

Electronic Supplementary Information For

Synthesis and structural characterization of pincer type bicyclic diacyloxy- and diazaselenuranes

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S1. Spectral Data

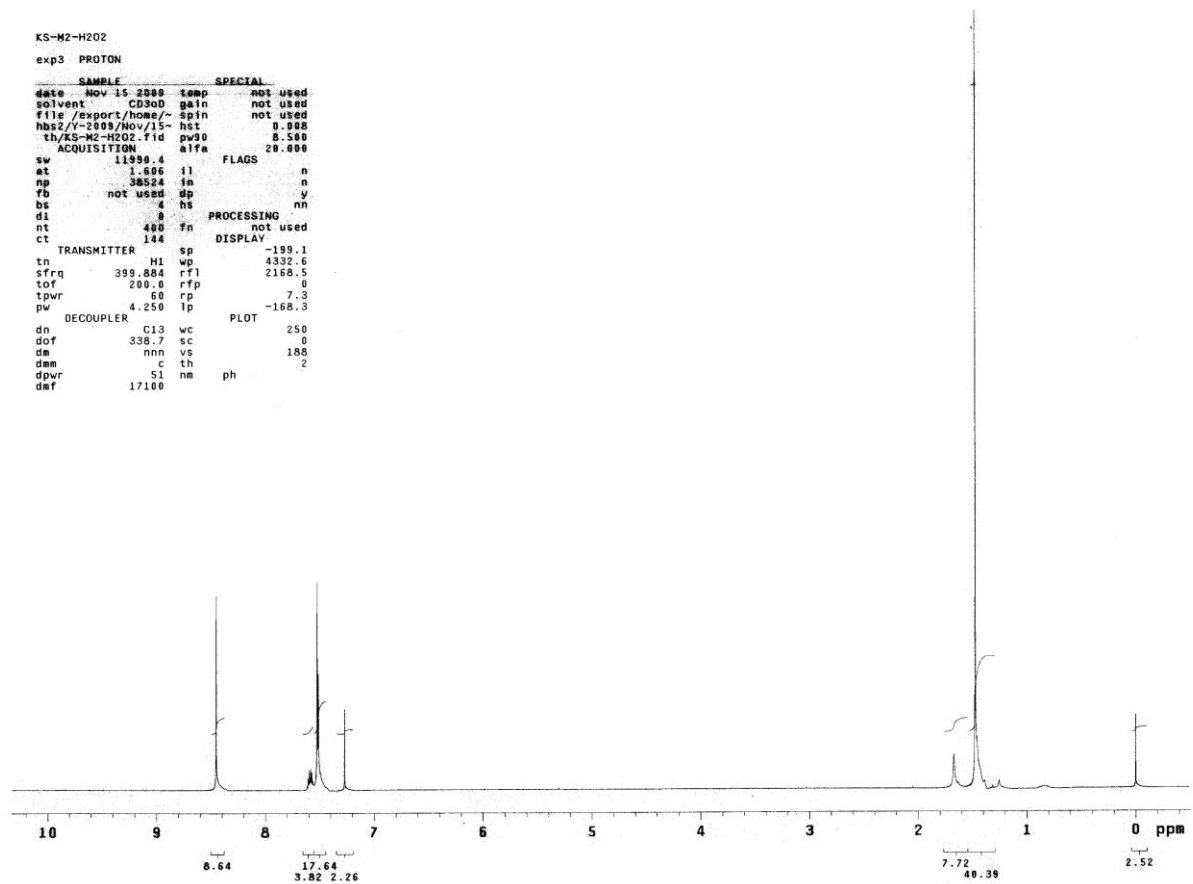


Fig. S1 ^1H NMR spectrum of **25**

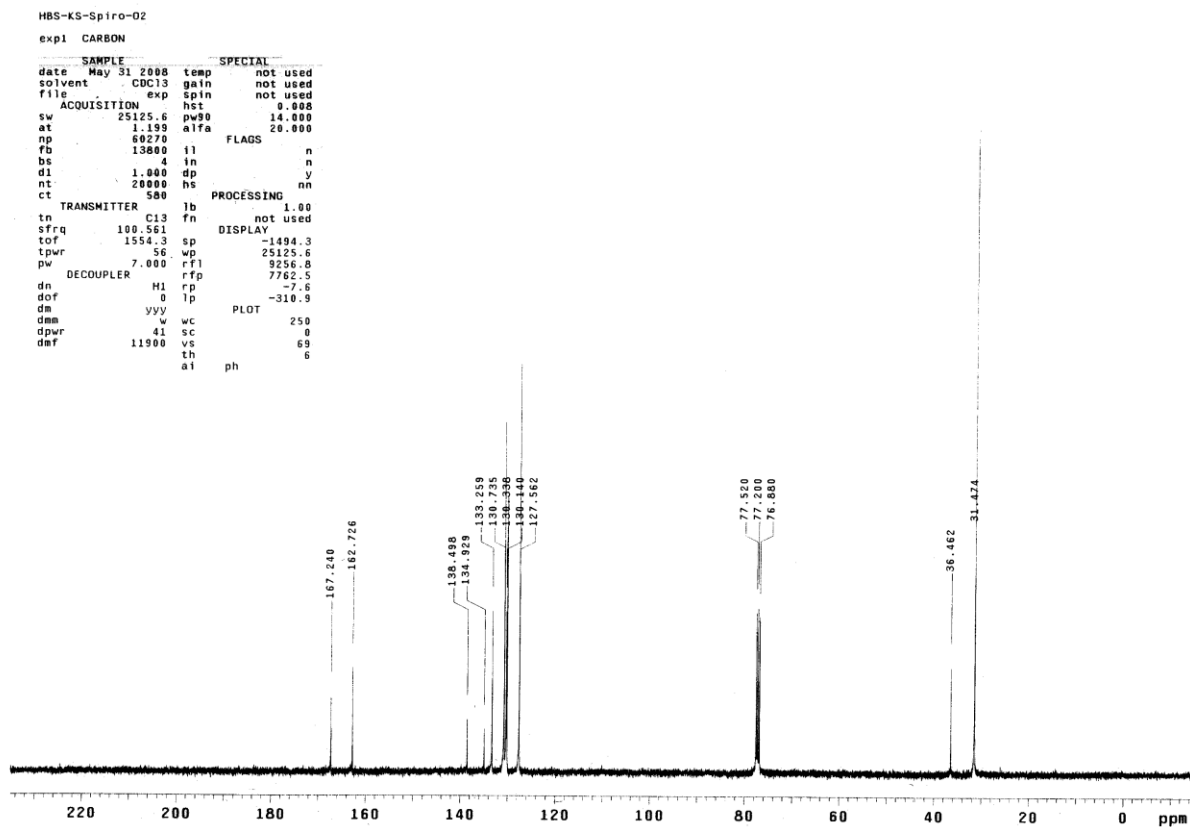


Fig. S2 ^{13}C NMR spectrum of 25

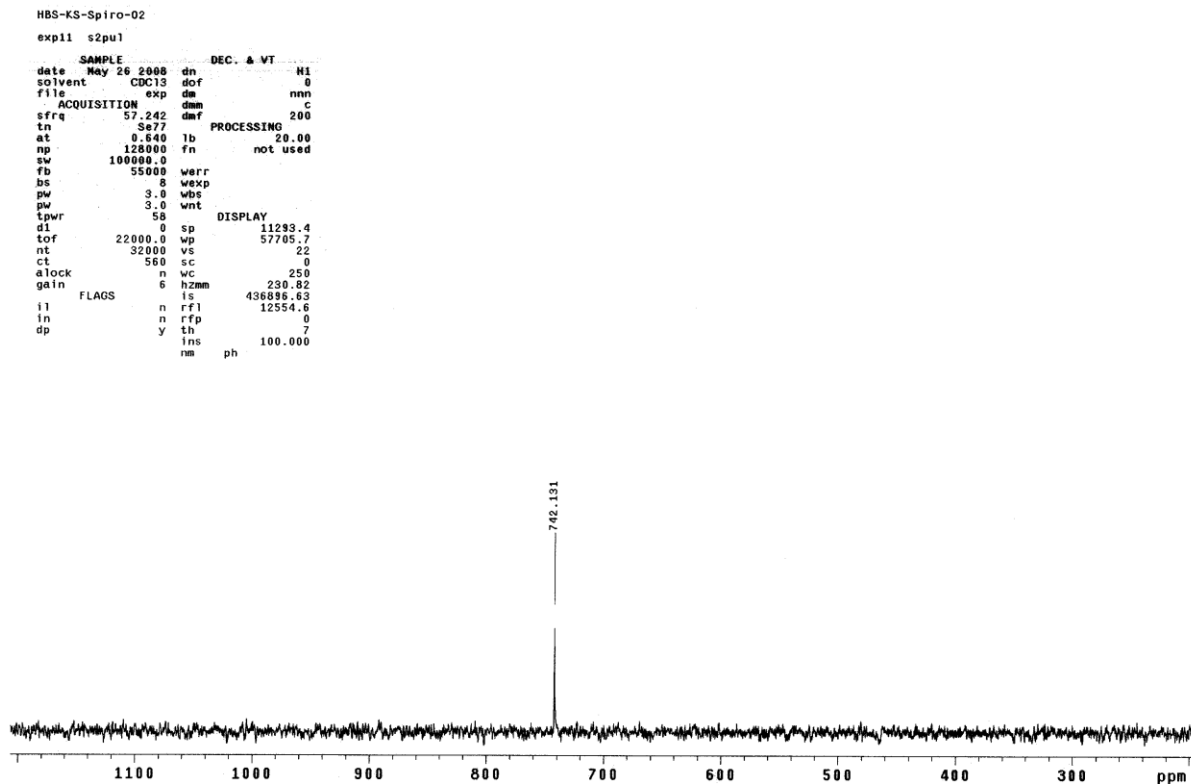


Fig. S3 ^{77}Se NMR spectrum of **25**

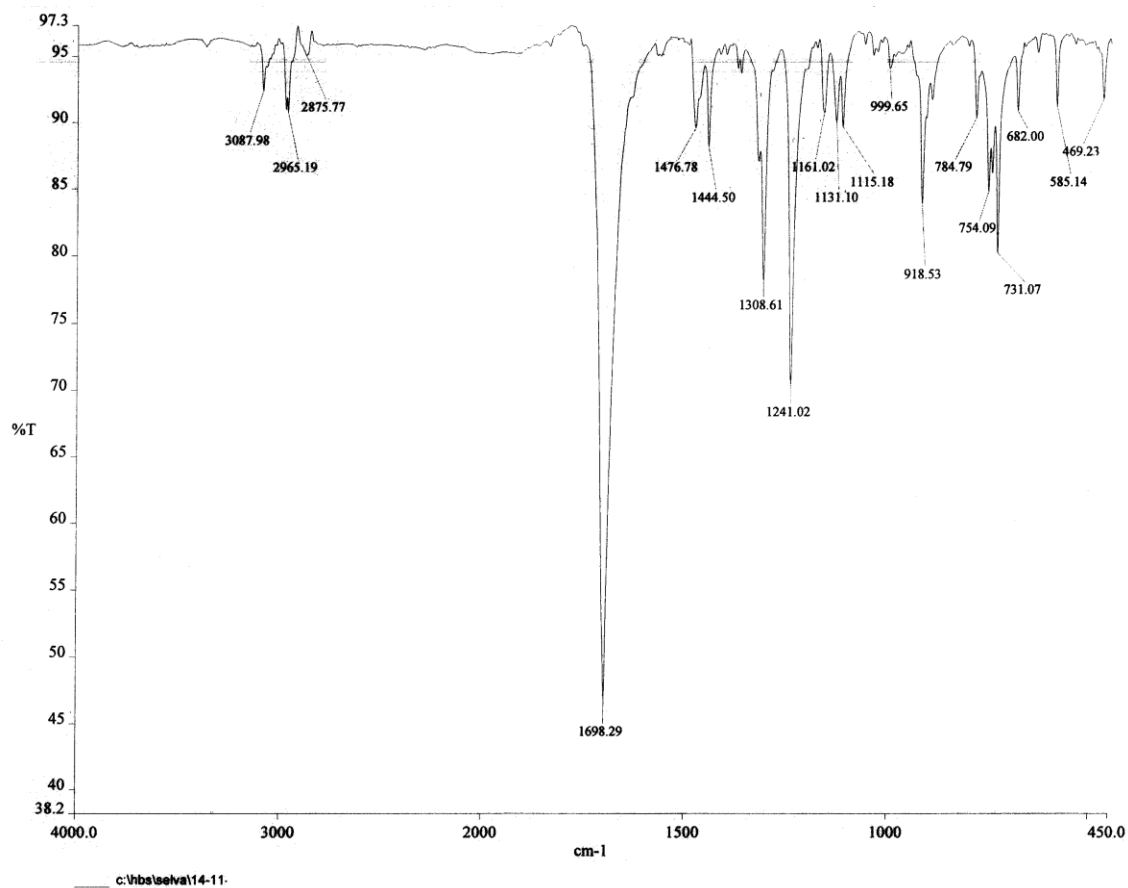


Fig. S4 FT-IR spectrum of **25**

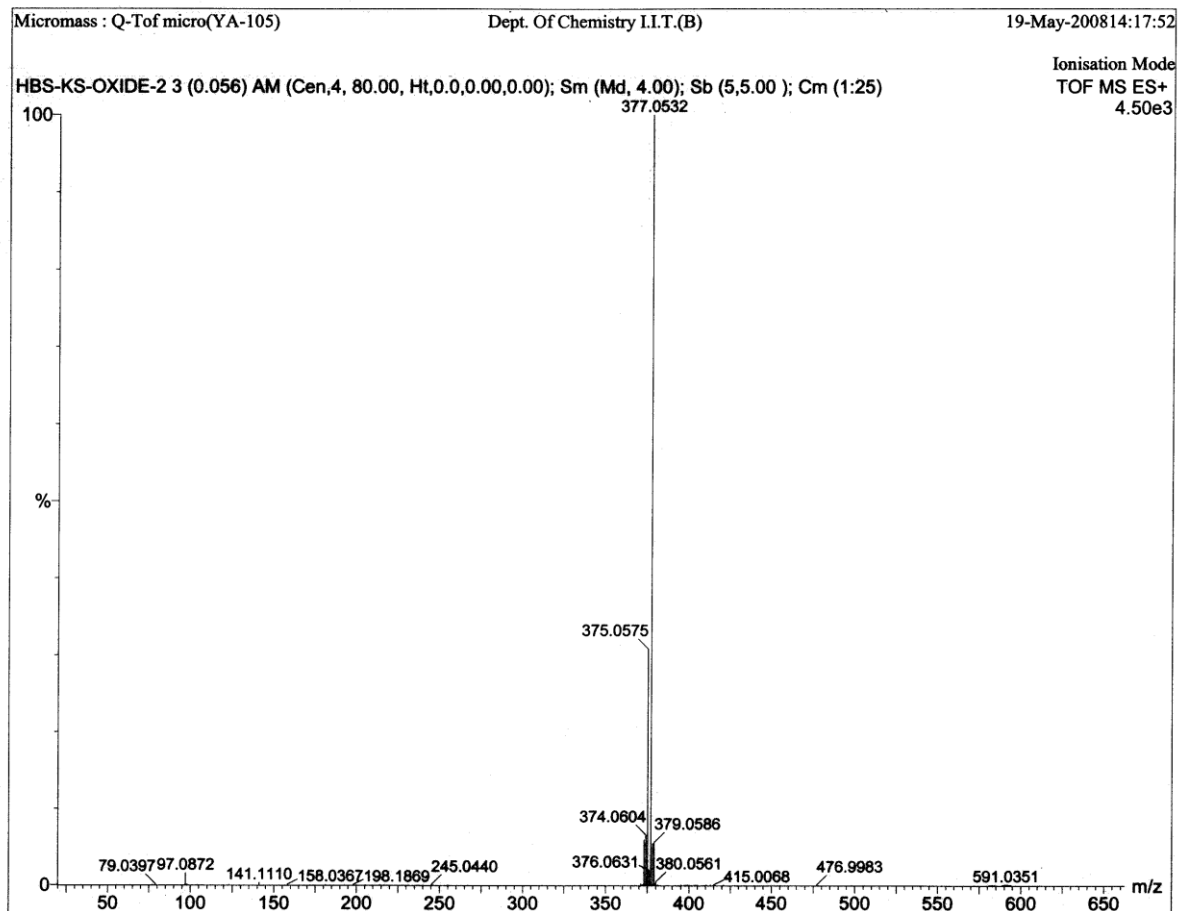


Fig. S5 ES-MS spectrum of **25**

Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

18 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-ToF micro (YA-105)

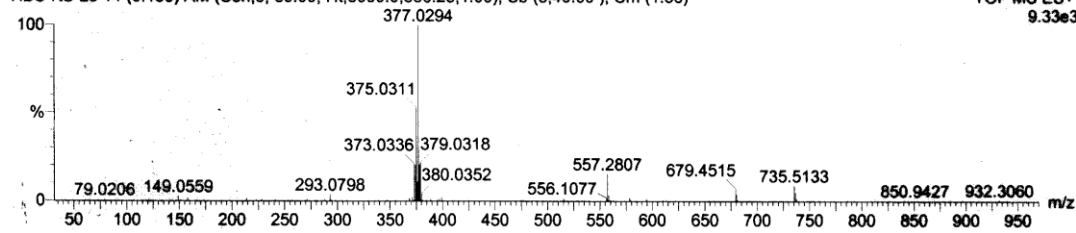
Dept. Of Chemistry I.I.T.(B)

13-Jun-2011 10:54:02

C₁₈H₁₆O₄Se

HBS-KS-25 14 (0.139) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sb (5,40.00); Cm (1:56)

TOF MS ES+
9.33e3



Minimum: -1.5
Maximum: 200.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
377.0294	377.0292	0.2	0.6	11.5	1	C ₁₈ H ₁₇ O ₄ Se

Fig. S6 ES-HRMS spectrum of 25

Eager 300 Report

Page: 1 Sample: KSSPIROSE1 (KSSPIROSE1)

Method Name : sp101008
Method File : D:\CHNS2008\SP101008.mth
Chromatogram : KSSPIROSE1
Operator ID : SP Company Name : C.E. Instruments
Analysed : 10/10/2008 15:40 Printed : 10/10/2008 16:57
Sample ID : KSSPIROSE1 (# 26) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : 1.877

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Warning Chromatogram has been subjected to manual integration.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Carbon	57.0184	64	2870223	mi	1.000000	.267485E+07
Hydrogen	4.1047	169	519678	mi	5.523079	.648699E+07
Totals	61.1231		3389901			

Fig. S7 Elemental analysis for 25

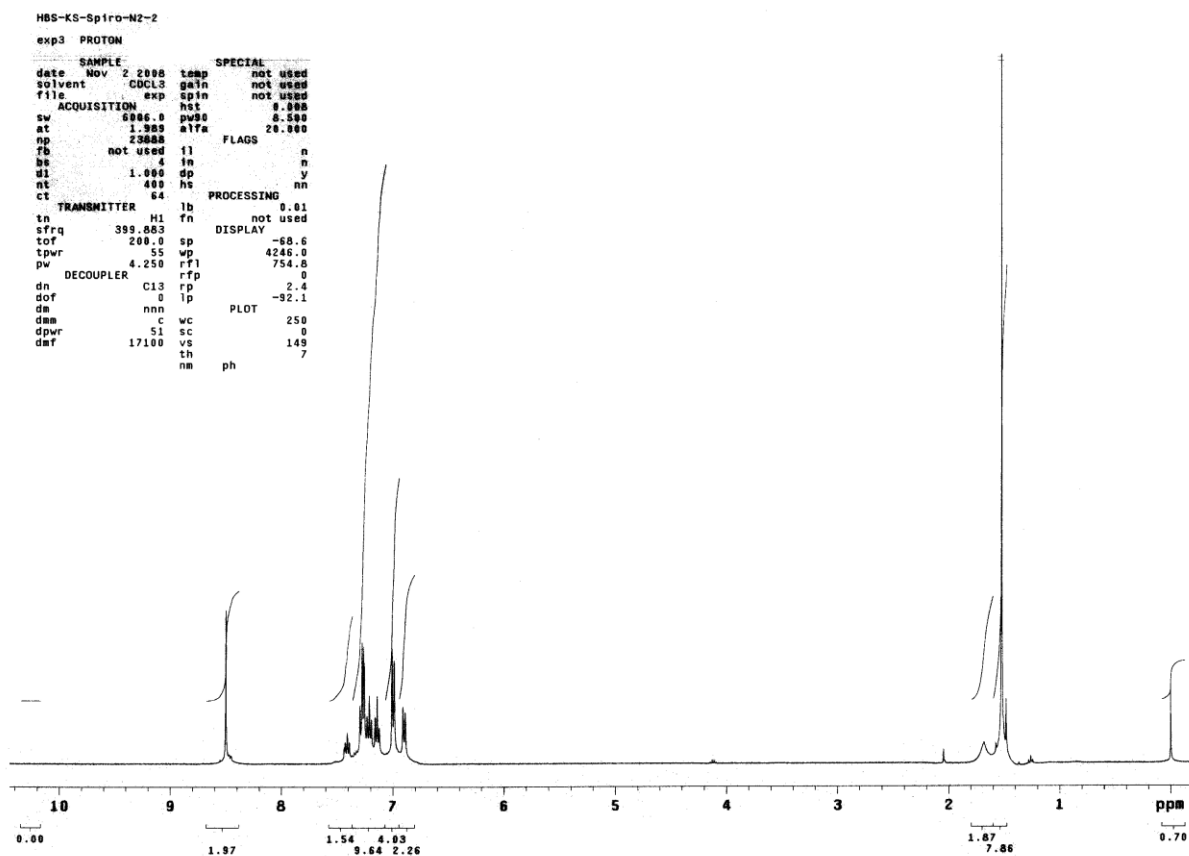


Fig. S8 ^1H NMR spectrum of **27**

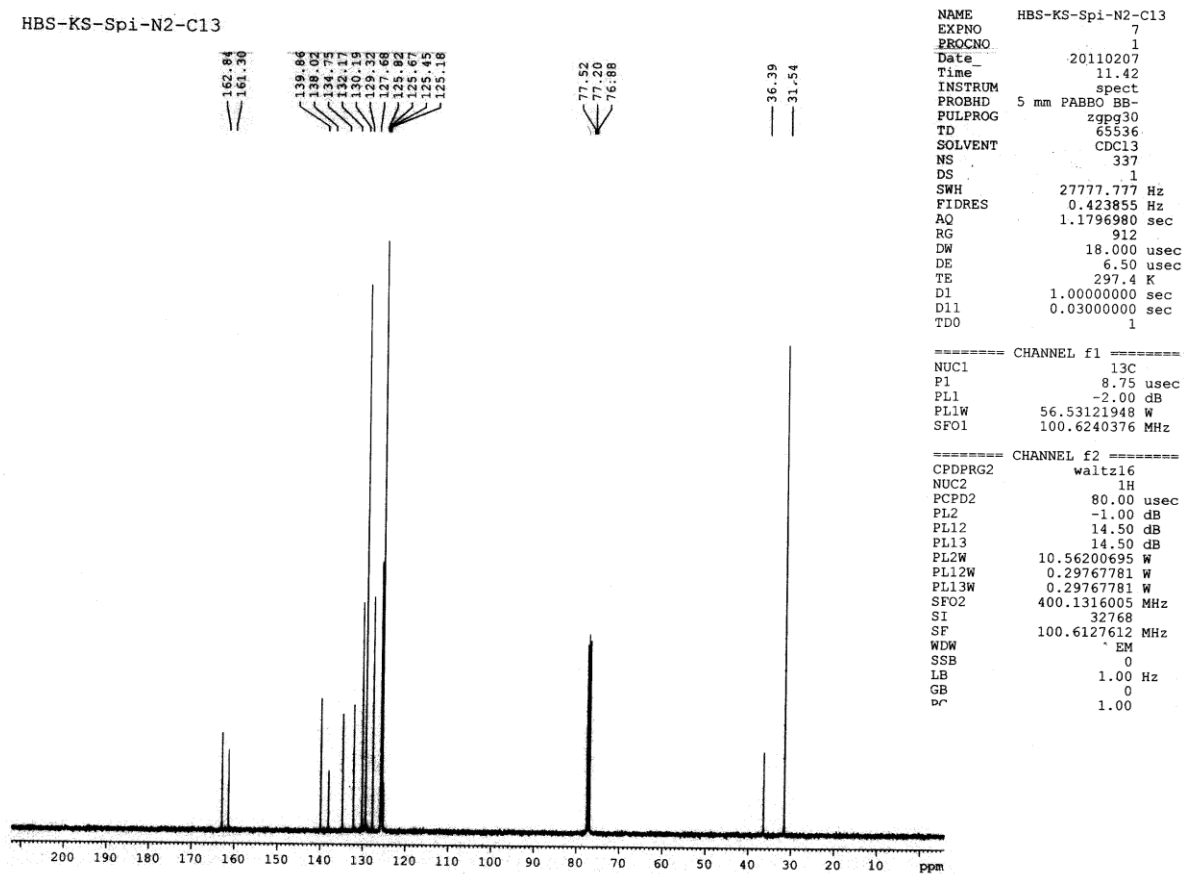


Fig. S9 ^{13}C NMR spectrum of 27

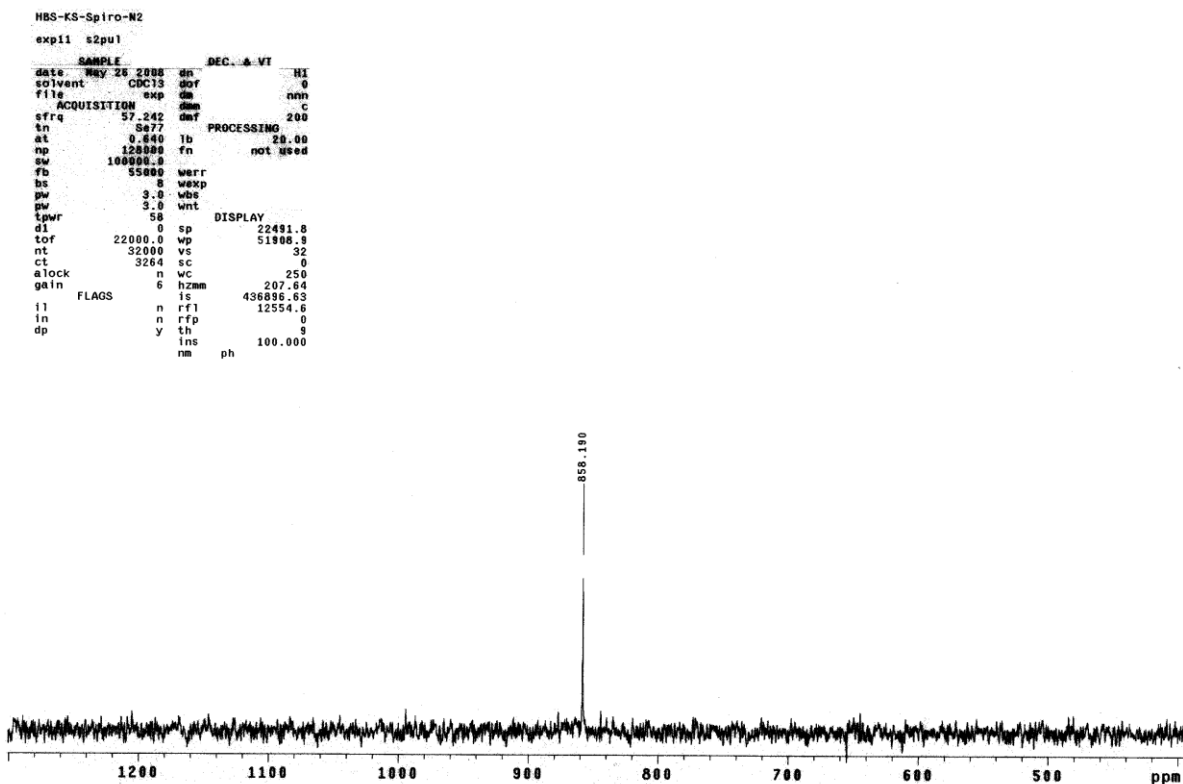


Fig. S10 ⁷⁷Se NMR spectrum of **27**

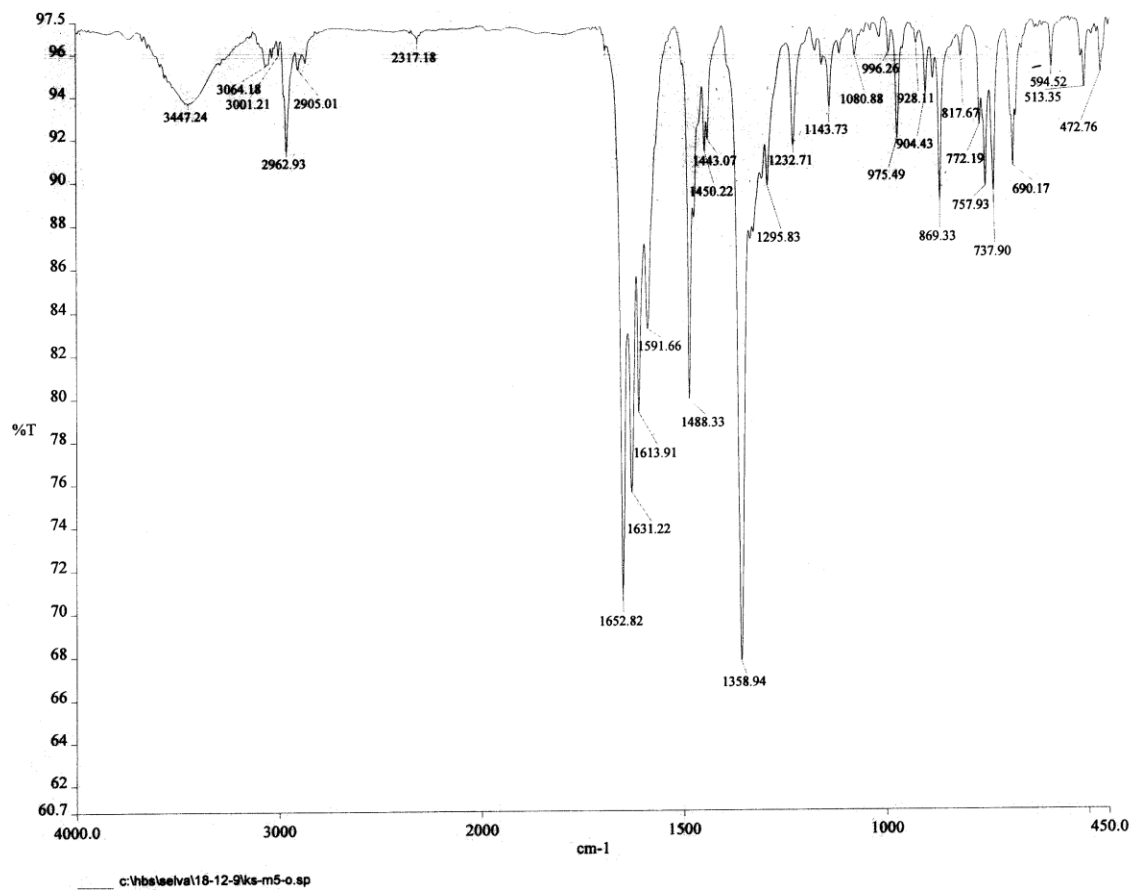


Fig. S11 FT-IR spectrum of **27**

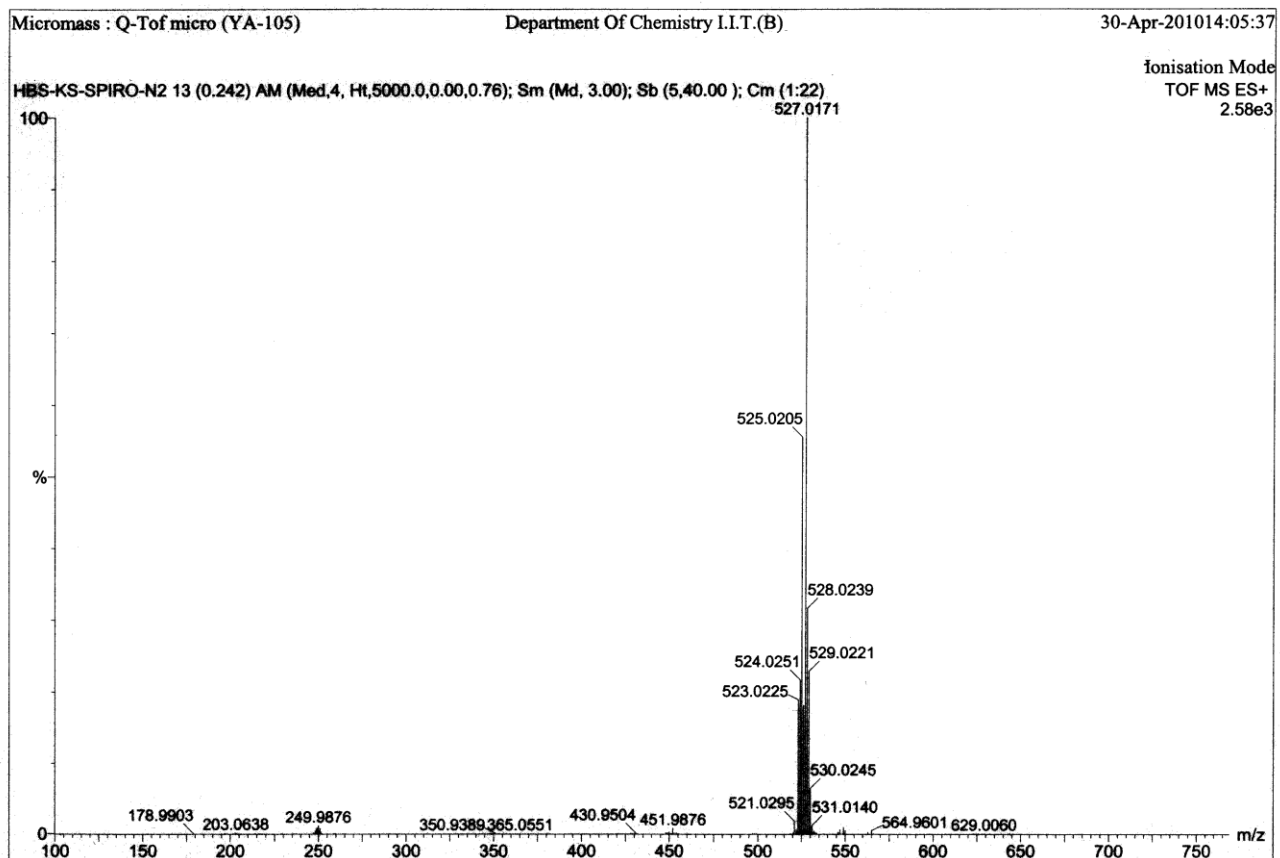


Fig. S12 ES-MS spectrum of 27

Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

28 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-ToF micro (YA-105)

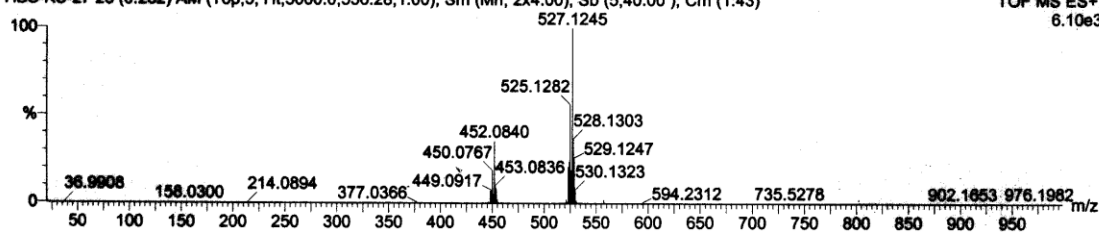
Dept. Of Chemistry I.I.T.(B)

13-Jun-201111:04:30

C₃₀H₂₈N₂O₂Se

HBS-KS-27 26 (0.262) AM (Top,5, Ht,5000.0,556.28,1.00); Sm (Mn, 2x4.00); Sb (5,40.00); Cm (1:43)

TOF MS ES+
6.10e3



Minimum:

Maximum:

200.0 20.0 -1.5
50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
527.1245	527.1238	0.7	1.4	19.5	1	C ₃₀ H ₂₇ N ₂ O ₂ Se

Fig. S13 ES-HRMS spectrum of 27

Eager 300 Report

SPTD N2-IMC

Page: 1 Sample: KS-RSEN2C (KS-RSEN2C)

Method Name : sp110209
Method File : D:\CHNS2008\sp110209.mth
Chromatogram : KS-RSEN2C
Operator ID : AGK
Analysed : 02/11/2009 14:49
Sample ID : KS-RSEN2C (# 28)
Analysis Type : UnkNown (Area)
Company Name : C.E. Instruments
Printed : 2/11/2009 16:04
Instrument N. : Instrument #1
Sample weight : 1.276

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	4.5646	43	60402	FU	38.151880	.103706E+07
2	0.0000	59	37046	FU		0.0000
Carbon	67.8109	65	2304462	FU	1.000000	.266330E+07
Hydrogen	4.6094	172	528119	RS	4.363528	.717613E+07
Totals	76.9849		2930029			

Fig. S14 Elemental analysis for 27

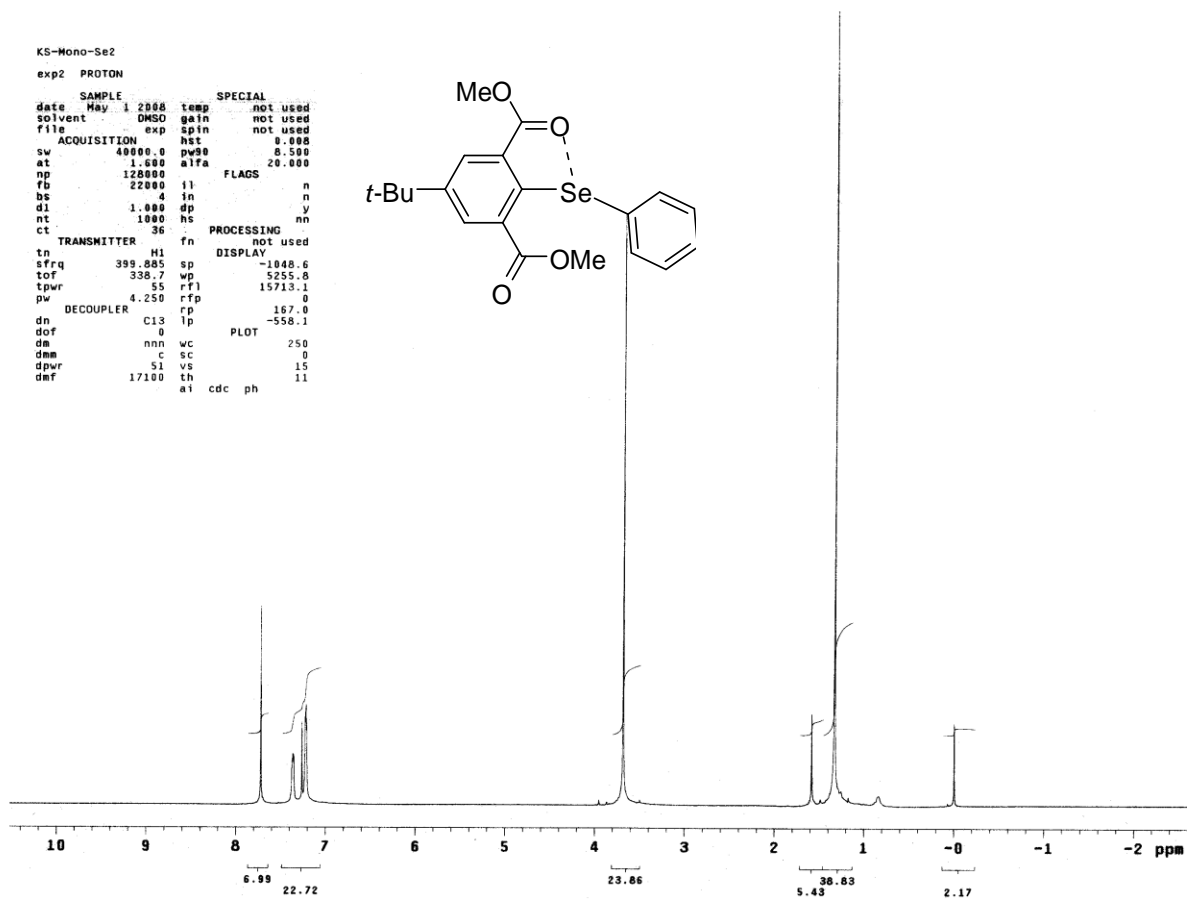


Fig. S15 ¹H NMR Spectrum of 29

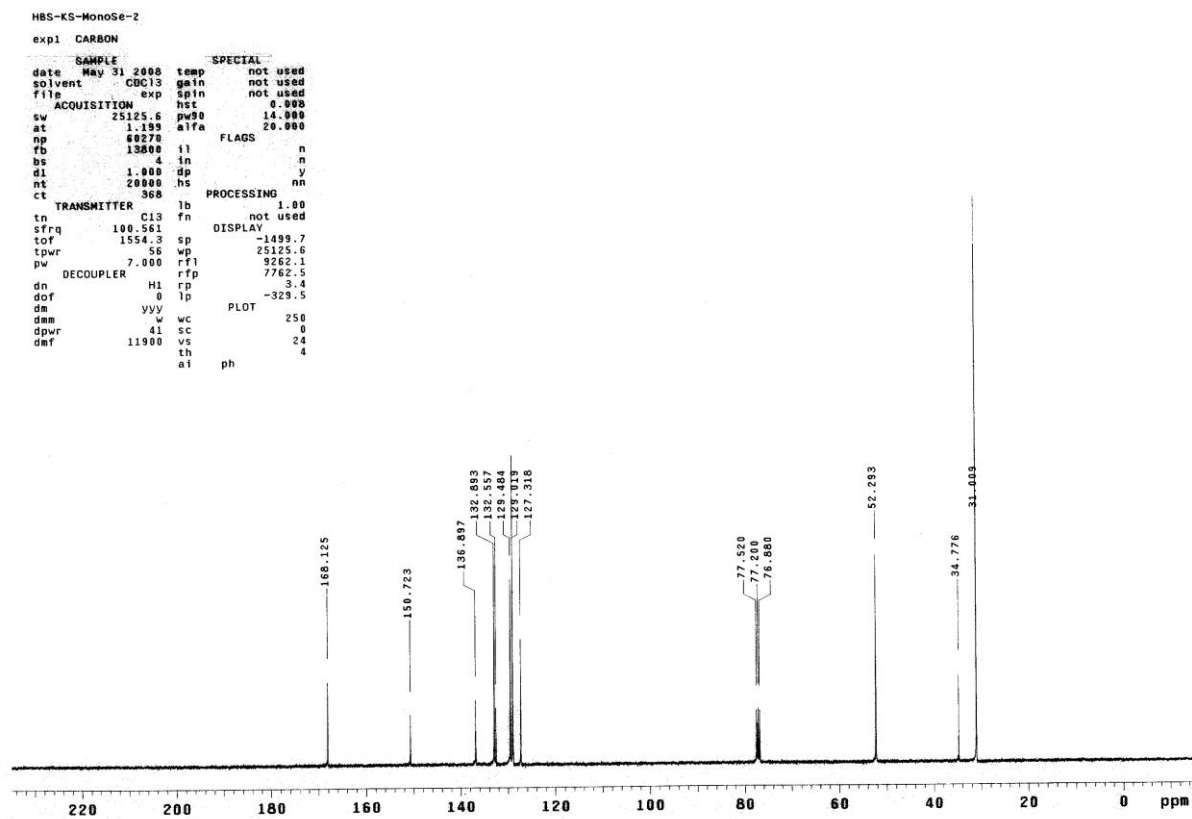


Fig. S16 ^{13}C NMR Spectrum of **29**

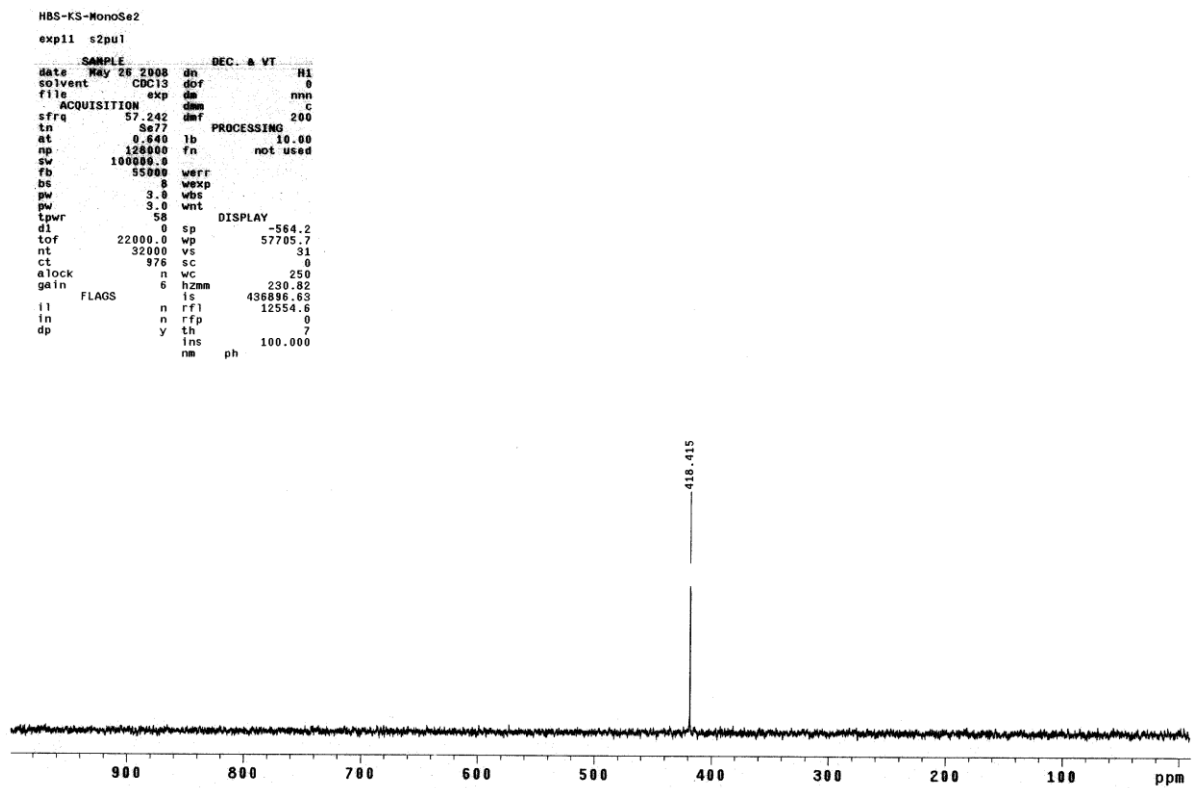


Fig. S17 ^{77}Se NMR Spectrum of **29**

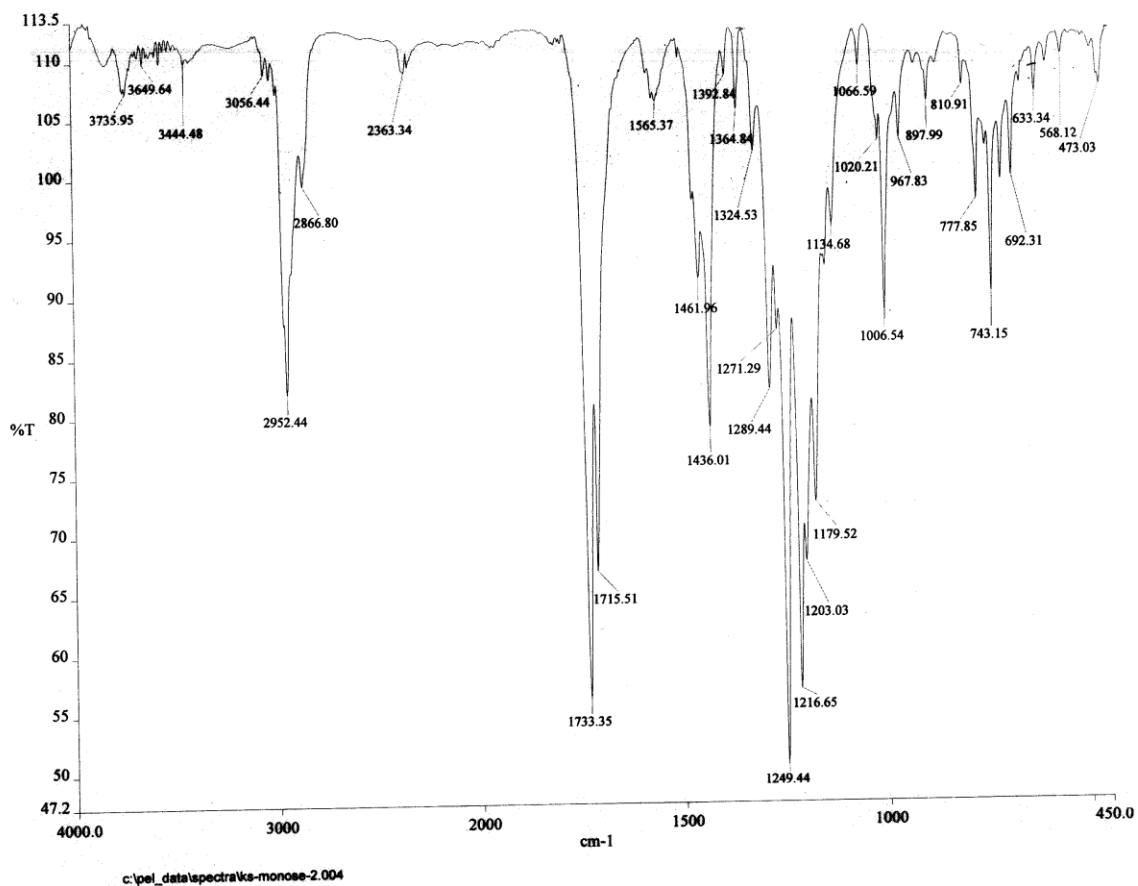


Fig. S18 FT-IR Spectrum of **29**

Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

19 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-ToF micro (YA-105)

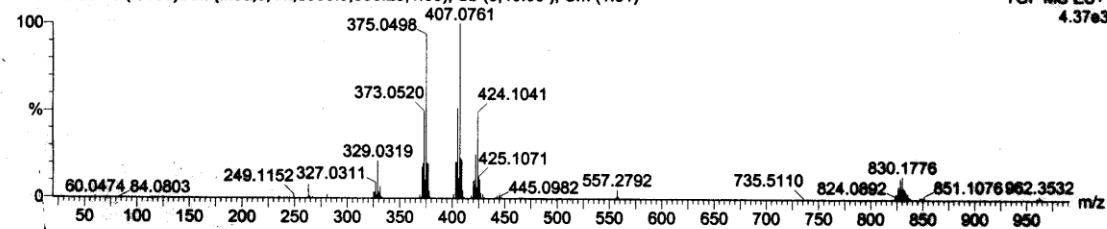
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13-Jun-2011 11:33:43

C₂₀H₂₂O₄Se

HBS-KS-29 16 (0.160) AM (Med,5, Ht,5000.0,556.28,1.00); Sb (5,40.00); Cm (1:31)

TOF MS ES+
4.37e3



Minimum:

Maximum: 200.0 20.0 -1.5

50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
407.0761	407.0762	-0.1	-0.2	10.5	1	C ₂₀ H ₂₃ O ₄ Se

Fig. S19 ES-HRMS spectrum of 29

Eager 300 Report

Page: 1 Sample: KSMONOSE2 (KSMONOSE2)

Method Name : sp101008
Method File : D:\CHNS2008\SP101008.mth
Chromatogram : KSMONOSE2
Operator ID : SP Company Name : C.E. Instruments
Analysed : 10/10/2008 15:48 Printed : 10/10/2008 16:57
Sample ID : KSMONOSE2 (# 27) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : 1.99

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Warning Chromatogram has been subjected to manual integration.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Carbon	58.5181	63	3122393	mi	1.000000	.267485E+07
Hydrogen	5.5355	174	734467	mi	4.251236	.646699E+07
Totals	64.0535		3856860			

Fig. S20 Elemental analysis for 29

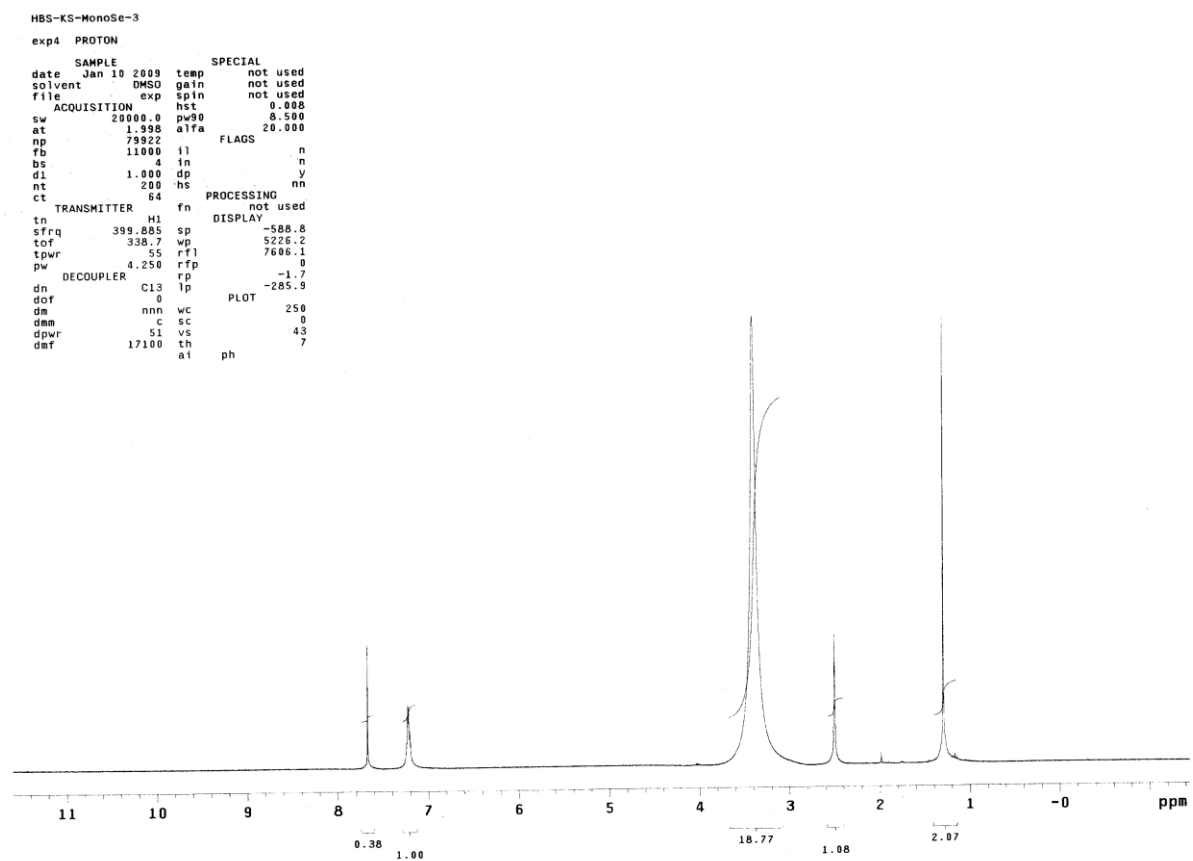


Fig. S21 ^1H NMR Spectrum of **30**

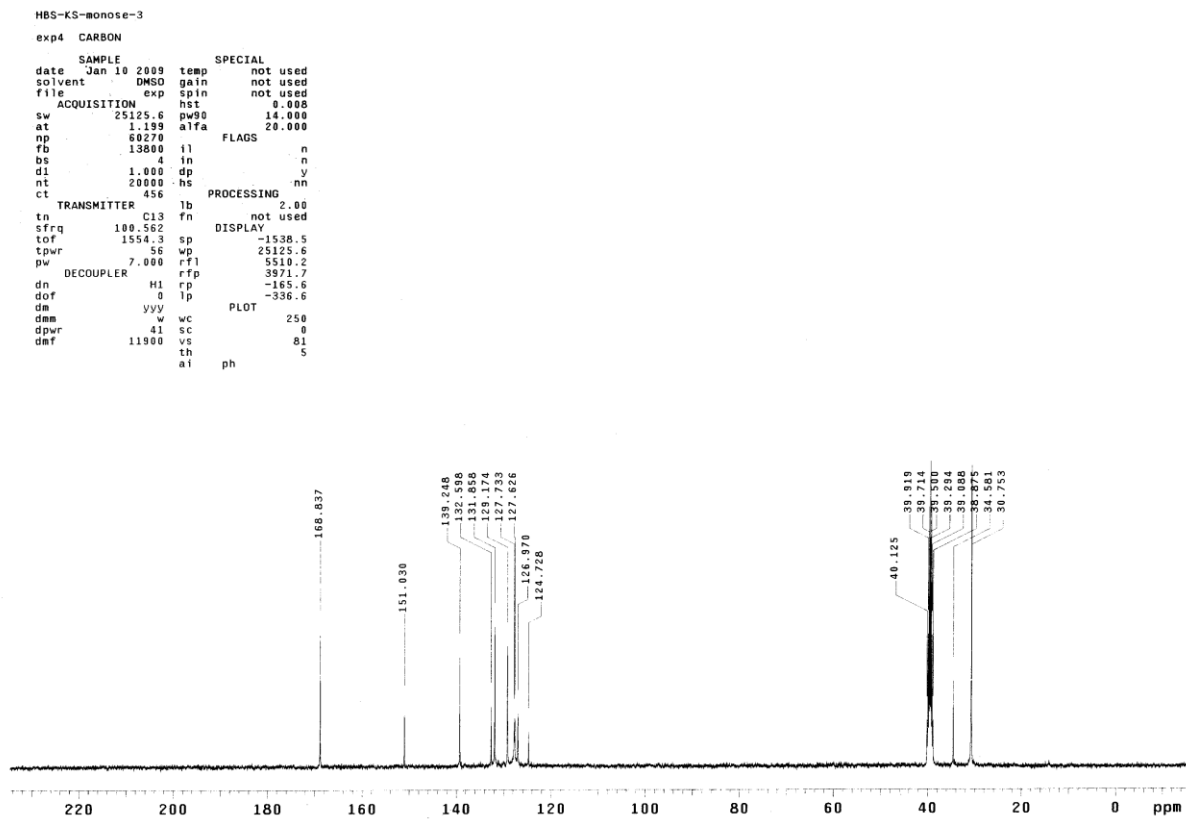


Fig. S22 ^{13}C NMR Spectrum of **30**

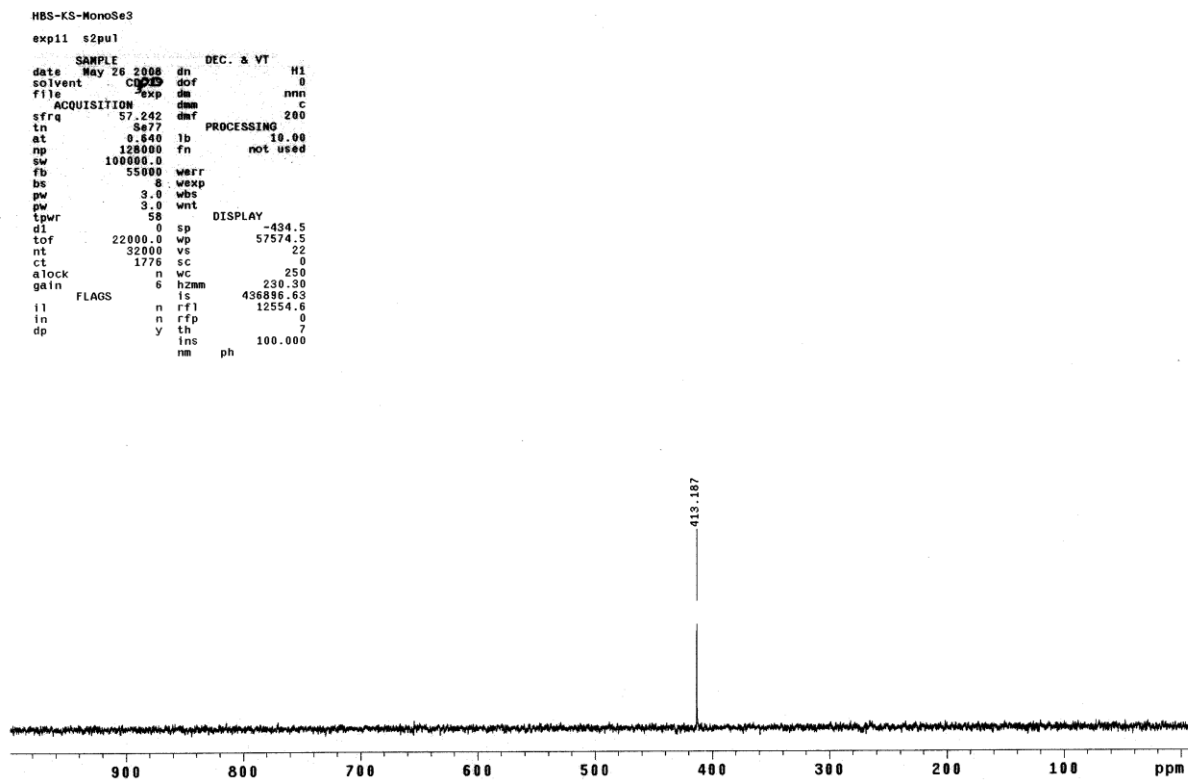


Fig. S23 ^{77}Se NMR Spectrum of 30

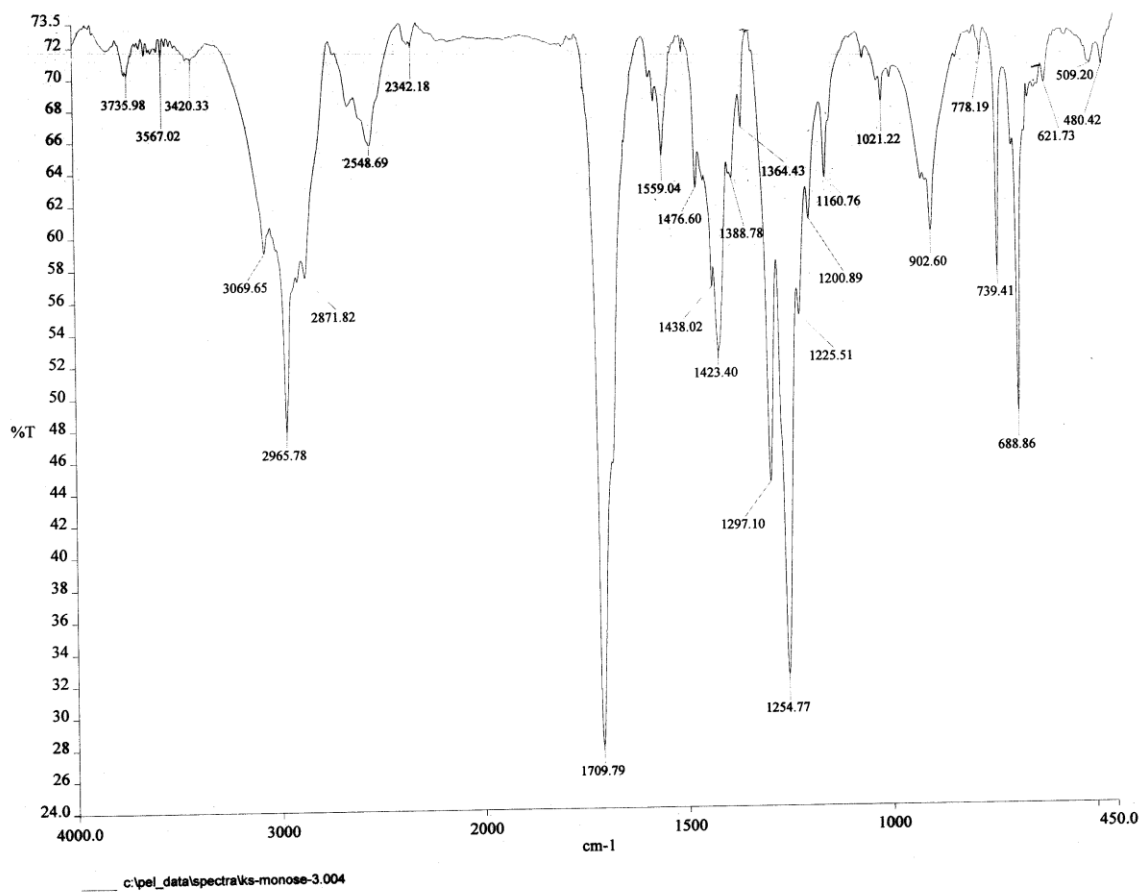


Fig. S24 FT-IR spectrum of **30**

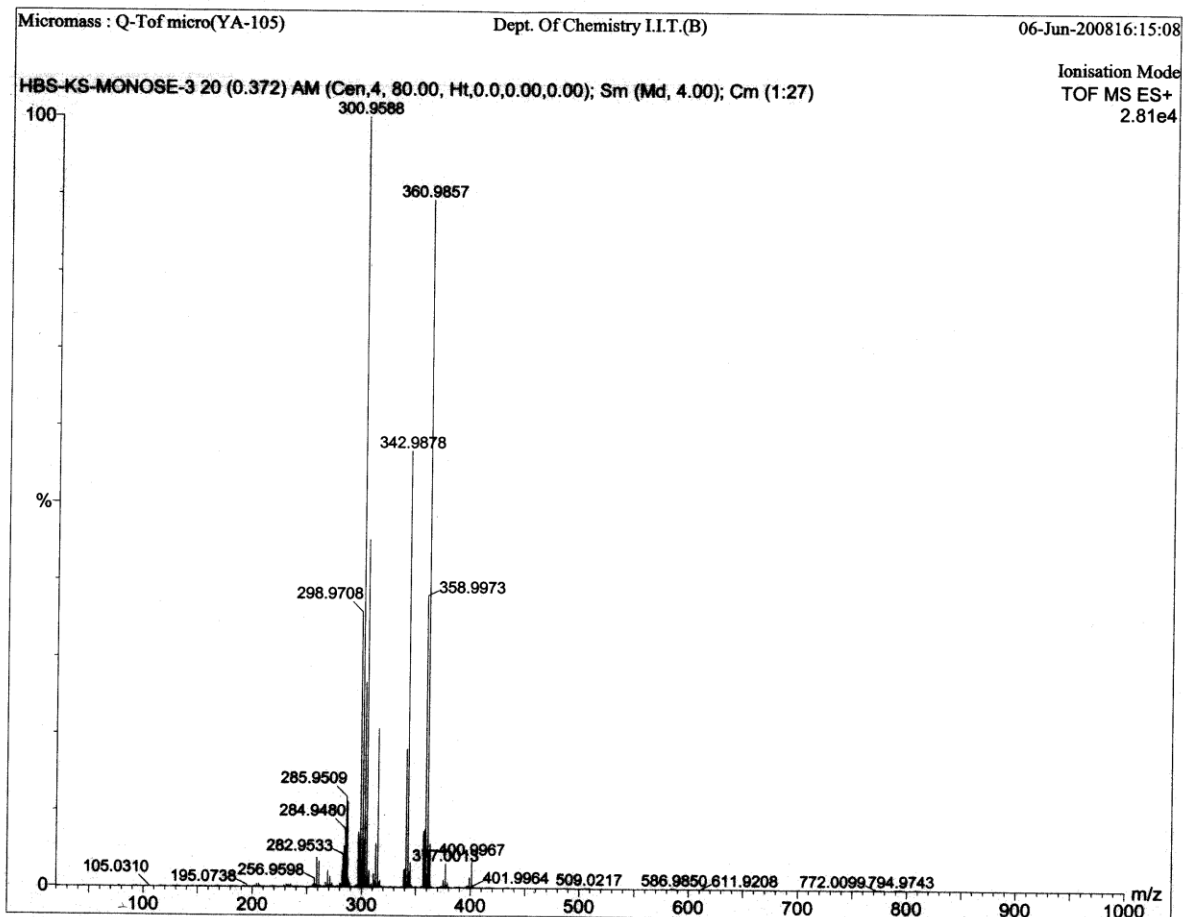


Fig. S25 ES-MS spectrum of 30

Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

22 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-ToF micro (YA-105)

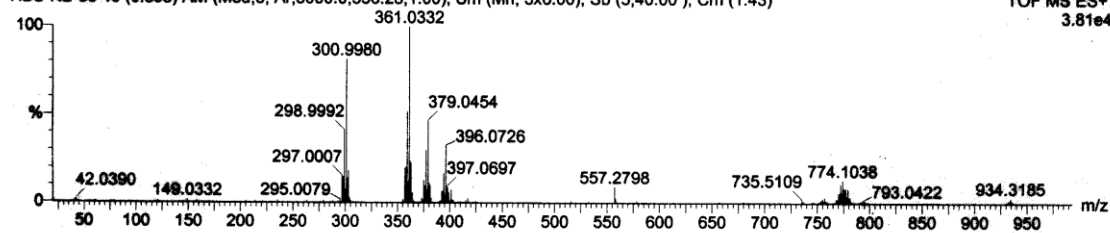
Dept. Of Chemistry I.I.T.(B)

13-Jun-2011 12:05:30

C₁₈H₁₈O₄Se

HBS-KS-30 40 (0.398) AM (Med,5, Ar,5000.0,556.28,1.00); Sm (Mn, 3x6.00); Sb (5,40.00); Cm (1:43)

TOF MS ES+
3.81e4



Minimum:

Maximum: 200.0 20.0 -1.5

Mass Calc. Mass mDa PPM DBE Score Formula

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
379.0454	379.0449	0.6	1.5	10.5	1	C ₁₈ H ₁₉ O ₄ Se

Fig. S26 ES-HRMS spectrum of 30

~~KS-M2~~ Eager 300 Report

Page: 1 Sample: ~~KS-M2~~ (KS-M2) KS-M3

Method Name : SP290410
Method File : D:\CHNS2008\SP290410.mth
Chromatogram : KS-M2
Operator ID : SP
Analysed : 04/29/2010 14:04
Sample ID : KS-M2 (# 21)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 4/29/2010 17:01
Instrument N. : Instrument #1
Sample weight : 1.561

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Carbon	57.8064	65	2238365	RS	1.000000	.247571E+07
Hydrogen	5.3952	172	623917	RS	3.587601	.653955E+07
Totals	63.2016		2862282			

Fig. S27 Elemental analysis for 30

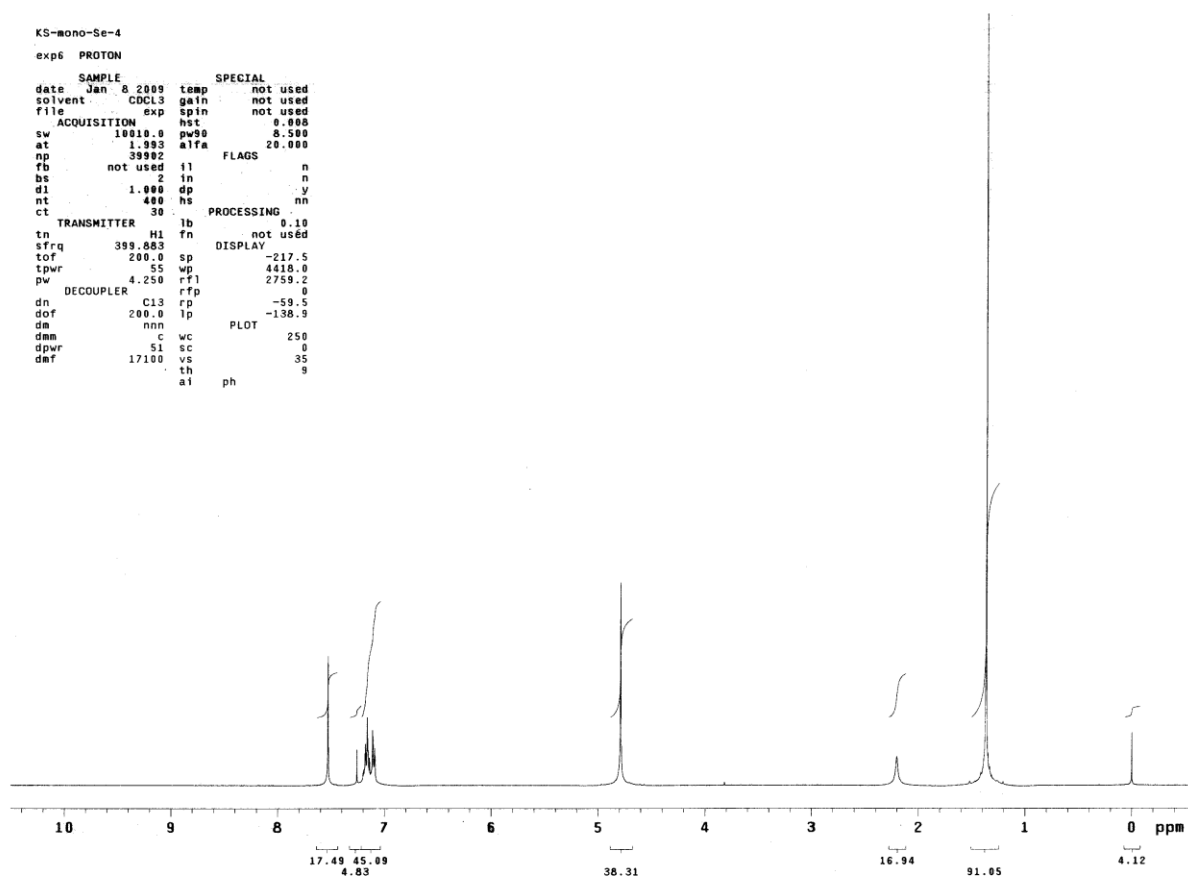


Fig. S28. ^1H NMR Spectrum of **31**

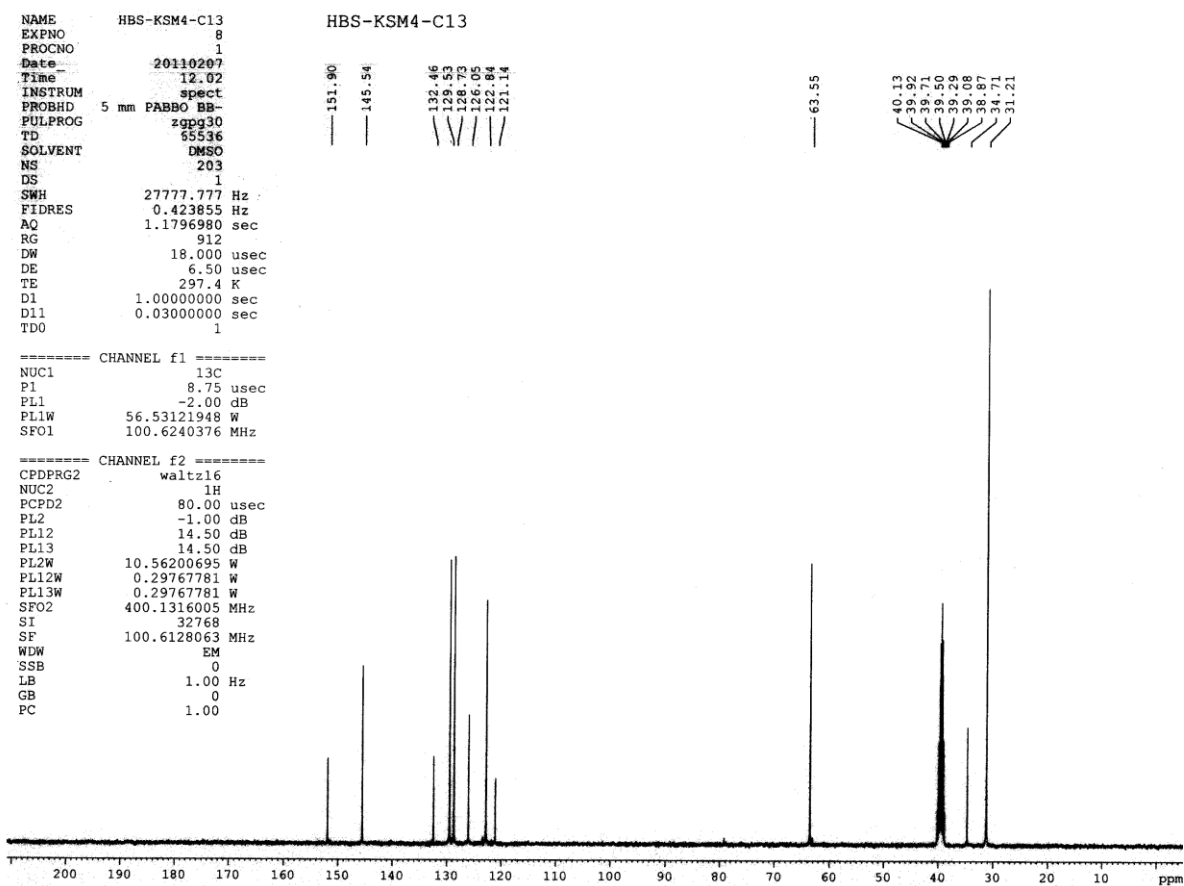


Fig. S29 ^{13}C NMR Spectrum of 31

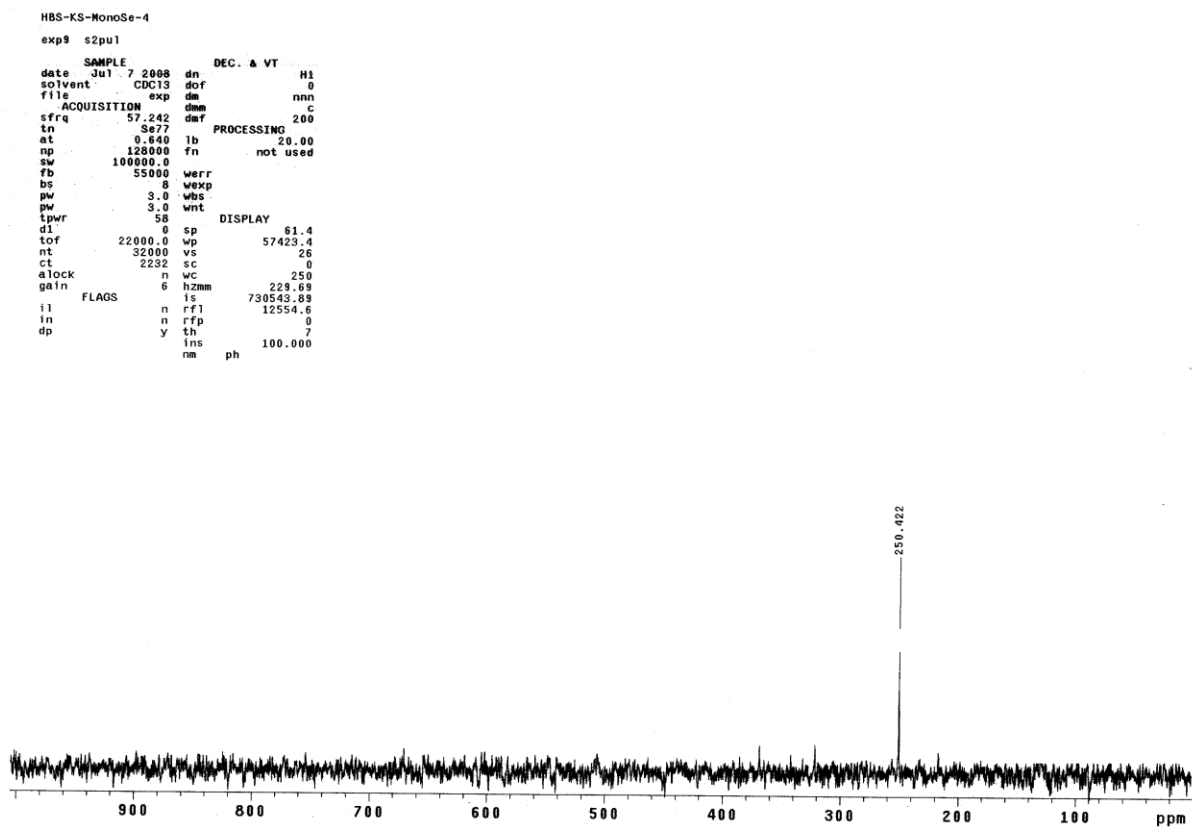


Fig. S30 ^{77}Se NMR Spectrum of **31**

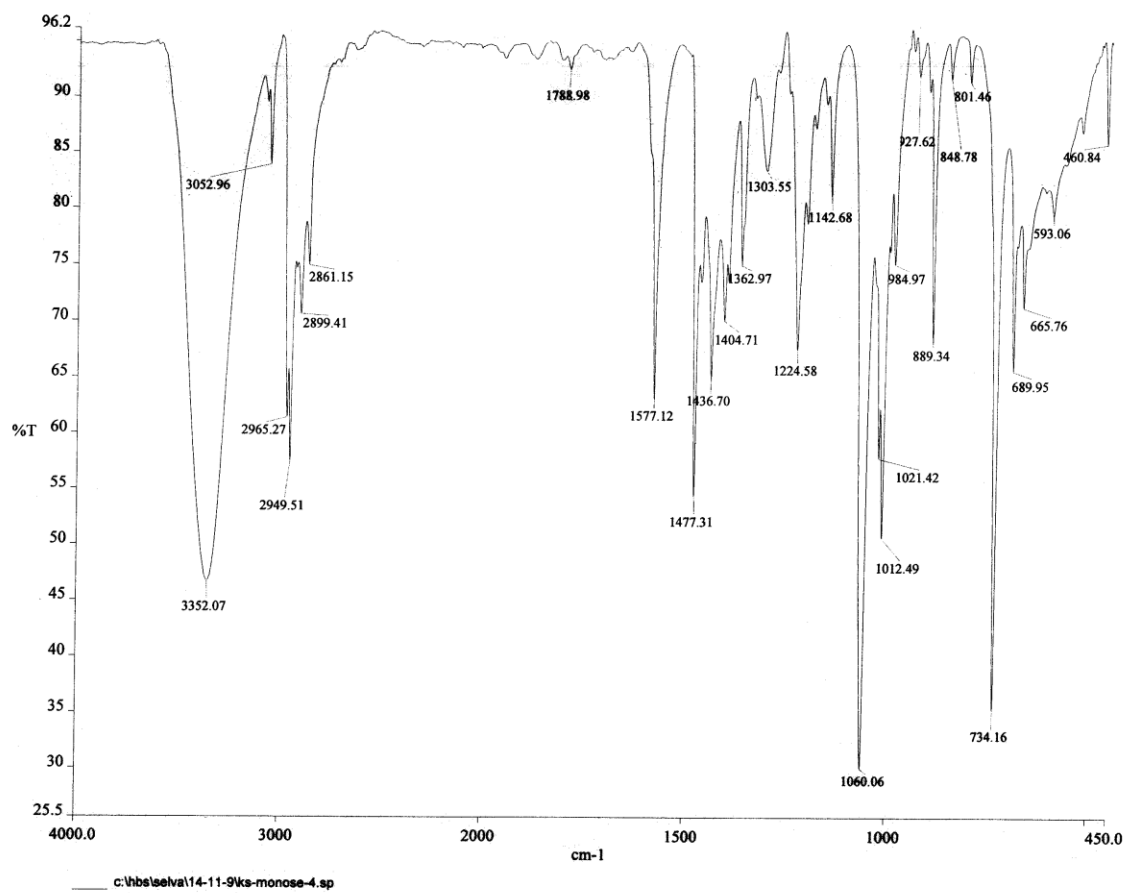


Fig. S31. FT-IR spectrum of **31**

Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

12 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-ToF micro (YA-105)

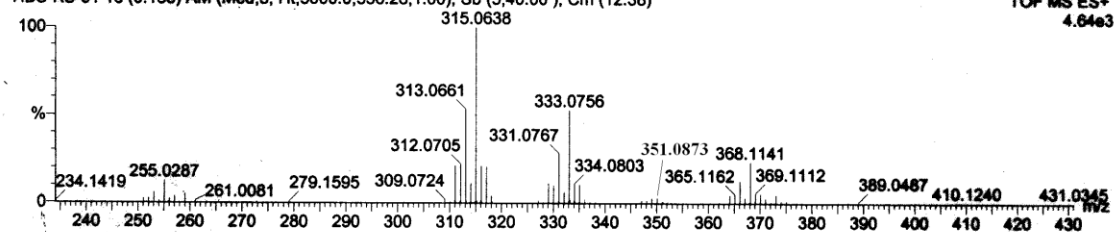
Dept. Of Chemistry I.I.T.(B)

13-Jun-2011 12:31:57

C₁₈H₂₂O₂Se

HBS-KS-31 16 (0.158) AM (Med,5, Ht,5000.0,556.28,1.00); Sb (5,40.00); Cm (12:38)

TOF MS ES+
4.64e3



Minimum:

Maximum: 200.0 20.0 -1.5

Mass Calc. Mass mDa PPM DBE Score Formula

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
351.0873	351.0863	1.0	2.7	8.5	1	C ₁₈ H ₂₃ O ₂ Se

Fig. S32. ES-HRMS spectrum of 31

Eager 300 Report

Page: 1 Sample: KSM4 (KSM4)

Method Name : SP061109
Method File : D:\CHNS2008\SP061109.mth
Chromatogram : KSM4
Operator ID : SP
Analysed : 11/06/2009 10:15
Sample ID : KSM4 (# 13)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 11/6/2009 13:10
Instrument N. : Instrument #1
Sample weight : .525

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Carbon	61.8350	67	803921	RS	1.000000	.246719E+07
Hydrogen	5.6762	178	164388	RS	4.890388	.525645E+07
Totals	67.5112		968309			

Fig. S33 Elemental analysis for 31

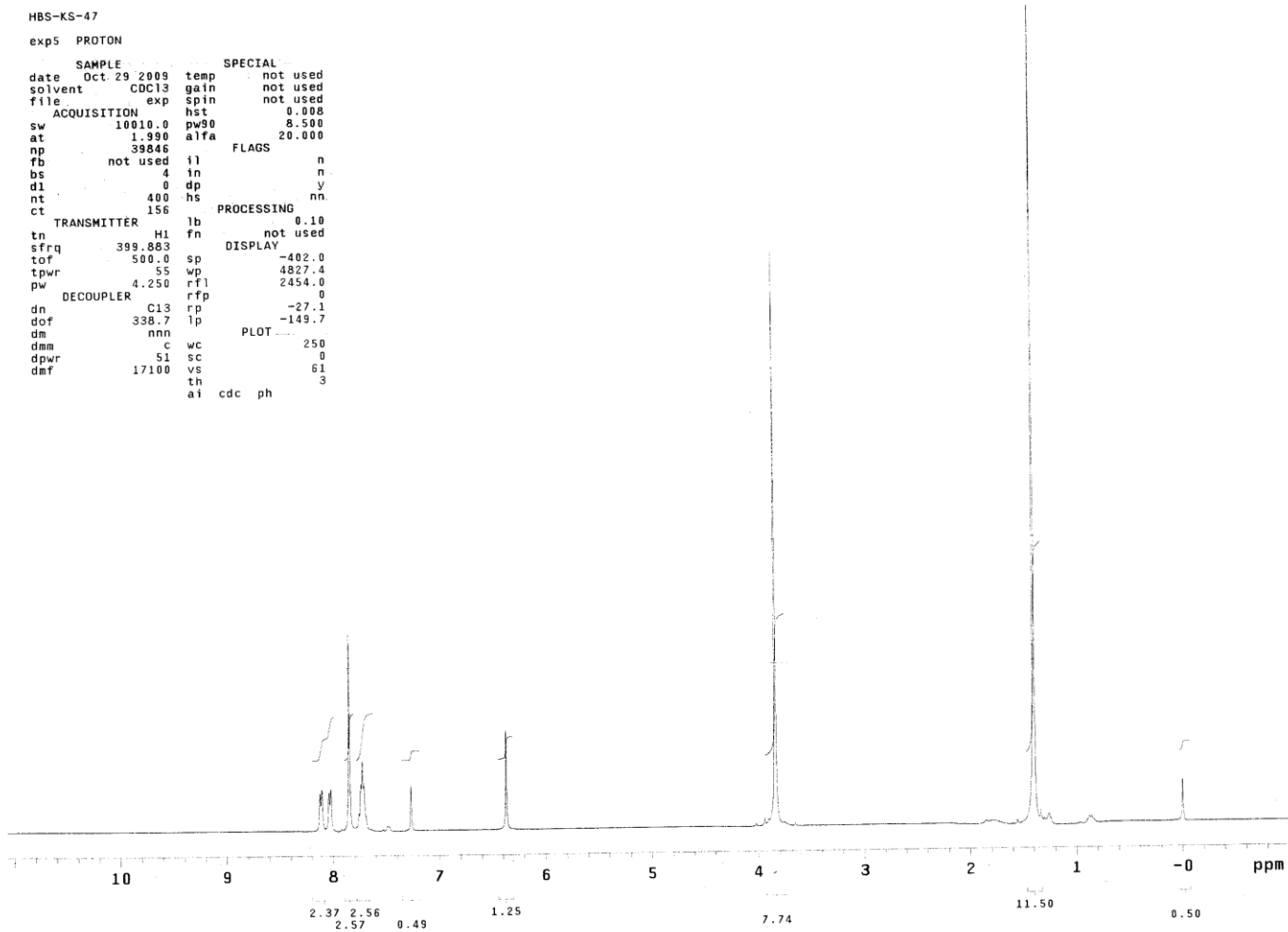


Fig. S34 ^1H NMR spectrum of **37**

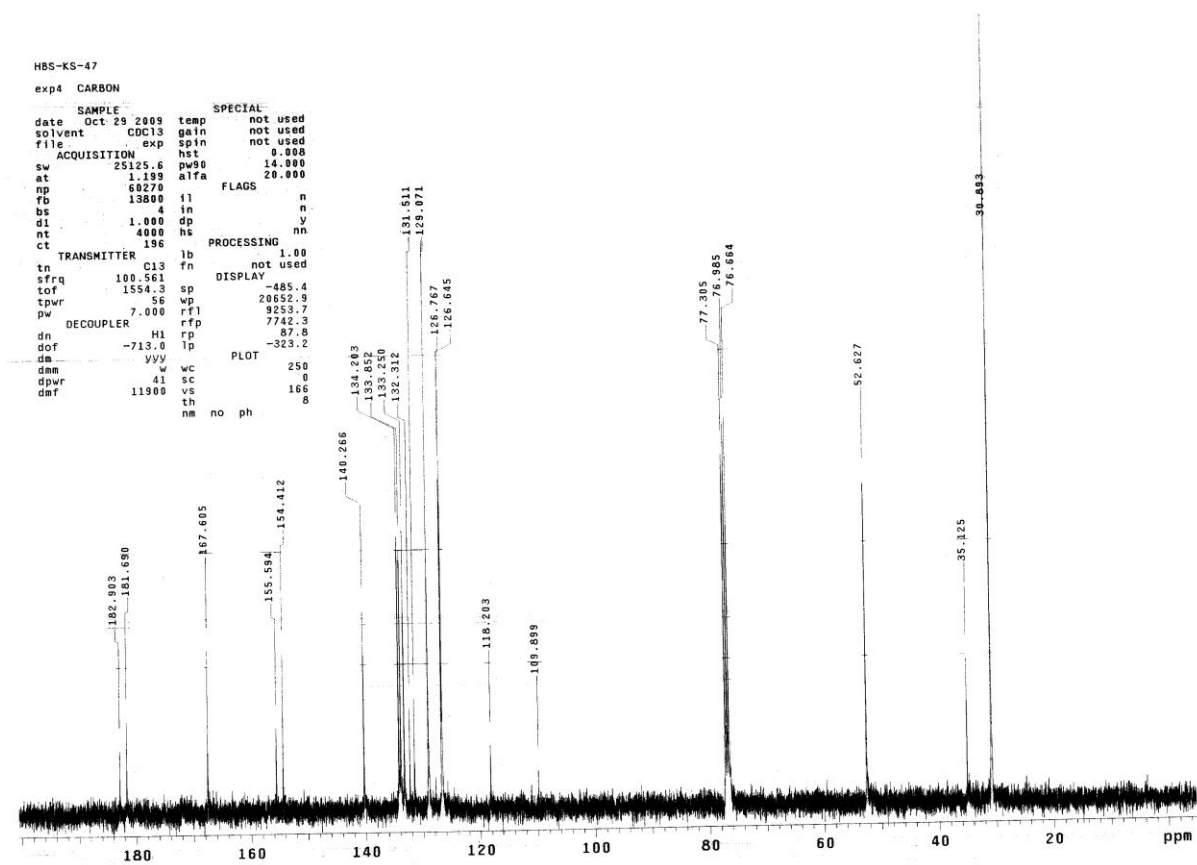


Fig. S35 ^{13}C NMR spectrum of **37**

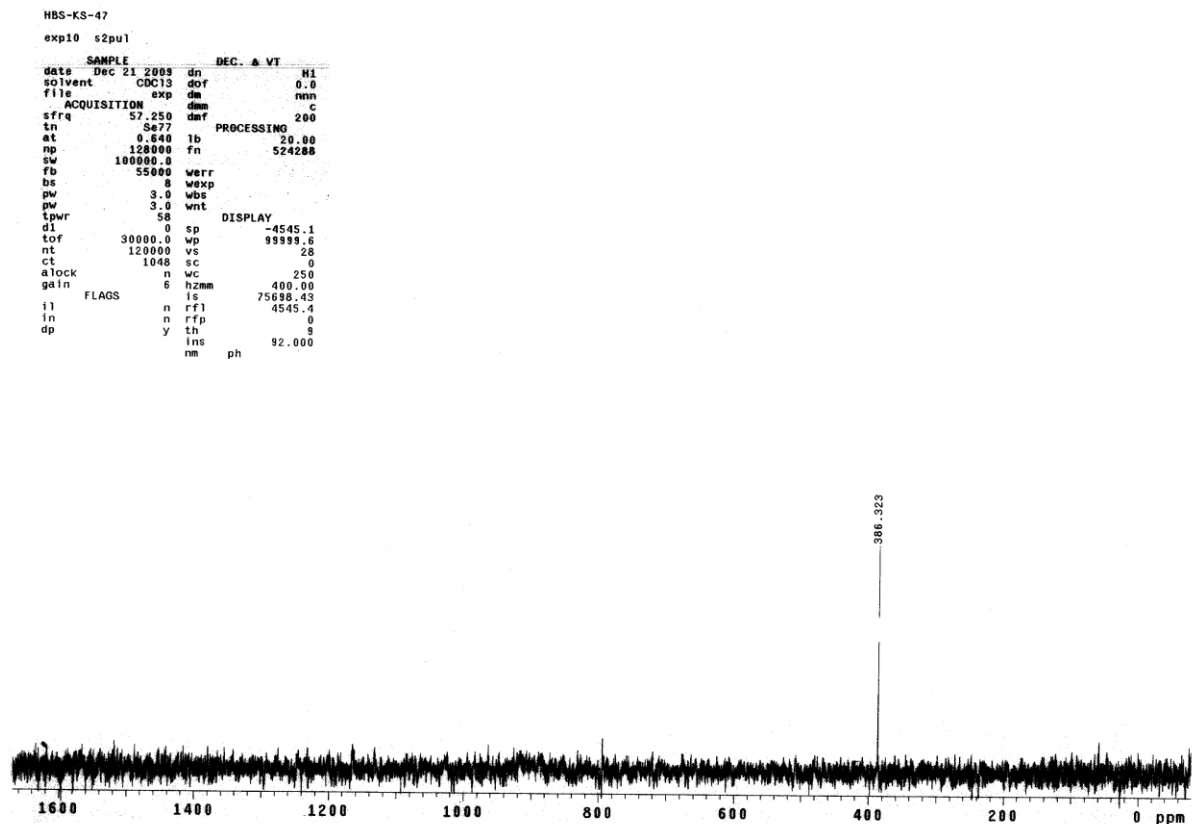


Fig. S36 ^{77}Se NMR spectrum of **37**

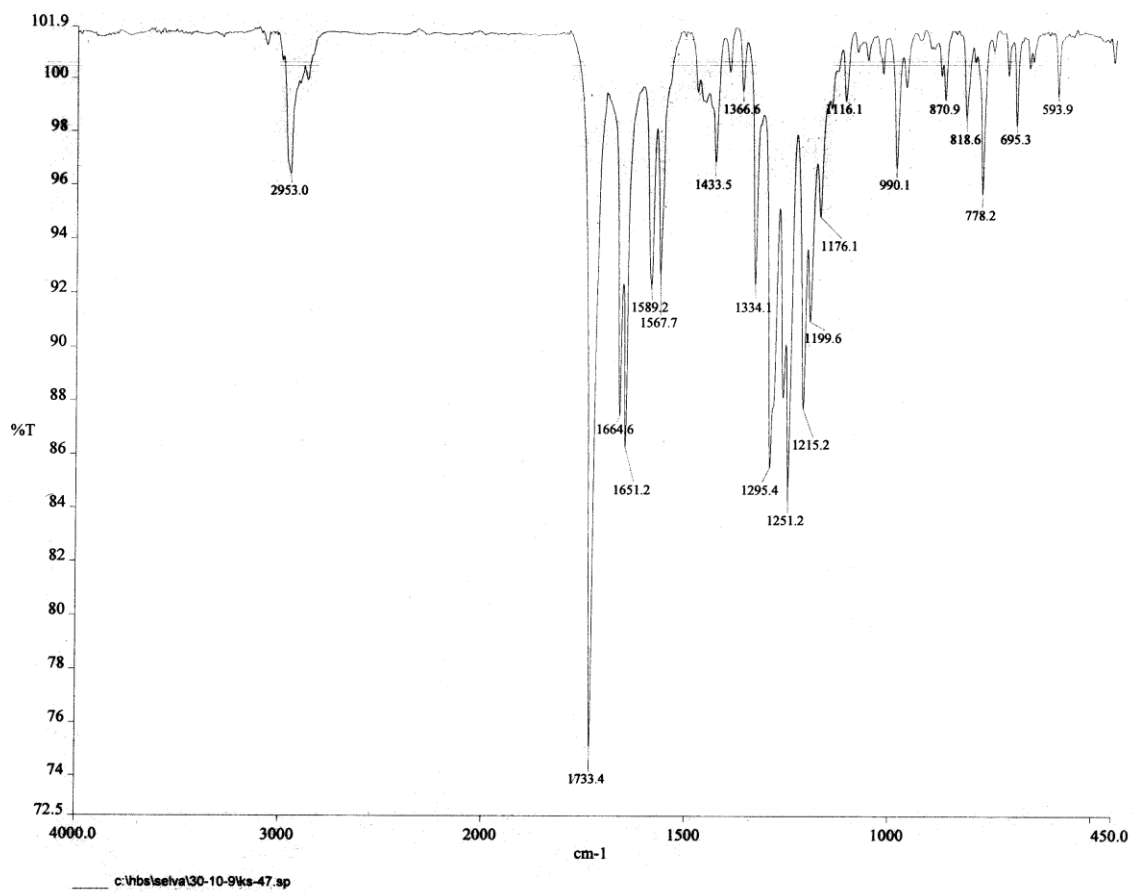


Fig. S37 FT-IR spectrum of **37**

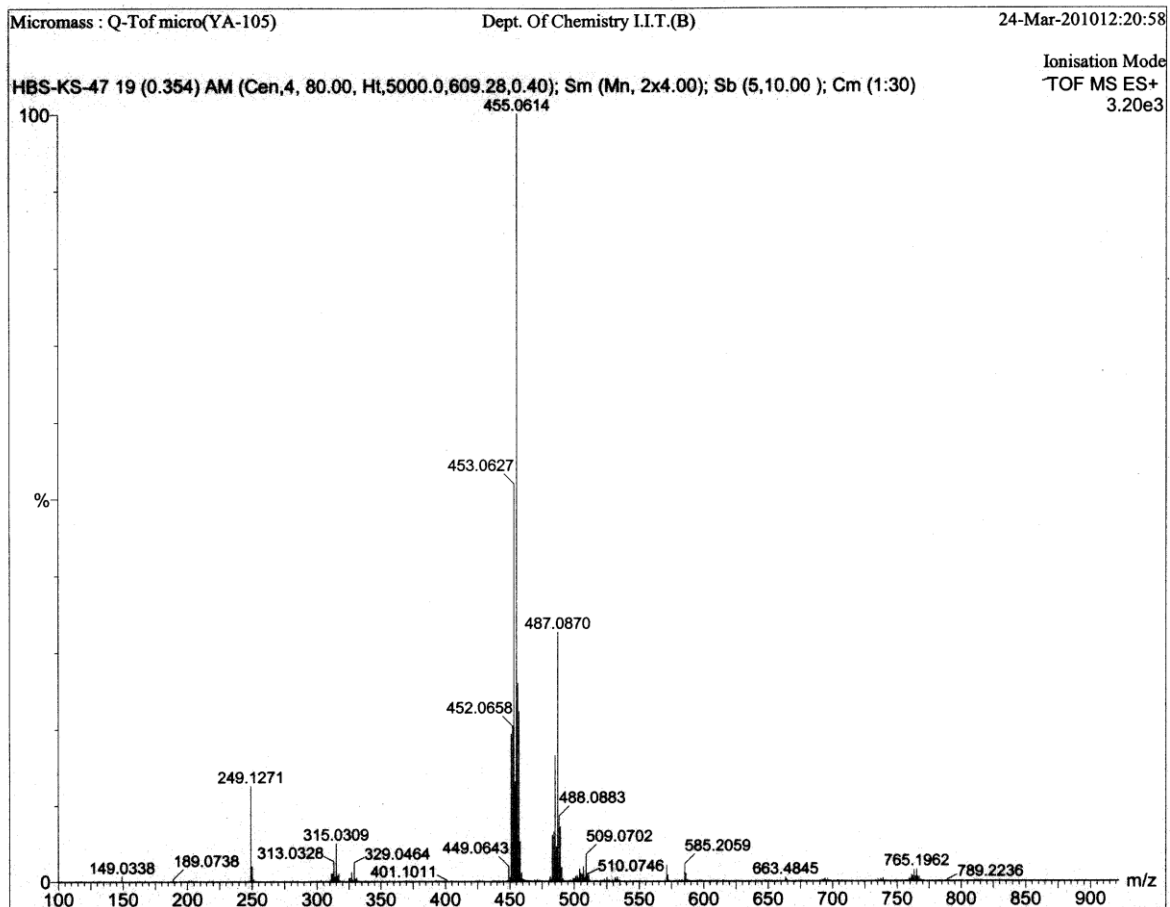


Fig. S38 ES-MS spectrum of **37**

Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-ToF micro (YA-105)

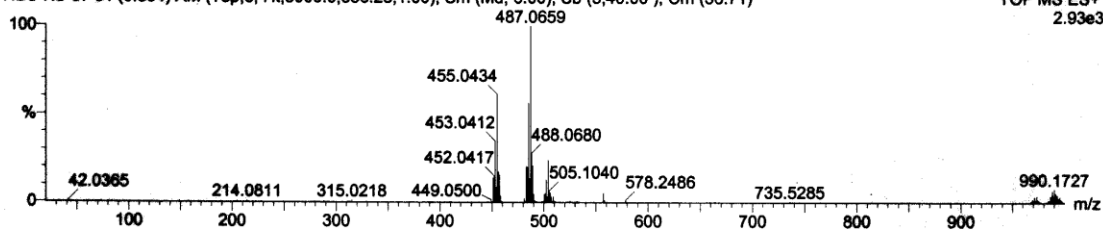
Dept. Of Chemistry I.I.T.(B)

13-Jun-2011 12:45:20

C₂₄H₂₂O₆Se

HBS-KS-37 51 (0.504) AM (Top,5, Ht,5000.0,556.28,1.00); Sm (Md, 6.00); Sb (5,40.00); Cm (36:71)

TOF MS ES+
2.93e3



Minimum:

Maximum:

200.0 20.0 -1.5

50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
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487.0659	487.0660	0.0	-0.1	14.5	1	C ₂₄ H ₂₃ O ₆ Se
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Fig. S39 ES-HRMS spectrum of 37

Eager 300 Report

Page: 1 Sample: KS-47 (KS-47)

Method Name : SP291009
Method File : D:\CHNS2008\SP291009.mth
Chromatogram : KS-47
Operator ID : MP
Analysed : 10/29/2009 15:05
Sample ID : KS-47 (# 28)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 10/29/2009 16:35
Instrument N. : Instrument #1
Sample weight : 1.395

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	11162	RS		0.0000
Carbon	58.9126	66	2033545	RS	1.000000	.247095E+07
Hydrogen	4.6161	172	366071	RS	5.555056	.552060E+07
Totals	63.5287		2410778			

Fig. S40 Elemental analysis for 37

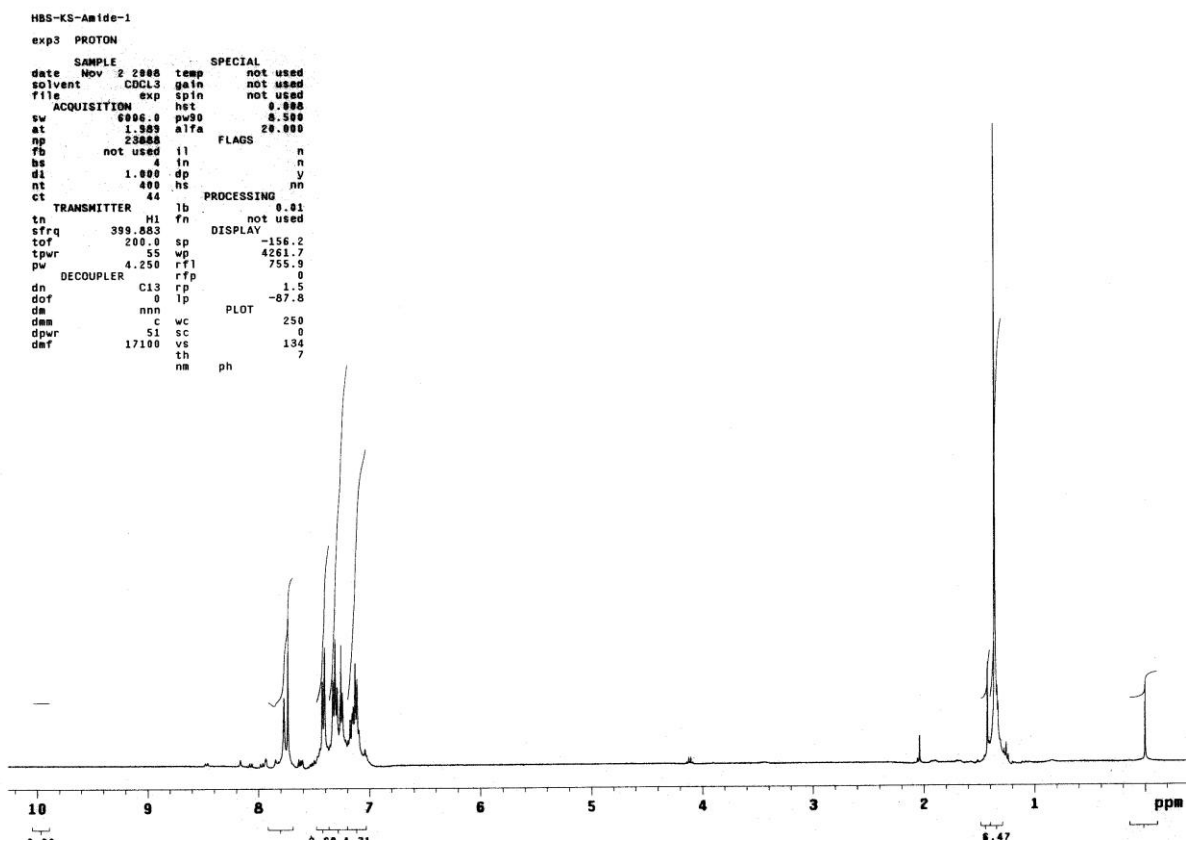


Fig. S41 ^1H NMR spectrum of **38**

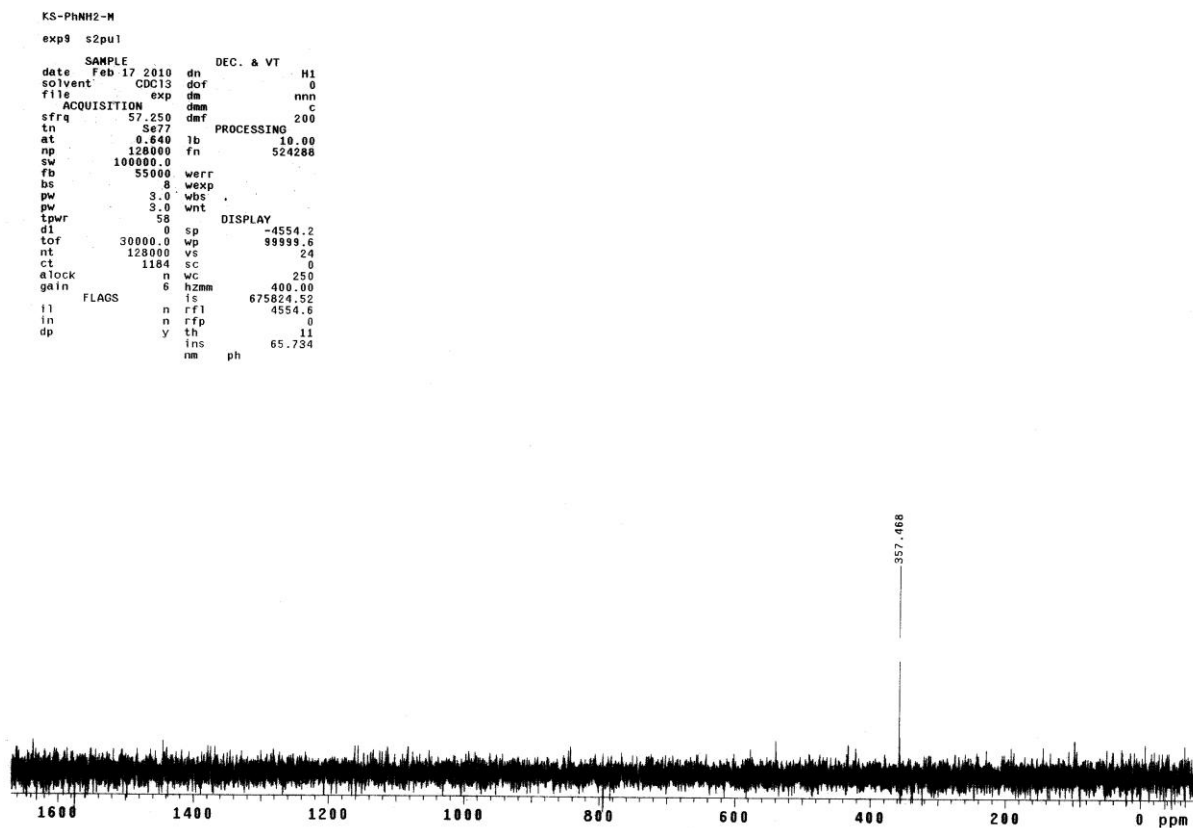


Fig. S42 ^{77}Se NMR spectrum of **38**

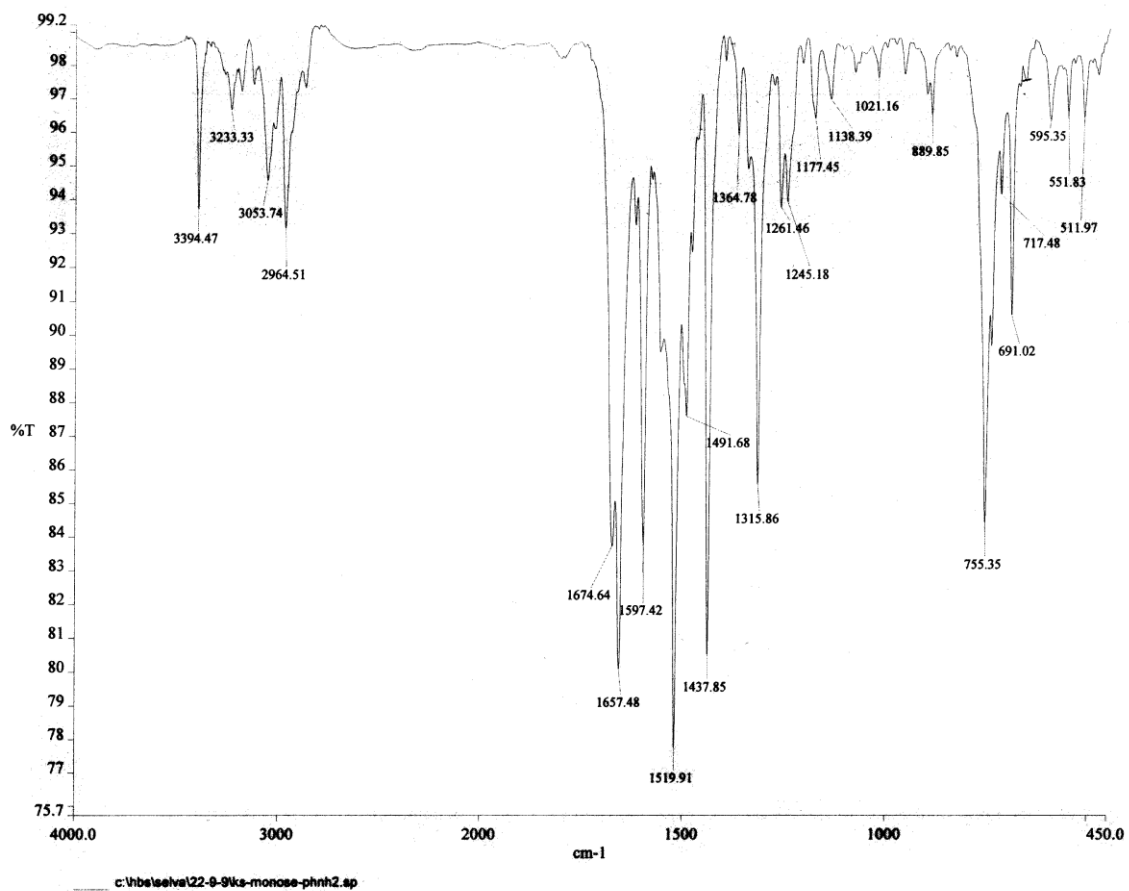


Fig. S43 FT-IR spectrum of **38**

Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

28 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-ToF micro (YA-105)

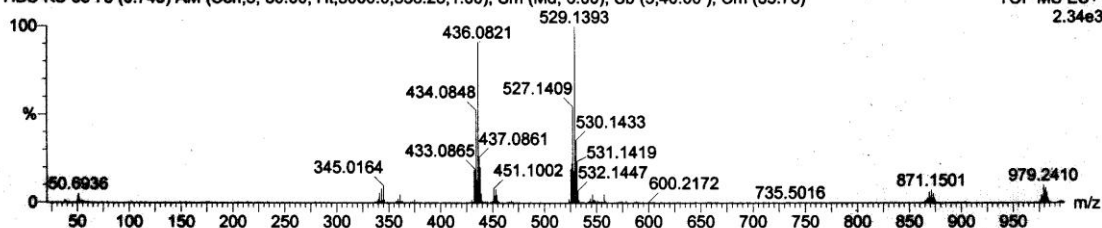
Dept. Of Chemistry I.I.T.(B)

13-Jun-201112:53:45

C₃₀H₂₉N₂O₂Se

HBS-KS-38 75 (0.749) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (Md, 6.00); Sb (5,40.00); Cm (35:76)

TOF MS ES+
2.34e3



Minimum:

Maximum: 200.0 20.0 -1.5

Mass Calc. Mass mDa PPM DBE Score Formula

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
529.1393	529.1394	-0.1	-0.3	18.5	1	C ₃₀ H ₂₉ N ₂ O ₂ Se

Fig. S44 ES-HRMS spectrum of 38

S2. GPx-Like activity of 25, 29, 30, 31, 37 and 47

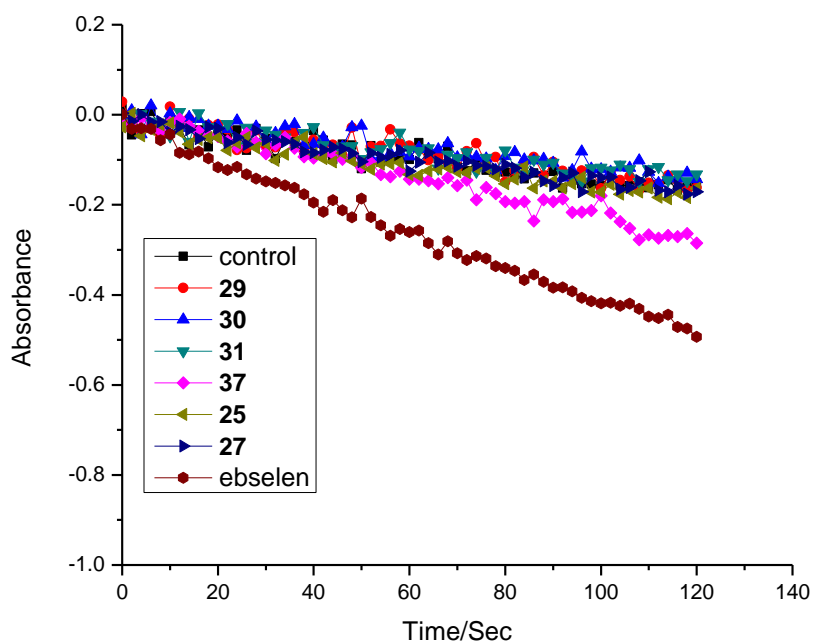


Fig. S45. Figure showing the decrease of absorbance (Depletion of NADH concentration) with respect to time at 340 nm.

Table S1. Glutathione peroxides like activity of control

S.No	$\Delta A/\text{Min}$	Initial reaction rates ($\mu\text{M min}^{-1}$)	Initial reaction rate ($\mu\text{M min}^{-1}$)
1	0.064	10.29	
2	0.068	10.93	10.56 ± 0.33
3	0.065	10.45	

Table S2. Glutathione peroxides like activity of ebselen

S.No	$\Delta A/\text{Min}$	Initial reaction rates ($\mu\text{M min}^{-1}$)	Initial reaction rate ($\mu\text{M min}^{-1}$)
1	0.229	36.82	
2	0.226	36.33	35.69 ± 1.55
3	0.211	33.92	

Table S3. Glutathione peroxides like activity of **25**

S.No	$\Delta A/\text{Min}$	Initial reaction rates ($\mu\text{M min}^{-1}$)	Initial reaction rate ($\mu\text{M min}^{-1}$)
1	0.080	12.86	
2	0.079	12.86	12.91 ± 0.09
3	0.081	13.02	

Table S4. Glutathione peroxides like activity of **27**

S.No	$\Delta A/\text{Min}$	Initial reaction rates ($\mu\text{M min}^{-1}$)	Initial reaction rate ($\mu\text{M min}^{-1}$)
1	0.083	13.34	
2	0.080	12.86	12.80 ± 0.57
3	0.076	12.21	

Table S5. Glutathione peroxides like activity of **29**

S.No	$\Delta A/\text{Min}$	Initial reaction rates ($\mu\text{M min}^{-1}$)	Initial reaction rate ($\mu\text{M min}^{-1}$)
1	0.072	11.58	
2	0.083	13.34	12.54 ± 0.89
3	0.079	12.70	

Table S6. Glutathione peroxides like activity of **30**

S.No	$\Delta A/\text{Min}$	Initial reaction rates ($\mu\text{M min}^{-1}$)	Initial reaction rate ($\mu\text{M min}^{-1}$)
1	0.084	13.50	
2	0.082	13.18	13.07 ± 0.49
3	0.078	12.54	

Table S7. Glutathione peroxides like activity of **31**

S.No	$\Delta A/\text{Min}$	Initial reaction rates ($\mu\text{M min}^{-1}$)	Initial reaction rate ($\mu\text{M min}^{-1}$)
1	0.073	11.58	
2	0.072	11.58	11.74 ± 0.28
3	0.075	12.06	

Table S8. Glutathione peroxides like activity of **37**

S.No	$\Delta A/\text{Min}$	Initial reaction rates ($\mu\text{M min}^{-1}$)	Initial reaction rate ($\mu\text{M min}^{-1}$)
1	0.132	21.22	
2	0.134	21.54	21.49 ± 0.24
3	0.135	21.70	

Table S9. Glutathione peroxides like activity of **47**

S.No	$\Delta A/\text{Min}$	Initial reaction rates ($\mu\text{M min}^{-1}$)	Initial reaction rate ($\mu\text{M min}^{-1}$)
1	0.116	18.64	
2	0.123	19.77	19.34 ± 0.61
3	0.122	19.61	

S3. Cyclic Voltammogram (CV) of 25, 27, 29, 30, 31, 37, 38 and 47.

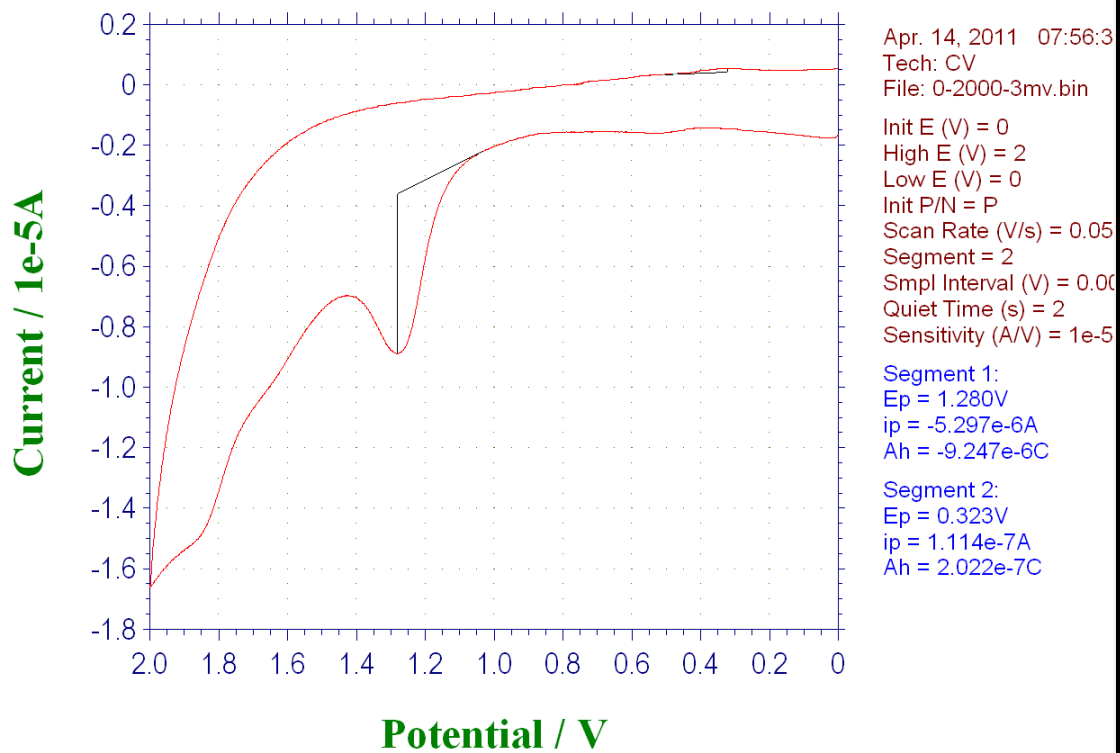


Fig. S46 CV of 25.

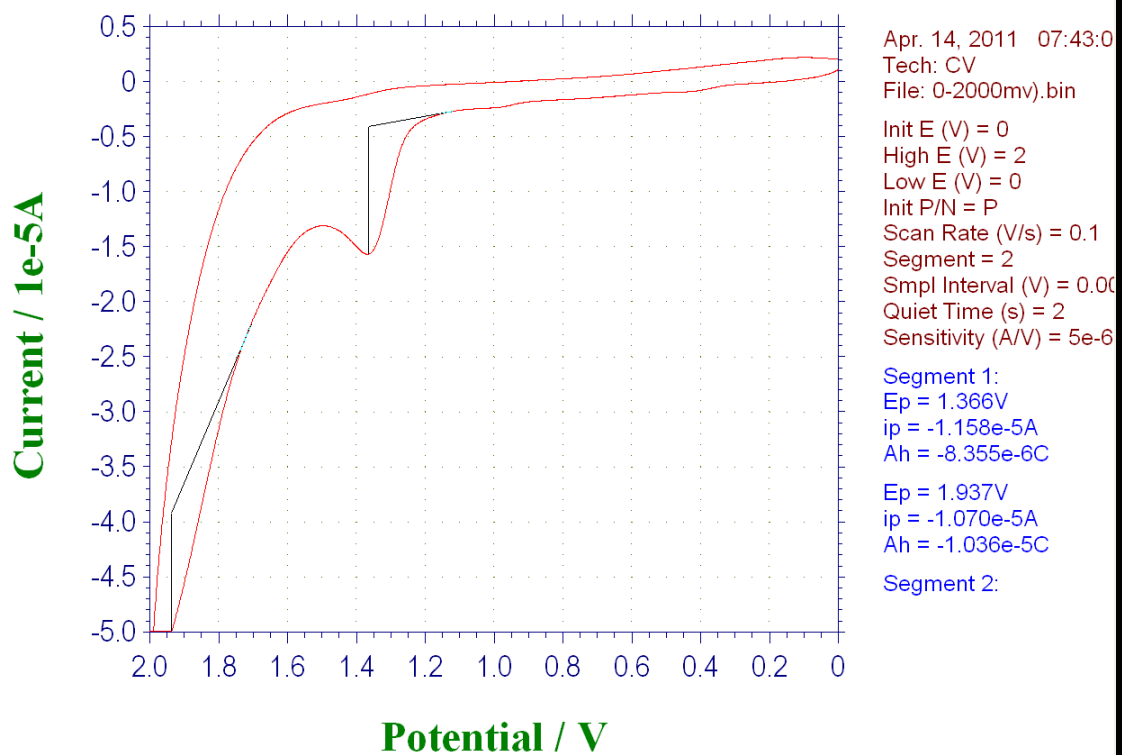


Fig. S47 CV of 27.

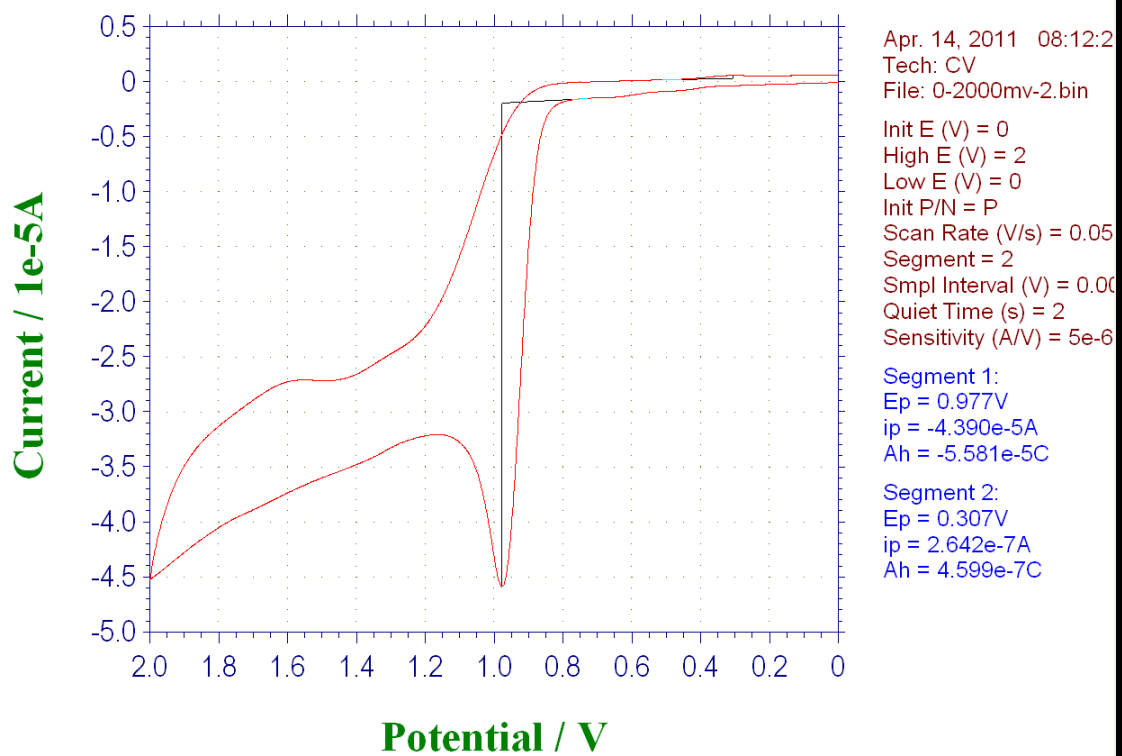


Fig. S48. CV of 29

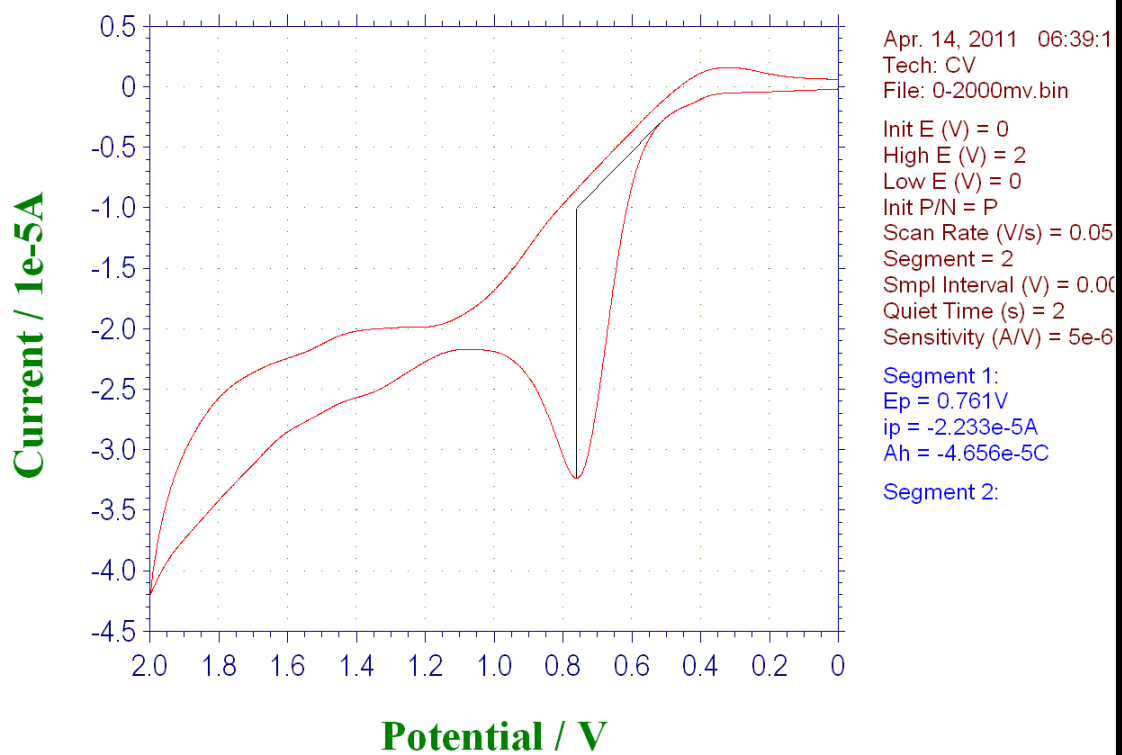


Fig. S49 CV of **30**

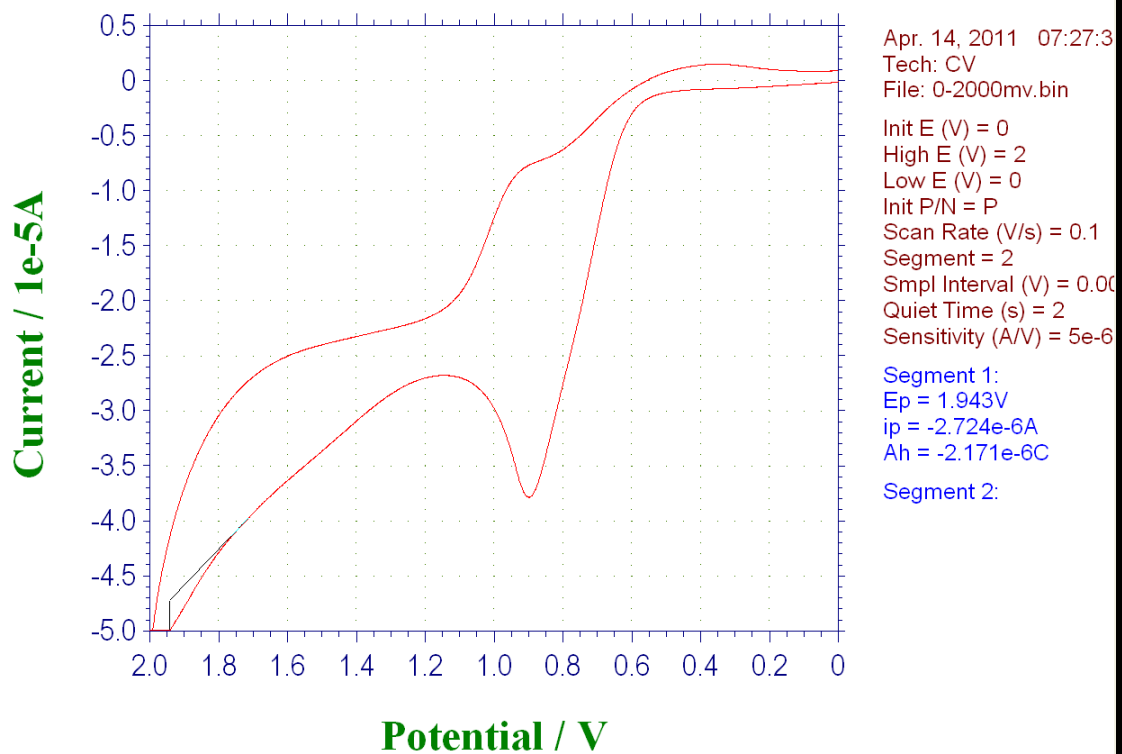


Fig. S50 CV of 31

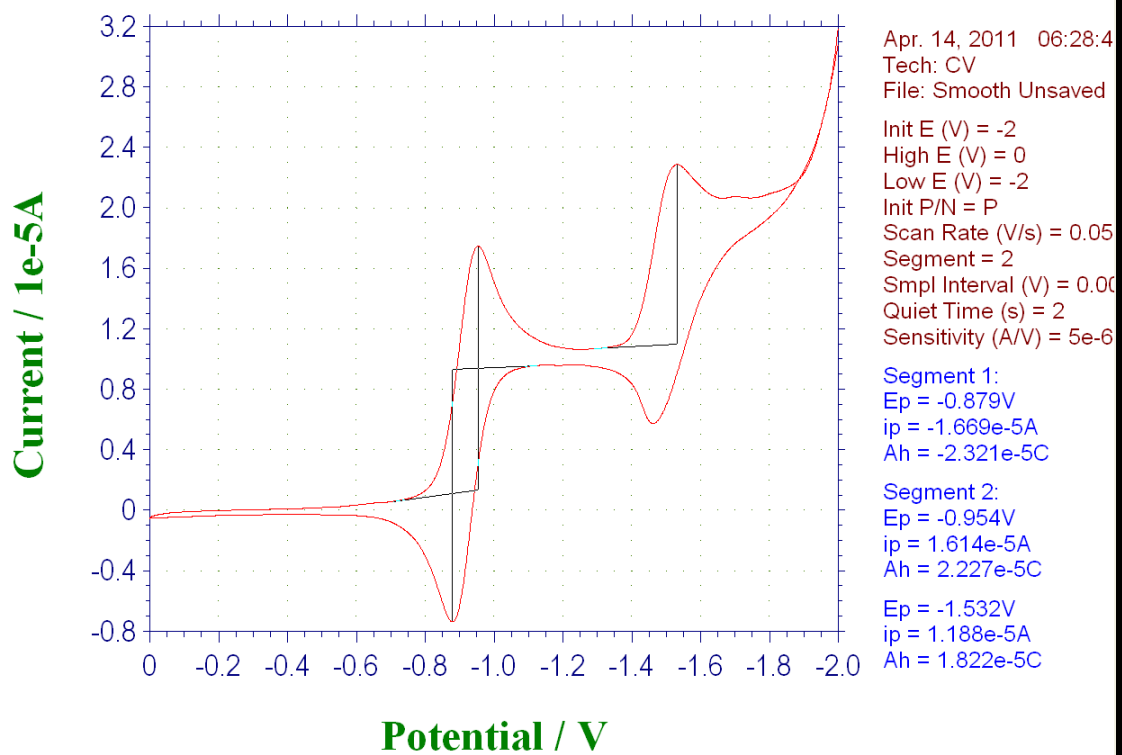


Fig. S51 CV for 37

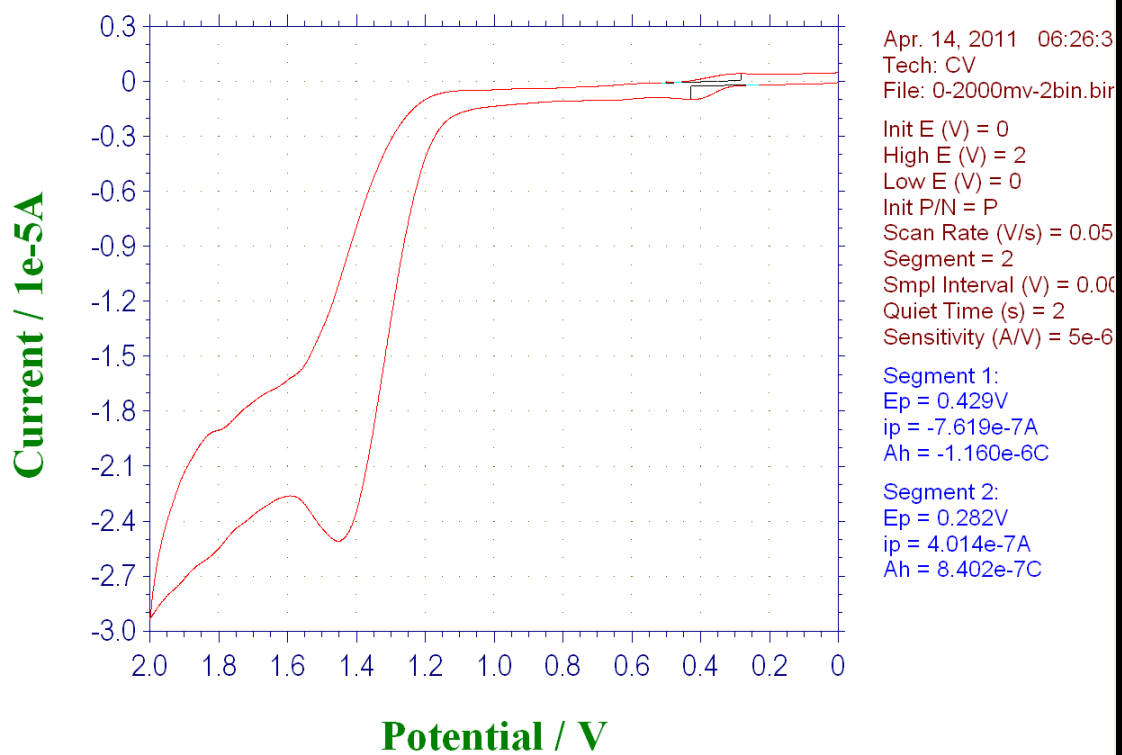


Fig. S52 CV of 37

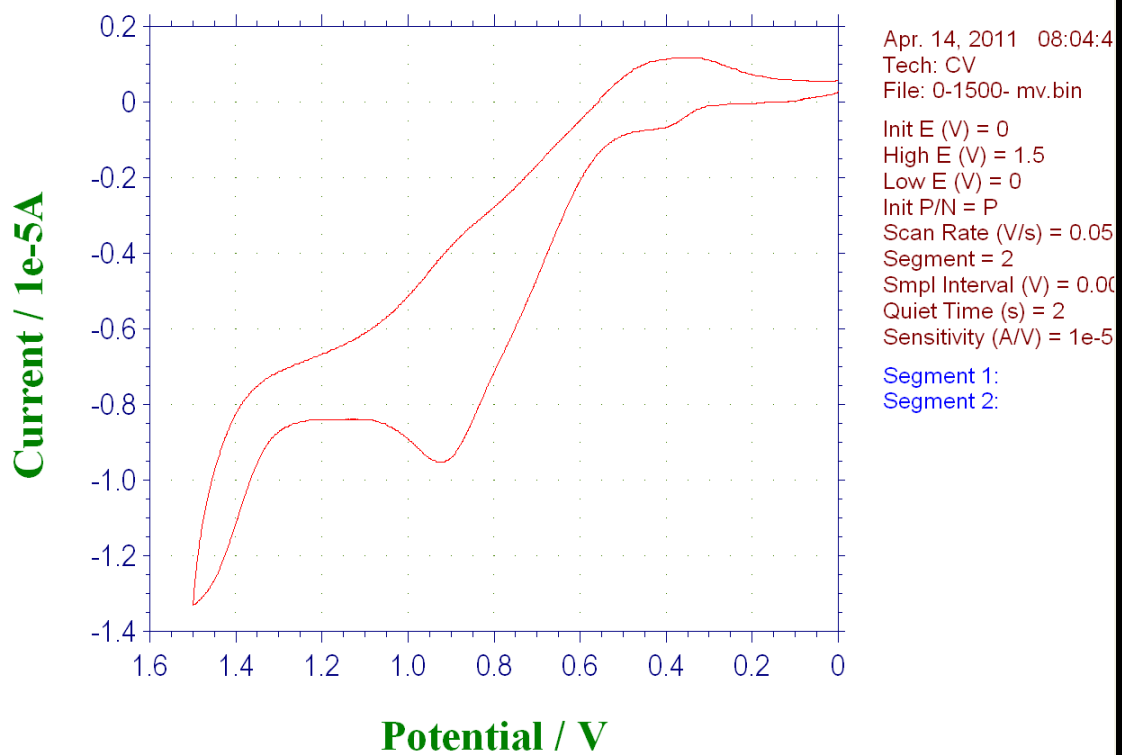


Fig. S53 CV of 38

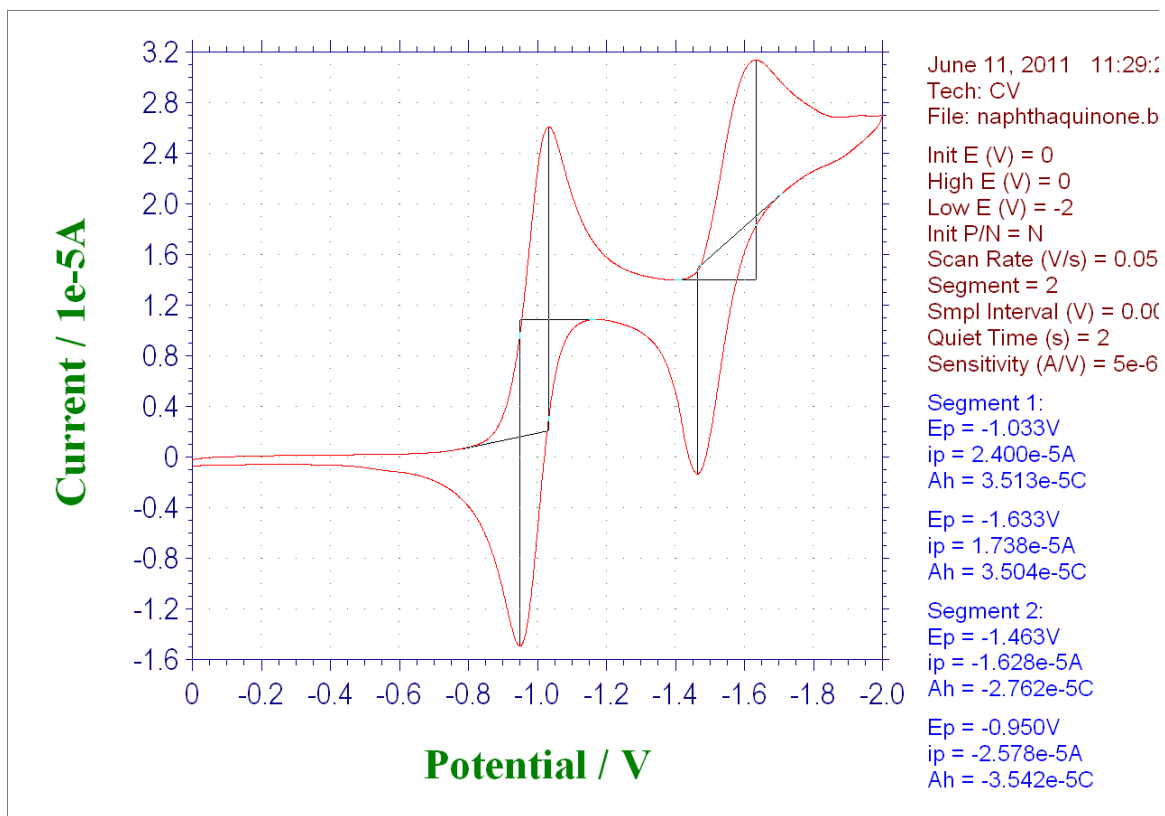
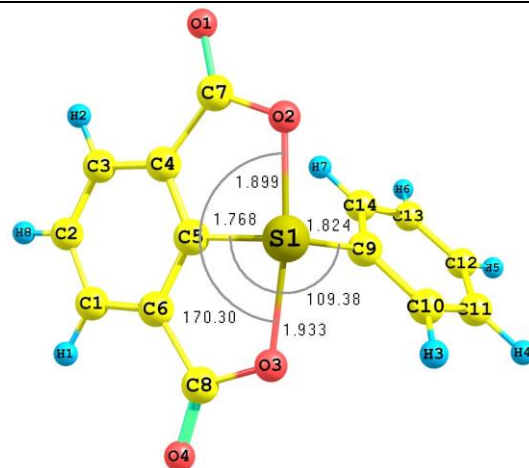


Fig. S54 CV of 47

S4. Geometries and coordinates for the optimized molecules

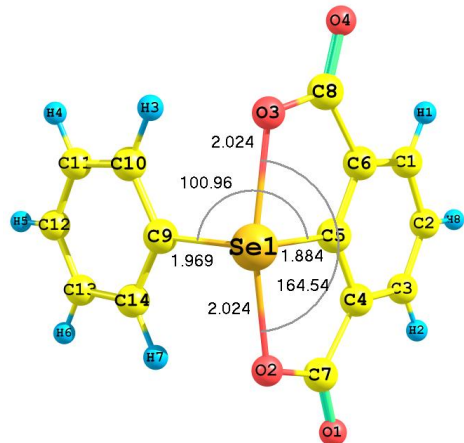


24

Electronic energy = -1237.35533758

No of imaginary frequency = 0

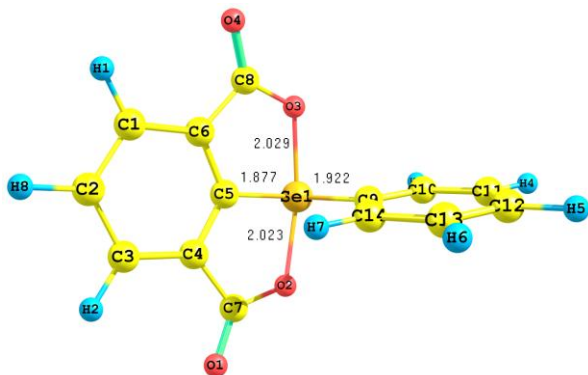
8	-1.562048000	-3.412214000	-0.513297000
8	-0.068402000	-1.861235000	-1.211884000
8	0.267984000	1.936078000	-0.993284000
8	-0.870454000	3.618013000	0.006325000
6	-2.777850000	1.402144000	1.022194000
1	-3.136909000	2.362937000	1.377935000
6	-3.466388000	0.213444000	1.312865000
6	-3.025744000	-1.034653000	0.846331000
1	-3.575259000	-1.945012000	1.064890000
6	-1.860057000	-1.093330000	0.078715000
6	-1.207910000	0.093815000	-0.166285000
6	-1.615653000	1.340393000	0.250511000
6	-1.180556000	-2.264092000	-0.563244000
6	-0.719128000	2.440154000	-0.236292000
6	1.713980000	-0.137503000	-0.209124000
6	2.778701000	0.701385000	-0.544672000
1	2.674323000	1.437996000	-1.332257000
6	3.969583000	0.593225000	0.173672000
1	4.804362000	1.239630000	-0.080118000
6	4.083923000	-0.331289000	1.212771000
1	5.012519000	-0.408597000	1.770893000
6	3.006681000	-1.158468000	1.534757000
1	3.092159000	-1.880396000	2.341491000
6	1.812879000	-1.074649000	0.817585000
1	0.989863000	-1.736904000	1.053399000
1	-4.372866000	0.262546000	1.909164000
16	0.206275000	0.017451000	-1.224187000



25a

Electronic Energy = -3238.58513312
No of imaginary frequency = 0

8	-1.287066000	-3.555131000	-0.023679000
8	-0.054306000	-2.005520000	-1.110019000
8	-0.051208000	2.005687000	-1.109266000
8	-1.280771000	3.556821000	-0.021483000
6	-2.785269000	1.229114000	1.276486000
1	-3.200452000	2.171934000	1.619094000
6	-3.303594000	0.002094000	1.718573000
6	-2.787439000	-1.225570000	1.275747000
1	-3.204293000	-2.167866000	1.617766000
6	-1.724397000	-1.225580000	0.368568000
6	-1.235894000	0.000798000	-0.014244000
6	-1.722257000	1.227804000	0.369278000
6	-1.017147000	-2.395839000	-0.254130000
6	-1.012999000	2.397199000	-0.252761000
6	1.735400000	-0.001184000	-0.100205000
6	2.307545000	1.217249000	0.268609000
1	1.874283000	2.153140000	-0.059283000
6	3.452567000	1.205076000	1.067610000
1	3.898328000	2.149349000	1.366714000
6	4.020139000	-0.002612000	1.474527000
1	4.911940000	-0.003171000	2.094862000
6	3.447820000	-1.209622000	1.072272000
1	3.889900000	-2.154472000	1.374996000
6	2.302799000	-1.220401000	0.273251000
1	1.866226000	-2.155852000	-0.051455000
1	-4.133122000	0.002614000	2.419682000
34	0.159422000	-0.000050000	-1.280244000

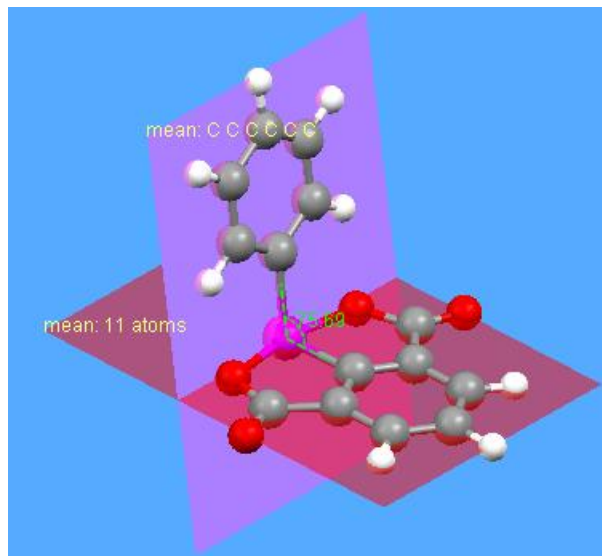


25b

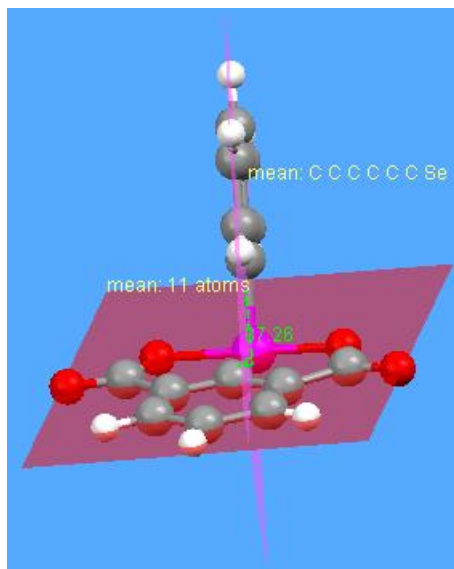
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No of imaginary frequency = 1 (-9.66)

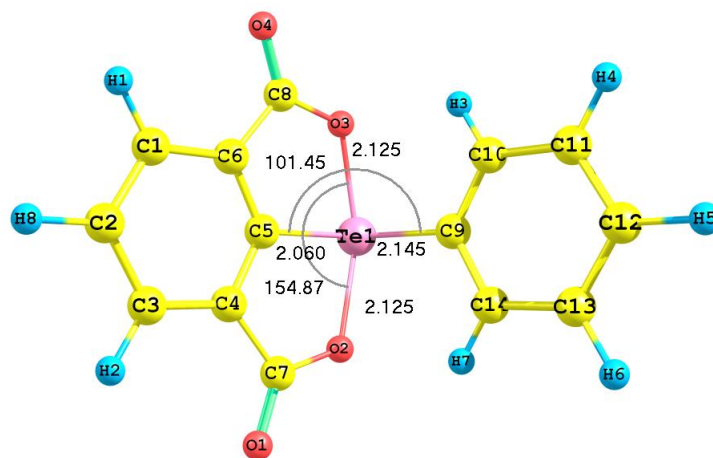
34	0.235692000	0.001974000	-1.222330000
8	-1.445900000	-3.504165000	-0.150634000
8	-0.021933000	-1.997480000	-1.051474000
8	0.166008000	2.012983000	-0.958975000
8	-1.077342000	3.598299000	0.064758000
6	-2.862271000	1.328687000	1.072833000
1	-3.256219000	2.282885000	1.409113000
6	-3.488444000	0.119545000	1.417192000
6	-2.990955000	-1.125795000	1.000579000
1	-3.483317000	-2.052068000	1.280441000
6	-1.839619000	-1.162837000	0.208995000
6	-1.266389000	0.049099000	-0.097706000
6	-1.712295000	1.293705000	0.279927000
6	-1.099238000	-2.356973000	-0.340438000
6	-0.853656000	2.435813000	-0.203646000
6	1.729160000	-0.068558000	-0.015082000
6	2.980581000	0.155044000	-0.585431000
1	3.072967000	0.369620000	-1.645976000
6	4.112773000	0.111465000	0.229082000
1	5.093071000	0.287445000	-0.203530000
6	3.979750000	-0.158190000	1.591567000
1	4.861212000	-0.193070000	2.225181000
6	2.716794000	-0.386144000	2.144303000
1	2.615979000	-0.598666000	3.204558000
6	1.577622000	-0.345013000	1.341293000
1	0.598153000	-0.527918000	1.769256000
1	-4.384937000	0.148492000	2.029968000



25a



25b

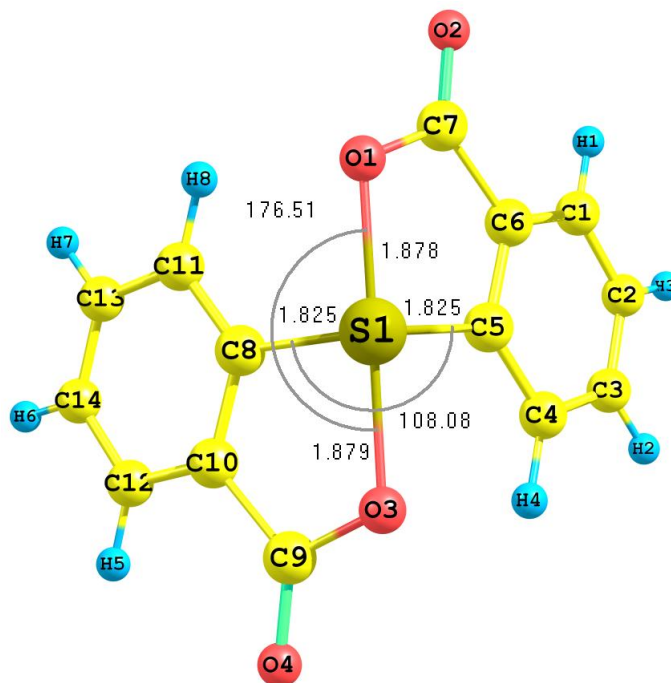


44

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No of imaginary frequency = 0

8	1.388749000	3.566448000	0.203331000
8	0.100186000	2.074450000	-0.896142000
8	0.100218000	-2.074439000	-0.895985000
8	1.388880000	-3.566378000	0.203459000
6	2.903298000	-1.228194000	1.409118000
1	3.301983000	-2.170177000	1.773190000
6	3.420950000	0.000131000	1.849492000
6	2.903254000	1.228402000	1.409022000
1	3.301904000	2.170430000	1.773015000
6	1.847438000	1.228320000	0.490739000
6	1.385559000	0.000034000	0.074844000
6	1.847479000	-1.228210000	0.490838000
6	1.109024000	2.418516000	-0.069170000
6	1.109131000	-2.418455000	-0.068988000
6	-1.870201000	-0.000017000	0.058210000
6	-2.423545000	-1.219893000	0.452614000
1	-1.981675000	-2.156488000	0.130680000
6	-3.547633000	-1.209787000	1.282222000
1	-3.981821000	-2.152421000	1.603292000
6	-4.107308000	0.000074000	1.696956000
1	-4.982147000	0.000116000	2.341217000
6	-3.547626000	1.209892000	1.282097000
1	-3.981797000	2.152556000	1.603100000
6	-2.423550000	1.219905000	0.452474000
1	-1.981672000	2.156458000	0.130425000
1	4.241656000	0.000173000	2.561184000
52	-0.180737000	-0.000108000	-1.263389000



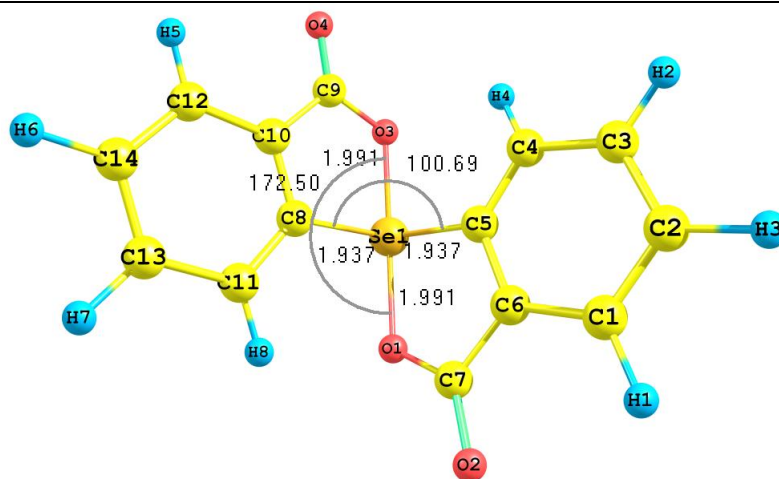
45

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No of imaginary frequency = 0

8	0.847769000	-1.675244000	-1.183904000
8	2.694595000	-2.696878000	-0.381272000
6	3.416661000	-0.077082000	0.859803000
1	4.140473000	-0.862394000	1.053766000
6	3.576526000	1.218980000	1.347287000
6	2.622331000	2.202712000	1.063659000
1	2.758637000	3.212156000	1.440644000
6	1.491333000	1.915331000	0.293043000
6	1.344815000	0.610699000	-0.169723000
6	2.291027000	-0.374290000	0.093400000
6	1.999657000	-1.710783000	-0.494259000
1	4.447940000	1.469870000	1.945014000
16	0.000211000	-0.000364000	-1.241307000
1	0.762027000	2.678069000	0.055829000
6	-1.344836000	-0.610898000	-0.169731000
8	-0.847787000	1.675304000	-1.184321000
6	-1.999427000	1.710796000	-0.494549000
6	-2.290935000	0.374250000	0.093075000
8	-2.694445000	2.696869000	-0.381206000
6	-1.491647000	-1.915446000	0.293271000

6	-3.416615000	0.077403000	0.859520000
6	-2.622730000	-2.202473000	1.063850000
6	-3.576738000	-1.218515000	1.347284000
1	-4.140180000	0.862992000	1.053270000
1	-4.448162000	-1.469113000	1.945118000
1	-2.759254000	-3.211865000	1.440900000
1	-0.762447000	-2.678403000	0.056422000



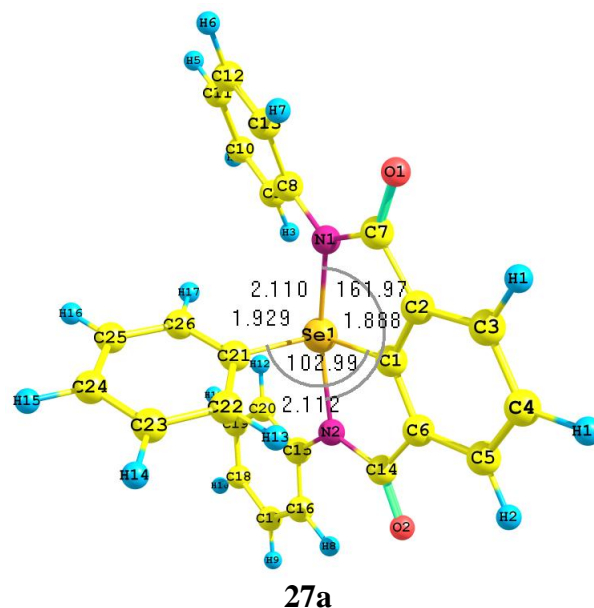
1

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No of imaginary frequency = 0

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6	-3.341458000	-0.027532000	1.115380000
1	-4.072702000	0.738914000	1.352613000
6	-3.430217000	-1.320273000	1.630738000
6	-2.471348000	-2.283741000	1.297903000
1	-2.553194000	-3.290168000	1.698149000
6	-1.405314000	-1.973292000	0.447393000
6	-1.330889000	-0.673324000	-0.036111000
6	-2.284664000	0.292970000	0.263261000
6	-2.096701000	1.651692000	-0.337837000
1	-4.251245000	-1.584069000	2.291049000
1	-0.665671000	-2.715369000	0.173220000
6	1.330776000	0.673050000	-0.035875000
8	1.026528000	-1.701702000	-1.141416000
6	2.096990000	-1.651891000	-0.337322000
6	2.284776000	-0.292980000	0.263513000
8	2.832120000	-2.594115000	-0.129452000
6	1.404531000	1.973164000	0.447348000
6	3.341481000	0.028187000	1.115520000
6	2.470353000	2.284167000	1.297850000

6	3.429616000	1.321053000	1.630695000
1	4.073082000	-0.737829000	1.353028000
1	4.250543000	1.585279000	2.290960000
1	2.551941000	3.290635000	1.698045000
1	0.664178000	2.714419000	0.172779000
34	0.000313000	-0.000135000	-1.272288000

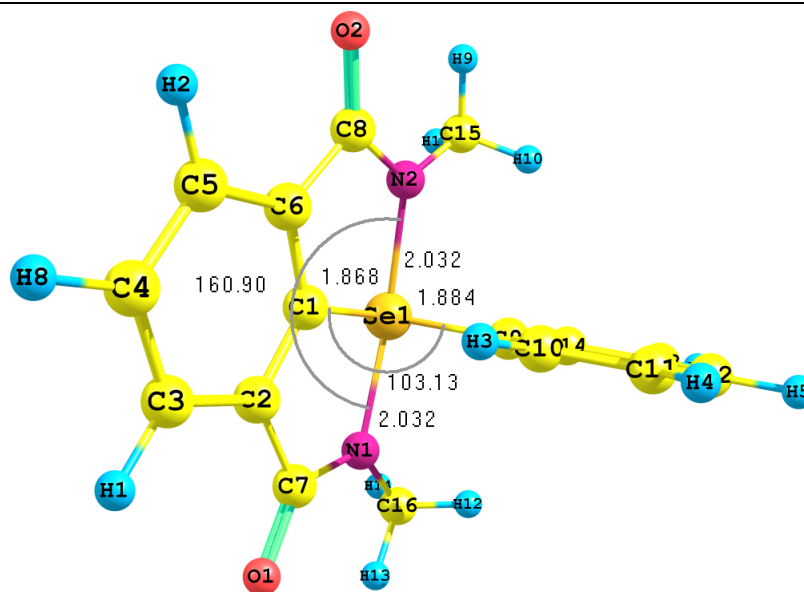


Electronic Energy = -3660.94345754

No of imaginary frequency = 0

34	0.020278000	0.086907000	-0.568886000
8	-3.492521000	2.282556000	-0.145668000
8	3.662753000	2.083879000	-0.323796000
7	-2.051859000	0.469774000	-0.465670000
7	2.115424000	0.328225000	-0.454569000
6	0.078299000	1.957328000	-0.321340000
6	-1.126649000	2.620385000	-0.196242000
6	-1.076949000	4.005806000	-0.023340000
1	-2.006679000	4.557352000	0.074412000
6	0.168182000	4.647148000	0.023717000
6	1.368610000	3.932608000	-0.085571000
1	2.333486000	4.427104000	-0.035087000
6	1.325211000	2.546162000	-0.255598000
6	-2.373055000	1.786861000	-0.257810000
6	-2.992902000	-0.559779000	-0.661699000
6	-2.628514000	-1.675011000	-1.440167000
1	-1.651902000	-1.702246000	-1.914895000
6	-3.518752000	-2.728430000	-1.639556000

1	-3.215703000	-3.574038000	-2.251722000
6	-4.792518000	-2.692197000	-1.071003000
1	-5.489482000	-3.510082000	-1.230145000
6	-5.161159000	-1.586389000	-0.302377000
1	-6.151713000	-1.542111000	0.143256000
6	-4.278526000	-0.528777000	-0.089935000
1	-4.577133000	0.330438000	0.494594000
6	2.516434000	1.637320000	-0.352850000
6	2.975164000	-0.779738000	-0.602097000
6	4.374339000	-0.697679000	-0.450586000
1	4.825994000	0.258800000	-0.232019000
6	5.160331000	-1.839640000	-0.596208000
1	6.237302000	-1.750643000	-0.476971000
6	4.593418000	-3.080168000	-0.890583000
1	5.217843000	-3.961885000	-1.003040000
6	3.209475000	-3.168015000	-1.041253000
1	2.741500000	-4.120822000	-1.275197000
6	2.411984000	-2.036583000	-0.896140000
1	1.339548000	-2.127490000	-1.032551000
6	-0.038958000	-0.587791000	1.237088000
6	0.382825000	0.186297000	2.315180000
1	0.754149000	1.193801000	2.167392000
6	0.324446000	-0.361182000	3.596192000
1	0.648146000	0.233303000	4.445542000
6	-0.142077000	-1.664074000	3.787569000
1	-0.181651000	-2.083955000	4.788518000
6	-0.553110000	-2.427113000	2.695018000
1	-0.915123000	-3.440946000	2.837689000
6	-0.501110000	-1.891511000	1.407002000
1	-0.835456000	-2.478727000	0.559028000
1	0.203992000	5.724809000	0.156247000



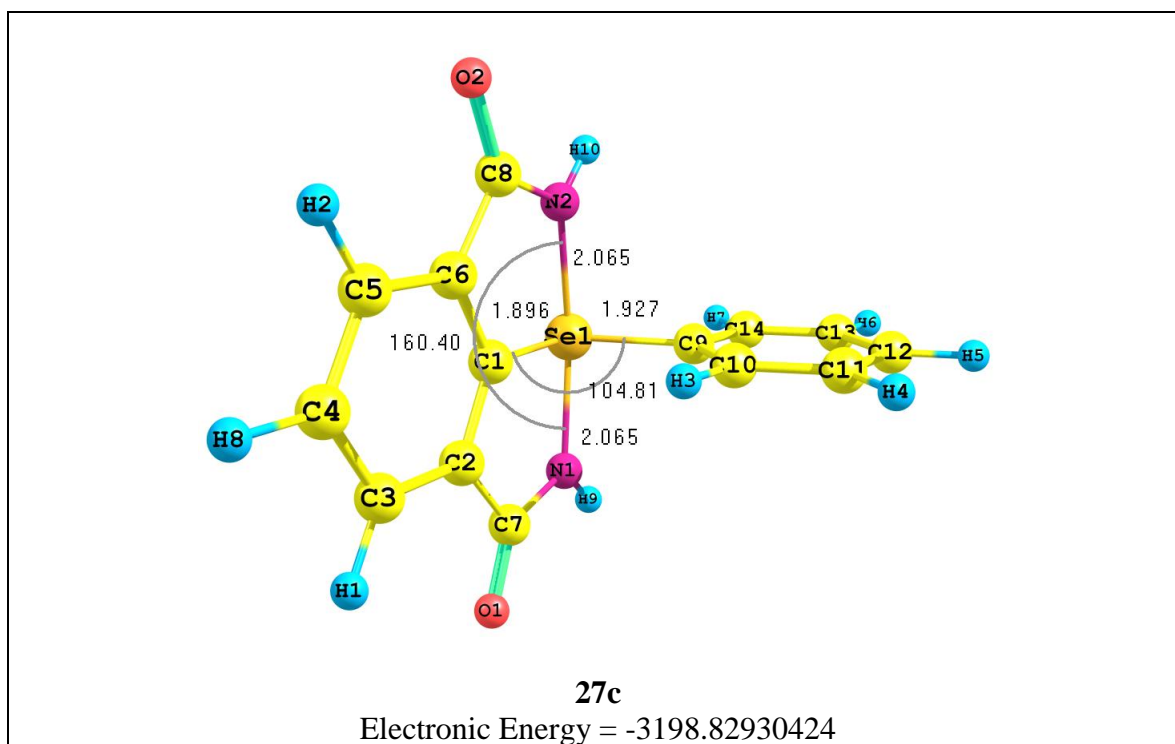
27b

Electronic Energy = -3269.98027899

No of imaginary frequency = 0

34	-0.222588000	-0.000222000	-1.103384000
8	1.397913000	3.571504000	0.091312000
8	1.404120000	-3.569508000	0.090049000
7	-0.033180000	2.003471000	-0.825538000
7	-0.029946000	-2.003554000	-0.825694000
6	1.348552000	0.001008000	-0.093331000
6	1.875424000	1.224998000	0.245805000
6	3.055869000	1.223070000	0.979607000
1	3.493531000	2.184816000	1.271557000
6	3.639190000	0.002740000	1.328096000
6	3.058031000	-1.218485000	0.979125000
1	3.497389000	-2.179582000	1.270664000
6	1.877581000	-1.222189000	0.245332000
6	1.076633000	2.411107000	-0.163469000
6	1.080764000	-2.409567000	-0.164236000
6	-1.574847000	-0.001158000	0.208592000
6	-1.276865000	-0.003215000	1.562655000
1	-0.233442000	-0.004390000	1.899751000
6	-2.327539000	-0.003807000	2.468316000
1	-2.113599000	-0.005365000	3.542649000
6	-3.647372000	-0.002495000	2.021166000
1	-4.467916000	-0.002981000	2.746725000
6	-3.926171000	-0.000693000	0.660907000
1	-4.962596000	0.000157000	0.306492000
6	-2.880995000	-0.000087000	-0.258311000

1	-3.076377000	0.001197000	-1.337586000
1	4.571237000	0.003454000	1.904433000
6	-0.989897000	-2.940188000	-1.299120000
1	-0.667892000	-3.947049000	-0.973861000
1	-1.995062000	-2.729154000	-0.881125000
1	-1.069047000	-2.933893000	-2.403463000
6	-0.994379000	2.938896000	-1.298826000
1	-1.999156000	2.726992000	-0.880288000
1	-0.673324000	3.946171000	-0.973885000
1	-1.074003000	2.932176000	-2.403126000



No of imaginary frequency = 0			
34	0.273575000	-0.000101000	-1.226868000
8	-1.399666000	-3.591249000	-0.027124000
8	-1.399194000	3.591489000	-0.026439000
7	0.060565000	-2.034579000	-0.947346000
7	0.061008000	2.034896000	-0.946938000
6	-1.261603000	0.000126000	-0.114818000
6	-1.791011000	-1.228963000	0.232756000
6	-2.953518000	-1.224310000	1.005885000
1	-3.395005000	-2.171544000	1.300002000
6	-3.524202000	0.000252000	1.380450000
6	-2.953262000	1.224722000	1.006049000
1	-3.394500000	2.172044000	1.300256000
6	-1.790726000	1.229247000	0.232926000
6	-1.036205000	-2.440268000	-0.253010000
6	-1.035702000	2.440535000	-0.252638000
6	1.764997000	-0.000121000	-0.007393000
6	1.602299000	-0.001097000	1.375405000
1	0.612545000	-0.001734000	1.818455000
6	2.739972000	-0.001187000	2.181147000
1	2.629005000	-0.001929000	3.261677000
6	4.015749000	-0.000345000	1.608936000
1	4.895072000	-0.000447000	2.246506000
6	4.160456000	0.000605000	0.221959000
1	5.148937000	0.001282000	-0.228203000
6	3.027410000	0.000705000	-0.594901000
1	3.130550000	0.001447000	-1.676897000
1	-4.430909000	0.000290000	1.979095000
1	0.627158000	-2.764212000	-1.368012000
1	0.627563000	2.764698000	-1.367382000