Supporting Information

Synthesis, structure and reactivity of [o-(2,6-diisopropylphenyl iminomethinyl)phenyl]selenenyl selenocyanate (RSeSeCN) and related derivatives

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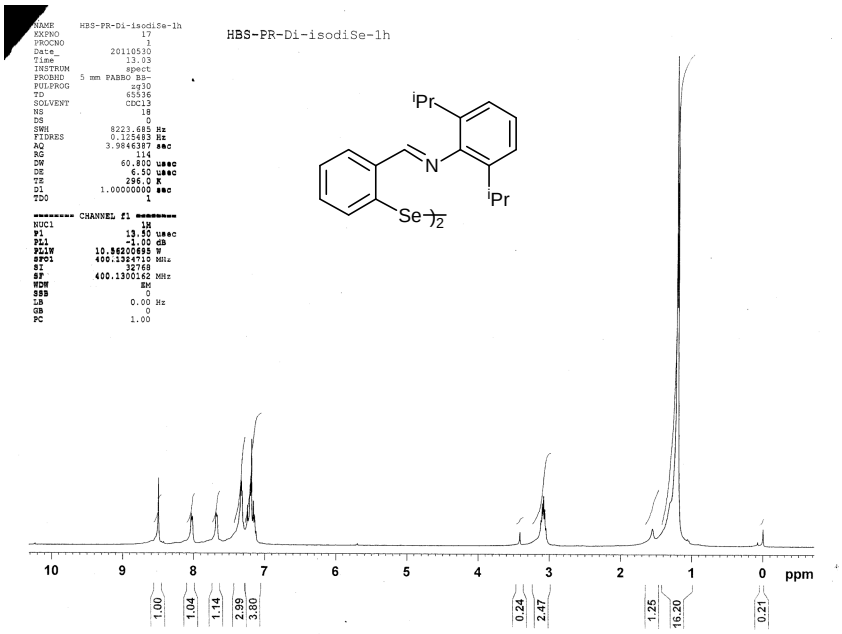


Figure S1. ^{1}H NMR spectrum of **11**

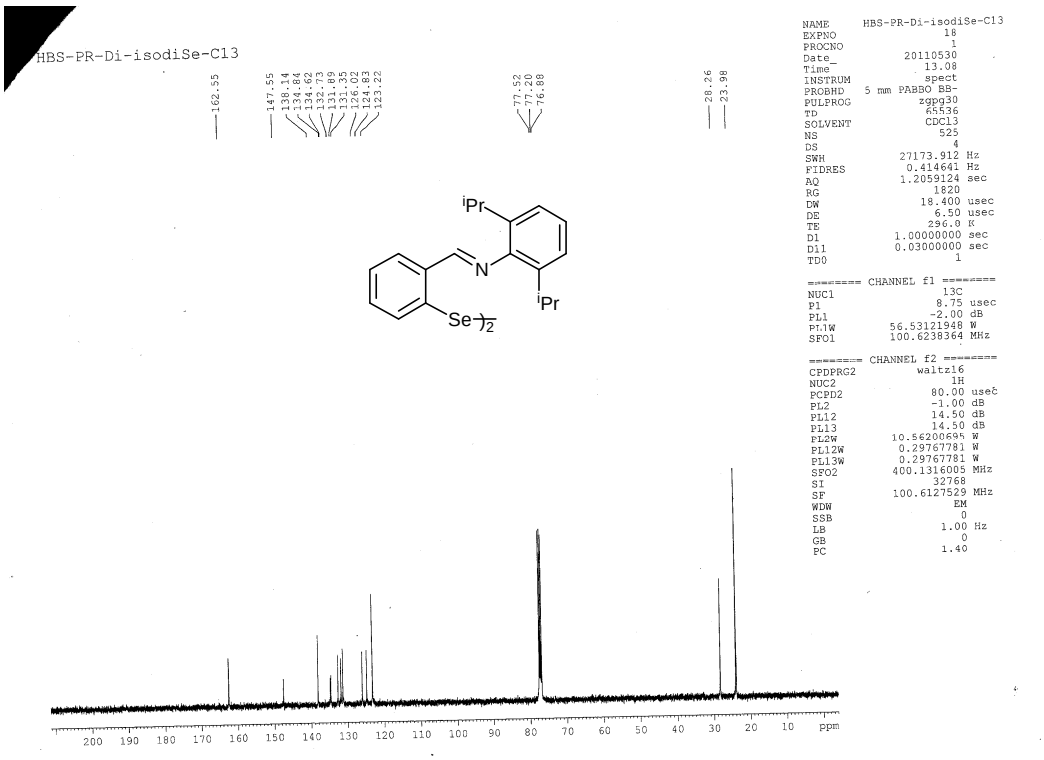


Figure S2. ^{13}C NMR spectrum of **11**

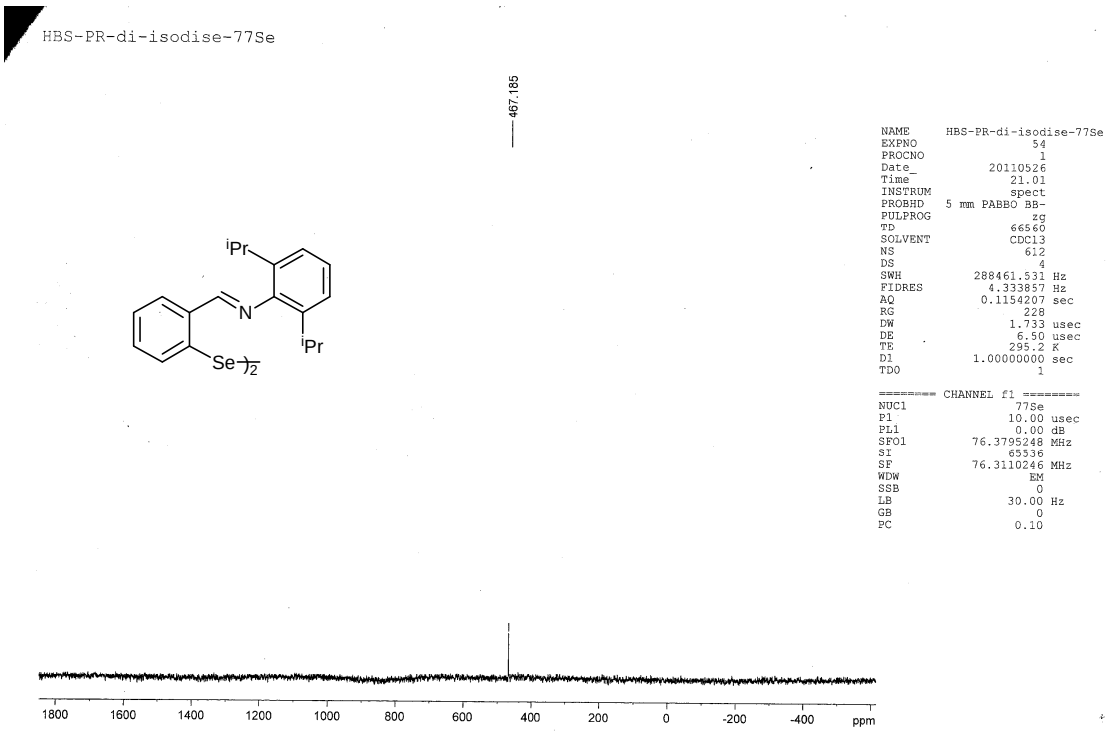


Figure S3. ^{77}Se NMR spectrum of **11**

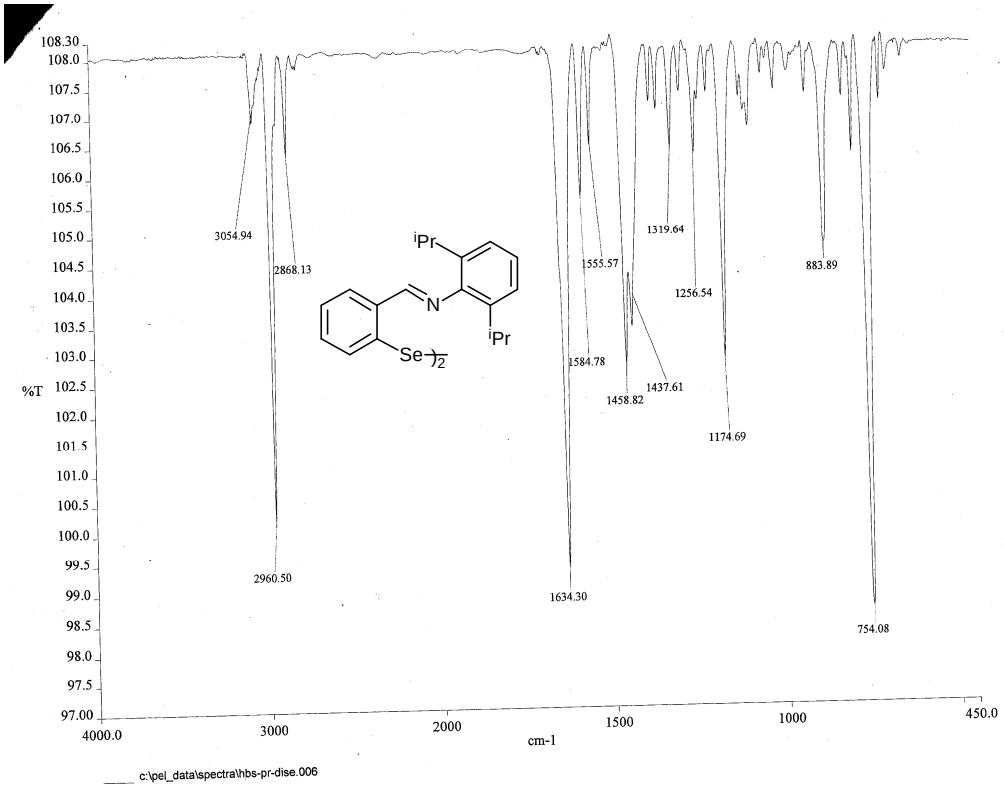


Figure S4. FT-IR spectrum of **11**

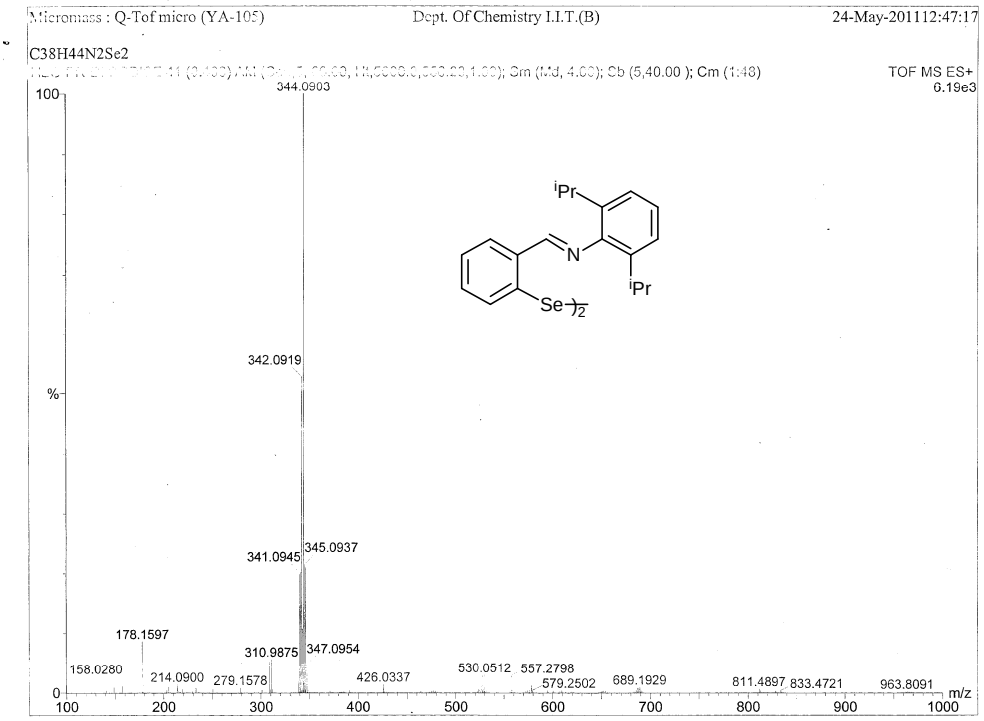


Figure S5. ESI-Mass spectrum of **11**

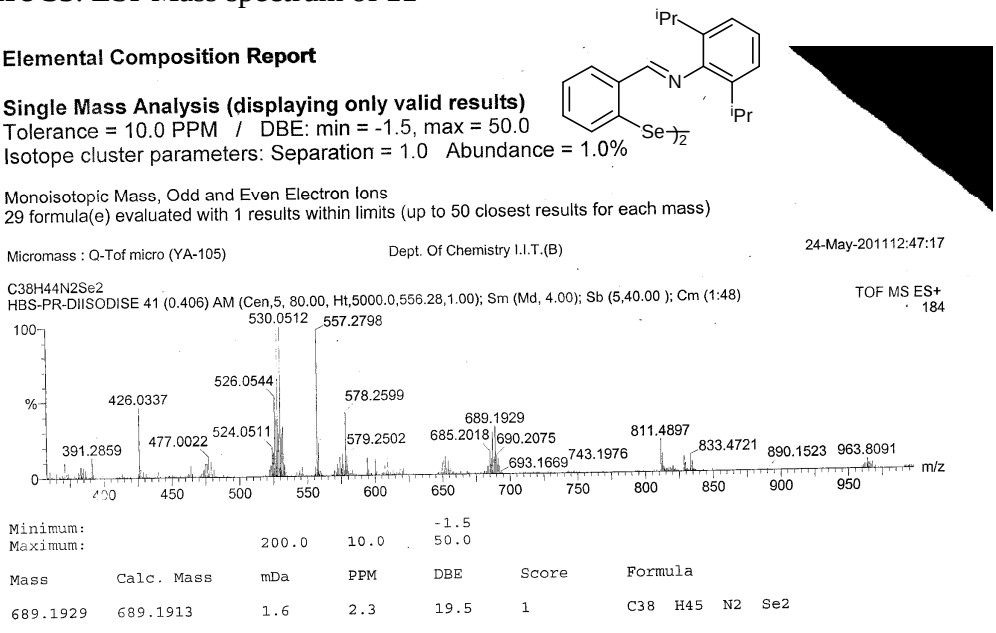


Figure S6. HRMS spectrum of **11**

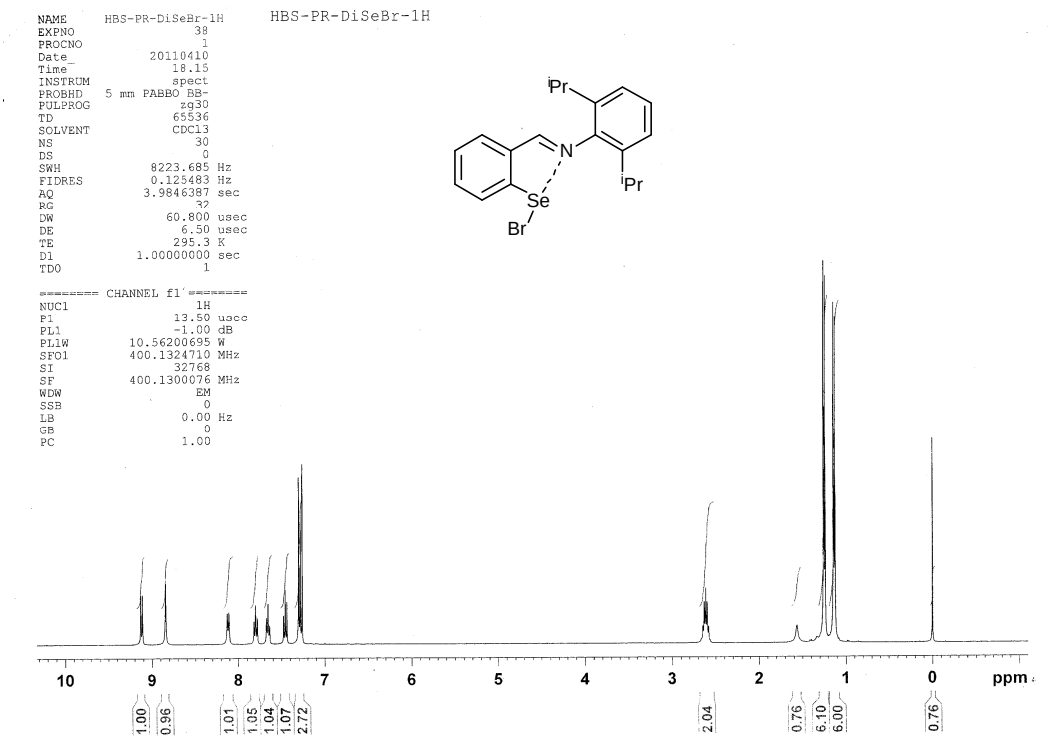


Figure S7. ^{1}H NMR spectrum of **13**

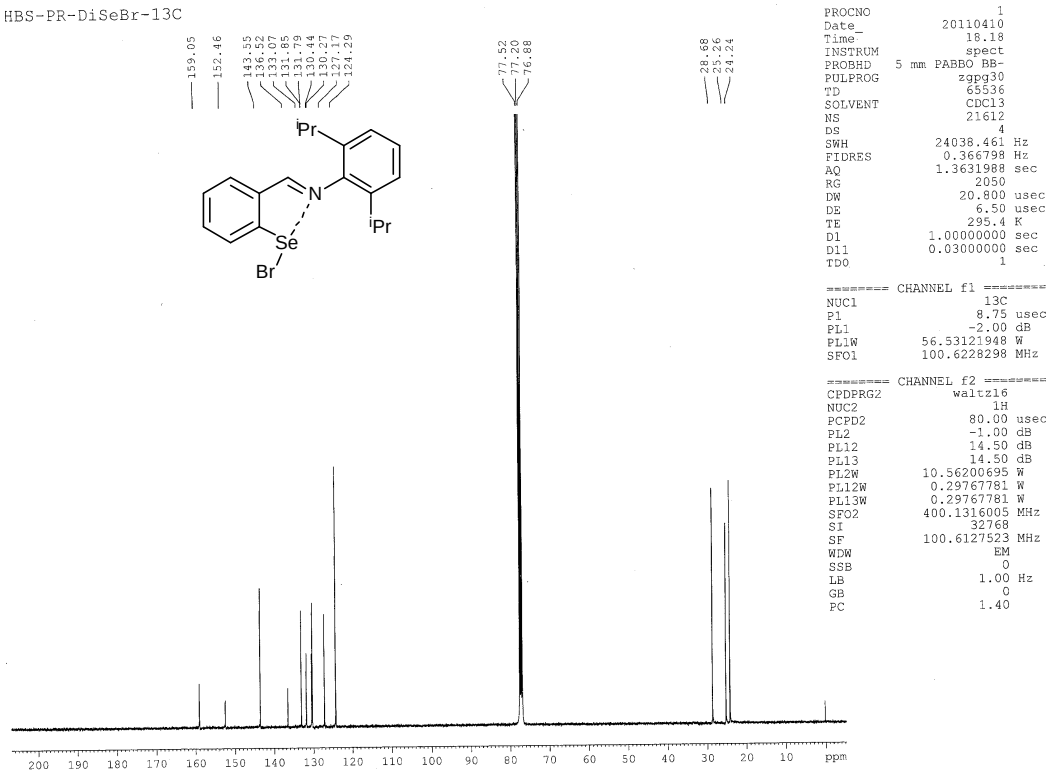
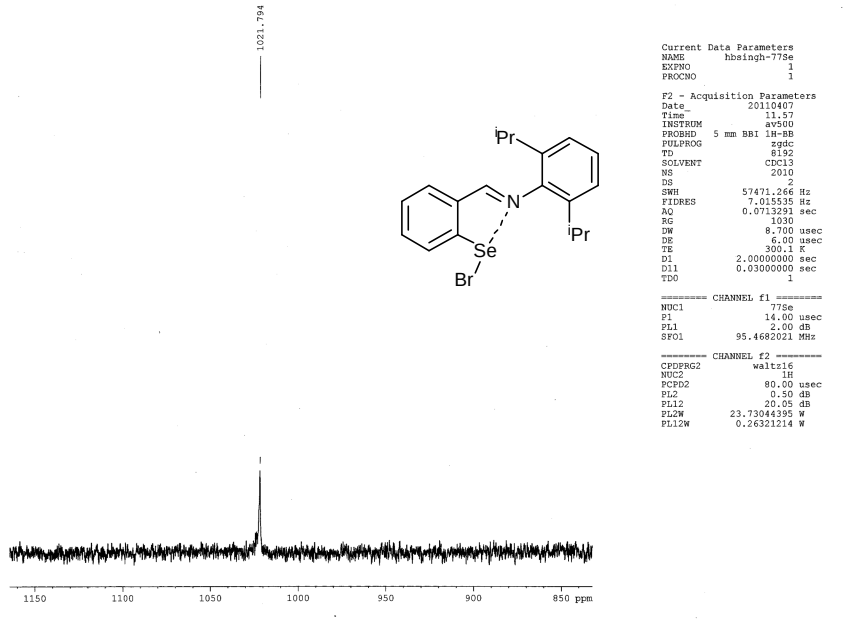


Figure S8. ^{13}C NMR spectrum of **13**



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PROCNO 1

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DE 6.00 usec
TE 300.1 K
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TD0 1

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PL1 2.00 dB
SFO1 95.4682021 MHz

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NUC2 1H
PCPD2 80.00 usec
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PL12 20.05 dB
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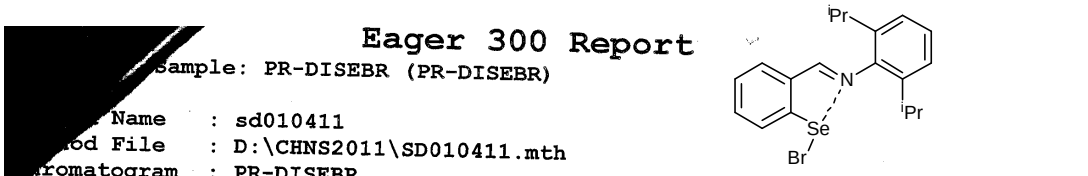
PL12W 0.26321214 W

Figure S9. ^{77}Se NMR spectrum of **13**



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Company Name : C.E. Instruments
Printed : 4/1/2011 15:13
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!!! Warning missing one or more peaks.

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Figure S10. CHN analysis of **13**

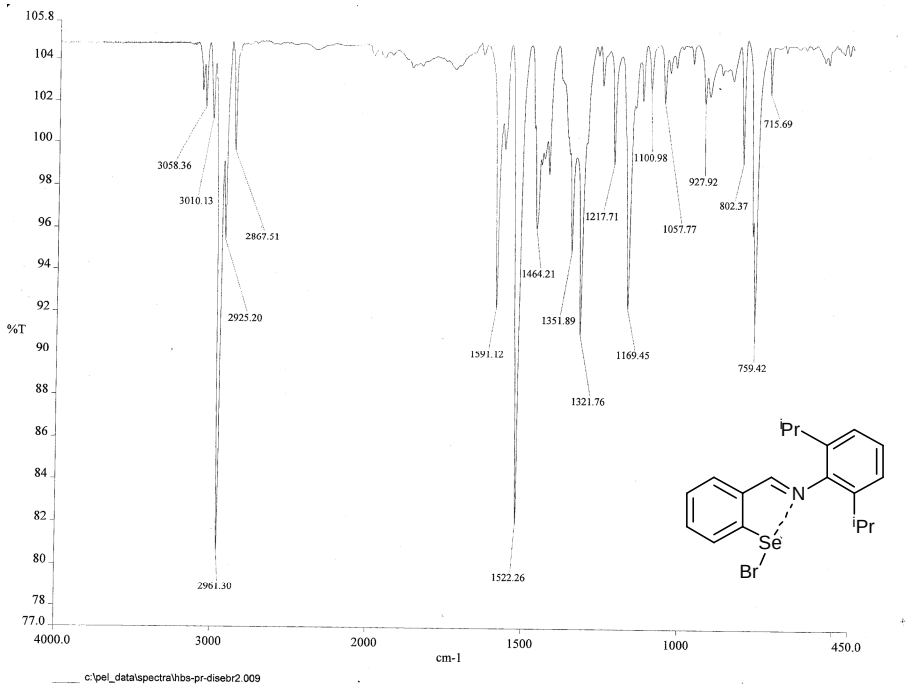


Figure S11. FT-IR spectrum of **13**

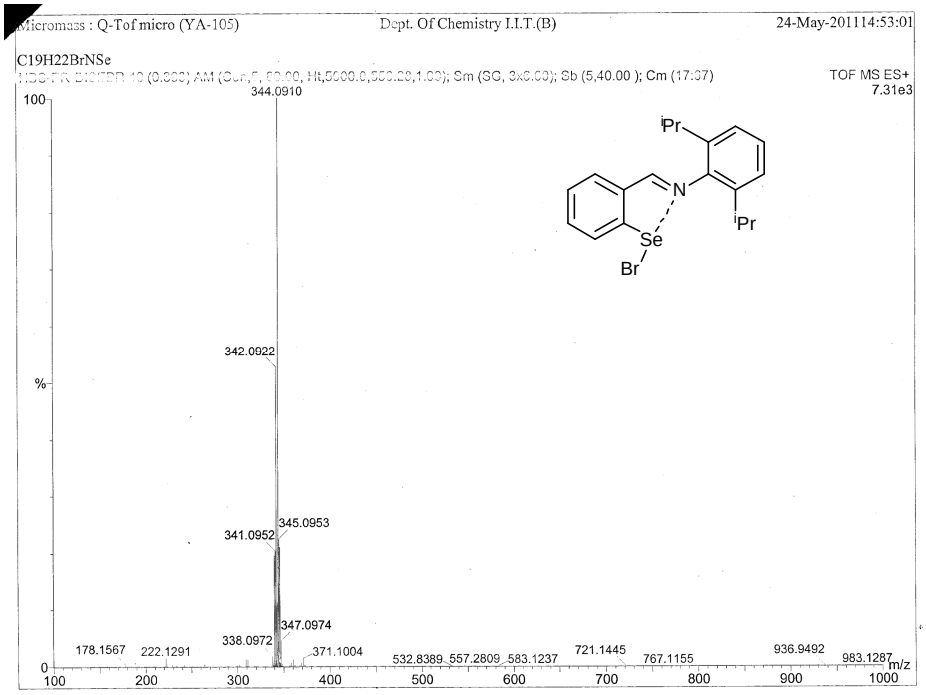


Figure S12. ESI-Mass spectrum of **13**

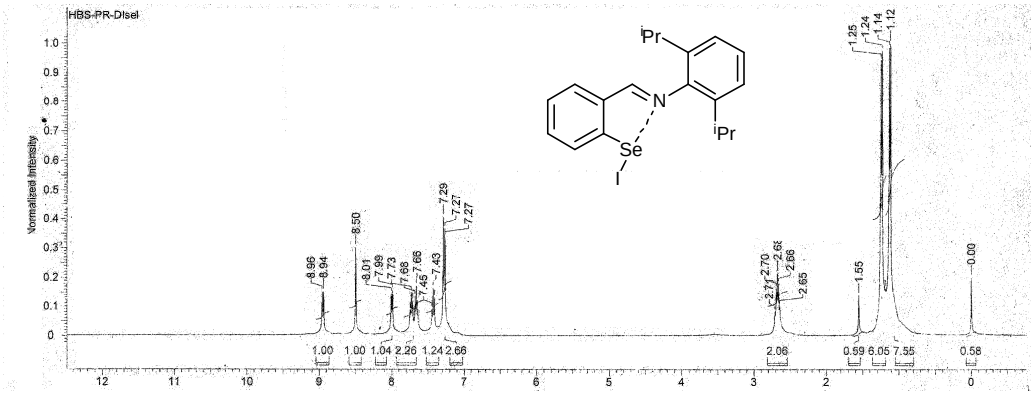


Figure S13. ^{1}H NMR spectrum of **14**

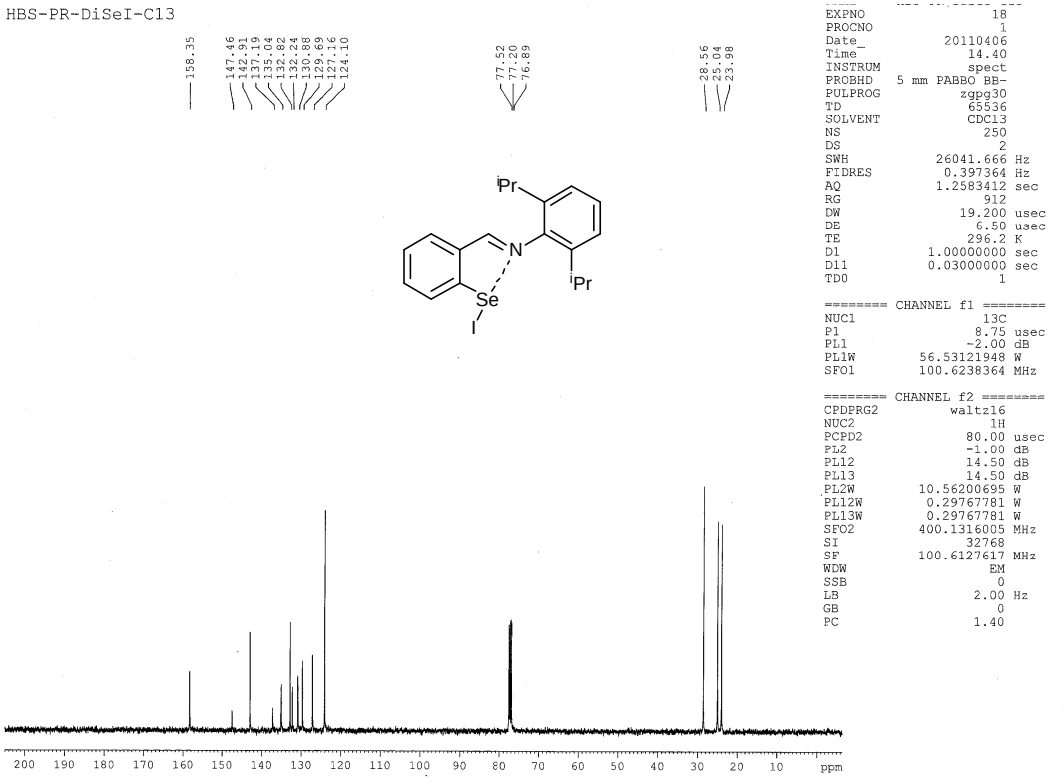


Figure S14. ^{13}C NMR spectrum of **14**

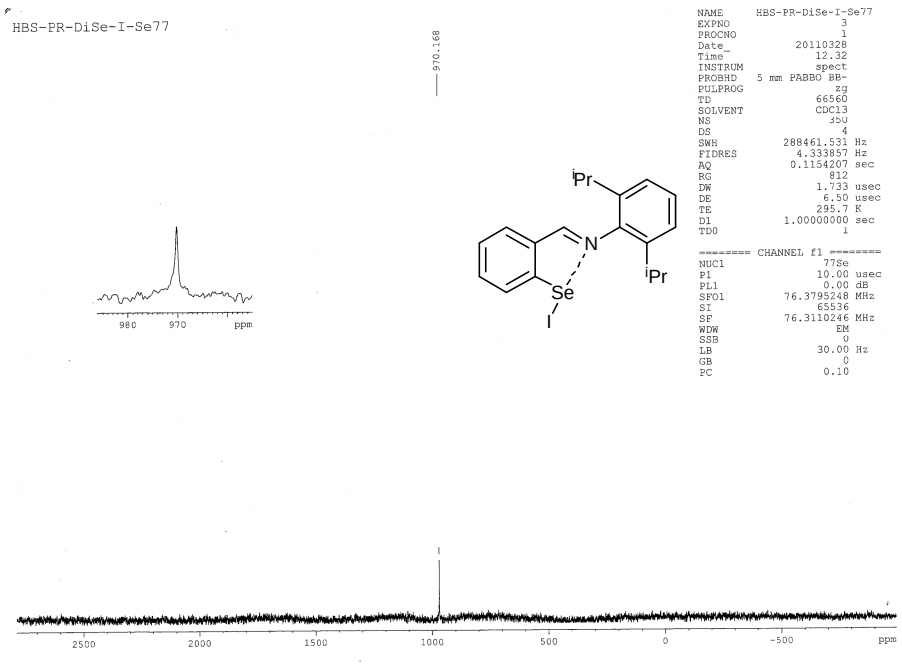


Figure S15. ^{77}Se NMR spectrum of **14**

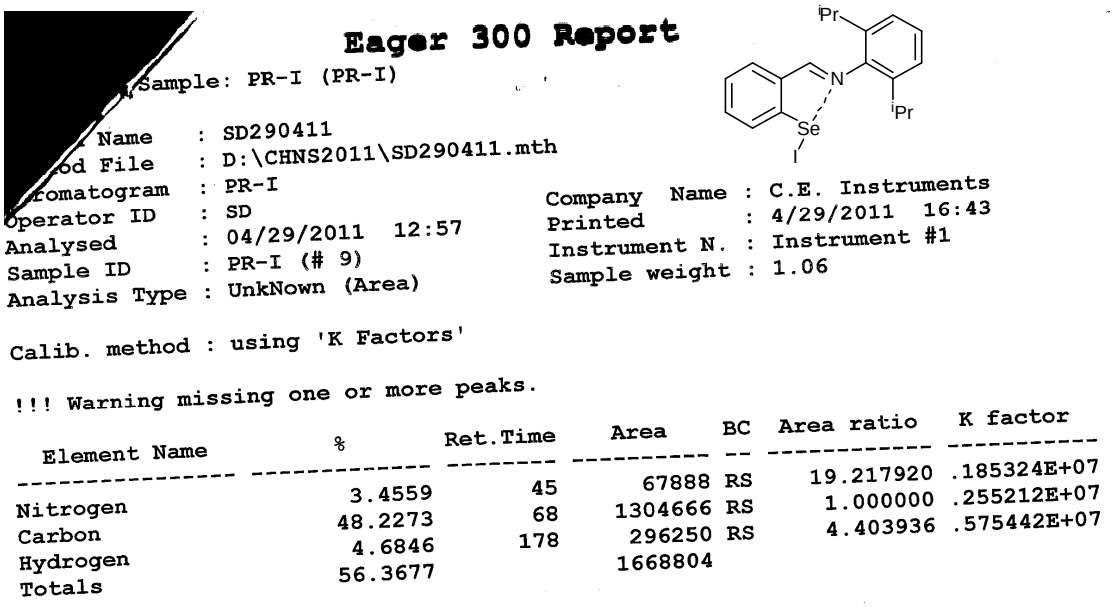


Figure S16. CHN analysis of **14**

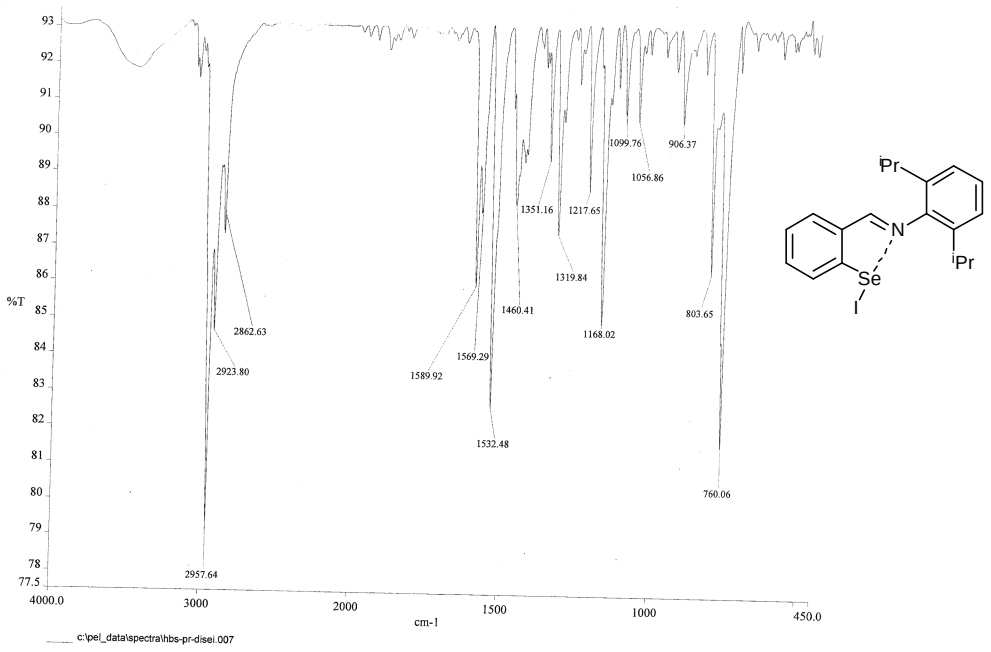


Figure S17. FT-IR spectrum of **14**

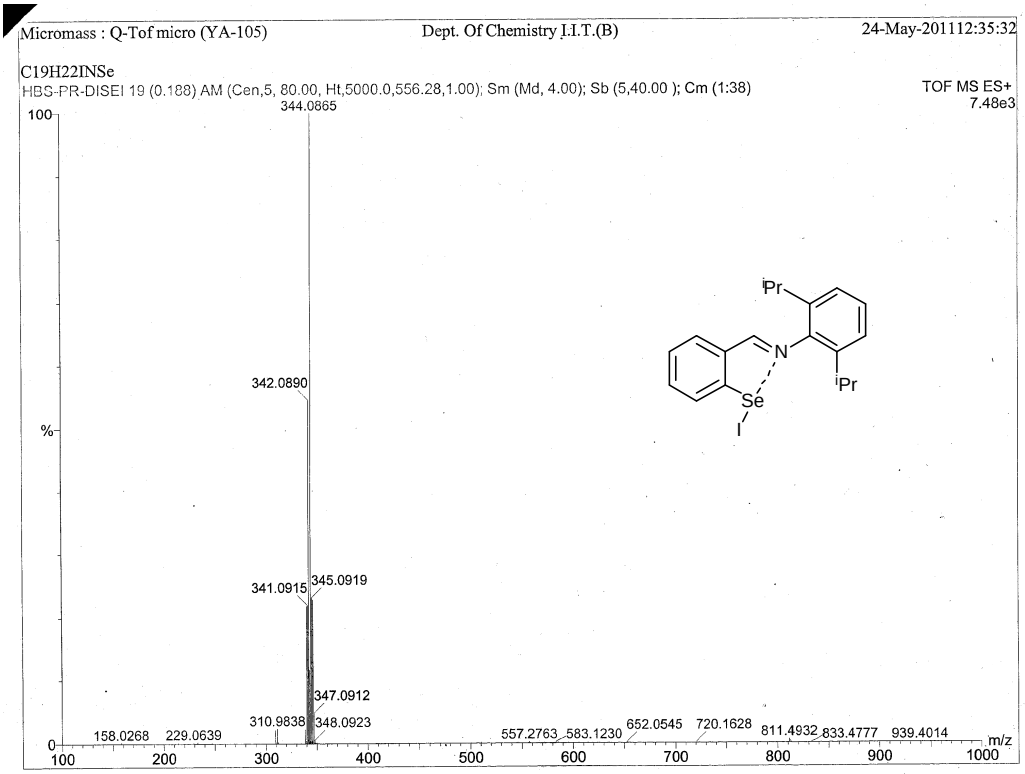


Figure S18. ESI-Mass spectrum of **14**

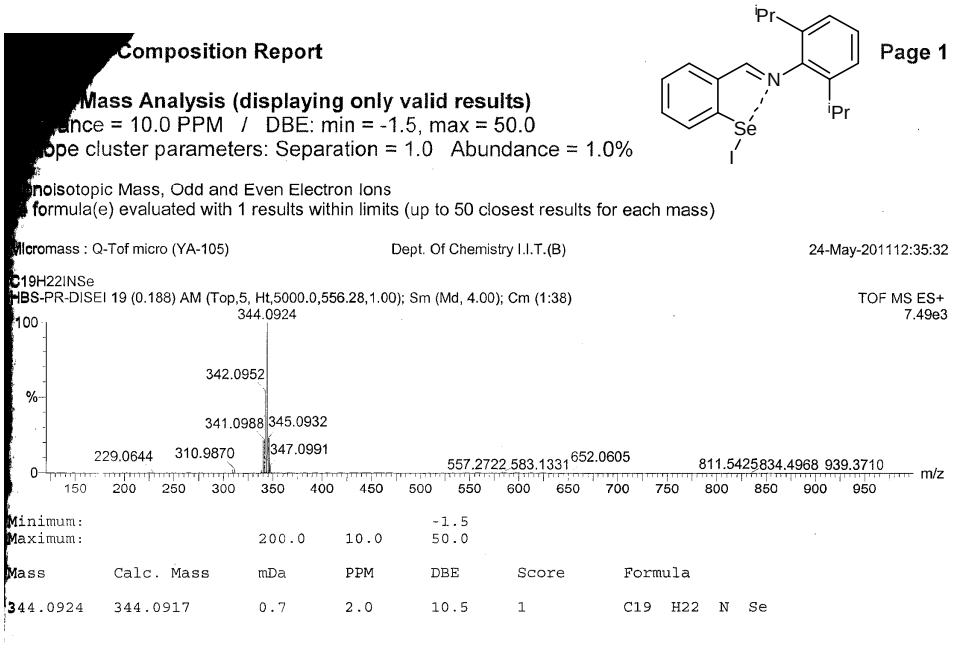


Figure S19. HRMS spectrum of **14**

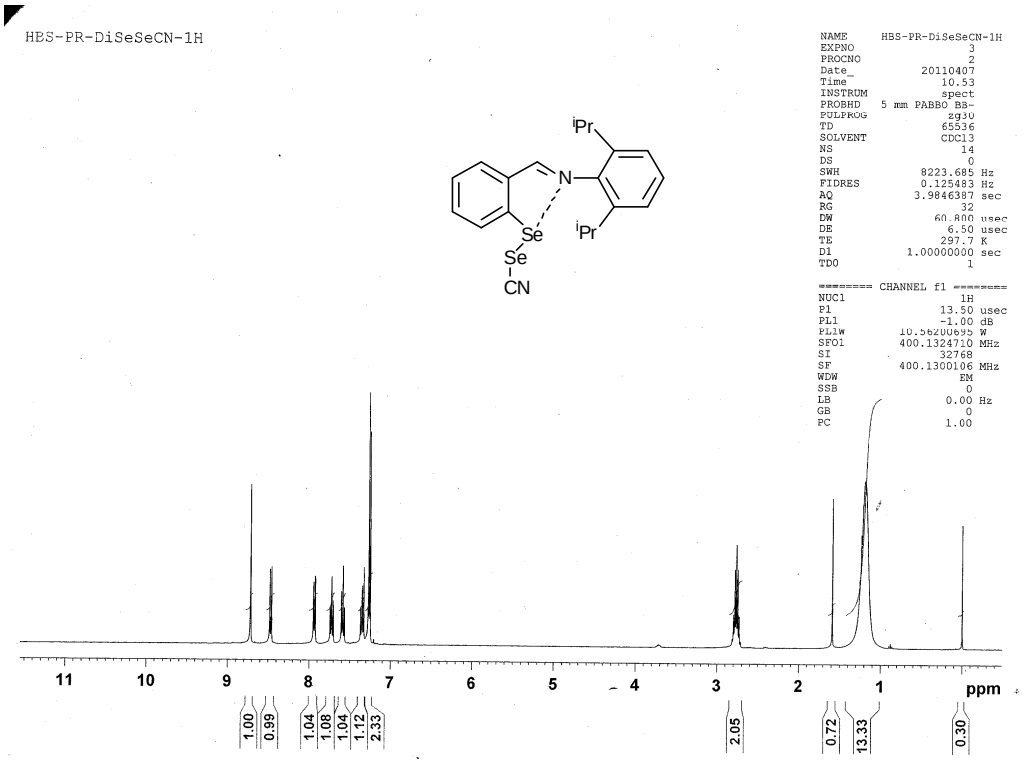


Figure S20. ^{1}H NMR spectrum of **15**

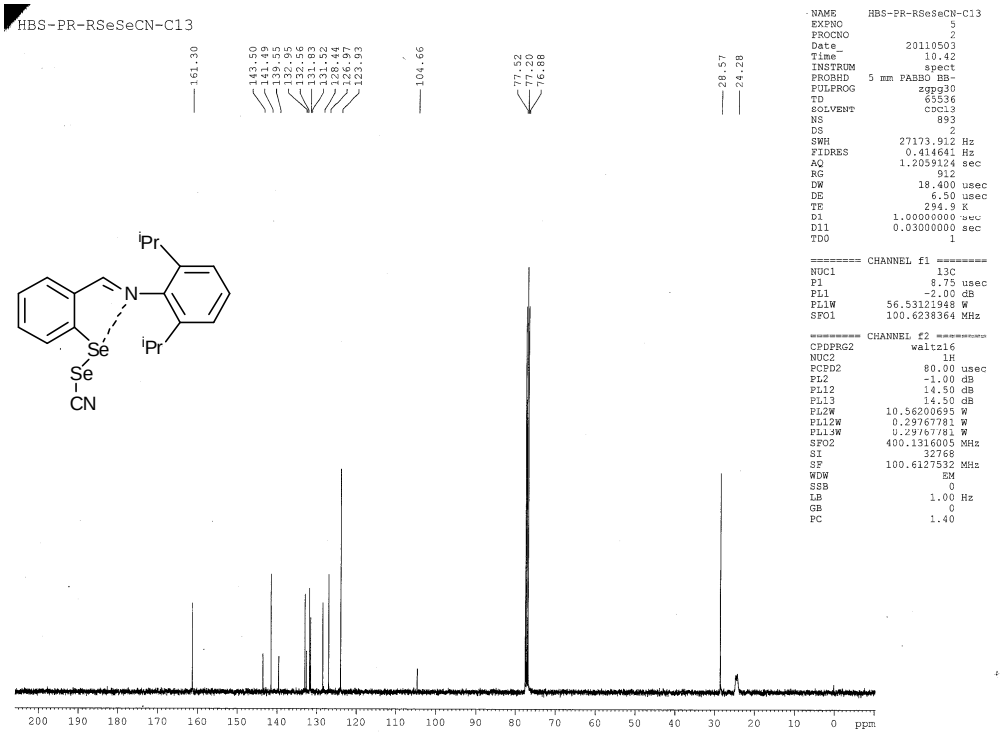


Figure S21. ^{13}C NMR spectrum of **15**

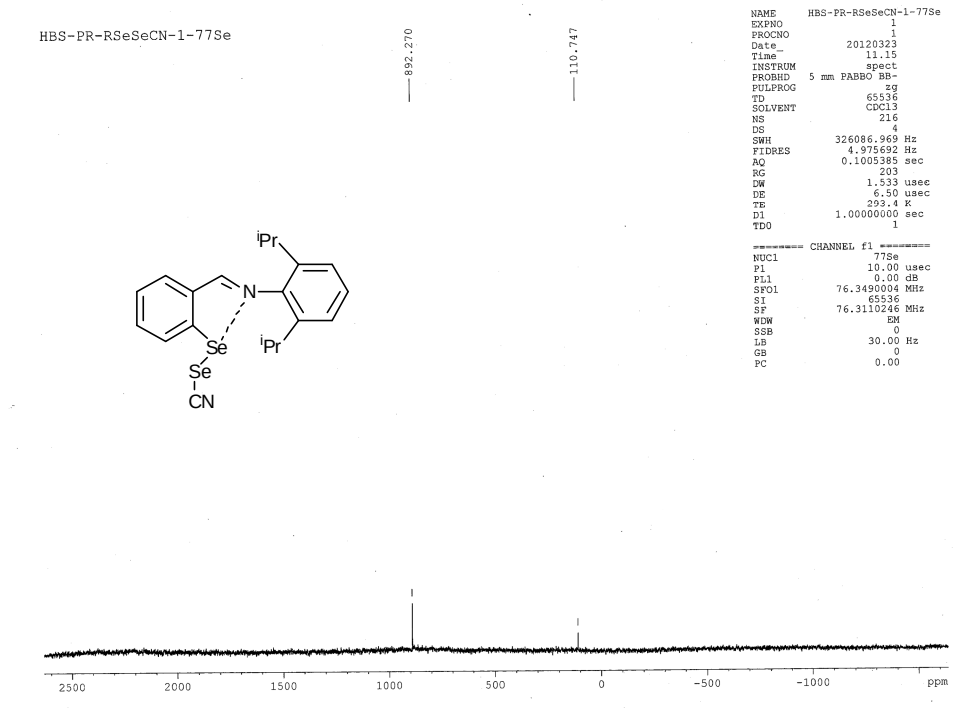
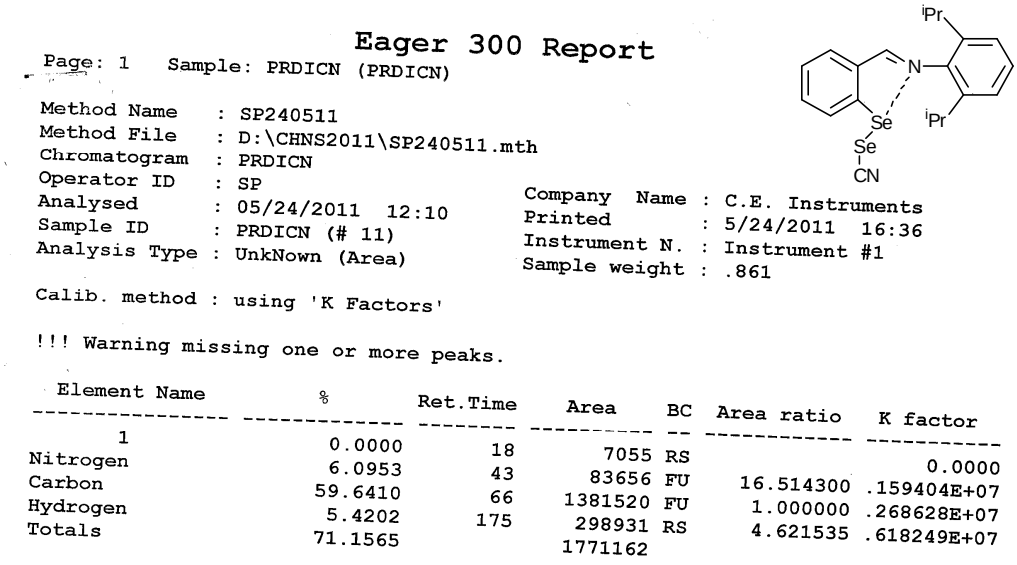


Figure S22. ^{77}Se NMR spectrum of **15**



Eager 300 Report

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Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 5/24/2011 16:36
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Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

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Hydrogen	5.4202	175	298931	RS	4.621535	.618249E+07
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Figure S23. CHN analysis of **15**

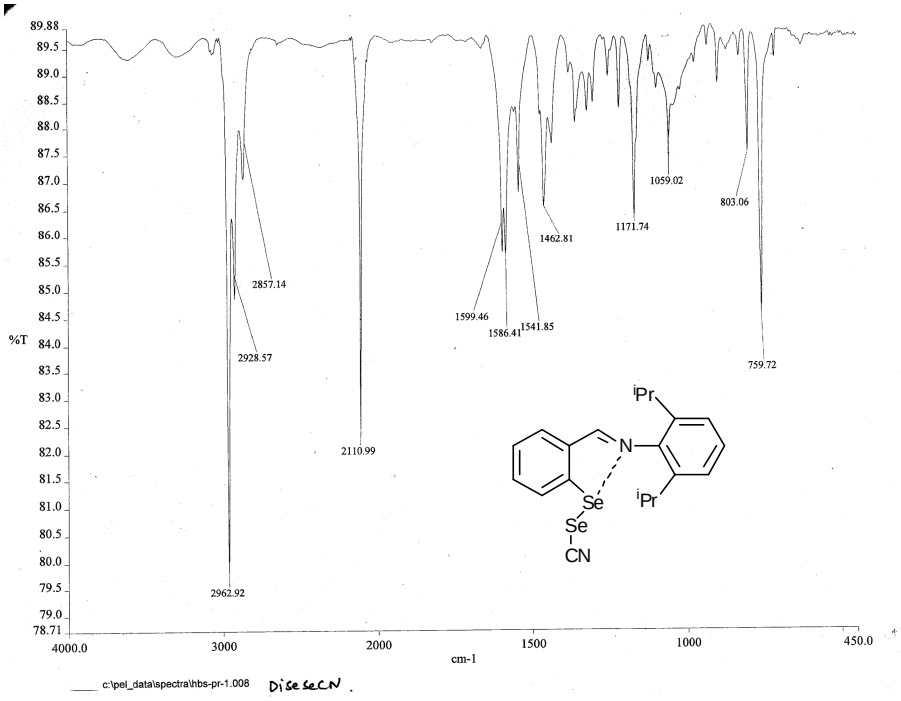


Figure S24. FT-IR spectrum of **15**

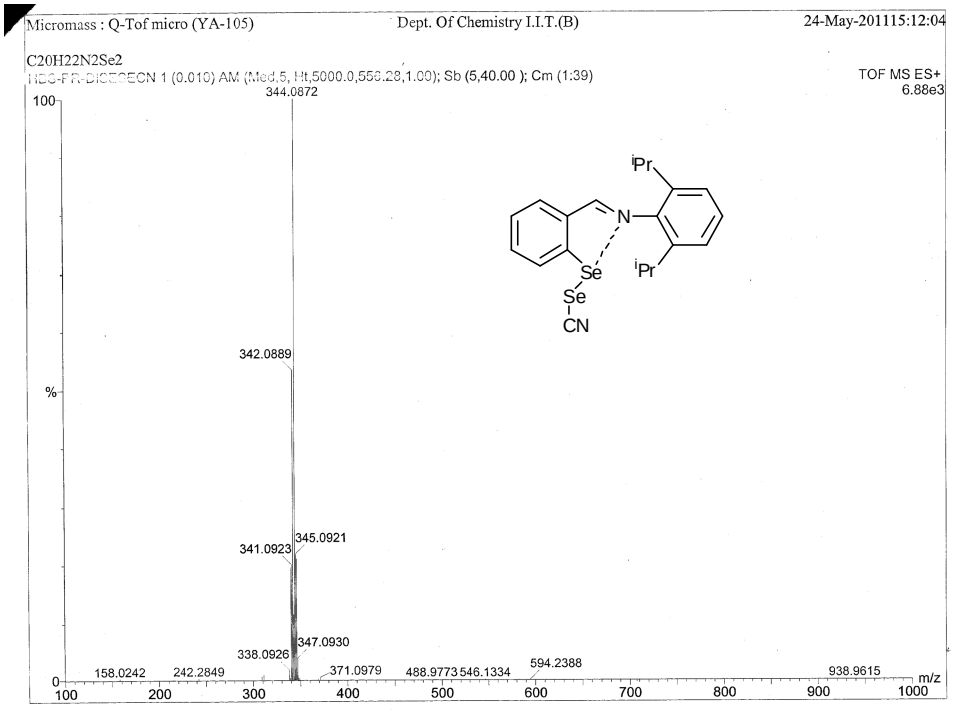


Figure S25. ESI-mass spectrum of **15**

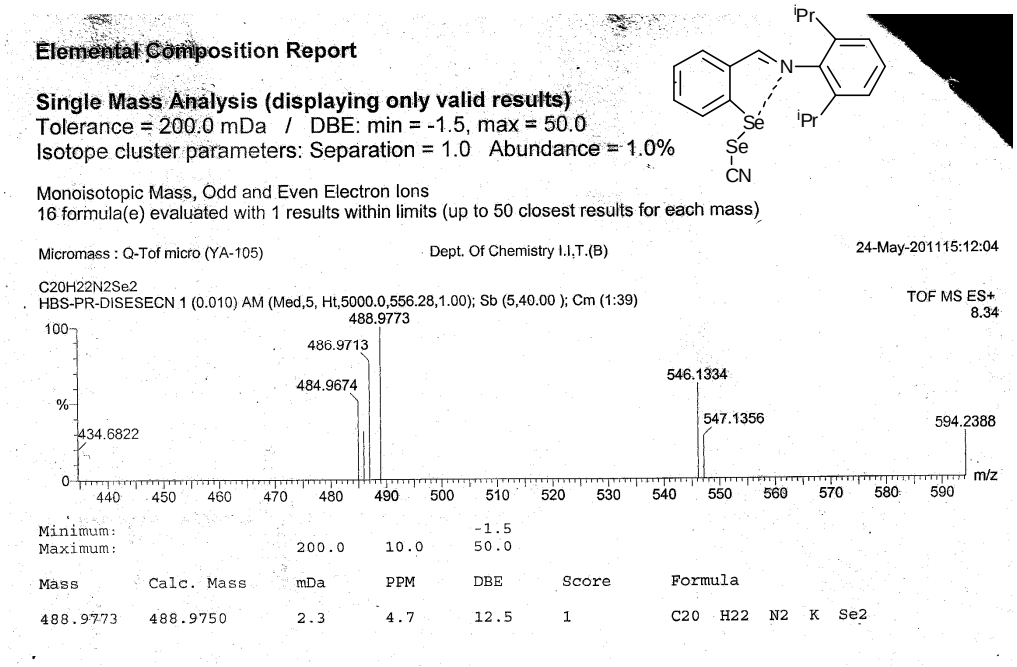


Figure S26. HRMS spectrum of **15**

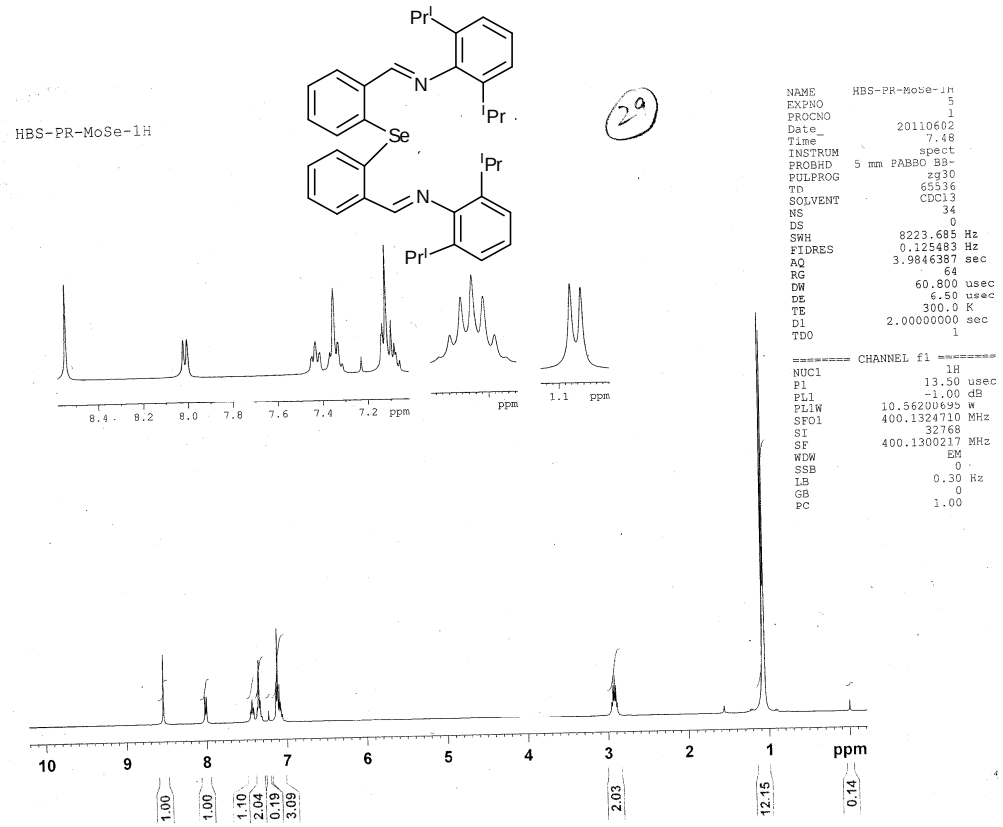


Figure S27. ^{1}H NMR spectrum of **17**

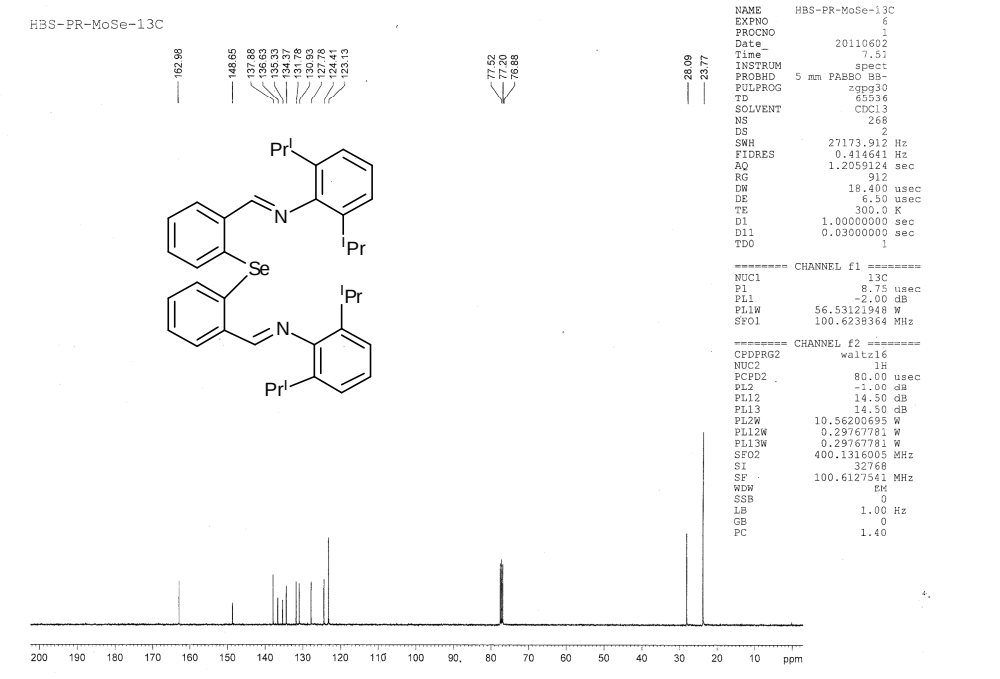


Figure S28. ^{13}C NMR spectrum of **17**

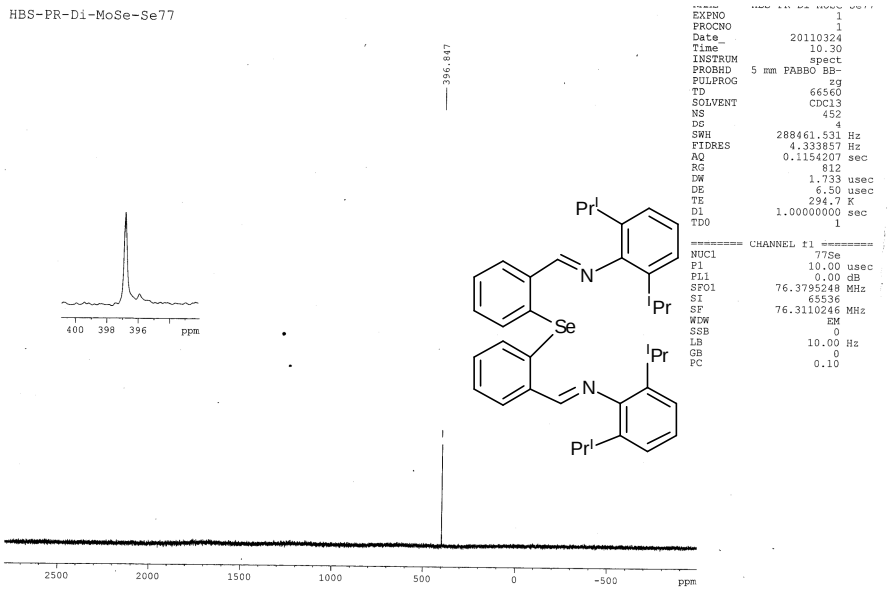


Figure S29. ^{77}Se NMR spectrum of **17**

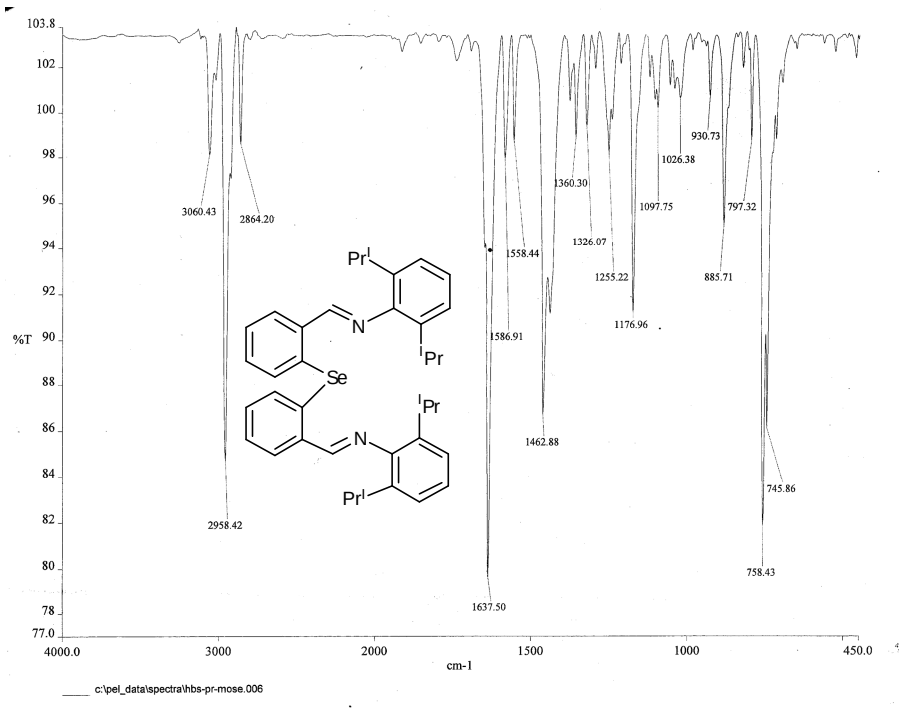


Figure S30. FT-IR spectrum of **17**

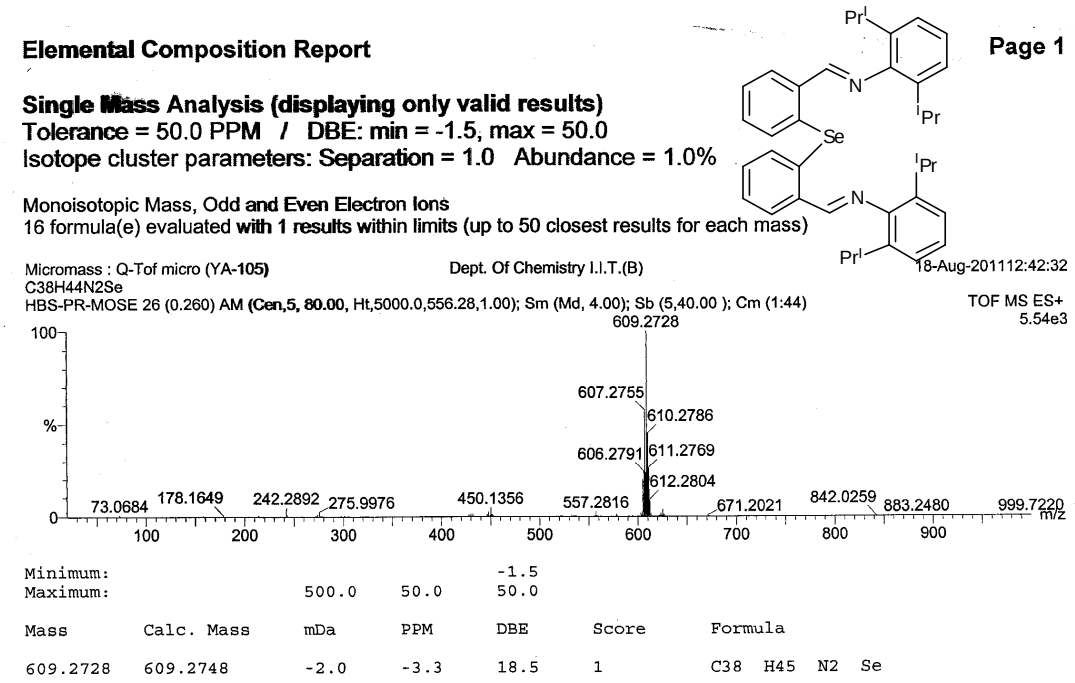


Figure S31. HRMS spectrum of **17**

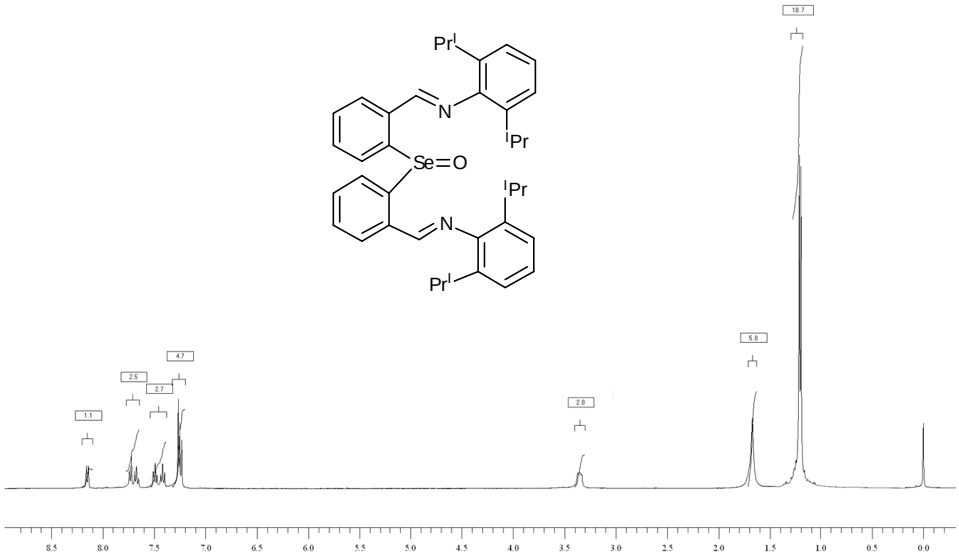
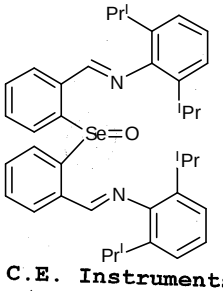


Figure S32. ^{1}H NMR spectrum of **18**



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Eager 300 Report

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Company Name : C.E. Instruments
Printed : 5/6/2011 17:14
Instrument N. : Instrument #1
Sample weight : .796

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

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2	0.0000	58	36014	FU		0.0000
Carbon	63.9283	67	1283553	FU	1.000000	.251772E+07
Hydrogen	6.0326	175	284070	RS	4.518438	.591571E+07
Totals	74.0300		1652802			

Figure S33. CHN analysis of **18**

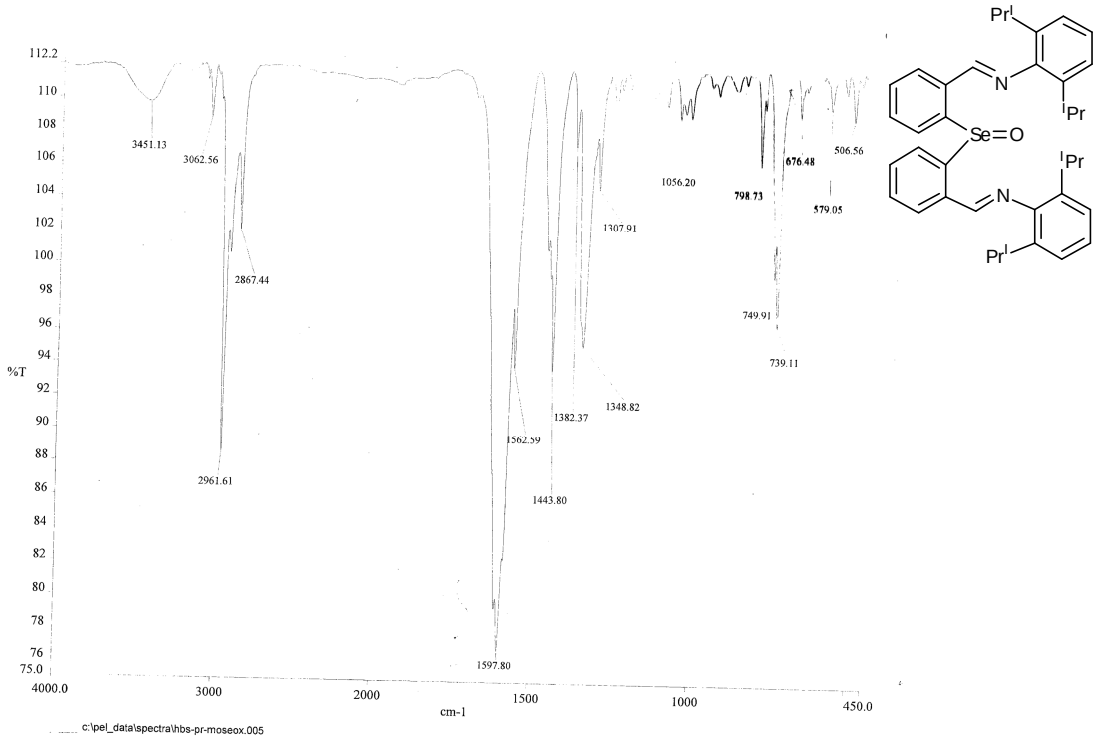

Figure S34. FT-IR spectrum of **18**

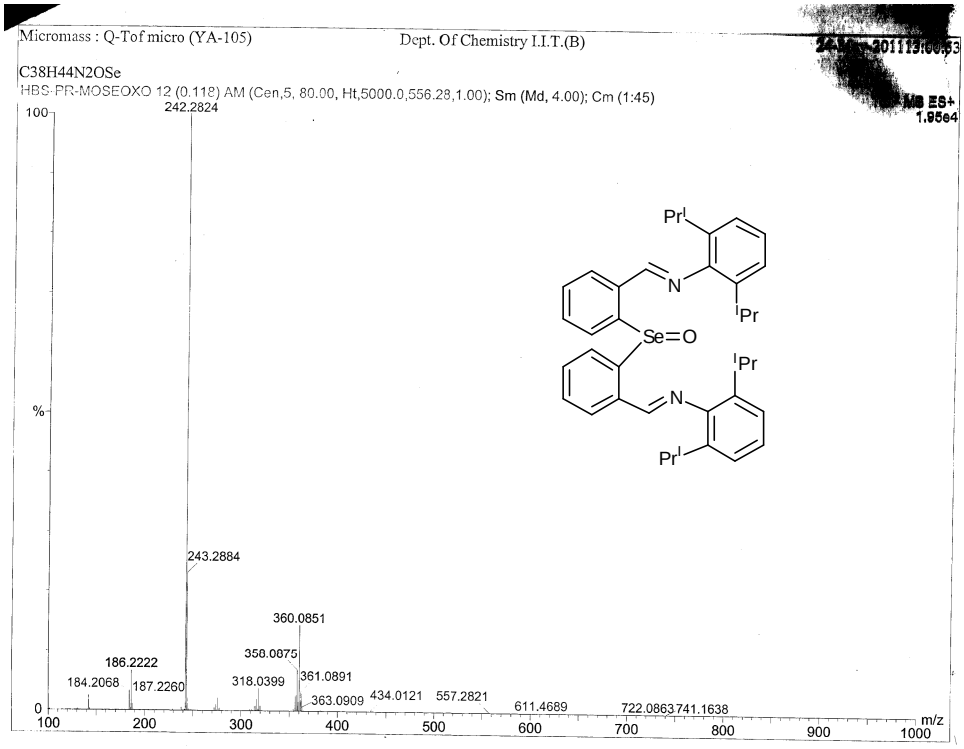

Figure S35. ESI-Mass spectrum of **18**

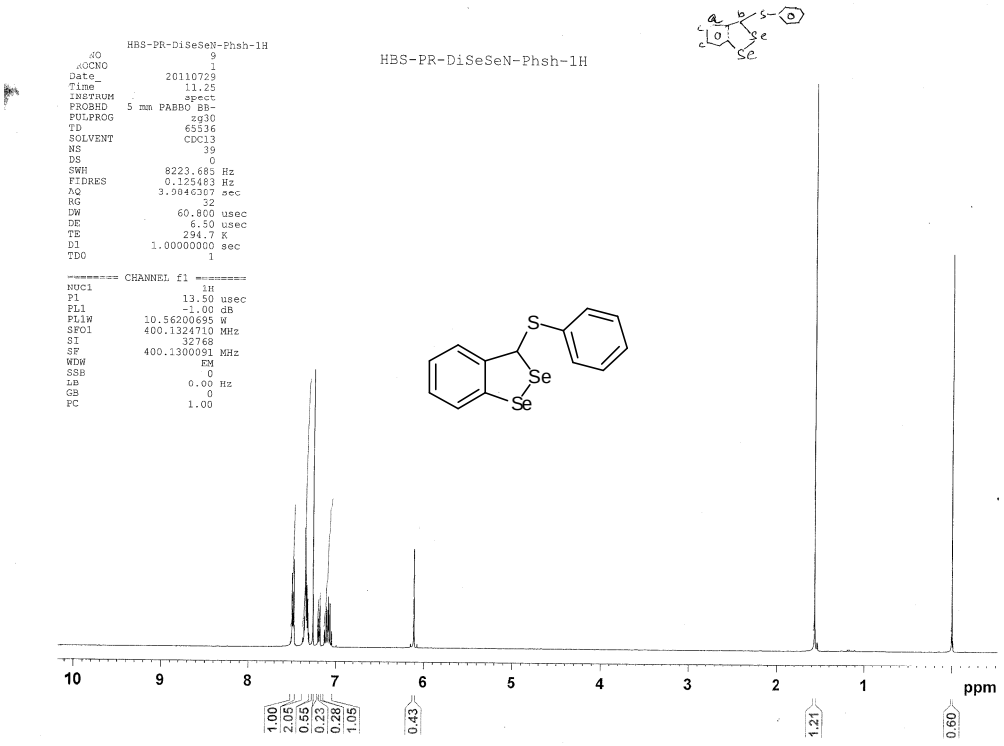

Figure S36. ^{1}H NMR spectrum of **22**

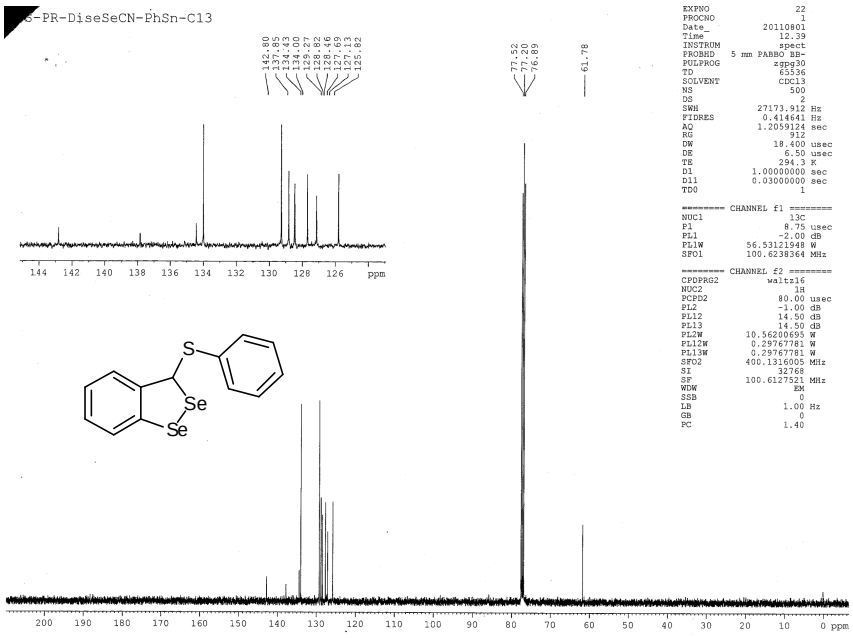

Figure S37. ^{13}C NMR spectrum of **22**

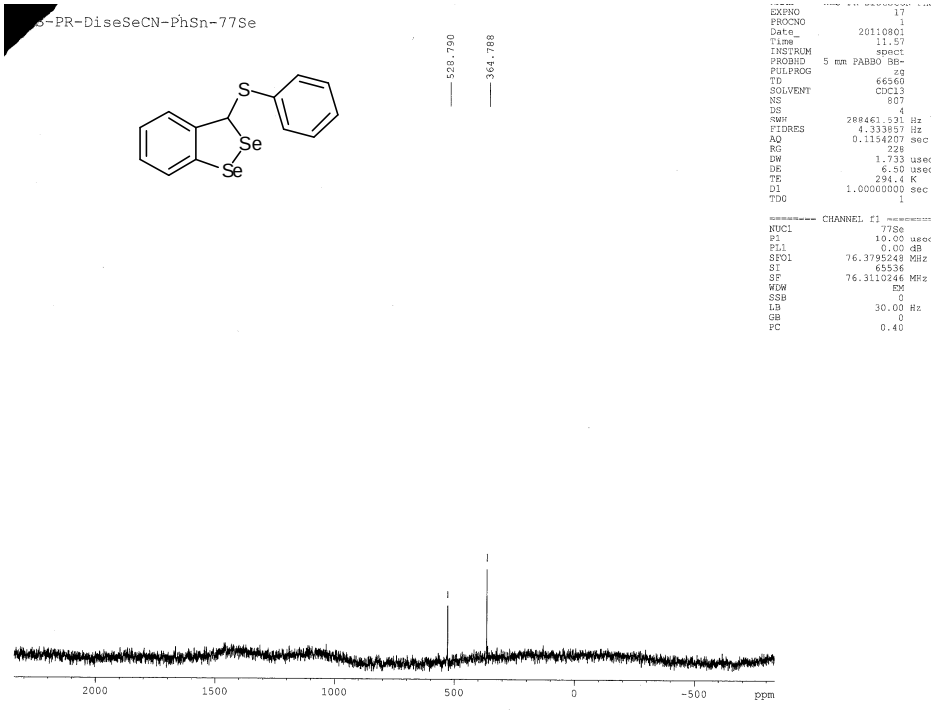

Figure S38. ^{77}Se NMR spectrum of **22**

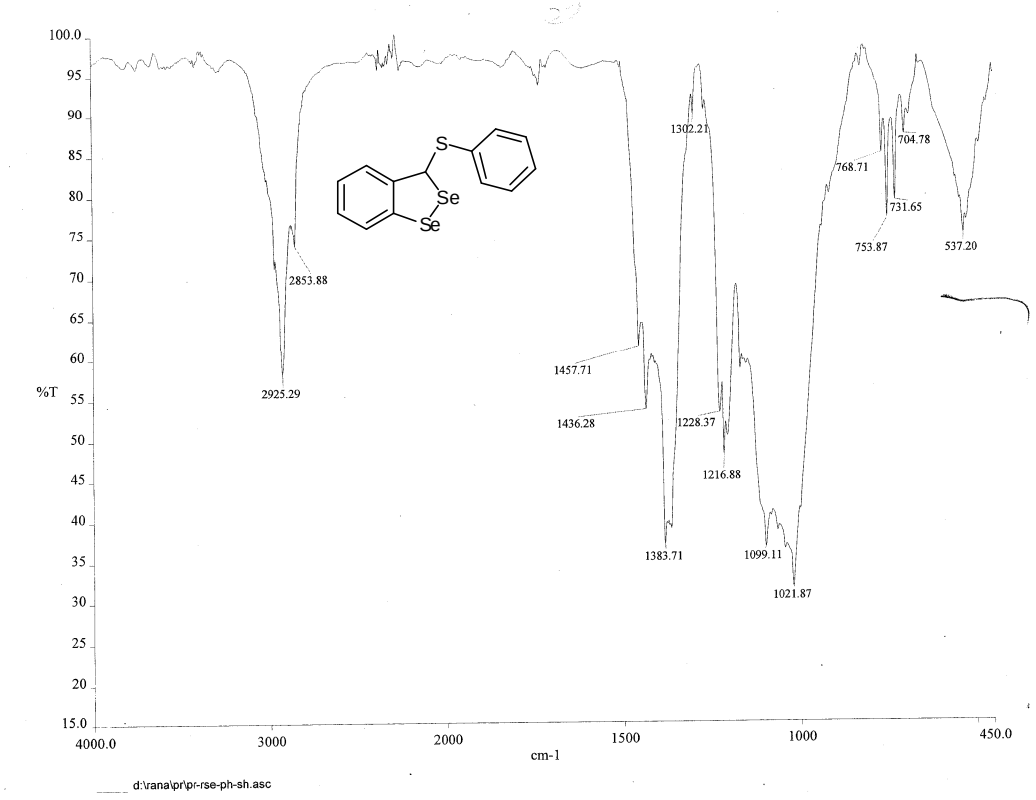

Figure S39. FT-IR spectrum of **22**

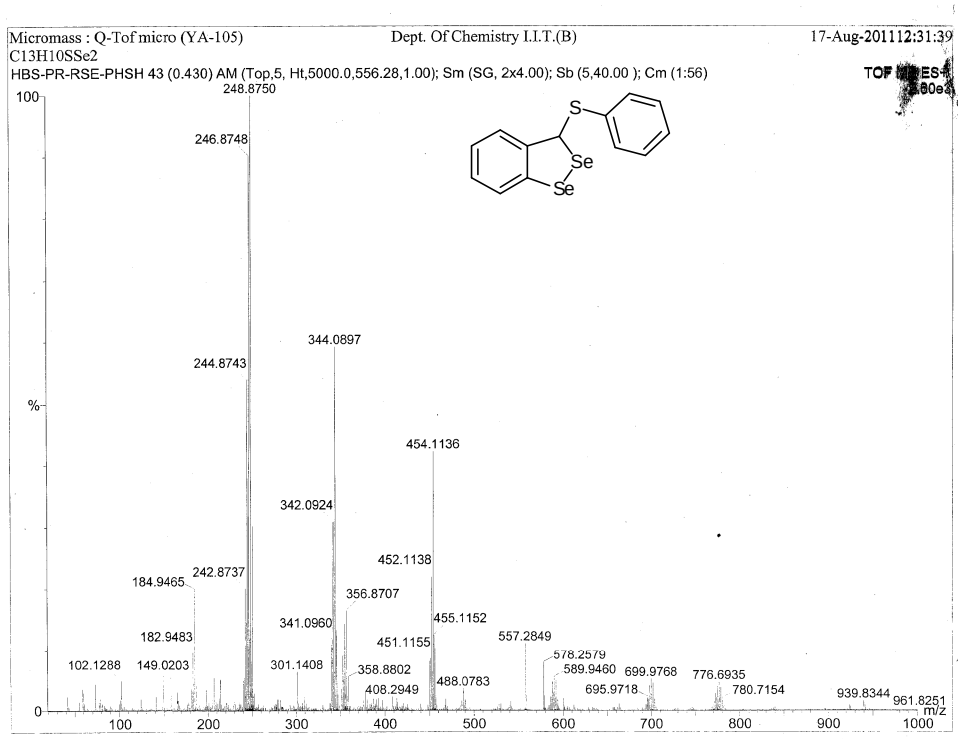

Figure S40. ESI-Mass spectrum of **22**

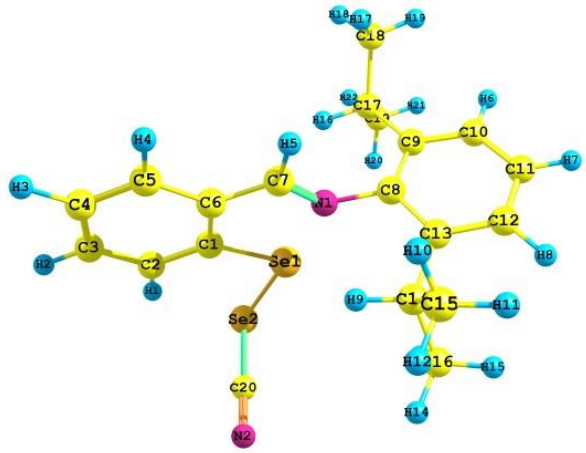

Figure S41. Optimized geometry of **15**.

Table S1. Comparison of the experimentally obtained structural parameters (Å and °) with that computed at B3LYP/6-31+G(d,p) level for **15**

Bond lengths (Å) / Bond Angle (°)	**15**	
	Optimized geometry	Crystal structure
Se1···N1	2.212	2.116(2)
Se1-Se2	2.546	2.6069(4)
Se1-C1	1.921	1.917(2)
N1-Se1-Se2	176.31	172.93(6)
C1-Se1-Se2	96.89	97.60(8)

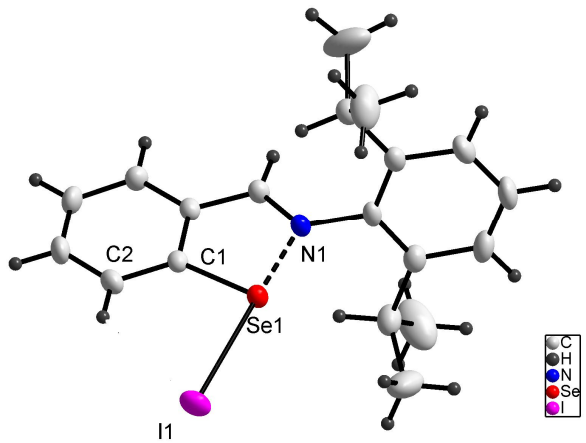

Figure S41. Molecular structure of **14** and selected bond lengths (Å) and angles (°). Se1-C1 1.895(2), Se1-I1 2.9029(3), Se1-N1 1.9993(17); N1-Se1-I1 177.66(6), C1-Se1-I1 97.14(6).

Table S2. Crystal data and structure refinement for **13**, **14**, **15** and **17**

Compound	**13**	**14**	**15**	**17**
Empirical formula	$C_{19}H_{22}BrNSe$	$C_{19}H_{22}INSe$	$C_{20}H_{22}N_2Se_2$	$C_{38}H_{44}N_2Se$
Formula weight	423.25	470.24	448.32	607.71
Crystal system	orthorhombic	orthorhombic	Monoclinic	Triclinic
Space group	Pbca	Pbca	P2(1)/c	P-1
a (Å)	9.5735(5)	9.5672(2)	10.0205(6)	9.5672(2)

b (Å)	16.5118(9)	17.2716(2)	11.4514(8)	11.1782(5)
c (Å)	23.4372(13)	23.5022(5)	16.4769(12)	17.0830(7)
α (deg)	90	90	90	89.666(3)
β (deg)	90	90	97.148(6)	75.815(3)
γ (deg)	90	90	90	75.815(3)
V ($Å^3$)	3704.9(3)	3883.52(12)	1876.0(2)	1607.85(11)
Z	8	8	4	2
D(calcd) Mg/m^3	1.518	1.609	1.587	1.255
Abs coeff (mm^{-1})	4.181	3.521	3.945	1.778
Reflens collected	45354	42681	18873	11196
final R(F) [$I > 2\sigma(I)$][a]	0.0264	0.0582	0.0248	0.0323
wR(F^2) indices [$I > 2\sigma$]	0.0764	0.0558	0.0754	0.0814
No. of data /restrains/ params	4597 / 0/ 203	5007 / 0/ 203	4851 / 0/ 221	6460 / 0/ 378
goodness of fit on F^2	1.028	1.057	1.041	1.039

[a] Definitions: $R(Fo) = \sum||Fo| - |Fc||/\sum|Fo|$ and $wR(Fo^2) = \{\sum[w(Fo^2 - Fc^2)^2]/\sum[w(Fc^2)^2]\}^{1/2}$