Supporting Information

Selone-stabilized aryltellurenyl cations

Sangeeta Yadav,[a] Saravanan Raju,[a] Harkesh B. Singh*[a] and Ray J. Butcher[b]

[a] Department of Chemistry, Indian Institute of Technology Bombay, Mumbai 400076, India.

[b] Department of Chemistry, Howard University, Washington, D. C. 20059, USA.

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Spectral data

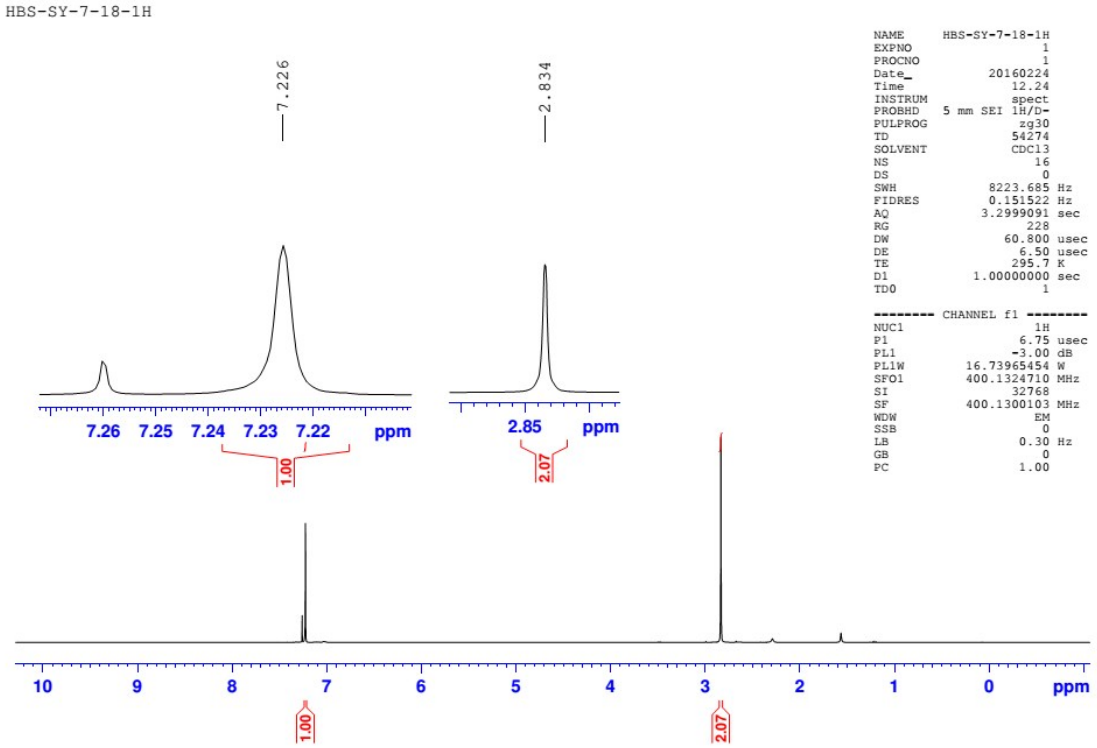


Figure S1. [1]H NMR spectrum of compound **7**.

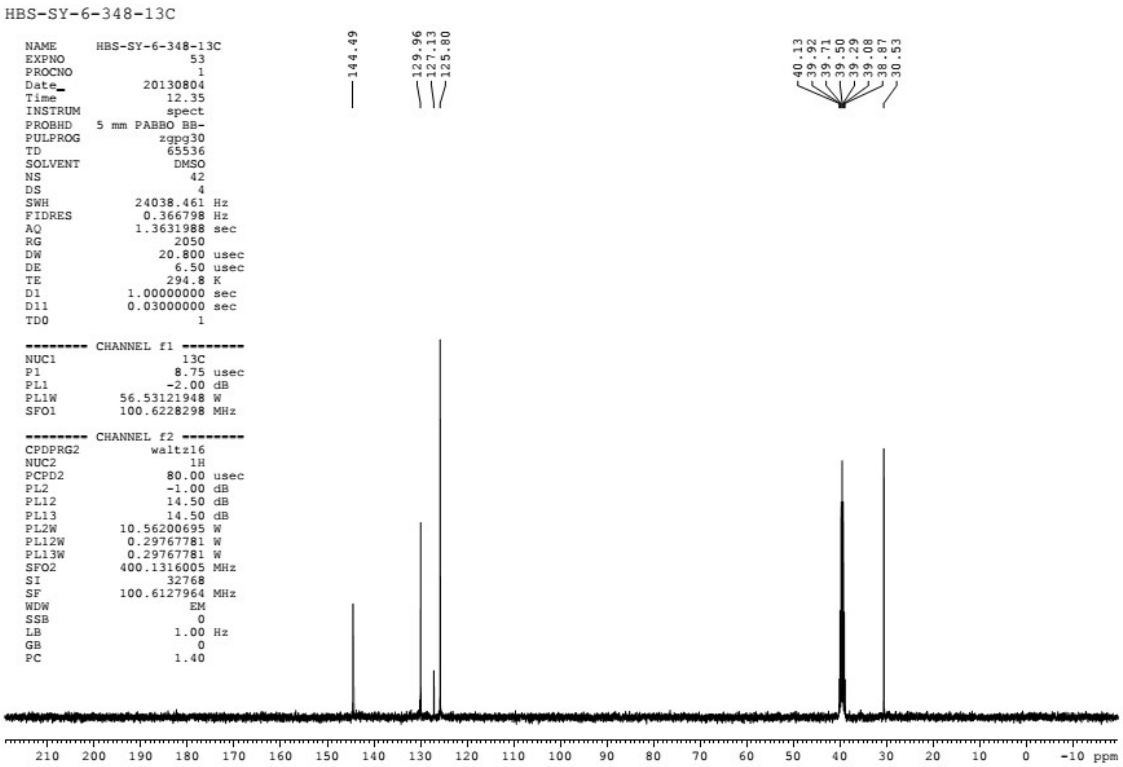


Figure S2. [13]C NMR spectrum of compound **7**.

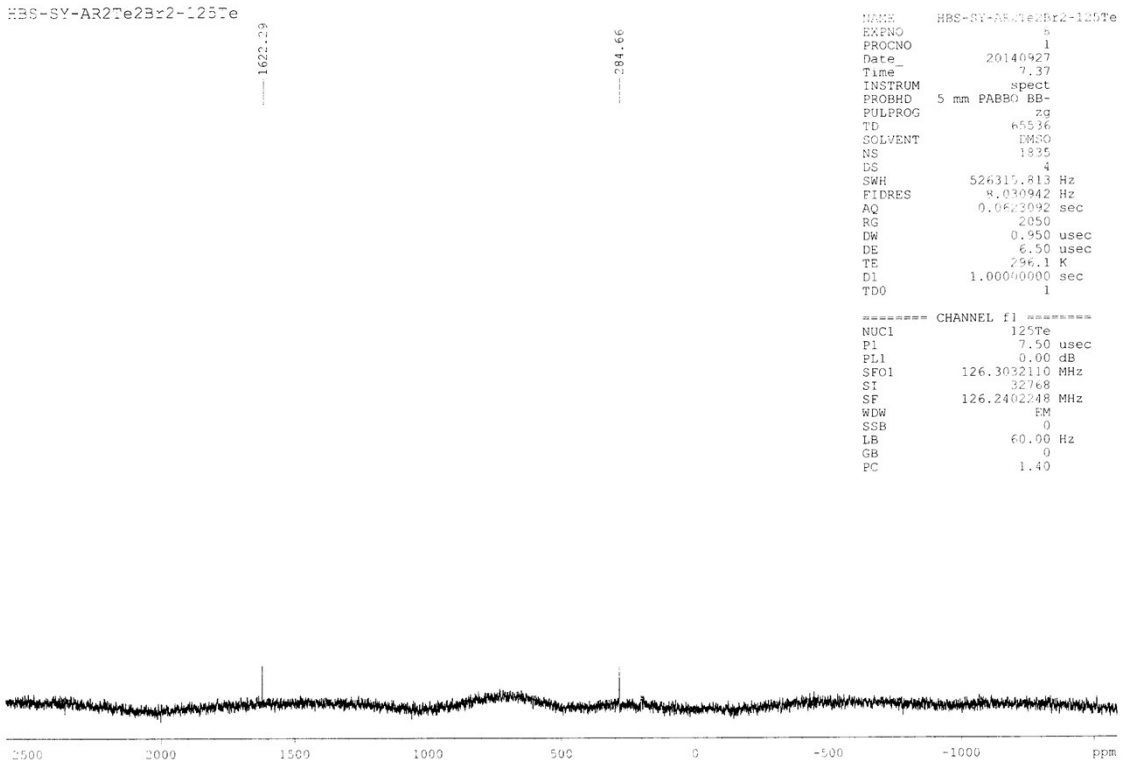


Figure S3. ^{125}Te NMR spectrum of compound **7**.

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**.

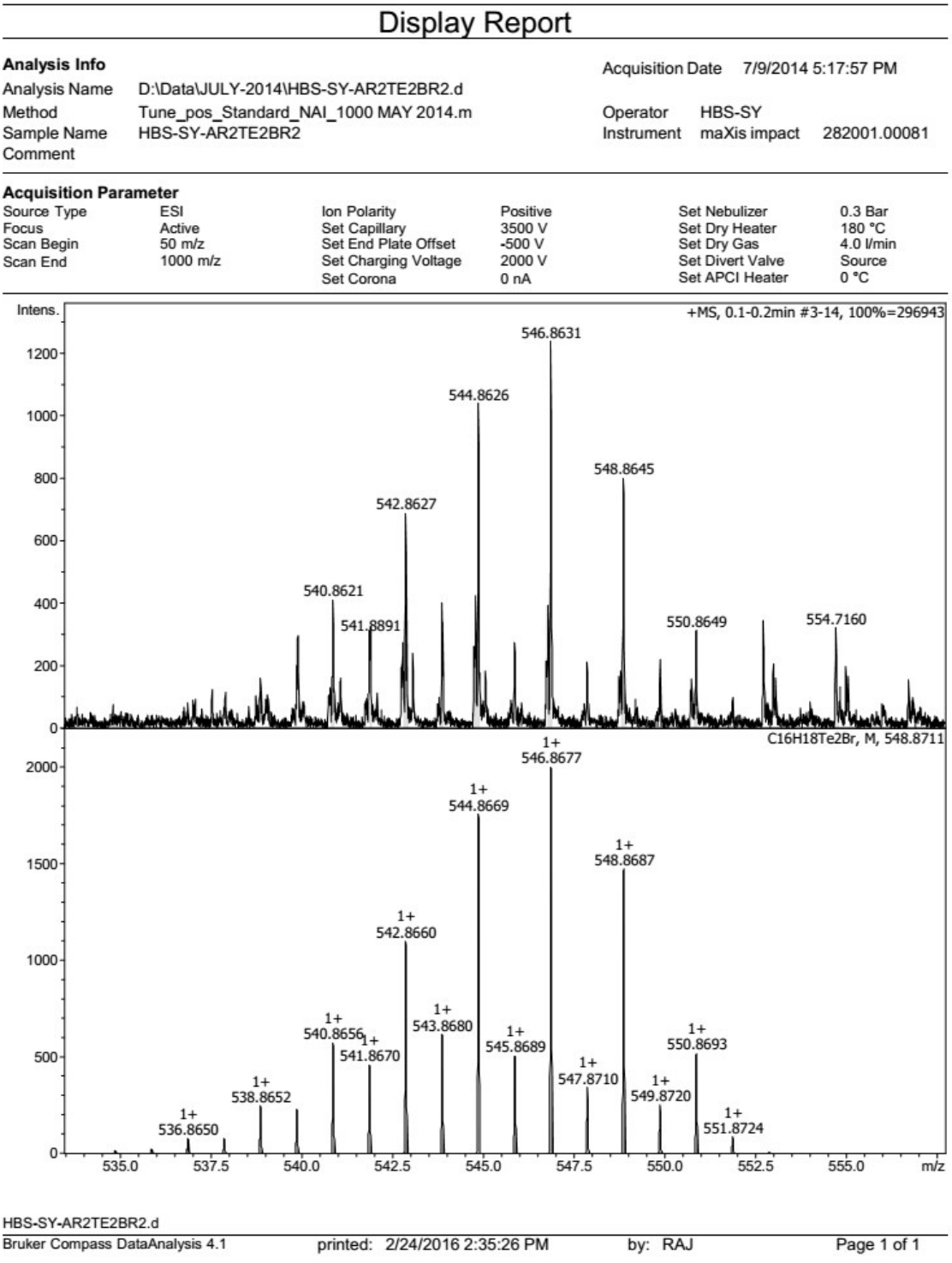


Figure S5. ESI-MS spectrum of compound **7**.

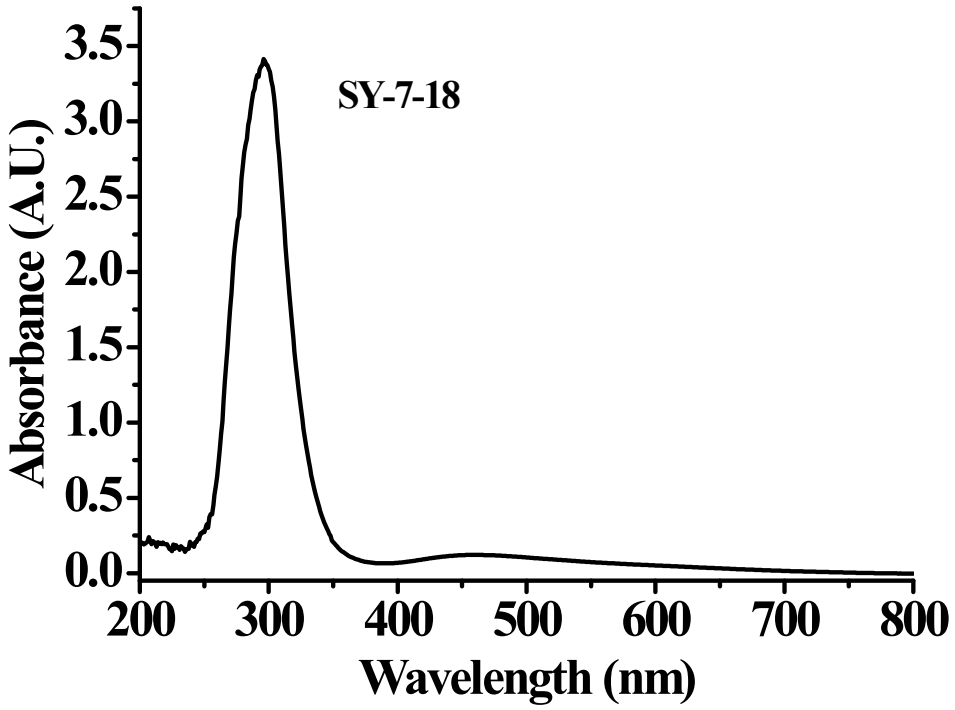


Figure S6. UV-Visible spectrum of compound **7**.

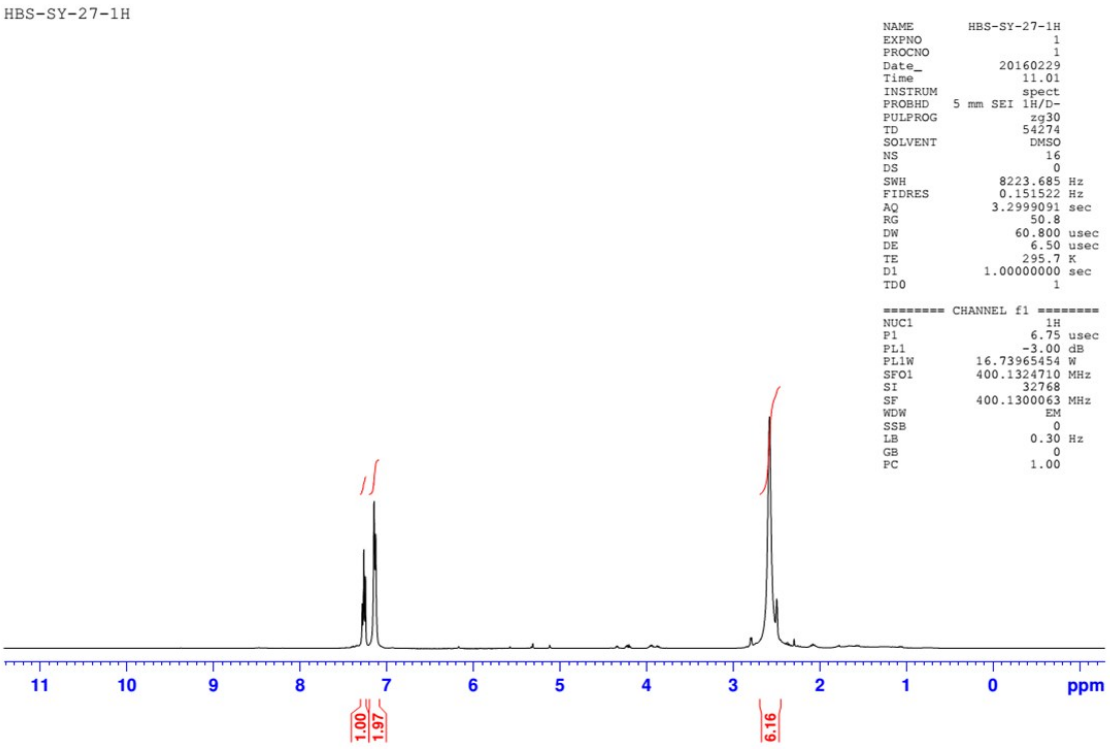


Figure S7. ^{1}H NMR spectrum of compound **8**.

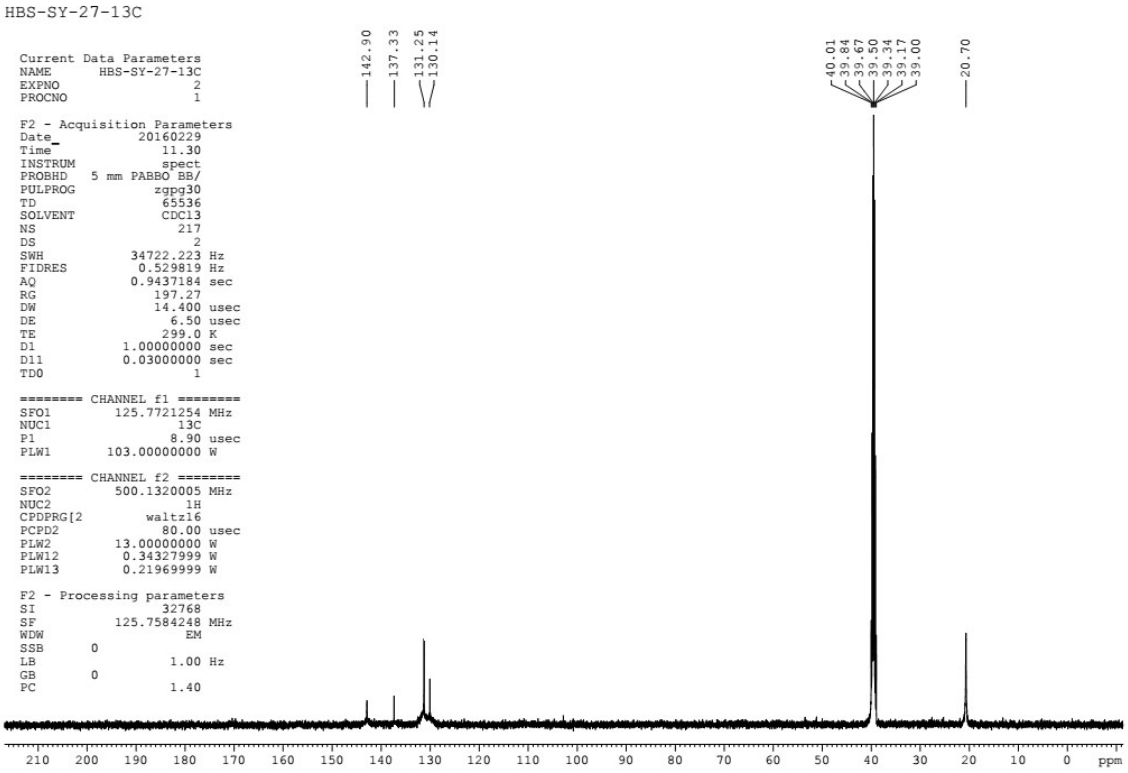


Figure S8. ^{13}C NMR spectrum of compound **8**.

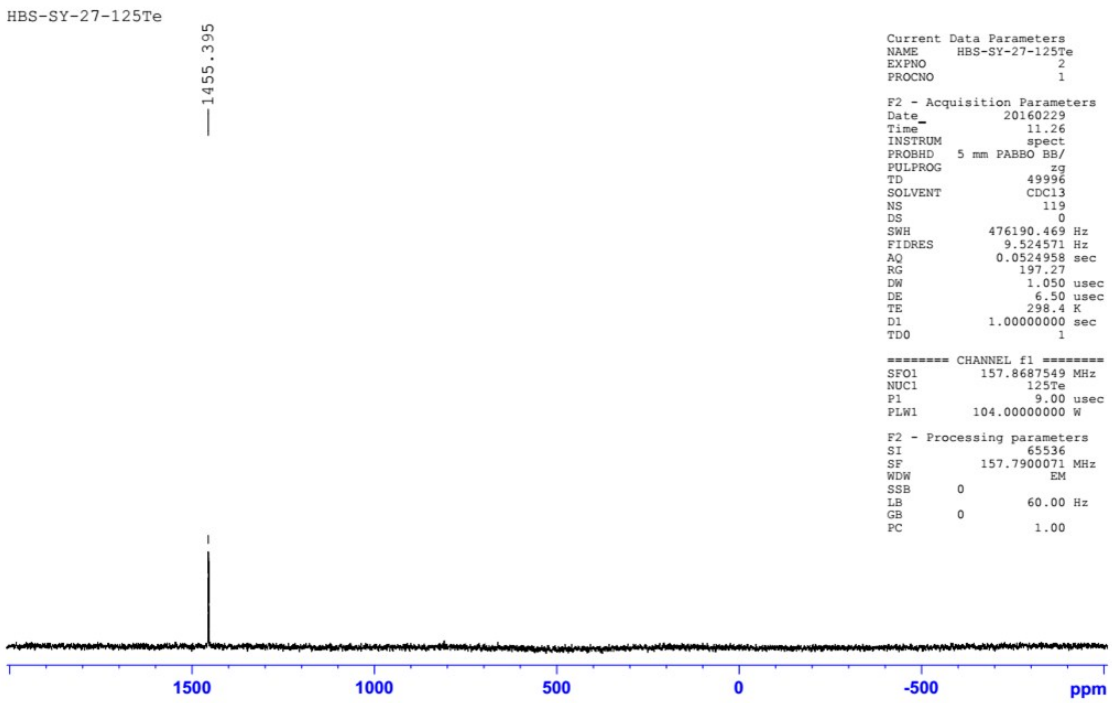
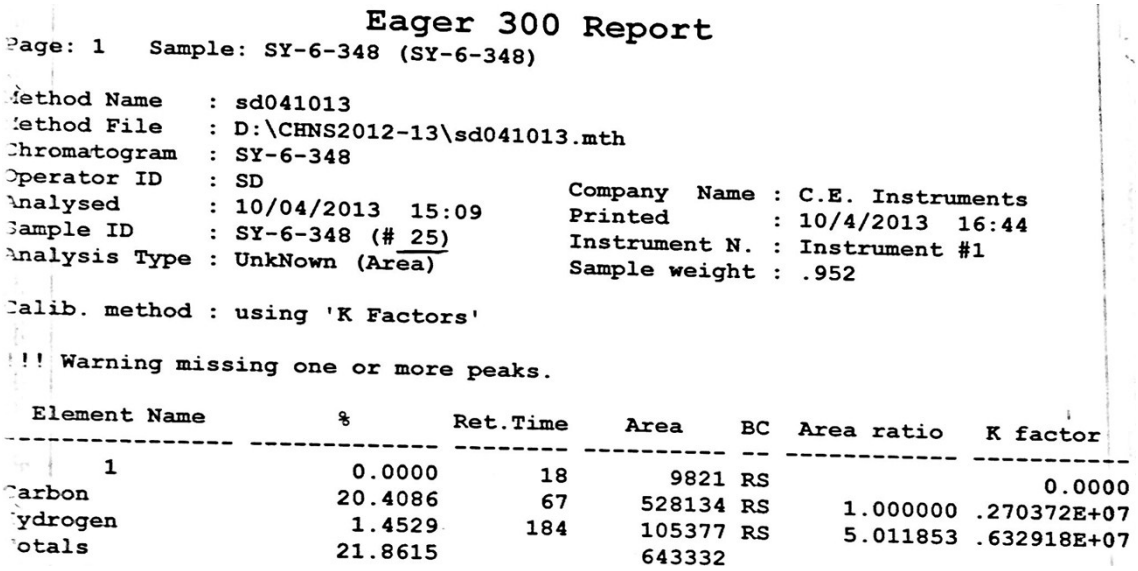


Figure S9. ^{125}Te NMR spectrum of compound **8**.



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**.

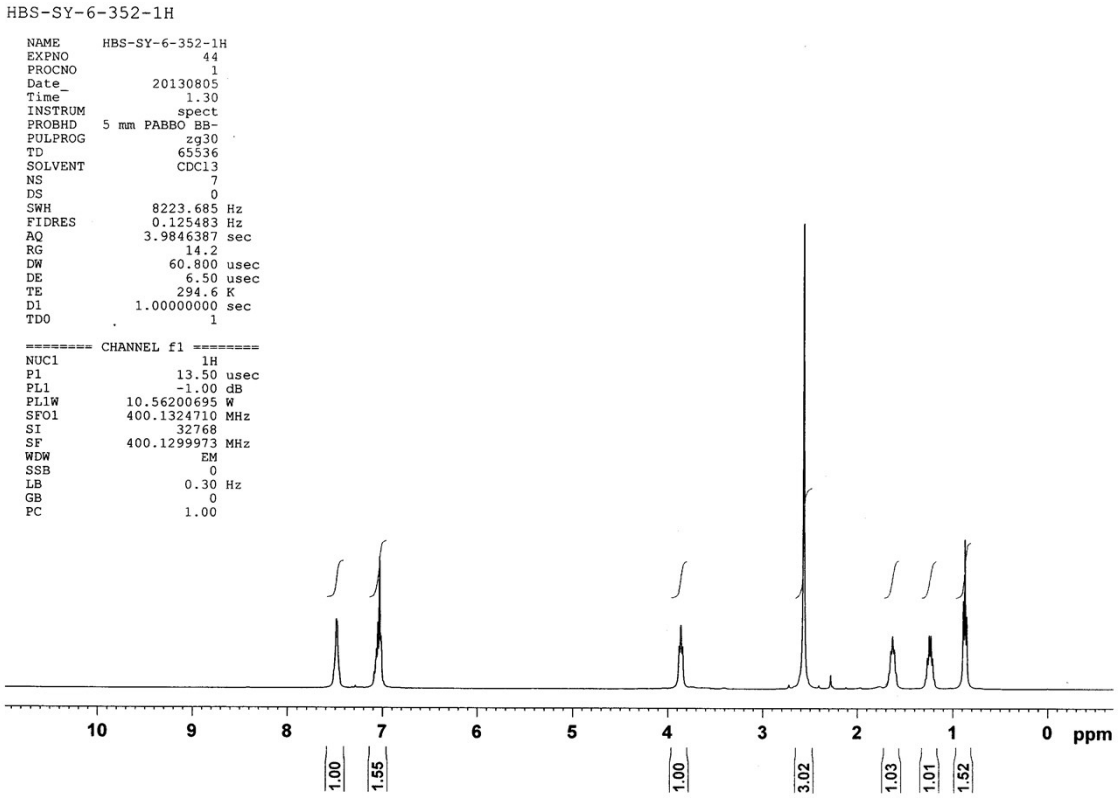


Figure S11. ^{1}H NMR spectrum of compound **10**.

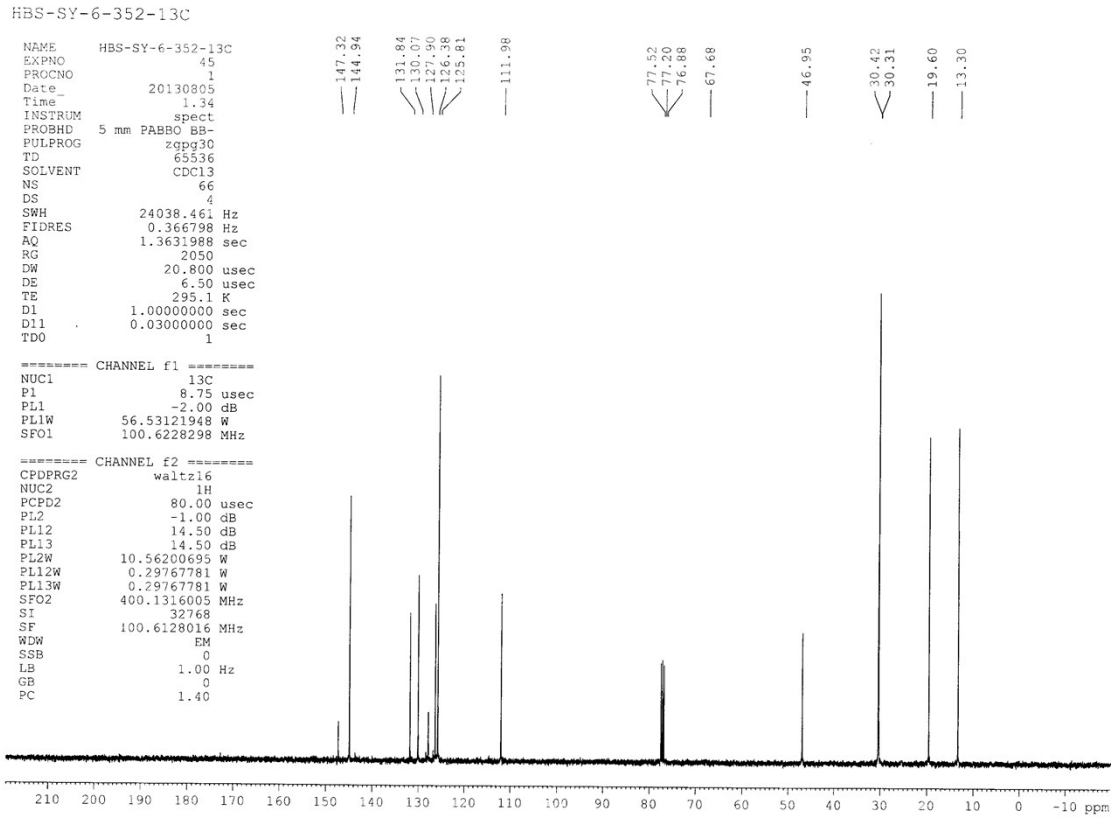


Figure S12. ^{13}C NMR spectrum of compound **10**.

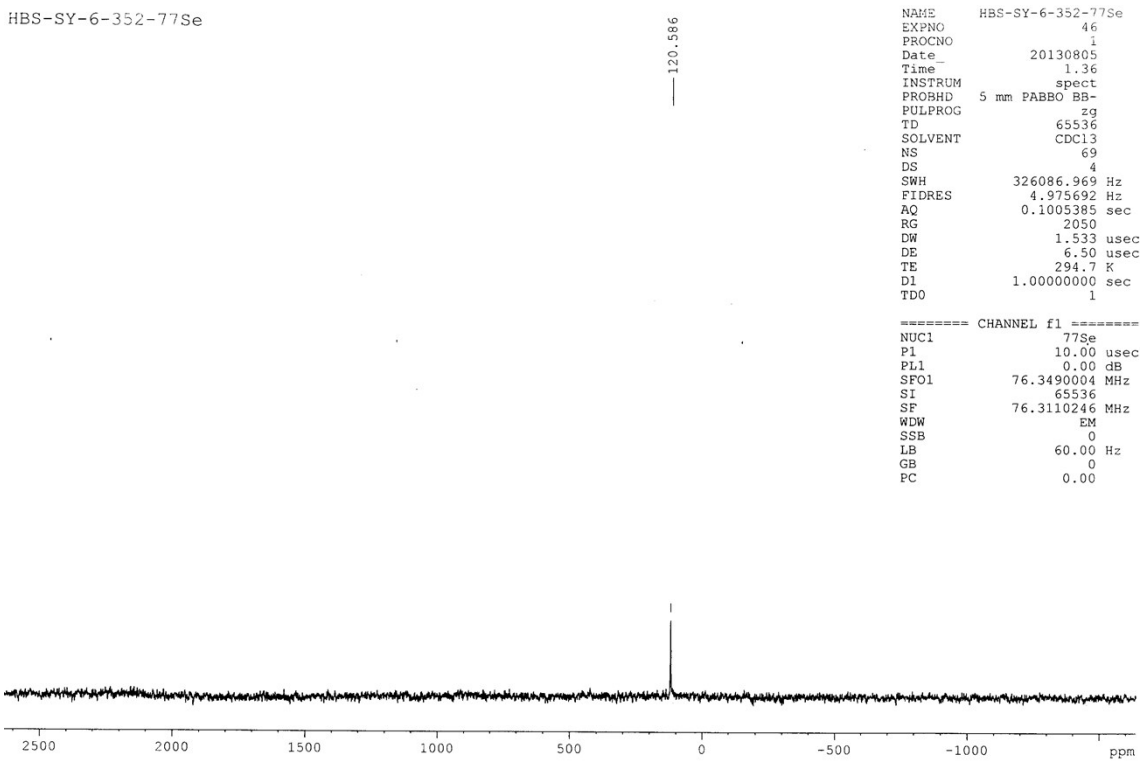


Figure S13. ^{77}Se NMR spectrum of compound **10**.

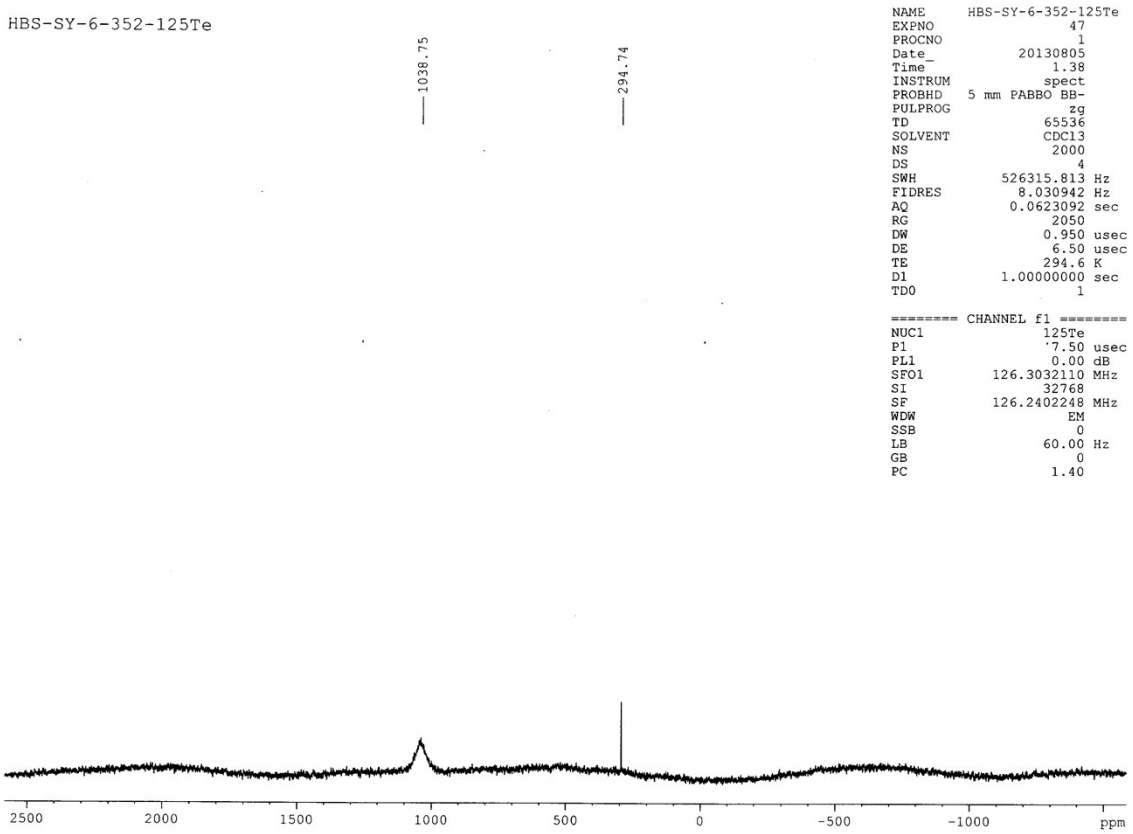


Figure S14. ^{125}Te NMR spectrum of compound **10**.

Eager 300 Report

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

Method Name : sd041013
Method File : D:\CHNS2012-13\sd041013.mth
Chromatogram : SY-6-350
Operator ID : SD
Analysed : 10/04/2013 14:58
Sample ID : SY-6-350 (# 24)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 10/4/2013 16:44
Instrument N. : Instrument #1
Sample weight : .882

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**.

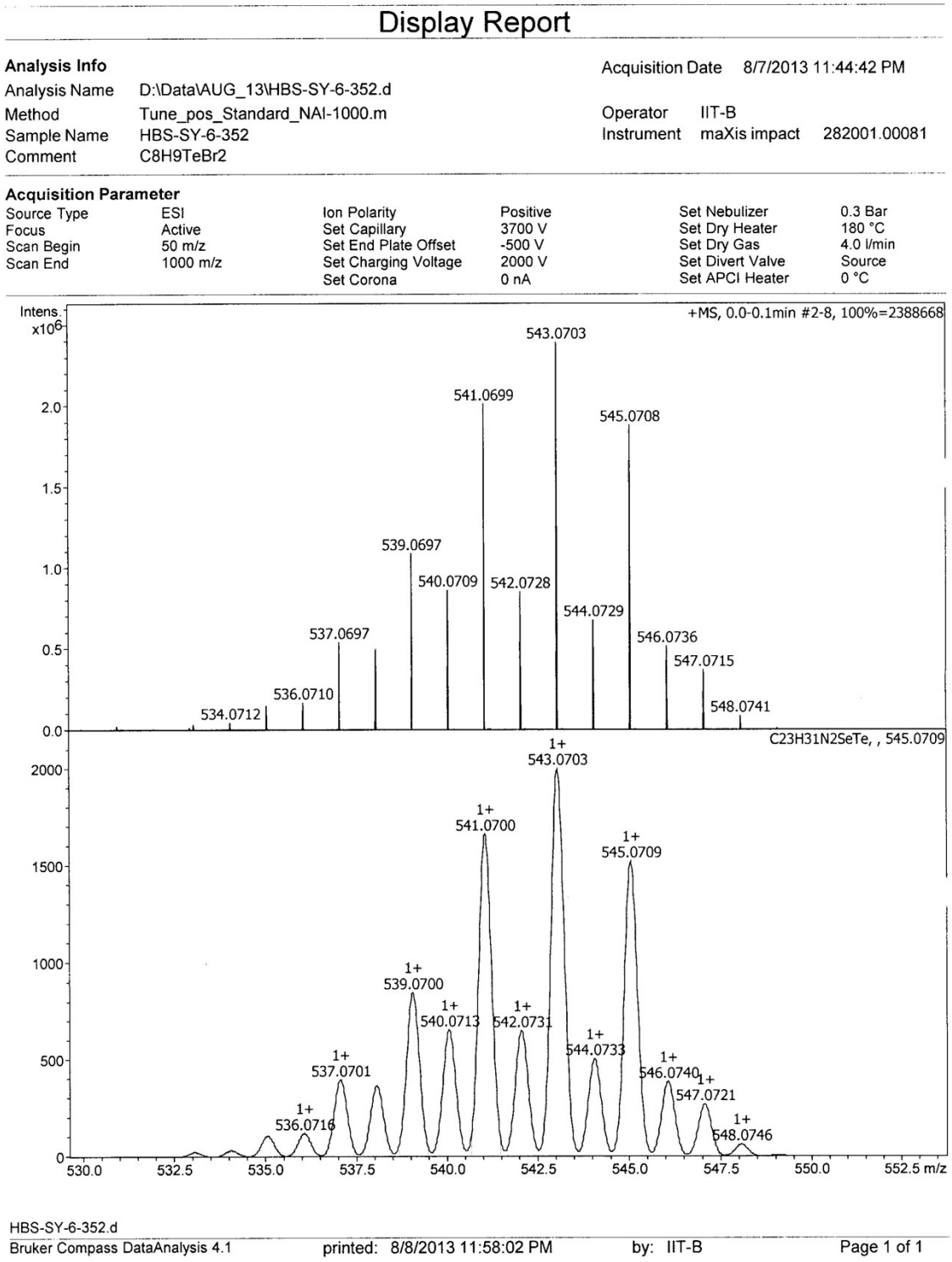


Figure S16. ESI-MS spectrum of compound **10** (positive mode of detection).

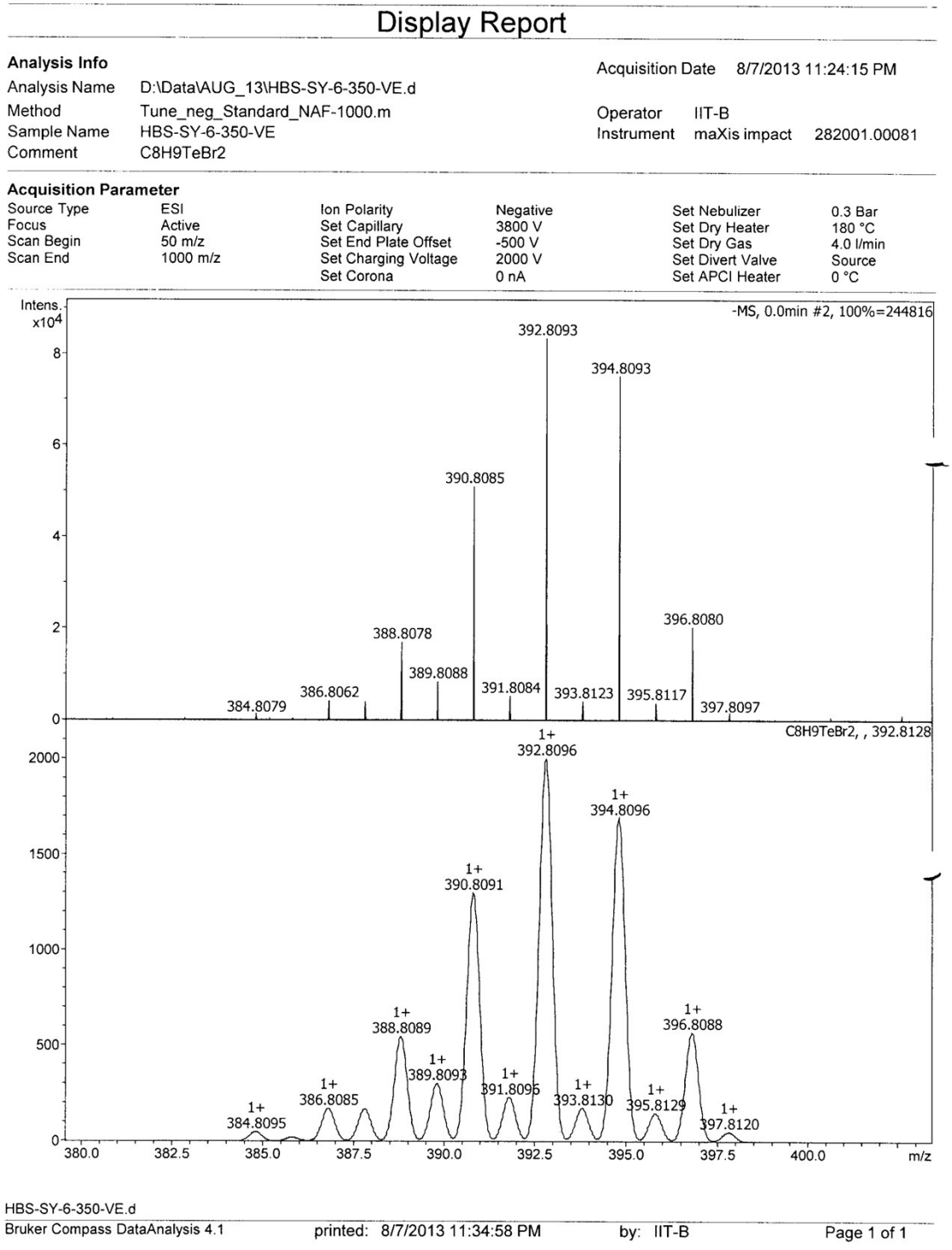


Figure S17. ESI-MS spectrum of compound **10 (**negative mode of detection**)**.

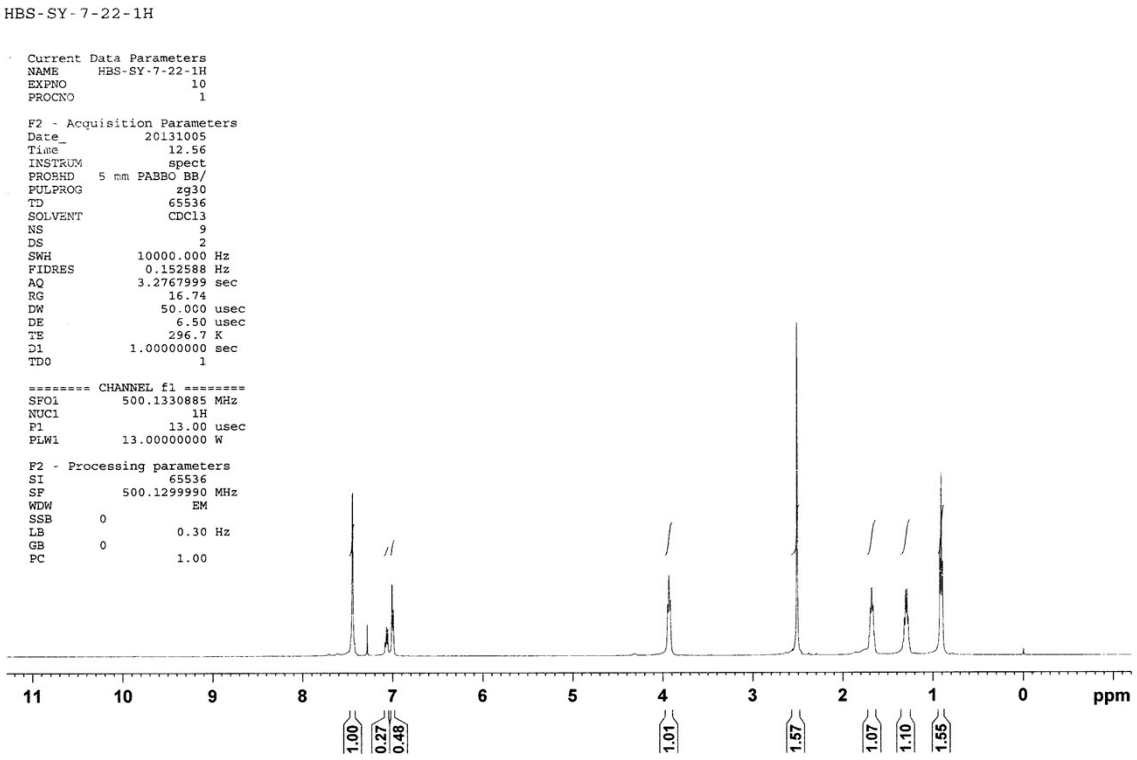


Figure S18. ^{1}H NMR spectrum of compound **11a**.

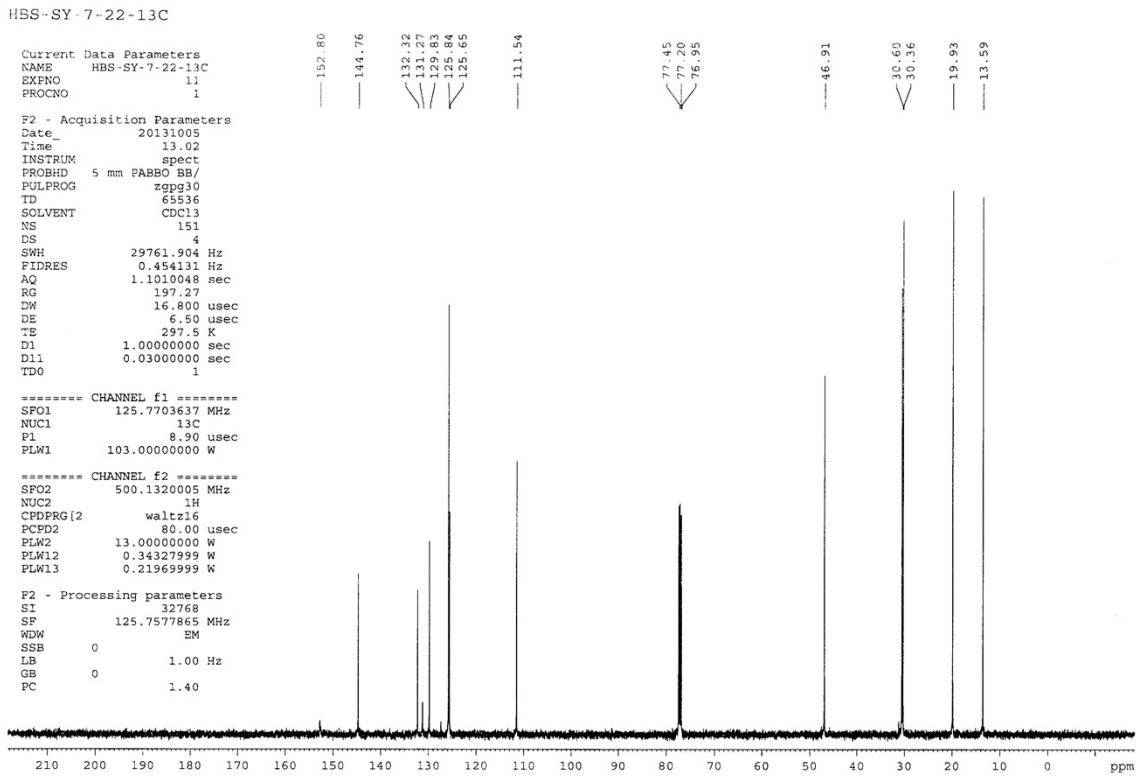


Figure S19. ^{13}C NMR spectrum of compound **11a**.

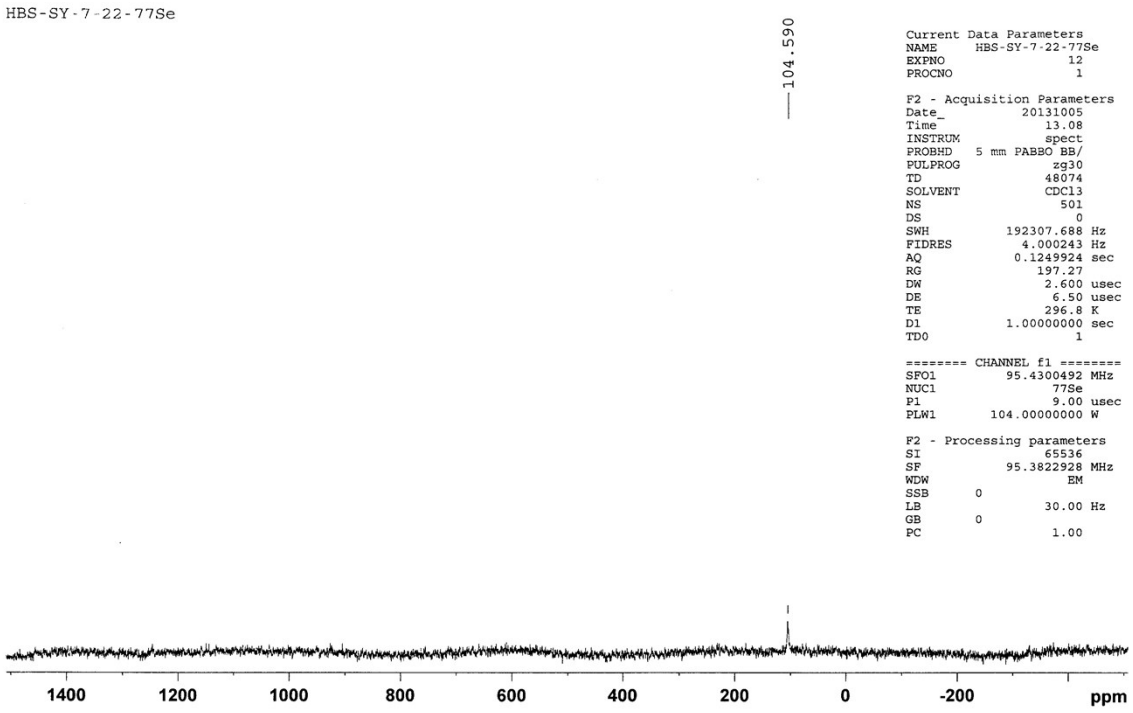


Figure S20. ^{77}Se NMR spectrum of compound **11a**.

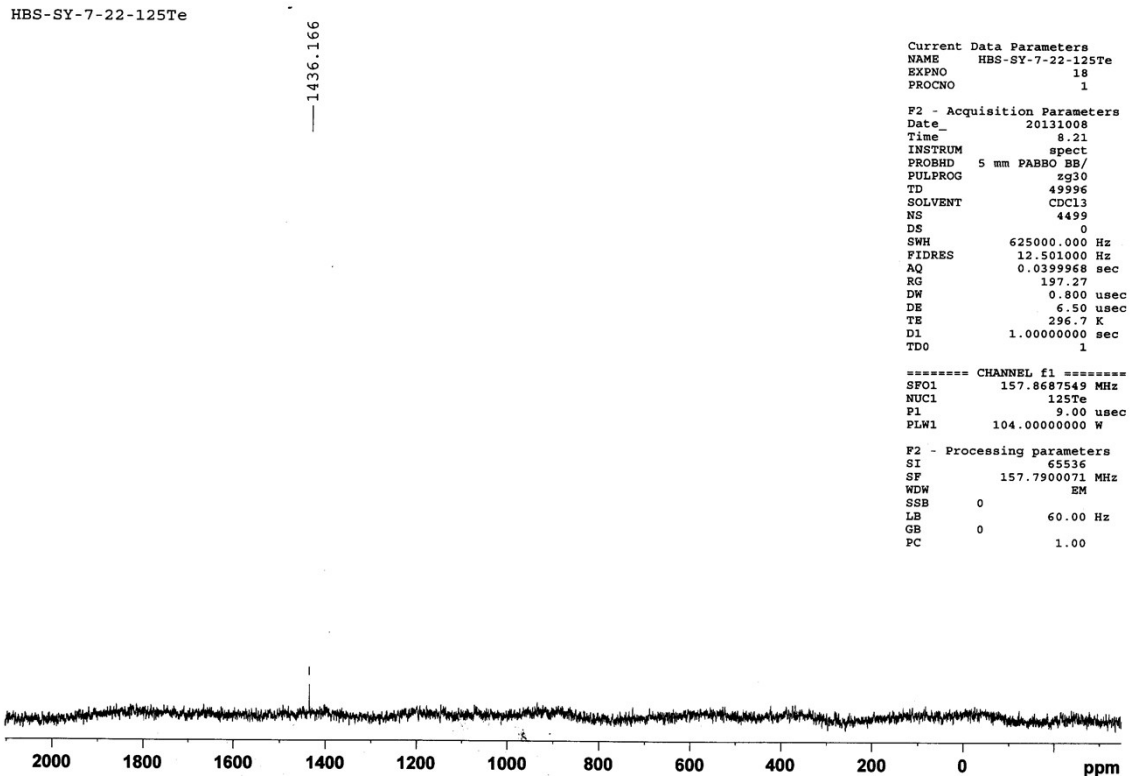


Figure S21. ^{125}Te NMR spectrum of compound **11a**.

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
Analysed : 10/12/2012 14:30
Sample ID : SY-5-4 (# 20)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 10/12/2012 16:55
Instrument N. : Instrument #1
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**.

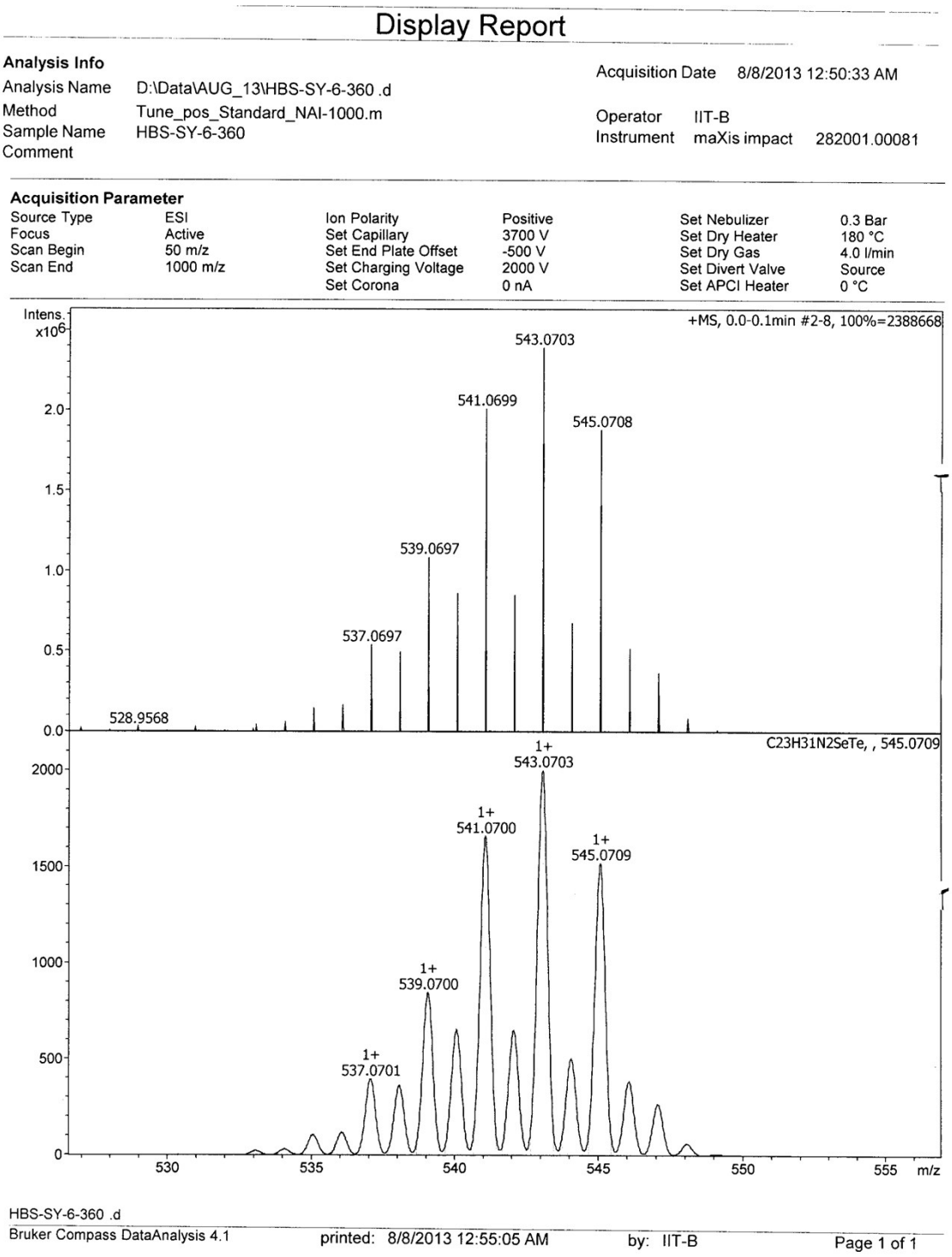


Figure S23. ESI-MS spectrum of compound **11a**.

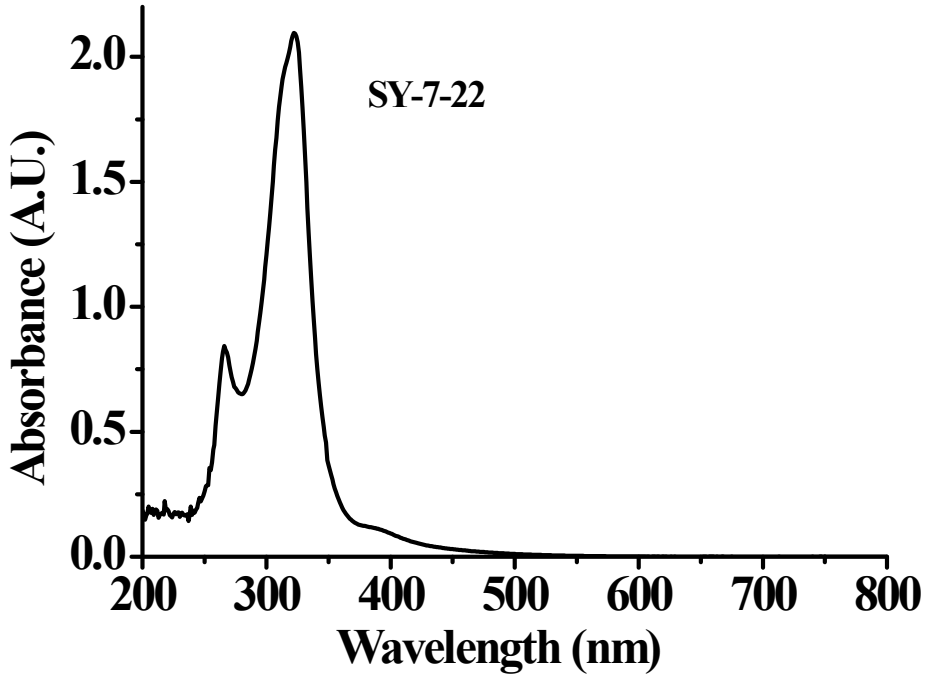


Figure S24. UV-Visible spectrum of compound **11a**.

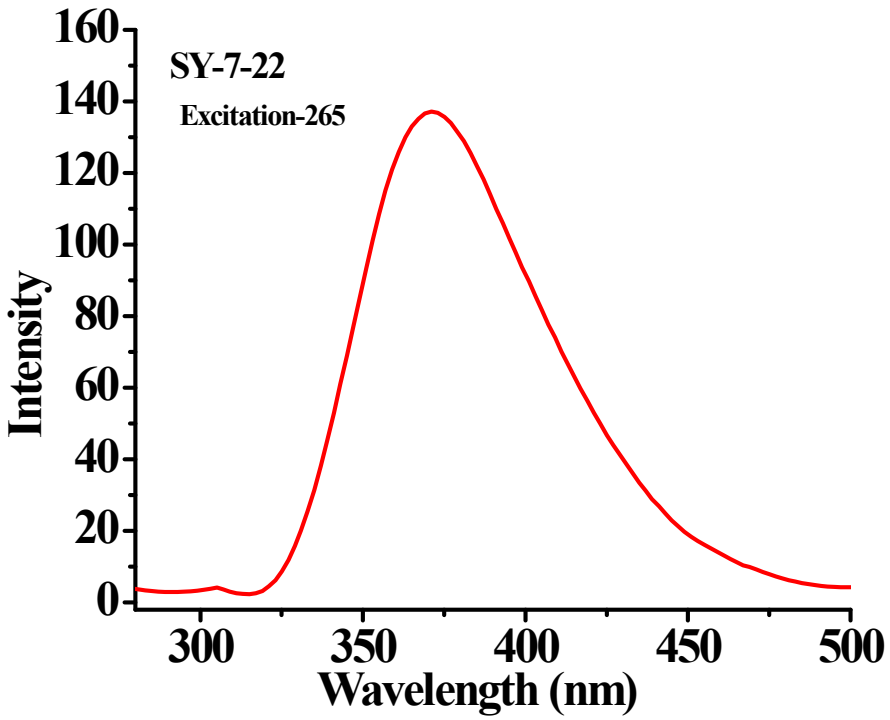


Figure S25. Emission spectrum of compound **11a**.

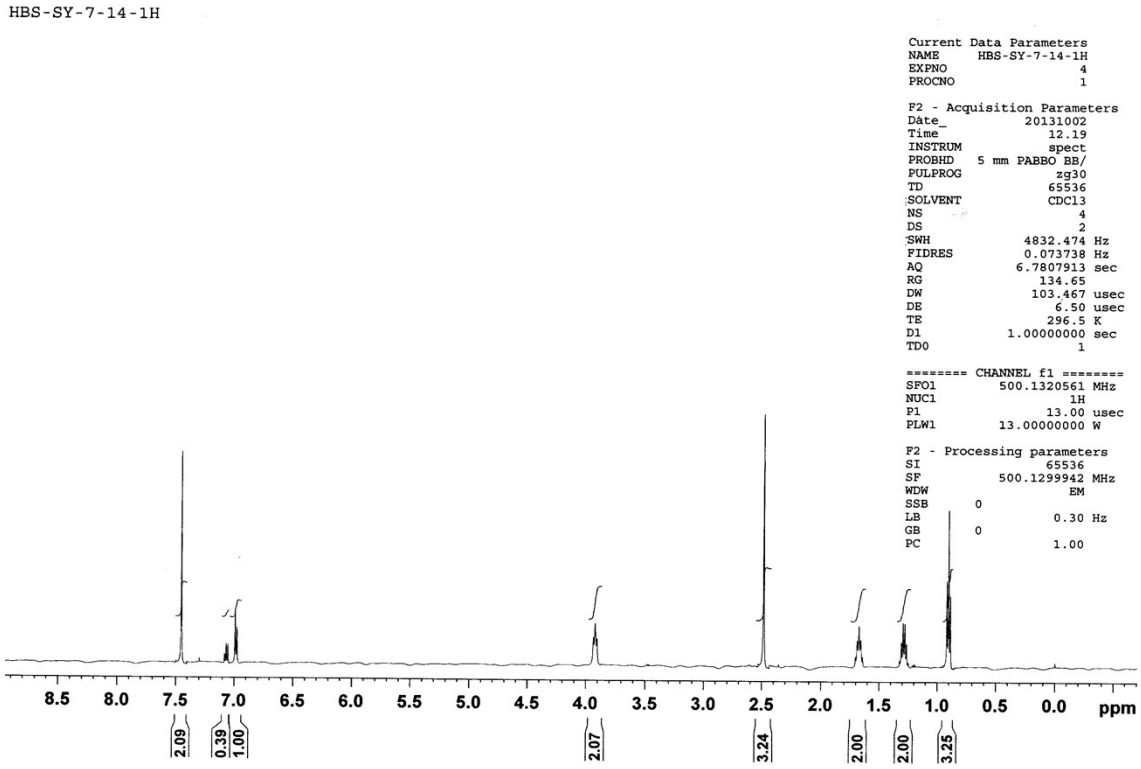


Figure S26. ^{1}H NMR spectrum of compound **11b**.

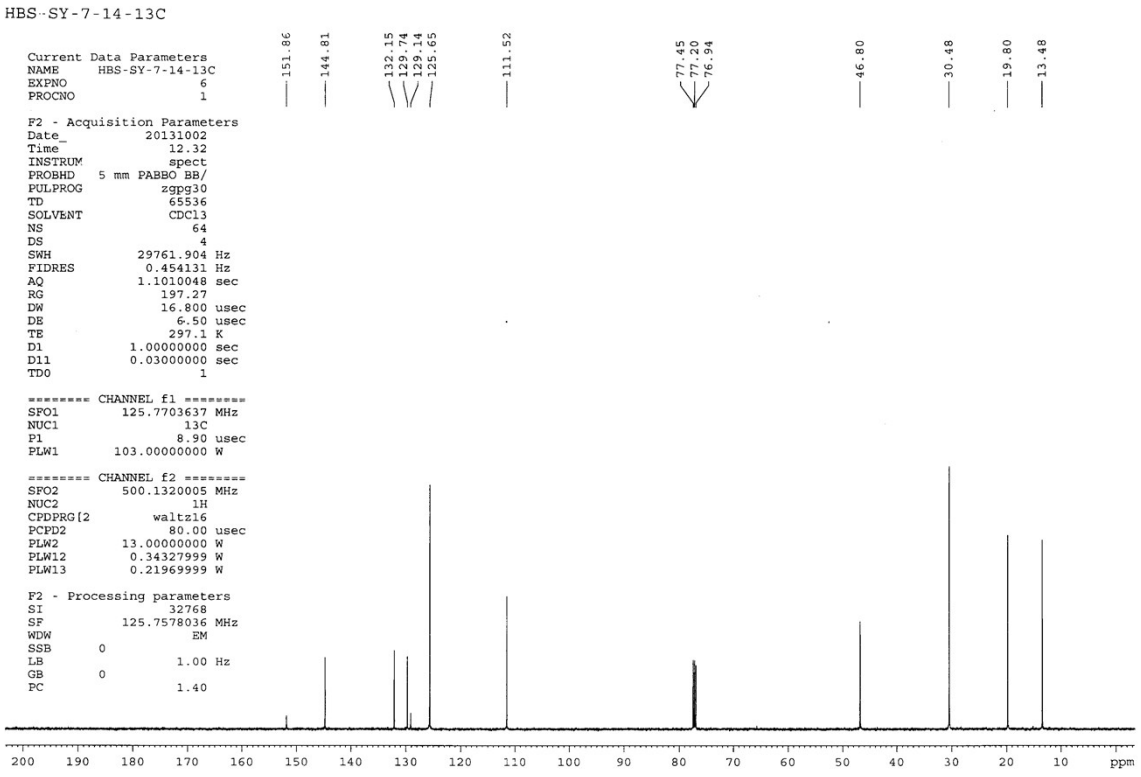


Figure S27. ^{13}C NMR spectrum of compound **11b**.

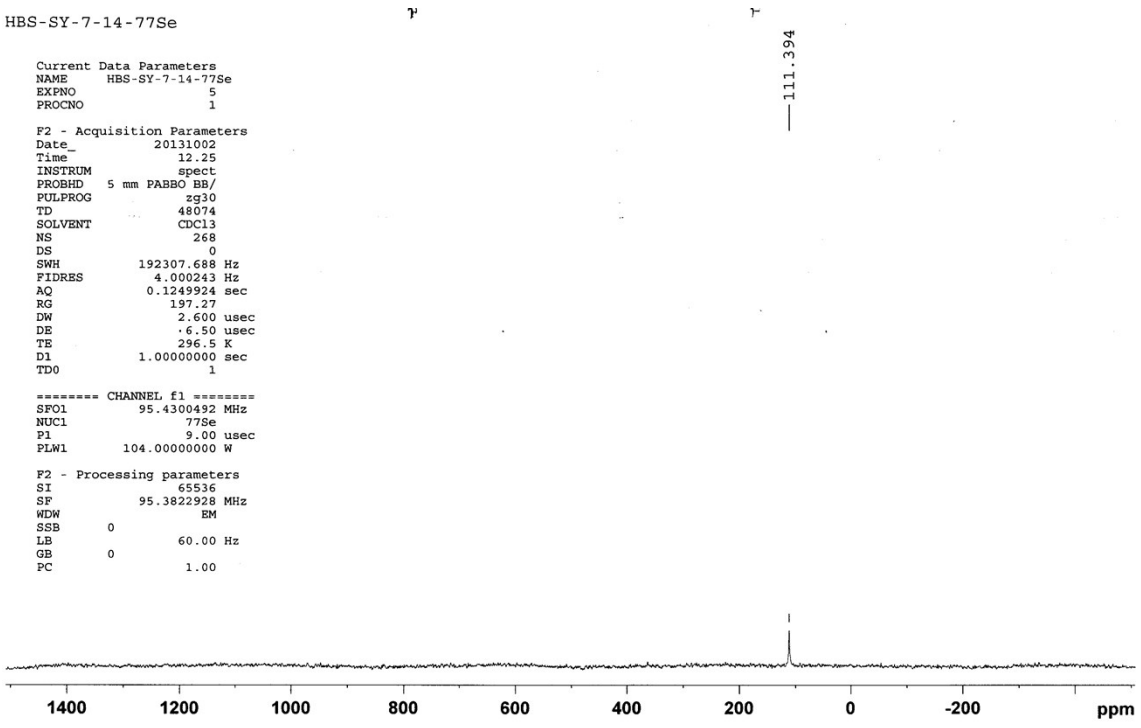


Figure S28. ^{77}Se NMR spectrum of compound **11b**.

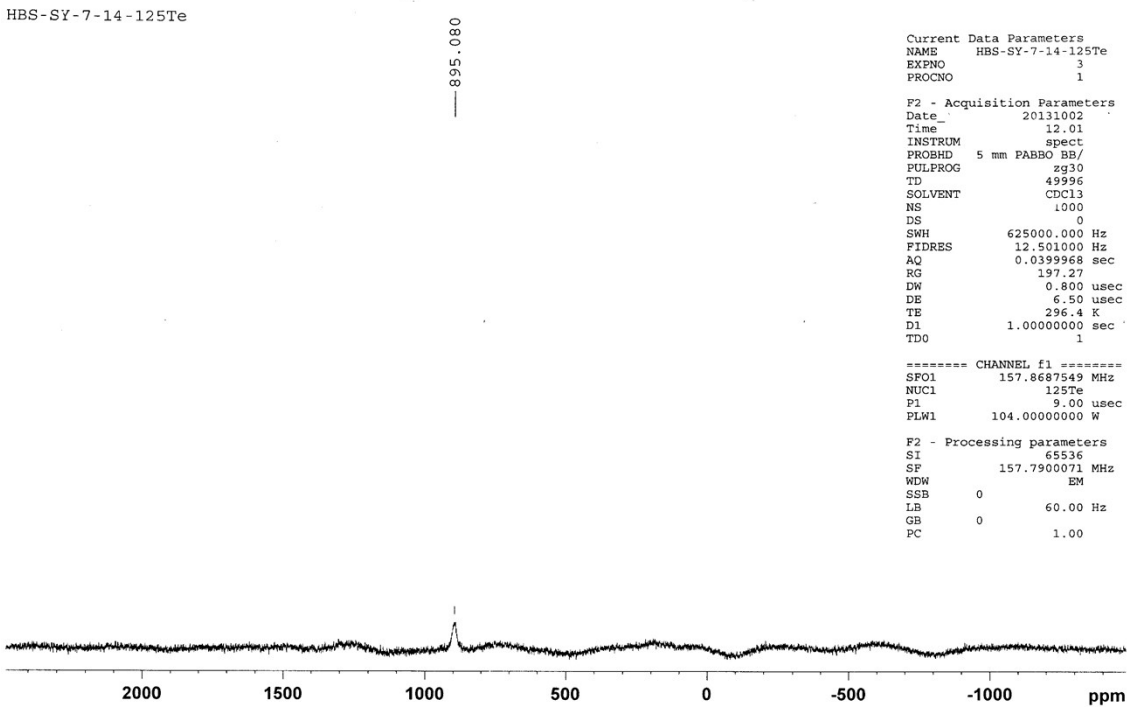
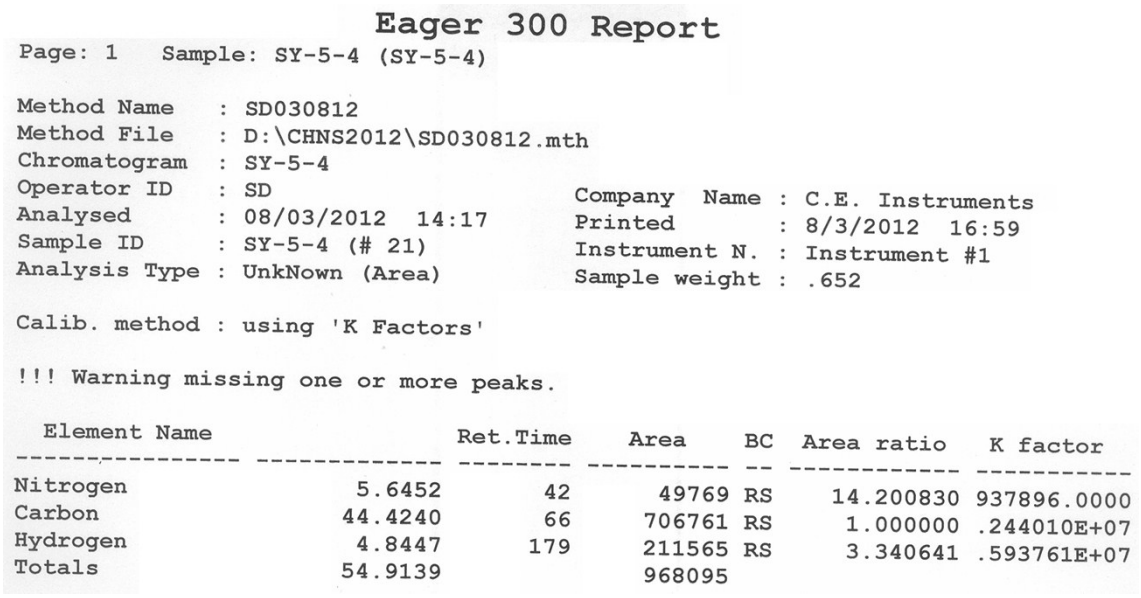


Figure S29. ^{125}Te NMR spectrum of compound **11b**.



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
Analysed : 08/03/2012 14:17
Sample ID : SY-5-4 (# 21)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 8/3/2012 16:59
Instrument N. : Instrument #1
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	49769	RS	14.200830	937896.0000
Carbon	44.4240	706761	RS	1.000000	.244010E+07
Hydrogen	4.8447	211565	RS	3.340641	.593761E+07
Totals	54.9139	968095			

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

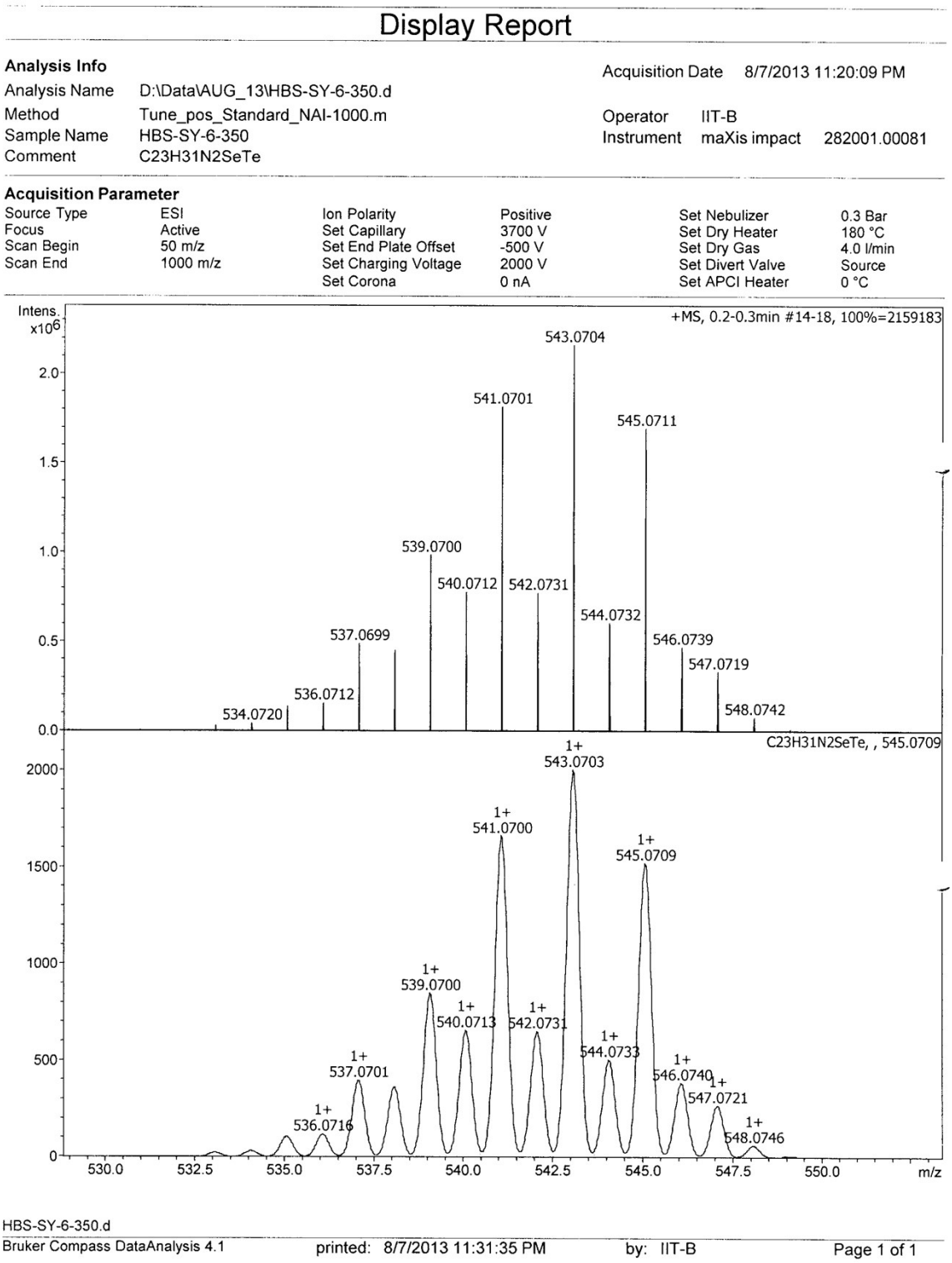


Figure S31. ESI-MS spectrum of compound **11b**.

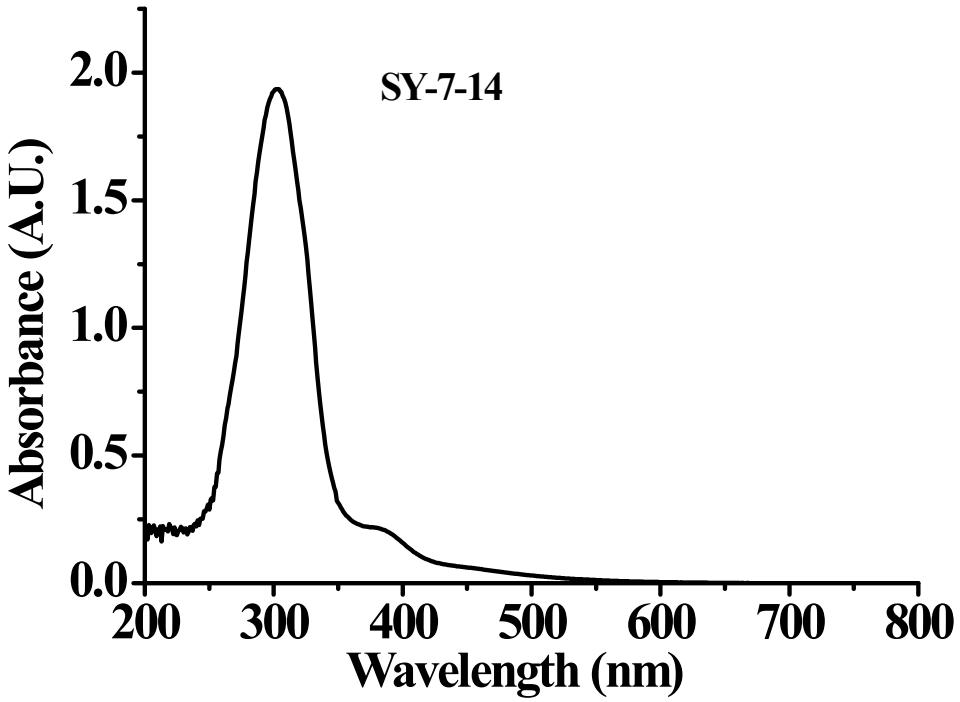


Figure S32. UV-Visible spectrum of compound **11b**.

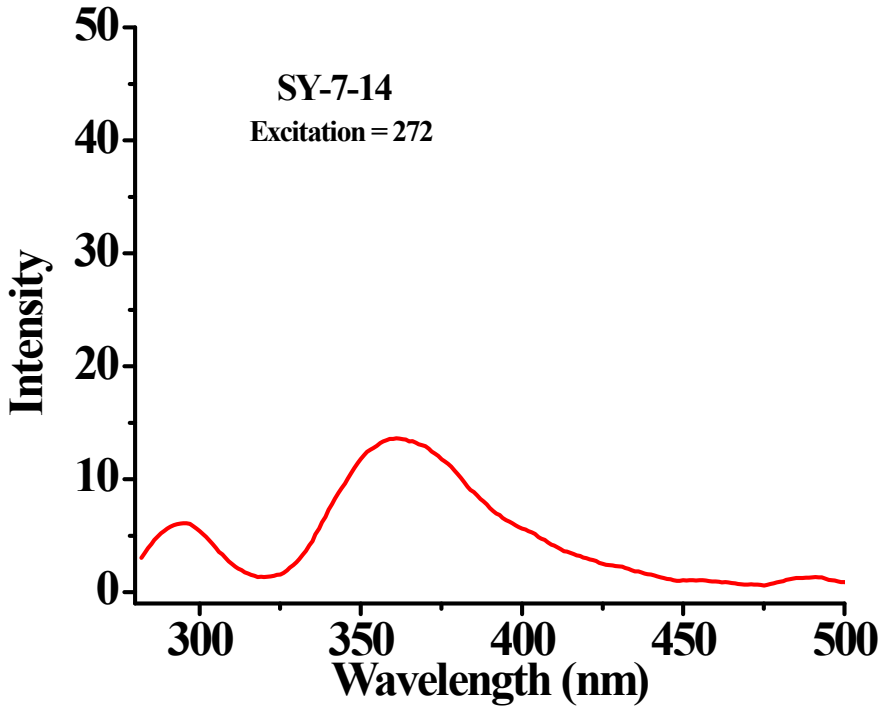


Figure S33. Emission spectrum of compound **11b**.

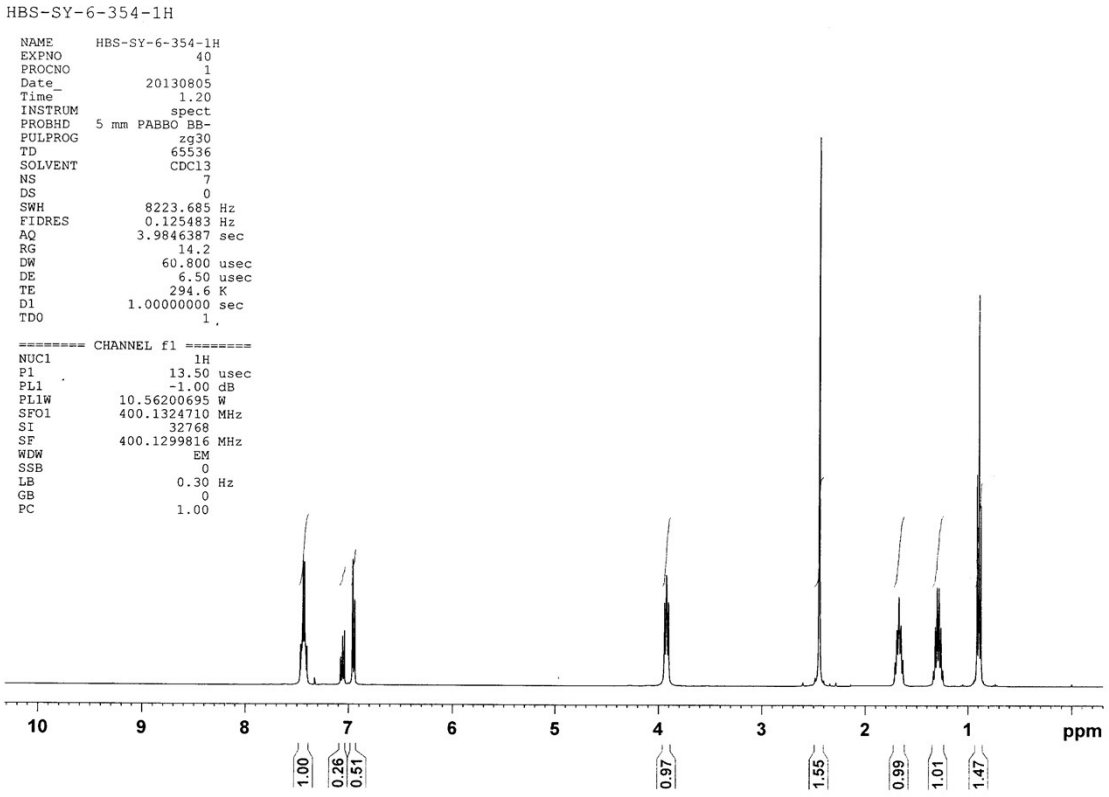


Figure S34. ^{1}H NMR spectrum of compound **11c**.

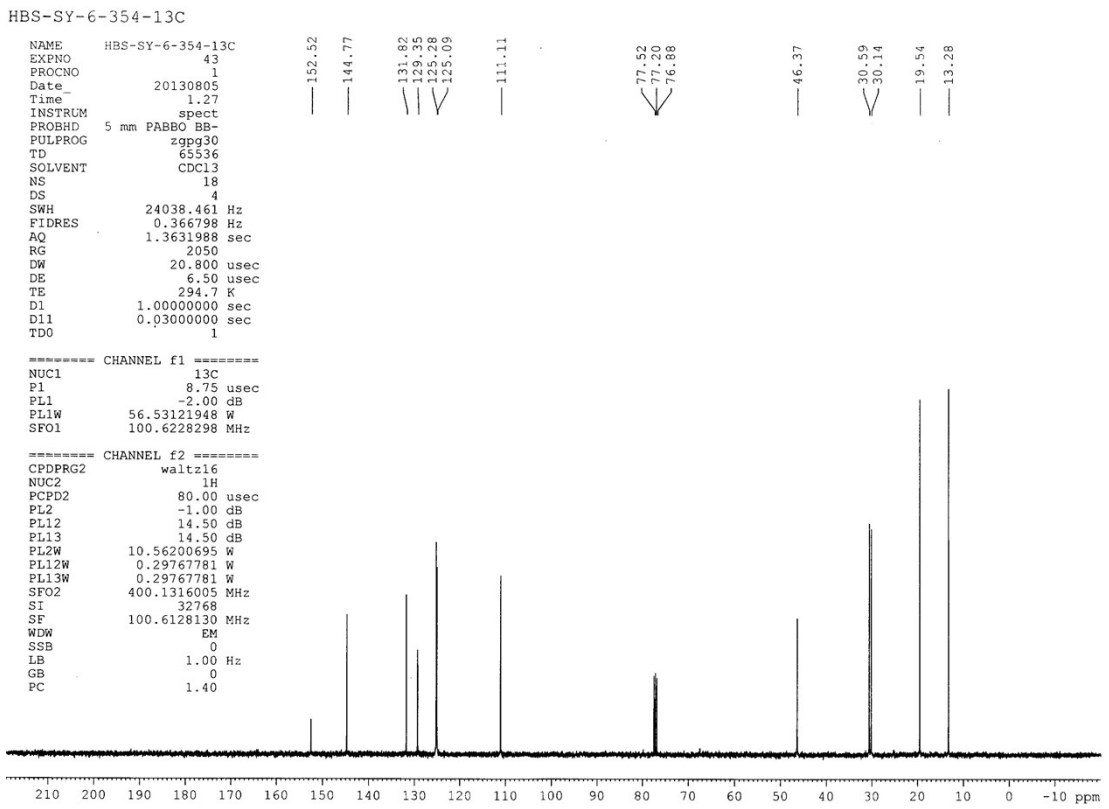


Figure S35. ^{13}C NMR spectrum of compound **11c**.

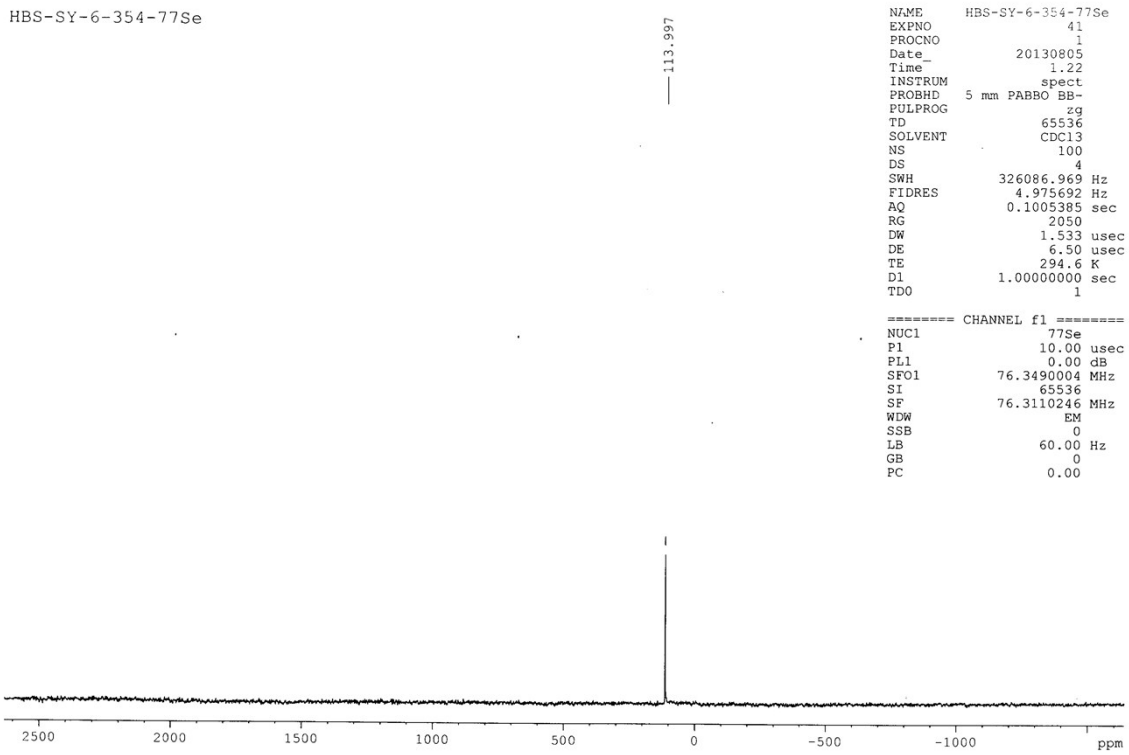


Figure S36. ^{77}Se NMR spectrum of compound **11c**.

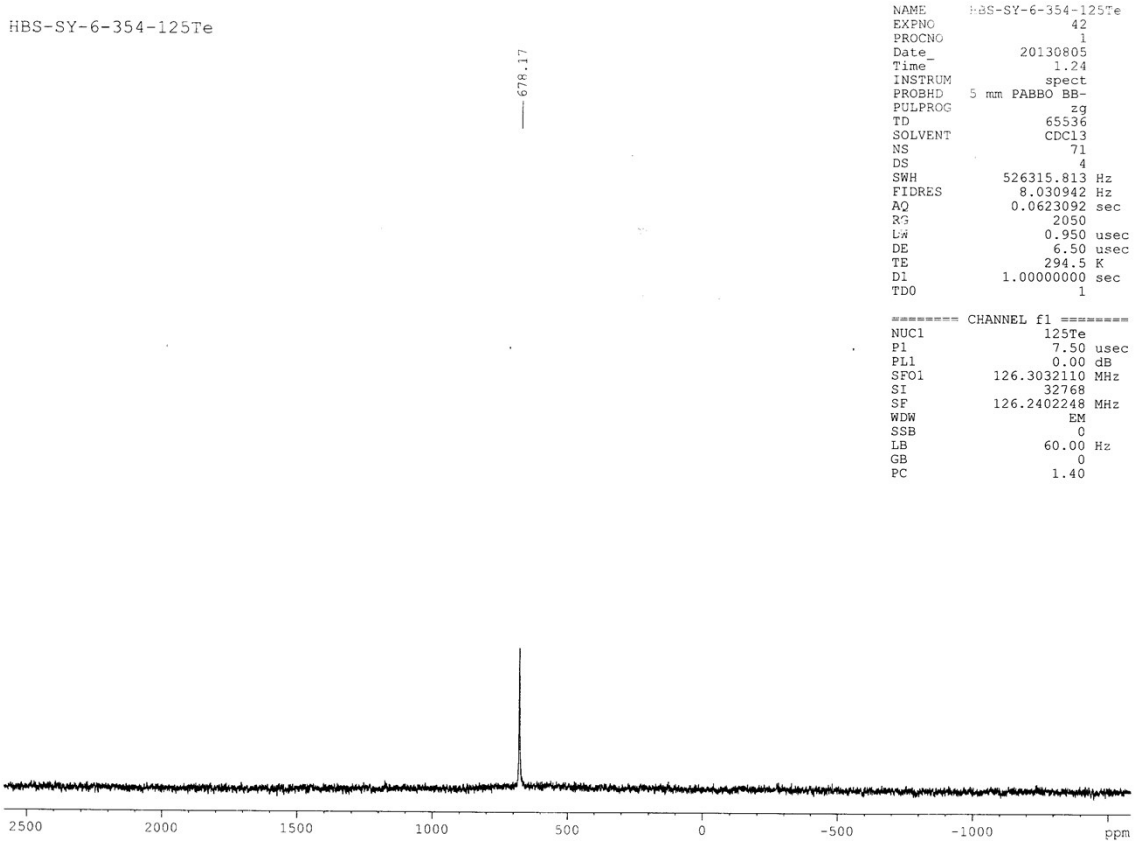


Figure S37. ^{125}Te NMR spectrum of compound **11c**.

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**.

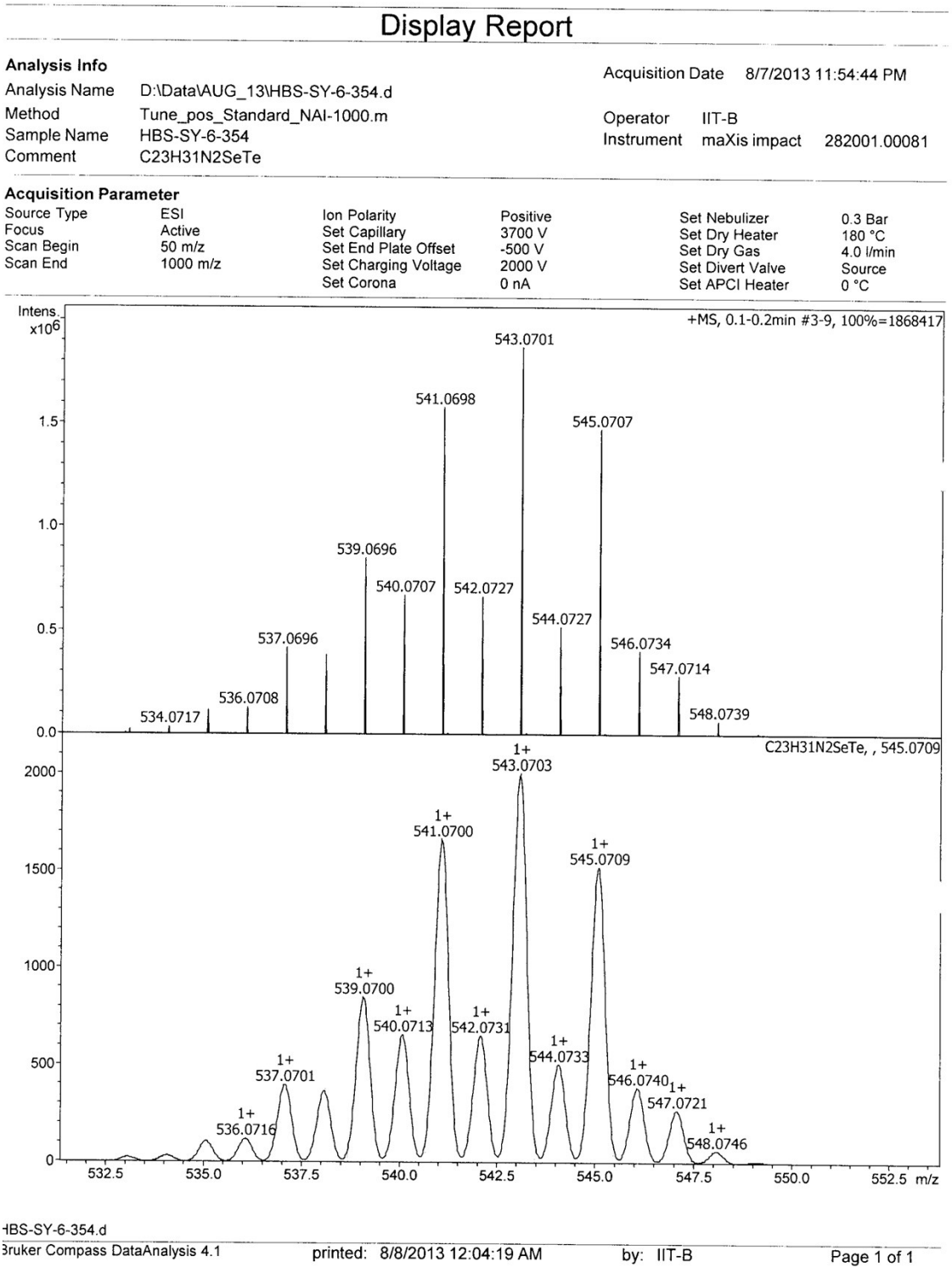


Figure S39. ESI-MS spectrum of compound **11c**.

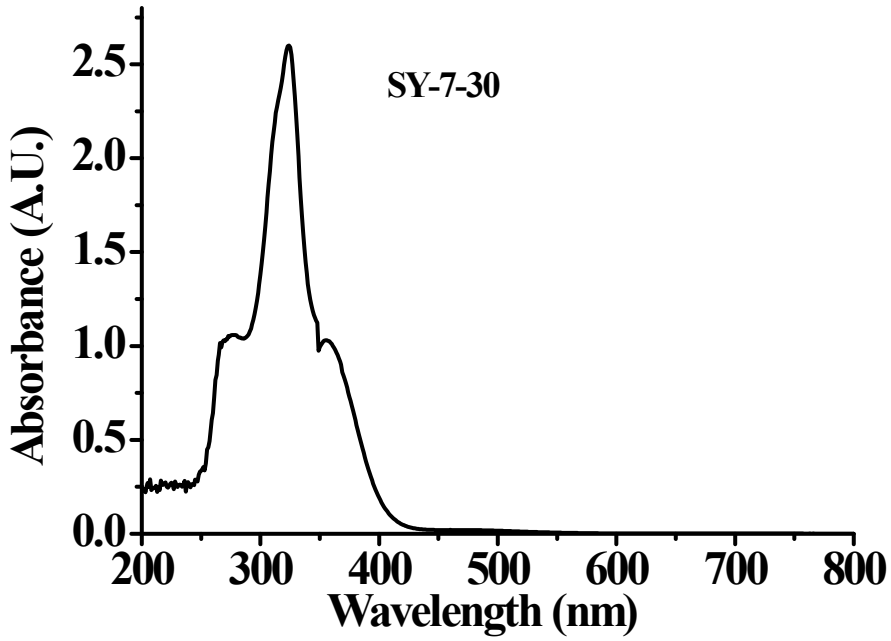


Figure S40. UV-Visible spectrum of compound **11c**.

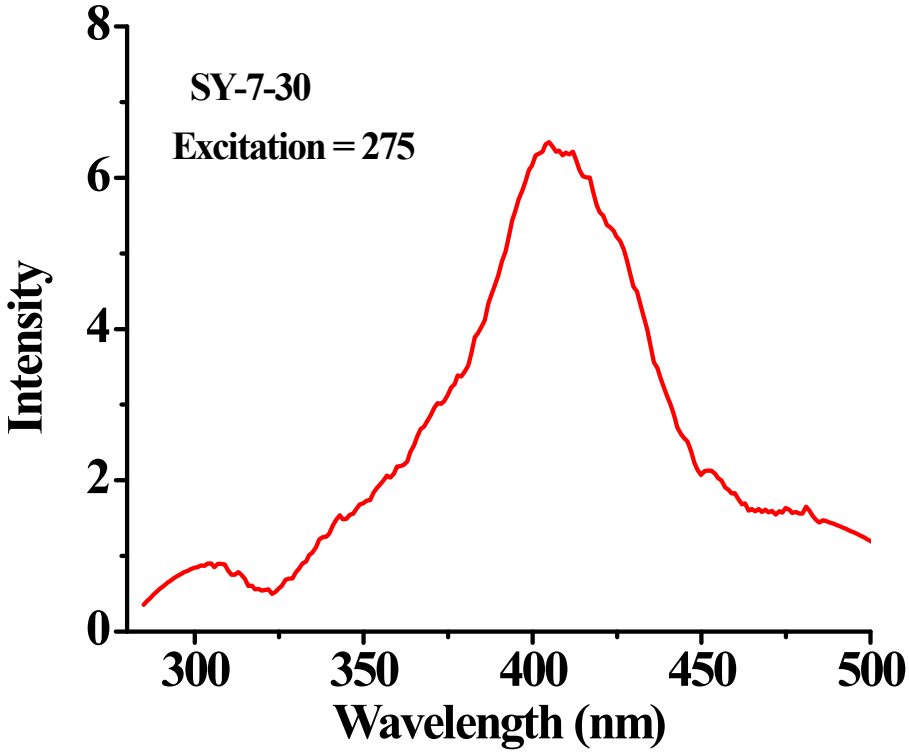


Figure S41. Emission spectrum of compound **11c**.

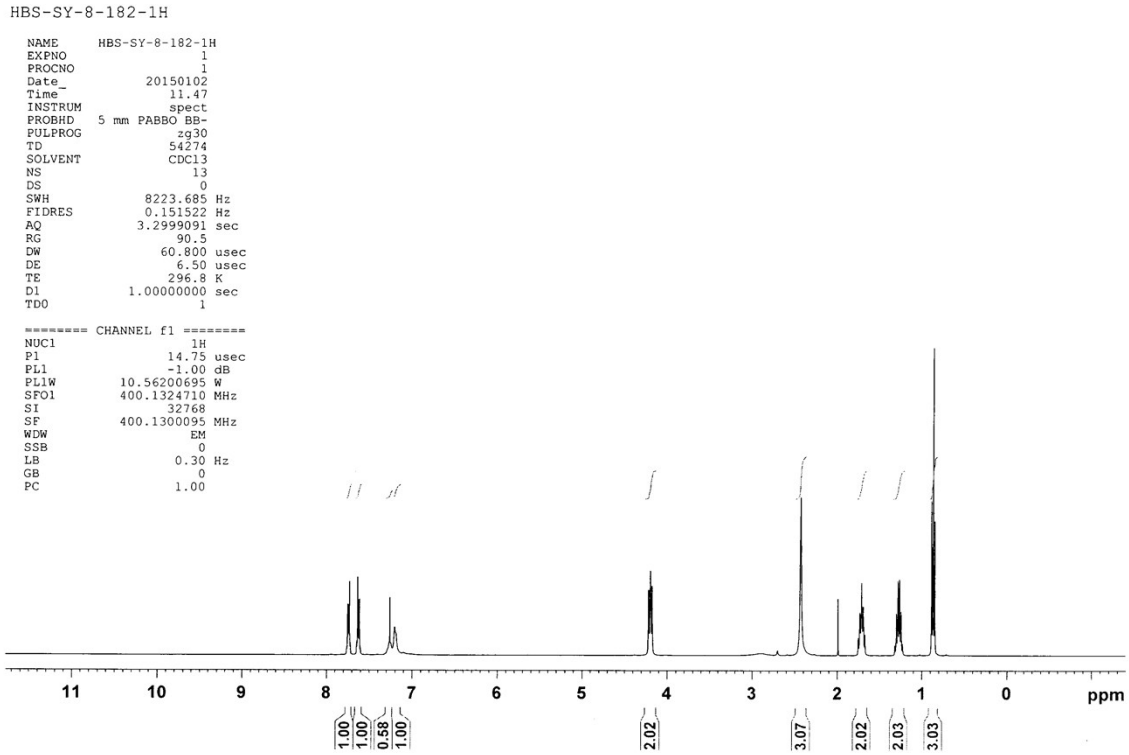


Figure S42. ^{1}H NMR spectrum of compound **15**.

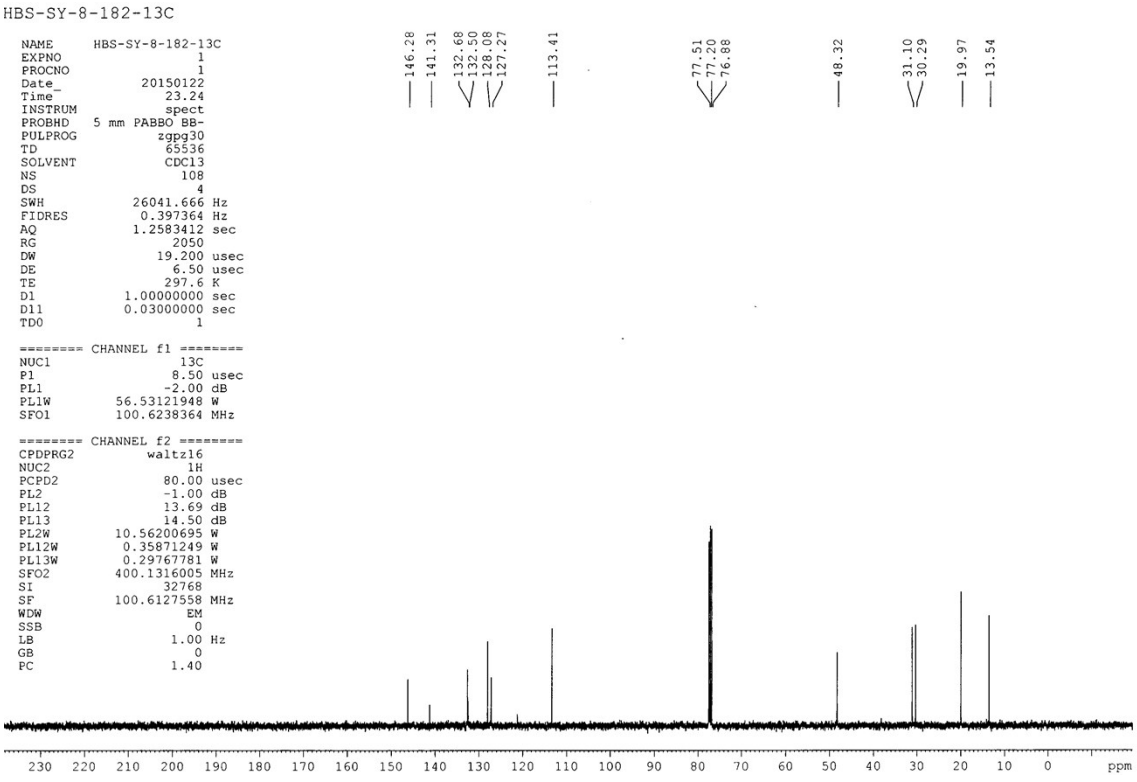


Figure S43. ^{13}C NMR spectrum of compound **15**.

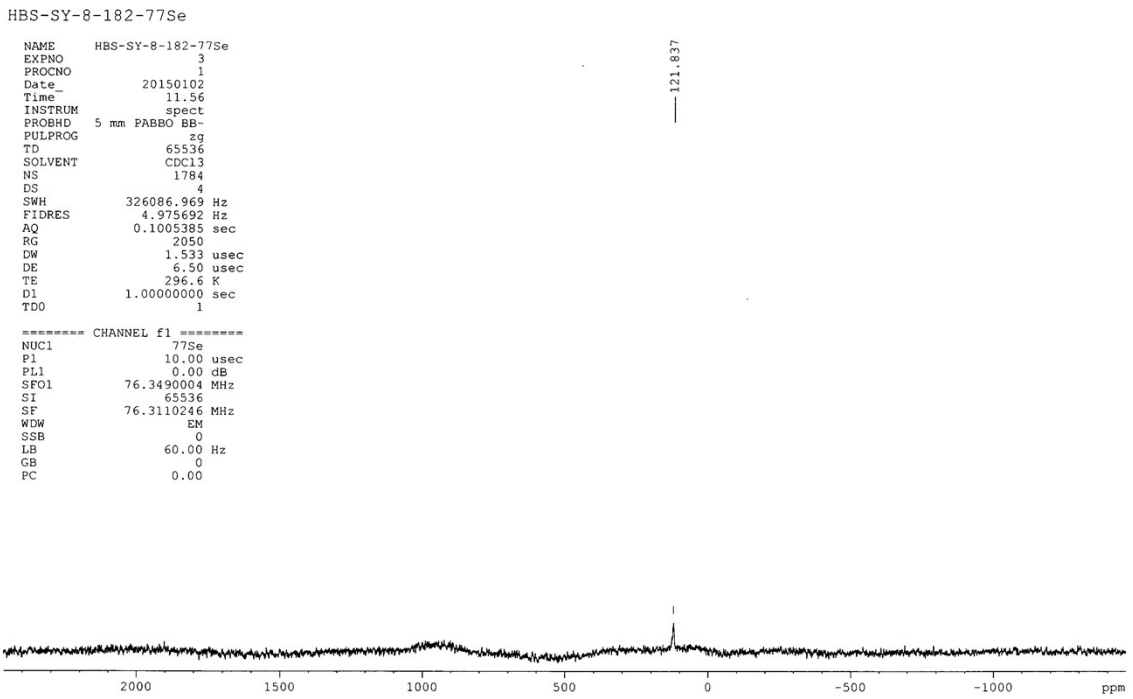


Figure S44. ^{77}Se NMR spectrum of compound **15**.

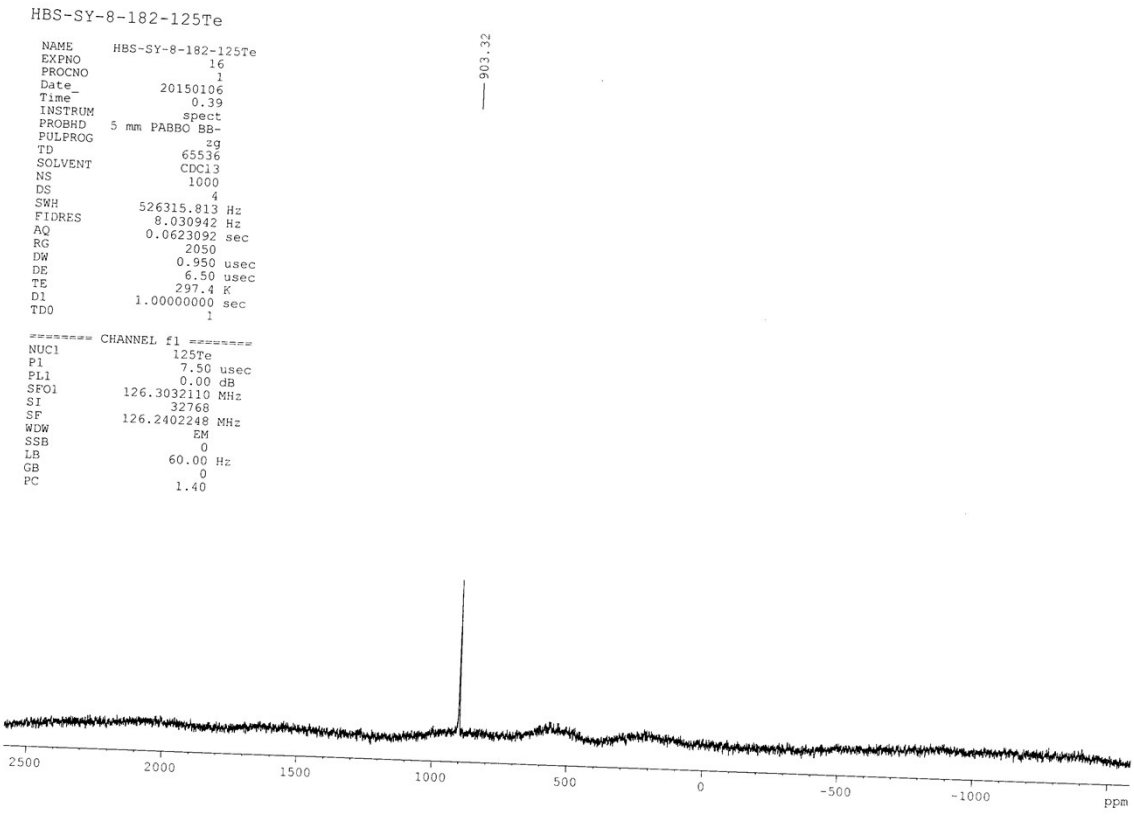


Figure S45. ^{125}Te NMR spectrum of compound **15**.

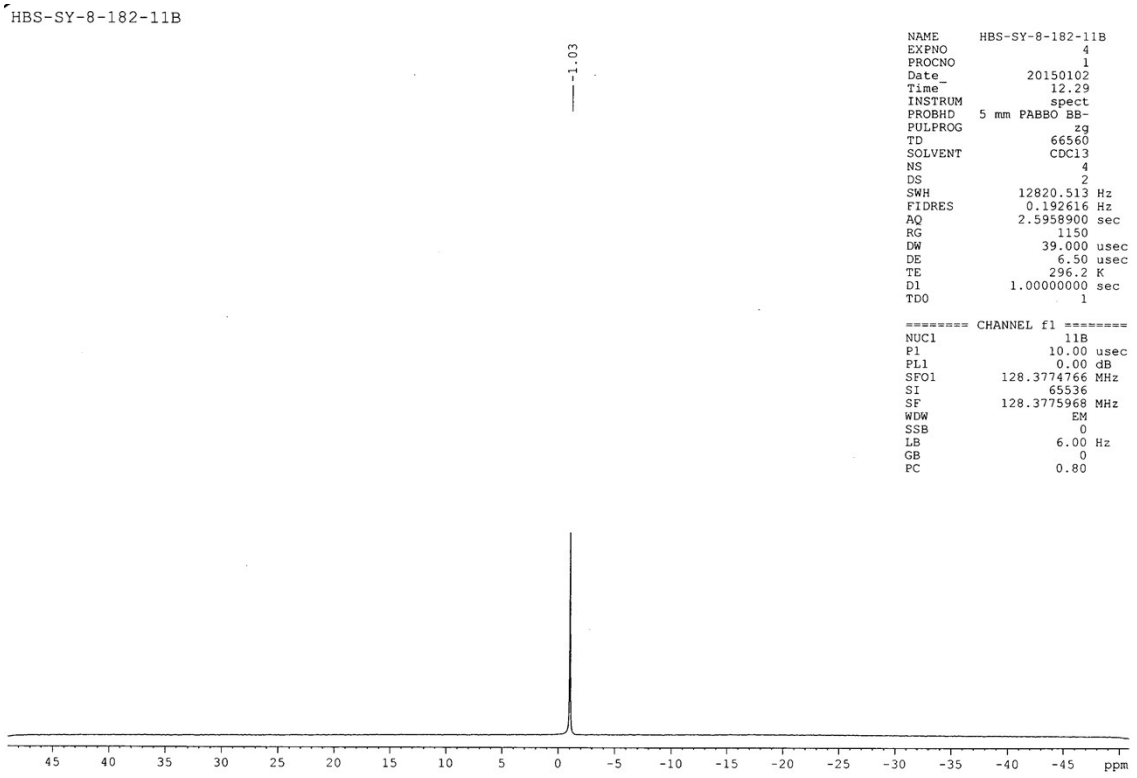


Figure S46. ^{15}B NMR spectrum of compound **15**.

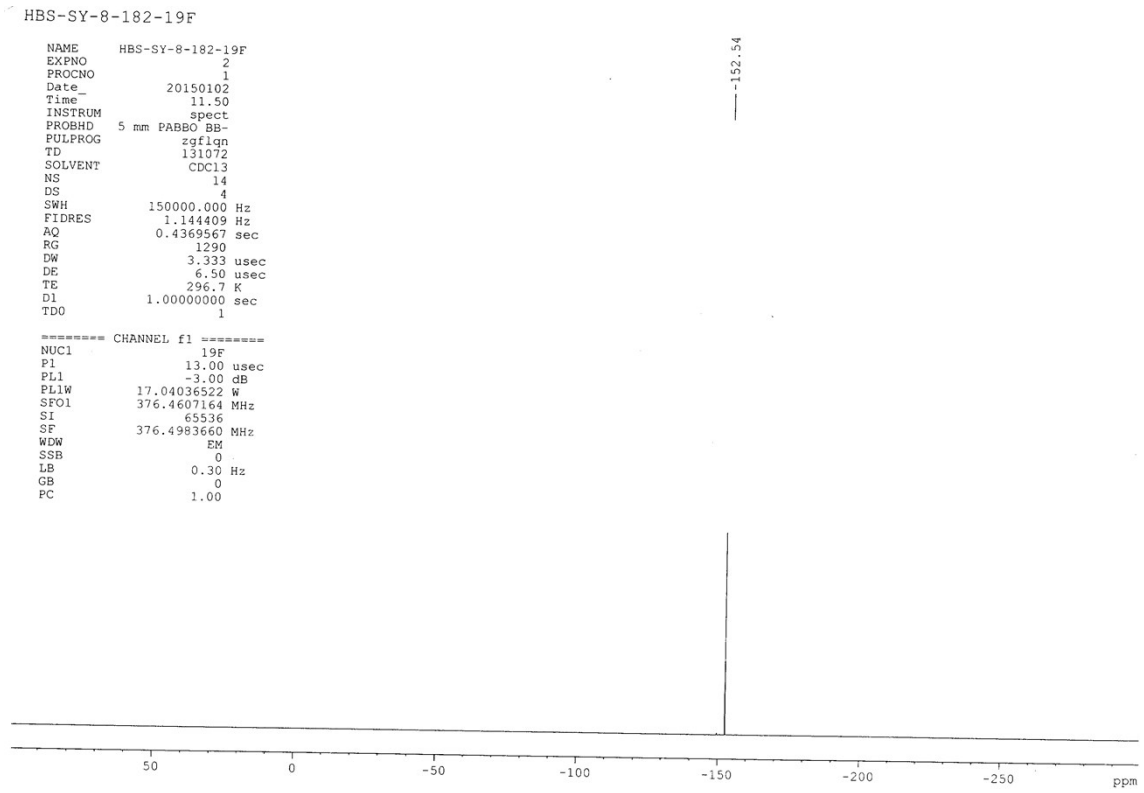


Figure S47. ^{19}F NMR spectrum of compound **15**.

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**.

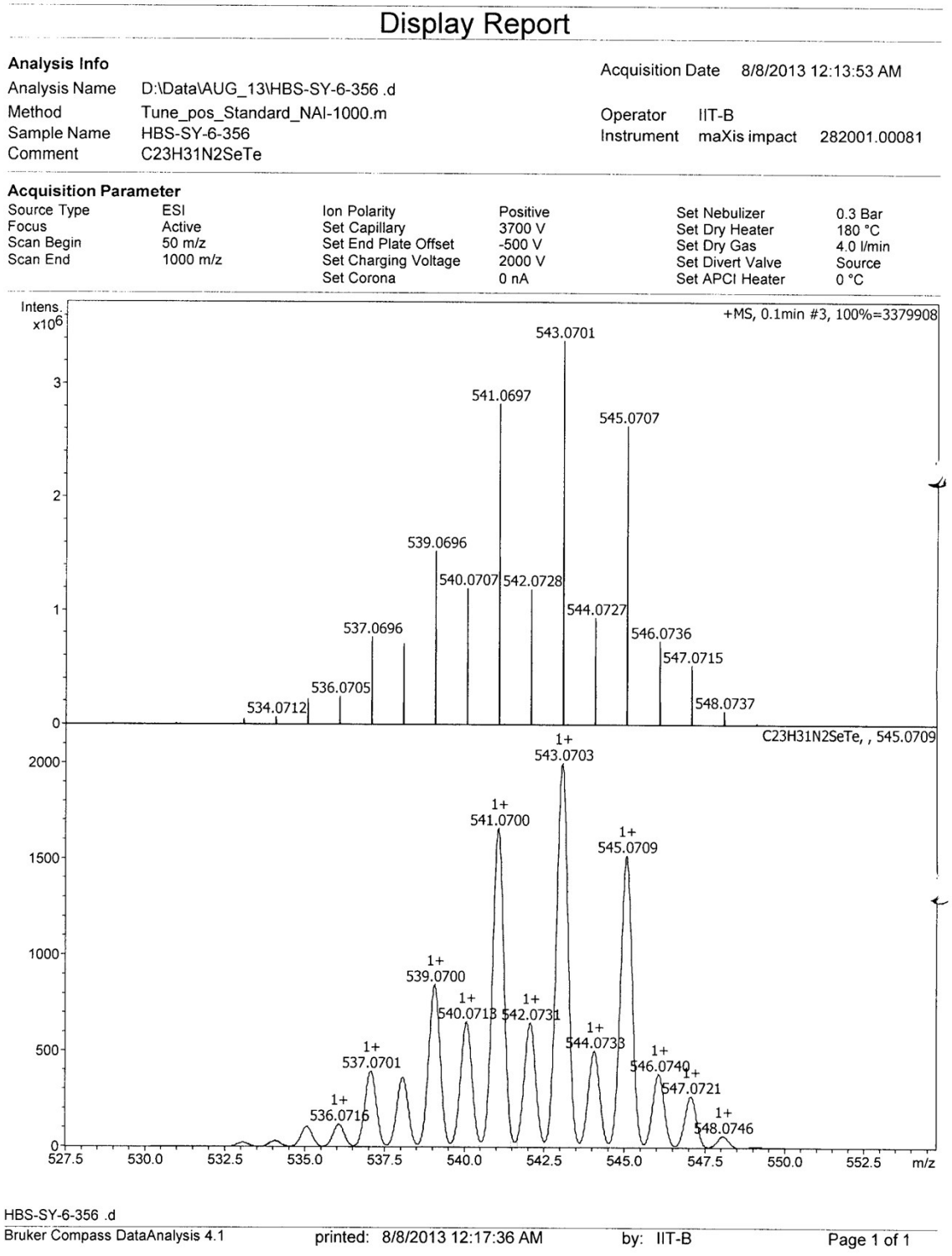


Figure S49. ESI-MS spectrum of compound **15**.

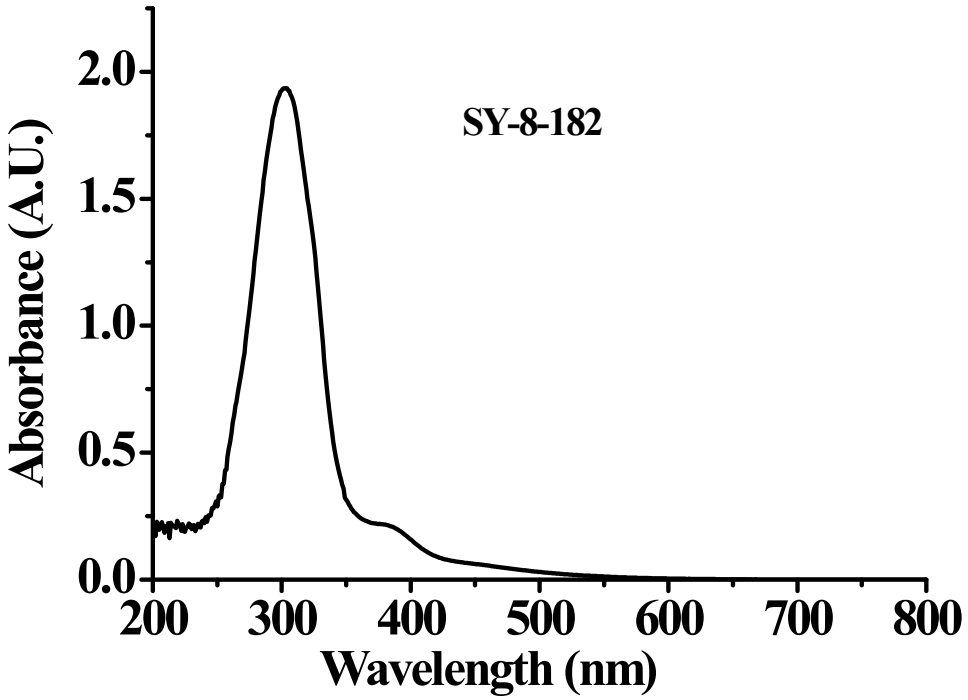


Figure S50. UV-Visible spectrum of compound **15**.

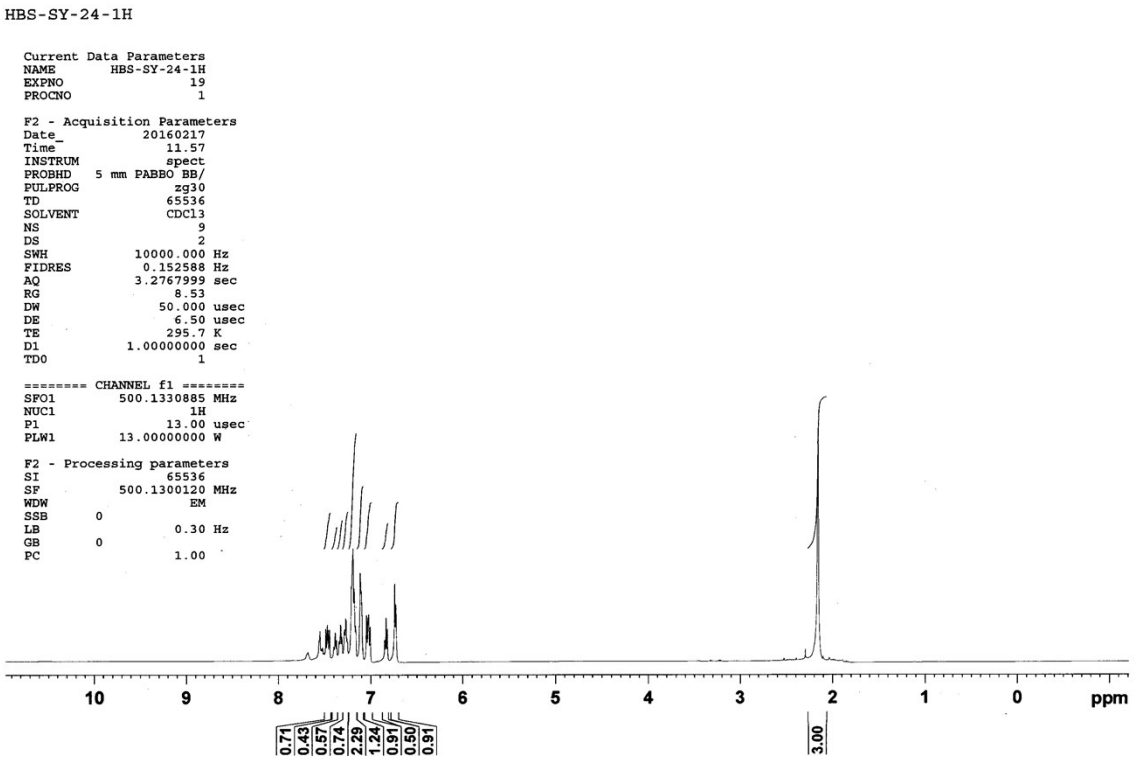


Figure S51. ^{1}H NMR spectrum of compound **16a**.

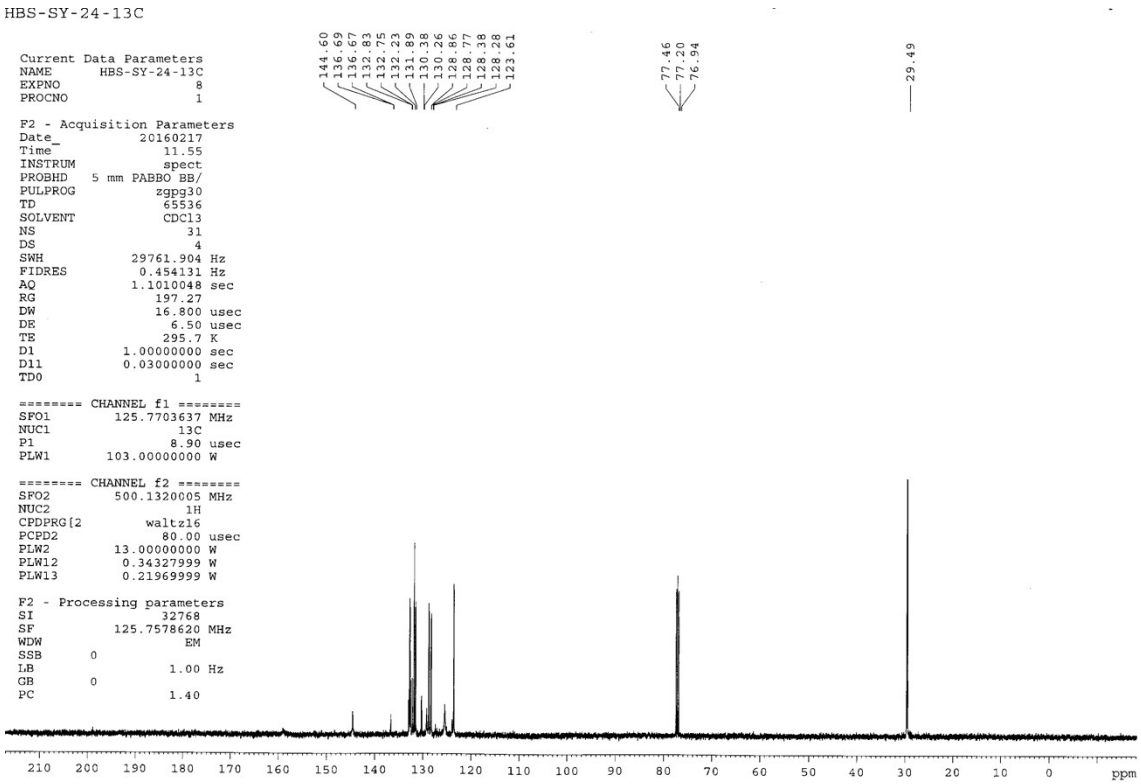


Figure S52. ^{13}C NMR spectrum of compound **16a**.

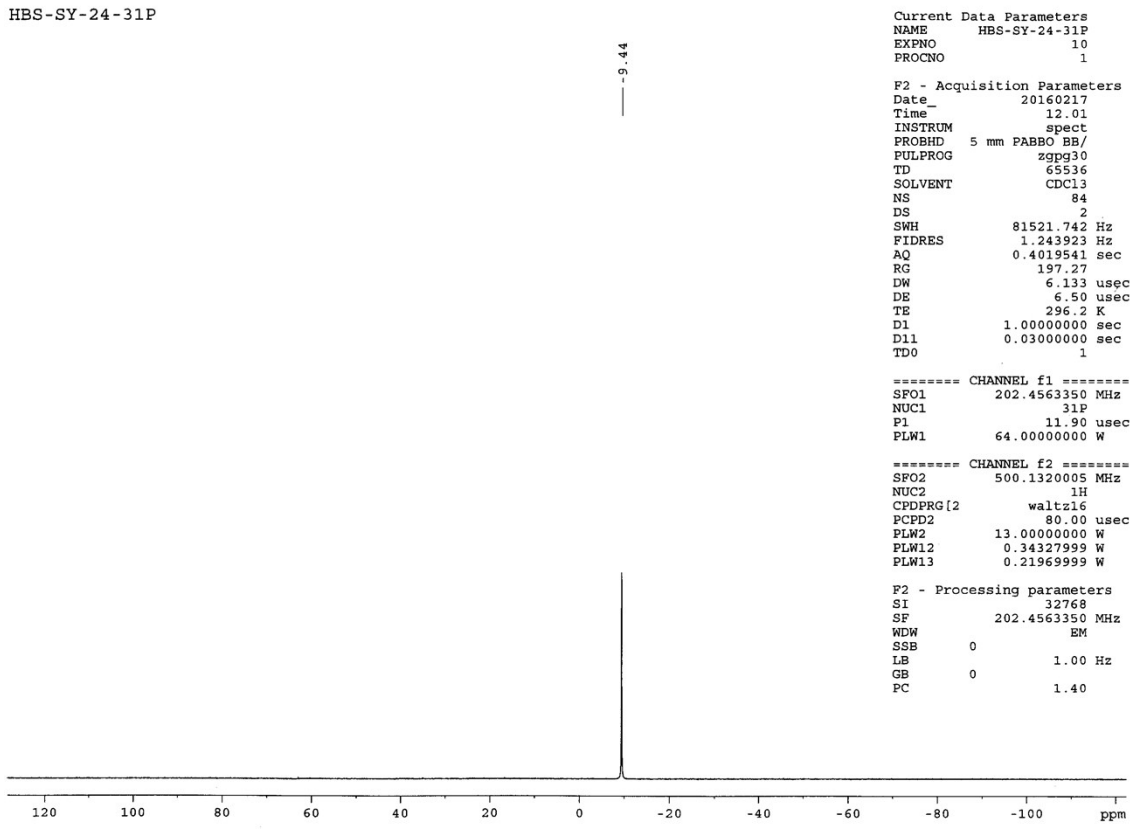


Figure S53. ^{31}P NMR spectrum of compound **16a**.

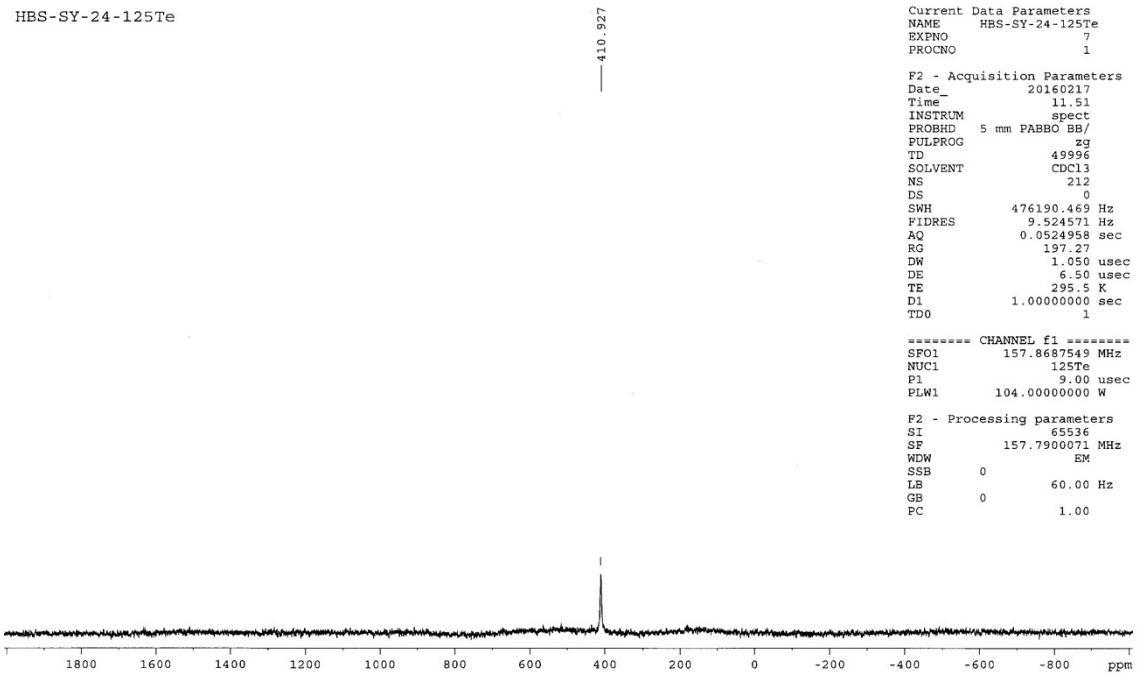


Figure S54. ^{125}Te NMR spectrum of compound **16a**.

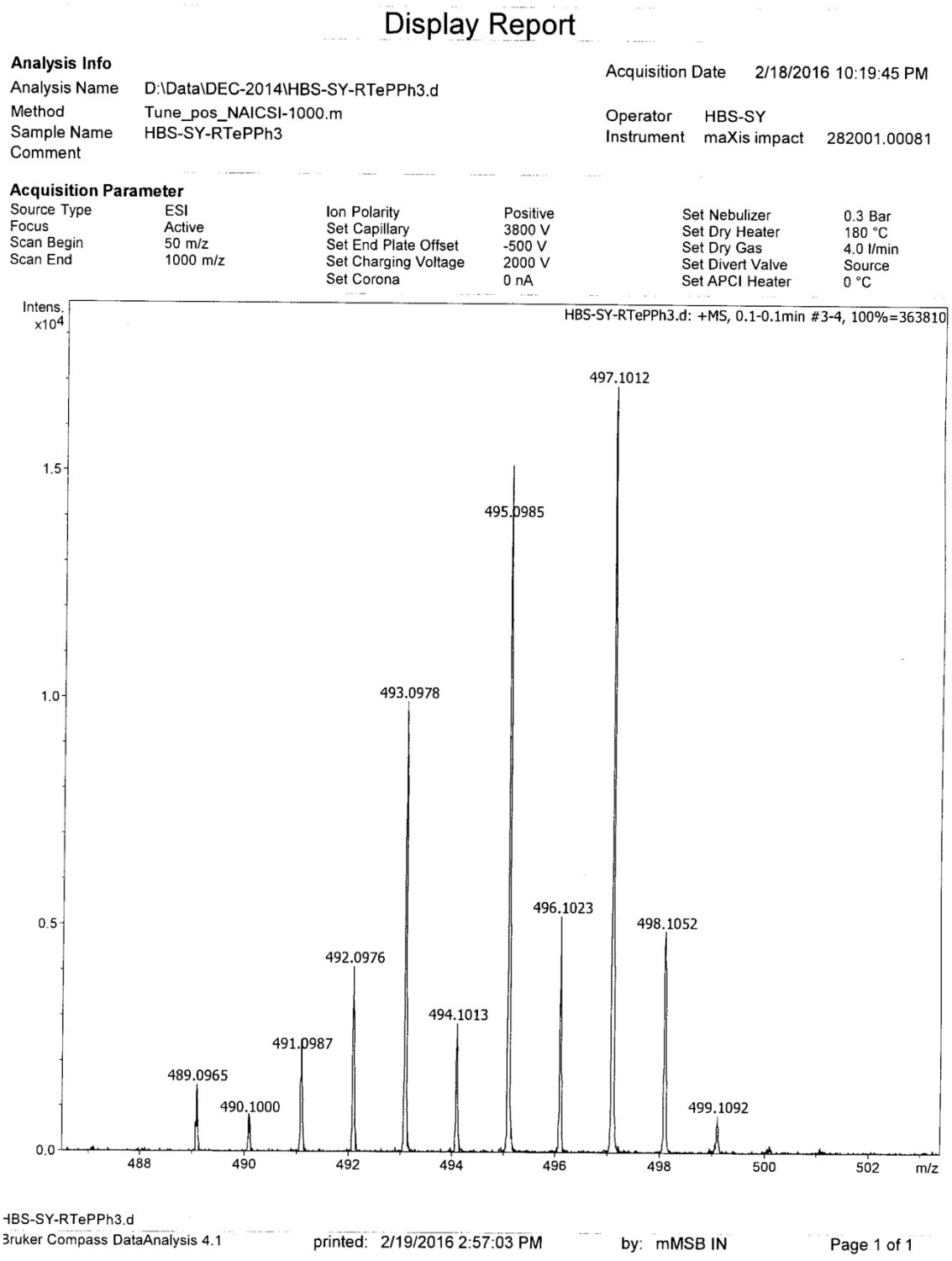


Figure S55. ESI-MS spectrum of compound **16a**.

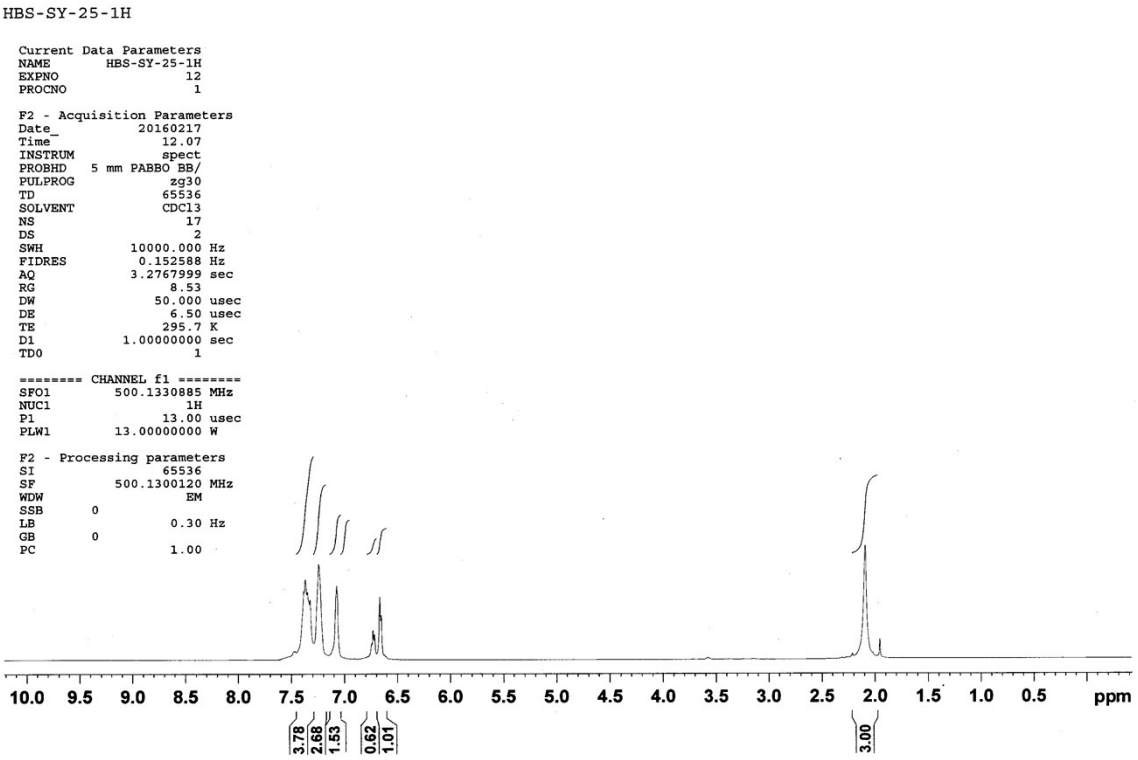


Figure S56. ^{1}H NMR spectrum of compound **16b**.

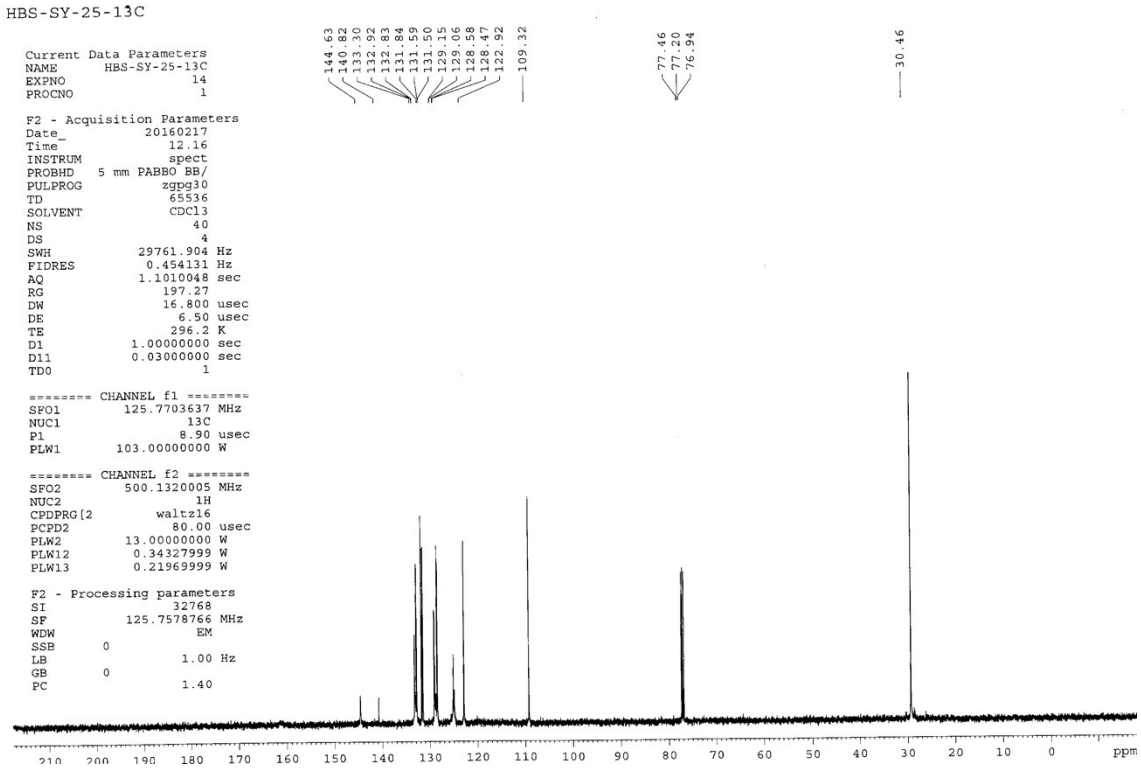


Figure S57. ^{13}C NMR spectrum of compound **16b**.

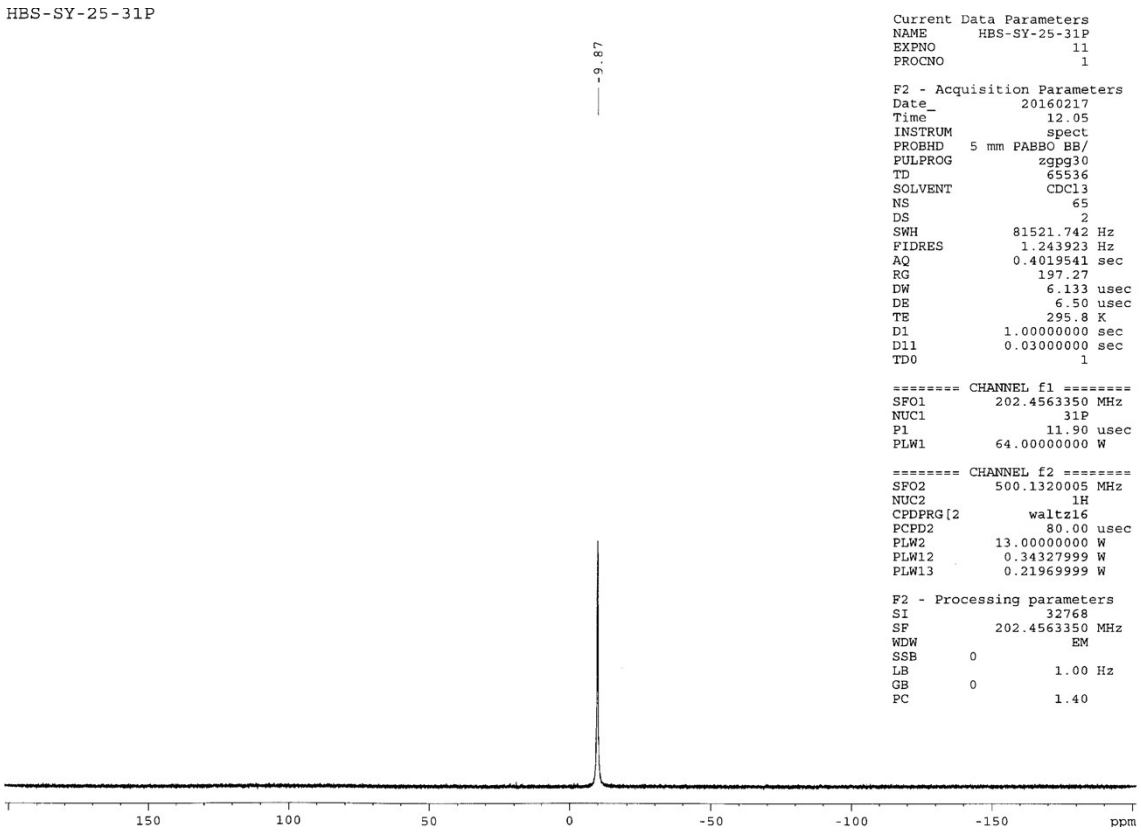


Figure S58. ^{31}P NMR spectrum of compound **16b**.

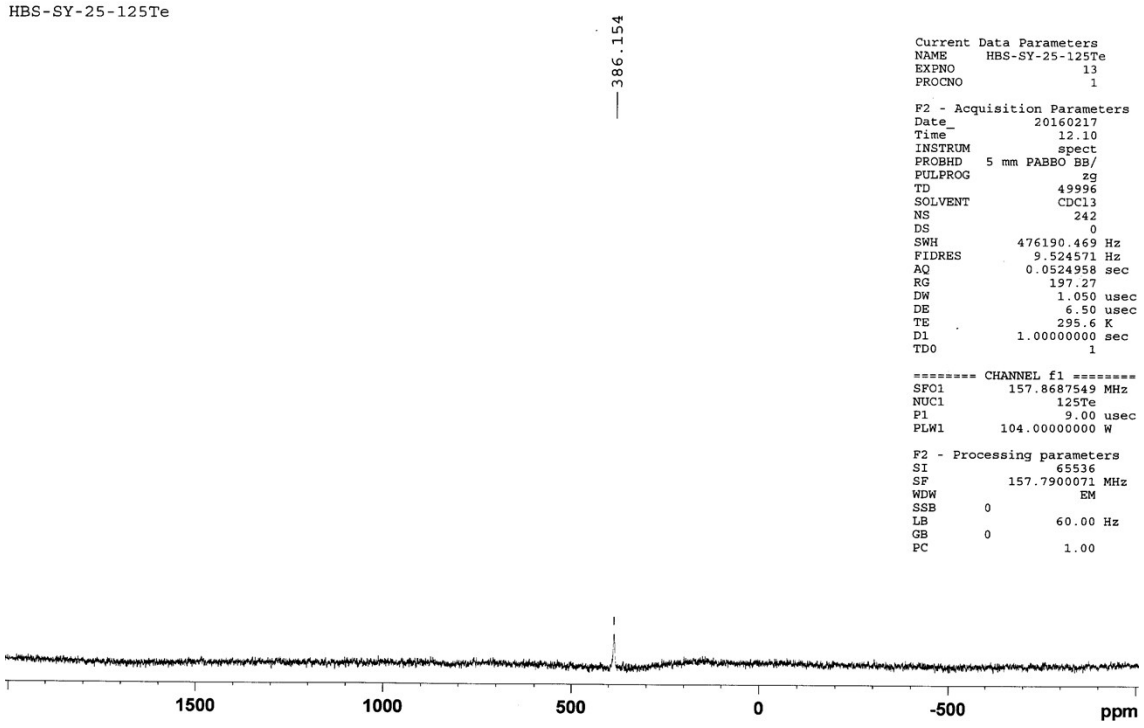


Figure S59. ^{125}Te NMR spectrum of compound **16b**.

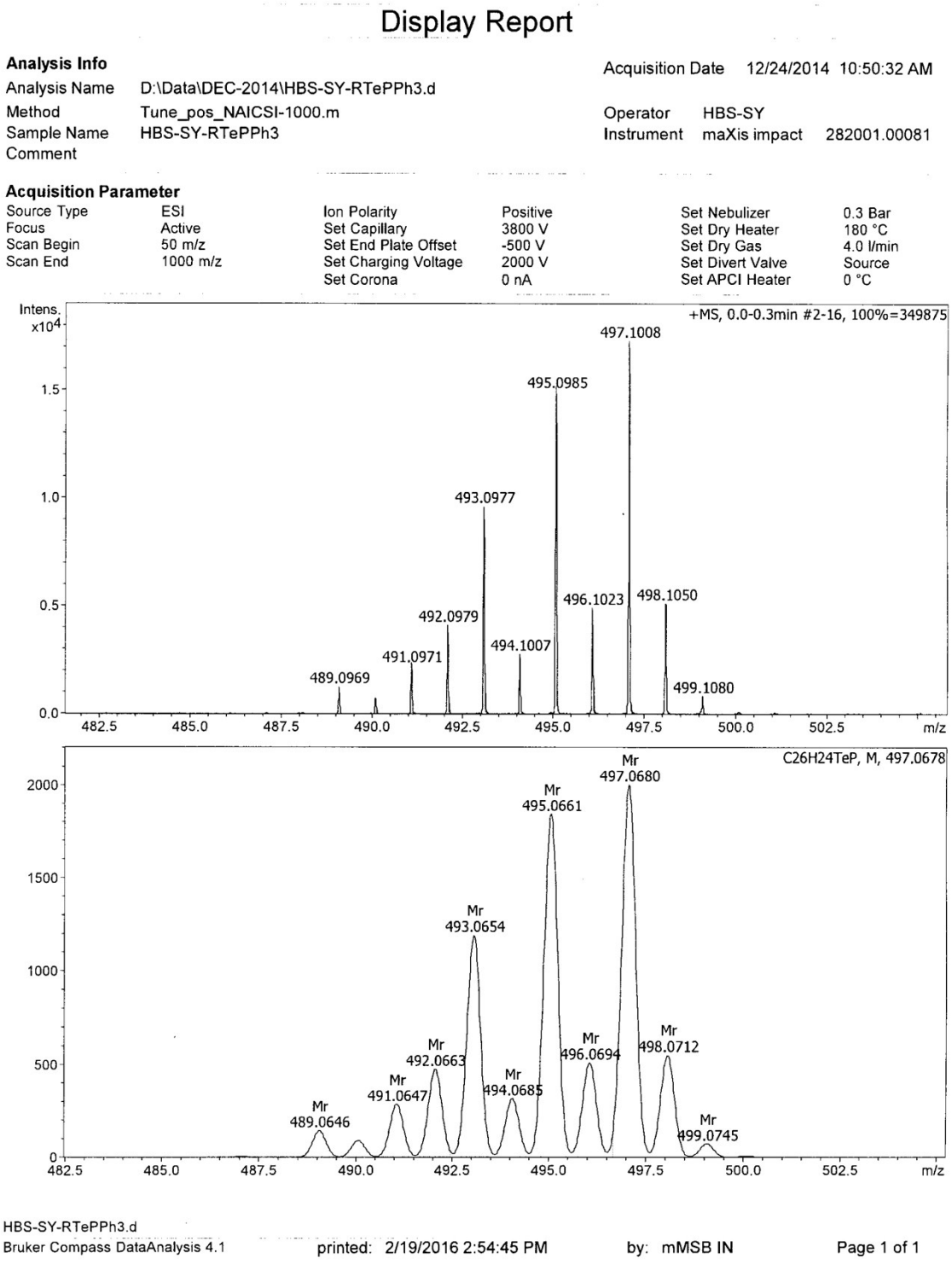


Figure S60. ESI-MS spectrum of compound **16b**.

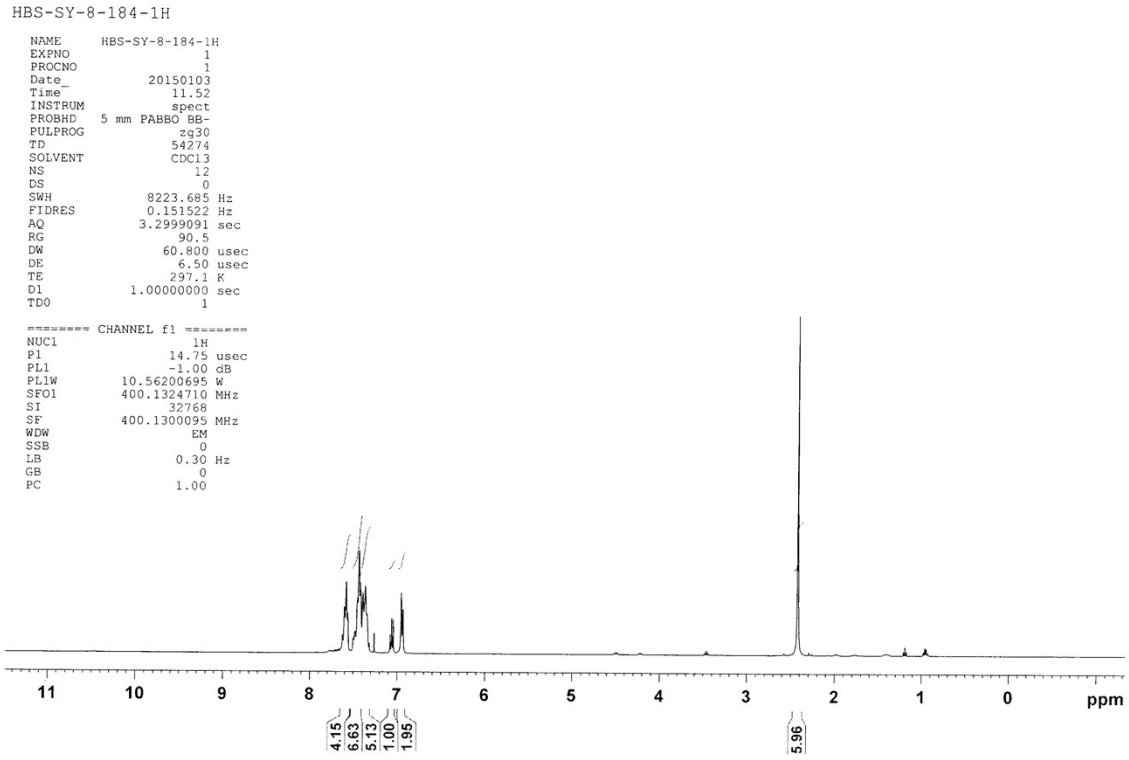


Figure S61. ^{1}H NMR spectrum of compound **16c**.

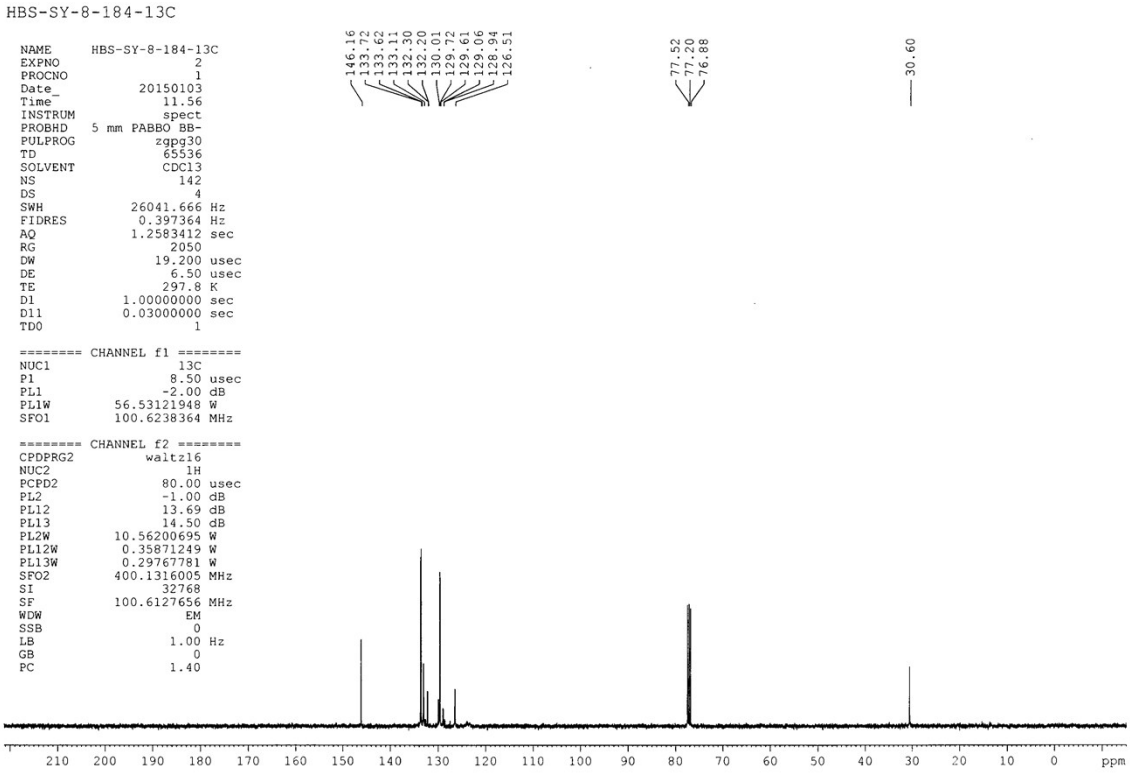


Figure S62. ^{13}C NMR spectrum of compound **16c**.

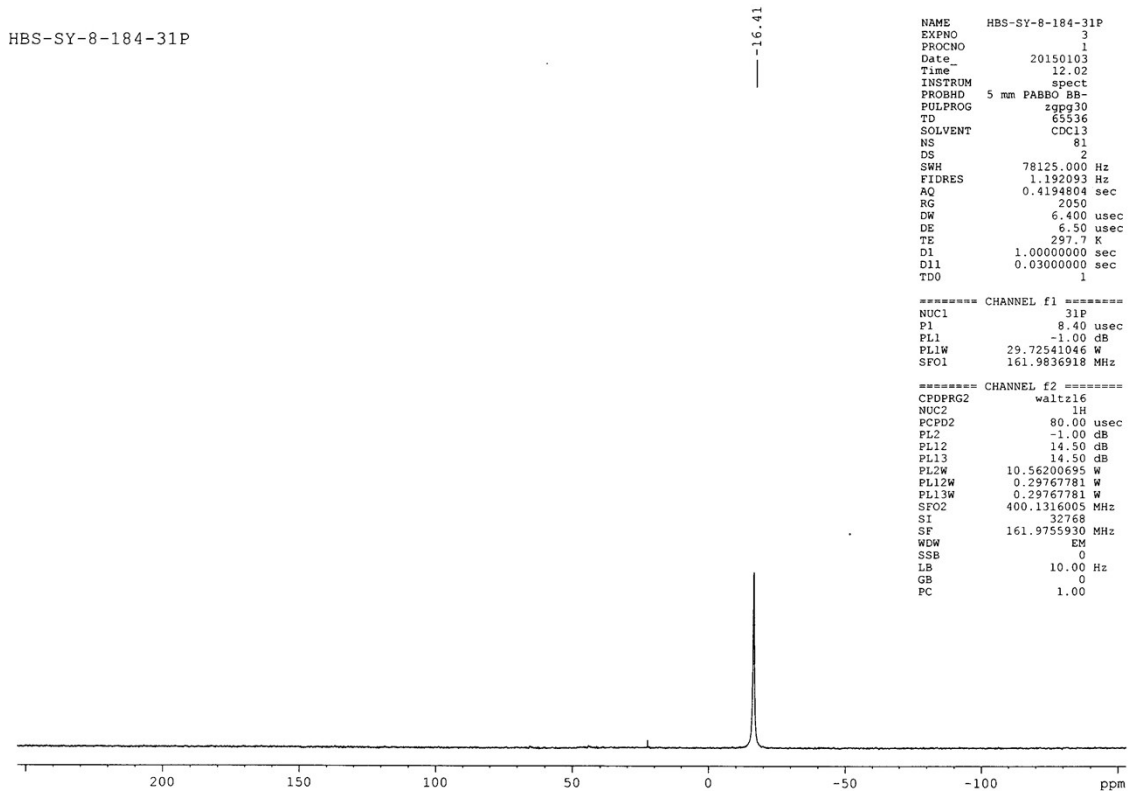


Figure S63. ^{31}P NMR spectrum of compound **16c**.

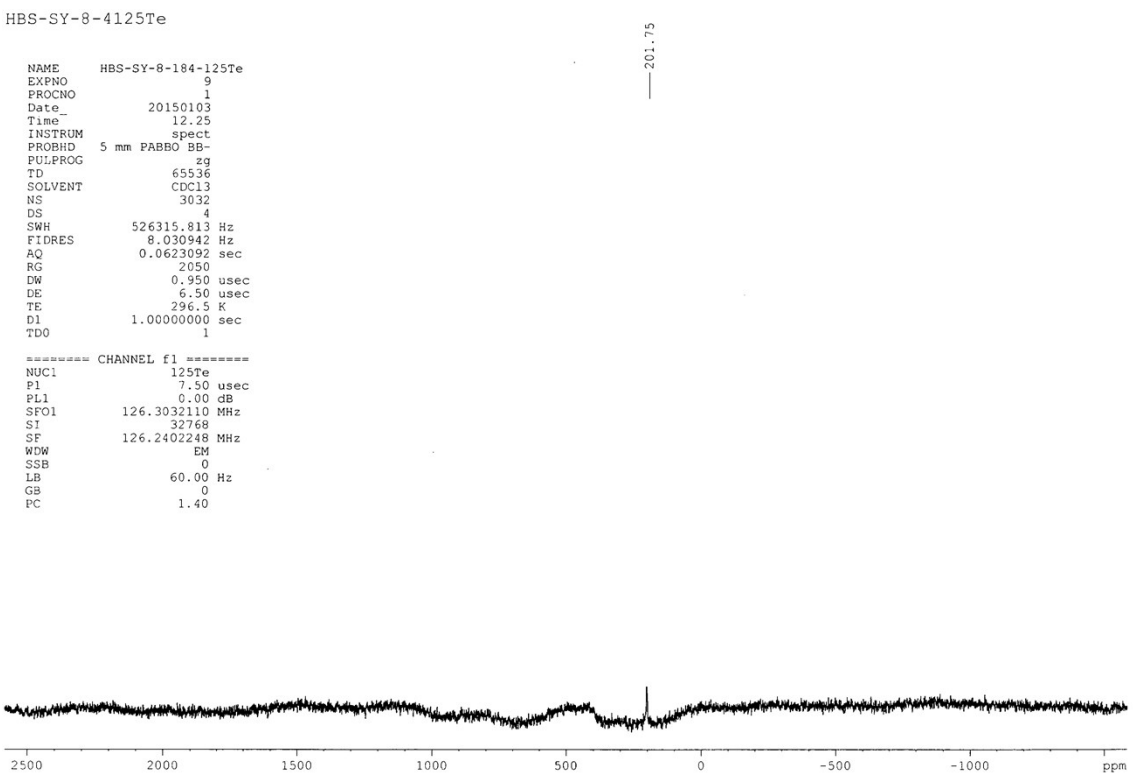


Figure S64. ^{125}Te NMR spectrum of compound **16c**.

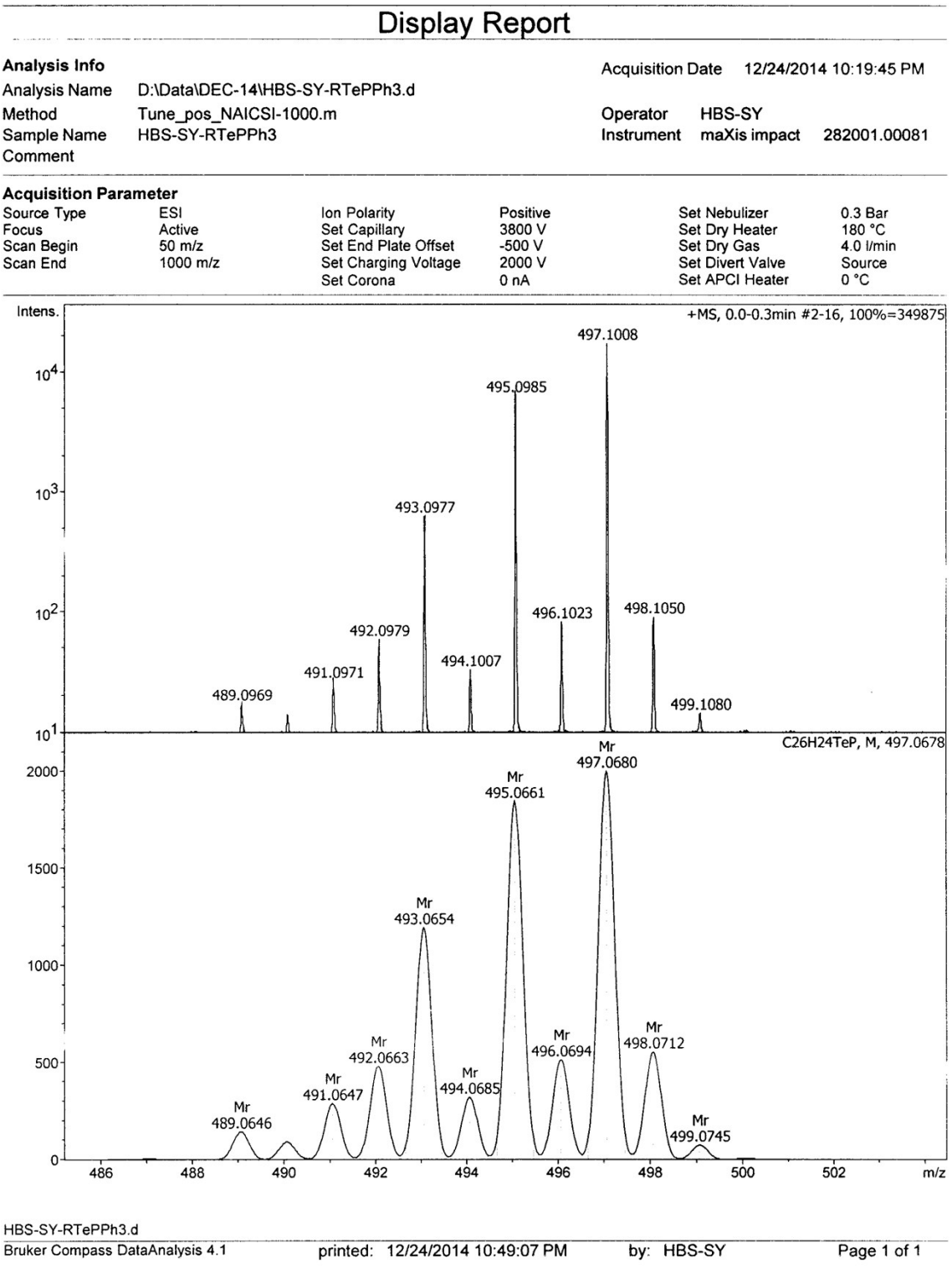


Figure S65. ESI-MS spectrum of compound **16c**.

Packing diagram of compound 8:

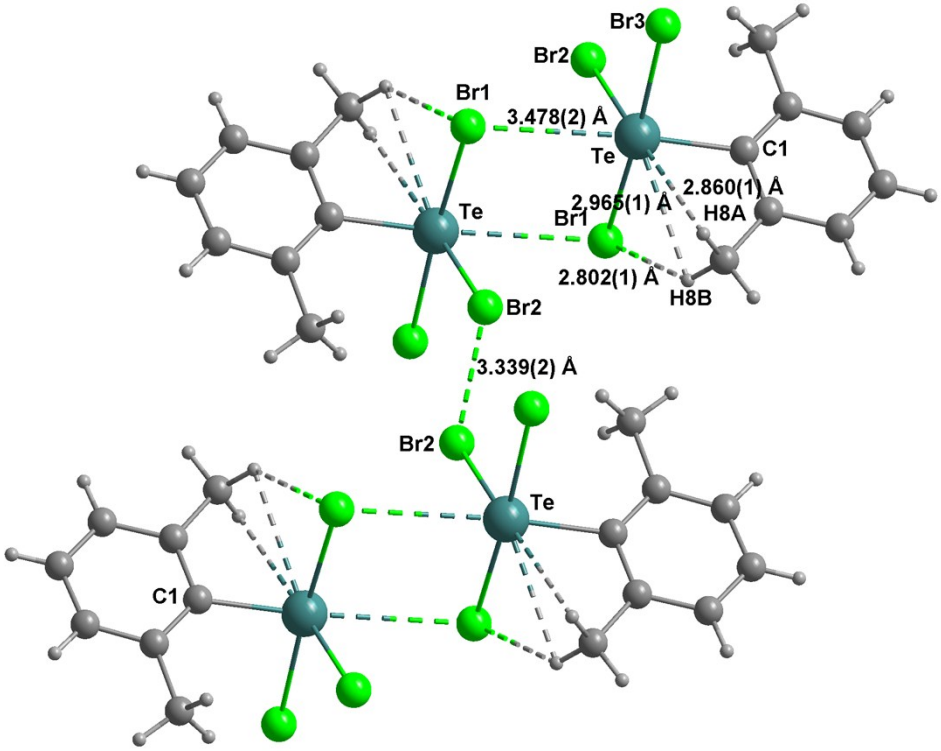
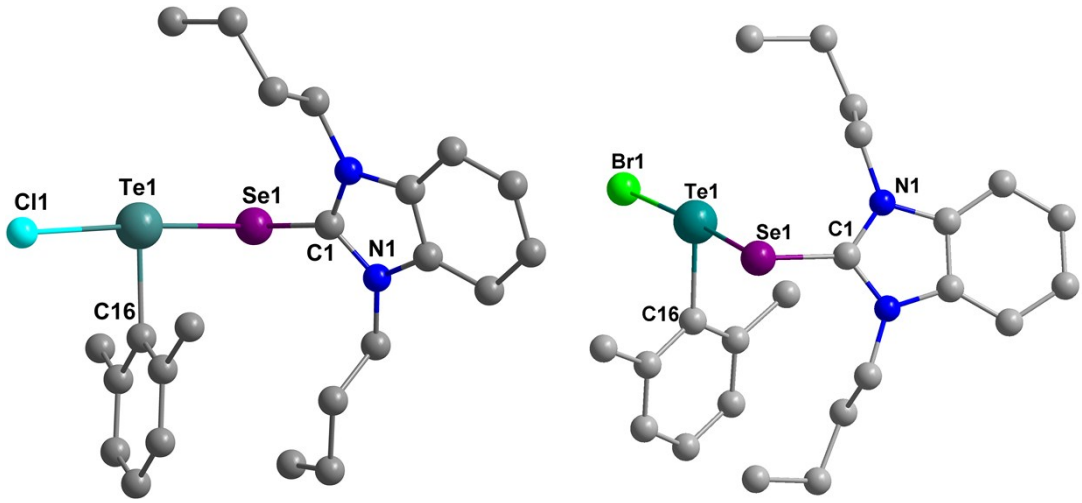


Figure S66. Packing diagram of compound **8**.

Molecular structure of compounds 11a and 11b:



(a) **(b)**

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**.[26] 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) º} and is comparatively smaller than the reported bond angle {177.6(1) º}. The C1-Te-C9 bond angle {113.13(31) º} is larger than the reported angle {112.6(7) º} 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.

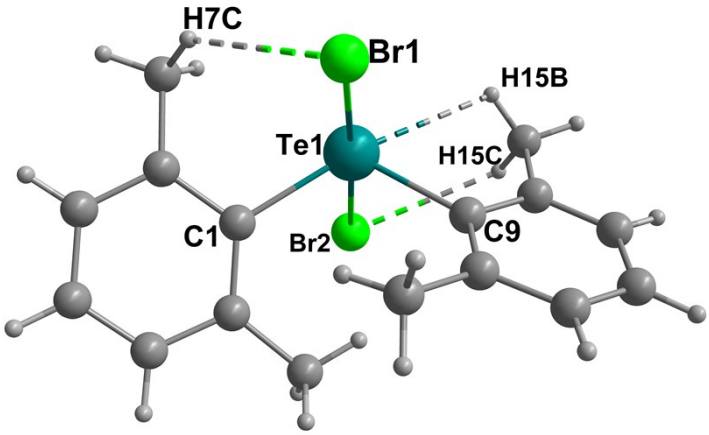


Figure S68. Molecular structure of compound **13**, Selected bond lengths [Å] and bond angles [º] Te1-C1 2.134(9), Te1-C9 2.141(8), Te1-Br1 2.668(1), Te1-Br2 2.693(1), Te1...H15B 2.781(1), Br1...H7C 2.7796(11), Br2... H15B 2.8117(10), C1-Te1-C9 113.13(31), Br1-Te1-Br2 177.05(3).

Summary of crystallographic data

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

	7	**8**	**11a**	**11b**
Chemical formula	$C_{16}H_{18}Br_2Te_2$	$C_8H_9Br_3Te$	$C_{23}H_{31}ClN_2SeTe$	$C_{23}H_{31}BrN_2SeTe$
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^3)	1771.6(6)	1136.5(9)	2354.9(11)	2369.1(17)
Z	4	4	4	4
D_{cal}, Mg/m^3	2.344	2.761	1.629	1.744
F(000)	1152	856	1144	1216
μ (mm^{-1})	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_1	0.0375	0.0425	0.0321	0.0543
wR_2	0.0949	0.0746	0.0706	0.1294
Final R (all data), R_1	0.0538	0.0507	0.0371	0.0599
wR_2	0.1184	0.0761	0.0722	0.1321
Goodness of fit on F^2	0.687	0.834	1.012	1.020

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

	11c	**15**	**16c**
Chemical formula	$C_{23}H_{31}IN_2SeTe$	$C_{23}H_{31}N_2SeTeBF_4$	$C_{26}H_{24}IPTe$
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 ($Å^3$)	2387.93(18)	2505.2(8)	4712.3(16)
Z	4	4	8
D_{cal}, Mg/m^3	1.861	1.667	1.753
F(000)	1288	1240	2400
μ (mm^{-1})	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_1	0.0419	0.0611	0.0223
wR_2	0.0930	0.1600	0.0678
Final R (all data), R_1	0.0543	0.0893	0.0249
wR_2	0.1029	0.2170	0.0863
Goodness of fit on F^2	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.

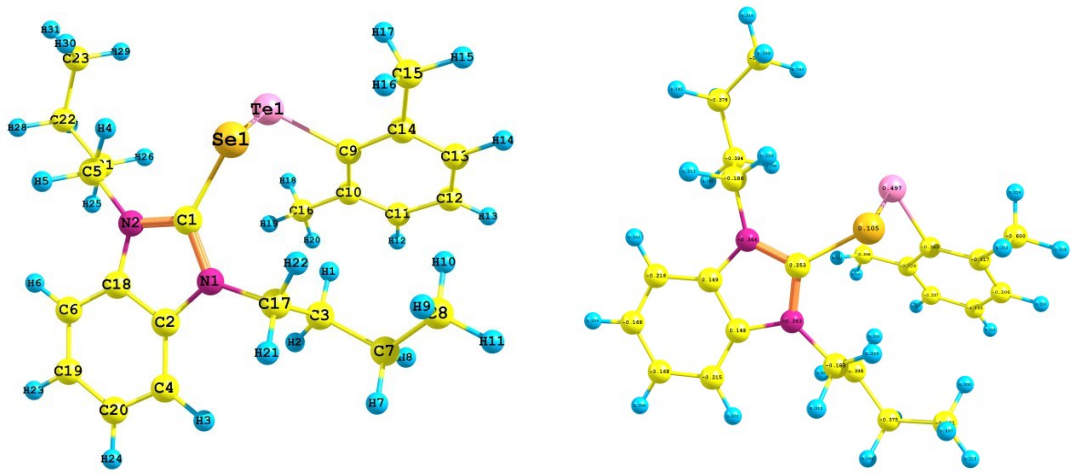
Table S3. Bond length and bond angle comparison between crystal structure of compound **15** and the optimized structure of selone complex of 2,6-dimethylphenyltellurenyl cation.

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



(a) (b)

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	0.163163000
Se	-0.097106000	-0.667882000	-1.776571000
N	-1.231484000	1.759439000	-0.685524000
N	-2.566583000	0.038608000	-0.415250000
C	-1.361461000	0.432081000	-0.871261000
C	-2.380880000	2.237638000	-0.080275000
C	0.811427000	2.930842000	0.118494000
C	-2.758678000	3.522528000	0.302162000
C	-3.126658000	-1.313624000	-0.451144000
C	-4.498277000	1.283129000	0.651809000
C	1.842831000	4.005970000	-0.220250000
C	2.813789000	3.621306000	-1.329112000
C	2.614301000	-0.636610000	0.668691000
C	2.590437000	-0.011136000	1.929777000
C	3.692075000	0.763372000	2.291929000
C	4.774055000	0.913964000	1.439267000
C	4.778771000	0.286553000	0.203518000
C	3.708747000	-0.506974000	-0.207240000
C	3.771929000	-1.167977000	-1.552973000
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