Supporting Information

Transition Metal Mediated Formation of Dicationic Diselenides Stabilised by N-Heterocyclic Carbenes: Designed Synthesis

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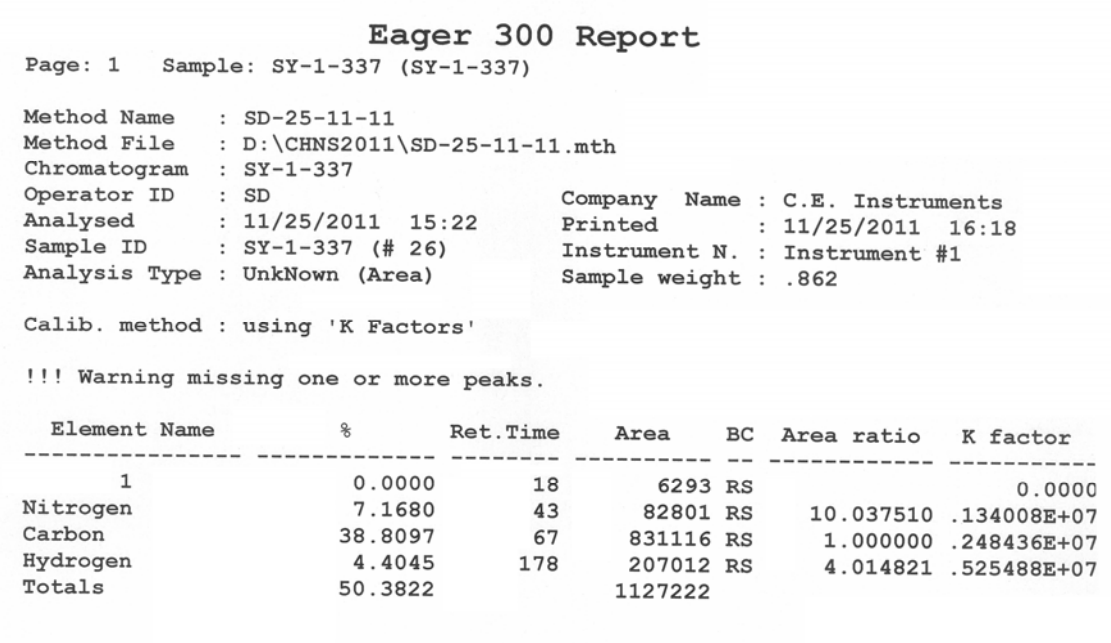
Spectroscopic data:



Eager 300 Report

Page: 1 Sample: SY-1-337 (SY-1-337)

Method Name : SD-25-11-11
Method File : D:\CHNS2011\SD-25-11-11.mth
Chromatogram : SY-1-337
Operator ID : SD
Analysed : 11/25/2011 15:22
Sample ID : SY-1-337 (# 26)
Analysis Type : UnkNown (Area)
Company Name : C.E. Instruments
Printed : 11/25/2011 16:18
Instrument N. : Instrument #1
Sample weight : .862

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	6293	RS		0.0000
Nitrogen	7.1680	43	82801	RS	10.037510	.134008E+07
Carbon	38.8097	67	831116	RS	1.000000	.248436E+07
Hydrogen	4.4045	178	207012	RS	4.014821	.525488E+07
Totals	50.3822		1127222			

Figure S1. Elemental analysis of compound **7**.

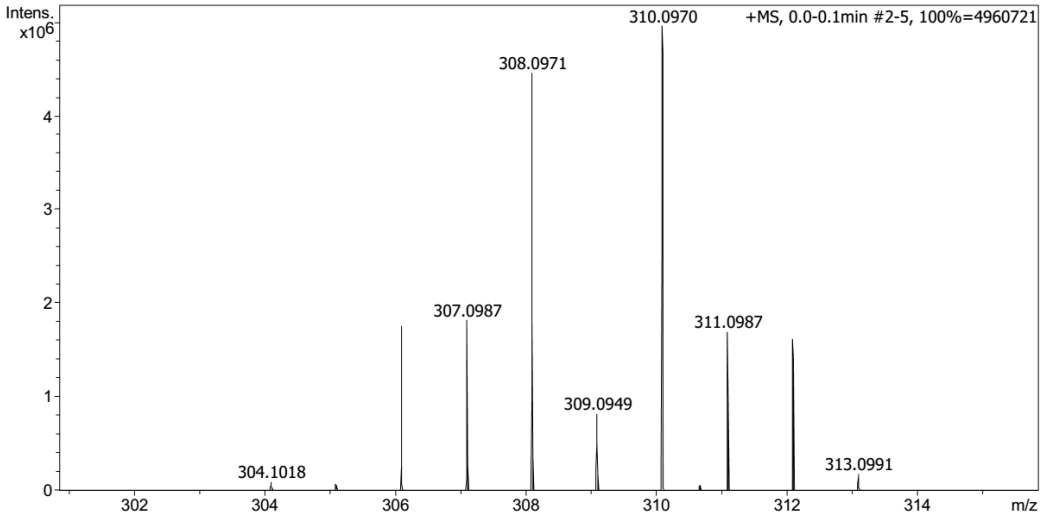
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\MARCH-2016\HBSSY-1.d	Acquisition Date	3/26/2016 10:20:38 PM
Method	Tune_pos_NAICSI-1000a.m	Operator	HBS-SY
Sample Name	HBSSY-1	Instrument	maXis impact 282001.00081
Comment			

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 Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
310.0970	1	C30H44N4Se2	310.0946	-7.8	324.8	1	100.00	11.0	even	ok

Figure S2. ESI-MS spectrum of compound **7**.

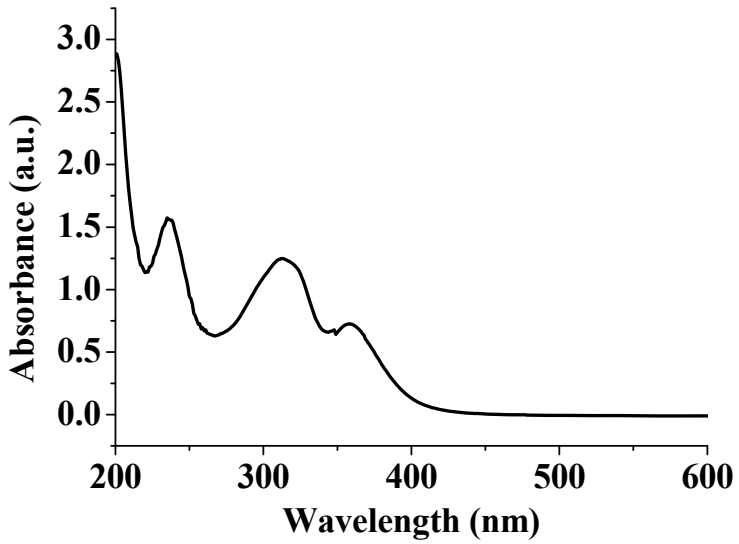


Figure S3. UV-Visible spectrum of compound **7**.

Eager 300 Report

Page: 1 Sample: SY-1-383 (SY-1-383)

Method Name : SD-25-11-11
Method File : D:\CHNS2011\SD-25-11-11.mth
Chromatogram : SY-1-383
Operator ID : SD Company Name : C.E. Instruments
Analysed : 11/25/2011 13:11 Printed : 11/25/2011 16:18
Sample ID : SY-1-383 (# 14) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : .966

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	10268	RS		0.0000
Nitrogen	5.4999	43	71197	RS	11.384700	.134008E+07
Carbon	33.7748	67	810557	RS	1.000000	.248436E+07
Hydrogen	3.9113	181	206048	RS	3.933824	.525488E+07
Totals	43.1859		1098070			

Figure S4. Elemental analysis of compound **8**.

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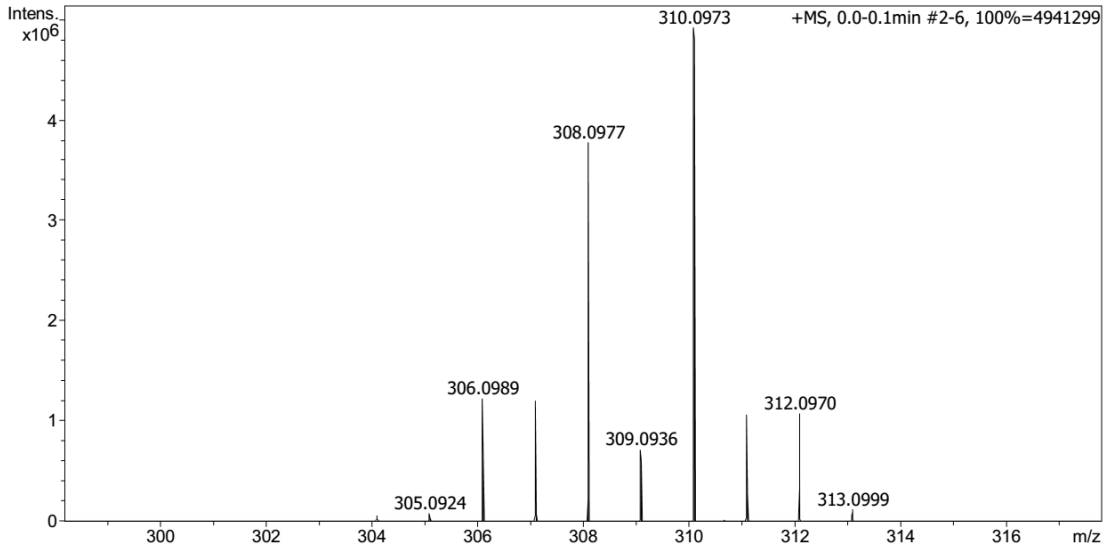
Analysis Info

Analysis Name D:\Data\MARCH-2016\HBS-SY-4.d
Method Tune_pos_NAICSI-1000a.m
Sample Name HBS-SY-4
Comment

Acquisition Date 3/26/2016 10:27:20 PM
Operator HBS-SY
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 Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
310.0973	1	C30H44N4Se2	310.0946	8.9	309.4	1	100.00	11.0	even	ok

Figure S5. ESI-MS spectrum of compound **8**.

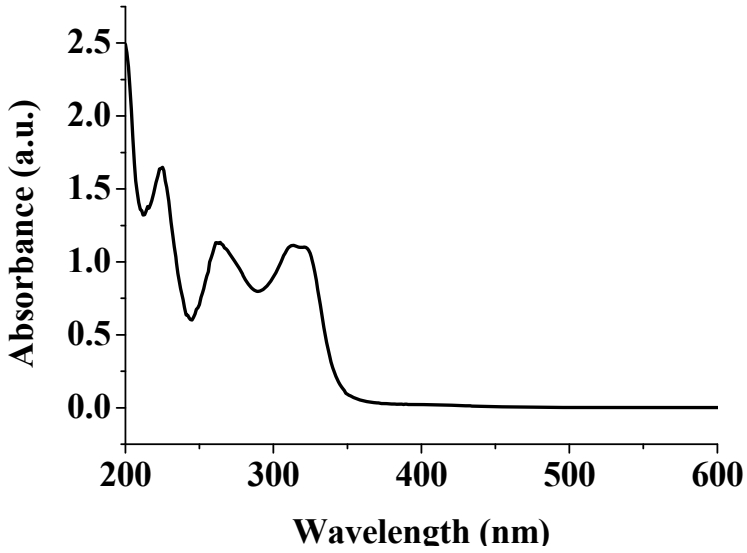


Figure S6. UV-Visible spectrum of compound **8**.

Eager 300 Report

Page: 1 Sample: SY-2-132 (SY-2-132)

Method Name : SP160312
Method File : D:\CHNS2012\SP160312.mth
Chromatogram : SY-2-132
Operator ID : SP
Analysed : 03/16/2012 13:40
Sample ID : SY-2-132 (# 17)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 3/16/2012 17:44
Instrument N. : Instrument #1
Sample weight : .938

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	16371	RS		0.0000
Nitrogen	6.9701	43	90677	RS	11.015590	.138694E+07
Carbon	39.3141	67	998861	RS	1.000000	.269880E+07
Hydrogen	4.2233	178	242325	RS	4.121989	.611708E+07
Totals	50.5075		1348234			

Figure S7. Elemental analysis of compound **9**.

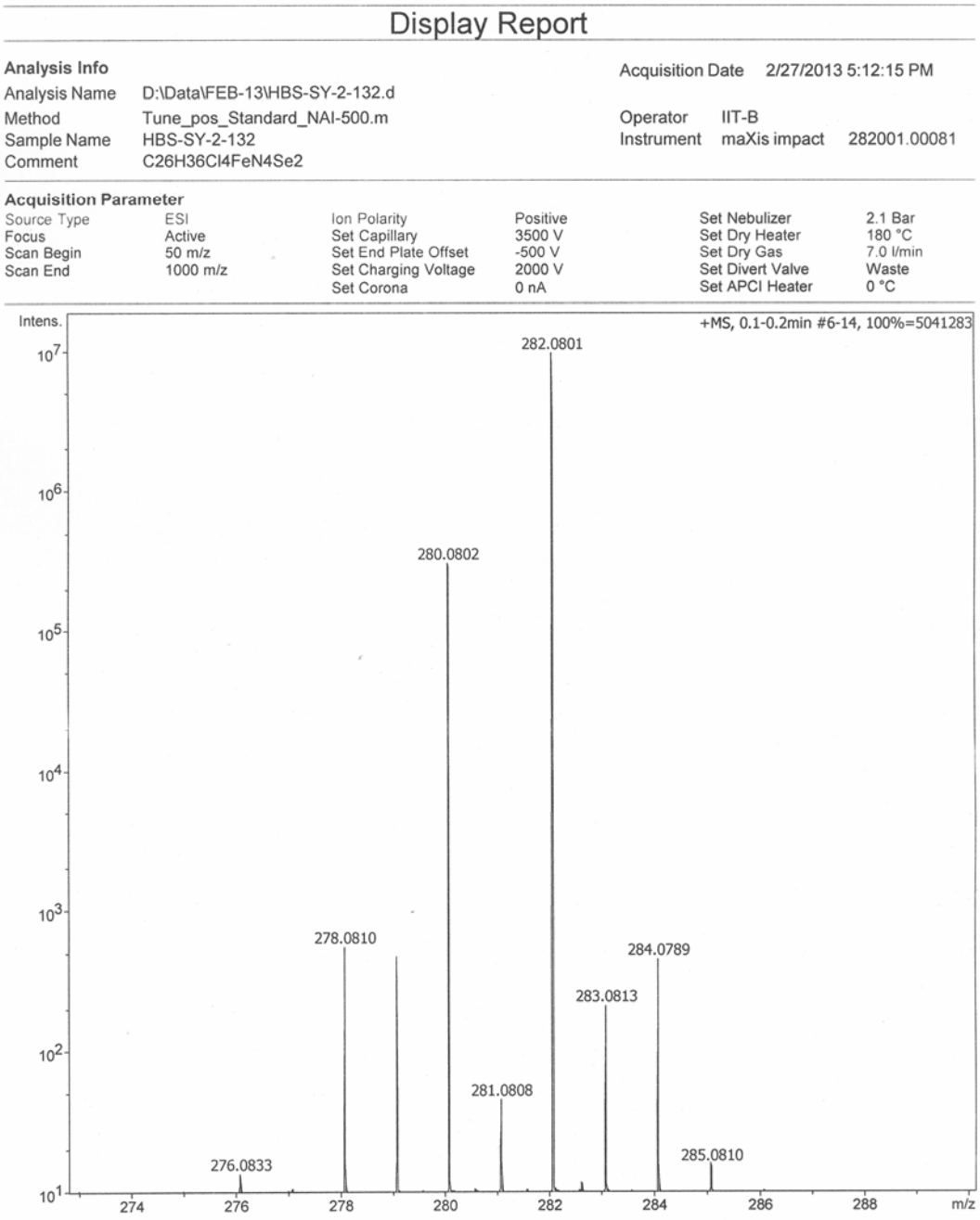


Figure S8. ESI-MS spectrum of compound **9**.

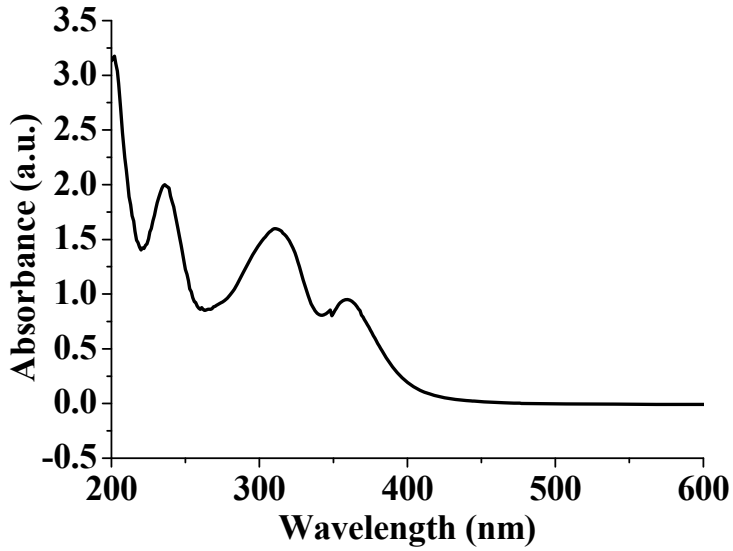


Figure S9. UV-Visible spectrum of compound **9**.

Eager 300 Report

Page: 1 Sample: SY-71-R (SY-71-R)

Method Name : HBS-VT-1-08-2014
Method File : D:\CHNS2012-13\HBS-VT-1-08-2014.mth
Chromatogram : SY-71-R
Operator ID : VARSHA Company Name : C.E. Instruments
Analysed : 08/01/2014 19:52 Printed : 8/1/2014 22:50
Sample ID : SY-71-R (# 41) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : 1.447

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	2.8515	42	54269	FU	21.959160	.131525E+07
Carbon	30.3573	66	1191702	FU	1.000000	.271291E+07
Hydrogen	3.4194	178	256595	RS	4.644289	.685809E+07
Totals	36.6282		1502566			

Figure S10. Elemental analysis of compound **10**.

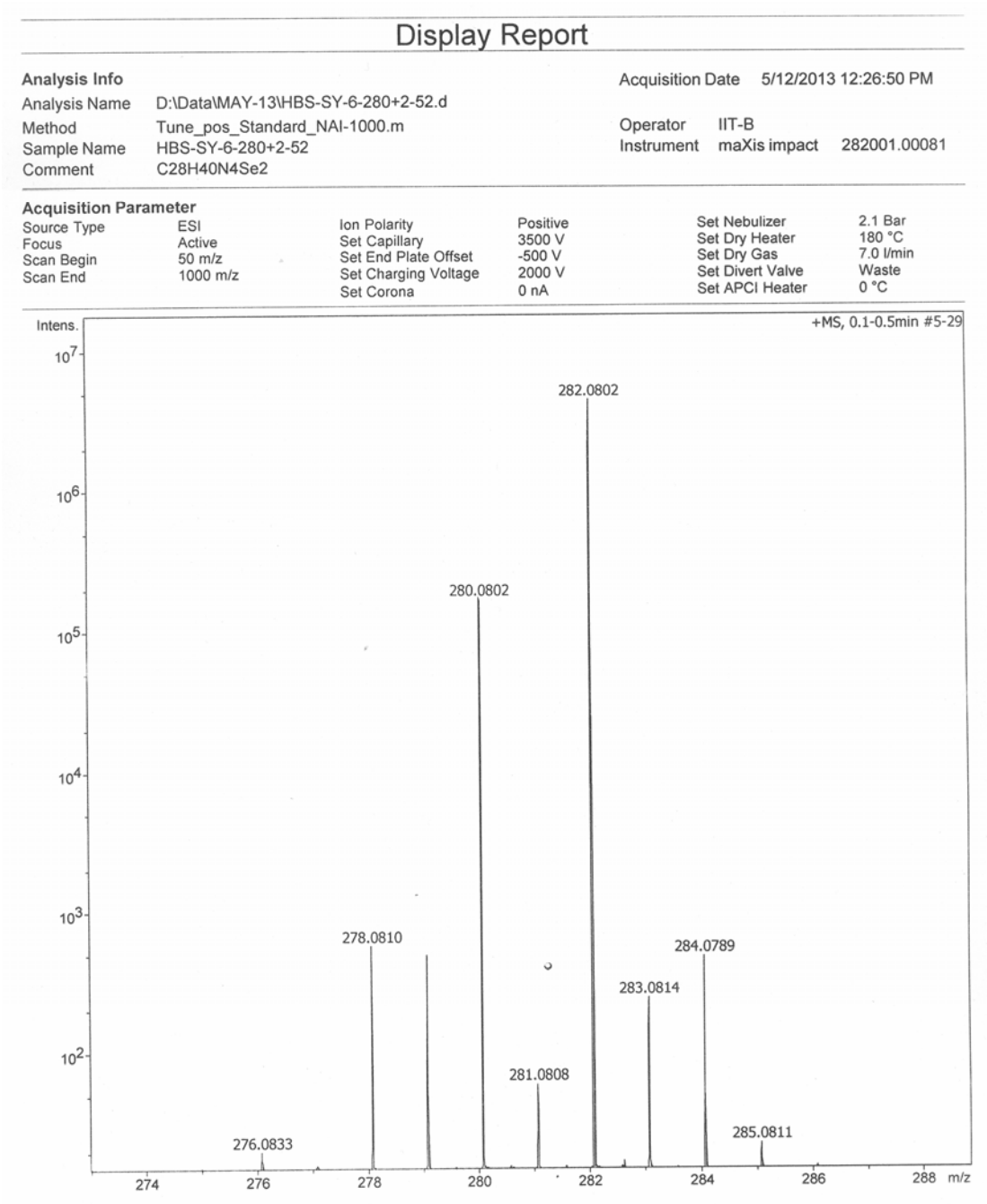


Figure S11. ESI-MS spectrum of compound **10**.

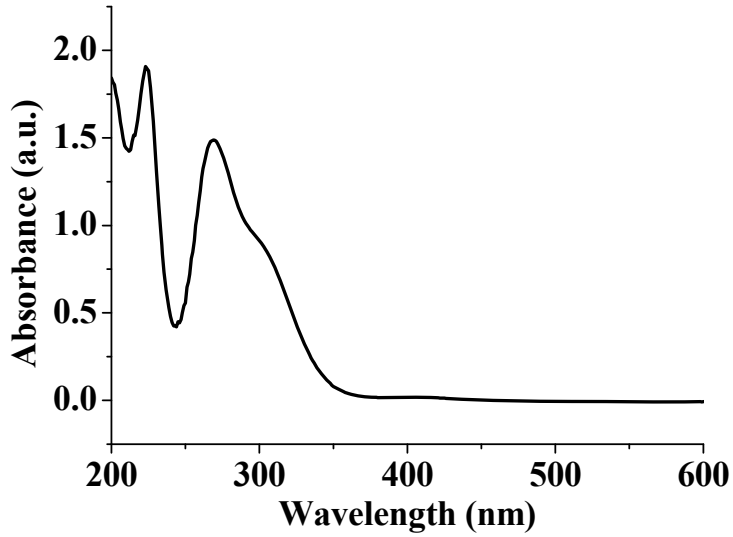


Figure S12. UV-Visible spectrum of compound **10**.

Eager 300 Report

Page: 1 Sample: SY-2-156 (SY-2-156)

Method Name : SD020312
Method File : D:\CHNS2012\SD020312.mth
Chromatogram : SY-2-156
Operator ID : SD
Analysed : 03/02/2012 14:45
Sample ID : SY-2-156 (# 27)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 3/2/2012 16:40
Instrument N. : Instrument #1
Sample weight : .629

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	8.1434	44	72341	FU	8.391951	.141232E+07
Carbon	38.8942	68	607085	FU	1.000000	.247227E+07
Hydrogen	4.2897	181	148548	RS	4.086792	.550538E+07
Totals	51.3273		827974			

Figure S13. Elemental analysis of compound **11**.

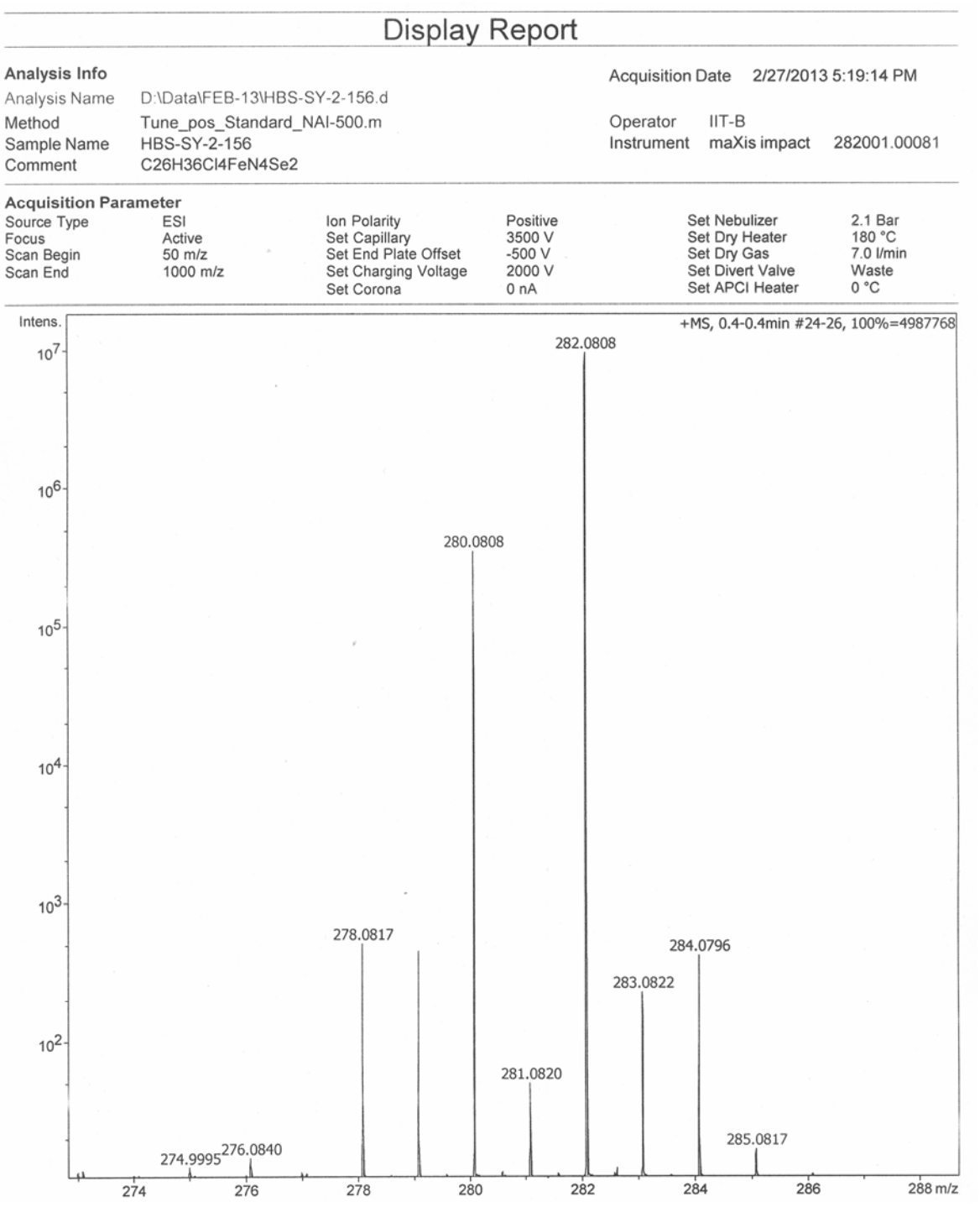


Figure S14. ESI-MS spectrum of compound **11**.

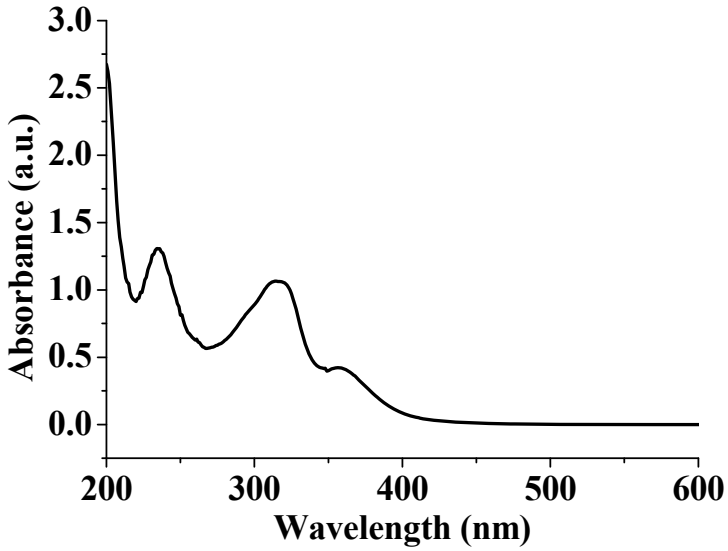


Figure S15. UV-Visible spectrum of compound **11**.

Eager 300 Report

Page: 1 Sample: SY-6-98 (SY-6-98)

Method Name : VT40113
Method File : D:\CHNS2012\VT40113.mth
Chromatogram : SY-6-98
Operator ID : VT
Analysed : 01/04/2013 13:41
Sample ID : SY-6-98 (# 11)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 1/4/2013 17:21
Instrument N. : Instrument #1
Sample weight : .643

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	6.5250	43	59373	FU	9.600132	.141514E+07
Carbon	30.3184	67	569991	FU	1.000000	.266261E+07
Hydrogen	3.6472	181	172377	RS	3.306652	.644079E+07
Totals	40.1906		801741			

Figure S16. Elemental analysis of compound **12**.

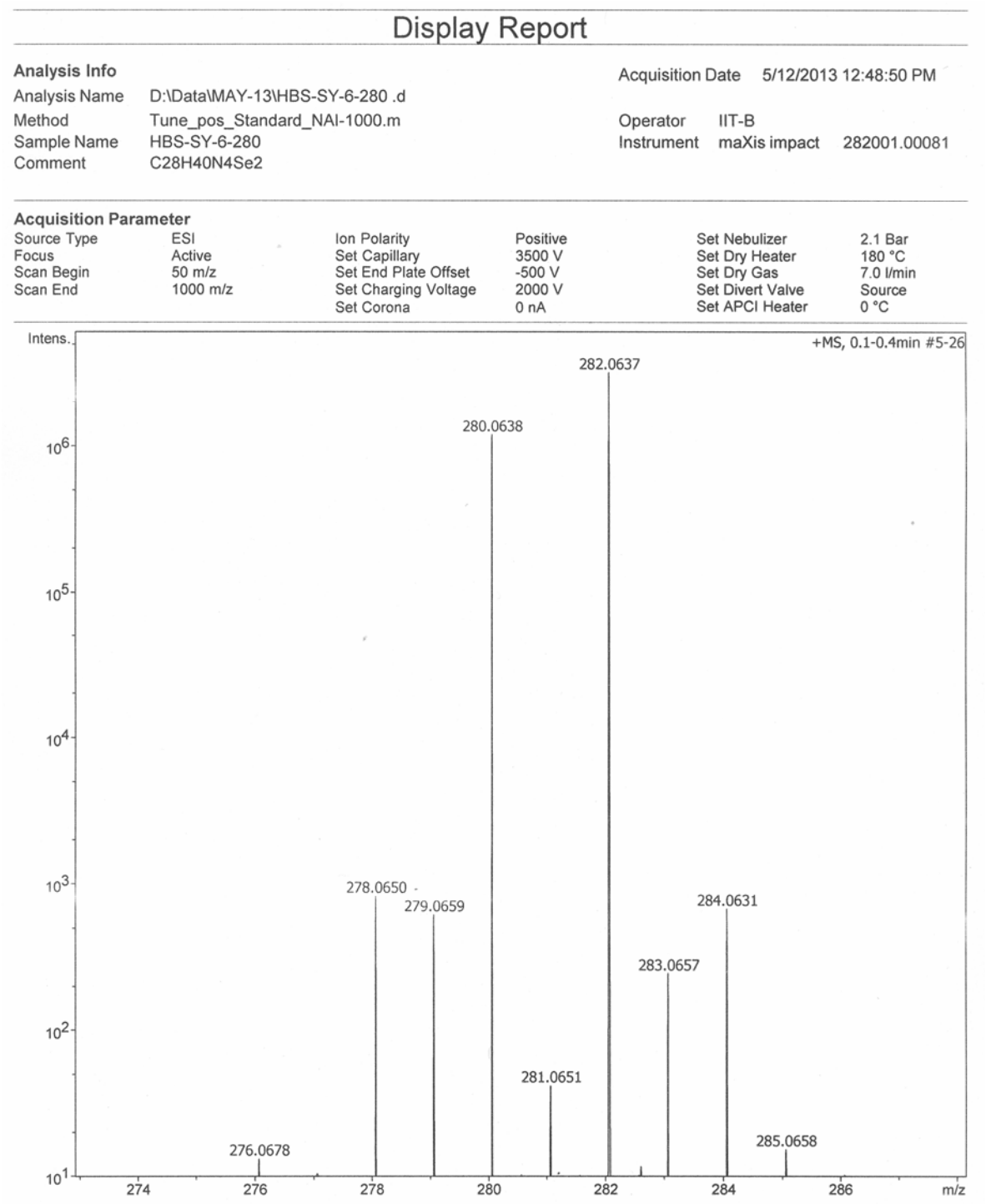


Figure S17. ESI-MS spectrum of compound **12**.

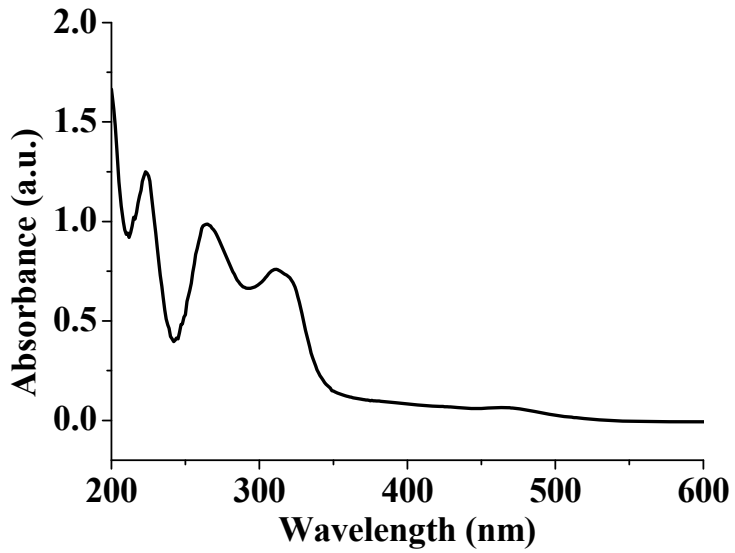


Figure S18. UV-Visible spectrum of compound **12**.

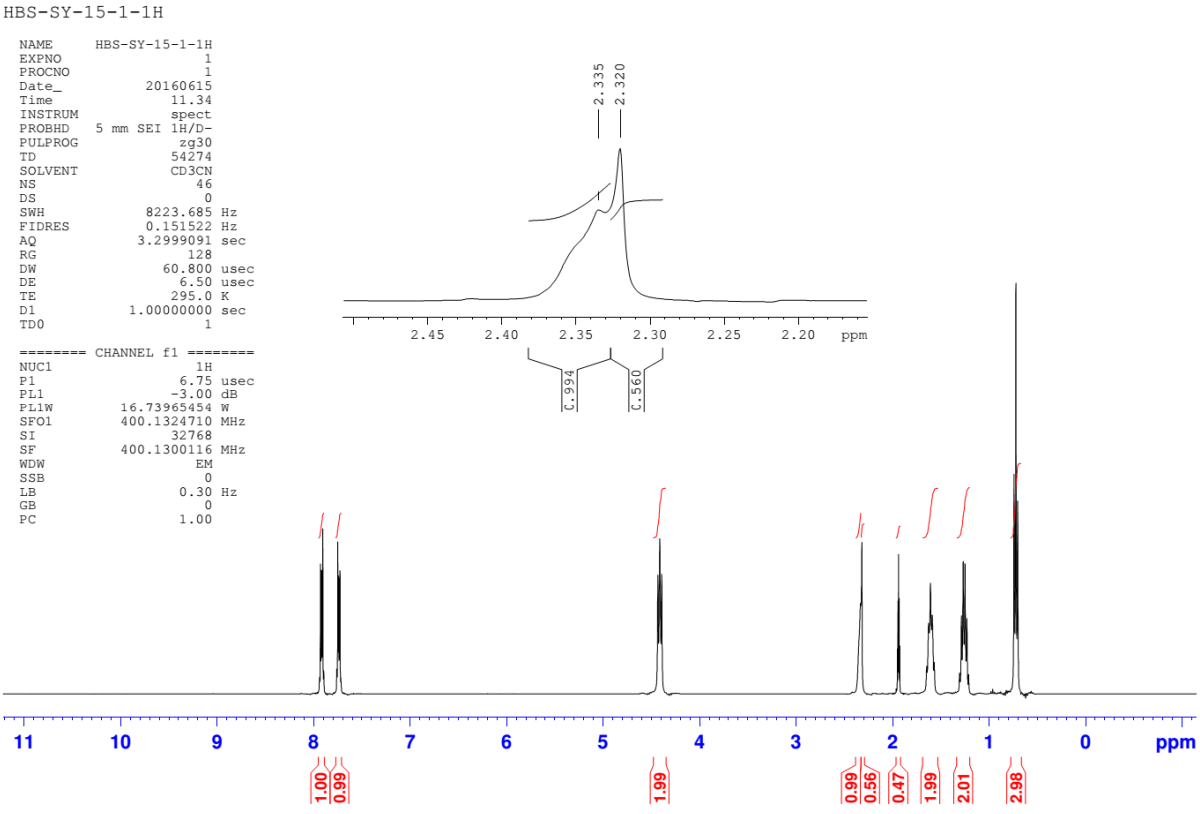


Figure S19a. ^{1}H NMR spectrum of compound **15**.

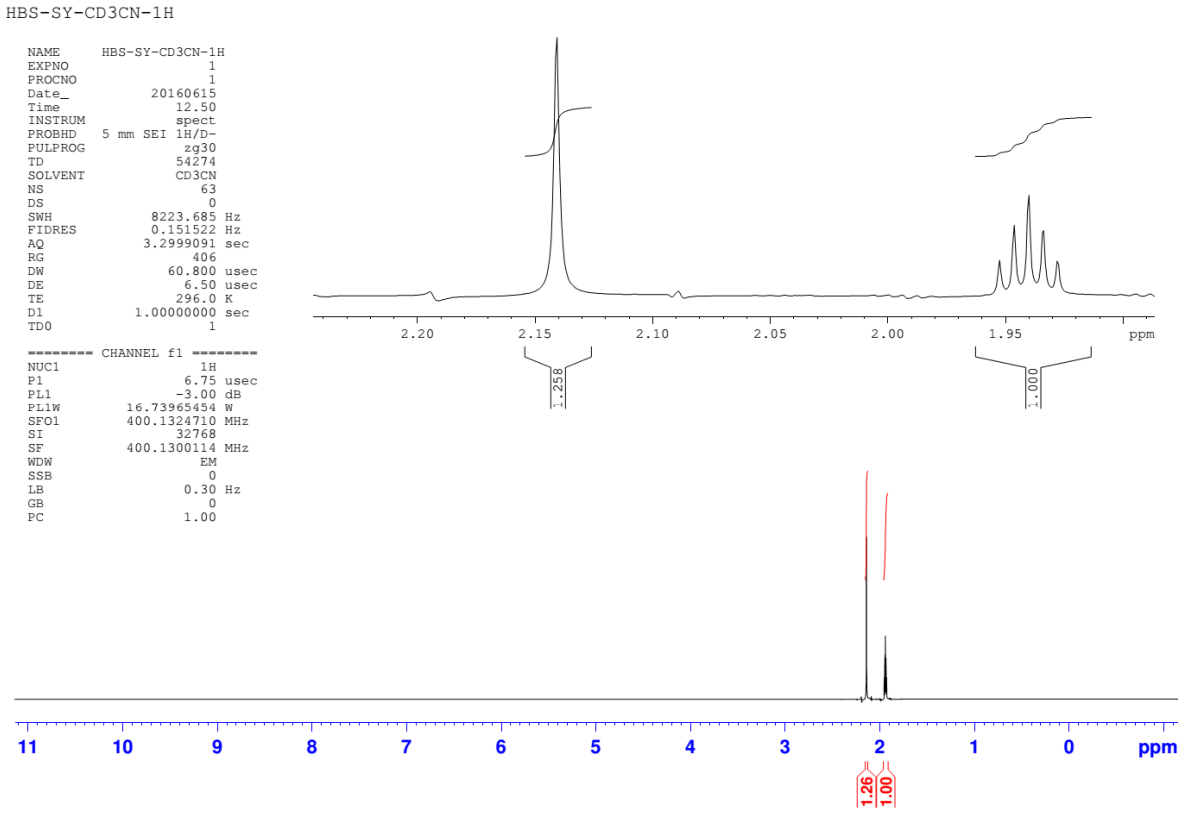


Figure S19b. ^{1}H NMR spectrum of CD_3CN.

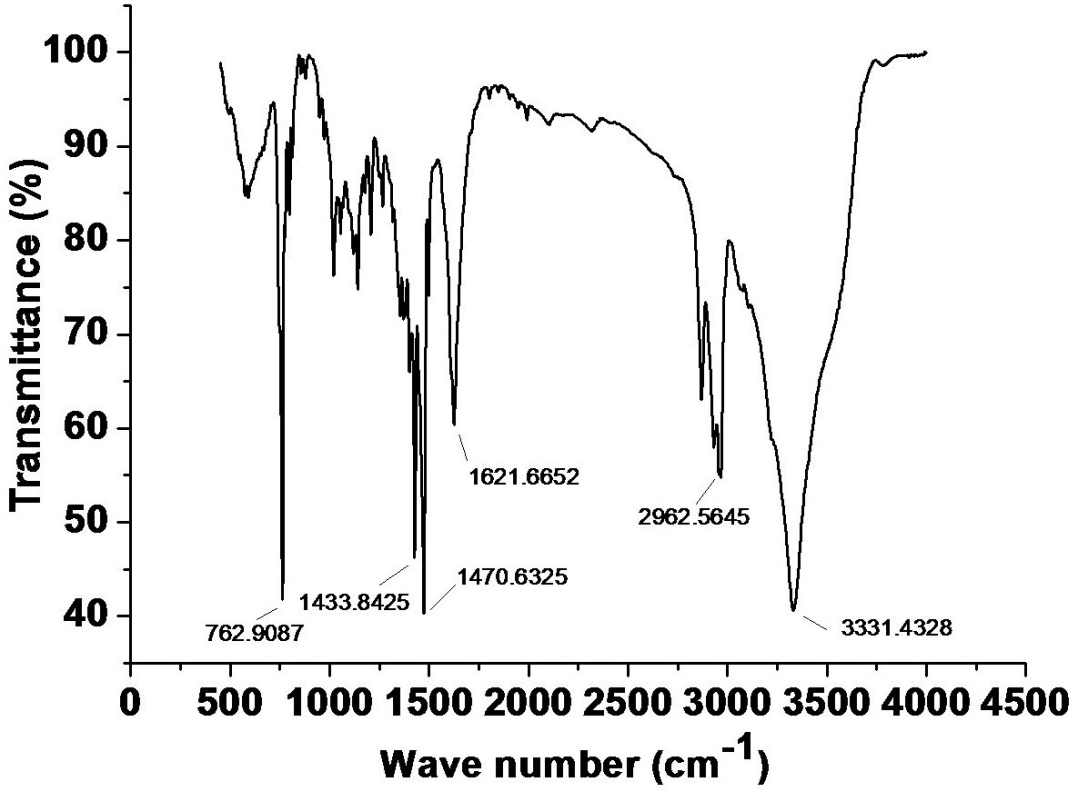


Figure S19c. IR spectrum of **15**.

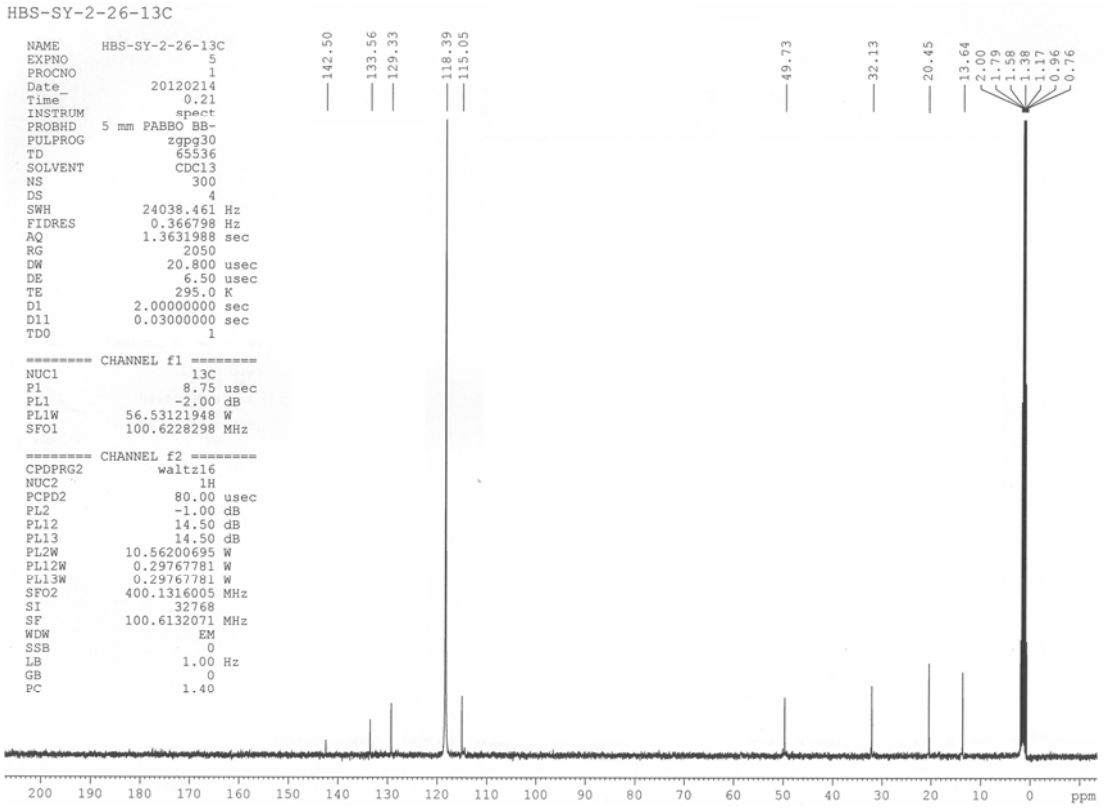


Figure S20. ^{13}C NMR spectrum of compound **15**.

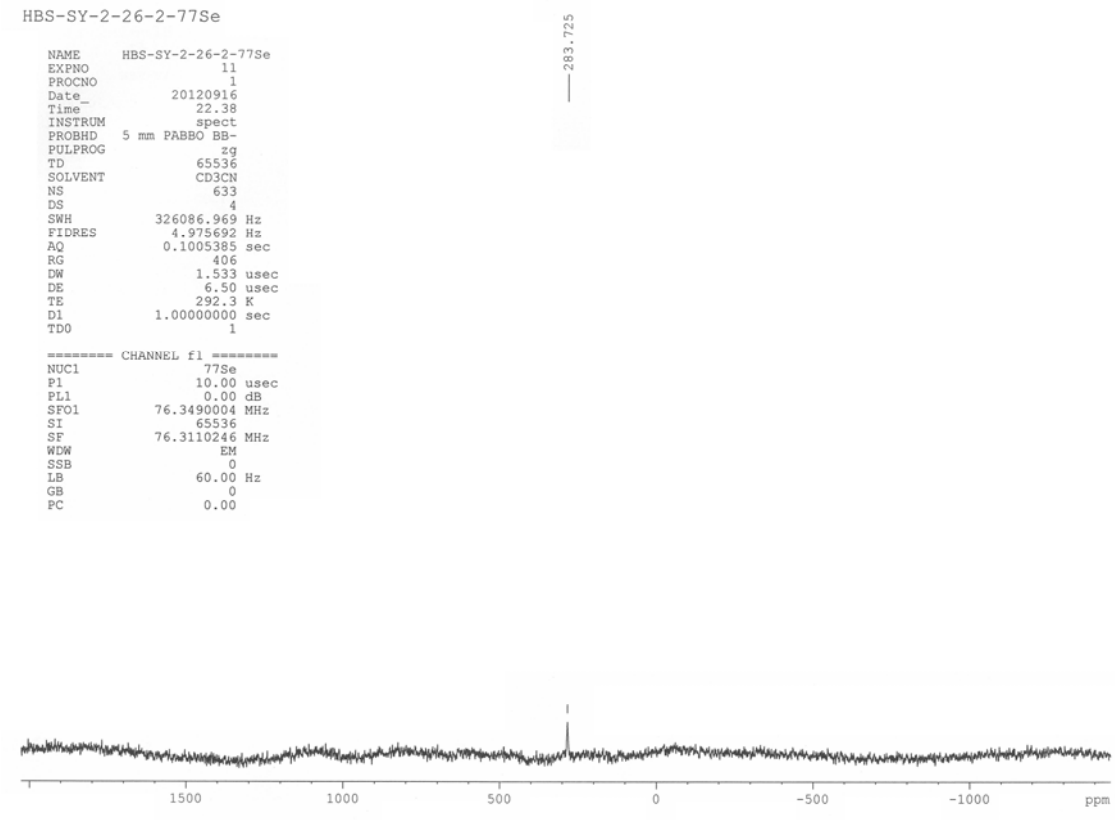


Figure S21. ^{77}Se NMR spectrum of compound **15**.

Eager 300 Report

Page: 1 Sample: HBS-SY-7-346 (HBS-SY-7-346)

Method Name : VT-1-30-05-2014
Method File : D:\CHNS-2014\VT-30-05-2014.mth
Chromatogram : HBS-SY-7-346
Operator ID : VARSHA Company Name : C.E. Instruments
Analysed : 05/30/2014 13:37 Printed : 5/30/2014 16:55
Sample ID : HBS-SY-7-346 (# 14) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : .813

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	9.2734	41	97415	FU	7.972095	.129209E+07
2	0.0000	56	190072	FU		0.0000
Carbon	35.7761	66	776601	FU	1.000000	.265371E+07
Hydrogen	4.3609	181	229487	RS	3.384073	.632629E+07
Totals	49.4104		1293574			

Figure S22. Elemental analysis of compound **15**.

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

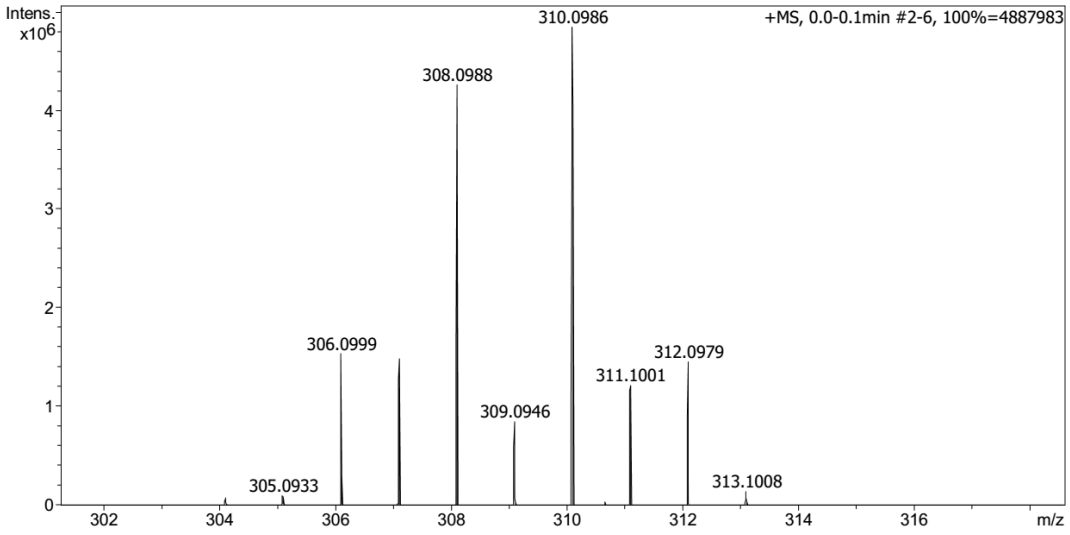
Analysis Info

Analysis Name D:\Data\MARCH-2016\HBS-SY-18.d
Method Tune_pos_NAICSI-1000a.m
Sample Name HBS-SY-18
Comment

Acquisition Date 3/26/2016 10:38:56 PM
Operator HBS-SY
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 Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
310.0986	1	C30H44N4Se2	310.0946	12.9	285.3	1	100.00	11.0	even	ok

Figure S23. ESI-MS spectrum of compound **15**.

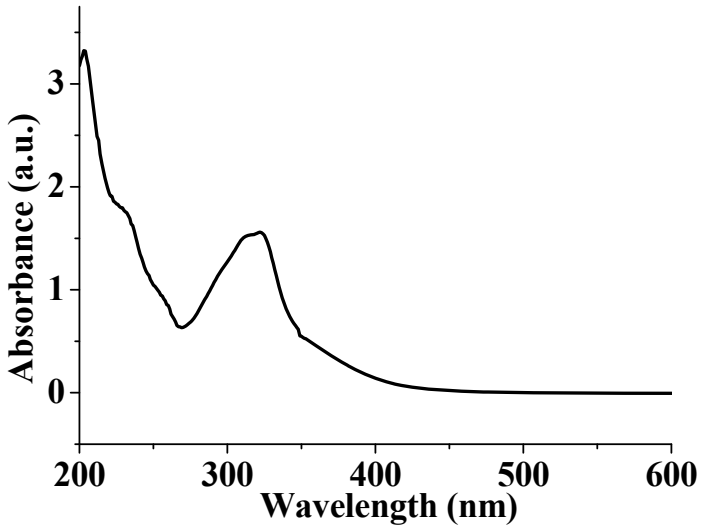


Figure S24. UV-Visible spectrum of compound **15**.

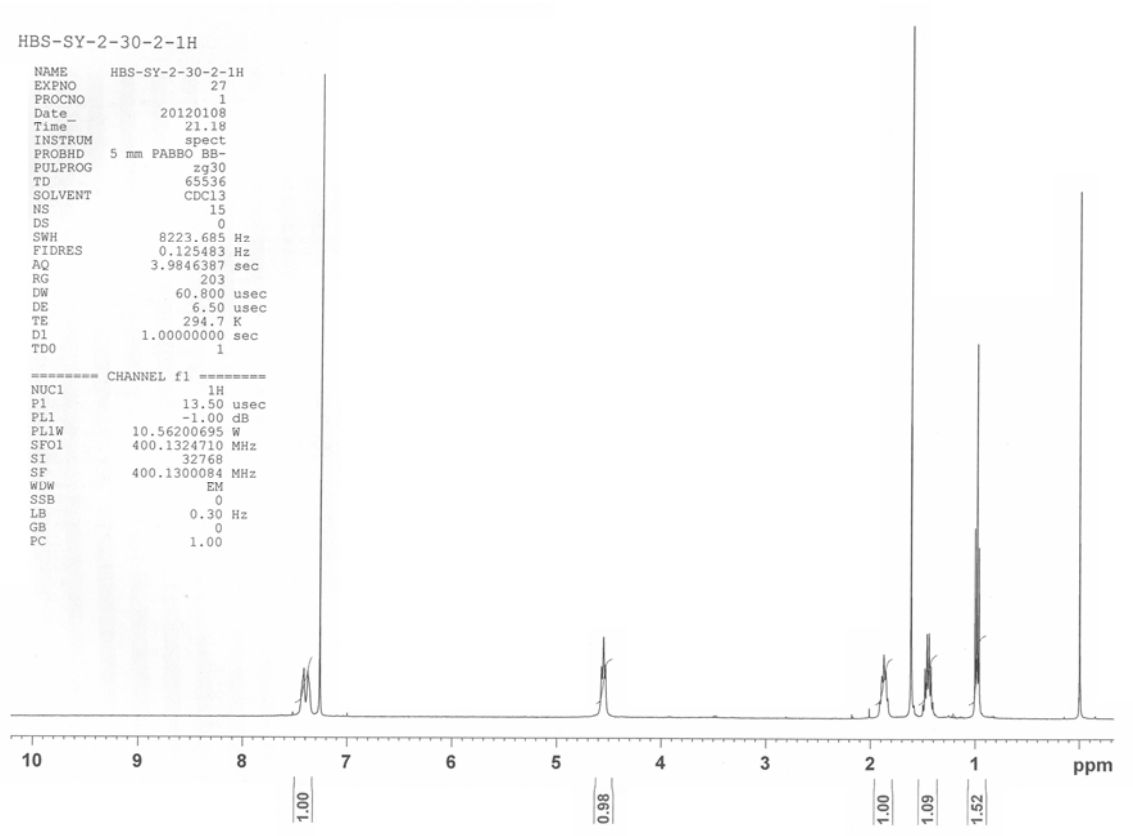


Figure S25. ^{1}H NMR spectrum of compound **17**.

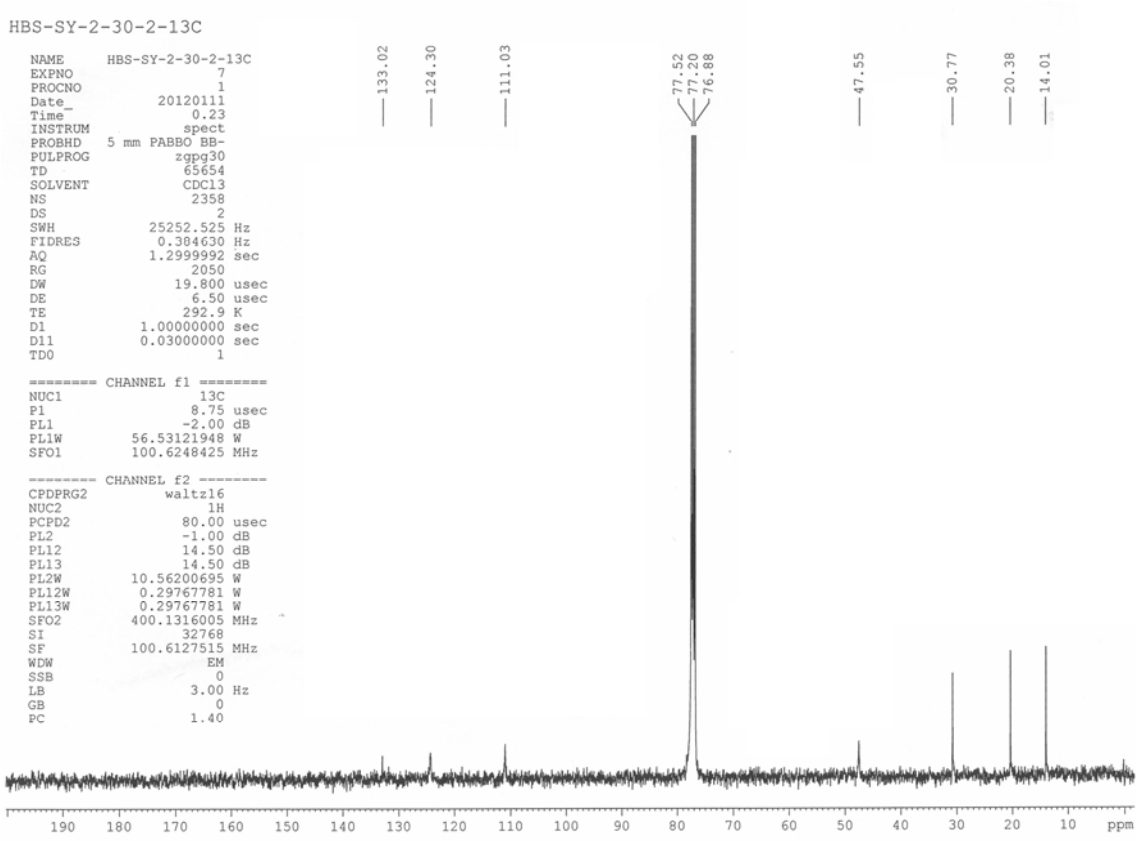


Figure S26. ^{13}C NMR spectrum of compound **17**.

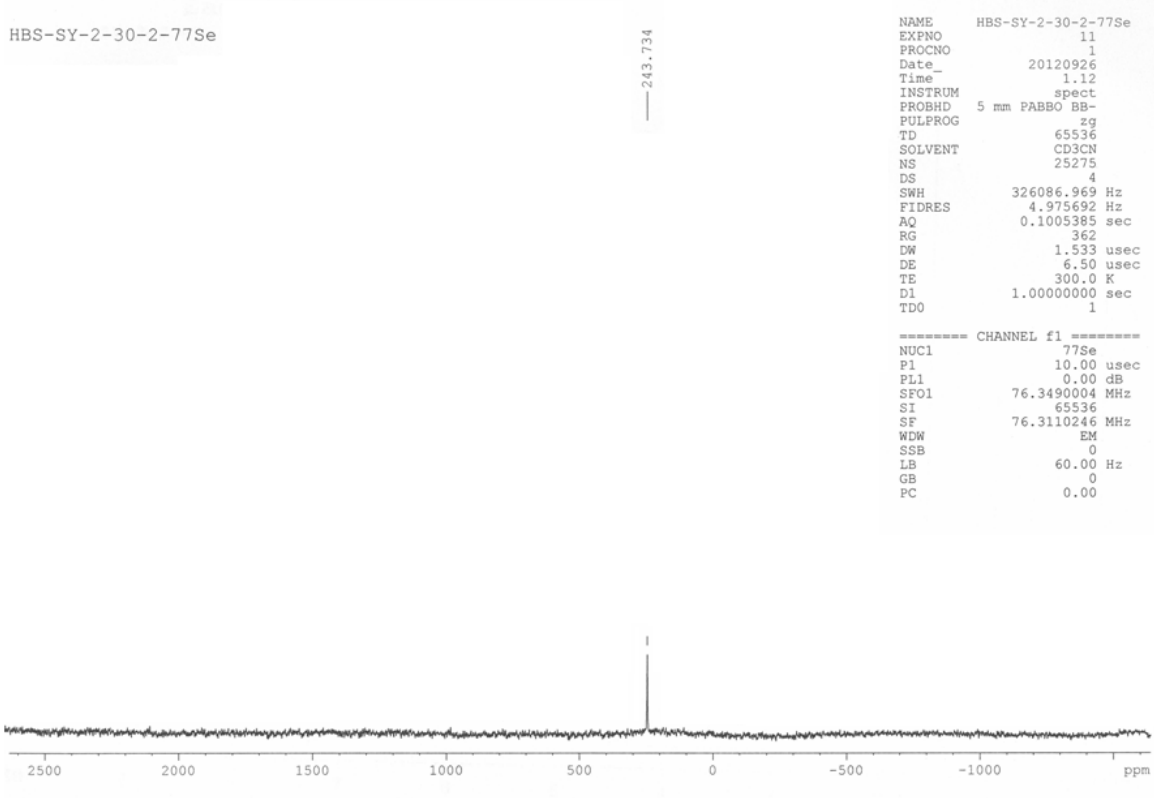


Figure S27. ^{77}Se NMR spectrum of compound **17**.

Eager 300 Report

Page: 1 Sample: SY-2-30-2 (SY-2-30-2)

Method Name : SP160312
Method File : D:\CHNS2012\SP160312.mth
Chromatogram : SY-2-30-2
Operator ID : SP Company Name : C.E. Instruments
Analysed : 03/16/2012 14:11 Printed : 3/16/2012 17:44
Sample ID : SY-2-30-2 (# 20) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : .958

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	17257	RS		0.0000
Nitrogen	5.8314	43	77481	RS	12.004650	.138694E+07
Carbon	35.8350	67	930132	RS	1.000000	.269880E+07
Hydrogen	4.1297	178	242005	RS	3.843441	.611708E+07
Totals	45.7961		1266875			

Figure S28. Elemental analysis of compound **17**.

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

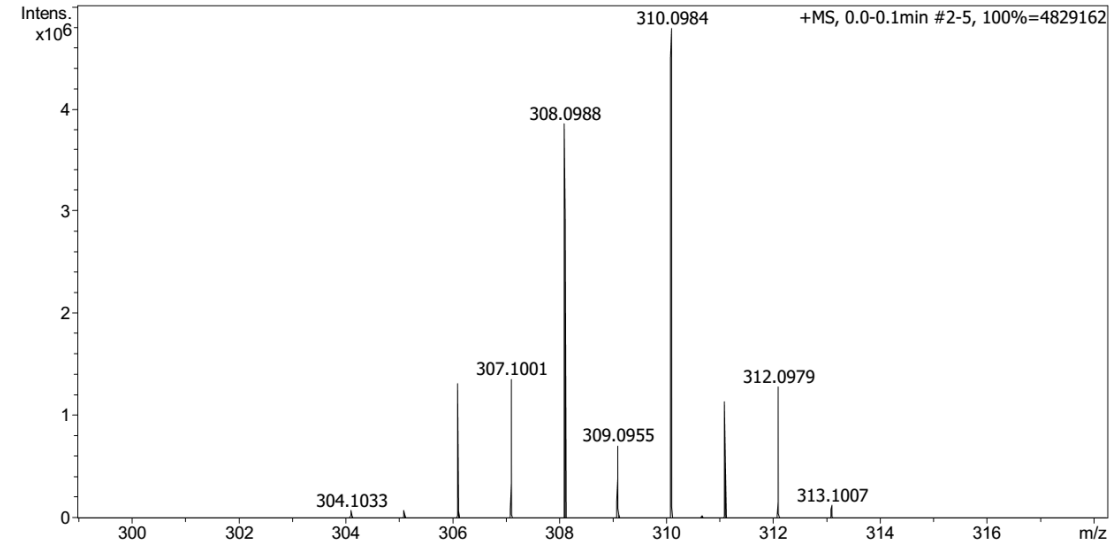
Analysis Info

Analysis Name D:\Data\MARCH-2016\HBS-SY-23.d
Method Tune_pos_NAICSI-1000a.m
Sample Name HBS-SY-23
Comment

Acquisition Date 3/26/2016 10:45:48 PM
Operator HBS-SY
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 Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
310.0984	1	C30H44N4Se2	310.0946	-12.4	280.9	1	100.00	11.0	even	ok

Figure S29. ESI-MS spectrum of compound 1**7**.

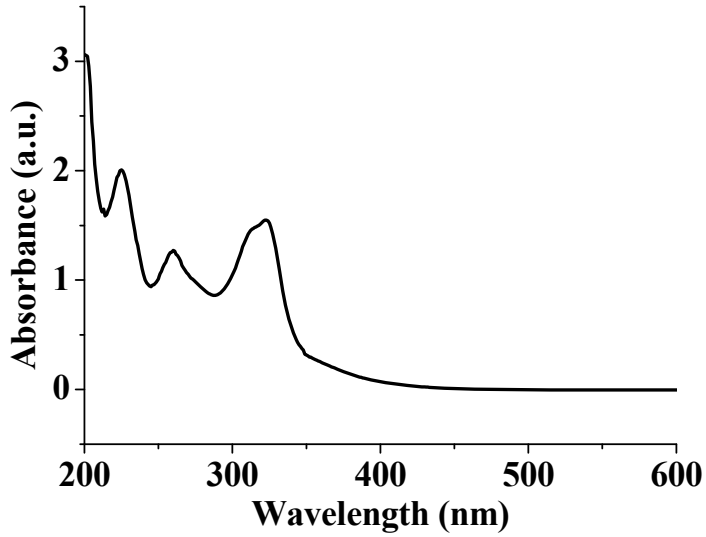


Figure S30. UV-Visible spectrum of compound 1**7**.

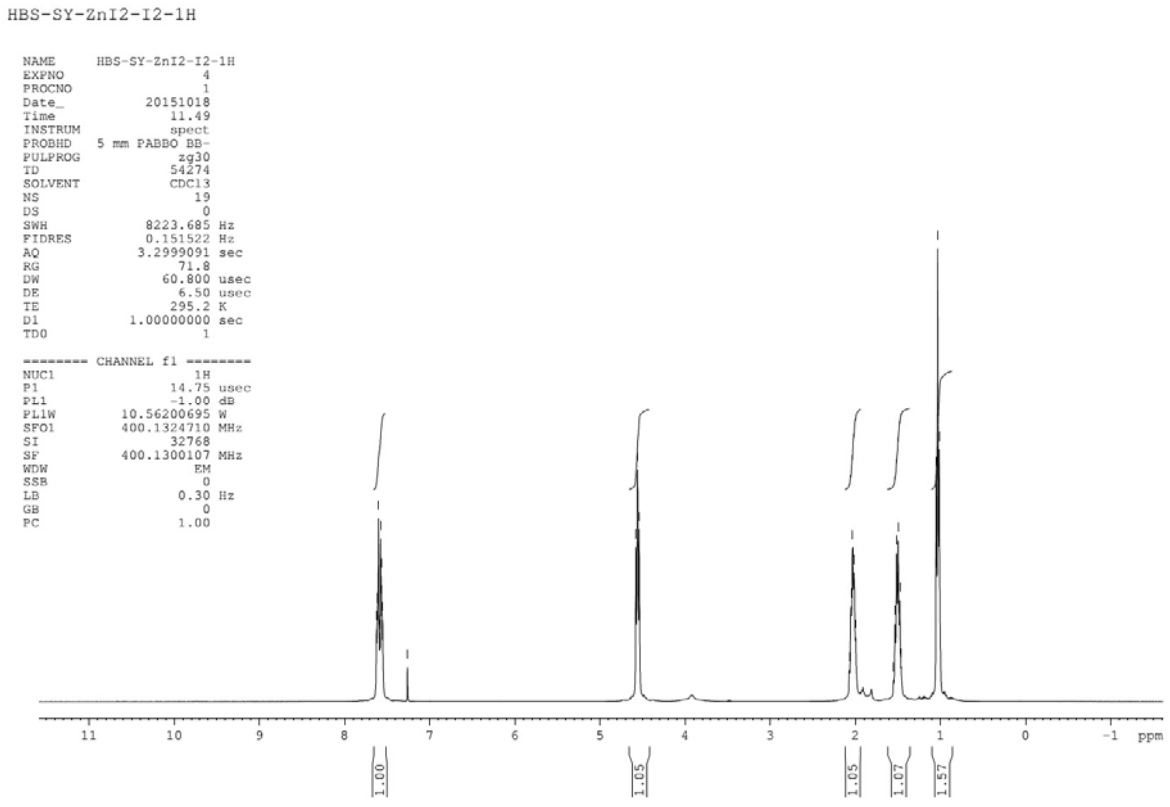


Figure S31. ^{1}H NMR spectrum of compound **19**.

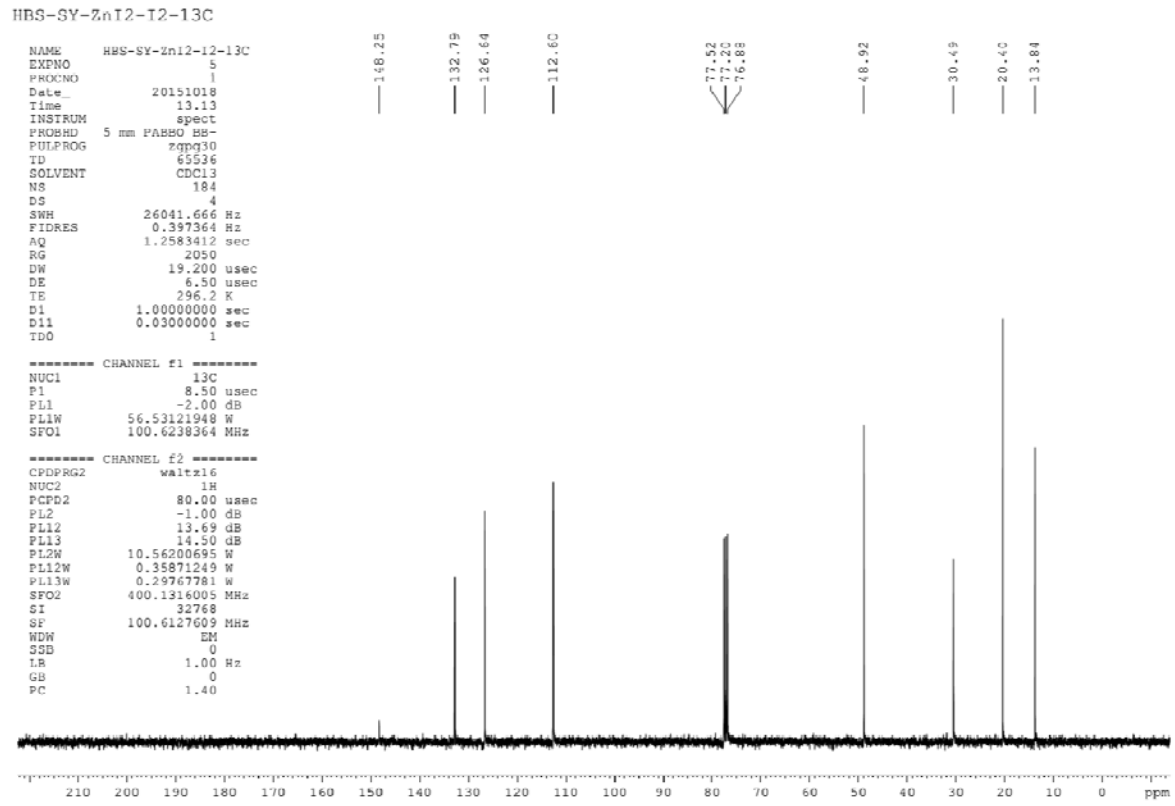


Figure S32. ^{13}C NMR spectrum of compound **19**.

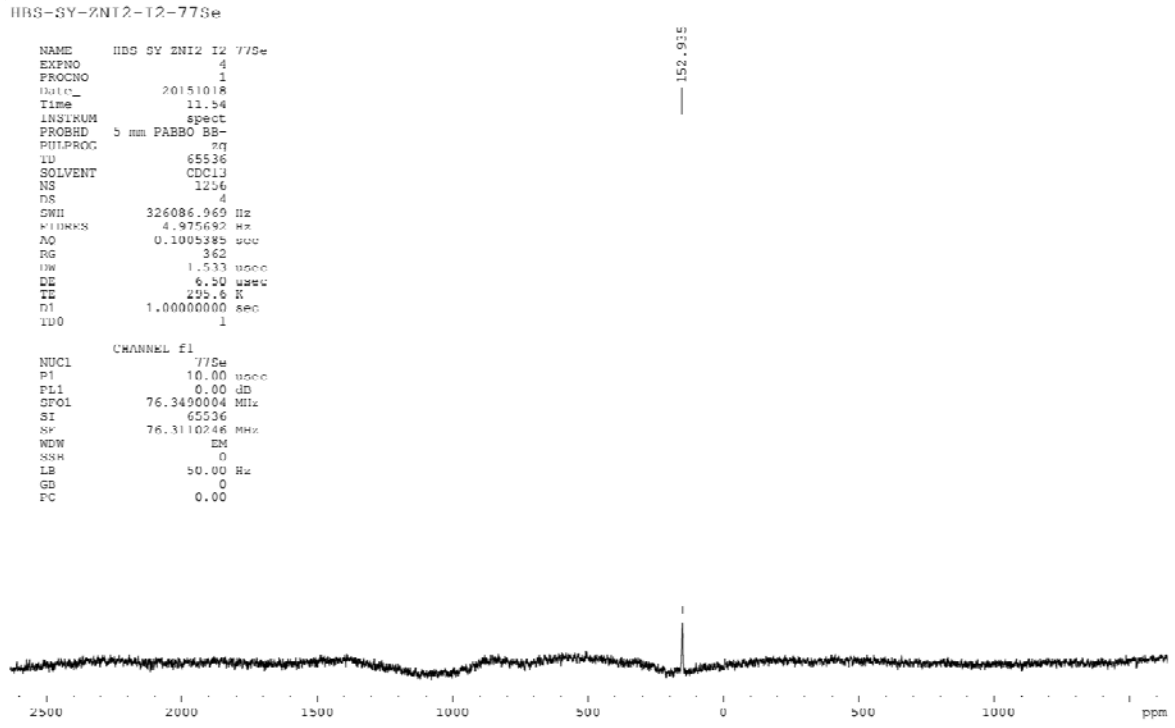


Figure S33. ^{77}Se NMR spectrum of compound **19**.

Eager 300 Report

Page: 1 Sample: SY-63 (SY-63)

Method Name : HBS-VT-1-08-2014
Method File : D:\CHNS2012-13\HBS-VT-1-08-2014.mth
Chromatogram : SY-63
Operator ID : VARSHA Company Name : C.E. Instruments
Analysed : 08/01/2014 20:02 Printed : 8/1/2014 22:50
Sample ID : SY-63 (# 42) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : 1.37

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	2.0595	42	37110	FU	39.269420	.131525E+07
Carbon	29.9088	65	1457269	FU	1.000000	.271291E+07
Hydrogen	3.6750	178	361791	RS	4.027929	.685809E+07
Totals	35.6432		1856169			

Figure S34. Elemental analysis of compound **19**.

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

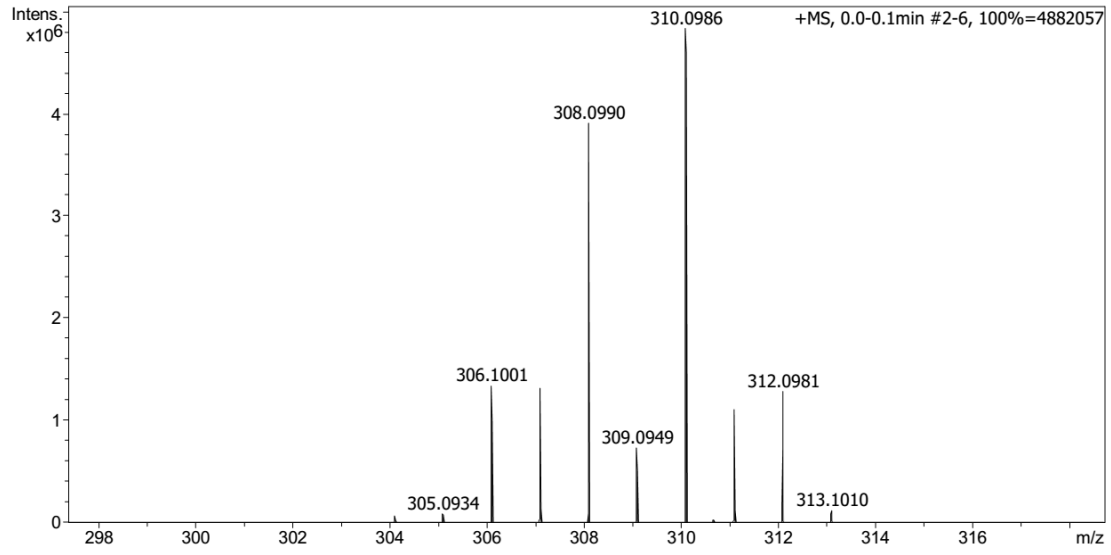
Analysis Info

Analysis Name D:\Data\MARCH-2016\HBS-SY-17.d
Method Tune_pos_NAICSI-1000a.m
Sample Name HBS-SY-17
Comment

Acquisition Date 3/26/2016 10:38:12 PM
Operator HBS-SY
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 Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
310.0986	1	C30H44N4Se2	310.0946	13.0	280.5	1	100.00	11.0	even	ok

Figure S35. ESI-MS spectrum of compound **19**.

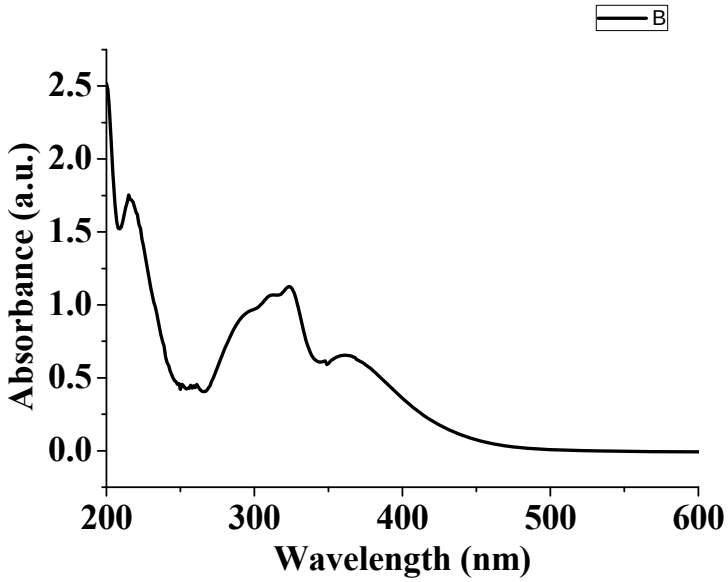


Figure S36. UV-Visible spectrum of compound **19**.

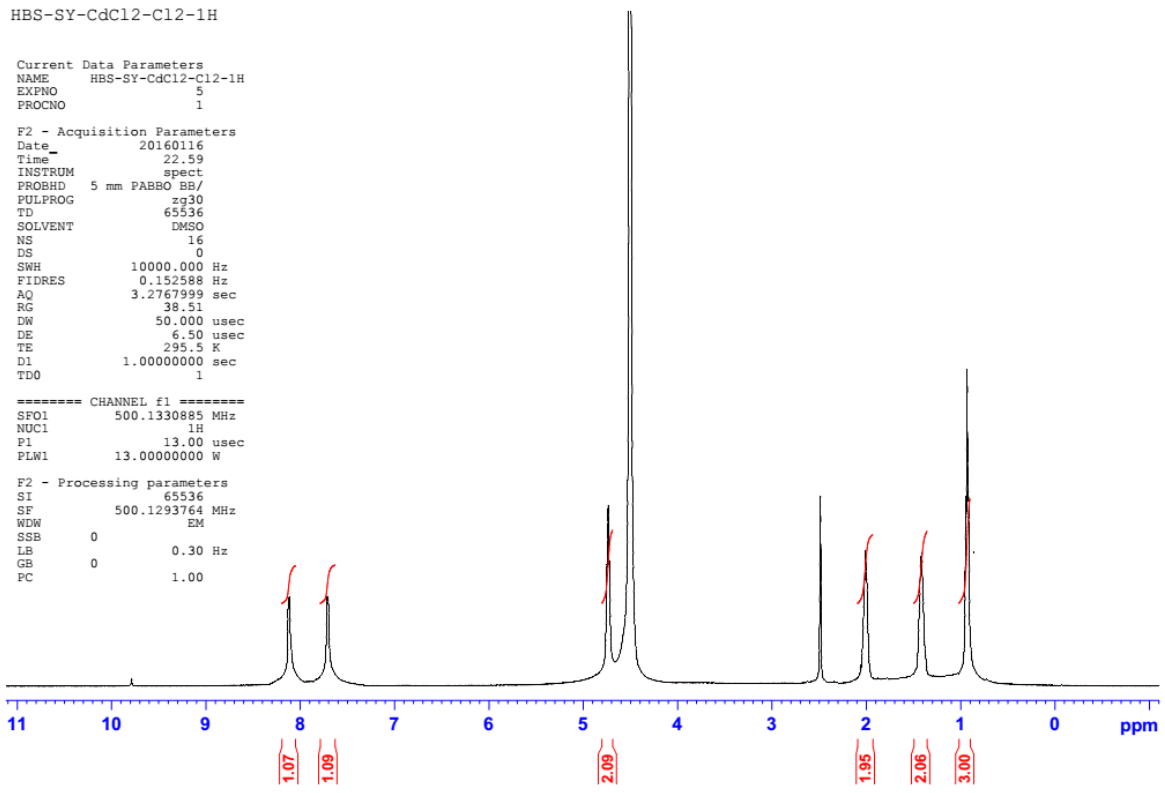


Figure S37. ^{1}H NMR spectrum of compound **21**.

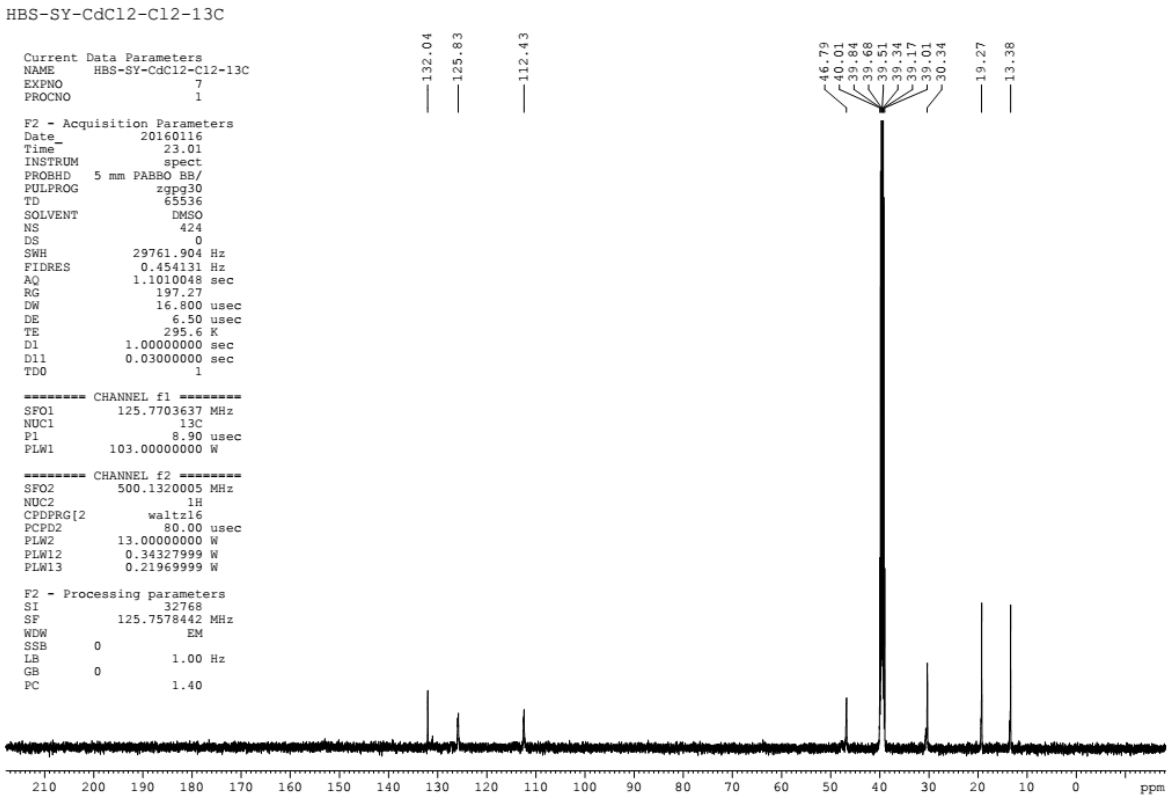


Figure S38. ^{13}C NMR spectrum of compound **21**.

Eager 300 Report

Page: 1 Sample: SY-5-34 (SY-5-34)

Method Name : SD030812
Method File : D:\CHNS2012\SD030812.mth
Chromatogram : SY-5-34
Operator ID : SD
Analysed : 08/03/2012 16:10
Sample ID : SY-5-34 (# 32)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 8/3/2012 16:59
Instrument N. : Instrument #1
Sample weight : 1.112

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	5.7206	42	74910 RS	14.977750	937896.0000
Carbon	41.3499	65	1121984 RS	1.000000	.244010E+07
Hydrogen	4.7592	177	338242 RS	3.317103	.593761E+07
Totals	51.8296		1535136		

Figure S39. Elemental analysis of compound **21**.

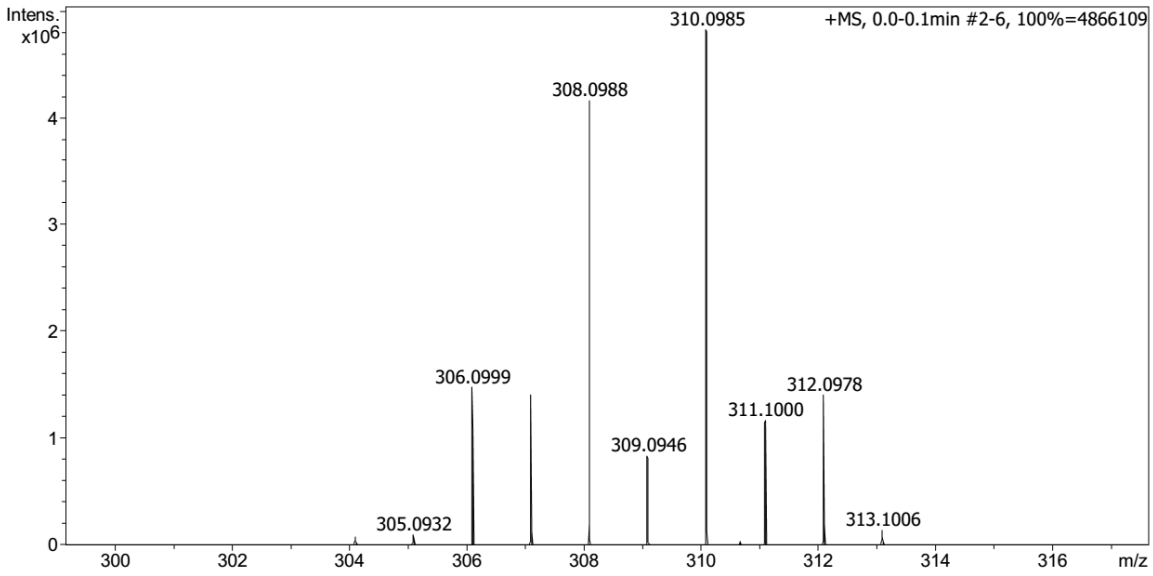
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\MARCH-2016\HBS-SY-16.d	Acquisition Date	3/26/2016 10:37:35 PM
Method	Tune_pos_NAICSI-1000a.m	Operator	HBS-SY
Sample Name	HBS-SY-16	Instrument	maXis impact 282001.00081
Comment			

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 Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
310.0985	1	C30H44N4Se2	310.0946	-12.7	283.3	1	100.00	11.0	even	ok

Figure S40. ESI-MS spectrum of compound **21**.

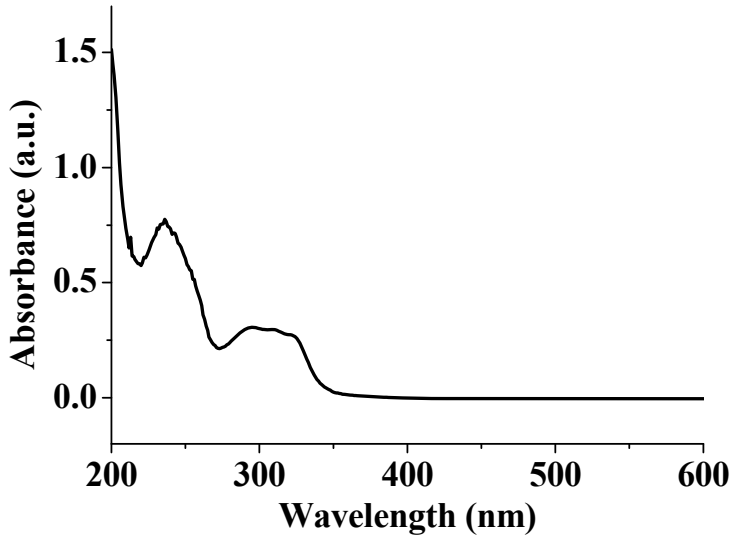


Figure S41. UV-Visible spectrum of compound **21**.

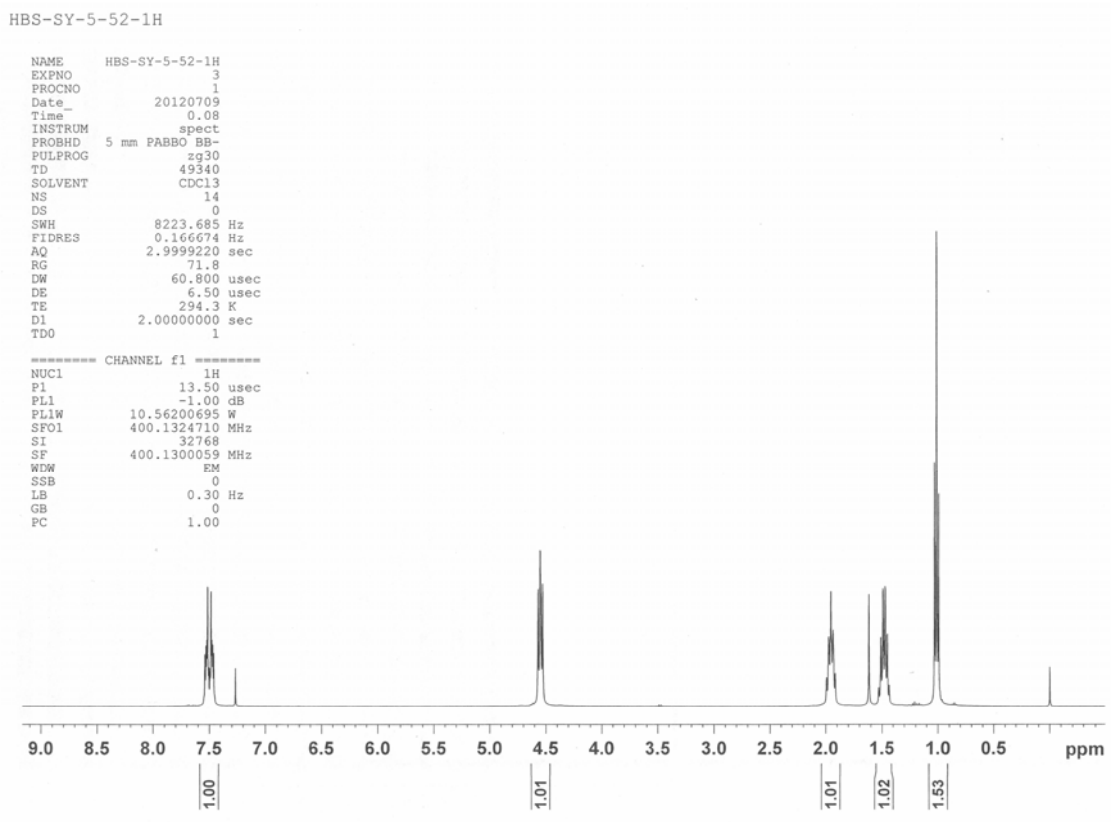


Figure S42. ^{1}H NMR spectrum of compound **22**.

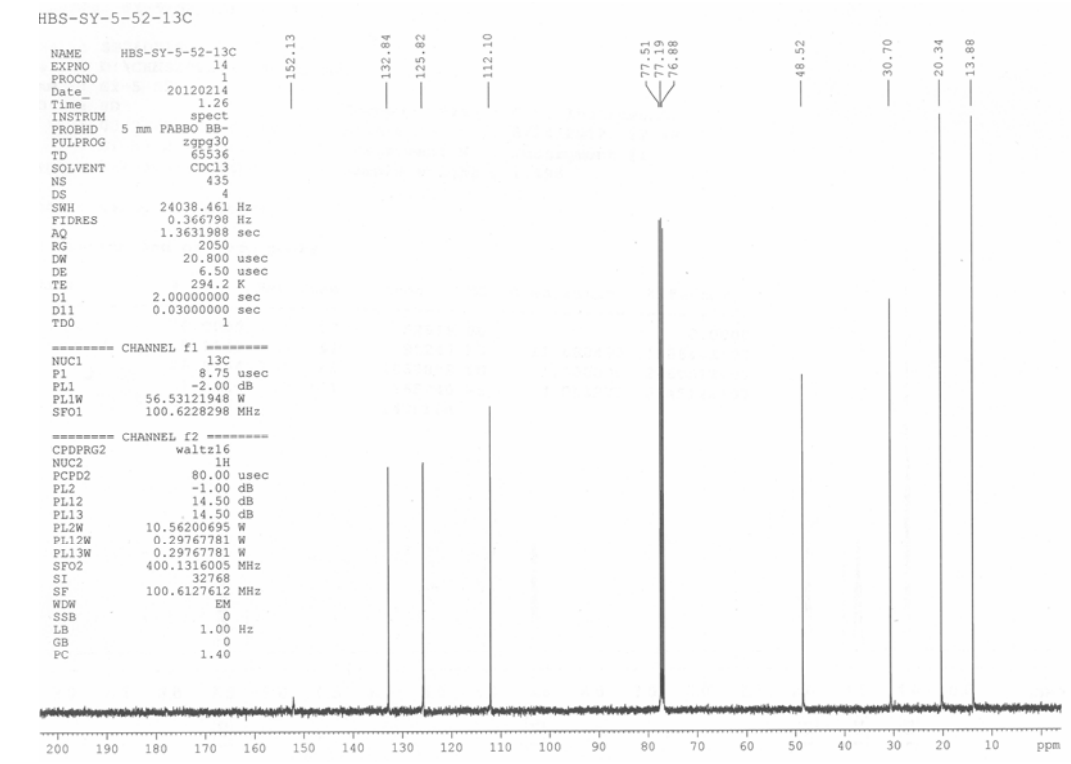


Figure S43. ^{13}C NMR spectrum of compound **22**.

Eager 300 Report

Page: 1 Sample: SY-5-52 (SY-5-52)

Method Name : SP240812
Method File : D:\CHNS2012\SP240812.mth
Chromatogram : SY-5-52
Operator ID : SD
Analysed : 08/24/2012 15:19
Sample ID : SY-5-52 (# 24)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 8/24/2012 22:48
Instrument N. : Instrument #1
Sample weight : 1.498

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	52819	FU		0.0000
Nitrogen	5.1342	42	91247	FU	11.680490	.118640E+07
Carbon	28.8384	65	1065808	FU	1.000000	.246051E+07
Hydrogen	3.3126	181	265240	RS	4.018277	.534512E+07
Totals	37.2853		1475114			

Figure S44. Elemental analysis of compound **22**.

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

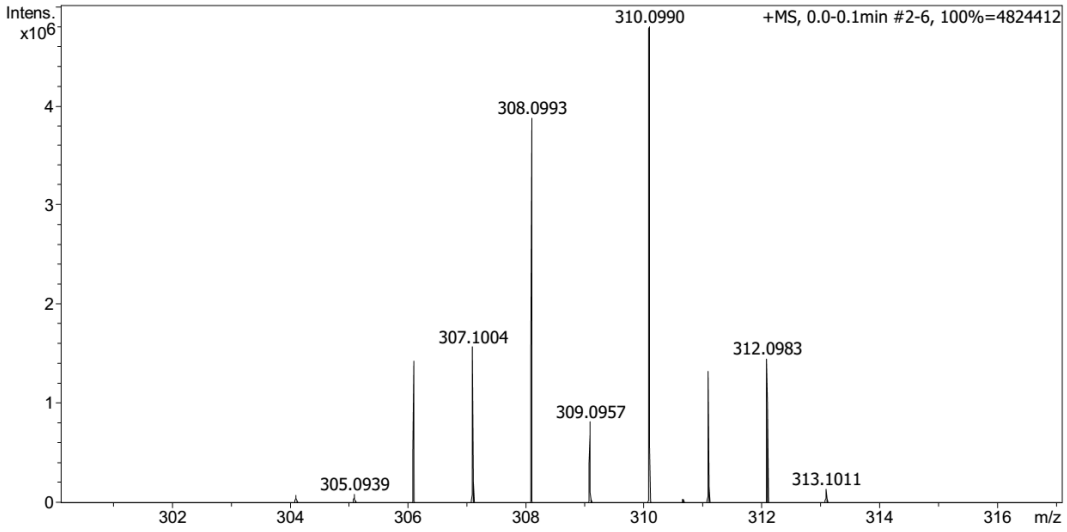
Analysis Info

Analysis Name D:\Data\MARCH-2016\HBS-SY-22.d
Method Tune_pos_NAICSI-1000a.m
Sample Name HBS-SY-22
Comment

Acquisition Date 3/26/2016 10:45:13 PM
Operator HBS-SY
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 Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
310.0990	1	C30H44N4Se2	310.0946	14.1	280.7	1	100.00	11.0	even	ok

Figure S45. ESI-MS spectrum of compound **22**.

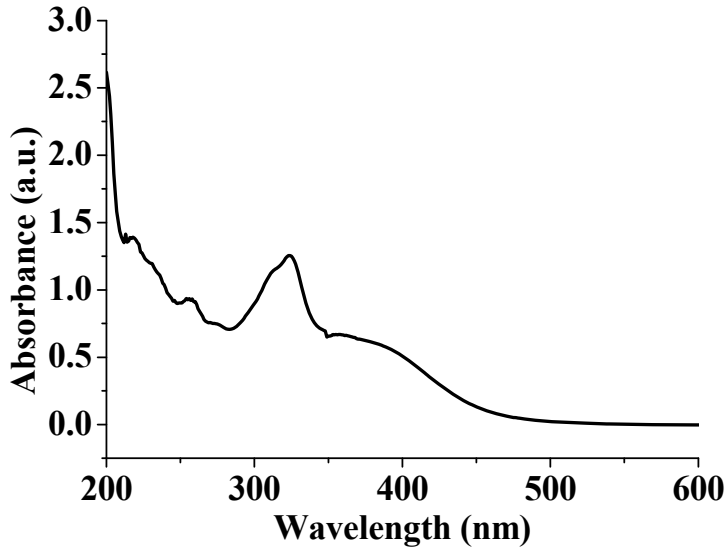


Figure S46. UV-Visible spectrum of compound **22**.

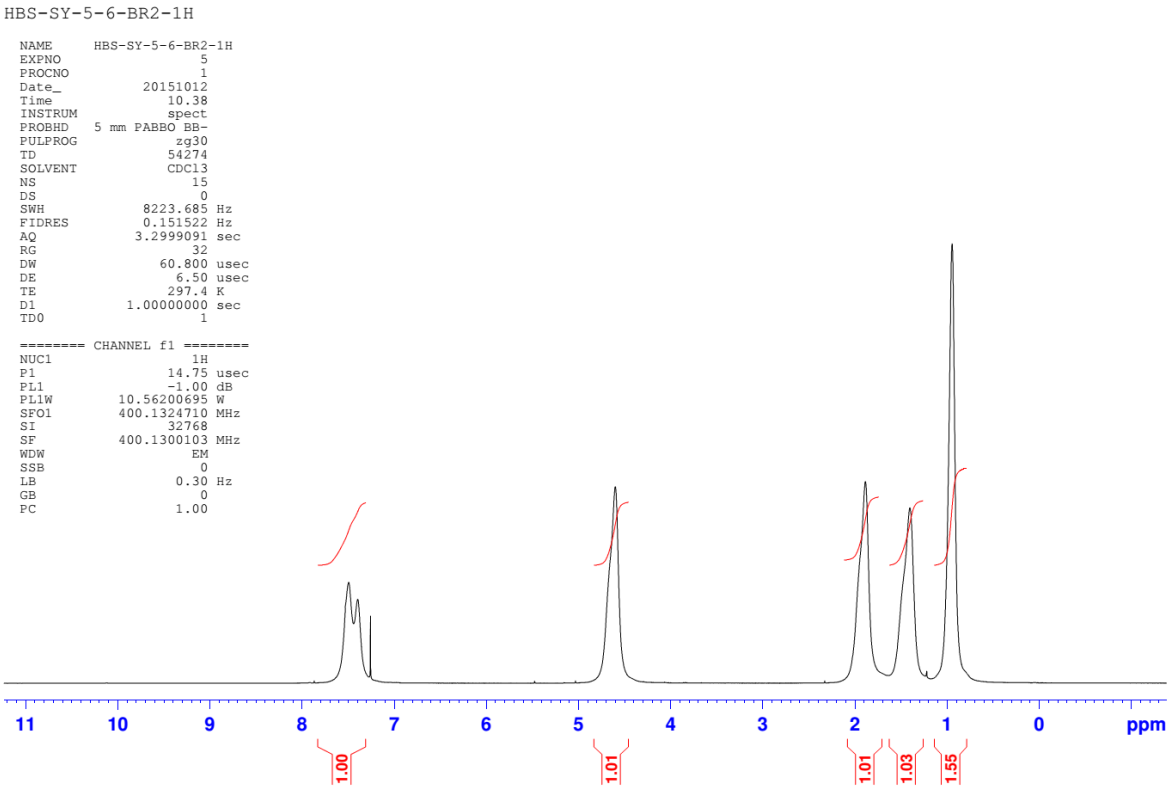


Figure S47. ^{1}H NMR spectrum of compound **23**.

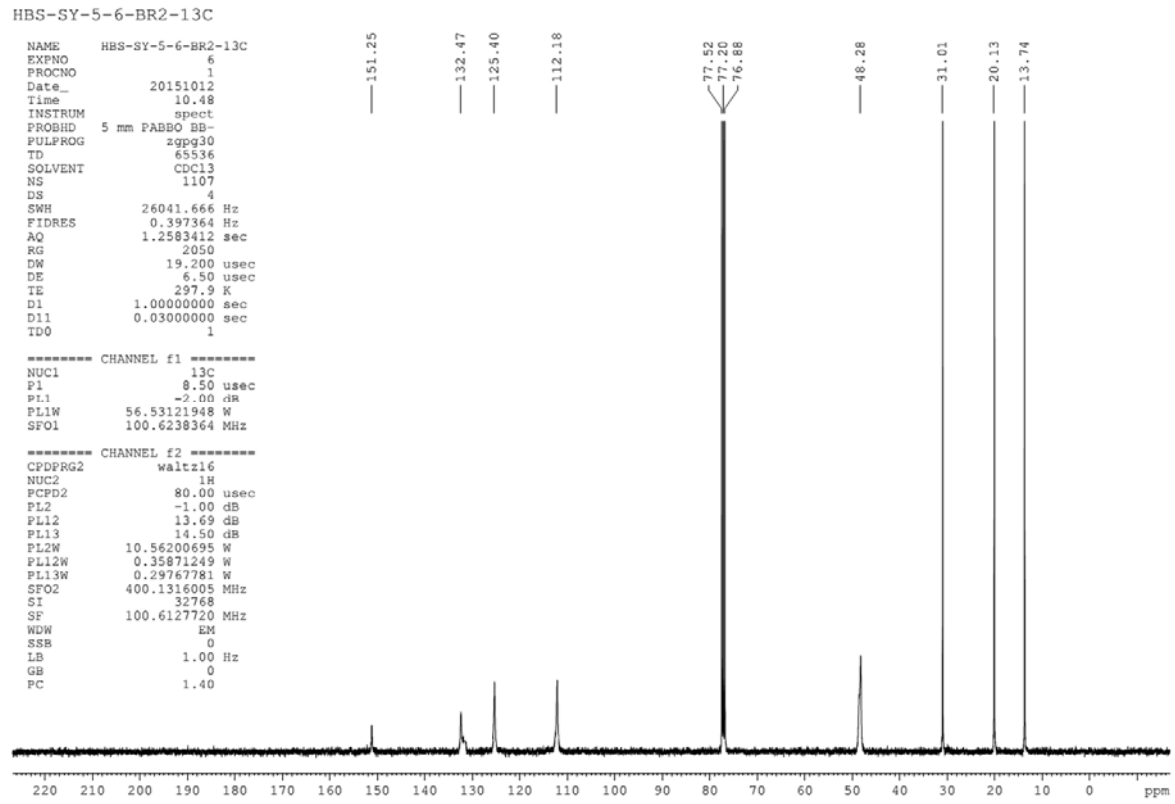


Figure S48. ^{13}C NMR spectrum of compound **23**.

Eager 300 Report

Page: 1 Sample: SY-63 (SY-63)

Method Name : HBS-VT-1-08-2014
Method File : D:\CHNS2012-13\HBS-VT-1-08-2014.mth
Chromatogram : SY-63
Operator ID : VARSHA
Company Name : C.E. Instruments
Analysed : 08/01/2014 20:02
Printed : 8/1/2014 22:50
Sample ID : SY-63 (# 42)
Instrument N. : Instrument #1
Analysis Type : UnkNown (Area)
Sample weight : 1.37

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	2.0595	42	37110	FU	39.269420	.131525E+07
Carbon	29.2088	65	1457269	FU	1.000000	.271291E+07
Hydrogen	3.6750	178	361791	RS	4.027929	.685809E+07
Totals	34.9432		1856169			

Figure S49. Elemental analysis of compound **23**.

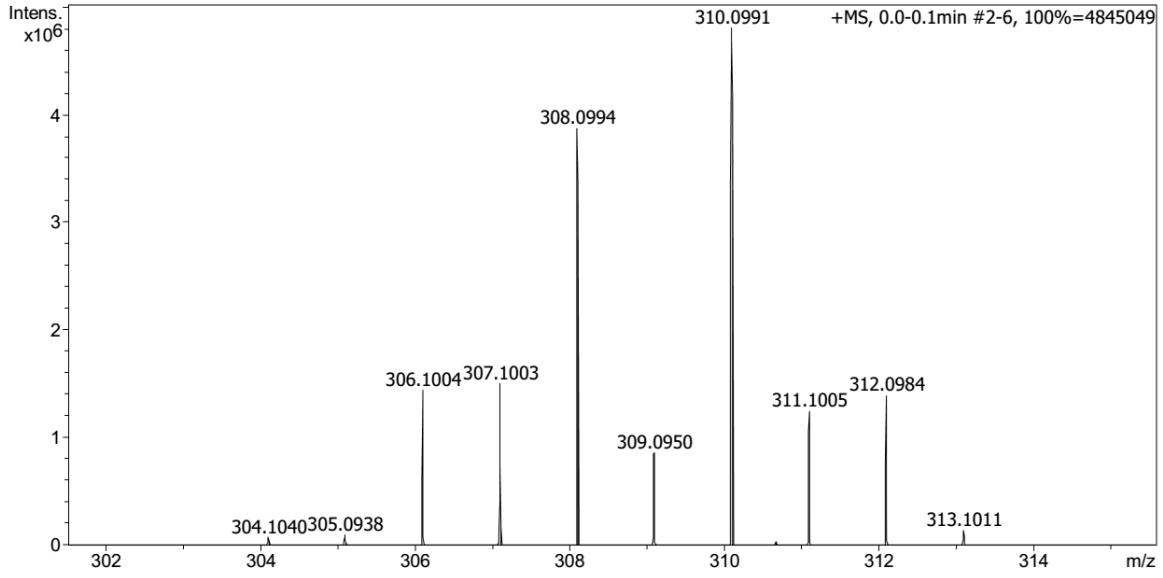
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\MARCH-2016\HBS-SY-15.d	Acquisition Date	3/26/2016 10:36:42 PM
Method	Tune_pos_NAICSI-1000a.m	Operator	HBS-SY
Sample Name	HBS-SY-15	Instrument	maXis impact 282001.00081
Comment			

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 Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
310.0991	1	C30H44N4Se2	310.0946	14.5	278.3	1	100.00	11.0	even	ok

Figure S50. ESI-MS spectrum of compound **23**.

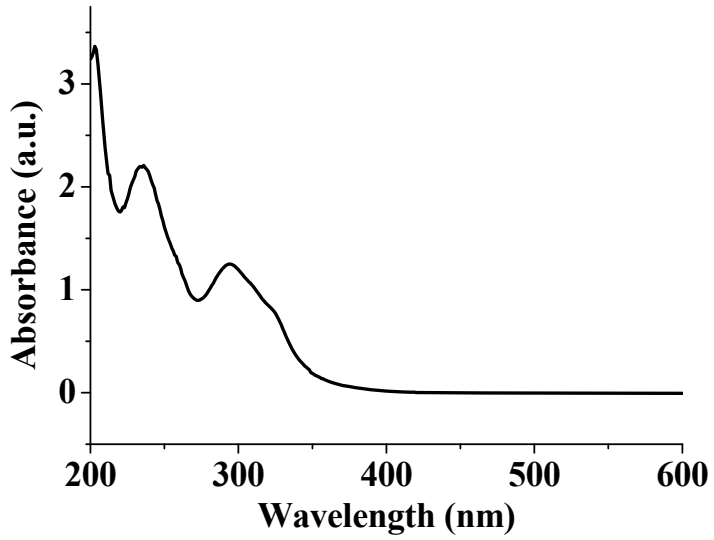


Figure S51. UV-Visible spectrum of compound **23**.

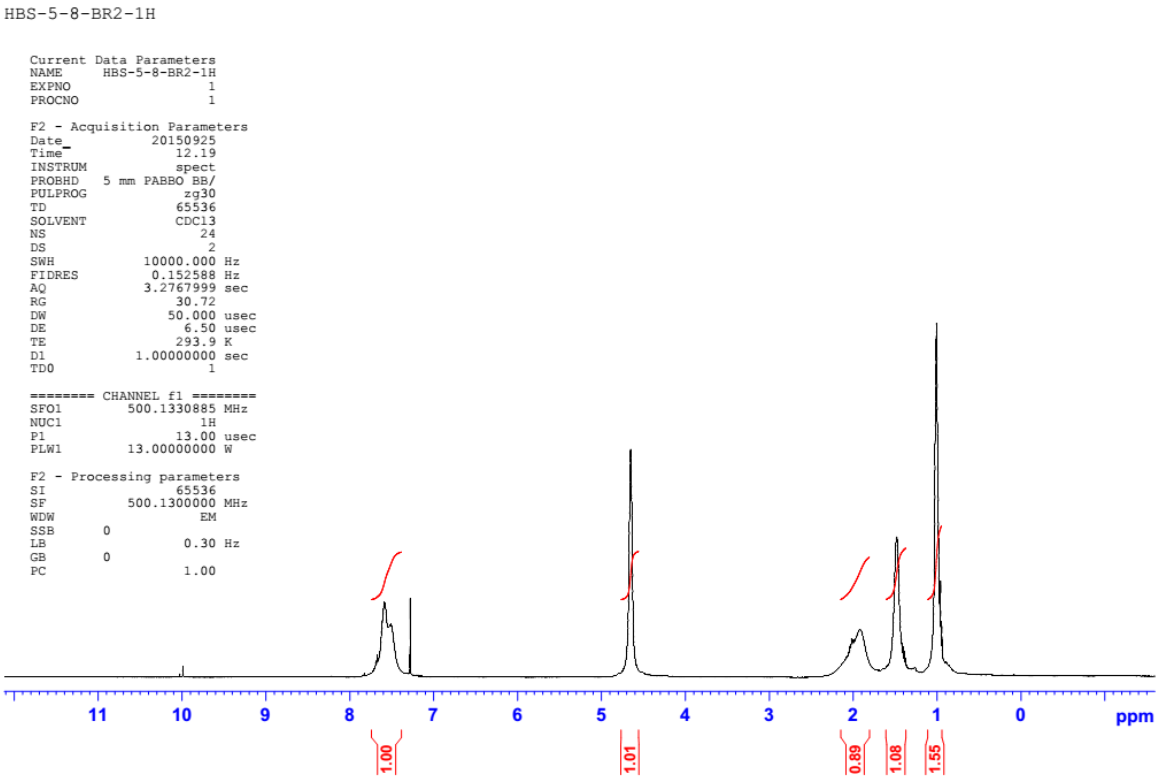


Figure S52. ^{1}H NMR spectrum of compound **24**.

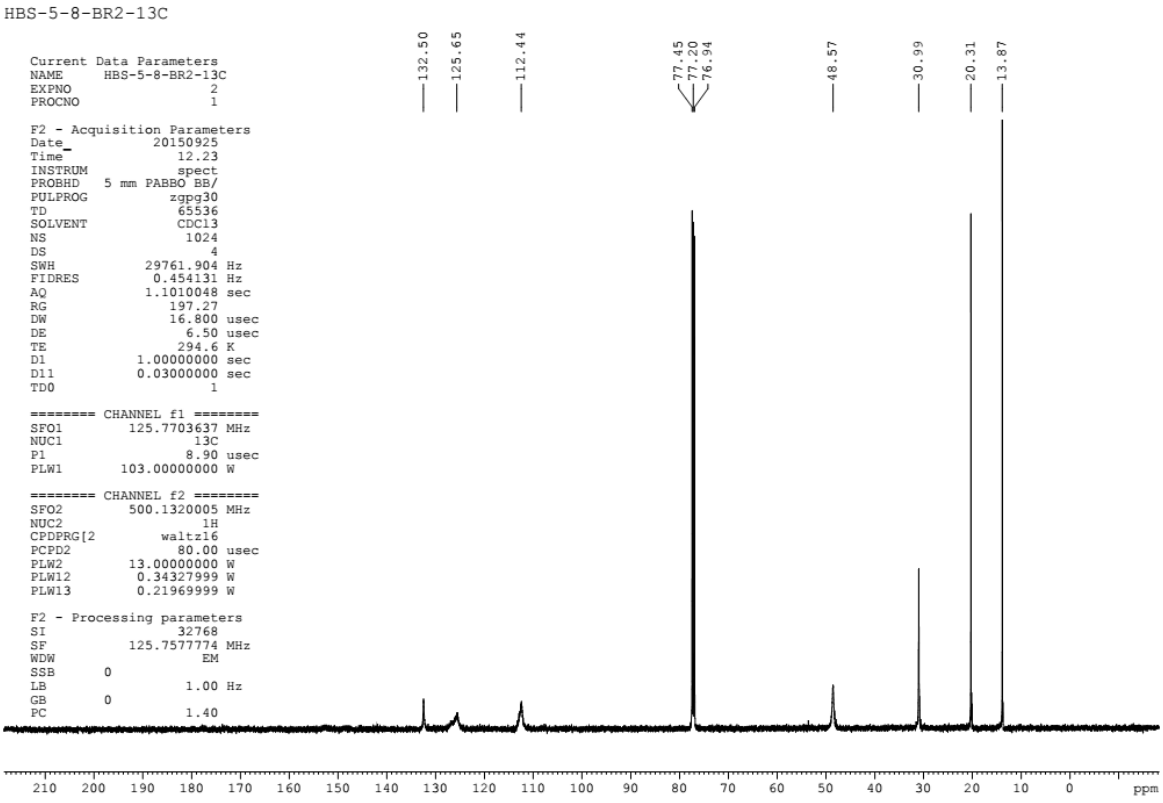


Figure S53. ^{13}C NMR spectrum of compound **24**.

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	5138	RS		0.0000
Nitrogen	4.7321	43	64591	RS	12.947190	.136224E+07
Carbon	31.3438	67	836272	RS	1.000000	.265382E+07
Hydrogen	3.7291	178	252391	RS	3.313399	.643434E+07
Totals	39.8050		1158392			

Figure S54. Elemental analysis of compound **24**.

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

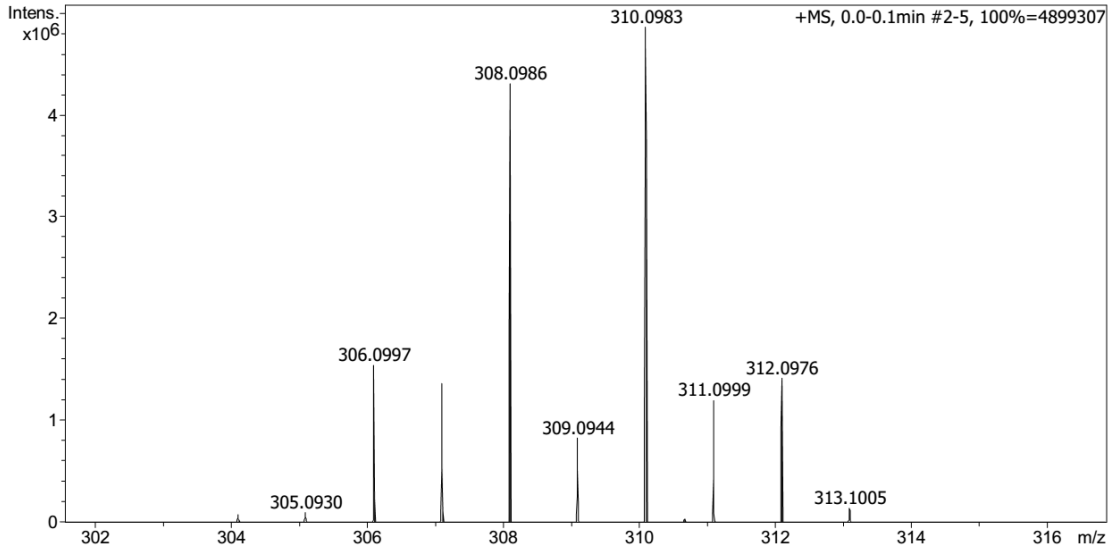
Analysis Info

Analysis Name D:\Data\MARCH-2016\HBS-SY-14.d
Method Tune_pos_NAICSI-1000a.m
Sample Name HBS-SY-14
Comment

Acquisition Date 3/26/2016 10:35:49 PM
Operator HBS-SY
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 Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
310.0983	1	C30H44N4Se2	310.0946	-11.9	318.3	1	100.00	11.0	even	ok

Figure S55. ESI-MS spectrum of compound **24**.

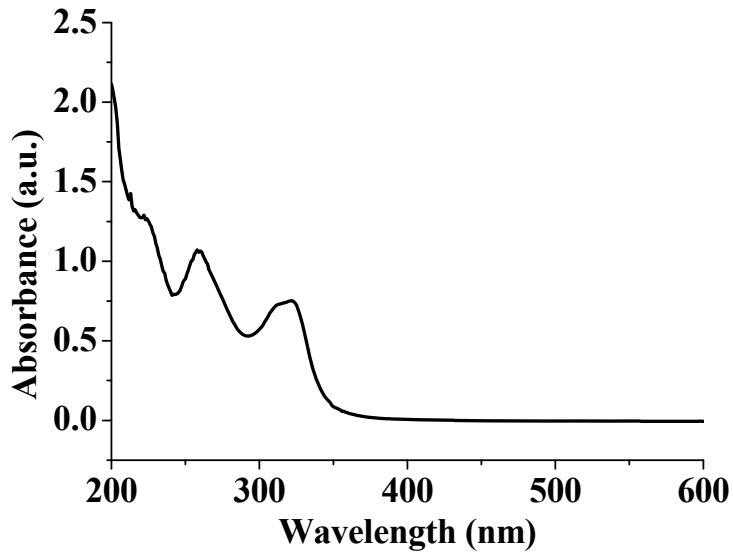


Figure S56. UV-Visible spectrum of compound **24**.

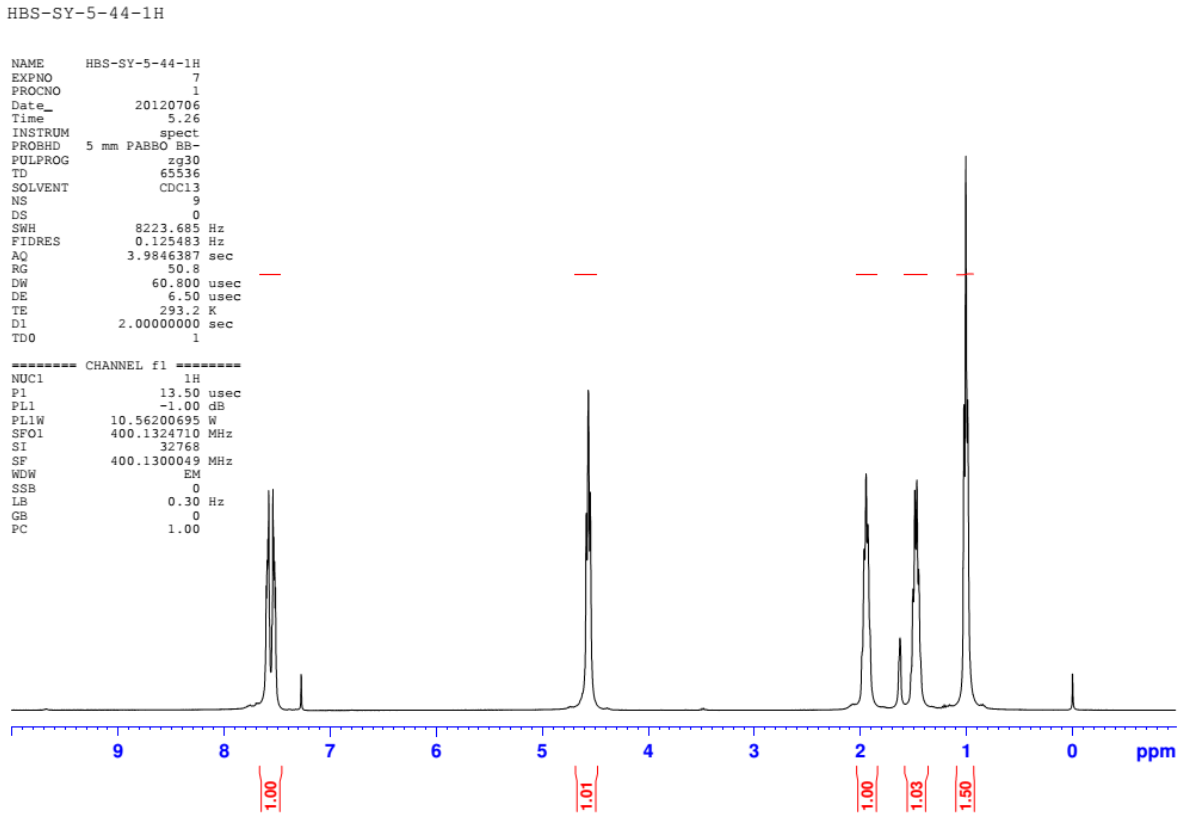


Figure S57. ^{1}H NMR spectrum of compound **25**.

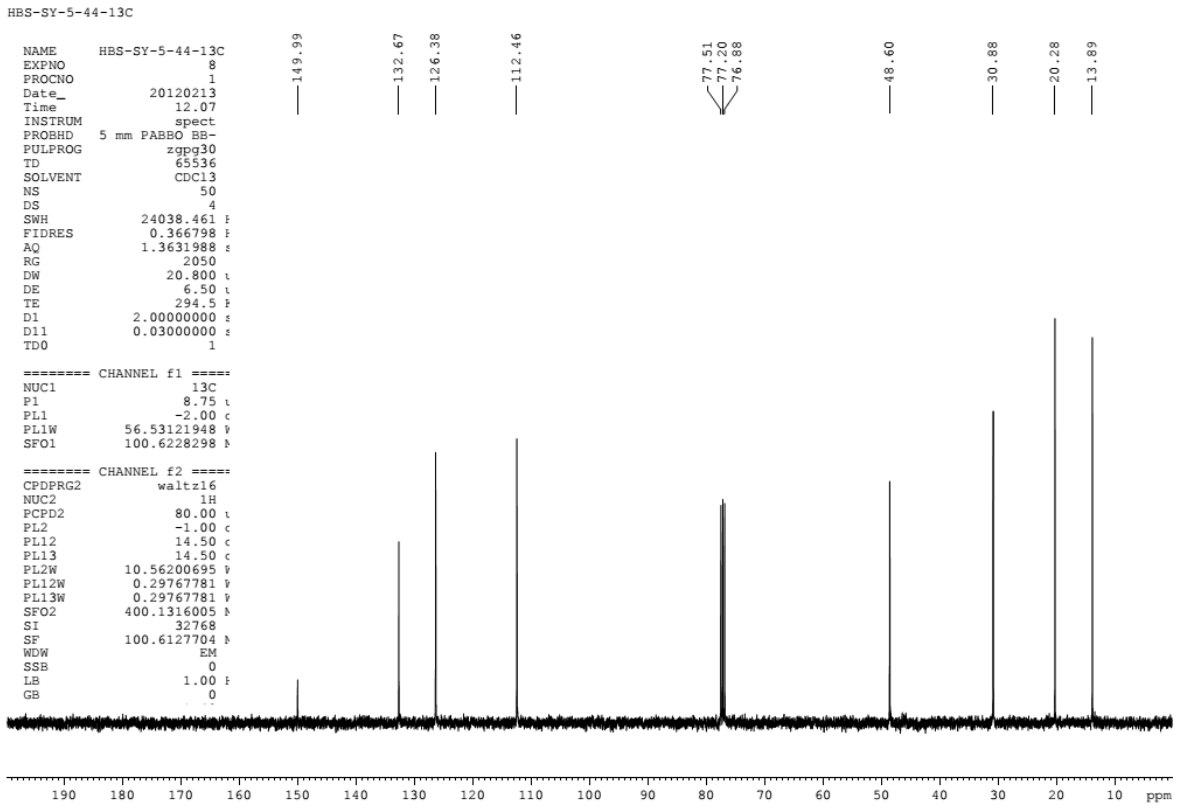


Figure S58. ^{13}C NMR spectrum of compound **25**.

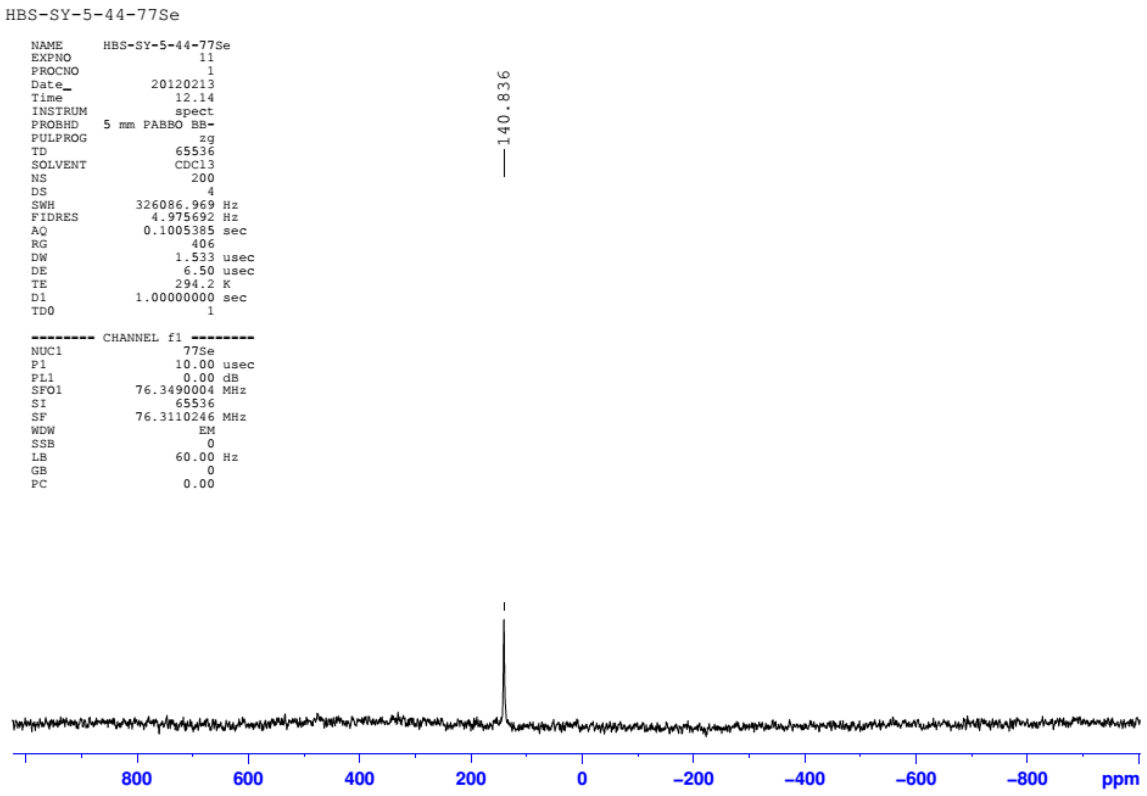


Figure S59. ^{77}Se NMR spectrum of compound **25**.

Eager 300 Report

Page: 1 Sample: SY-75 (SY-75)

Method Name : HBS-VT-18-07-2014
Method File : D:\CHNS-2014\HBS-VT-18-07-2014.mth
Chromatogram : SY-75
Operator ID : VARSHA Company Name : C.E. Instruments
Analysed : 07/18/2014 13:28 Printed : 7/18/2014 18:41
Sample ID : SY-75 (# 13) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : .717

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	12.8469	41	133617	FU	5.485007	.105591E+07
Carbon	27.4615	66	732891	FU	1.000000	.270944E+07
Hydrogen	3.5163	178	247261	RS	2.964037	.679637E+07
Totals	43.8247		1113769			

Figure S60. Elemental analysis of compound **25**.

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

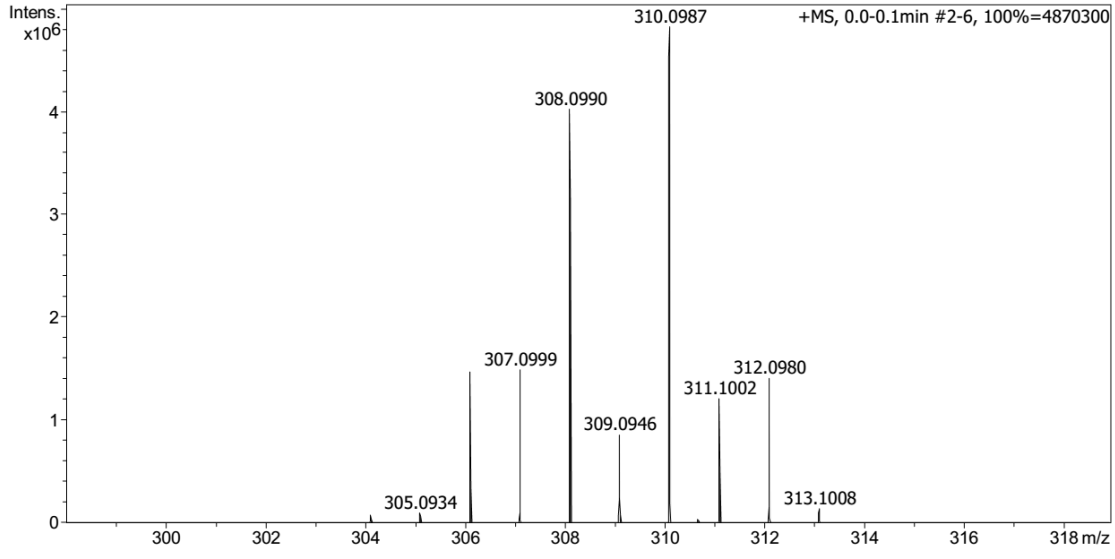
Analysis Info

Analysis Name D:\Data\MARCH-2016\HBS-SY-20.d
Method Tune_pos_NAICSI-1000a.m
Sample Name HBS-SY-20
Comment

Acquisition Date 3/26/2016 10:40:23 PM
Operator HBS-SY
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 Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
310.0987	1	C30H44N4Se2	310.0946	13.2	280.7	1	100.00	11.0	even	ok

Figure S61. ESI-MS spectrum of compound **25**.

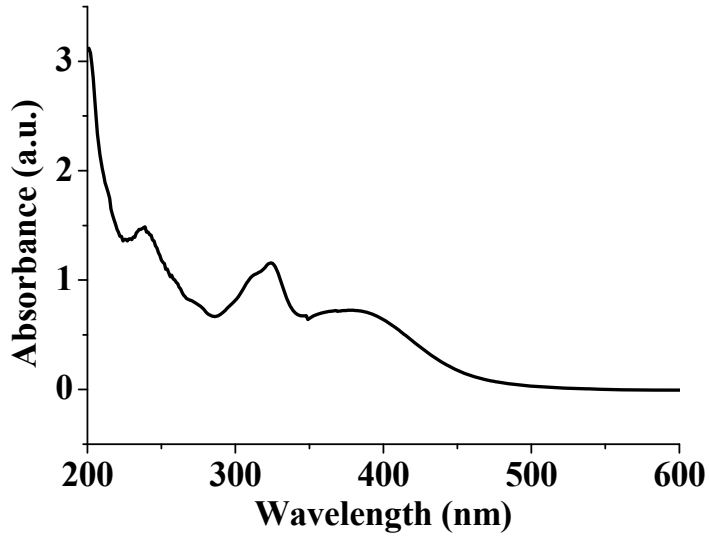


Figure S62. UV-Visible spectrum of compound **25**.

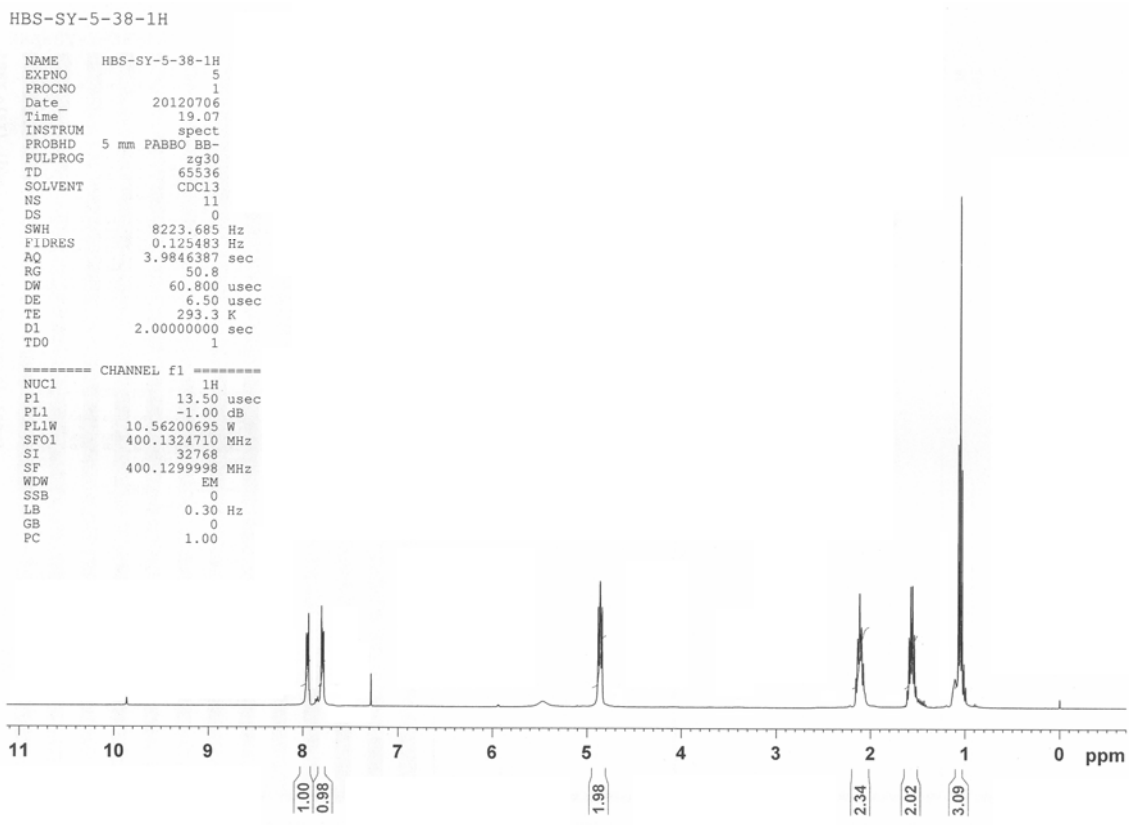


Figure S63. ^{1}H NMR spectrum of compound **26**.

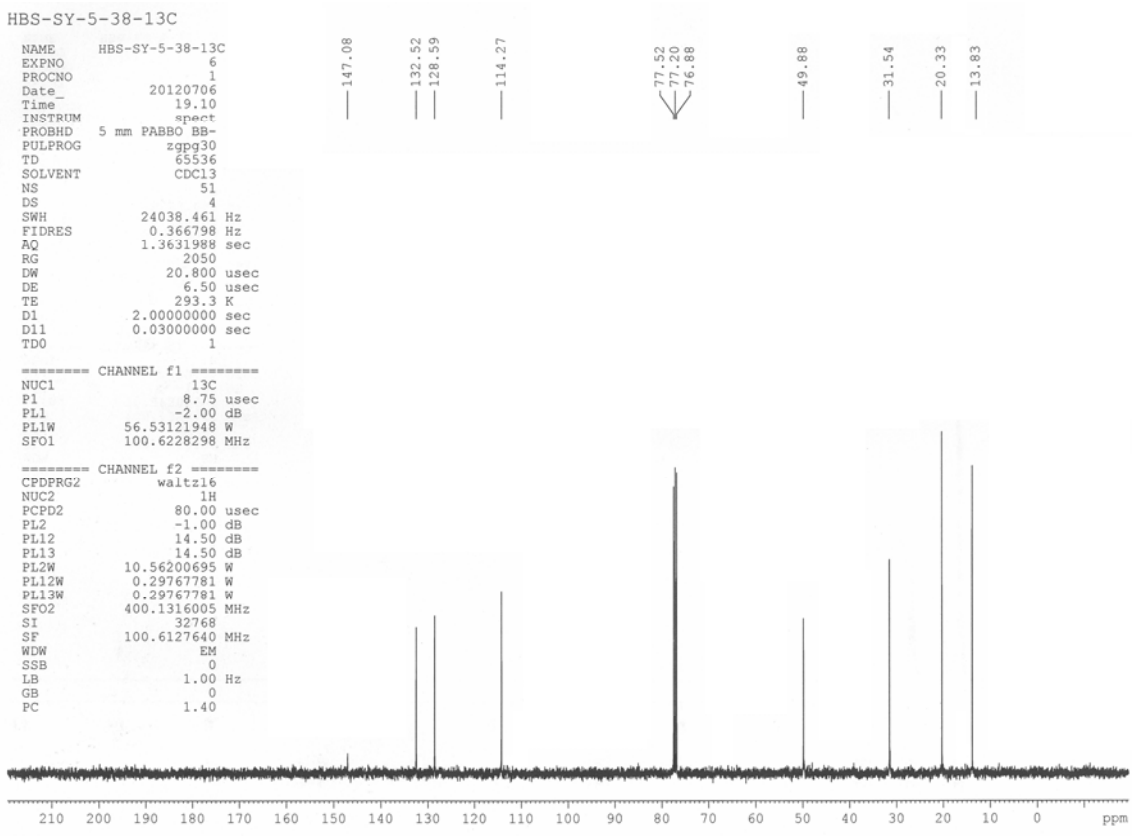


Figure S64. ^{13}C NMR spectrum of compound **26**.

Eager 300 Report

Page: 1 Sample: SY-2-30-1 (SY-2-30-1)

Method Name : SP160312
Method File : D:\CHNS2012\SP160312.mth
Chromatogram : SY-2-30-1
Operator ID : SP
Analysed : 03/16/2012 14:00
Sample ID : SY-2-30-1 (# 19)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 3/16/2012 17:44
Instrument N. : Instrument #1
Sample weight : 1.19

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	6.2490	43	103136	RS	12.999900	.138694E+07
Carbon	41.6345	66	1340758	RS	1.000000	.269880E+07
Hydrogen	4.9561	175	360774	RS	3.716338	.611708E+07
Totals	52.8396		1804668			

Figure S65. Elemental analysis of compound **26**.

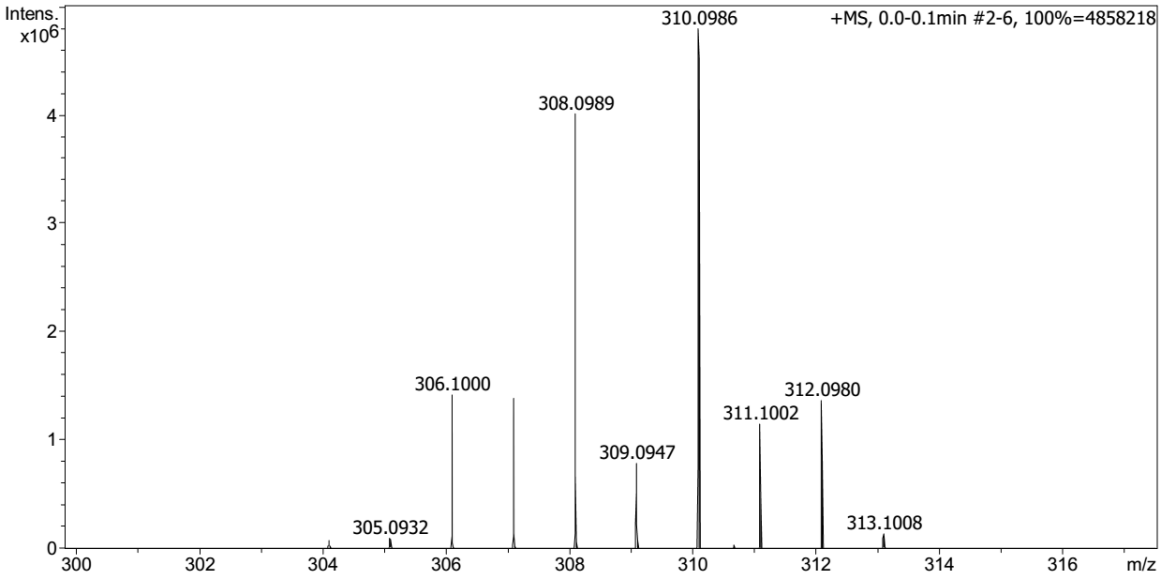
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\MARCH-2016\HBS-SY-19.d	Acquisition Date	3/26/2016 10:39:42 PM
Method	Tune_pos_NAICSI-1000a.m	Operator	HBS-SY
Sample Name	HBS-SY-19	Instrument	maXis impact 282001.00081
Comment			

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 Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
310.0986	1	C30H44N4Se2	310.0946	-12.9	282.2	1	100.00	11.0	even	ok

Figure S66. ESI-MS spectrum of compound **26**.

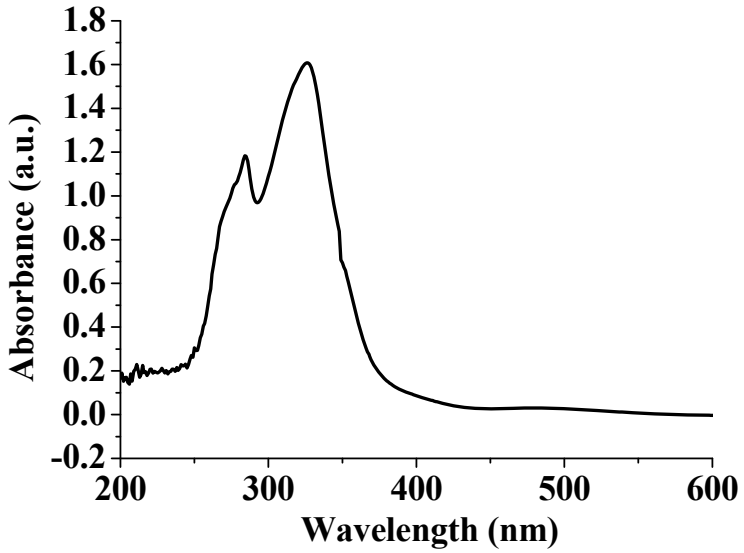


Figure S67. UV-Visible spectrum of compound **26**.

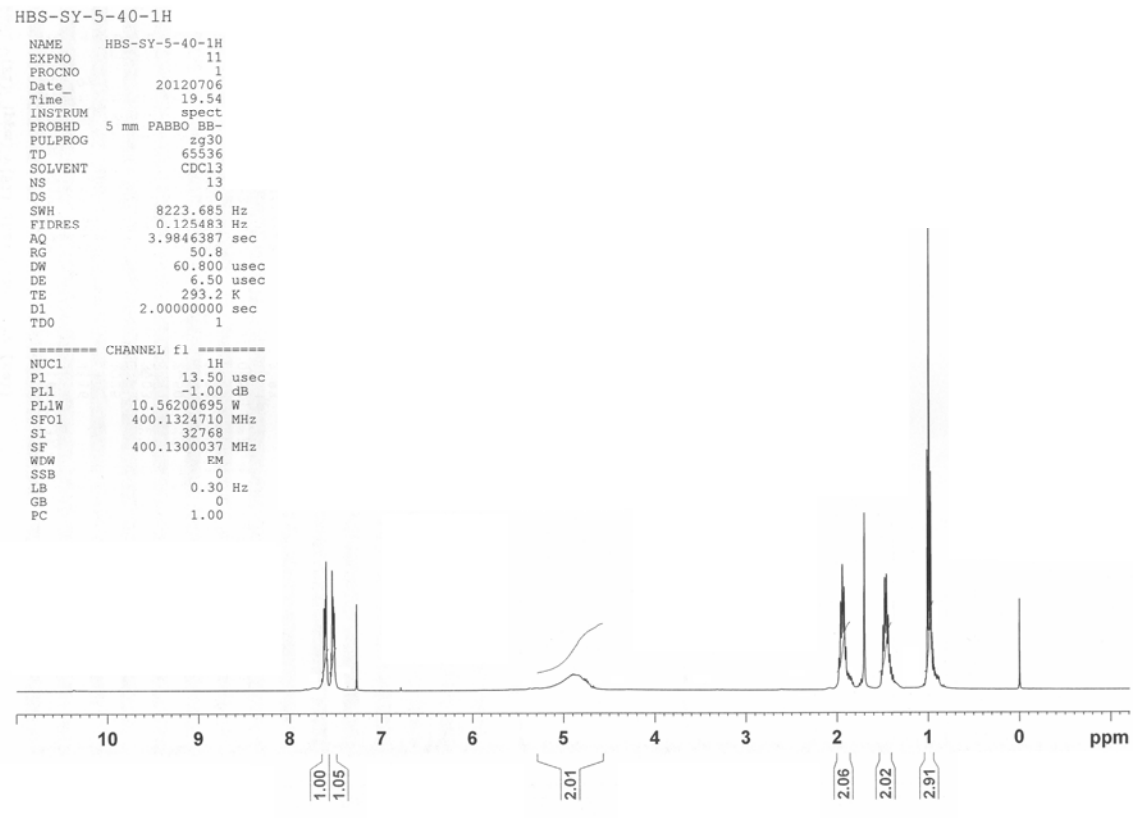


Figure S68. ^{1}H NMR spectrum of compound **27**.

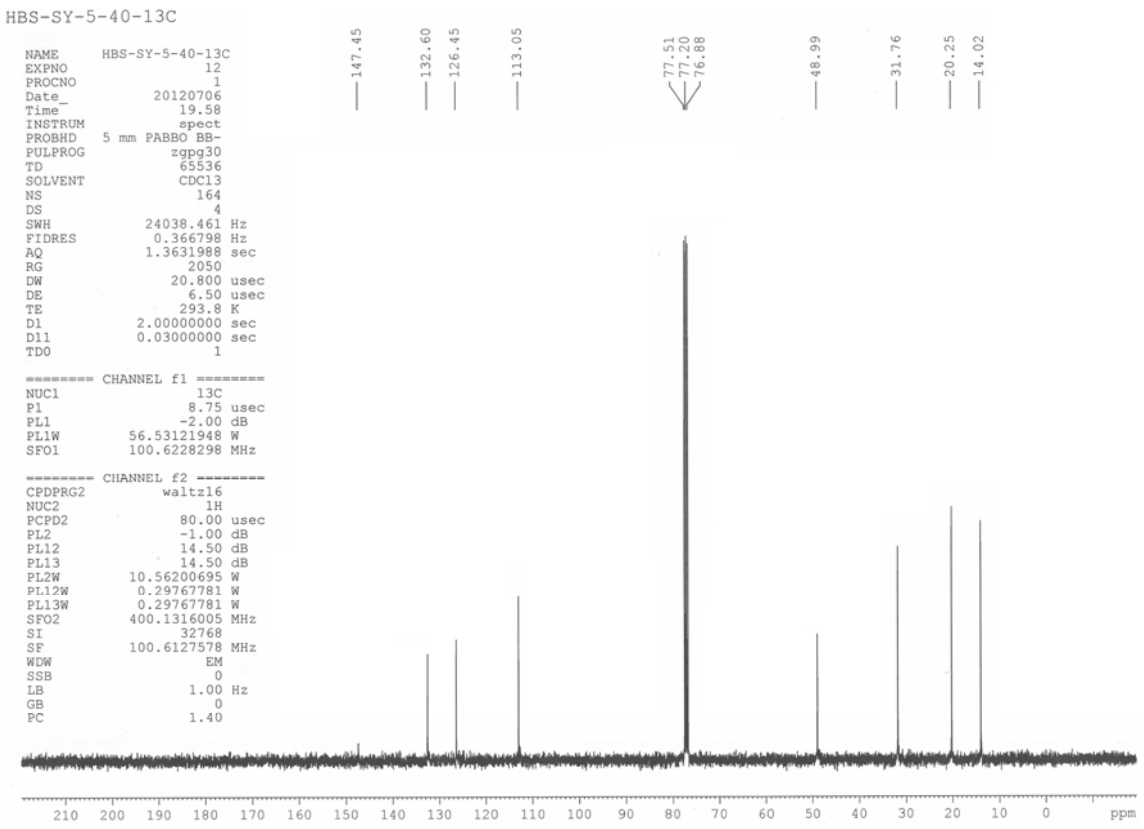


Figure S69. ^{13}C NMR spectrum of compound **27**.

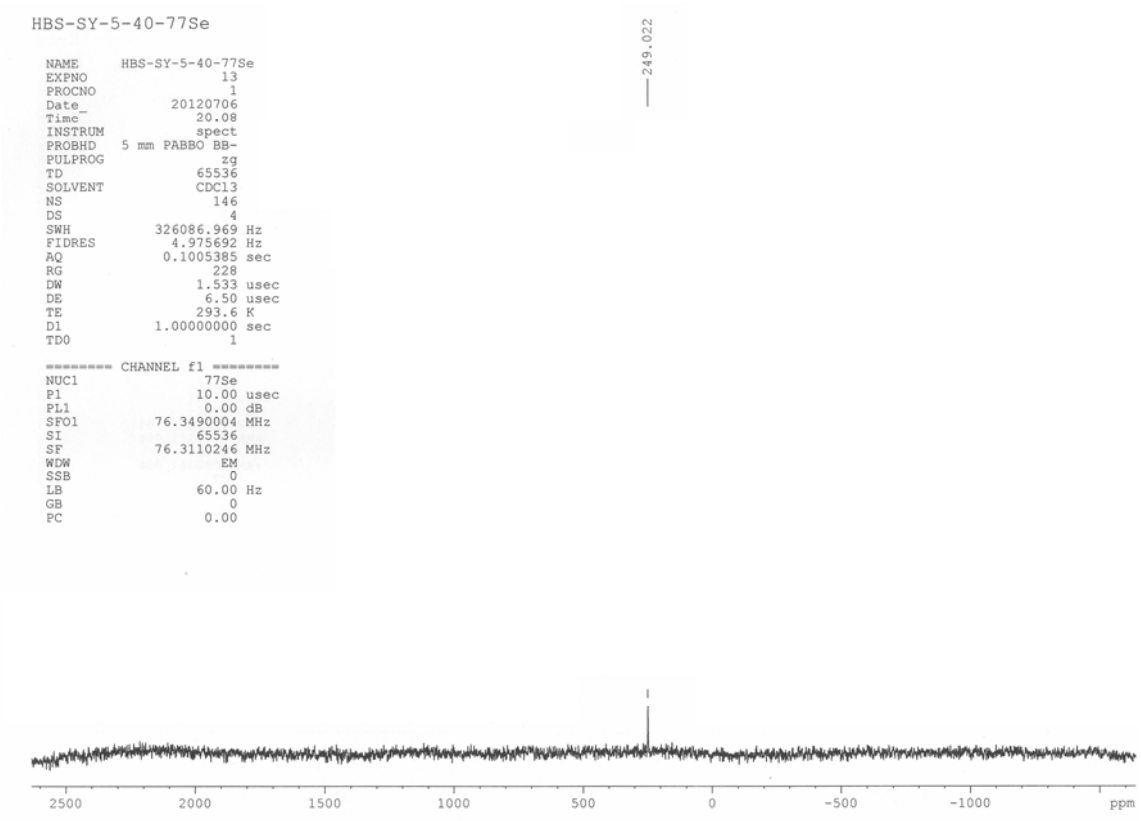


Figure S70. ^{77}Se NMR spectrum of compound **27**.

Eager 300 Report

Page: 1 Sample: HBS-SY-2-18 (HBS-SY-2-18)

Method Name : SP141211
Method File : D:\CHNS2011\SP141211.mth
Chromatogram : HBS-SY-2-18
Operator ID : SP
Analysed : 12/14/2011 14:36
Sample ID : HBS-SY-2-18 (# 22)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 12/14/2011 15:54
Instrument N. : Instrument #1
Sample weight : .831

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	5696	RS		0.0000
Nitrogen	7.2823	43	87755	RS	9.662236	.145011E+07
Carbon	38.0873	67	847910	RS	1.000000	.267152E+07
Hydrogen	4.4468	181	219551	RS	3.862016	.562667E+07
Totals	49.8164		1160912			

Figure S71. Elemental analysis of compound **27**.

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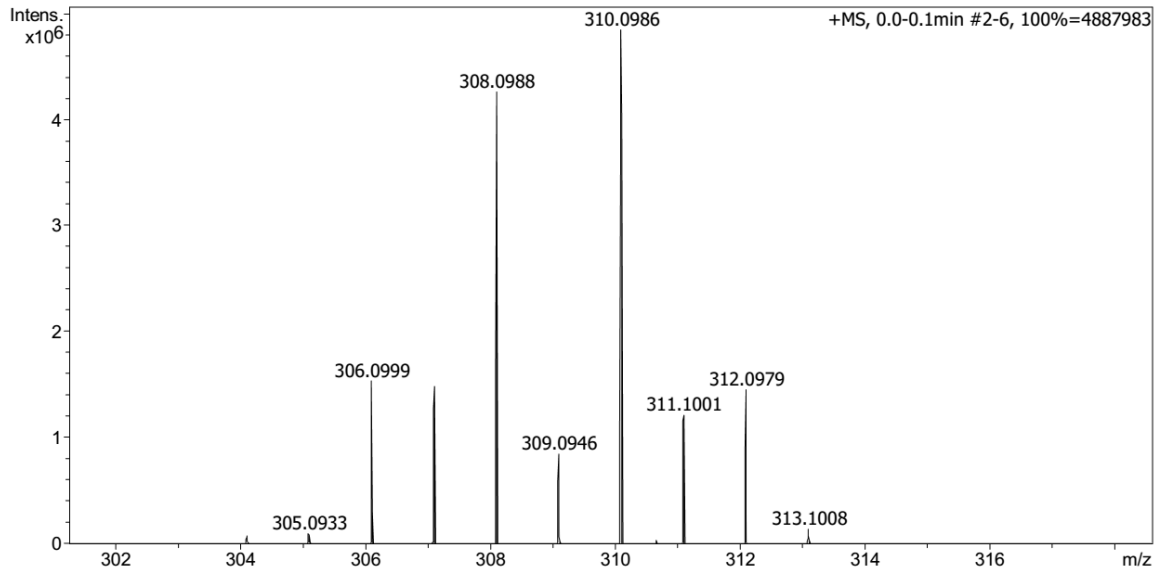
Analysis Info

Analysis Name	D:\Data\MARCH-2016\HBS-SY-18.d	Acquisition Date	3/26/2016 10:38:56 PM
Method	Tune_pos_NAICSI-1000a.m	Operator	HBS-SY
Sample Name	HBS-SY-18	Instrument	maXis impact 282001.00081
Comment			

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 Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
310.0986	1	C30H44N4Se2	310.0946	12.9	285.3	1	100.00	11.0	even	ok

Figure S72. ESI-MS spectrum of compound **27**.

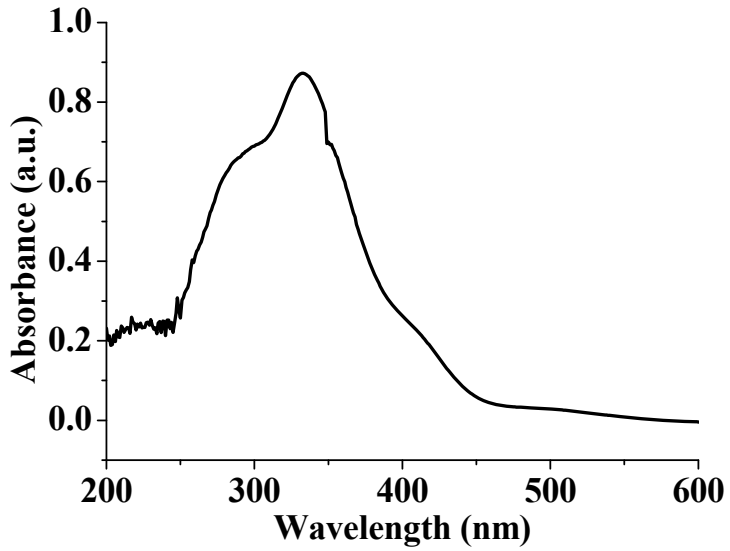
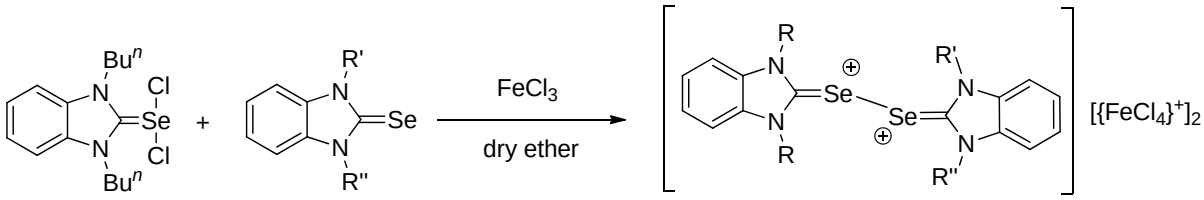


Figure S73. UV-Visible spectrum of compound **27**.

Unsymmetrical dicationic diselenides:



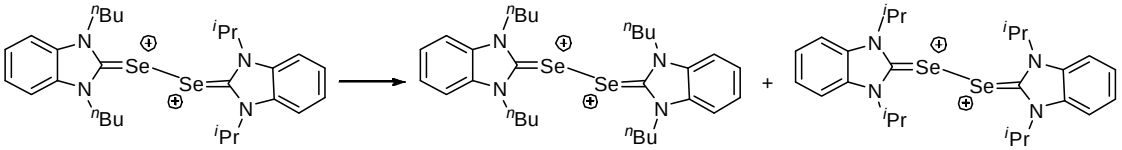
4b

3c R', R'' = *n*-Pr
3d R', R'' = *i*-Pr
S1 R', R'' =2-(2'-methoxyethoxy) ethyl
S2 R' = *n*-Bu, R'' = 2-bromobenzyl
S3 R' = Py, R'' = *n*-Bu

S4 R, R' = *n*-Pr
S5 R, R' = *i*-Pr
S6 R, R' =2-(2'-methoxyethoxy) ethyl
S7 R, R' = *n*-Bu, R'' = 2-bromobenzyl$^-$
S8 R = *n*-Bu, R' = Py

Scheme S1. Synthesis of unsymmetrical dicationic diselenide.

The unsymmetrical dicationic diselenides could not be characterized completely. The formation of these compounds was inferred by mass spectrometry (Table S1). This disproportionation of unsymmetrical dicationic diselenides is energetically favoured (Scheme S2, Table S5). The total energy of respective symmetrical dicationic diselenides is 5.73 kcal/mol lower than the energy of 2 molecules of unsymmetrical dicationic diselenides. The energy difference indicates that in the solution form both unsymmetrical and symmetrical dicationic diselenides are present therefore, in mass spectra the presence of unsymmetrical dicationic diselenides was observed.



SA **SB** **SC**

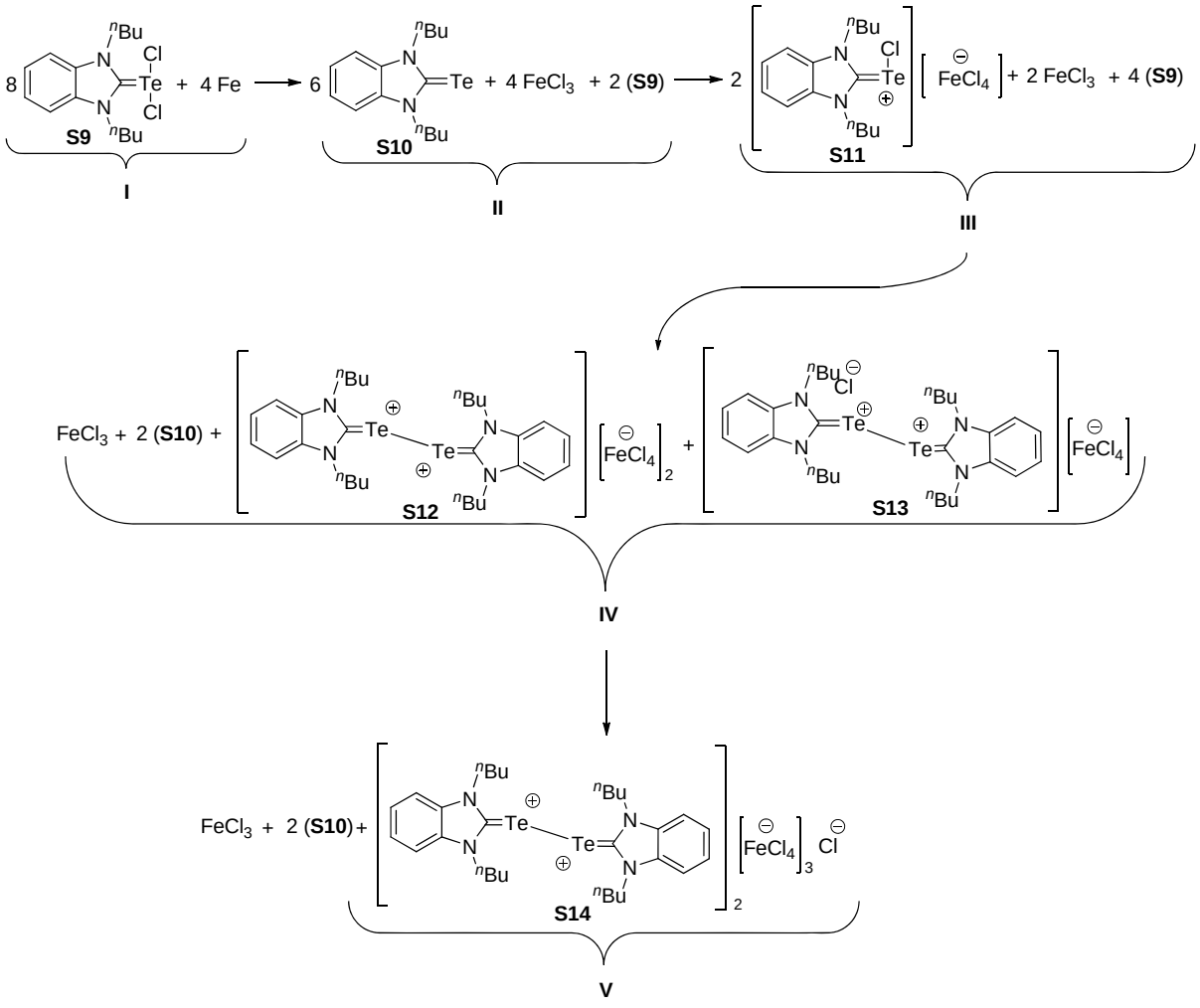
Scheme S2. Disproportionation of unsymmetrical dicationic diselenide.

Table S1. ESI-MS spectra of unsymmetrical dicationic diselenides.

Compound	Experimental *m/z*	Calculated *m/z*
S4	296.0789	296.0789
S5	296.0785	296.0789
S6	356.1002	356.1001
S7	366.0408	366.0418
S8	295.5689	295.5687

Attempted synthesis of dicationic ditelluride: Mechanism D

Attempted synthesis of dicationic ditellurides by following the same reaction conditions (Mechanism D, Scheme S3) was unsuccessful. DFT calculations indicated that this path is not energetically favourable for dicationic ditellurides (Table S7). The energy profile for the synthesis of dicationic ditelluride (Figure S74) shows that in the first step itself the products have very high energy *i.e.* ΔE = 213.76 kcal/mol, which does not allow the reaction to proceed further.



Scheme S3. Synthetic route for dicationic ditelluride.

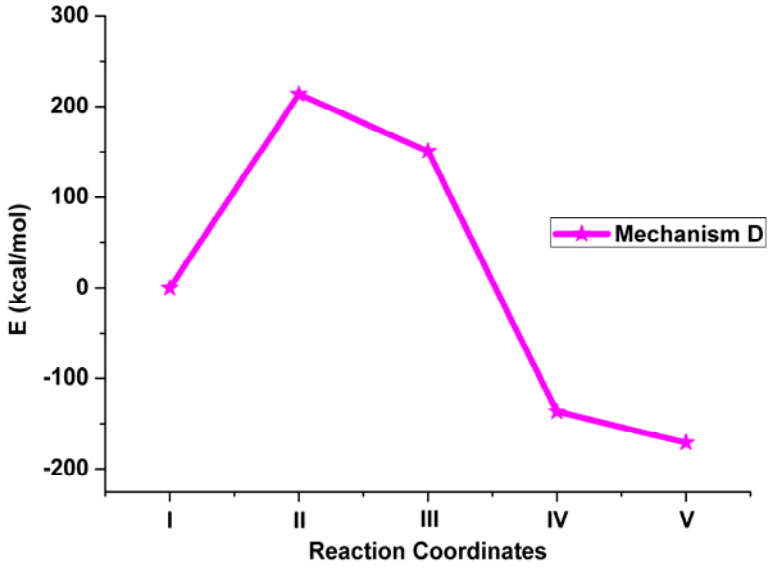


Figure S74. Energy profile for the synthesis of dicationic ditelluride.

Mechanistic studies for the synthesis of 15 by NMR spectroscopy at -40 °C:

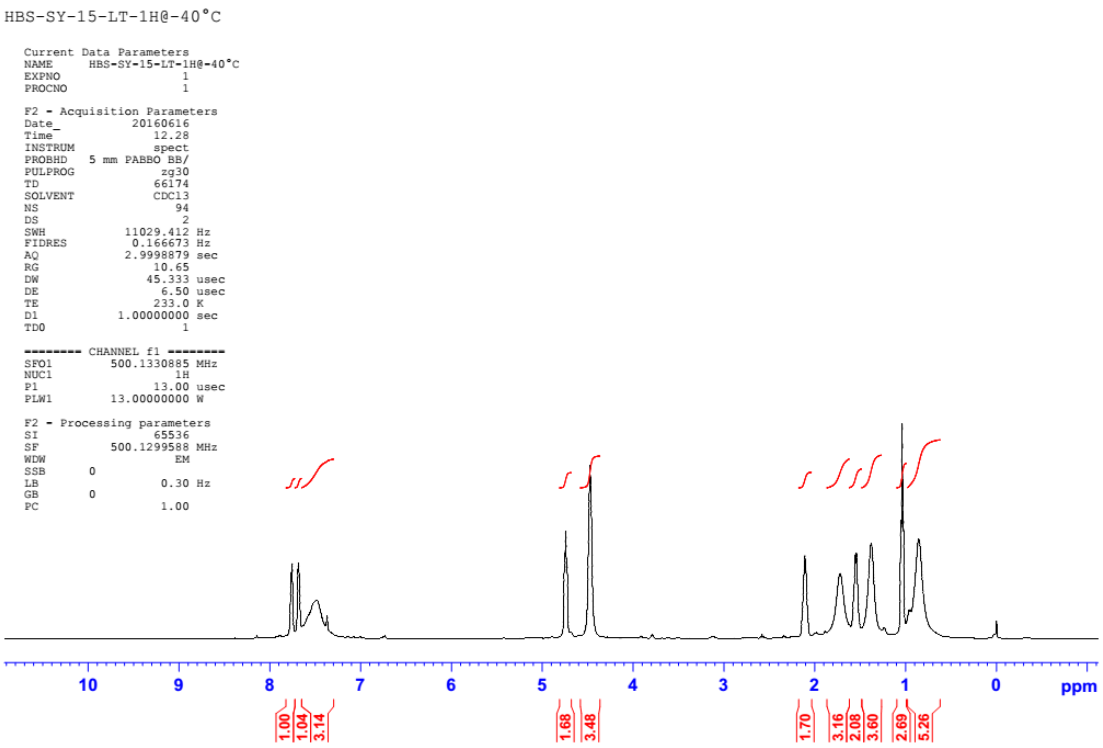


Figure S75. ^{1}H NMR spectrum of a mixture of **3b**, **4b** and $ZnCl_2$ at -40 °C.

Packing diagram of compound 15:

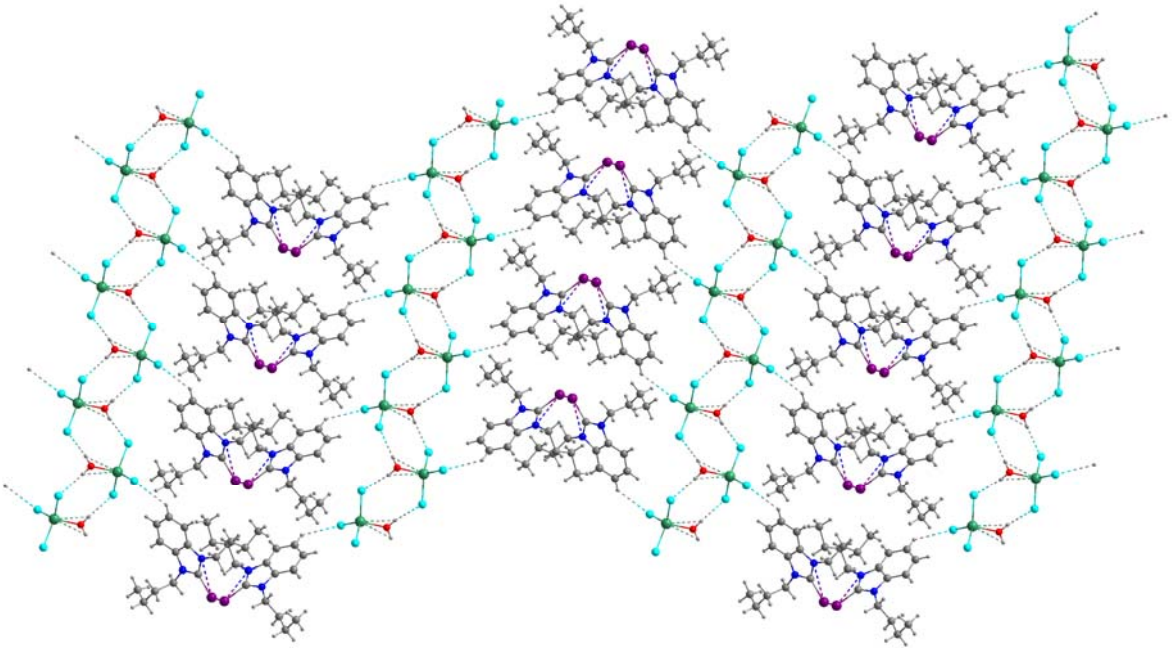


Figure S76. Packing diagram of compound **15**.

New Crystal data for 15 on freshly prepared sample (123 K): $C_{30}H_{44}Cl_6N_4O_2Se_2Zn_2$, fw 994.06, monoclinic, space group *C*2/*c*, Yellow crystals, a= 25.1245(9), b= 8.3466(2), c= 22.6386(7) Å, α = 90, β= 123.457(3), γ =90 °, V= 3960.8(2) $Å^3$, Z = 8, D_{calcd}= 1.667 Mg/m^3, R1= 0.0232, wR2 = 0.0702 (all data), GOF = 1.210.

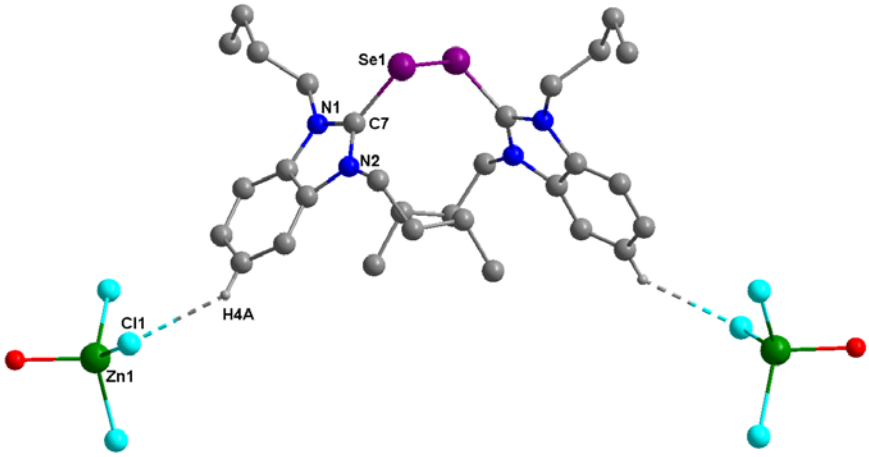


Figure S77. Molecular structure of compound **15**.

Computational Data:

All the structures were optimized with Gaussian 09 program by using MPW1PW91 method and TZVP basis set for Fe, 3-21g(d) basis set for Te and 6-311g(d) basis set for rest of the atoms.

Table S2. Comparison of bond lengths of compound **7**.

	Crystal structure of **7**	Optimized geometry of **7**	Crystal structure of **15**	Optimized geometry of $[L_2Se_2]^{2+}$
Se-Se (Å)	2.411	2.434	2.363	2.381
Se-C (Å)	1.903	1.903	1.901	1.897
C-N (Å)	1.347	1.347	1.348	1.348
Se···Cl (Å)	2.818	2.855	-	-
Se-Se-C (°)	93.34	97.38	104.29	103.87
Se-C-N (°)	124.39	125.07	123.65	124.95
N-C-N (°)	109.53	109.63	109.40	109.53

Energy of optimized steps:

Table S3. Mechanism A (Synthesis of dicationic diselenides):

	AU	**kcal/mol**	Normalized Energy (round figure) **kcal/mol**	ΔE **kcal/mol**
I	-37187.27230176	-23335370.66580434	0.00	----
II	-37188.09125344	-23335884.56585204	-513.90	-513.90
III	-37188.18808284	-23335945.32723089	-574.66	-60.76
IV	-37188.26448844	-23335993.27247899	-622.61	-33.25
V	-37188.31402544	-23336024.3574225	-653.69	-31.08

Table S4. Mechanism B (alternative mechanism for the synthesis of dicationic diselenide):

	AU	**kcal/mol**	Normalized Energy (round figure) **kcal/mol**	ΔE **kcal/mol**
I	-37187.27230176	-23335370.66580434	0.00	----
II	-37188.09125344	-23335884.56585204	-513.90	-513.90
III	-37188.05262744	-23335860.32766593	-489.66	24.24
IV	-37188.26448844	-23335993.27247899	-622.61	-132.95
V	-37188.31402544	-23336024.3574225	-653.69	-31.08

Table S5. Mechanism C (synthesis of selone adduct of ferric chloride)

	AU	**kcal/mol**	Normalized Energy (round figure) **kcal/mol**	ΔE (**kcal/mol**)
I	-37187.27230176	-23335370.66580434	0.00	-----
II	-37188.09125344	-23335884.56585204	-513.90	-513.90
III	-37188.26083588	-23335990.9804625	-620.31	-106.41
IV	-37188.28977157	-23336009.137886	-638.47	-18.16

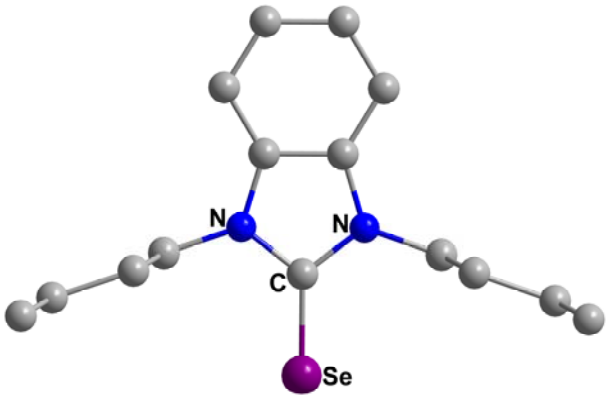
Table S6. Energy of unsymmetric dicationic diselenide and the products of its disproportionation

Compound	**E (kcal/mol)**	**Normalized Energy (kcal/mol)**	**ΔE (kcal/mol)**
2SA	-7671922.1501436	0.00	--
SB+SC	-7671927.8776622	5.73	5.73

Table S7. Mechanism D (Synthesis of dicationic ditelluride)

	A. U.	**kcal/mol**	Normalized Energy (round figure) **kcal/mol**	ΔE (**kcal/mol**)
I	-70660.07488712	-44339875.895829	0.00	-----
II	-70659.73424478	-44339662.13948775	213.76	213.76
III	-70659.83461128	-44339725.12043082	150.78	-62.98
IV	-70660.29324384	-44340012.91676878	-137.02	-287.80
V	-70660.34672268	-44340046.4752547	-170.58	-33.56

Compound 3b

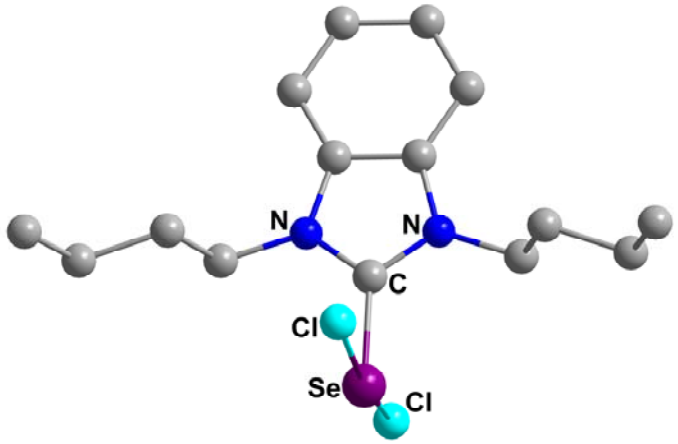


MPW1PW91/6-311G* E(RmPW1PW91) = -3096.07525870

C	0.699892000	1.685529000	-0.345686000
C	-0.700550000	1.685210000	-0.345789000
N	-1.096637000	0.378953000	-0.562418000
C	0.000177000	-0.429419000	-0.682140000
N	1.096600000	0.379465000	-0.562362000
C	1.420264000	2.856079000	-0.159117000
C	0.696748000	4.029468000	0.025222000
C	-0.698555000	4.029148000	0.025115000
C	-1.421497000	2.855425000	-0.159342000
C	2.470229000	-0.083411000	-0.615419000
C	3.034370000	-0.412620000	0.759772000
C	4.477377000	-0.895013000	0.685260000
C	5.054776000	-1.240287000	2.050395000
C	-2.470055000	-0.084528000	-0.615531000
C	-3.034325000	-0.413385000	0.759692000
C	-4.477273000	-0.895955000	0.685161000
C	-5.054663000	-1.241256000	2.050295000
Se	0.000620000	-2.230499000	-0.950366000
H	2.503305000	2.861599000	-0.153298000
H	1.229207000	4.961351000	0.174621000
H	-1.231464000	4.960785000	0.174442000
H	-2.504542000	2.860433000	-0.153665000
H	2.476659000	-0.968976000	-1.252582000
H	3.060205000	0.690865000	-1.113061000
H	2.966569000	0.468925000	1.407430000
H	2.405469000	-1.185700000	1.211618000
H	4.529651000	-1.773729000	0.033056000
H	5.098619000	-0.127204000	0.208538000
H	6.086554000	-1.589399000	1.970961000
H	5.050762000	-0.373252000	2.716613000
H	4.476113000	-2.030036000	2.536101000
H	-3.060278000	0.689260000	-1.113645000
H	-2.475949000	-0.970385000	-1.252291000
H	-2.405382000	-1.186246000	1.211859000

H	-2.966712000	0.468356000	1.407102000
H	-5.098581000	-0.128222000	0.208406000
H	-4.529452000	-1.774694000	0.032980000
H	-6.086450000	-1.590340000	1.970867000
H	-4.476009000	-2.031030000	2.535970000
H	-5.050617000	-0.374239000	2.716537000

Compound 4b

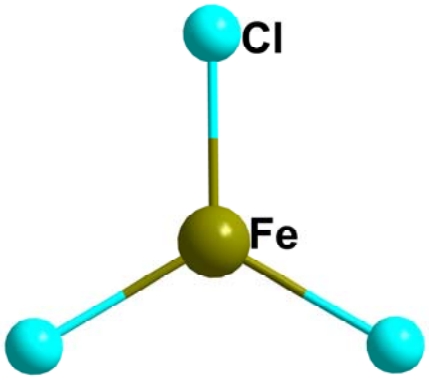


MPW1PW91/6-311G* E(RmPW1PW91) = -4016.55148494

C	-0.698435000	1.971499000	0.336700000
C	0.699135000	1.971160000	0.336618000
N	1.095027000	0.649025000	0.425750000
C	-0.000138000	-0.125537000	0.472619000
N	-1.094947000	0.649536000	0.425868000
C	-1.425022000	3.155472000	0.275768000
C	-0.699965000	4.333059000	0.215052000
C	0.701885000	4.332708000	0.214985000
C	1.426337000	3.154748000	0.275624000
C	-2.480591000	0.190461000	0.464094000
C	-3.112300000	0.115683000	-0.918773000
C	-4.554475000	-0.372576000	-0.848281000
C	-5.204048000	-0.467469000	-2.221394000
C	2.480458000	0.189380000	0.464076000
C	3.112504000	0.114840000	-0.918640000
C	4.554555000	-0.373769000	-0.847784000
C	5.204580000	-0.468607000	-2.220682000
Se	-0.000514000	-2.011447000	0.617586000
Cl	-0.000757000	-1.552846000	3.000824000
Cl	-0.000162000	-1.981426000	-1.822099000
H	-2.507433000	3.160608000	0.275910000
H	-1.228207000	5.277565000	0.166262000
H	1.230596000	5.276949000	0.166150000
H	2.508753000	3.159292000	0.275660000
H	-2.475791000	-0.785473000	0.947242000
H	-3.022312000	0.874664000	1.121239000

H	-3.075855000	1.099918000	-1.398838000
H	-2.516835000	-0.557856000	-1.540583000
H	-4.579263000	-1.354568000	-0.363754000
H	-5.142826000	0.295952000	-0.208320000
H	-6.232716000	-0.826545000	-2.150186000
H	-5.227999000	0.505394000	-2.719644000
H	-4.656916000	-1.155825000	-2.869647000
H	3.022347000	0.873102000	1.121591000
H	2.475138000	-0.786740000	0.946838000
H	2.517092000	-0.558393000	-1.540838000
H	3.076467000	1.099207000	-1.398468000
H	5.142838000	0.294530000	-0.207517000
H	4.578956000	-1.355837000	-0.363390000
H	6.233130000	-0.827962000	-2.149165000
H	4.657507000	-1.156724000	-2.869240000
H	5.228968000	0.504325000	-2.718775000

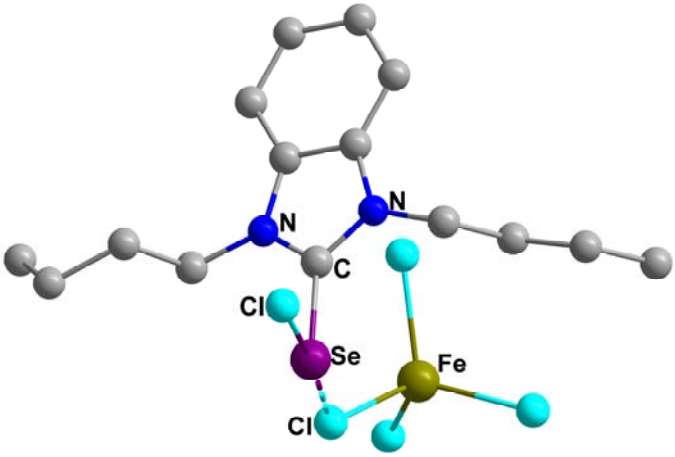
FeCl3



mpw1pw91/gen E(UmPW1PW91) = -2644.63418284

Fe	0.000674000	-0.000137000	0.000874000
Cl	-1.238079000	-1.745023000	-0.000445000
Cl	-0.894648000	1.943197000	-0.000445000
Cl	2.131695000	-0.197964000	-0.000446000

Compound A

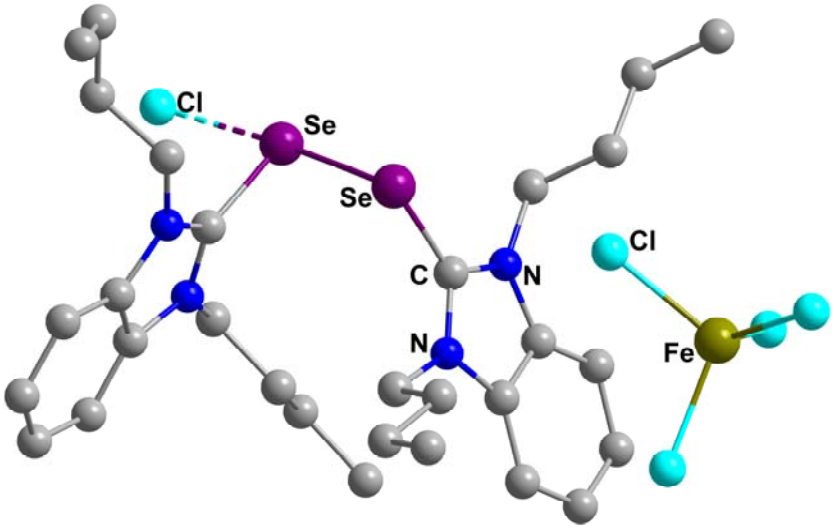


umpw1pw91/gen E(UmPW1PW91) = -6661.23408097

Cl	2.206610000	2.046687000	-2.844422000
Se	0.781053000	0.383096000	-2.254327000
C	1.039287000	0.736092000	-0.407584000
Cl	-0.747496000	-1.785225000	-1.482439000
Fe	-2.323142000	-1.778328000	0.206978000
Cl	-1.302950000	-0.825924000	1.928358000
Cl	-4.014778000	-0.564571000	-0.474870000
Cl	-2.833237000	-3.854279000	0.602407000
N	1.790530000	-0.001861000	0.423272000
C	1.811909000	0.615837000	1.657759000
C	2.502405000	-1.236996000	0.096671000
N	0.572581000	1.813623000	0.242745000
C	1.041063000	1.775303000	1.541140000
C	-0.316215000	2.849002000	-0.288015000
C	2.426320000	0.265734000	2.856467000
C	2.242914000	1.125127000	3.921909000
H	3.014753000	-0.636979000	2.955309000
C	1.473902000	2.294602000	3.803043000
H	2.699458000	0.889938000	4.875506000
C	0.858230000	2.640688000	2.616023000
H	1.354105000	2.936081000	4.667490000
H	0.255131000	3.535280000	2.533932000
C	3.965192000	-0.981271000	-0.243164000
H	1.980832000	-1.705005000	-0.735611000
H	2.380163000	-1.896919000	0.955542000
C	4.712700000	-2.260948000	-0.612116000
H	4.462305000	-0.490678000	0.600785000
H	4.006756000	-0.278875000	-1.080627000
C	4.855005000	-3.261951000	0.528049000
H	4.217216000	-2.737734000	-1.464761000
H	5.707213000	-1.977343000	-0.967912000
H	5.466862000	-4.113141000	0.224177000

H	3.893369000	-3.665593000	0.853869000
H	5.338644000	-2.808003000	1.397897000
C	-1.762332000	2.662711000	0.145667000
H	-0.226625000	2.829435000	-1.372416000
H	0.086657000	3.807356000	0.047383000
C	-2.644933000	3.789978000	-0.378992000
H	-1.824603000	2.613156000	1.236917000
H	-2.129944000	1.701343000	-0.220841000
C	-4.096990000	3.634411000	0.049801000
H	-2.258498000	4.756042000	-0.031483000
H	-2.587488000	3.816699000	-1.472861000
H	-4.715151000	4.439332000	-0.352745000
H	-4.194613000	3.654500000	1.138225000
H	-4.511681000	2.686405000	-0.297742000

Compound B



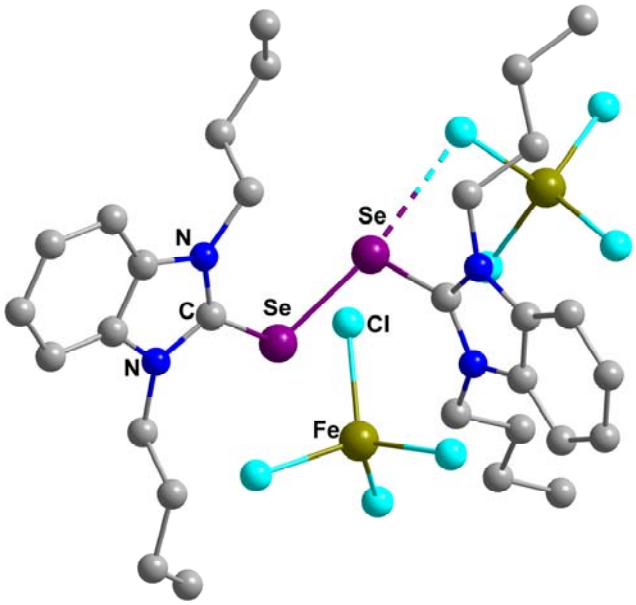
umpw1pw91/gen E(UmPW1PW91) = -9757.32105700

Cl	-4.843191000	-2.959892000	0.046812000
Se	-2.656773000	-1.934493000	-0.616404000
C	-3.478721000	-0.367551000	0.066860000
Se	-0.601855000	-0.582154000	-1.406427000
C	0.497438000	-0.507596000	0.114639000
Cl	3.133686000	0.442582000	-1.860478000
Fe	5.085912000	0.883671000	-0.830752000
Cl	4.742872000	2.577318000	0.578475000
Cl	5.660042000	-0.927311000	0.324570000
Cl	6.610896000	1.398074000	-2.315980000
N	-4.021131000	0.610868000	-0.676755000
C	-4.564741000	1.562059000	0.169631000
C	-4.150835000	0.626251000	-2.132416000

N	-3.645442000	-0.079853000	1.369436000
C	-4.327806000	1.120039000	1.473428000
C	-3.295433000	-0.933668000	2.503179000
N	0.724921000	0.596579000	0.852761000
C	1.656704000	0.294796000	1.830959000
C	0.125570000	1.914139000	0.656415000
N	1.226966000	-1.523756000	0.610348000
C	1.967078000	-1.059098000	1.683391000
C	1.320560000	-2.878713000	0.068926000
C	-5.239998000	2.750802000	-0.085557000
C	-5.669597000	3.473544000	1.013683000
H	-5.431049000	3.095266000	-1.093705000
C	-5.438820000	3.026530000	2.322417000
H	-6.201074000	4.404569000	0.859331000
C	-4.765705000	1.844439000	2.577238000
H	-5.797633000	3.620358000	3.154160000
H	-4.593510000	1.503318000	3.589843000
C	-5.467452000	0.010537000	-2.590176000
H	-3.303383000	0.080195000	-2.542901000
H	-4.044223000	1.665418000	-2.445200000
C	-5.595666000	-0.036757000	-4.110888000
H	-6.302708000	0.577291000	-2.164268000
H	-5.535731000	-0.999716000	-2.178238000
C	-5.649515000	1.328880000	-4.784854000
H	-4.771128000	-0.625292000	-4.527850000
H	-6.505539000	-0.593452000	-4.351075000
H	-5.832637000	1.229086000	-5.856149000
H	-4.715972000	1.886909000	-4.676201000
H	-6.455236000	1.943661000	-4.373103000
C	-2.054468000	-0.466170000	3.247351000
H	-3.174477000	-1.944125000	2.118156000
H	-4.169873000	-0.954050000	3.157114000
C	-1.762327000	-1.352594000	4.453369000
H	-2.177153000	0.572572000	3.572815000
H	-1.201643000	-0.476895000	2.562429000
C	-0.533900000	-0.902883000	5.230535000
H	-2.634193000	-1.362777000	5.117472000
H	-1.628823000	-2.386727000	4.118024000
H	-0.347030000	-1.557608000	6.083665000
H	-0.656710000	0.112351000	5.617054000
H	0.362507000	-0.910513000	4.606421000
C	2.246326000	1.074233000	2.820111000
C	3.142633000	0.439479000	3.659530000
H	2.048440000	2.133968000	2.908951000
C	3.446231000	-0.922152000	3.518153000
H	3.645922000	1.015654000	4.425816000
C	2.869274000	-1.695732000	2.528488000
H	4.176392000	-1.371253000	4.179711000
H	3.140465000	-2.734939000	2.398826000

C	0.968255000	2.843423000	-0.202546000
H	-0.032869000	2.332666000	1.653458000
H	-0.856878000	1.754189000	0.210616000
C	0.358517000	4.238077000	-0.277458000
H	1.985175000	2.896566000	0.194443000
H	1.064721000	2.416175000	-1.203395000
C	1.176480000	5.176529000	-1.153668000
H	0.276988000	4.659851000	0.731940000
H	-0.667442000	4.175367000	-0.662273000
H	0.735224000	6.175080000	-1.187890000
H	1.240904000	4.804628000	-2.178824000
H	2.197955000	5.273378000	-0.780311000
C	2.500458000	-3.060067000	-0.874181000
H	0.378223000	-3.092149000	-0.434119000
H	1.386326000	-3.552606000	0.926308000
C	2.633768000	-4.509242000	-1.327098000
H	3.421980000	-2.730255000	-0.386477000
H	2.370927000	-2.402410000	-1.736945000
C	3.792190000	-4.704784000	-2.295146000
H	2.773711000	-5.157713000	-0.453557000
H	1.700415000	-4.837111000	-1.800615000
H	3.881272000	-5.749324000	-2.601210000
H	4.740503000	-4.405987000	-1.843298000
H	3.659144000	-4.103514000	-3.197339000

Compound C



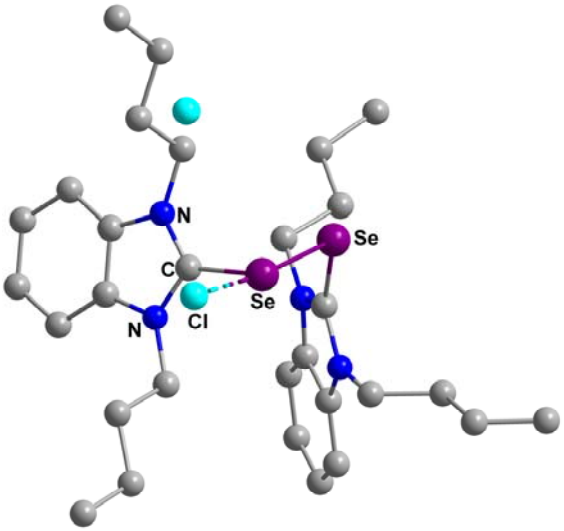
umpw1pw91/gen E(UmPW1PW91) = -12402.0082138

Se	1.093122000	1.029719000	-1.025547000
C	1.223095000	-0.378600000	0.260645000
Se	-1.020114000	0.419982000	-2.007897000

Cl	3.673104000	2.196493000	-0.258220000
C	-2.478720000	1.443252000	-1.334683000
Fe	-3.092201000	-1.989395000	1.808955000
Cl	-2.710978000	-3.069953000	3.674019000
Cl	-2.056767000	0.018080000	1.873872000
Cl	-2.223114000	-3.095087000	0.066625000
Cl	-5.238381000	-1.629913000	1.462905000
Fe	5.145823000	0.561512000	-0.891515000
Cl	4.859606000	-1.044654000	0.606854000
Cl	4.470547000	-0.144418000	-2.872083000
Cl	7.162961000	1.370596000	-0.894559000
N	1.212831000	-1.691010000	-0.029735000
C	1.208584000	-2.396196000	1.157720000
C	1.230022000	-2.316636000	-1.354673000
N	1.281602000	-0.210520000	1.592275000
C	1.264013000	-1.454903000	2.187650000
C	1.361588000	1.046791000	2.332967000
N	-3.699656000	1.199911000	-1.851752000
C	-4.613214000	2.055836000	-1.257137000
C	-4.058444000	0.195056000	-2.854705000
N	-2.567695000	2.443485000	-0.445852000
C	-3.893343000	2.850860000	-0.369366000
C	-1.497334000	3.083090000	0.310597000
C	1.111983000	-3.760855000	1.422939000
C	1.088022000	-4.133997000	2.749576000
H	1.021514000	-4.491772000	0.632051000
C	1.146044000	-3.186413000	3.785889000
H	0.994701000	-5.182985000	3.001071000
C	1.231262000	-1.835160000	3.527866000
H	1.094351000	-3.525999000	4.812642000
H	1.234514000	-1.109850000	4.329385000
C	2.496872000	-3.116787000	-1.625096000
H	1.156074000	-1.515196000	-2.087765000
H	0.325990000	-2.924930000	-1.429456000
C	2.498994000	-3.661421000	-3.049206000
H	2.592830000	-3.941548000	-0.914407000
H	3.364434000	-2.472536000	-1.473712000
C	3.755292000	-4.463540000	-3.355646000
H	2.423892000	-2.825832000	-3.753423000
H	1.611567000	-4.284979000	-3.211544000
H	3.743698000	-4.839943000	-4.380463000
H	3.852440000	-5.324242000	-2.688646000
H	4.649987000	-3.848754000	-3.237799000
C	2.688103000	1.224421000	3.061015000
H	0.509090000	1.066893000	3.015490000
H	1.227762000	1.848966000	1.608792000
C	2.784049000	2.604854000	3.699784000
H	2.806247000	0.454773000	3.828428000
H	3.506495000	1.082857000	2.353391000

C	4.092268000	2.802517000	4.451805000
H	1.938912000	2.760662000	4.381275000
H	2.696804000	3.368649000	2.919206000
H	4.149480000	3.799847000	4.892358000
H	4.949930000	2.683969000	3.786150000
H	4.200227000	2.077146000	5.262399000
C	-5.985497000	2.199559000	-1.420225000
C	-6.603308000	3.176748000	-0.658879000
H	-6.552541000	1.570424000	-2.093813000
C	-5.879436000	3.978535000	0.232983000
H	-7.673461000	3.317330000	-0.747652000
C	-4.512347000	3.831890000	0.395380000
H	-6.402579000	4.727034000	0.815252000
H	-3.961354000	4.452232000	1.090069000
C	-4.582267000	-1.091091000	-2.233922000
H	-3.182243000	0.021898000	-3.480924000
H	-4.806307000	0.660670000	-3.501240000
C	-5.067212000	-2.094364000	-3.277133000
H	-5.397329000	-0.850147000	-1.547275000
H	-3.800030000	-1.544564000	-1.620592000
C	-3.967778000	-2.651551000	-4.173381000
H	-5.857046000	-1.643052000	-3.890203000
H	-5.541354000	-2.919553000	-2.740144000
H	-4.357611000	-3.430271000	-4.831640000
H	-3.167961000	-3.096682000	-3.576442000
H	-3.520566000	-1.889092000	-4.817762000
C	-0.923561000	4.291679000	-0.418026000
H	-0.736525000	2.334113000	0.505397000
H	-1.924079000	3.346312000	1.277474000
C	0.186470000	4.989872000	0.364930000
H	-1.728965000	5.002463000	-0.633248000
H	-0.534140000	3.965955000	-1.388030000
C	-0.266932000	5.619219000	1.676508000
H	1.004658000	4.285762000	0.549138000
H	0.611727000	5.765709000	-0.277303000
H	0.547144000	6.179732000	2.139157000
H	-0.595283000	4.877048000	2.408575000
H	-1.093322000	6.318071000	1.517783000

Compound D



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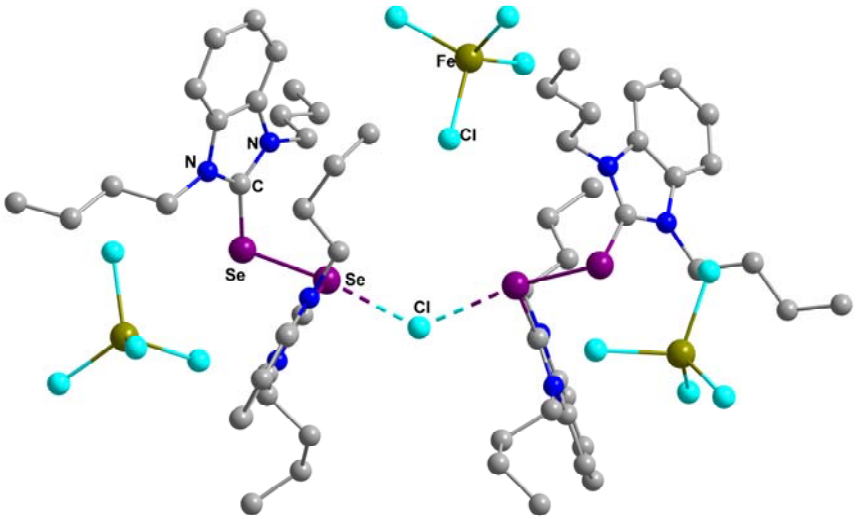
C	3.464738000	1.471818000	3.378076000
C	2.810610000	0.466311000	4.107806000
C	2.062587000	-0.515132000	3.484536000
C	2.005817000	-0.462369000	2.093353000
C	2.671210000	0.528616000	1.368360000
C	3.401972000	1.532443000	1.999223000
N	1.328390000	-1.241404000	1.172544000
C	1.581625000	-0.755716000	-0.061734000
N	2.398485000	0.297936000	0.030362000
C	2.959381000	1.082635000	-1.072987000
C	4.417141000	0.731759000	-1.333212000
C	4.981982000	1.571687000	-2.473328000
C	6.446968000	1.268910000	-2.752279000
C	0.529243000	-2.411196000	1.513445000
C	1.370649000	-3.604865000	1.947169000
C	0.497448000	-4.805849000	2.291010000
C	1.315274000	-6.014872000	2.722270000
Se	0.857207000	-1.460236000	-1.666862000
C	-4.954655000	-0.332516000	2.900655000
C	-4.512712000	0.924217000	3.333772000
C	-3.541383000	1.629268000	2.642136000
C	-3.021642000	1.033210000	1.498429000
C	-3.463526000	-0.220959000	1.066409000
C	-4.439109000	-0.927851000	1.760425000
N	-2.055059000	1.452298000	0.601597000
C	-1.910518000	0.515064000	-0.356374000
N	-2.753704000	-0.513251000	-0.084248000
C	-2.998878000	-1.666026000	-0.940727000
C	-4.138311000	-1.428505000	-1.922216000
C	-4.404253000	-2.650678000	-2.793064000

C	-5.523108000	-2.419307000	-3.798539000
C	-1.387206000	2.758978000	0.657518000
C	-2.169238000	3.822335000	-0.102131000
C	-1.601197000	5.217012000	0.136155000
C	-2.279325000	6.271603000	-0.725348000
Se	-0.775985000	0.662737000	-1.831021000
Cl	2.496227000	-3.234589000	-1.569956000
H	4.009764000	2.241041000	3.911094000
H	2.882378000	0.467772000	5.189232000
H	1.543923000	-1.276576000	4.052653000
H	3.834556000	2.351409000	1.442418000
H	2.351647000	0.874619000	-1.951344000
H	2.805344000	2.135252000	-0.803908000
H	5.008383000	0.902488000	-0.427496000
H	4.504740000	-0.334139000	-1.570029000
H	4.392844000	1.394191000	-3.380129000
H	4.858600000	2.632832000	-2.235048000
H	6.828198000	1.877222000	-3.575237000
H	7.068927000	1.474592000	-1.876905000
H	6.593516000	0.219357000	-3.021232000
H	-0.166041000	-2.109282000	2.301970000
H	-0.058431000	-2.660516000	0.630233000
H	2.057626000	-3.860043000	1.137414000
H	1.985305000	-3.334453000	2.811390000
H	-0.208111000	-4.536782000	3.086565000
H	-0.111732000	-5.071438000	1.419618000
H	0.673496000	-6.866189000	2.958137000
H	2.002763000	-6.326819000	1.932849000
H	1.912209000	-5.795444000	3.611359000
H	-5.719821000	-0.849351000	3.467360000
H	-4.942855000	1.357046000	4.228849000
H	-3.206835000	2.602490000	2.976686000
H	-4.790513000	-1.896248000	1.426805000
H	-2.070718000	-1.884665000	-1.466096000
H	-3.208488000	-2.516226000	-0.287638000
H	-5.046121000	-1.155385000	-1.373374000
H	-3.882185000	-0.570800000	-2.551587000
H	-3.486228000	-2.924907000	-3.324119000
H	-4.653579000	-3.508348000	-2.157394000
H	-5.694755000	-3.305833000	-4.411887000
H	-6.464793000	-2.176138000	-3.299508000
H	-5.284734000	-1.593164000	-4.472772000
H	-1.288666000	3.012923000	1.713691000
H	-0.367543000	2.668973000	0.276517000
H	-2.131802000	3.585235000	-1.171165000
H	-3.227038000	3.789017000	0.189388000
H	-1.717674000	5.476277000	1.195151000
H	-0.523366000	5.201779000	-0.047931000
H	-1.867293000	7.263287000	-0.527947000

H	-2.134342000	6.065737000	-1.789410000
H	-3.357754000	6.318954000	-0.542242000
Cl	1.861382000	3.947882000	0.380450000

Compound 7



umpw1pw91/gen E(UmPW1PW91) = -22159.3788078

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Se	-2.729217000	-0.559221000	-0.663092000
Cl	-7.291054000	-2.882228000	0.393908000
C	-2.955939000	-1.890332000	0.677102000
Cl	-0.144387000	-1.759689000	-0.496625000
Se	2.455425000	-0.754718000	0.324443000
C	2.810592000	-1.684108000	-1.294331000
Se	4.750759000	-0.299502000	0.947659000
C	5.066270000	1.329281000	0.017167000
Cl	7.154692000	-3.237233000	-0.221497000
Fe	0.434906000	5.443285000	-0.378828000
Cl	1.425560000	5.901862000	-2.289032000
Cl	-1.558003000	6.411005000	-0.266939000
Cl	0.187375000	3.220279000	-0.217262000
Cl	1.725463000	6.108609000	1.302900000
Fe	-8.071196000	-2.065474000	-1.551318000
Cl	-8.543601000	0.094365000	-1.254460000
Cl	-6.407383000	-2.177074000	-3.037532000
Cl	-9.811149000	-3.201048000	-2.205685000
Fe	7.358340000	-2.848056000	1.979969000
Cl	7.926173000	-0.704309000	2.246880000
Cl	5.328975000	-3.104788000	2.887774000
Cl	8.812790000	-4.199265000	2.873727000
N	-4.367432000	2.740925000	0.392438000
C	-4.555215000	3.482734000	1.545246000

C	-3.698157000	3.237786000	-0.813768000
N	-5.596029000	1.515678000	1.738494000
C	-5.339517000	2.703869000	2.400371000
C	-6.437102000	0.441519000	2.275533000
N	-2.528783000	-1.787410000	1.949970000
C	-2.824358000	-2.969461000	2.604733000
C	-1.753902000	-0.697478000	2.538234000
N	-3.531172000	-3.085222000	0.490806000
C	-3.476045000	-3.788401000	1.679965000
C	-3.999337000	-3.654378000	-0.775445000
N	3.333265000	-2.914959000	-1.384401000
C	3.431495000	-3.250018000	-2.722053000
C	3.606351000	-3.844917000	-0.285015000
N	2.564038000	-1.203963000	-2.526487000
C	2.931102000	-2.167008000	-3.448640000
C	1.904421000	0.054939000	-2.874893000
N	5.909425000	1.475357000	-1.023923000
C	5.919223000	2.808396000	-1.396885000
C	6.734486000	0.442492000	-1.656592000
N	4.538864000	2.524378000	0.332277000
C	5.042177000	3.475808000	-0.537154000
C	3.670976000	2.819288000	1.474517000
C	-4.094437000	4.743357000	1.916546000
C	-4.453456000	5.185114000	3.176263000
H	-3.472584000	5.342572000	1.263252000
C	-5.237471000	4.402611000	4.039380000
H	-4.113703000	6.159110000	3.506330000
C	-5.693872000	3.150311000	3.671324000
H	-5.490758000	4.790026000	5.018855000
H	-6.295470000	2.550385000	4.341407000
C	-4.637381000	4.057434000	-1.686732000
H	-3.317465000	2.374393000	-1.354728000
H	-2.834547000	3.818021000	-0.490412000
C	-3.947532000	4.527740000	-2.962431000
H	-4.999330000	4.922347000	-1.121428000
H	-5.515247000	3.452196000	-1.937228000
C	-4.865117000	5.365607000	-3.840914000
H	-3.597282000	3.655714000	-3.526175000
H	-3.056005000	5.106336000	-2.702646000
H	-4.353645000	5.685323000	-4.750657000
H	-5.199462000	6.266161000	-3.319768000
H	-5.754553000	4.805312000	-4.140546000
C	-7.909199000	0.828414000	2.333566000
H	-6.048563000	0.200314000	3.268796000
H	-6.297787000	-0.434231000	1.641841000
C	-8.747491000	-0.263705000	2.988832000
H	-8.033023000	1.769249000	2.879676000
H	-8.265862000	1.002277000	1.316077000
C	-10.229636000	0.080867000	3.000291000

H	-8.398260000	-0.431311000	4.015418000
H	-8.595980000	-1.204713000	2.452929000
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H	-10.423762000	1.010023000	3.543850000
C	-2.566720000	-3.400006000	3.903479000
C	-3.005861000	-4.667942000	4.237525000
H	-2.043572000	-2.780447000	4.620067000
C	-3.682690000	-5.480550000	3.314471000
H	-2.825009000	-5.043023000	5.237515000
C	-3.928130000	-5.059570000	2.021062000
H	-4.019387000	-6.462512000	3.623393000
H	-4.451078000	-5.686819000	1.311573000
C	-2.548607000	0.102963000	3.562520000
H	-1.400832000	-0.076089000	1.718767000
H	-0.870228000	-1.153994000	2.991224000
C	-1.677365000	1.072843000	4.359063000
H	-3.049236000	-0.582534000	4.252714000
H	-3.340454000	0.653329000	3.045338000
C	-1.065246000	2.196387000	3.533367000
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H	-2.291921000	1.504538000	5.154412000
H	-0.485620000	2.872819000	4.163968000
H	-1.836107000	2.794849000	3.042205000
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C	-2.922920000	-4.506315000	-1.436069000
H	-4.300359000	-2.835620000	-1.423733000
H	-4.908098000	-4.209232000	-0.549050000
C	-3.372520000	-5.061564000	-2.786380000
H	-2.643648000	-5.331503000	-0.770874000
H	-2.025266000	-3.894838000	-1.564381000
C	-4.545999000	-6.030305000	-2.713955000
H	-3.625872000	-4.231379000	-3.453519000
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H	-4.744646000	-6.473613000	-3.691410000
H	-5.469057000	-5.538840000	-2.400427000
H	-4.344585000	-6.851038000	-2.018294000
C	3.905859000	-4.396579000	-3.352399000
C	3.843544000	-4.417791000	-4.733138000
H	4.307145000	-5.230102000	-2.791163000
C	3.323503000	-3.337587000	-5.463617000
H	4.203393000	-5.290038000	-5.264957000
C	2.859984000	-2.194307000	-4.838997000
H	3.286540000	-3.400885000	-6.544370000
H	2.460312000	-1.365183000	-5.408272000
C	2.437903000	-4.795401000	-0.055692000
H	3.812765000	-3.261930000	0.609090000
H	4.534013000	-4.357657000	-0.533542000
C	2.688145000	-5.746389000	1.113515000

H	2.245173000	-5.372458000	-0.967291000
H	1.539010000	-4.200865000	0.130045000
C	3.833445000	-6.727218000	0.895107000
H	2.874748000	-5.164595000	2.021626000
H	1.763141000	-6.302786000	1.293839000
H	3.899446000	-7.437531000	1.721191000
H	4.802012000	-6.226599000	0.835041000
H	3.693280000	-7.306148000	-0.023110000
C	2.856292000	1.083404000	-3.467304000
H	1.416711000	0.432577000	-1.978727000
H	1.109542000	-0.200100000	-3.579090000
C	2.106517000	2.299459000	-4.000894000
H	3.444486000	0.629337000	-4.272267000
H	3.571543000	1.394248000	-2.699083000
C	3.034150000	3.333402000	-4.620113000
H	1.374265000	1.970503000	-4.747821000
H	1.532128000	2.762686000	-3.193332000
H	2.469441000	4.186789000	-4.997024000
H	3.604285000	2.912679000	-5.453947000
H	3.744927000	3.719199000	-3.886094000
C	6.590474000	3.479495000	-2.416278000
C	6.346625000	4.835504000	-2.531238000
H	7.265360000	2.969024000	-3.090653000
C	5.463568000	5.503085000	-1.667335000
H	6.843493000	5.396674000	-3.313356000
C	4.794310000	4.840600000	-0.656090000
H	5.287690000	6.562599000	-1.804117000
H	4.098597000	5.358331000	-0.008274000
C	8.213232000	0.590027000	-1.321171000
H	6.559994000	0.515676000	-2.733451000
H	6.362943000	-0.525940000	-1.322941000
C	9.067488000	-0.392325000	-2.114971000
H	8.543835000	1.614282000	-1.522456000
H	8.349627000	0.418100000	-0.250974000
C	10.544259000	-0.281906000	-1.763907000
H	8.928516000	-0.217281000	-3.189225000
H	8.723145000	-1.411293000	-1.917726000
H	11.140738000	-0.988971000	-2.343464000
H	10.712714000	-0.498455000	-0.706966000
H	10.931959000	0.720898000	-1.964467000
C	4.470057000	3.242104000	2.698990000
H	3.083011000	1.926517000	1.675943000
H	2.972776000	3.593681000	1.159290000
C	3.561972000	3.523397000	3.890614000
H	5.054375000	4.136834000	2.460376000
H	5.187255000	2.454496000	2.952649000
C	4.340880000	3.969421000	5.119644000
H	2.829867000	4.289021000	3.616248000
H	2.988961000	2.619800000	4.128907000

H	3.673819000	4.156926000	5.963365000
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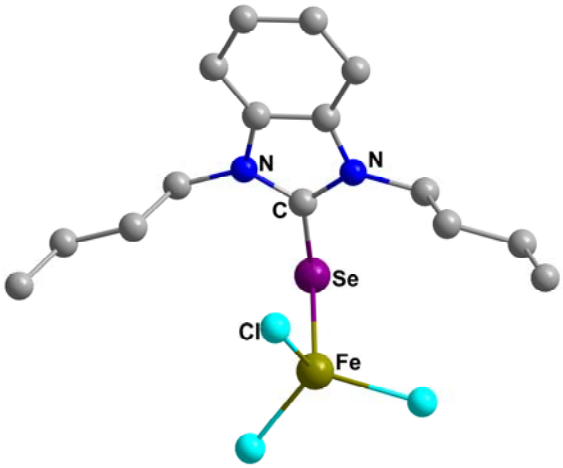
Compound E



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C	-2.670232000	1.175138000	-0.233921000
C	-1.751374000	2.227010000	-0.254960000
C	-2.111214000	3.511292000	0.137561000
N	-2.007679000	0.059817000	-0.714141000
C	-0.734050000	0.396732000	-1.007523000
N	-0.563551000	1.708843000	-0.741343000
C	0.661563000	2.482116000	-0.934274000
C	1.347253000	2.860804000	0.371026000
C	2.617071000	3.663523000	0.114741000
C	3.340277000	4.028479000	1.402784000
C	-2.606400000	-1.265065000	-0.853000000
C	-2.625135000	-2.050157000	0.450103000
C	-3.267169000	-3.420393000	0.268180000
C	-3.273020000	-4.233961000	1.554397000
Se	0.526058000	-0.760844000	-1.769244000
Fe	1.865111000	-1.284259000	0.297616000
Cl	2.195215000	-3.435617000	0.137913000
Cl	3.711195000	-0.102037000	0.160047000
Cl	0.603966000	-0.664183000	1.997562000
H	-3.735479000	4.682908000	0.875404000
H	-5.347097000	2.825937000	0.928578000
H	-4.693711000	0.547238000	0.214498000
H	-1.406654000	4.332381000	0.117373000
H	1.320750000	1.873039000	-1.552493000
H	0.392204000	3.369013000	-1.514702000

H	0.664783000	3.435365000	1.005880000
H	1.590806000	1.951971000	0.924897000
H	3.287336000	3.078474000	-0.522882000
H	2.373774000	4.575083000	-0.445134000
H	4.245114000	4.604398000	1.198648000
H	2.707647000	4.629412000	2.062017000
H	3.635933000	3.131943000	1.951588000
H	-3.614739000	-1.116930000	-1.247253000
H	-2.033261000	-1.795224000	-1.612870000
H	-1.600085000	-2.161015000	0.811164000
H	-3.160746000	-1.483668000	1.219329000
H	-4.294121000	-3.303691000	-0.099084000
H	-2.727431000	-3.972454000	-0.508991000
H	-3.732897000	-5.212377000	1.402078000
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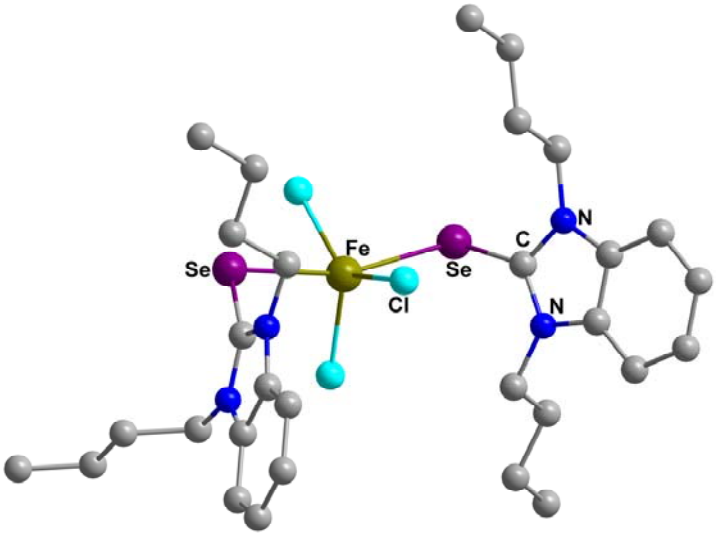
Compound F



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C	-3.476729000	0.701122000	2.285336000
C	-3.861983000	-0.613411000	2.003323000
C	-4.425366000	-1.427388000	2.978101000
N	-2.956432000	1.220559000	1.115432000
C	-3.009809000	0.280422000	0.142802000
N	-3.556354000	-0.838946000	0.674613000
C	-3.846968000	-2.066610000	-0.054832000
C	-5.274213000	-2.103637000	-0.581941000
C	-5.566168000	-3.399118000	-1.329465000
C	-6.984157000	-3.453268000	-1.879360000

C	-2.467528000	2.581782000	0.951316000
C	-3.591714000	3.572118000	0.683080000
C	-3.070220000	4.997106000	0.542836000
C	-4.178992000	6.005509000	0.278461000
Se	-2.461685000	0.495428000	-1.621582000
Fe	0.079475000	-0.388802000	-1.500096000
C	5.147086000	0.124498000	3.964564000
C	5.666785000	1.297749000	3.407193000
C	5.435808000	1.632565000	2.081042000
C	4.666689000	0.752823000	1.330324000
C	4.145684000	-0.419323000	1.887682000
C	4.378368000	-0.753959000	3.215426000
N	4.261356000	0.775011000	0.009532000
C	3.507539000	-0.322532000	-0.249053000
N	3.438036000	-1.054514000	0.885724000
C	2.743666000	-2.326502000	1.026447000
C	3.651609000	-3.520092000	0.767740000
C	2.905703000	-4.838766000	0.932266000
C	3.778095000	-6.048252000	0.629396000
C	4.539958000	1.848869000	-0.933241000
C	3.555394000	3.003888000	-0.818318000
C	3.845794000	4.094348000	-1.841872000
C	2.865455000	5.255228000	-1.752830000
Se	2.751243000	-0.730712000	-1.894314000
Cl	0.070401000	0.156760000	-3.676978000
Cl	0.484121000	0.764084000	0.417753000
Cl	-0.397639000	-2.526945000	-1.019864000
H	-5.022998000	-1.485689000	5.028307000
H	-4.341719000	0.825378000	5.525185000
H	-3.338082000	2.263652000	3.775431000
H	-4.724943000	-2.445799000	2.765290000
H	-3.124282000	-2.135324000	-0.865665000
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H	-5.982904000	-1.980959000	0.245130000
H	-5.420553000	-1.249381000	-1.250586000
H	-4.849184000	-3.510713000	-2.149349000
H	-5.397994000	-4.253421000	-0.663282000
H	-7.168025000	-4.387469000	-2.413967000
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H	-7.169803000	-2.633020000	-2.577413000
H	-1.909373000	2.835868000	1.854888000
H	-1.753254000	2.564017000	0.130519000
H	-4.107399000	3.273313000	-0.235231000
H	-4.333258000	3.524449000	1.488509000
H	-2.526886000	5.279834000	1.452245000
H	-2.337411000	5.034625000	-0.270145000
H	-3.781840000	7.017907000	0.179923000
H	-4.716178000	5.771543000	-0.644143000
H	-4.910441000	6.015754000	1.091095000

H	5.348938000	-0.103441000	5.004444000
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H	5.834732000	2.545016000	1.655865000
H	3.980083000	-1.661681000	3.650784000
H	2.320614000	-2.351408000	2.032848000
H	1.906996000	-2.320148000	0.330229000
H	4.044157000	-3.442253000	-0.250857000
H	4.515333000	-3.488994000	1.442337000
H	2.515135000	-4.914220000	1.954128000
H	2.031375000	-4.839499000	0.273618000
H	3.222851000	-6.980489000	0.752892000
H	4.148620000	-6.020485000	-0.398436000
H	4.647459000	-6.092005000	1.291607000
H	5.567591000	2.176958000	-0.756802000
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H	2.544318000	2.612837000	-0.959223000
H	3.587812000	3.420202000	0.194521000
H	4.868787000	4.467050000	-1.708055000
H	3.808598000	3.662964000	-2.847894000
H	3.088626000	6.023348000	-2.496342000
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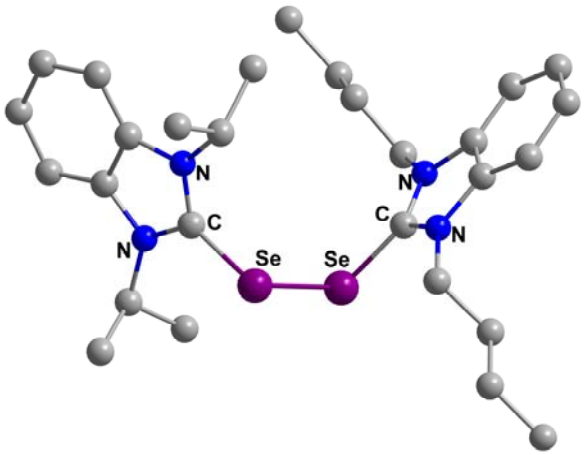
Compound G



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C	3.592838000	1.149592000	0.602011000
C	3.025471000	2.129012000	-0.220866000
C	3.497787000	3.441013000	-0.230602000
N	2.916906000	-0.030334000	0.345300000
C	1.969209000	0.215296000	-0.576339000
N	2.017971000	1.511936000	-0.940591000

C	1.219151000	2.186269000	-1.973163000
C	0.061530000	2.997825000	-1.413009000
C	-0.653894000	3.781344000	-2.510245000
C	-1.830245000	4.587852000	-1.980302000
C	3.321834000	-1.336799000	0.880733000
C	4.483741000	-1.945376000	0.106254000
C	4.915944000	-3.282350000	0.701929000
C	6.076425000	-3.906396000	-0.059946000
Se	0.834138000	-1.065434000	-1.400911000
Se	-0.475526000	-1.961902000	0.370279000
C	-2.083105000	-0.945604000	0.399878000
N	-2.357403000	0.002941000	1.323753000
C	-3.655574000	0.437535000	1.126253000
C	-4.159620000	-0.283474000	0.034117000
N	-3.158513000	-1.141180000	-0.388040000
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C	-5.731001000	1.556165000	1.339811000
C	-6.231815000	0.838310000	0.237994000
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C	-3.400957000	-2.184531000	-1.430392000
C	-1.468975000	0.408911000	2.445273000
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C	-2.416635000	-2.135836000	-2.587937000
C	-1.167131000	1.899519000	2.413565000
C	-2.035140000	-0.079860000	3.771516000
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H	5.939985000	3.011626000	2.097635000
H	5.104782000	0.688271000	2.095130000
H	3.070562000	4.205119000	-0.866766000
H	1.912694000	2.818401000	-2.530133000
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H	0.425669000	3.686830000	-0.644182000
H	0.058671000	4.453560000	-2.999276000
H	-0.999603000	3.092141000	-3.288542000
H	-2.316309000	5.142415000	-2.783330000
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H	3.575189000	-1.182341000	1.930538000
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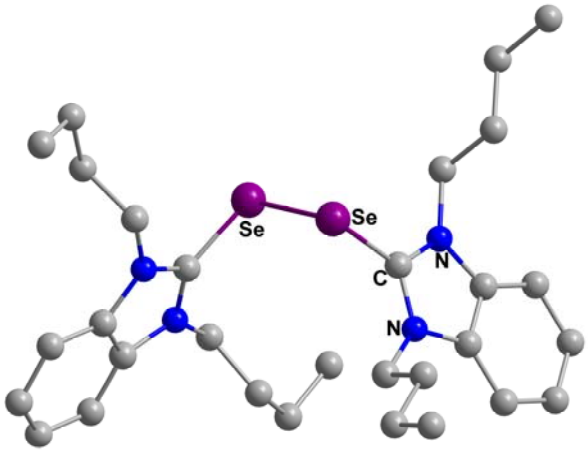
H	6.365726000	-4.859125000	0.384271000
H	5.815716000	-4.096687000	-1.103550000
H	6.956515000	-3.259720000	-0.049344000
H	-4.086874000	1.928607000	2.654831000
H	-6.374327000	2.269715000	1.839267000

H	-7.248549000	1.016222000	-0.089011000
H	-5.871197000	-0.636279000	-1.269381000
H	-4.372144000	-1.897487000	-1.829008000
H	-0.538954000	-0.126514000	2.254285000
H	-3.876514000	-4.268737000	-1.554712000
H	-4.280459000	-3.559149000	0.005522000
H	-2.592474000	-3.928247000	-0.402444000
H	-2.846370000	-2.685895000	-3.426057000
H	-2.234058000	-1.114959000	-2.925967000
H	-1.470364000	-2.620495000	-2.349270000
H	-0.401583000	2.115028000	3.160082000
H	-0.785458000	2.211128000	1.441093000
H	-2.030024000	2.518291000	2.654024000
H	-1.322404000	0.141754000	4.566661000
H	-2.200259000	-1.158126000	3.762988000
H	-2.975247000	0.406605000	4.030396000

Compound H



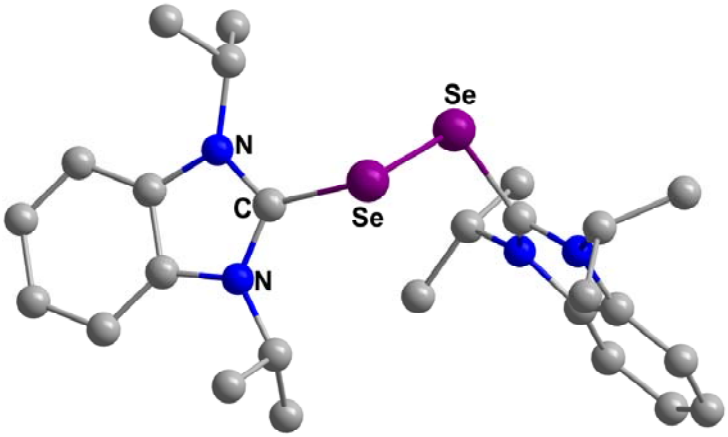
umpw1pw91/6-311g* E(UmPW1PW91) = -6191.62352337

Se	0.486612000	1.407458000	0.723434000
Se	-0.848673000	1.323922000	-1.245885000
N	-2.360017000	-1.141000000	-1.335106000
N	-3.285511000	0.367709000	-0.028536000
C	1.299142000	-1.549189000	2.020083000
H	1.310906000	-2.627572000	1.855113000
H	0.275403000	-1.209253000	1.864995000
C	1.789800000	-1.195516000	3.418192000
H	1.755670000	-0.108136000	3.548587000
C	0.952524000	-1.873303000	4.498751000
H	0.990013000	-2.959570000	4.362008000
H	-0.099011000	-1.587715000	4.380874000
C	1.422682000	-1.520940000	5.902883000
H	0.811004000	-2.019413000	6.655340000
H	2.457714000	-1.828110000	6.067359000

C	-2.225357000	0.093332000	-0.810205000
C	-3.544451000	-1.683928000	-0.873895000
C	-4.159699000	-2.910749000	-1.124625000
H	-3.720173000	-3.656359000	-1.774175000
C	-5.371063000	-3.130042000	-0.501825000
H	-5.888257000	-4.066864000	-0.667142000
C	-5.957967000	-2.167501000	0.342704000
H	-6.911535000	-2.388535000	0.805585000
C	-5.355985000	-0.950904000	0.588733000
H	-5.821613000	-0.213454000	1.229294000
C	-4.131600000	-0.724515000	-0.040033000
C	-1.447253000	-1.828216000	-2.254764000
H	-0.845006000	-1.066970000	-2.746377000
H	-2.069954000	-2.288738000	-3.023963000
C	-3.604500000	1.643808000	0.625698000
H	-2.666264000	2.148604000	0.851574000
H	-4.070220000	1.393517000	1.578295000
C	-4.501401000	2.522983000	-0.238176000
H	-5.407876000	1.970580000	-0.504451000
H	-3.980123000	2.739637000	-1.175967000
C	-4.879954000	3.831281000	0.455996000
H	-3.971994000	4.385227000	0.719176000
C	-5.764681000	3.661573000	1.684447000
H	-6.073972000	4.632364000	2.072671000
H	-5.260599000	3.144714000	2.505715000
H	-6.675993000	3.106845000	1.445657000
C	1.923330000	0.228809000	0.347647000
N	2.951408000	0.486707000	-0.480354000
N	2.125348000	-0.951854000	0.964903000
C	3.848673000	-0.561302000	-0.400882000
C	3.182090000	1.707710000	-1.264116000
C	3.328606000	-1.472295000	0.526947000
C	5.060578000	-0.790350000	-1.052077000
H	2.212844000	2.156944000	-1.473927000
H	3.599244000	1.391680000	-2.221368000
C	4.097802000	2.694443000	-0.551537000
C	4.001344000	-2.650477000	0.851568000
H	5.472806000	-0.091048000	-1.767717000
C	5.720911000	-1.958364000	-0.730619000
H	5.042642000	2.204421000	-0.297203000
H	3.637169000	2.993775000	0.395791000
C	4.368238000	3.926507000	-1.410509000
C	5.200362000	-2.872528000	0.205917000
H	3.614752000	-3.356986000	1.574495000
H	6.668200000	-2.178182000	-1.206802000
H	3.419226000	4.409739000	-1.668213000
H	4.820292000	3.618562000	-2.359625000
C	5.278075000	4.928851000	-0.714809000
H	5.760537000	-3.772556000	0.426465000

H	5.458342000	5.796492000	-1.349983000
H	6.249614000	4.490238000	-0.476598000
H	4.838603000	5.290731000	0.217547000
H	2.839436000	-1.485940000	3.524907000
H	1.361366000	-0.446304000	6.089300000
C	-0.579014000	-2.866750000	-1.554710000
H	-1.213496000	-3.527876000	-0.957690000
H	0.086973000	-2.353469000	-0.851396000
C	0.242162000	-3.700772000	-2.538023000
H	-0.434004000	-4.229594000	-3.217679000
H	0.753748000	-4.481802000	-1.969717000
C	1.264250000	-2.907913000	-3.341958000
H	1.868830000	-3.572854000	-3.959395000
H	1.950058000	-2.361288000	-2.687306000
H	0.800289000	-2.187952000	-4.020451000
H	-5.399940000	4.452158000	-0.277436000

Compound I



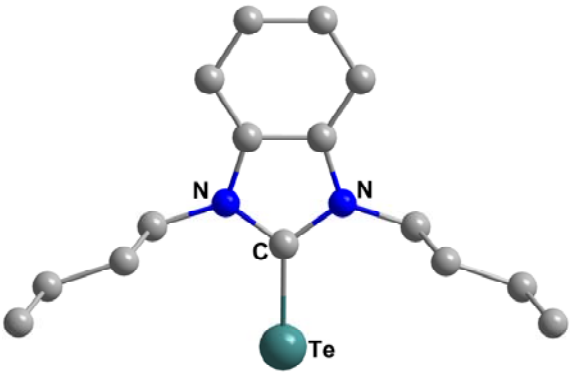
mpw1pw91/6-311g* E(RmPW1PW91) = -6034.36916176

Se	0.709796000	-1.611657000	0.954256000
C	2.118328000	-0.409434000	0.514827000
Se	-0.709809000	-1.611565000	-0.954240000
C	-2.118322000	-0.409348000	-0.514765000
N	3.086108000	-0.641844000	-0.392299000
C	3.995446000	0.400818000	-0.327090000
C	3.199367000	-1.845587000	-1.258758000
N	2.371022000	0.737521000	1.178088000
C	3.550496000	1.268523000	0.682535000
C	1.577732000	1.276951000	2.313981000
C	5.168259000	0.660051000	-1.041254000
C	5.871817000	1.795018000	-0.700739000
H	5.526432000	0.008000000	-1.823761000
C	5.434124000	2.656429000	0.320957000
H	6.788259000	2.026345000	-1.228979000

C	4.276166000	2.412232000	1.026914000
H	6.023558000	3.532569000	0.560466000
H	3.962805000	3.083744000	1.812137000
C	3.080945000	-1.473029000	-2.729295000
C	4.446066000	-2.646934000	-0.912380000
H	2.335251000	-2.451597000	-0.985895000
H	2.168651000	-0.907644000	-2.926775000
H	3.045385000	-2.386368000	-3.324089000
H	3.927397000	-0.887615000	-3.086394000
H	4.477559000	-2.894944000	0.149220000
H	5.370012000	-2.132130000	-1.171969000
H	4.426879000	-3.582937000	-1.471695000
C	2.359359000	1.156486000	3.614547000
C	1.068432000	2.680743000	2.023273000
H	0.714156000	0.613515000	2.371549000
H	2.666025000	0.126554000	3.802870000
H	1.725102000	1.472367000	4.443581000
H	3.250722000	1.783382000	3.627330000
H	0.541246000	2.725555000	1.069370000
H	1.857409000	3.430674000	2.011108000
H	0.366629000	2.966706000	2.807601000
N	-2.370900000	0.737695000	-1.177919000
C	-3.550423000	1.268666000	-0.682447000
C	-1.577444000	1.277292000	-2.313629000
N	-3.086241000	-0.641865000	0.392178000
C	-3.995551000	0.400821000	0.326978000
C	-3.199592000	-1.845695000	1.258494000
C	-4.275957000	2.412487000	-1.026729000
C	-5.433998000	2.656640000	-0.320900000
H	-3.962437000	3.084107000	-1.811797000
C	-5.871895000	1.795069000	0.700579000
H	-6.023332000	3.532870000	-0.560329000
C	-5.168460000	0.660004000	1.041009000
H	-6.788399000	2.026361000	1.228727000
H	-5.526800000	0.007837000	1.823344000
C	-1.068577000	2.681228000	-2.022854000
C	-2.358716000	1.156606000	-3.614387000
H	-0.713690000	0.614070000	-2.370940000
H	-0.541938000	2.726313000	-1.068661000
H	-1.857694000	3.431023000	-2.011286000
H	-0.366384000	2.967182000	-2.806830000
H	-2.665032000	0.126587000	-3.802805000
H	-1.724352000	1.472692000	-4.443261000
H	-3.250258000	1.783241000	-3.627352000
C	-4.446303000	-2.646950000	0.911951000
C	-3.081242000	-1.473293000	2.729073000
H	-2.335479000	-2.451712000	0.985620000
H	-2.168932000	-0.907968000	2.926656000
H	-3.045753000	-2.386685000	3.323787000

H	-3.927684000	-0.887872000	3.086177000
H	-4.477768000	-2.894786000	-0.149690000
H	-5.370240000	-2.132162000	1.171600000
H	-4.427158000	-3.583044000	1.471118000

Compound 36

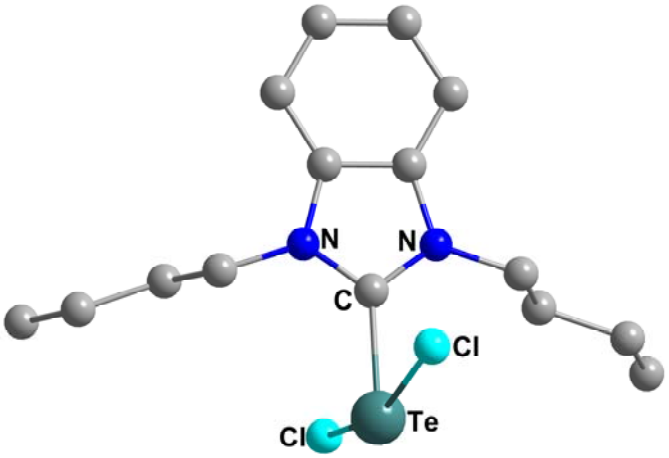


mpw1pw91/gen E(RmPW1PW91) = -7279.98231620

C	0.701828000	1.997280000	-0.377005000
C	-0.701791000	1.997294000	-0.377005000
N	-1.100296000	0.667852000	-0.498283000
C	-0.000003000	-0.152104000	-0.561643000
N	1.100306000	0.667830000	-0.498283000
C	1.424866000	3.179972000	-0.277456000
C	0.700409000	4.366422000	-0.178953000
C	-0.700323000	4.366436000	-0.178953000
C	-1.424804000	3.180001000	-0.277455000
C	2.481167000	0.202509000	-0.524121000
C	3.034608000	-0.077244000	0.870825000
C	4.473480000	-0.592098000	0.822555000
C	5.038325000	-0.895561000	2.208452000
C	-2.481167000	0.202557000	-0.524118000
C	-3.034605000	-0.077202000	0.870827000
C	-4.473481000	-0.592045000	0.822560000
C	-5.038329000	-0.895496000	2.208458000
H	2.504379000	3.185140000	-0.273343000
H	1.230744000	5.304059000	-0.098589000
H	-1.230639000	5.304084000	-0.098588000
H	-2.504318000	3.185192000	-0.273343000
H	2.492489000	-0.710698000	-1.119421000
H	3.077294000	0.954002000	-1.044147000
H	2.981830000	0.830450000	1.479668000
H	2.392929000	-0.822433000	1.347144000
H	4.506703000	-1.497222000	0.208710000
H	5.110705000	0.144088000	0.320699000
H	6.060046000	-1.271974000	2.146254000
H	5.050488000	-0.001186000	2.834850000

H	4.435915000	-1.649410000	2.718253000
H	-3.077283000	0.954069000	-1.044130000
H	-2.492511000	-0.710641000	-1.119430000
H	-2.392929000	-0.822400000	1.347138000
H	-2.981817000	0.830487000	1.479678000
H	-5.110700000	0.144142000	0.320699000
H	-4.506709000	-1.497172000	0.208719000
H	-6.060050000	-1.271907000	2.146260000
H	-4.435922000	-1.649342000	2.718266000
H	-5.050491000	-0.001115000	2.834848000
Te	-0.000025000	-2.222006000	-0.715885000

Compound 37

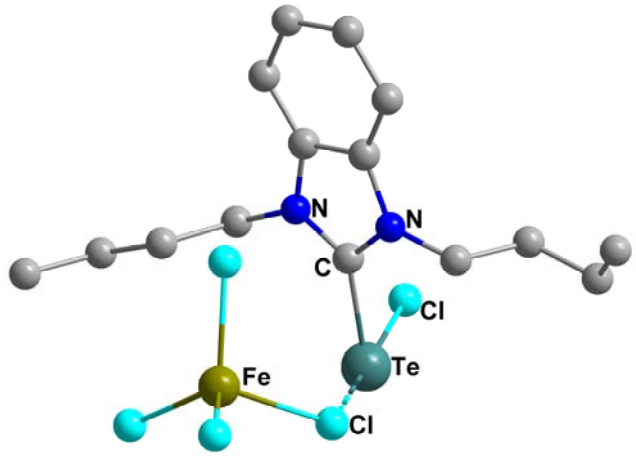


mpw1pw91/gen E(RmPW1PW91) = -8200.65180811

C	-1.089575000	2.033204000	0.395755000
C	0.278261000	2.308151000	0.321636000
N	0.926181000	1.086662000	0.343403000
C	0.010250000	0.112195000	0.419971000
N	-1.214443000	0.656257000	0.455404000
C	-2.036107000	3.051898000	0.421646000
C	-1.560779000	4.350024000	0.363199000
C	-0.188426000	4.625850000	0.280903000
C	0.754573000	3.613483000	0.260053000
C	-2.485744000	-0.056861000	0.541952000
C	-3.237153000	-0.090769000	-0.781513000
C	-4.549562000	-0.855522000	-0.654654000
C	-5.313737000	-0.917693000	-1.969197000
C	2.373349000	0.898190000	0.277552000
C	2.872702000	0.741342000	-1.150561000
C	4.381459000	0.533391000	-1.198284000
C	4.900102000	0.366965000	-2.619296000
Cl	0.919788000	-1.240622000	3.024423000
Cl	-0.143656000	-1.815292000	-2.063345000
H	-3.096169000	2.843719000	0.486615000

H	-2.265172000	5.172801000	0.380865000
H	0.141435000	5.656637000	0.234314000
H	1.812584000	3.833288000	0.197845000
H	-2.255175000	-1.066105000	0.881575000
H	-3.070524000	0.425211000	1.329336000
H	-3.435374000	0.929364000	-1.127722000
H	-2.599114000	-0.561126000	-1.533835000
H	-4.342028000	-1.872421000	-0.304753000
H	-5.178174000	-0.391952000	0.115185000
H	-6.247597000	-1.472631000	-1.859682000
H	-5.564949000	0.082585000	-2.332284000
H	-4.723688000	-1.411218000	-2.744718000
H	2.826603000	1.758521000	0.772827000
H	2.613026000	0.025998000	0.884271000
H	2.362001000	-0.108614000	-1.612390000
H	2.596180000	1.624609000	-1.736793000
H	4.888231000	1.379164000	-0.718382000
H	4.642777000	-0.350935000	-0.607038000
H	5.980020000	0.206694000	-2.631524000
H	4.431850000	-0.487880000	-3.112598000
H	4.690580000	1.251819000	-3.226126000
Te	0.460743000	-1.961549000	0.516924000

Compound 38

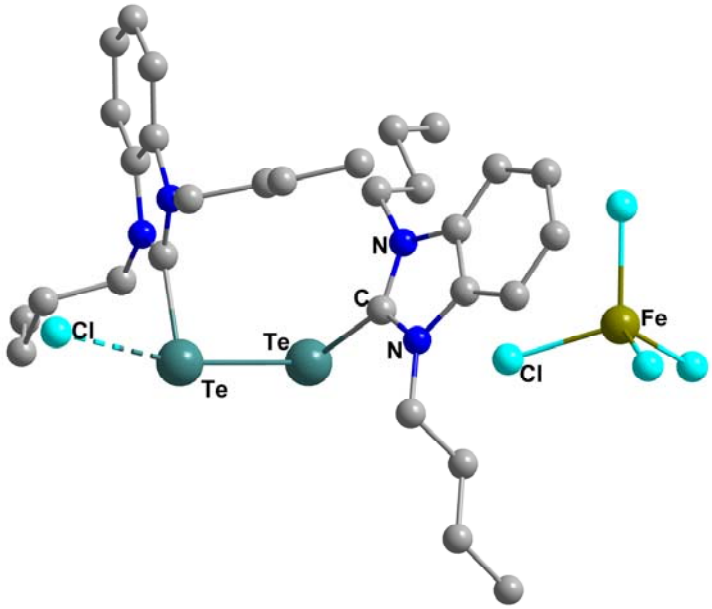


mpw1pw91/gen E(UmPW1PW91) = -10845.3361742

Cl	2.263543000	2.101964000	-2.741549000
C	1.059888000	0.633155000	-0.152559000
Cl	-0.829470000	-2.085653000	-1.198556000
Fe	-2.519650000	-1.650334000	0.325262000
Cl	-1.499641000	-0.639569000	2.011330000
Cl	-3.922338000	-0.296064000	-0.674402000
Cl	-3.379695000	-3.560839000	0.893217000
N	1.748503000	-0.143578000	0.694471000
C	1.831426000	0.501548000	1.913518000

C	2.384699000	-1.423788000	0.387908000
N	0.693720000	1.762527000	0.468886000
C	1.159783000	1.717368000	1.768654000
C	-0.113053000	2.855820000	-0.076851000
C	2.425222000	0.135686000	3.117770000
C	2.320651000	1.035501000	4.160711000
H	2.941934000	-0.807359000	3.238887000
C	1.647356000	2.259225000	4.014408000
H	2.765028000	0.789722000	5.117394000
C	1.054937000	2.622718000	2.820515000
H	1.585384000	2.931099000	4.861690000
H	0.526607000	3.561362000	2.716534000
C	3.817477000	-1.245840000	-0.096588000
H	1.773363000	-1.930873000	-0.355761000
H	2.322776000	-2.023049000	1.295661000
C	4.478430000	-2.570384000	-0.470565000
H	4.406871000	-0.737268000	0.674050000
H	3.806062000	-0.584335000	-0.967924000
C	4.676995000	-3.529975000	0.696391000
H	3.891858000	-3.058663000	-1.256301000
H	5.449162000	-2.345340000	-0.921037000
H	5.226621000	-4.418363000	0.380361000
H	3.730720000	-3.878236000	1.117628000
H	5.249810000	-3.062777000	1.502744000
C	-1.580459000	2.753301000	0.306746000
H	0.013088000	2.852779000	-1.157488000
H	0.336435000	3.783413000	0.283499000
C	-2.376861000	3.933040000	-0.239236000
H	-1.681252000	2.700803000	1.394958000
H	-1.989592000	1.816680000	-0.079451000
C	-3.849548000	3.859765000	0.138021000
H	-1.947638000	4.872918000	0.129078000
H	-2.279009000	3.962870000	-1.330151000
H	-4.406075000	4.701188000	-0.279534000
H	-3.983227000	3.879632000	1.222588000
H	-4.305537000	2.939170000	-0.230984000
Te	0.704029000	0.203280000	-2.204240000

Compound 39



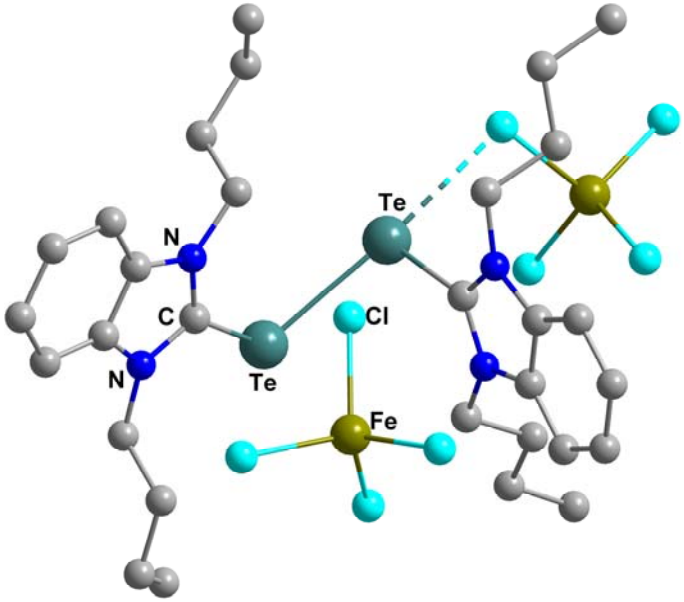
mpw1pw91/gen E(UmPW1PW91) = -18125.5190212

Cl	-5.304431000	-2.545385000	0.798770000
C	-3.483283000	-0.086299000	0.248632000
C	0.732760000	-0.456094000	0.206787000
Cl	3.323740000	0.257499000	-1.820086000
Fe	5.275898000	0.792682000	-0.831158000
Cl	4.937206000	2.629050000	0.385055000
Cl	5.833647000	-0.893637000	0.507249000
Cl	6.806788000	1.135243000	-2.357729000
N	-3.888668000	0.867656000	-0.602901000
C	-4.237437000	1.994681000	0.122080000
C	-4.080397000	0.712263000	-2.041922000
N	-3.555443000	0.381283000	1.503437000
C	-4.023082000	1.683804000	1.466883000
C	-3.280283000	-0.364059000	2.729875000
N	0.932593000	0.724735000	0.816496000
C	1.837114000	0.545948000	1.849069000
C	0.320743000	2.001025000	0.456909000
N	1.446000000	-1.402737000	0.837011000
C	2.159347000	-0.812959000	1.866454000
C	1.534466000	-2.814426000	0.469130000
C	-4.717196000	3.240058000	-0.269829000
C	-4.971360000	4.156189000	0.735651000
H	-4.892540000	3.485456000	-1.309349000
C	-4.758681000	3.843401000	2.085994000
H	-5.346725000	5.137792000	0.473603000
C	-4.282571000	2.604314000	2.476891000
H	-4.974024000	4.589530000	2.841034000
H	-4.122252000	2.367665000	3.520884000
C	-5.465131000	0.172842000	-2.374352000

H	-3.303140000	0.040997000	-2.403135000
H	-3.890490000	1.686252000	-2.492728000
C	-5.663923000	-0.050086000	-3.871285000
H	-6.225830000	0.862983000	-1.993952000
H	-5.605057000	-0.768986000	-1.836689000
C	-5.640156000	1.221959000	-4.710125000
H	-4.906552000	-0.751781000	-4.237926000
H	-6.624069000	-0.554466000	-4.008904000
H	-5.869868000	1.005238000	-5.754840000
H	-4.664287000	1.714345000	-4.698139000
H	-6.382201000	1.943906000	-4.357160000
C	-1.894540000	-0.098511000	3.295016000
H	-3.430981000	-1.418683000	2.508167000
H	-4.061013000	-0.088759000	3.441371000
C	-1.677141000	-0.853239000	4.601881000
H	-1.754429000	0.975759000	3.458207000
H	-1.144428000	-0.402691000	2.558151000
C	-0.315736000	-0.579193000	5.223203000
H	-2.465417000	-0.582024000	5.313518000
H	-1.793777000	-1.927118000	4.421161000
H	-0.184511000	-1.143930000	6.148053000
H	-0.193496000	0.479685000	5.464833000
H	0.498539000	-0.855345000	4.549602000
C	2.393246000	1.438823000	2.758324000
C	3.275269000	0.914178000	3.684194000
H	2.184075000	2.499539000	2.720403000
C	3.594823000	-0.451044000	3.705239000
H	3.755065000	1.579151000	4.391429000
C	3.046861000	-1.339073000	2.798787000
H	4.313588000	-0.813362000	4.429556000
H	3.330756000	-2.382974000	2.793973000
C	1.168785000	2.840342000	-0.484310000
H	0.126290000	2.528715000	1.393828000
H	-0.645378000	1.770048000	0.005529000
C	0.533388000	4.201331000	-0.741042000
H	2.174014000	2.963555000	-0.073301000
H	1.298696000	2.298095000	-1.423867000
C	1.350773000	5.043741000	-1.710233000
H	0.421006000	4.740930000	0.207514000
H	-0.482428000	4.068300000	-1.134675000
H	0.890152000	6.020173000	-1.875876000
H	1.445073000	4.550173000	-2.680198000
H	2.361715000	5.209623000	-1.332400000
C	2.687976000	-3.113676000	-0.474855000
H	0.579852000	-3.091024000	0.021249000
H	1.624104000	-3.375148000	1.402243000
C	2.798129000	-4.606012000	-0.762672000
H	3.623178000	-2.737344000	-0.051423000
H	2.537348000	-2.558448000	-1.403842000

C	3.931410000	-4.923464000	-1.727990000
H	2.952663000	-5.153174000	0.175331000
H	1.850504000	-4.973701000	-1.174870000
H	4.001144000	-5.996317000	-1.919682000
H	4.893161000	-4.590723000	-1.331637000
H	3.785027000	-4.422110000	-2.687451000
Te	-2.865311000	-2.047089000	-0.292795000
Te	-0.399900000	-0.738369000	-1.548079000

Compound 40



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C	-2.959642000	1.332177000	-1.195360000
Fe	-2.891550000	-2.022365000	1.900072000
Cl	-2.426066000	-3.065167000	3.767291000
Cl	-1.799320000	-0.045754000	1.842709000
Cl	-2.180321000	-3.186271000	0.130866000
Cl	-5.046997000	-1.587259000	1.710670000
Fe	5.398802000	0.490434000	-0.778824000
Cl	4.993807000	-1.108654000	0.692762000
Cl	4.723113000	-0.138647000	-2.780356000
Cl	7.447684000	1.206633000	-0.724503000
N	1.324970000	-1.687836000	0.086087000
C	1.342640000	-2.412888000	1.262378000
C	1.291379000	-2.291698000	-1.246314000
N	1.485453000	-0.237158000	1.722937000
C	1.456277000	-1.489281000	2.302617000
C	1.564203000	1.007513000	2.481985000
N	-4.209544000	0.962528000	-1.528769000
C	-5.107434000	1.661260000	-0.737466000
C	-4.593537000	0.002947000	-2.563658000

N	-3.019047000	2.267535000	-0.238733000
C	-4.349172000	2.497836000	0.080053000
C	-1.902996000	3.005797000	0.334489000
C	1.226443000	-3.778674000	1.509937000
C	1.243945000	-4.172702000	2.831329000
H	1.094596000	-4.495167000	0.711405000
C	1.361486000	-3.243272000	3.878095000
H	1.139281000	-5.223610000	3.070111000
C	1.465273000	-1.889618000	3.636609000
H	1.344555000	-3.597911000	4.900969000
H	1.520108000	-1.177395000	4.448177000
C	2.551479000	-3.075827000	-1.582418000
H	1.173996000	-1.478601000	-1.959695000
H	0.389185000	-2.904821000	-1.296038000
C	2.500194000	-3.596763000	-3.014312000
H	2.680829000	-3.910952000	-0.888999000
H	3.420797000	-2.428266000	-1.455134000
C	3.748540000	-4.383601000	-3.386032000
H	2.388835000	-2.749763000	-3.700161000
H	1.611327000	-4.224270000	-3.151046000
H	3.698201000	-4.742035000	-4.416158000
H	3.877715000	-5.255088000	-2.738891000
H	4.643315000	-3.764674000	-3.292828000
C	2.910685000	1.209682000	3.163626000
H	0.738764000	0.993934000	3.197504000
H	1.371981000	1.818825000	1.780269000
C	2.991168000	2.580002000	3.825697000
H	3.078966000	0.428087000	3.909685000
H	3.706750000	1.105946000	2.424825000
C	4.325484000	2.807729000	4.521099000
H	2.173495000	2.694240000	4.547633000
H	2.841275000	3.354906000	3.065633000
H	4.369483000	3.796886000	4.981185000
H	5.154567000	2.733158000	3.814065000
H	4.495666000	2.069304000	5.308863000
C	-6.494612000	1.633833000	-0.667547000
C	-7.088728000	2.481071000	0.251360000
H	-7.086843000	0.968354000	-1.281963000
C	-6.327477000	3.324544000	1.071202000
H	-8.167453000	2.482693000	0.347882000
C	-4.945276000	3.349491000	1.001996000
H	-6.832132000	3.966089000	1.783116000
H	-4.363579000	3.997332000	1.644779000
C	-4.788839000	-1.408564000	-2.032706000
H	-3.830348000	0.042595000	-3.342960000
H	-5.509704000	0.387775000	-3.017820000
C	-5.239672000	-2.382645000	-3.118355000
H	-5.520180000	-1.388793000	-1.221492000
H	-3.857050000	-1.762886000	-1.584801000

C	-4.214795000	-2.607656000	-4.223604000
H	-6.188892000	-2.045749000	-3.552625000
H	-5.456706000	-3.336857000	-2.631914000
H	-4.543116000	-3.391522000	-4.908768000
H	-3.252878000	-2.917068000	-3.807049000
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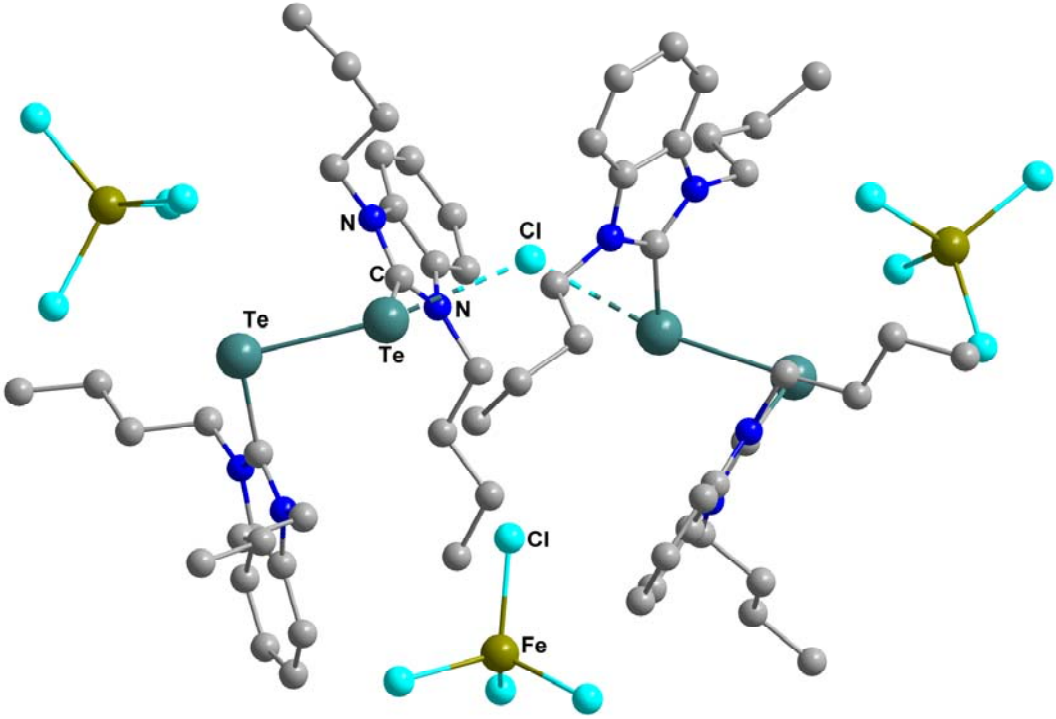
C	-1.584150000	4.263538000	-0.463206000
H	-1.047564000	2.336353000	0.370011000
H	-2.166267000	3.220199000	1.368939000
C	-0.445777000	5.082766000	0.142130000
H	-2.484544000	4.881728000	-0.546700000
H	-1.318651000	3.966089000	-1.483398000
C	-0.767292000	5.704195000	1.495690000
H	0.450535000	4.458579000	0.222002000
H	-0.189022000	5.876955000	-0.564385000
H	0.051710000	6.340848000	1.834806000
H	-0.928711000	4.955010000	2.274779000
H	-1.664239000	6.327822000	1.443157000
Te	-1.304163000	0.474327000	-2.215844000
Te	1.273542000	1.223139000	-1.000359000

Compound 41



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Cl	0.108492000	-2.035549000	0.414825000
C	-2.937306000	-1.839238000	1.230390000

C	-5.330448000	1.635969000	0.130143000
Cl	-7.413734000	-3.304952000	0.461534000
Fe	-0.356799000	5.626897000	0.433309000
Cl	-1.147861000	6.071206000	2.436724000
Cl	1.615196000	6.587760000	0.111788000
Cl	-0.125942000	3.404711000	0.233051000
Cl	-1.803367000	6.310439000	-1.108006000
Fe	8.402218000	-2.191946000	1.428307000
Cl	9.248094000	-0.171408000	1.081411000
Cl	6.724956000	-1.974300000	2.917945000
Cl	9.882165000	-3.609316000	2.169462000
Fe	-7.811032000	-3.033015000	-1.725823000
Cl	-8.761193000	-1.048332000	-2.024617000
Cl	-5.816398000	-2.977846000	-2.782544000
Cl	-9.024802000	-4.669563000	-2.494072000
N	4.402796000	2.904495000	-0.672245000
C	4.485904000	3.599870000	-1.867073000
C	3.726251000	3.386345000	0.533744000
N	5.709951000	1.737297000	-1.984966000
C	5.327380000	2.858275000	-2.701267000
C	6.640139000	0.719946000	-2.475117000
N	2.732204000	-2.107505000	-1.947054000
C	3.221183000	-3.248945000	-2.557613000
C	1.867962000	-1.124562000	-2.593910000
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C	3.927239000	-3.952984000	-1.579121000
C	4.306627000	-3.664037000	0.895707000
N	-3.553761000	-3.024565000	1.294667000
C	-3.668597000	-3.389576000	2.623579000
C	-3.894559000	-3.888774000	0.163574000
N	-2.641370000	-1.416372000	2.469523000
C	-3.082886000	-2.366388000	3.372822000
C	-1.920724000	-0.201549000	2.841848000
N	-6.135794000	1.782215000	1.198421000
C	-6.020727000	3.079387000	1.668716000
C	-7.052345000	0.784183000	1.750988000
N	-4.690168000	2.793054000	-0.097923000
C	-5.091081000	3.723256000	0.847198000
C	-3.812950000	3.079774000	-1.233365000
C	3.896562000	4.787617000	-2.290642000
C	4.192600000	5.200085000	-3.577248000
H	3.237687000	5.362198000	-1.651333000
C	5.040761000	4.459164000	-4.415285000
H	3.756495000	6.120683000	-3.945316000
C	5.623023000	3.276387000	-3.995787000
H	5.246486000	4.824161000	-5.414367000
H	6.280468000	2.710888000	-4.643757000
C	4.636051000	4.250584000	1.393229000
H	3.387037000	2.511231000	1.084571000

H	2.834772000	3.926553000	0.219336000
C	3.951063000	4.671110000	2.688270000
H	4.937936000	5.137103000	0.826402000
H	5.549076000	3.690103000	1.621576000
C	4.841901000	5.548572000	3.555176000
H	3.660873000	3.775247000	3.249103000
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H	4.334643000	5.832338000	4.479054000
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C	8.093875000	1.155998000	-2.361005000
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H	6.467566000	-0.188763000	-1.898261000
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H	8.237508000	2.113268000	-2.874252000
H	8.331016000	1.321539000	-1.306298000
C	10.500046000	0.510714000	-2.798428000
H	8.799160000	-0.067286000	-3.989907000
H	8.875052000	-0.844171000	-2.417656000
H	11.158563000	-0.249982000	-3.221703000
H	10.774462000	0.634882000	-1.749076000
H	10.706676000	1.452491000	-3.315039000
C	3.110969000	-3.726109000	-3.860747000
C	3.738220000	-4.926669000	-4.138391000
H	2.566976000	-3.187351000	-4.626021000
C	4.454619000	-5.628811000	-3.156361000
H	3.680046000	-5.333542000	-5.140658000
C	4.563562000	-5.157435000	-1.861840000
H	4.939532000	-6.560157000	-3.421662000
H	5.128390000	-5.693484000	-1.111007000
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H	1.160988000	-0.776787000	-1.843893000
H	1.286155000	-1.668874000	-3.340172000
C	1.748462000	0.927593000	-4.076495000
H	3.449156000	-0.379263000	-3.840526000
H	3.107199000	0.605257000	-2.424447000
C	0.594796000	1.573191000	-3.318830000
H	1.358222000	0.351843000	-4.923988000
H	2.376971000	1.709661000	-4.511832000
H	0.052856000	2.271280000	-3.959118000
H	0.940229000	2.133327000	-2.447396000
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C	3.237556000	-4.464403000	1.627110000
H	4.599181000	-2.786325000	1.467043000
H	5.221720000	-4.226323000	0.723990000
C	3.672766000	-4.857482000	3.036998000
H	2.989905000	-5.361471000	1.048302000
H	2.323981000	-3.863856000	1.672735000
C	4.865787000	-5.803674000	3.087701000

H	3.898999000	-3.952576000	3.610327000
H	2.816195000	-5.324344000	3.532697000
H	5.062459000	-6.126391000	4.111660000
H	5.782960000	-5.333819000	2.726956000
H	4.686828000	-6.702993000	2.490526000
C	-4.227366000	-4.510342000	3.230118000
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H	-2.560078000	-1.639222000	5.348099000
C	-2.728985000	-4.792692000	-0.213981000
H	-4.187057000	-3.251788000	-0.668090000
H	-4.789011000	-4.439713000	0.446558000
C	-3.030506000	-5.645318000	-1.444388000
H	-2.477299000	-5.438766000	0.634845000
H	-1.849459000	-4.168197000	-0.395556000
C	-4.154528000	-6.655123000	-1.249272000
H	-3.270380000	-4.991232000	-2.288520000
H	-2.111335000	-6.172398000	-1.718078000
H	-4.251083000	-7.303135000	-2.122176000
H	-5.124610000	-6.173776000	-1.109475000
H	-3.966904000	-7.297771000	-0.383560000
C	-2.837342000	0.908274000	3.330791000
H	-1.341247000	0.116891000	1.977627000
H	-1.201474000	-0.490162000	3.610934000
C	-2.041881000	2.103990000	3.843662000
H	-3.492018000	0.527988000	4.122922000
H	-3.490500000	1.215132000	2.506871000
C	-2.928310000	3.199795000	4.414226000
H	-1.340639000	1.764880000	4.615527000
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H	-2.330653000	4.042637000	4.762443000
H	-3.522056000	2.835640000	5.257976000
H	-3.617641000	3.587803000	3.661546000
C	-6.628835000	3.735549000	2.735214000
C	-6.264129000	5.053592000	2.942101000
H	-7.352228000	3.243759000	3.372742000
C	-5.324536000	5.696165000	2.120804000
H	-6.710705000	5.602862000	3.762106000
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H	-5.054989000	6.724454000	2.326525000
H	-3.986635000	5.547826000	0.439946000
C	-8.486454000	0.986799000	1.282853000
H	-6.973195000	0.848005000	2.838779000
H	-6.688481000	-0.198853000	1.452212000
C	-9.431731000	-0.027961000	1.915559000

H	-8.814167000	2.005351000	1.517951000
H	-8.521406000	0.885197000	0.194399000
C	-10.865742000	0.142686000	1.436168000
H	-9.392820000	0.064641000	3.008011000
H	-9.086334000	-1.038133000	1.676967000
H	-11.525908000	-0.589009000	1.905507000
H	-10.935453000	0.002014000	0.355635000
H	-11.253324000	1.137890000	1.672183000
C	-4.587948000	3.605081000	-2.432426000
H	-3.285526000	2.159199000	-1.476366000
H	-3.061278000	3.792188000	-0.896574000
C	-3.678444000	3.835613000	-3.633086000
H	-5.088001000	4.540025000	-2.159741000
H	-5.373209000	2.887291000	-2.692766000
C	-4.432252000	4.386487000	-4.834622000
H	-2.875187000	4.523361000	-3.352510000
H	-3.195622000	2.889737000	-3.905144000
H	-3.765070000	4.533535000	-5.686202000
H	-4.889193000	5.352670000	-4.606620000
H	-5.229611000	3.709708000	-5.152600000
Te	-5.271521000	-0.119702000	-1.086827000
Te	-2.459990000	-0.797805000	-0.556388000
Te	2.673292000	-0.593996000	0.758003000
Te	5.473438000	0.357037000	0.782260000