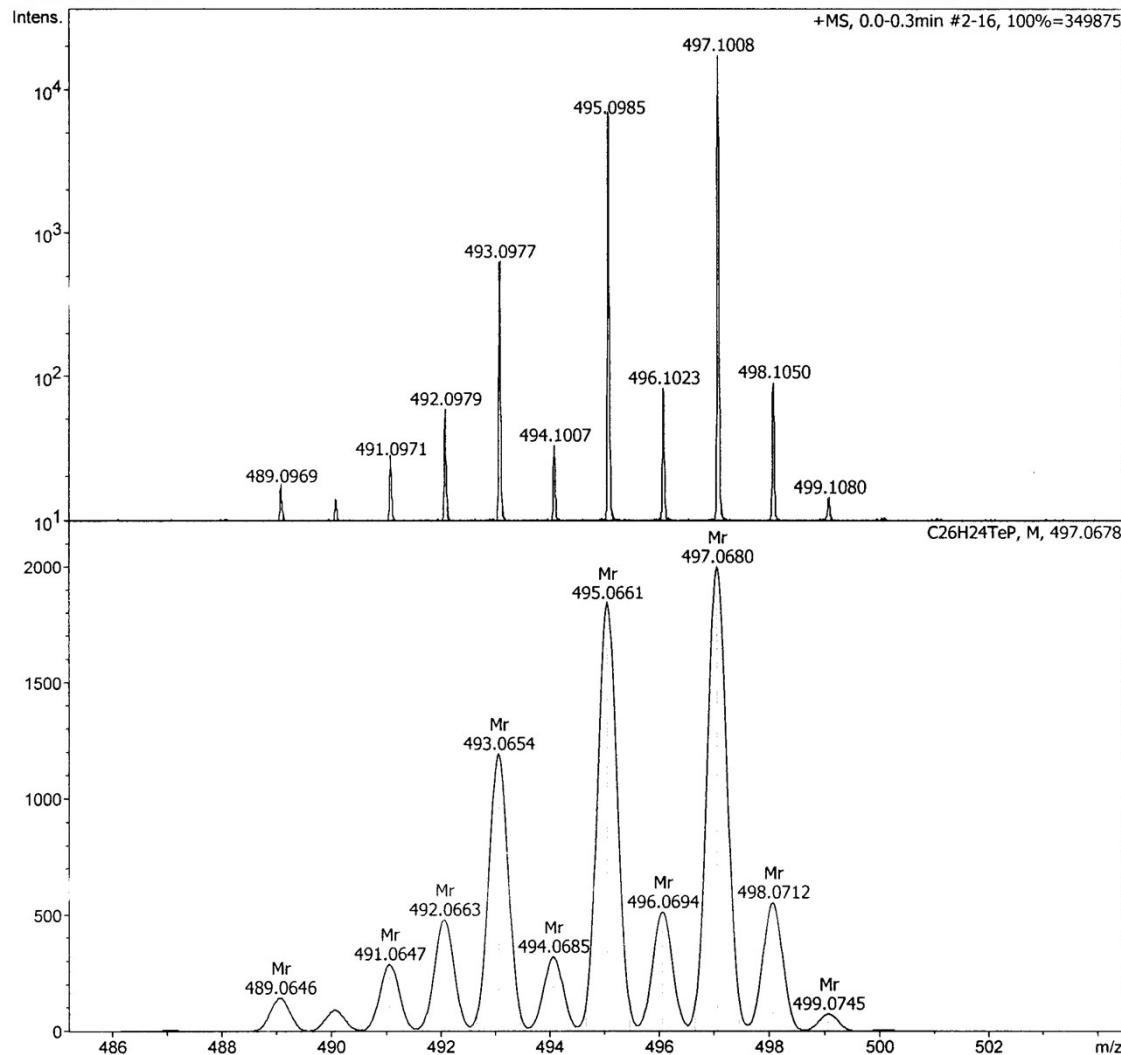
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 Operator HBS-SY  
 Instrument maXis impact 282001.00081

**Acquisition Parameter**

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



HBS-SY-RTePPh3.d

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by: HBS-SY

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**Figure S65.** ESI-MS spectrum of compound **16c**.

Packing diagram of compound 8:

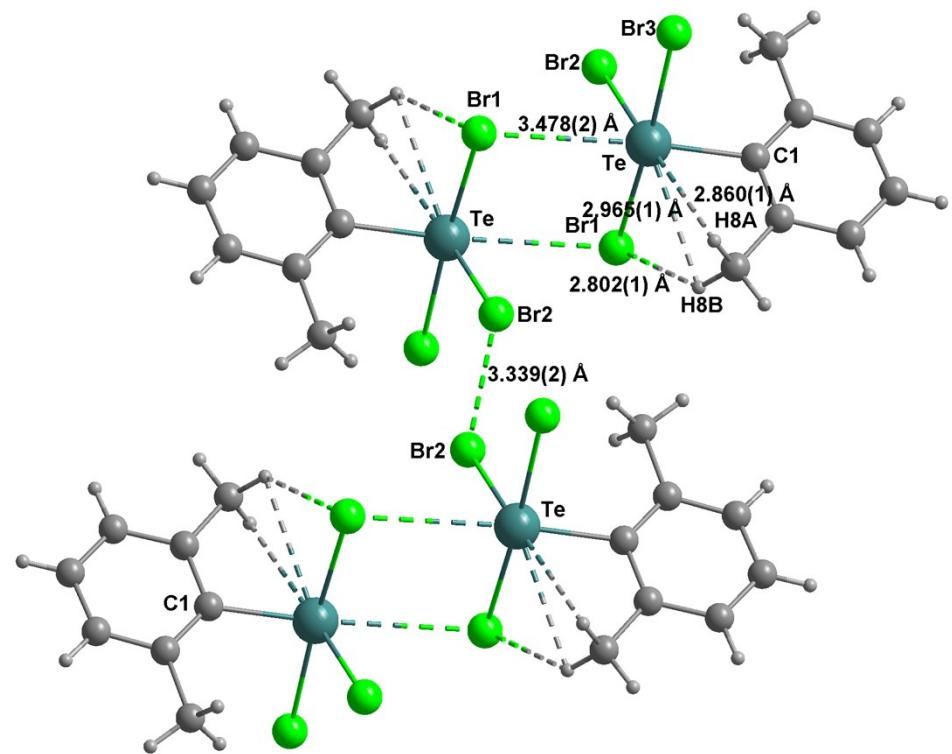


Figure S66. Packing diagram of compound 8.

Molecular structure of compounds 11a and 11b:

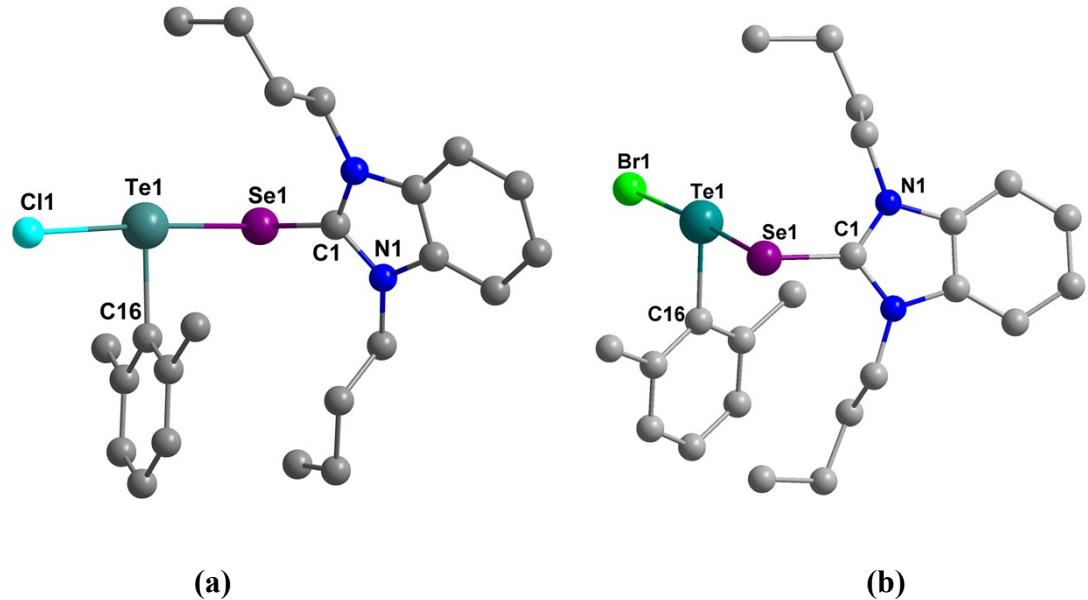
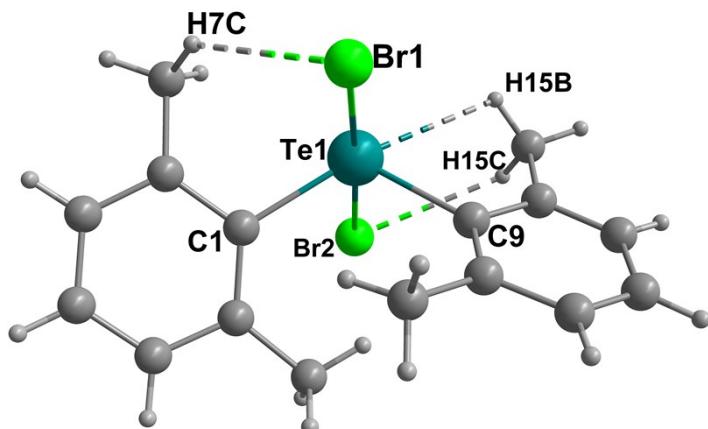


Figure S67 Molecular structure of compounds (a) 11a and (b) 11b. Hydrogen atoms have been omitted for clarity.

**Molecular structure of compound 13:** Compound **13** was characterized by X-ray crystallographic structure. Furukawa and coworkers have reported the molecular structure of compound **13**.<sup>26</sup> The molecular structure of compound **13** is shown in Figure S68. The compound crystallizes in orthorhombic system with  $P2_1P2_1P2_1$  space group. It has distorted tetrahedral (see-saw) geometry around tellurium. The Te1-Br1 {2.668(1)} and Te1-Br2 {2.693(1)} bond lengths are comparable with the reported bond lengths {2.663(3) and 2.697(3) Å respectively}, Br1-Te1-Br2 bond is almost linear {177.05(3) °} and is comparatively smaller than the reported bond angle {177.6(1) °}. The C1-Te-C9 bond angle {113.13(31) °} is larger than the reported angle {112.6(7) °} for the same. There are three types of intramolecular hydrogen bonds namely Te1···H15B 2.7809(7), Br1···H7C 2.7796(11) and Br2··· H15B 2.8117(10) Å.



**Figure S68.** Molecular structure of compound **13**, Selected bond lengths [Å] and bond angles [°] Te1-C1 2.134(9), Te1-C9 2.141(8), Te1-Br1 2.668(1), Te1-Br2 2.693(1), Te1...H15B 2.781(1), Br1...H7C 2.7796(11), Br2... H15B 2.8117(10), C1-Te1-C9 113.13(31), Br1-Te1-Br2 177.05(3).

## Summary of crystallographic data

**Table S1** Summary of crystallographic data of compounds **7**, **8**, **11a** and **11b**.

	<b>7</b>	<b>8</b>	<b>11a</b>	<b>11b</b>
Chemical formula	C <sub>16</sub> H <sub>18</sub> Br <sub>2</sub> Te <sub>2</sub>	C <sub>8</sub> H <sub>9</sub> Br <sub>3</sub> Te	C <sub>23</sub> H <sub>31</sub> ClN <sub>2</sub> SeTe	C <sub>23</sub> H <sub>31</sub> BrN <sub>2</sub> SeTe
F. W. (g/mol)	625.32	472.48	577.51	621.97
Space group	P 1 21/c 1	P 1 21/c	P 1 21/c 1	P 1 21/c 1
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
a (Å)	10.334(2)	8.996(4)	7.4430(19)	7.455(3)
b (Å)	18.758(4)	14.280(6)	16.986(5)	17.000(7)
c (Å)	9.1880(18)	9.201(4)	18.627(5)	18.707(8)
α (deg)	90.00	90.00	90.00	90
β (deg)	95.90(3)	105.946(5)	90.382(6)	92.214(7)
γ (deg)	90.00	90.00	90.00	90
V (Å <sup>3</sup> )	1771.6(6)	1136.5(9)	2354.9(11)	2369.1(17)
Z	4	4	4	4
D <sub>cal</sub> , Mg/m <sup>3</sup>	2.344	2.761	1.629	1.744
F(000)	1152	856	1144	1216
μ (mm <sup>-1</sup> )	7.793	13.113	2.934	4.490
2θ range (deg)	3.03 to 29.19	3.14 to 25.37	3.18 to 25.35	3.14 to 25.02
Collected reflections	4764	2065	4266	4165
Unique reflections	3799	1444	3507	3271
Final R (obs. data), R <sub>1</sub>	0.0375	0.0425	0.0321	0.0543
wR <sub>2</sub>	0.0949	0.0746	0.0706	0.1294
Final R (all data), R <sub>1</sub>	0.0538	0.0507	0.0371	0.0599
wR <sub>2</sub>	0.1184	0.0761	0.0722	0.1321
Goodness of fit on F <sup>2</sup>	0.687	0.834	1.012	1.020

**Table S2** Summary of crystallographic data of compound **11c**, **15** and **16c**.

	<b>11c</b>	<b>15</b>	<b>16c</b>
Chemical formula	C <sub>23</sub> H <sub>31</sub> IN <sub>2</sub> SeTe	C <sub>23</sub> H <sub>31</sub> N <sub>2</sub> SeTeBF <sub>4</sub>	C <sub>26</sub> H <sub>24</sub> IPTe
F. W. (g/mol)	668.98	628.87	621.92
Space group	P 1 21/c 1	P 1 21/c 1	Pbca
Crystal system	Monoclinic	Monoclinic	orthorhombic
a (Å)	7.4903(3)	7.806(1)	11.579(2)
b (Å)	17.1048(8)	16.228(3)	15.339(3)
c (Å)	18.6895(8)	19.817(4)	26.530(5)
α (deg)	90	90	90.00
β (deg)	94.244(4)	93.629(3)	90.00
γ (deg)	90	90	90.00
V (Å <sup>3</sup> )	2387.93(18)	2505.2(8)	4712.3(16)
Z	4	4	8
D <sub>cal</sub> , Mg/m <sup>3</sup>	1.861	1.667	1.753
F(000)	1288	1240	2400
μ (mm <sup>-1</sup> )	4.074	2.683	2.651
2θ range (deg)	2.19 to 31.35	3.02 to 29.40	3.07 to 29.19
Collected reflections	7311	6820	6347
Unique reflections	6086	4294	6177
Final R (obs. data), R <sub>1</sub>	0.0419	0.0611	0.0223
wR <sub>2</sub>	0.0930	0.1600	0.0678
Final R (all data), R <sub>1</sub>	0.0543	0.0893	0.0249
wR <sub>2</sub>	0.1029	0.2170	0.0863
Goodness of fit on F <sup>2</sup>	1.045	1.002	1.295

**Computational data:** All the structures were optimized with Gaussian 09 program by using MPW1PW91 method and Lanl2dz ECP basis set for Te and 6-311g(d) basis set for rest of the atoms.

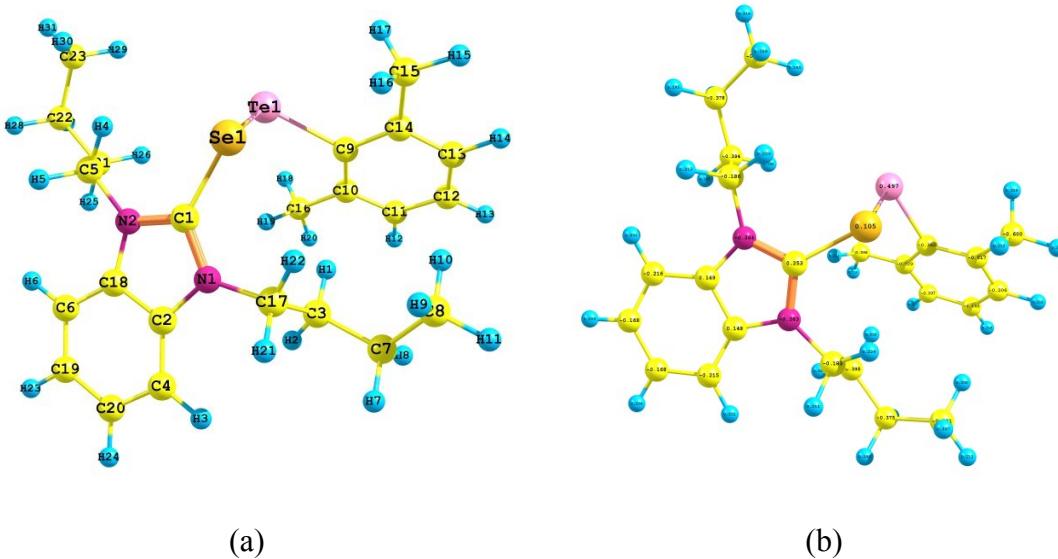
**Table S3.** Bond length and bond angle comparison between crystal structure of compound **15** and the optimized structure of selone complex of 2,6-dimethylphenyltellurenyl cation.

Bond length (Å) and bond angle (°)	Crystal structure	Optimized structure
Se1-Te1	2.54339	2.58672
Se1-C2	1.88987	1.90476
C2-N1	1.34446	1.34658
C2-N2	1.33914	1.34725
Te1-C12	2.12702	2.13551
Se1-Te1-C12	97.212	100.854
Te1-Se1-C2	100.96443	102.690

**Table S4.** Calculated charge on atoms in selone complex of 2,6-dimethylphenyltellurenyl cation .

Atom	Mulliken Charge	NPA Charge	Atom	Mulliken Charge	NPA Charge
Te	0.553	0.497	C2	0.230	0.148
Se	-0.136	0.105	C18	0.235	0.149
C1	0.319	0.253	N1	-0.429	-0.363
C9	-0.672	-0.362	N2	-0.425	-0.364

## Compound 15



**Figure S69.** (a) Optimized geometry of selone complex of 2,6-dimethylphenyltellurenyl cation and (b) NPA charge distribution on selone complex of 2,6-dimethylphenyltellurenyl cation.

**Table S5:** Coordinates of the optimized geometry of selone complex of 2,6-dimethylphenyltellurenyl cation.

E(RmPW1PW91) = -1021.74728874		
Te	1.019936000	-1.964331000
Se	-0.097106000	-0.667882000
N	-1.231484000	1.759439000
N	-2.566583000	0.038608000
C	-1.361461000	0.432081000
C	-2.380880000	2.237638000
C	0.811427000	2.930842000
C	-2.758678000	3.522528000
C	-3.126658000	-1.313624000
C	-4.498277000	1.283129000
C	1.842831000	4.005970000
C	2.813789000	3.621306000
C	2.614301000	-0.636610000
C	2.590437000	-0.011136000
C	3.692075000	0.763372000
C	4.774055000	0.913964000
C	4.778771000	0.286553000
C	3.708747000	-0.506974000
C	3.771929000	-1.167977000
C	1.455479000	-0.147519000
		2.906400000

C	-0.093636000	2.602238000	-1.062002000
C	-3.230363000	1.142077000	0.092509000
C	-4.870686000	2.558519000	1.031923000
C	-4.014835000	3.659120000	0.861834000
C	-3.130518000	-1.987514000	0.916078000
C	-3.771407000	-3.374317000	0.881463000
C	-3.008376000	-4.401740000	0.054788000
H	1.319835000	2.017367000	0.441900000
H	0.200254000	3.267288000	0.961619000
H	-2.107289000	4.376548000	0.169551000
H	-2.542407000	-1.876744000	-1.176732000
H	-4.139874000	-1.225299000	-0.850202000
H	-5.166803000	0.441965000	0.780474000
H	1.327765000	4.937123000	-0.483021000
H	2.405153000	4.225871000	0.691016000
H	2.318606000	3.498875000	-2.295985000
H	3.329645000	2.686570000	-1.095560000
H	3.574759000	4.391897000	-1.461724000
H	3.699319000	1.247908000	3.262052000
H	5.622588000	1.516143000	1.743244000
H	5.632064000	0.402313000	-0.455345000
H	4.745114000	-1.007497000	-2.015771000
H	3.017672000	-0.768210000	-2.236421000
H	3.607493000	-2.244964000	-1.485772000
H	1.378832000	-1.162314000	3.304136000
H	0.490950000	0.090623000	2.453289000
H	1.600978000	0.520380000	3.755123000
H	-0.512680000	3.507910000	-1.506219000
H	0.449035000	2.079347000	-1.846354000
H	-5.848483000	2.714814000	1.470222000
H	-4.350377000	4.640096000	1.174428000
H	-3.665576000	-1.356638000	1.631483000
H	-2.101338000	-2.060863000	1.280482000
H	-3.850542000	-3.730057000	1.912018000
H	-4.801739000	-3.294377000	0.517100000
H	-1.971749000	-4.491846000	0.391337000
H	-2.993879000	-4.160528000	-1.011013000
H	-3.464306000	-5.388428000	0.146679000