

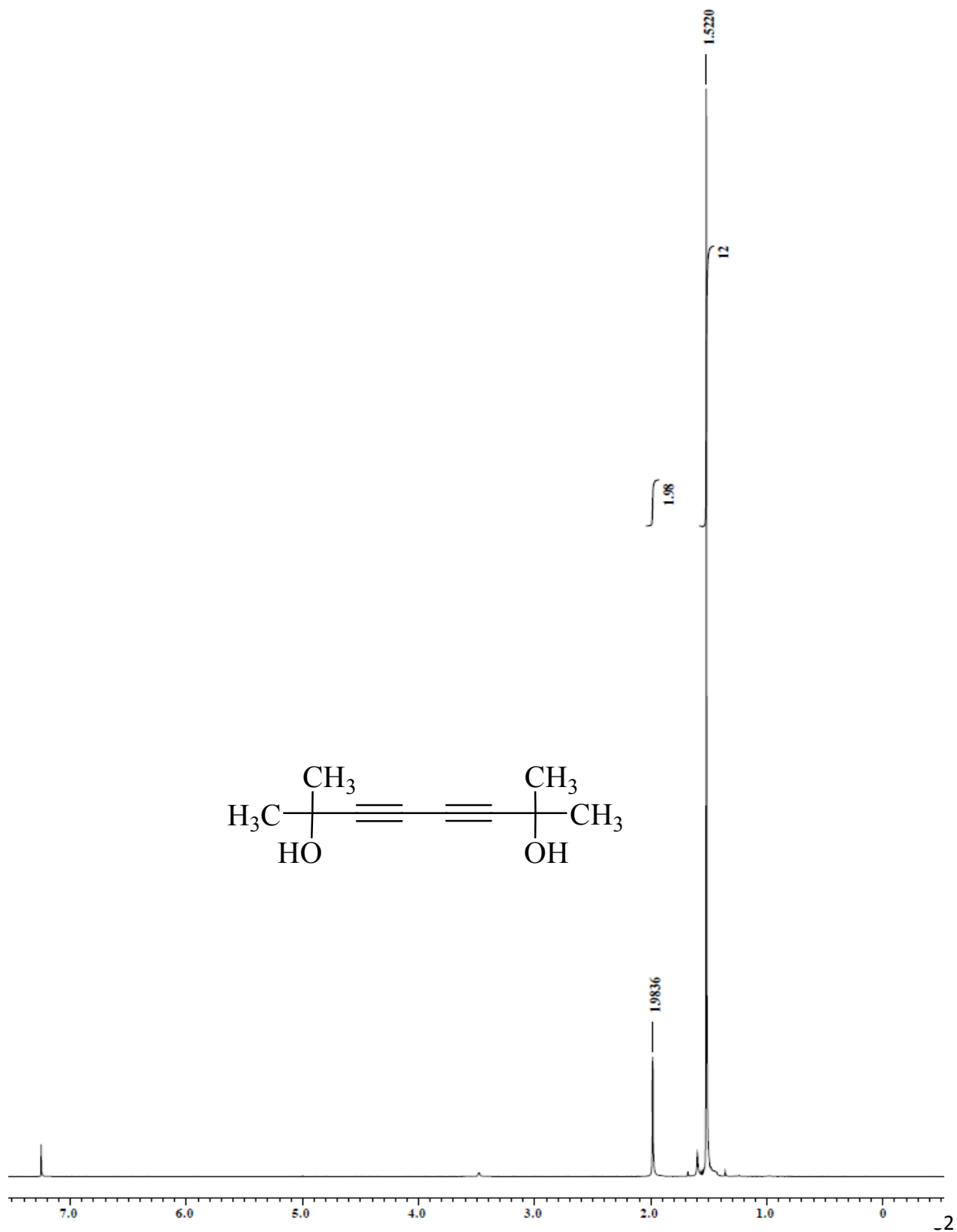
Supplementary Information for publication

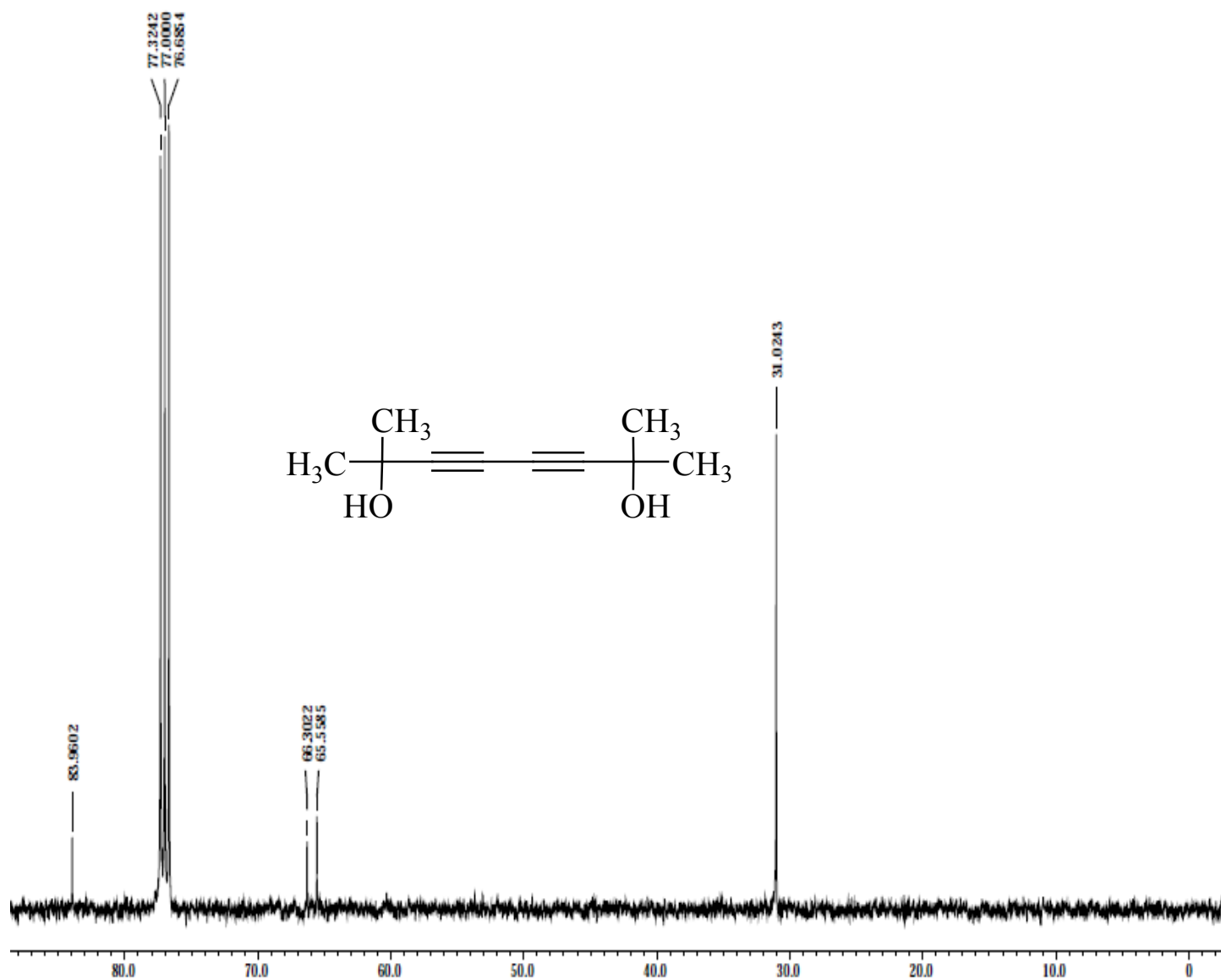
**Synthesis of 5,10,15,20-*meso*-unsubstituted and 5,10,15,20-*meso*-substituted-21,23-ditellura/diselena core-modified porphyrinogens: oxidation and detection of mercury(II)**

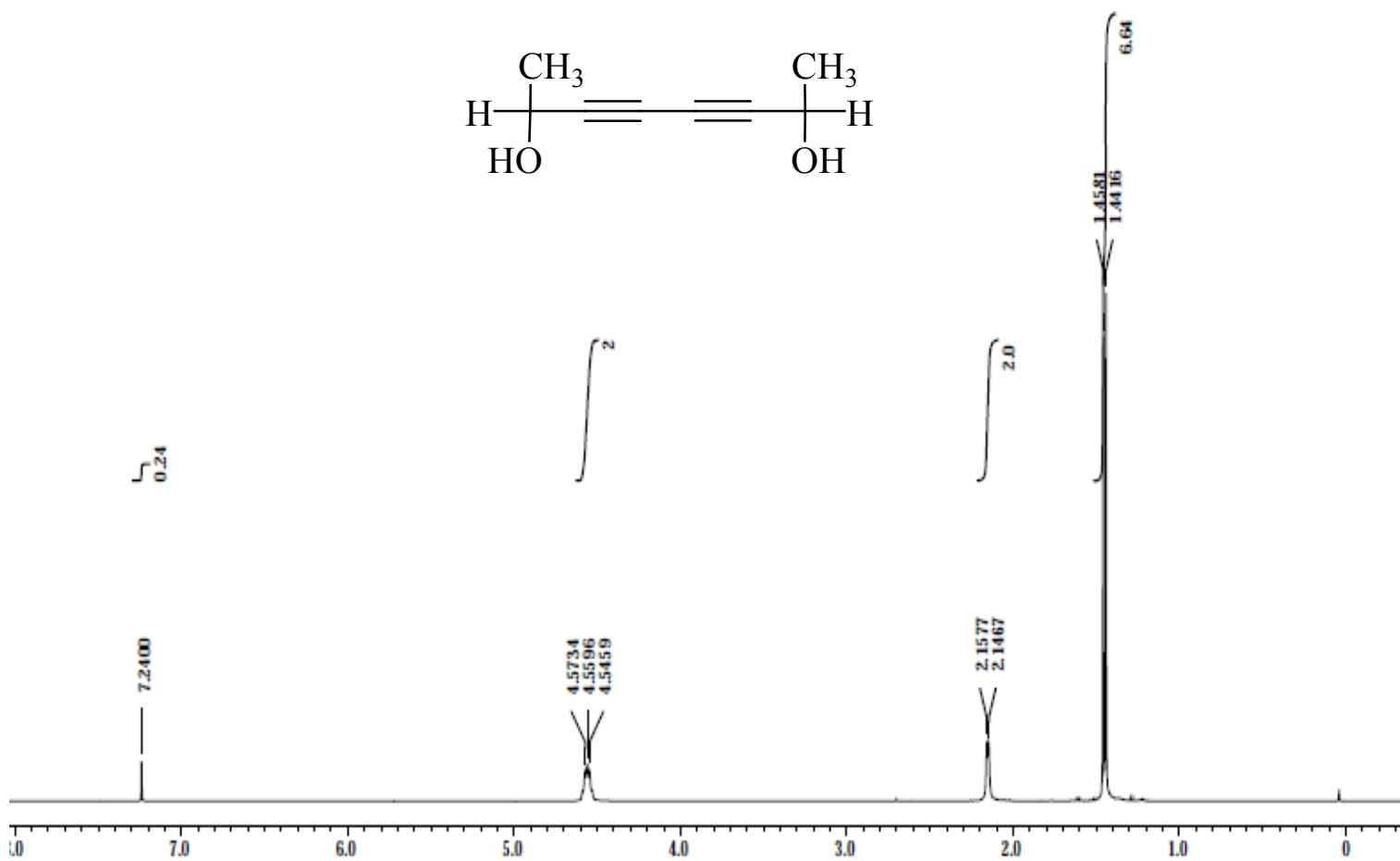
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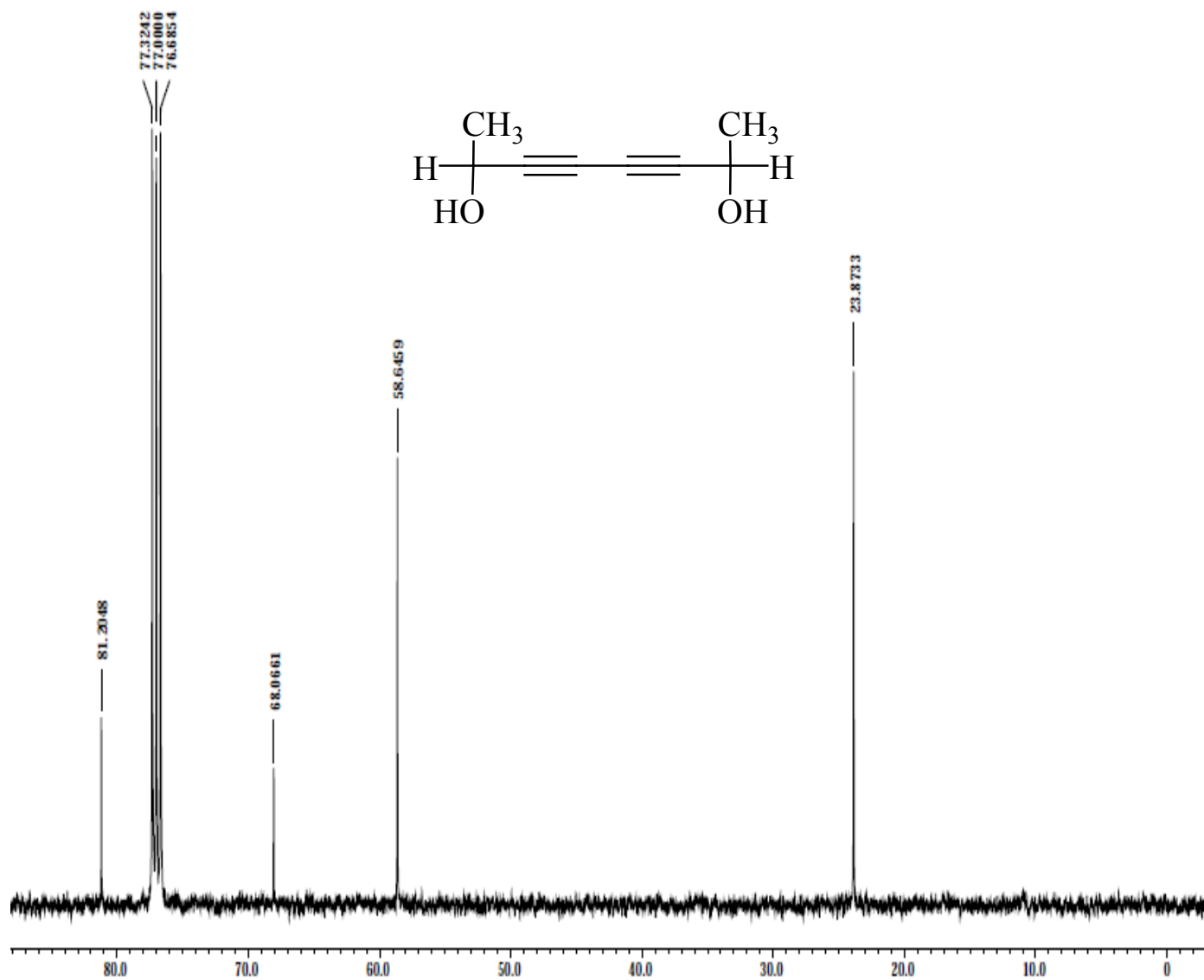
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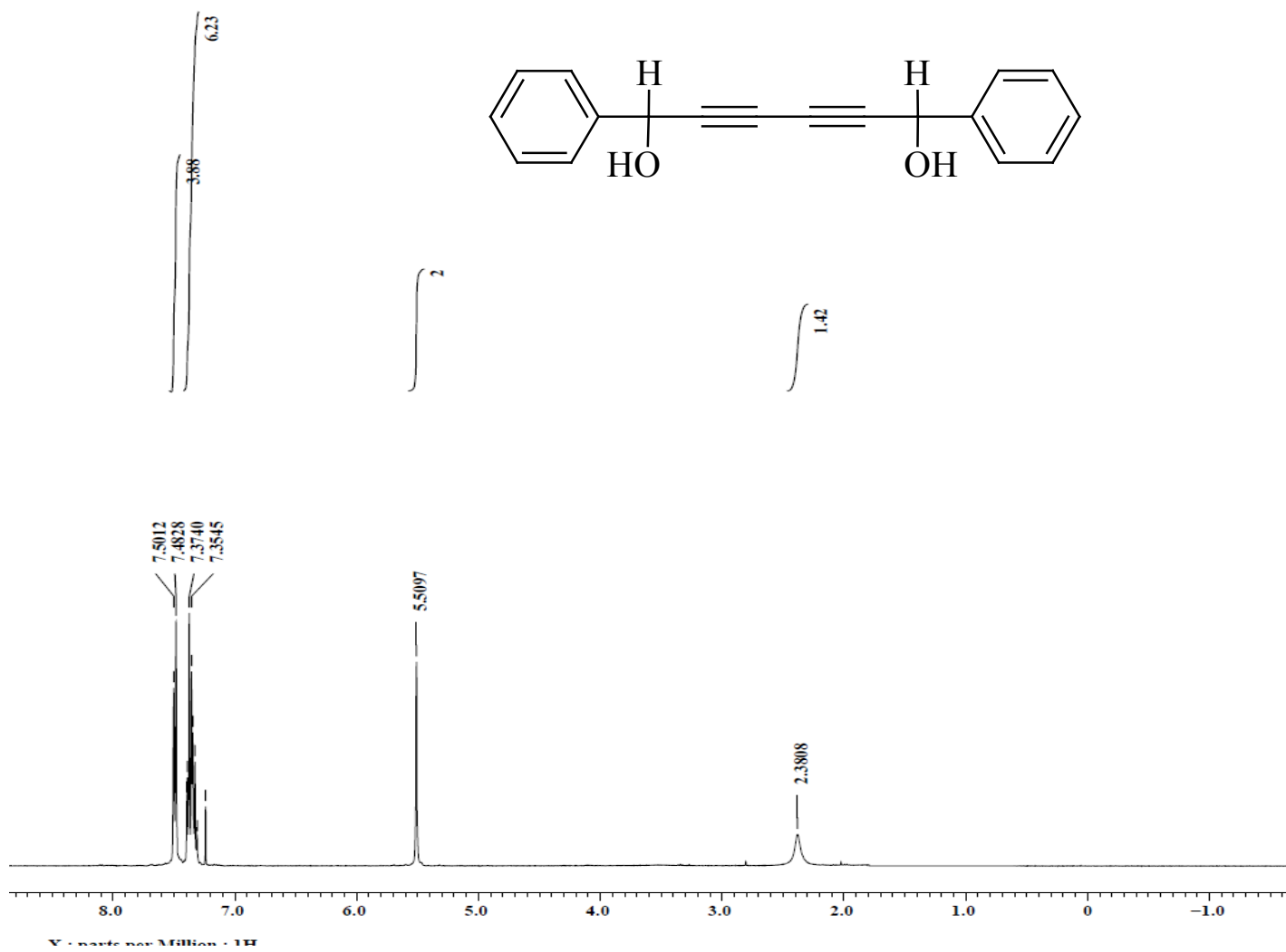
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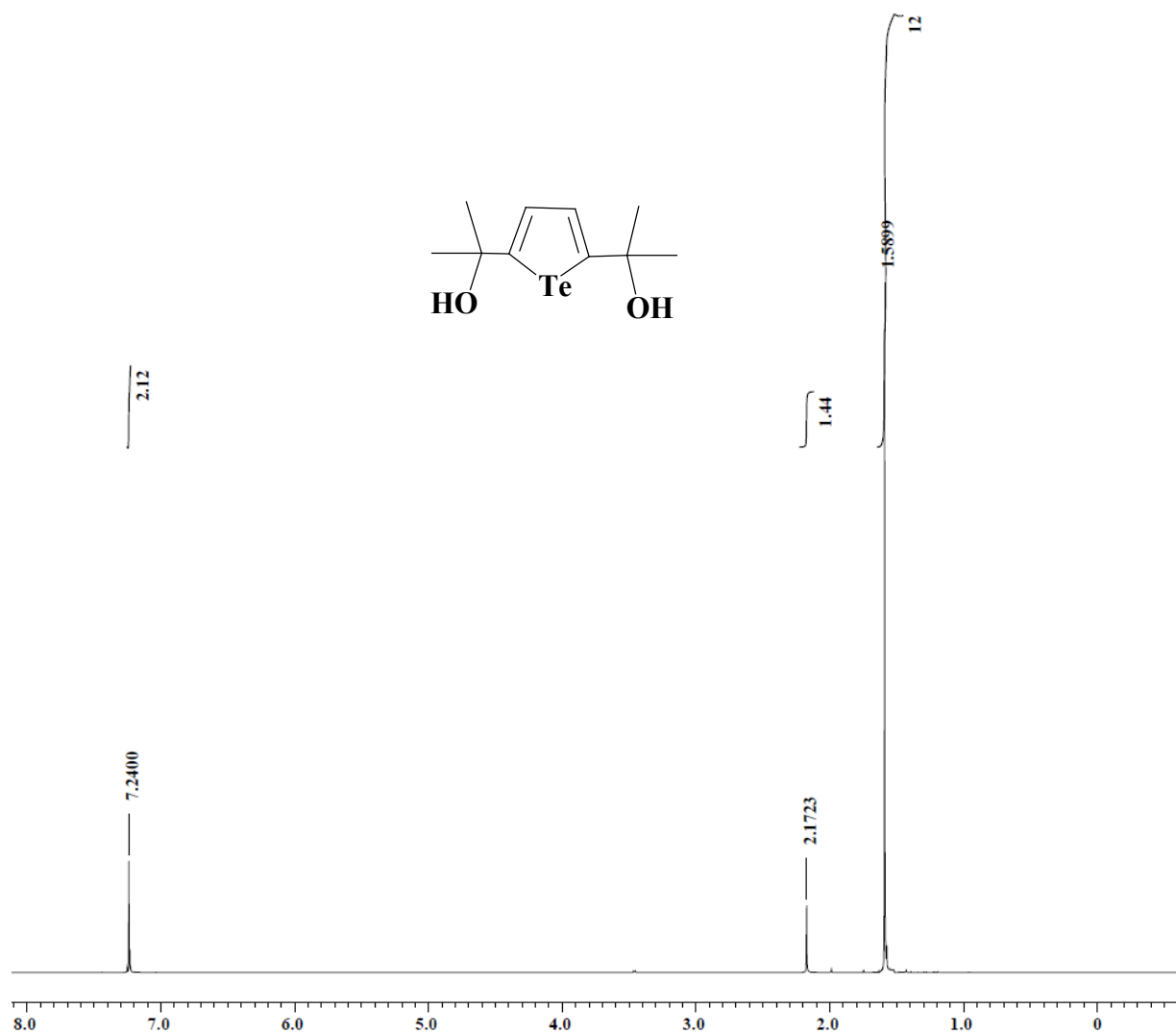


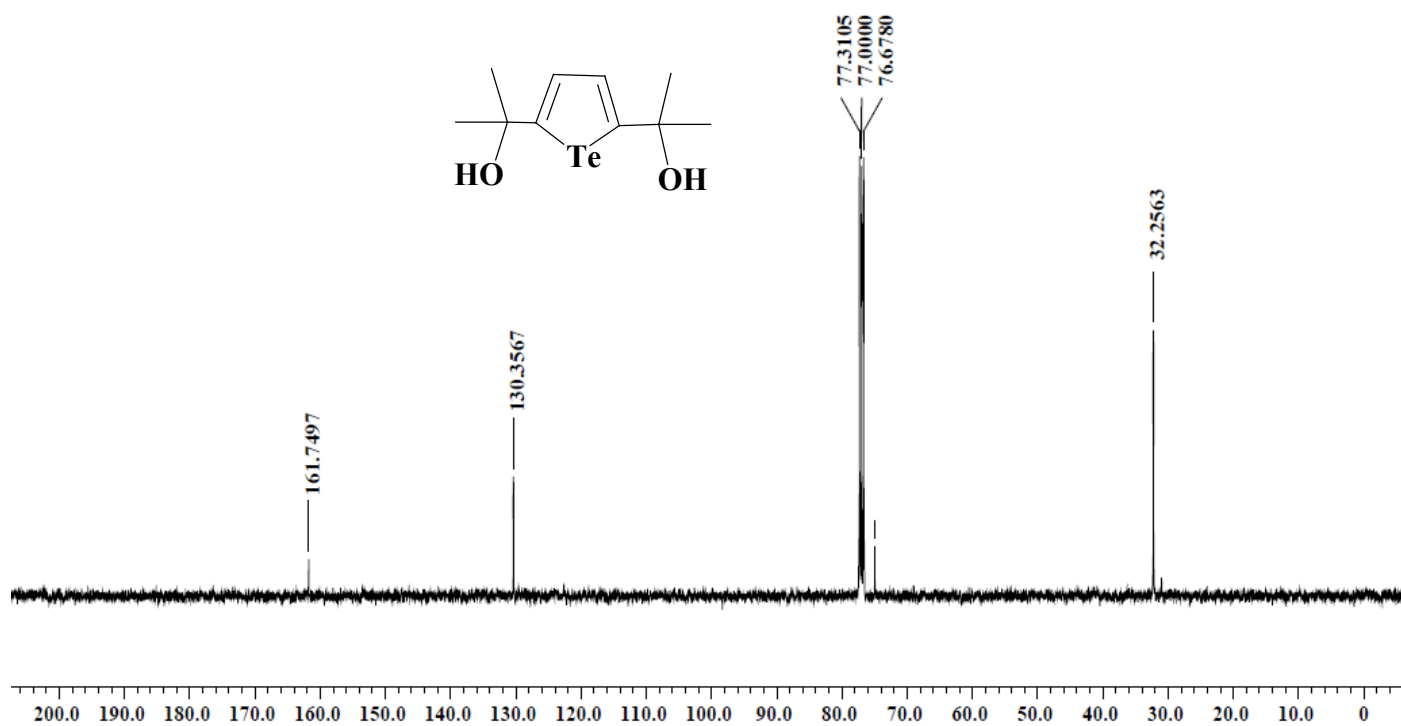




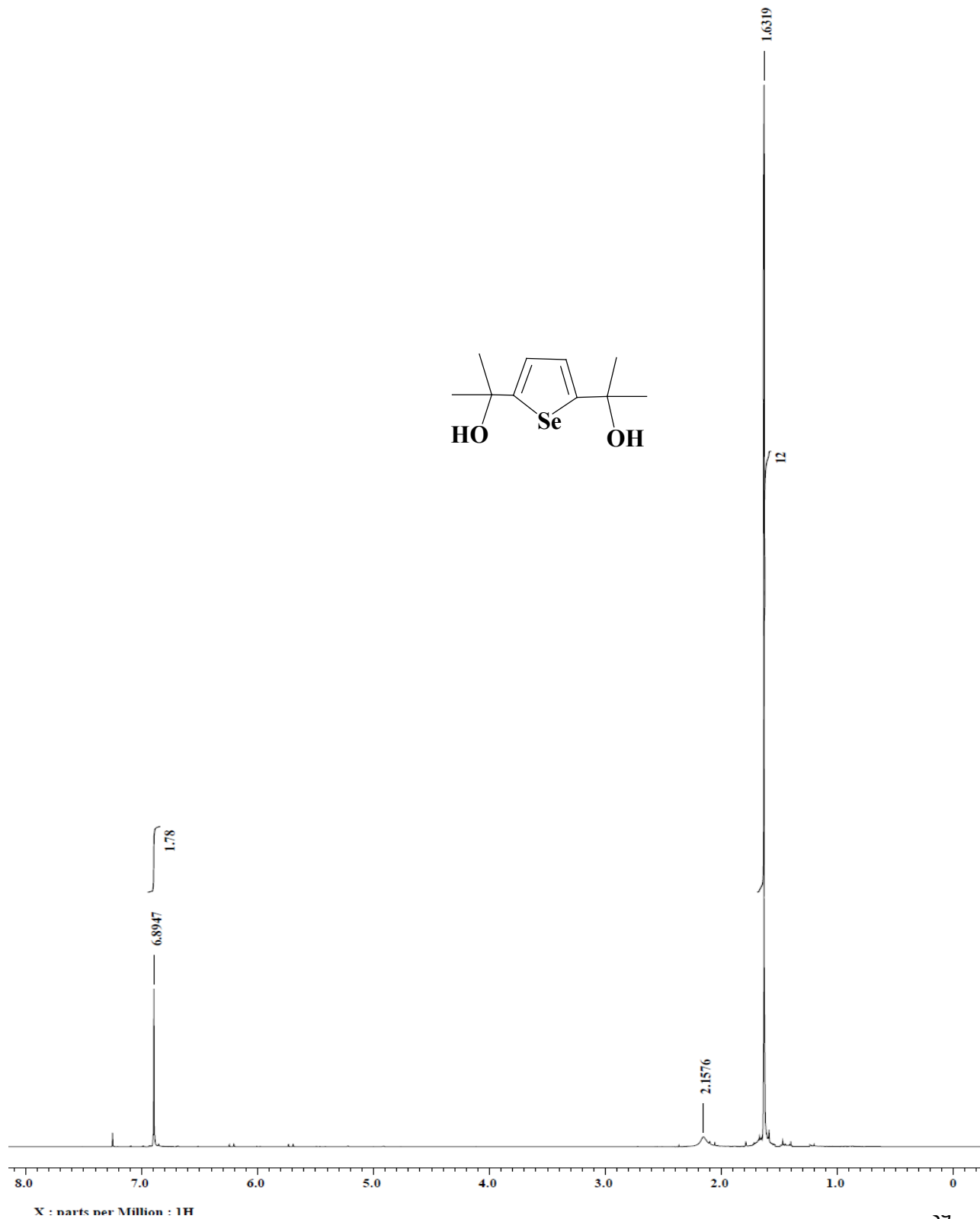
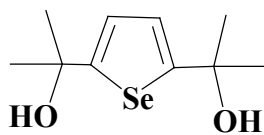


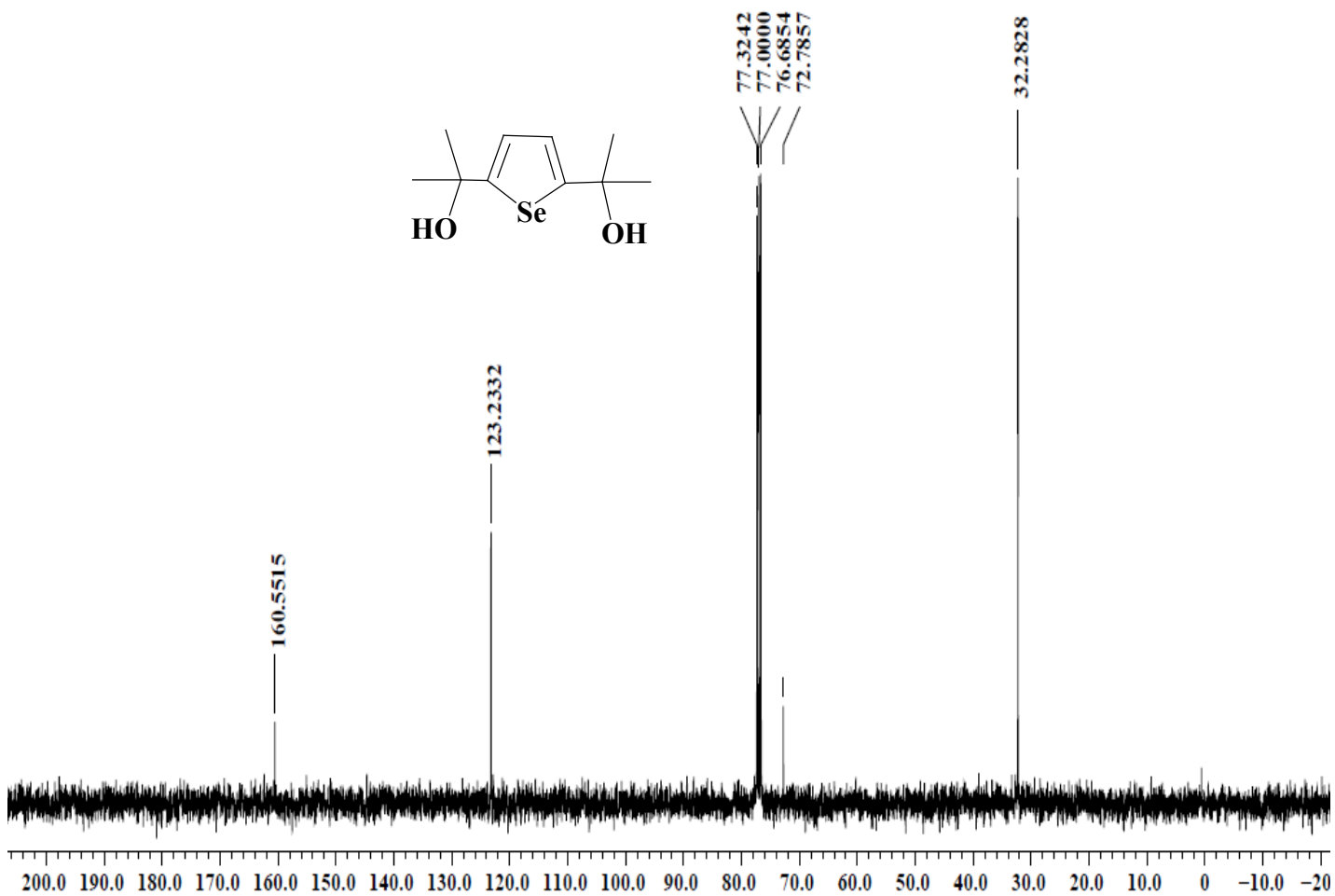


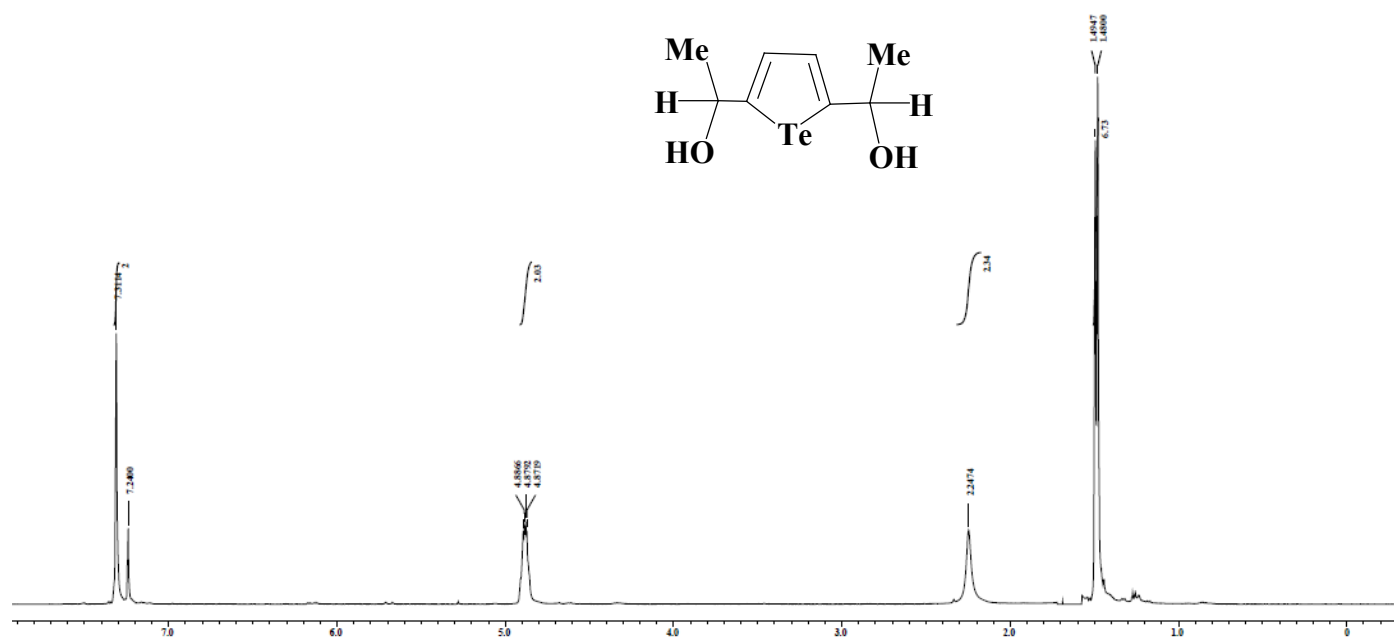


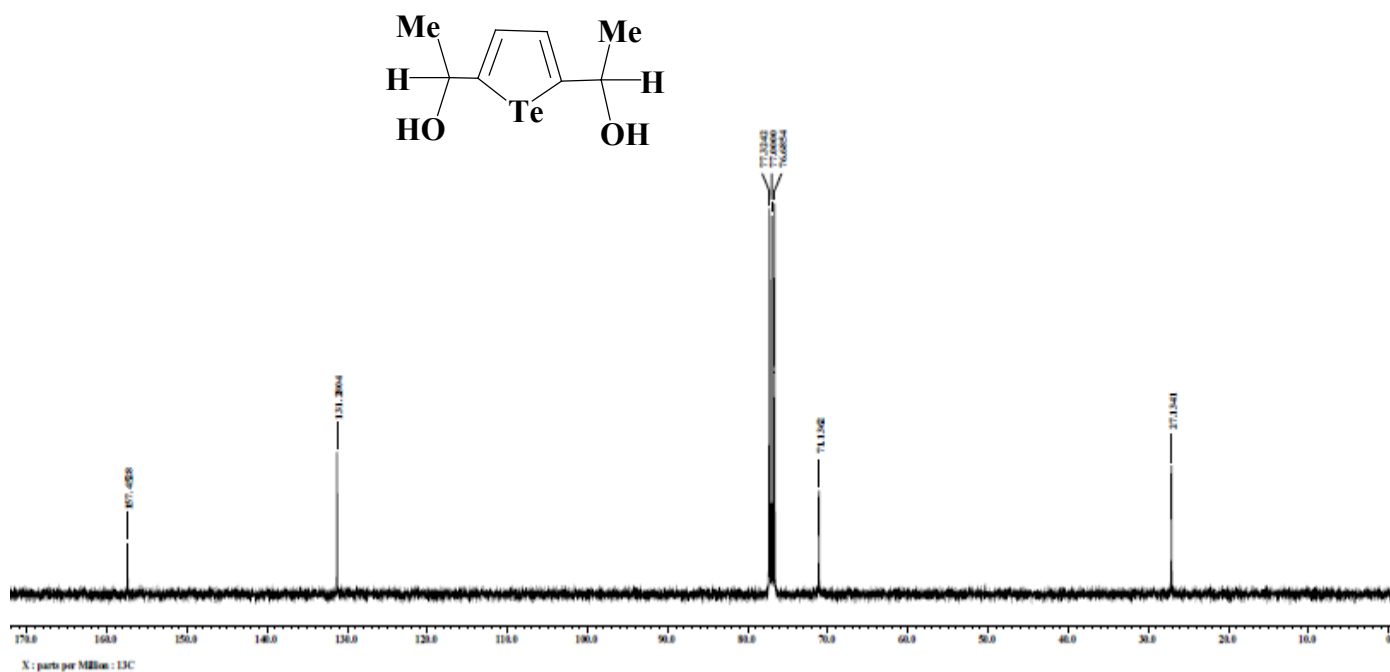


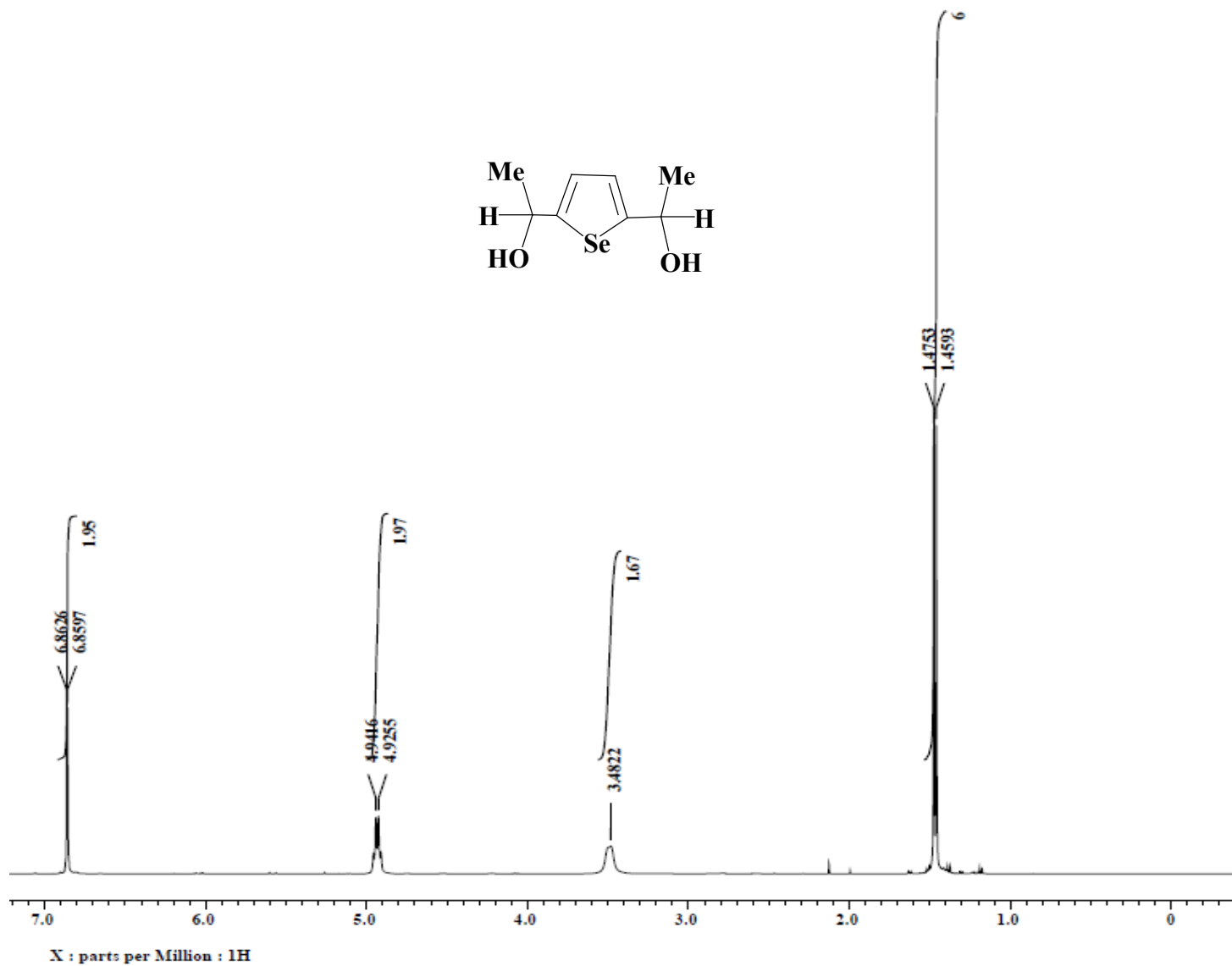
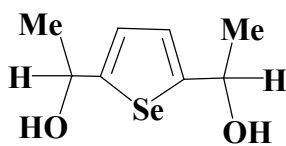


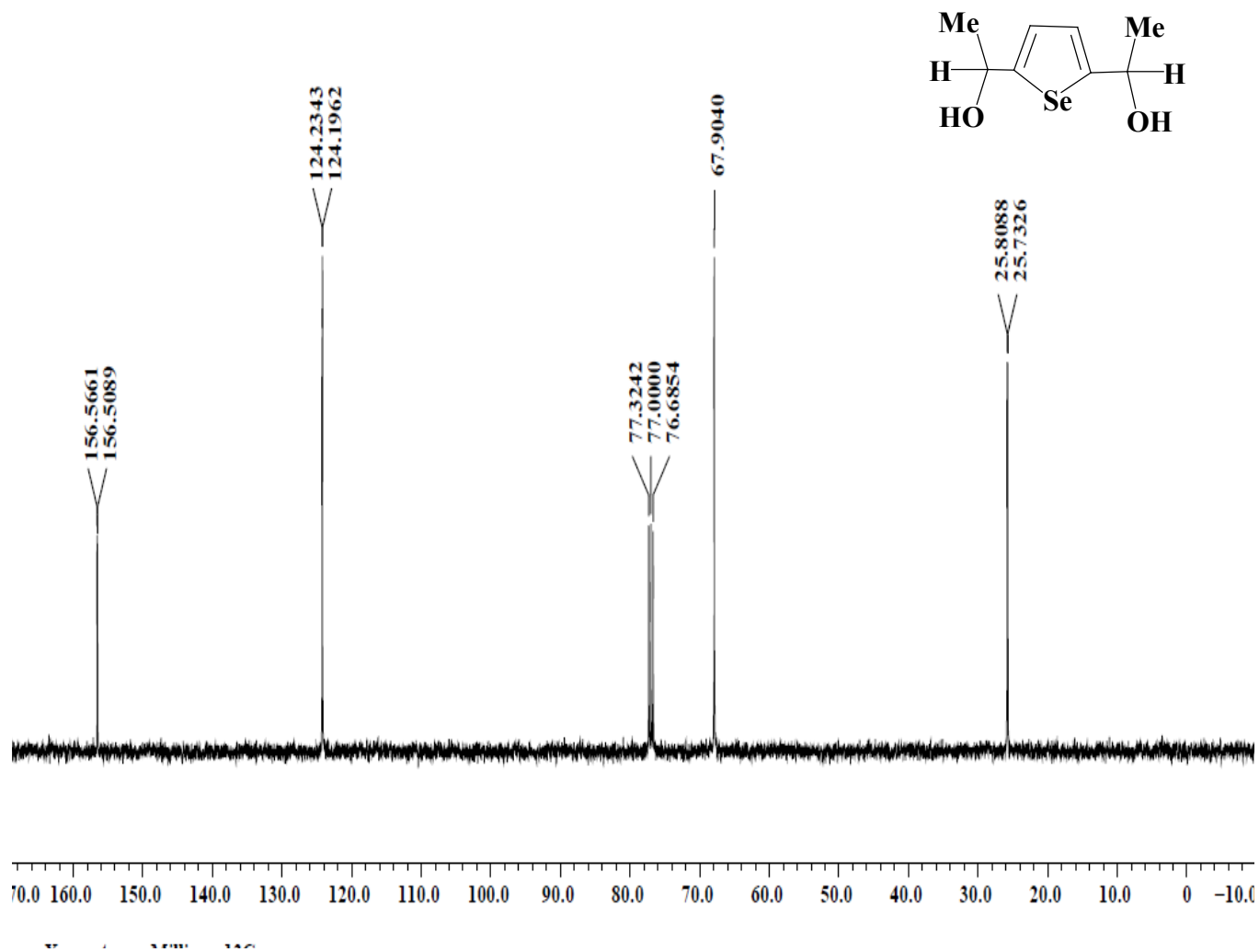


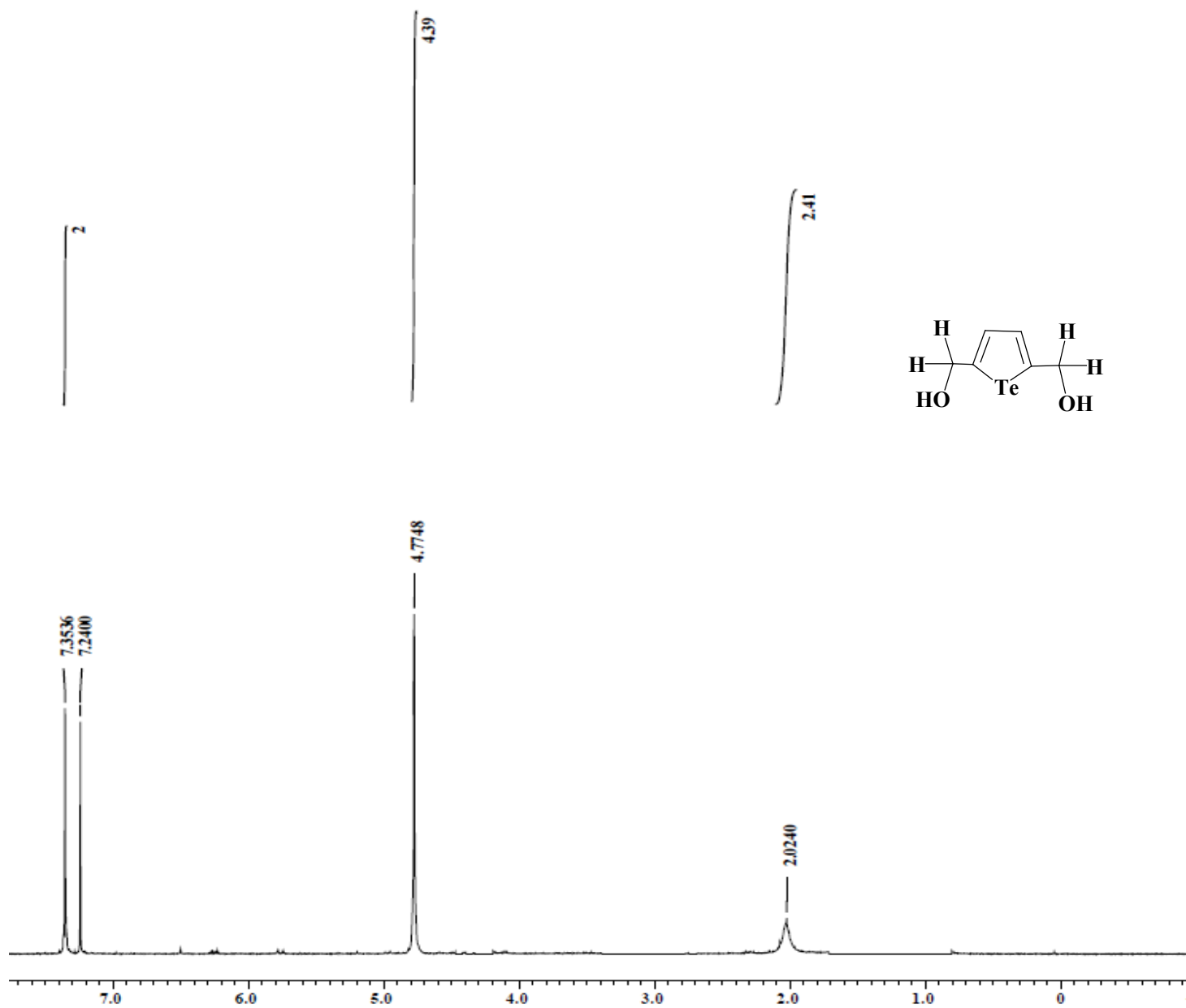


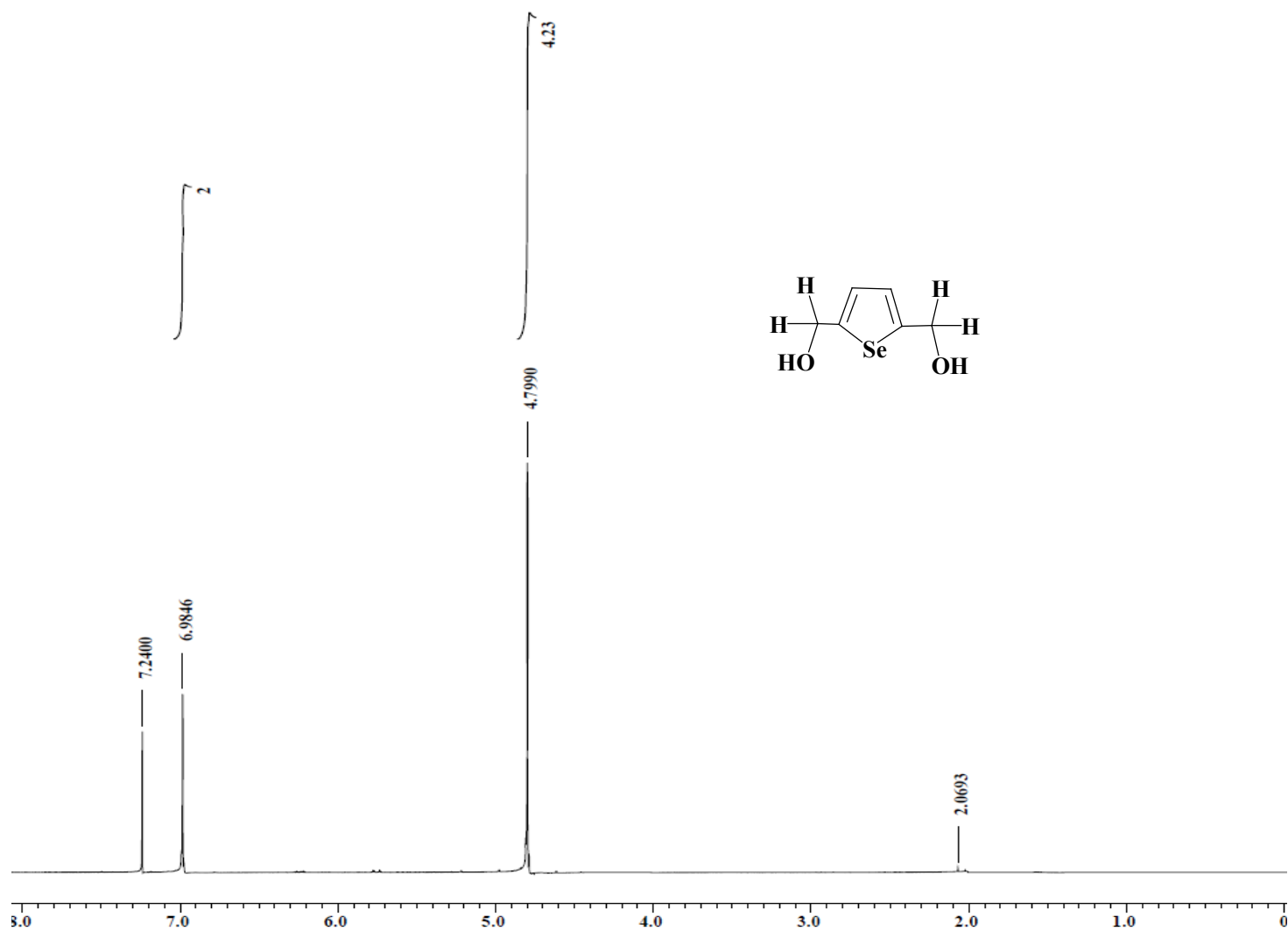




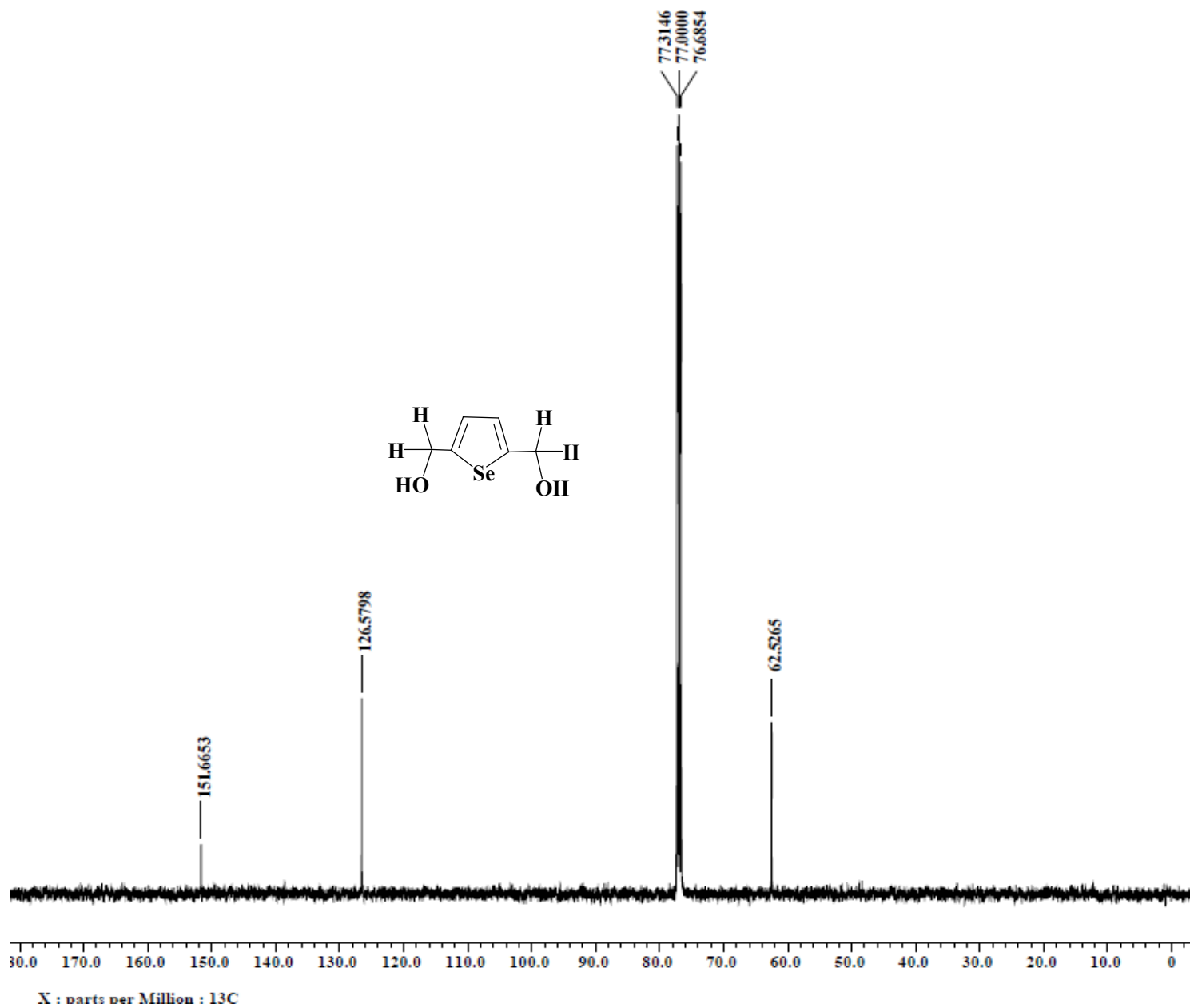


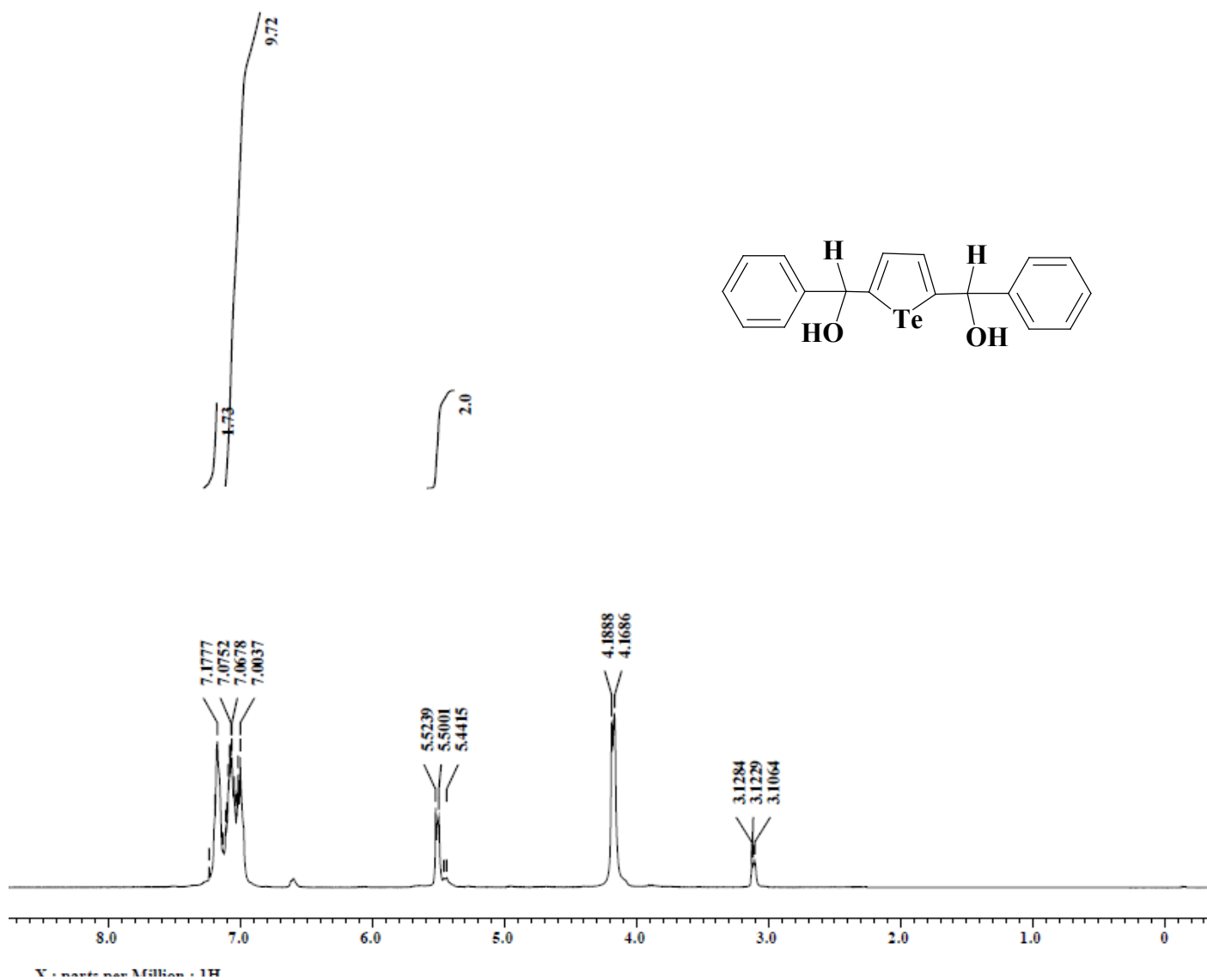


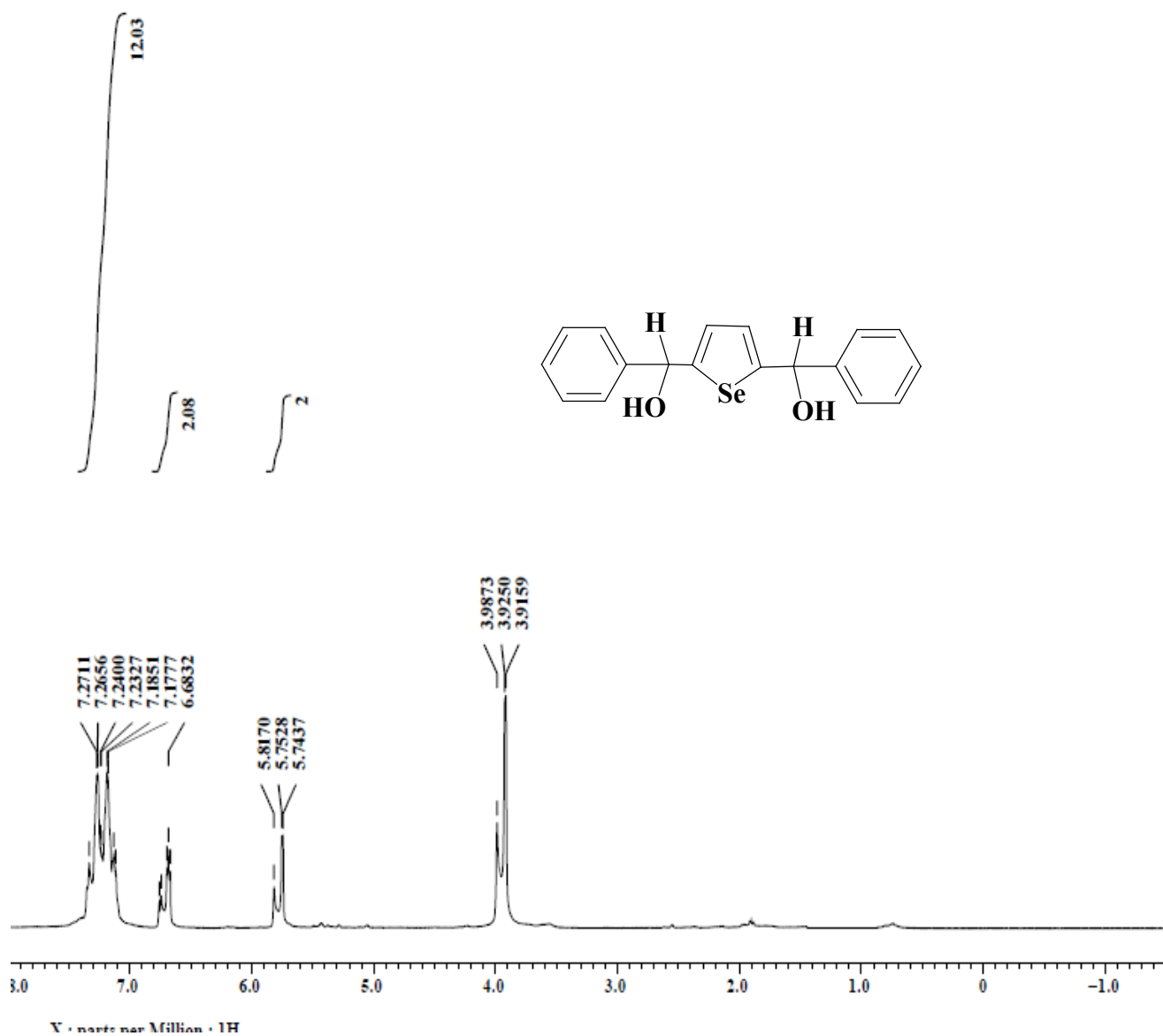


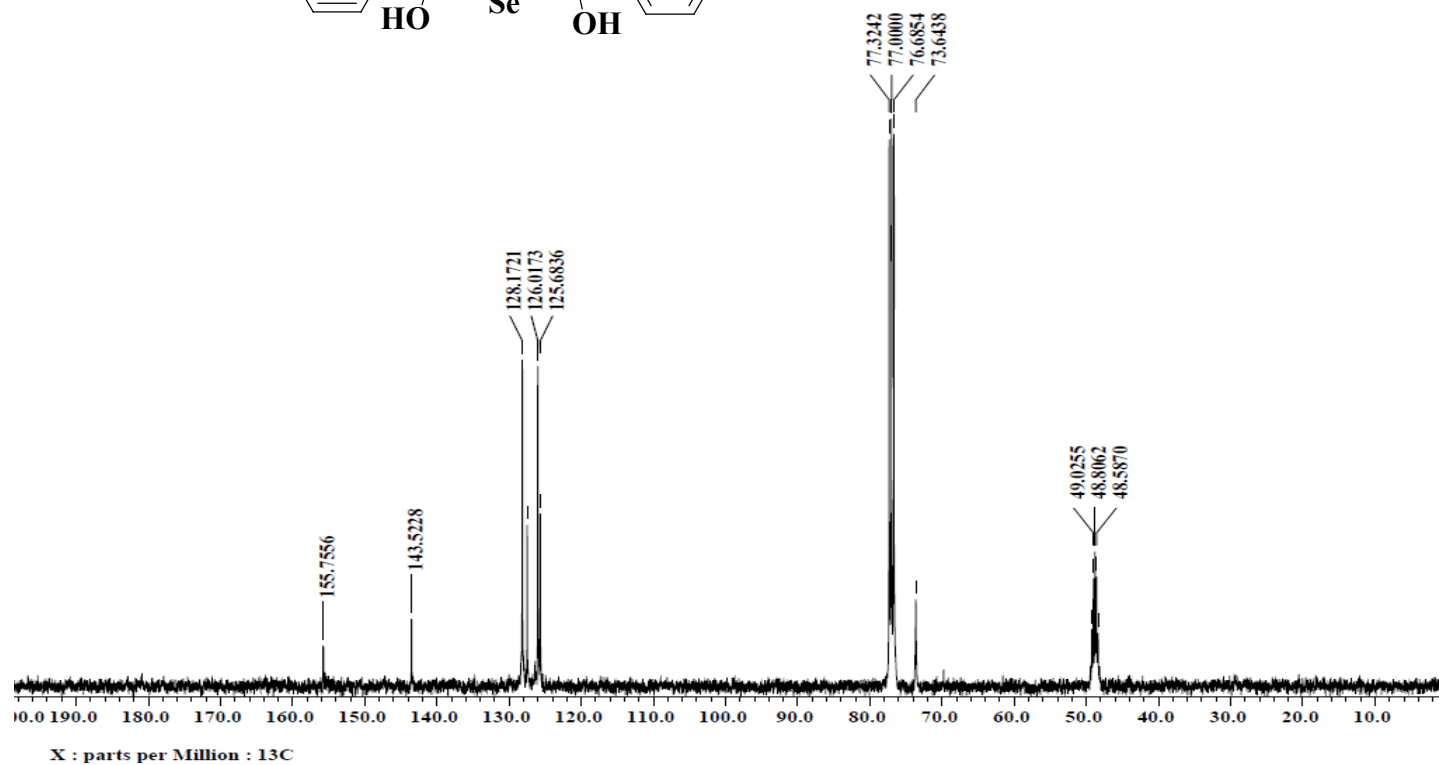
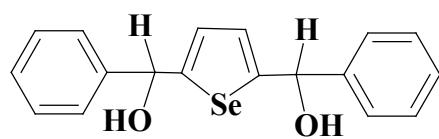




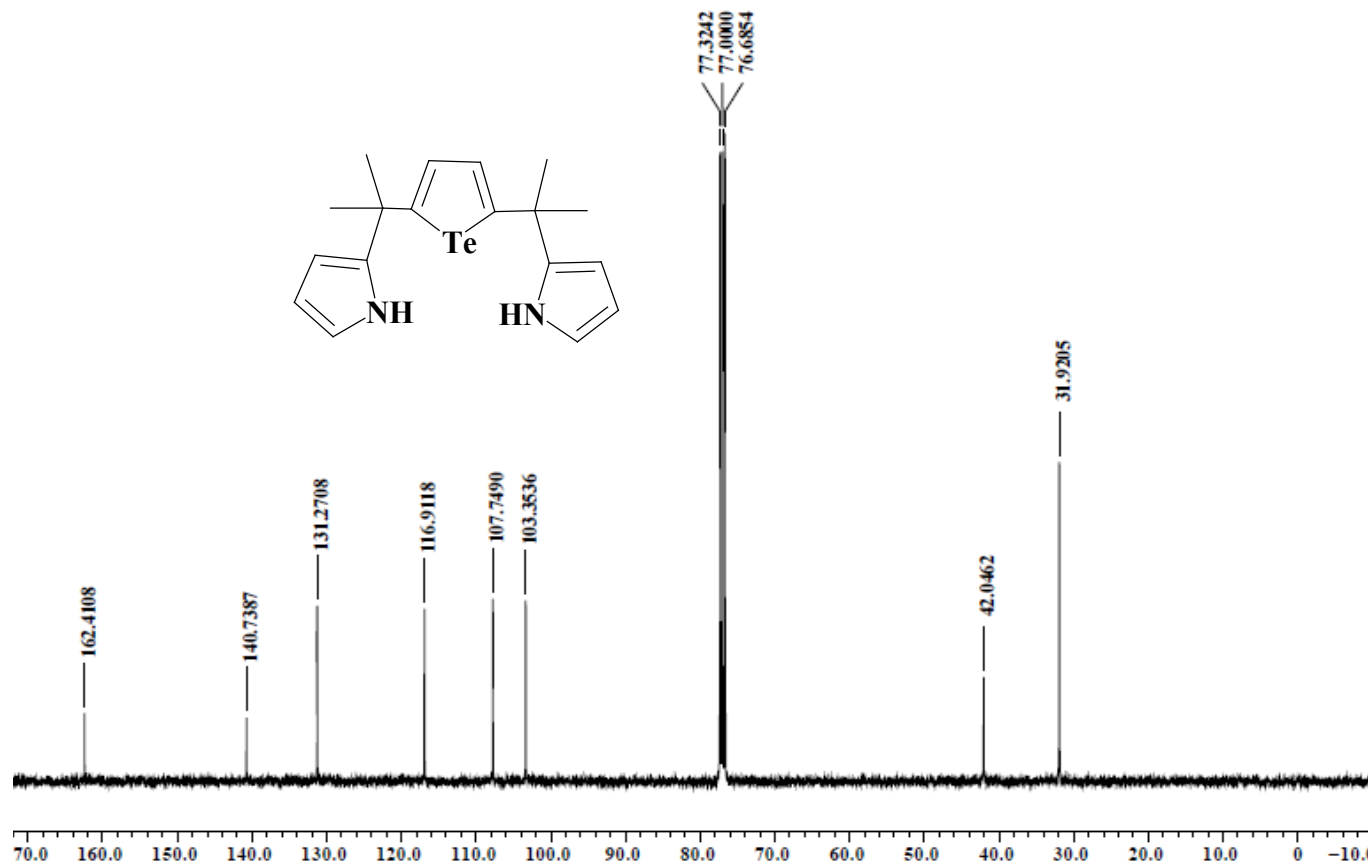


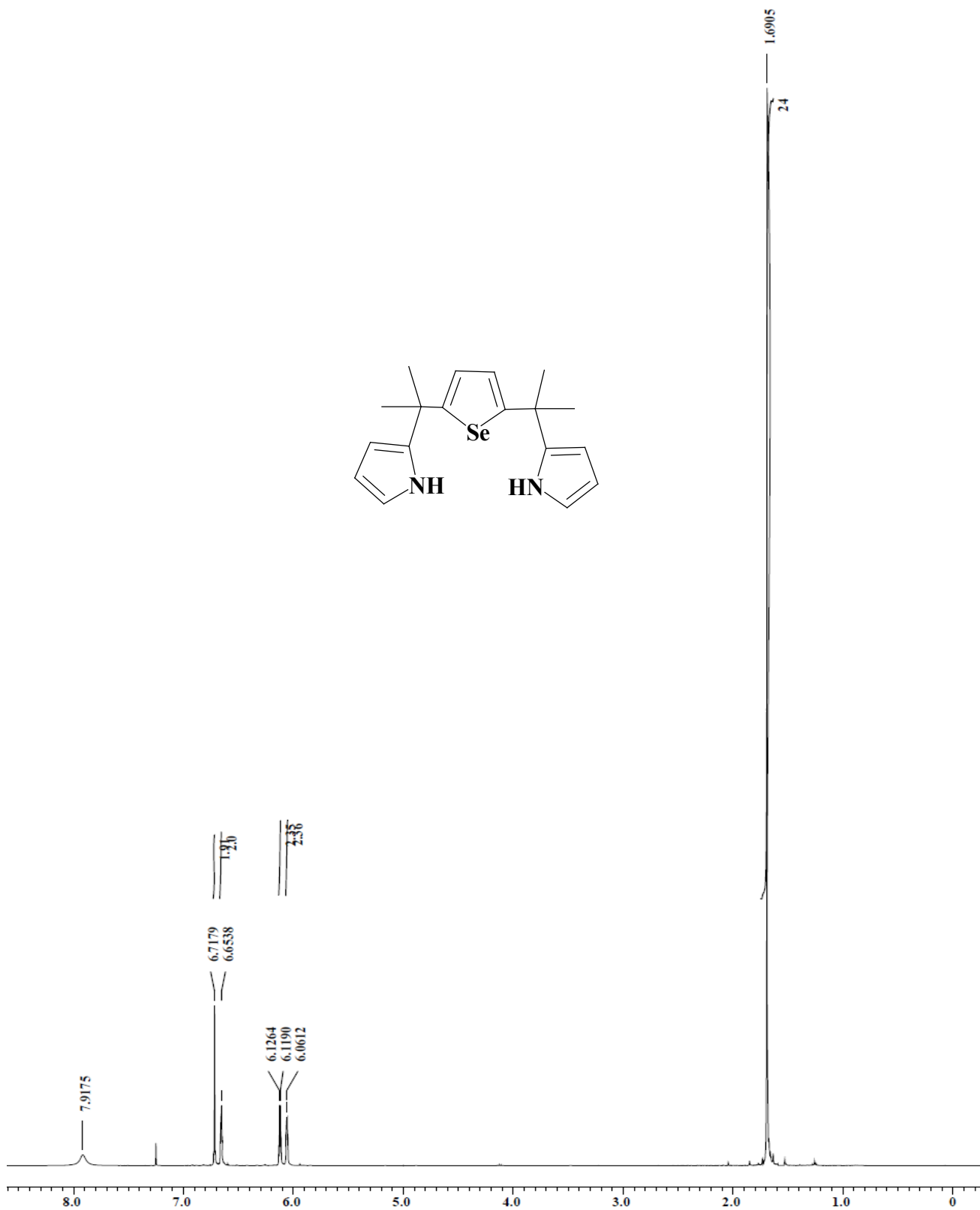
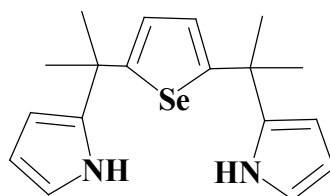


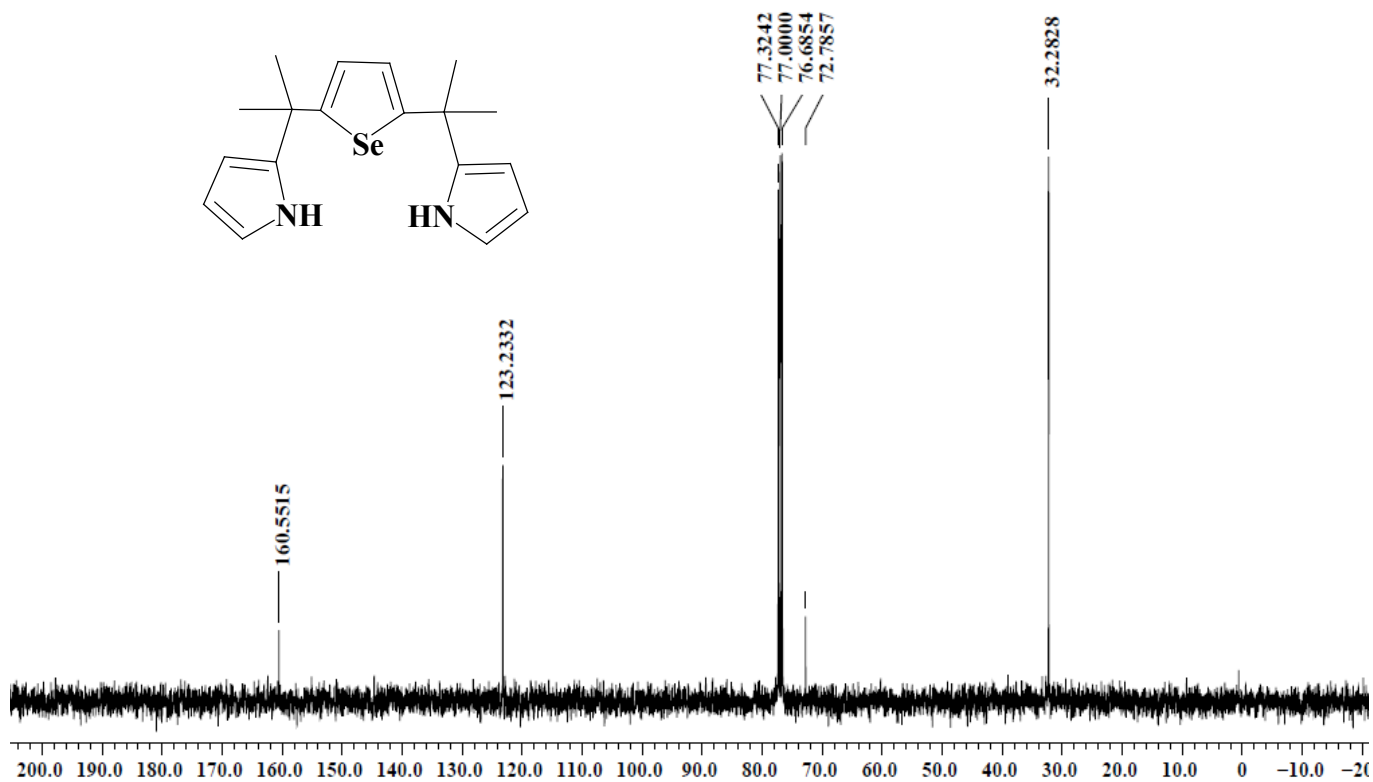




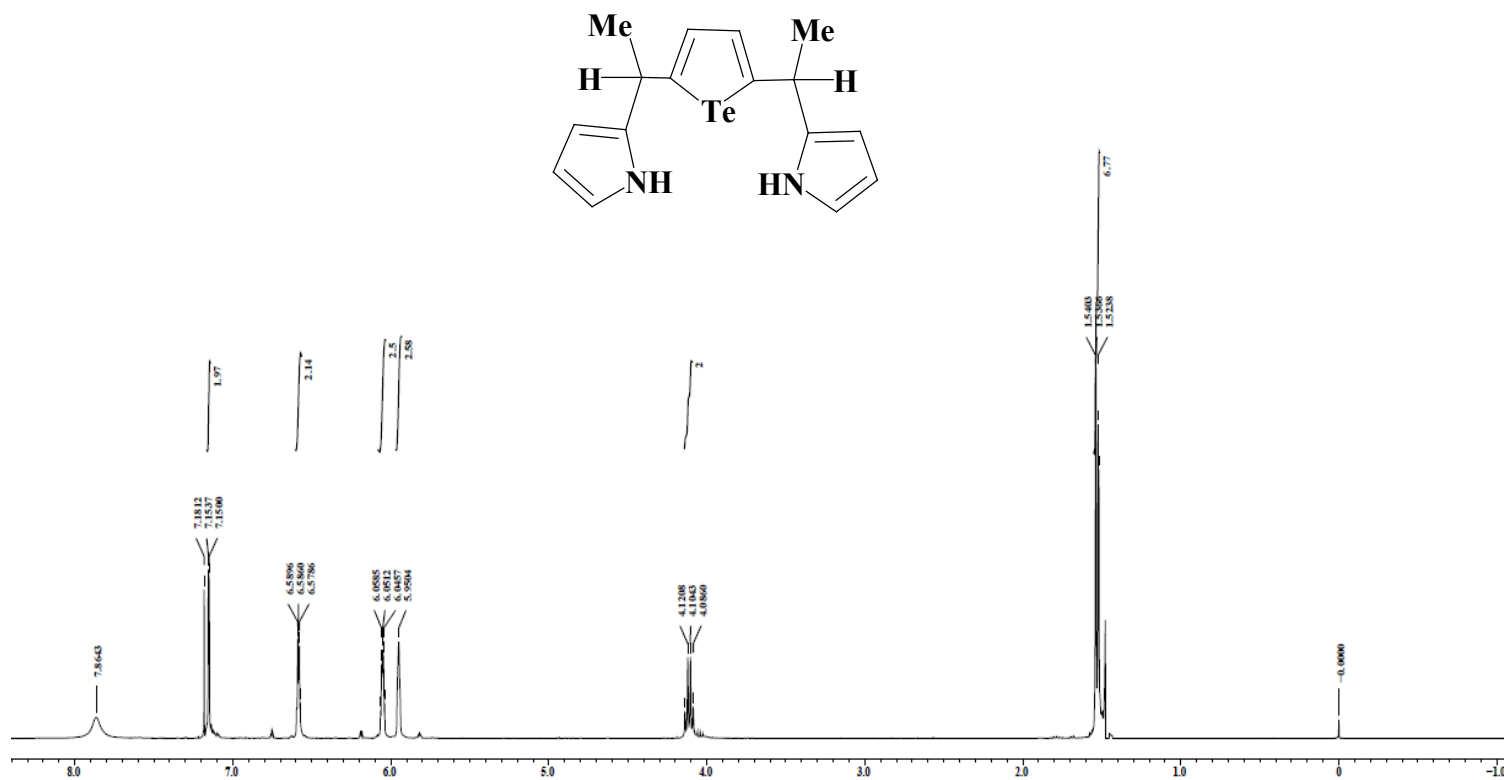


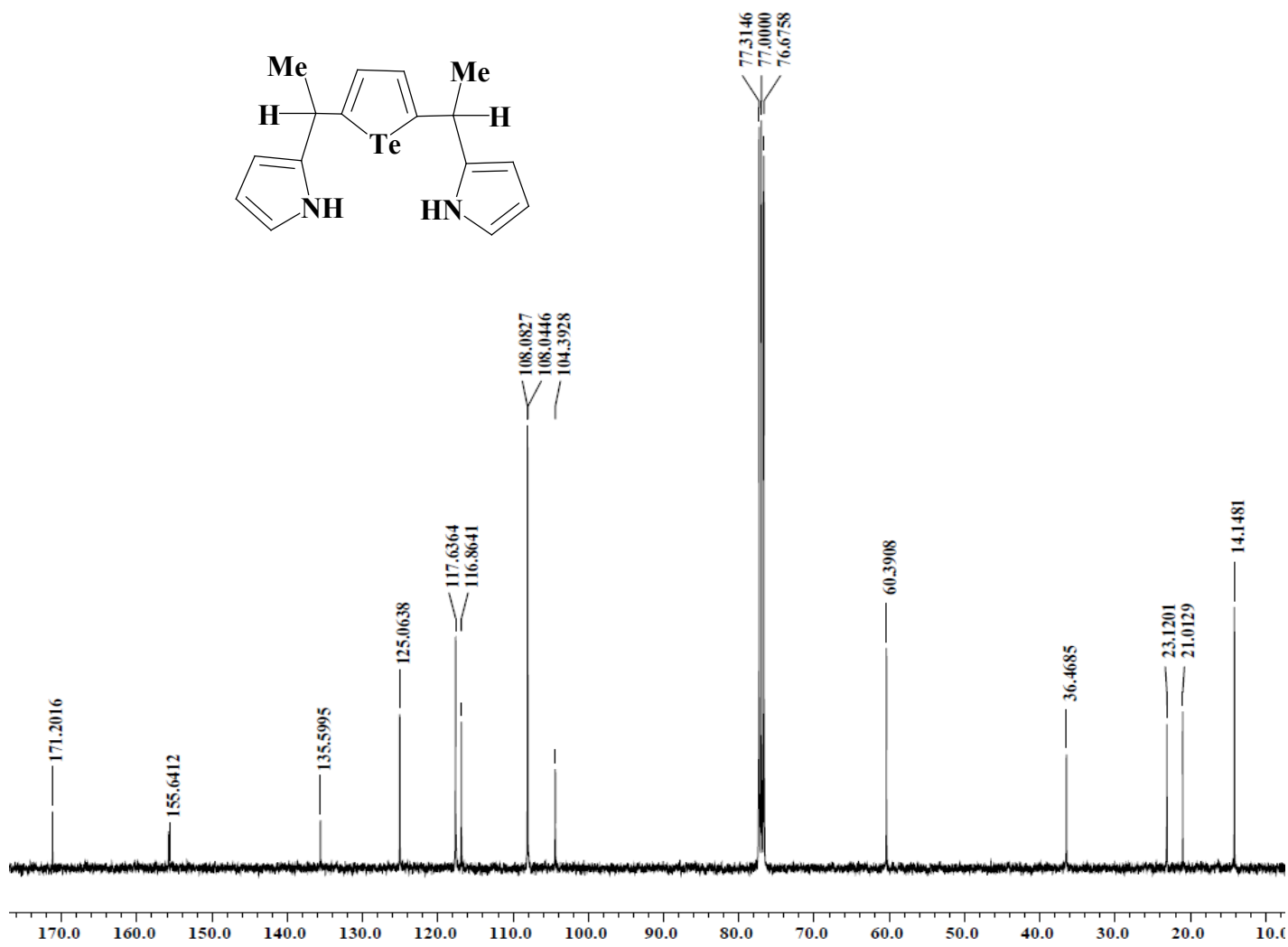


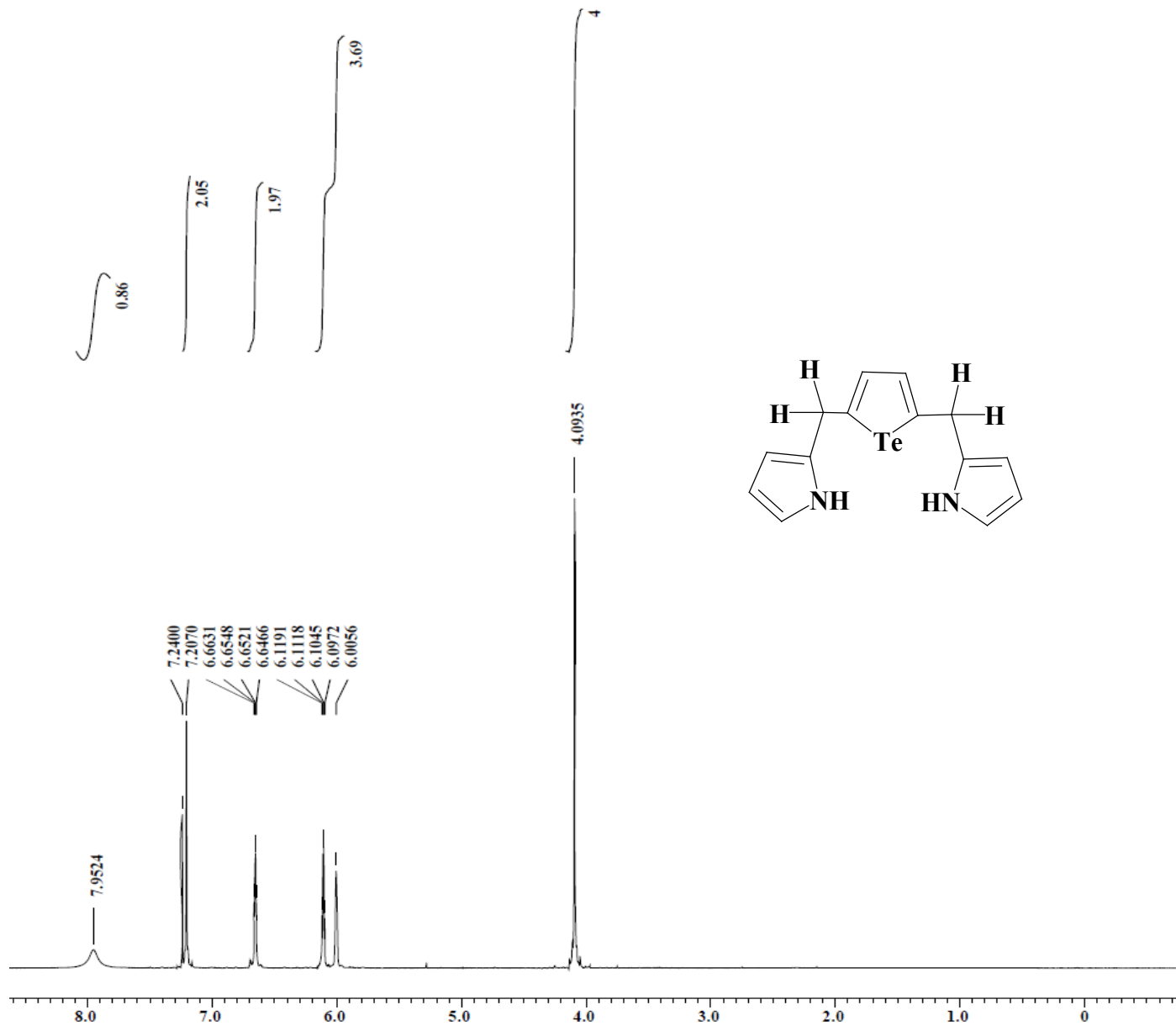


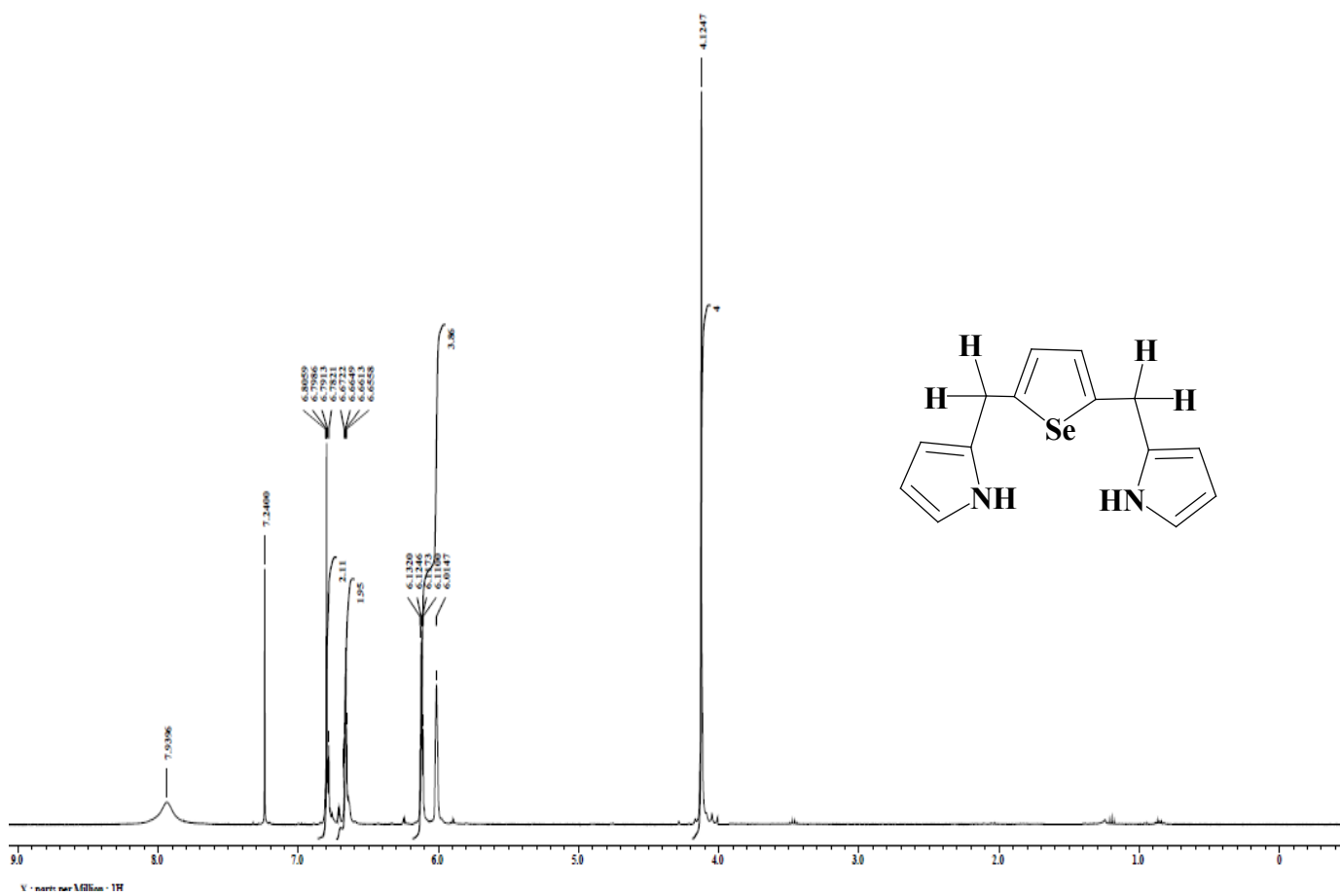


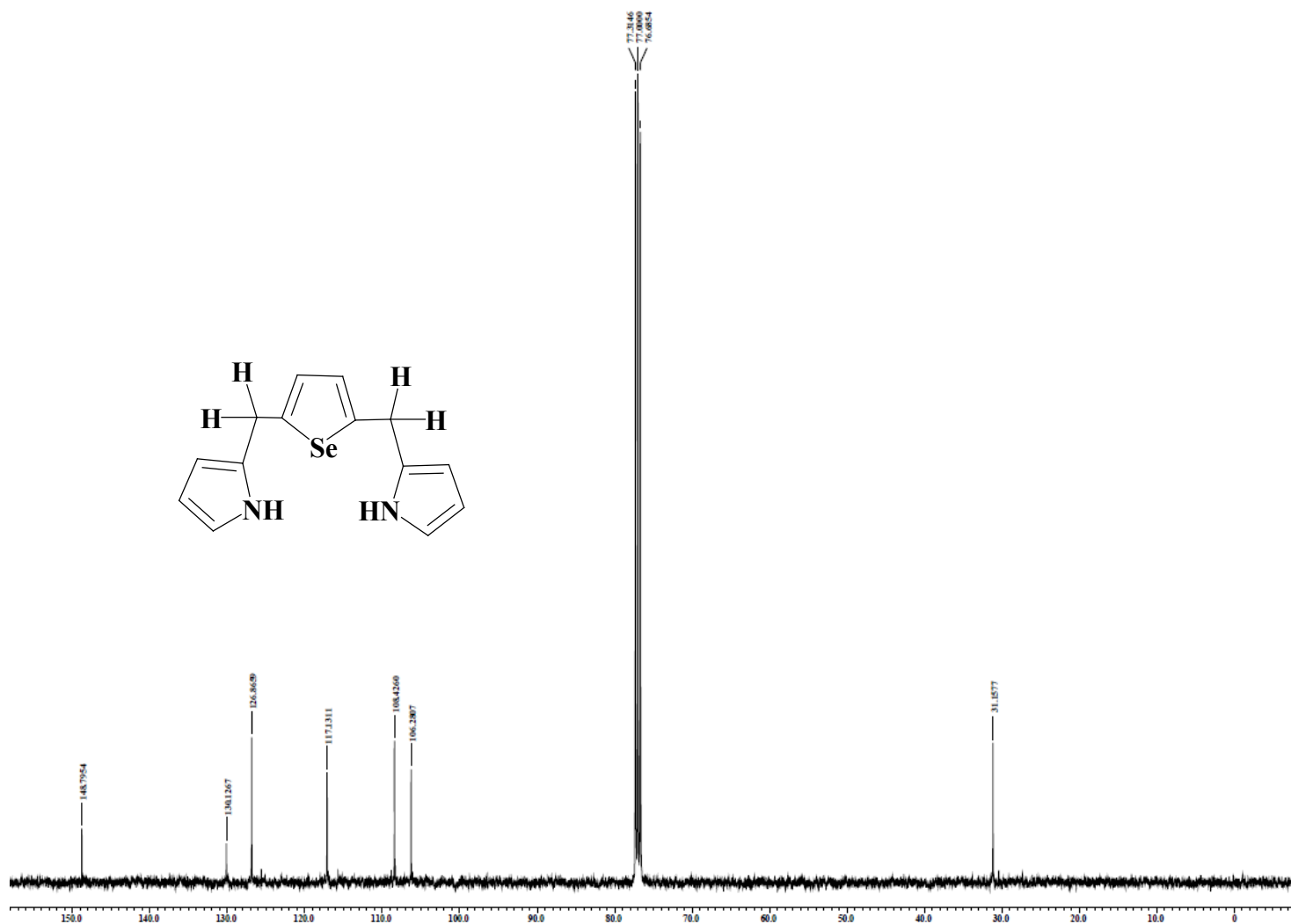


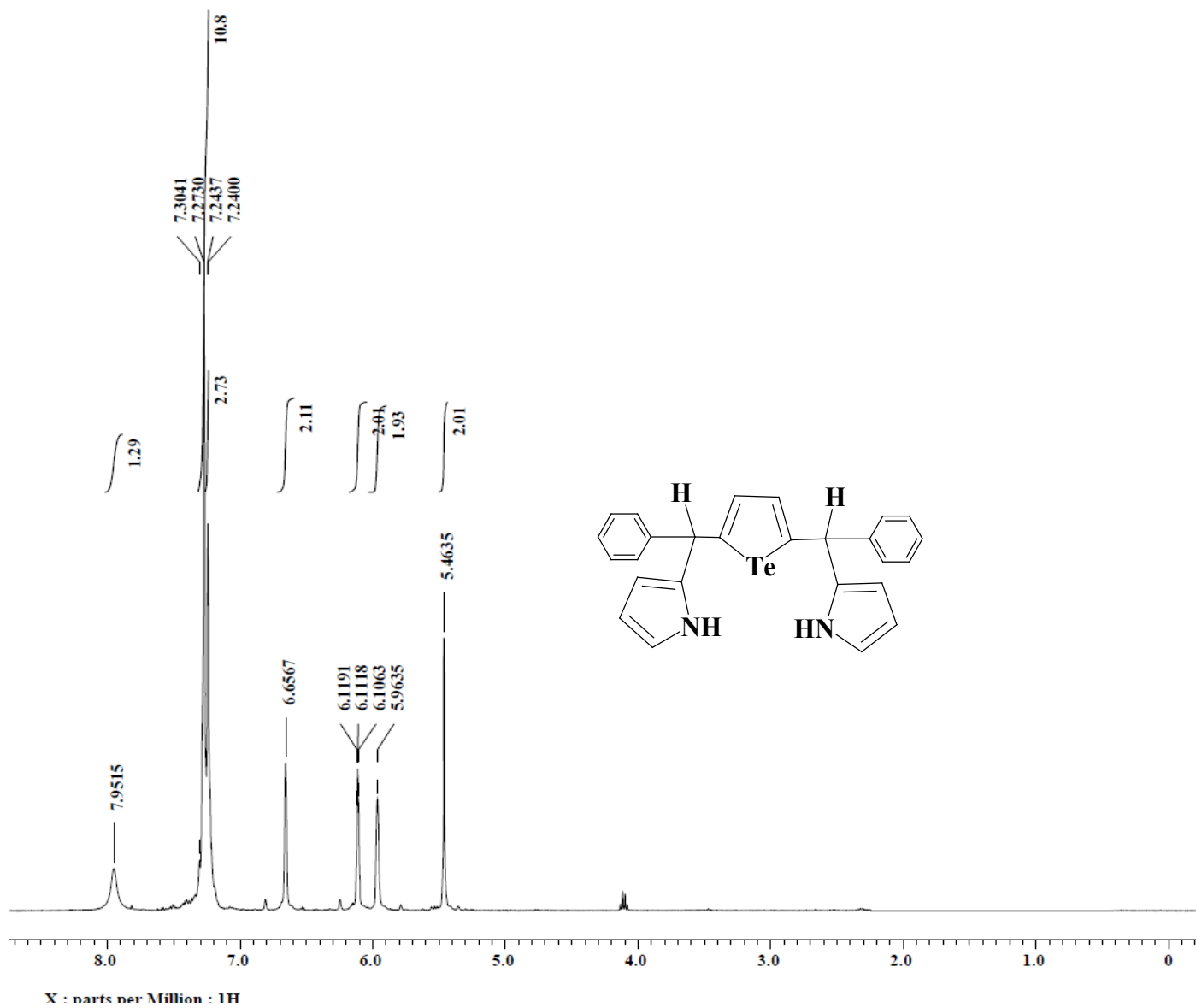


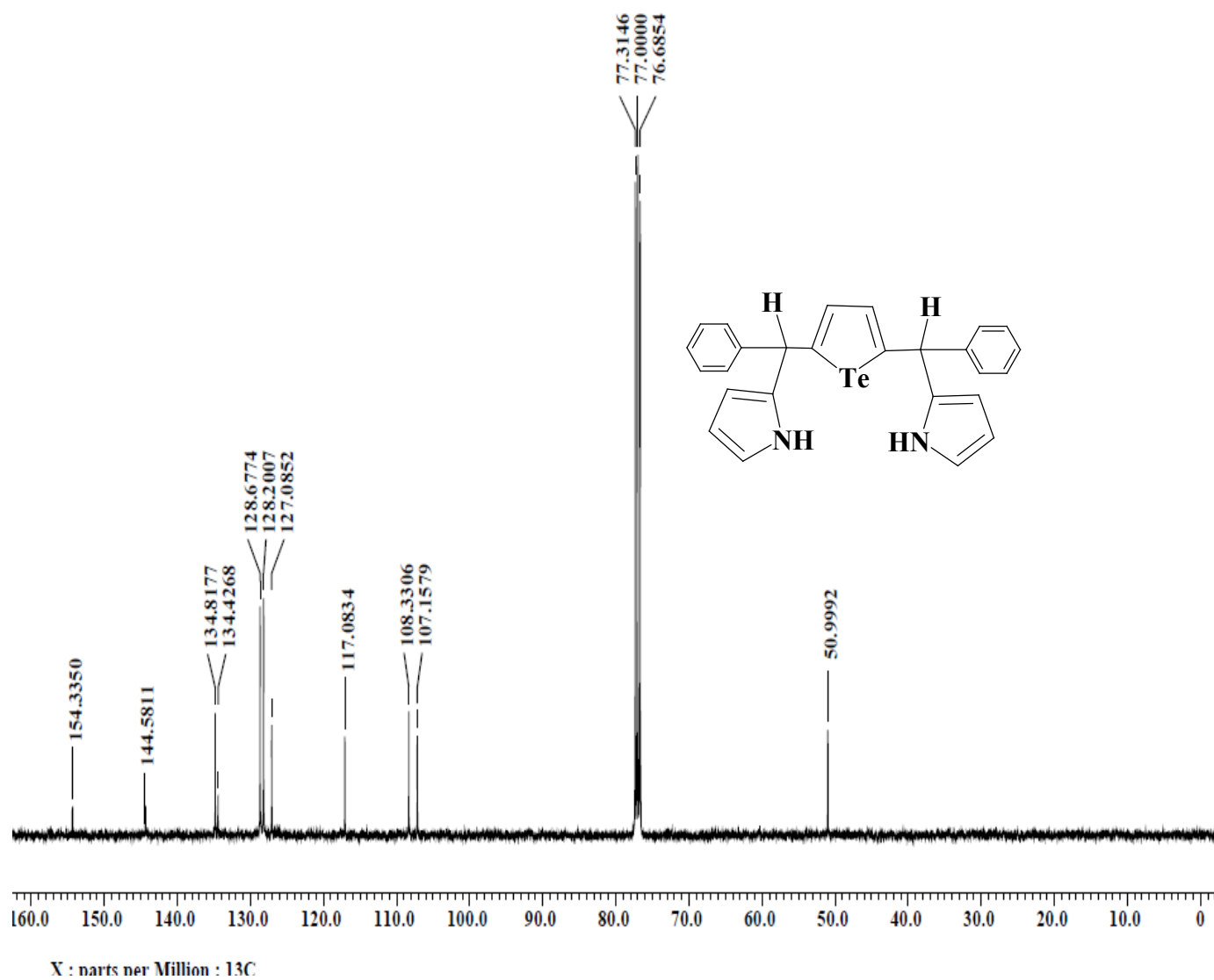


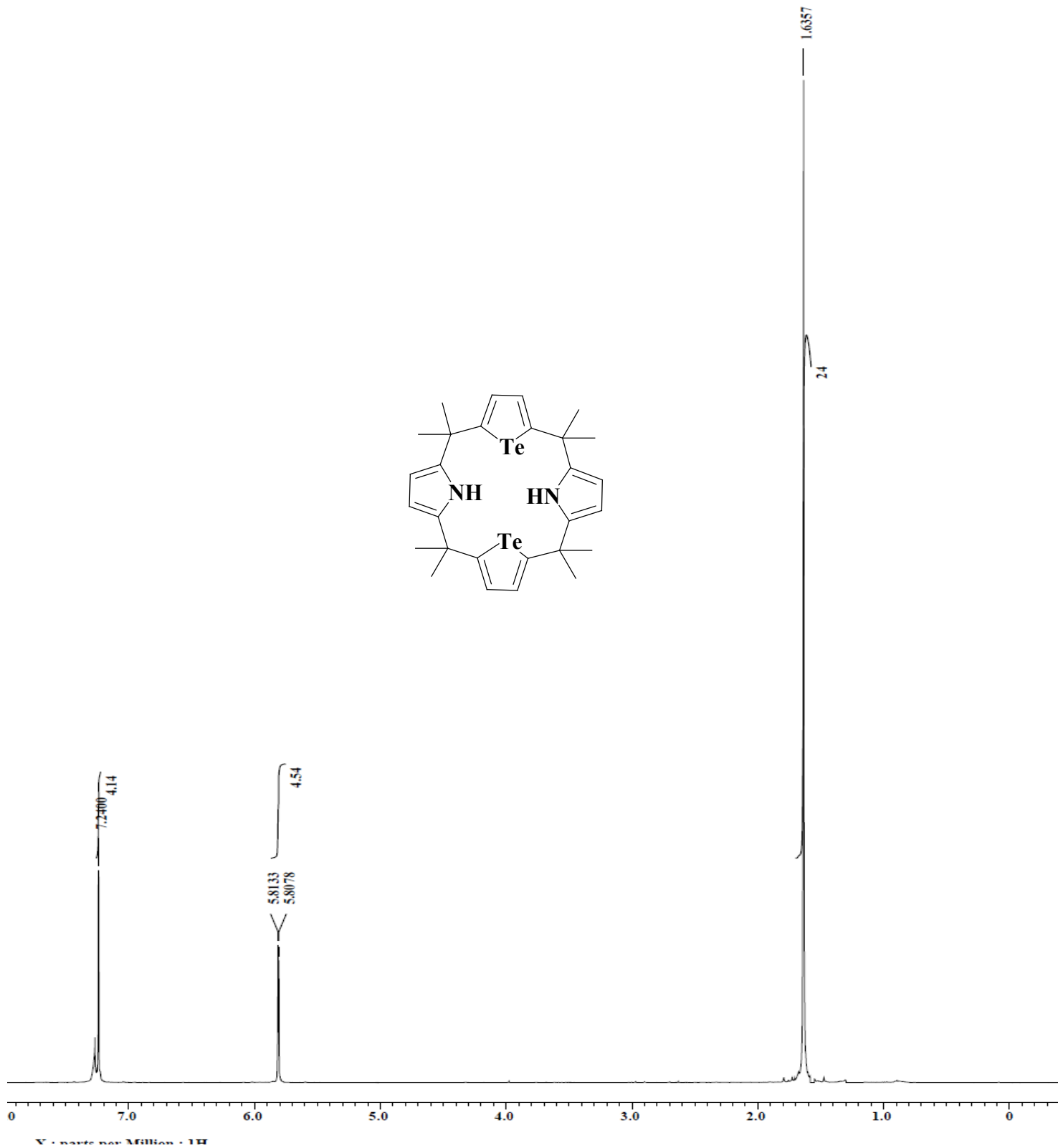
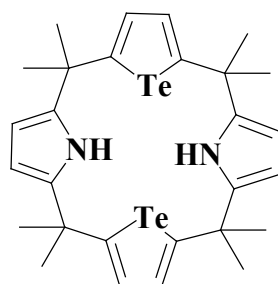




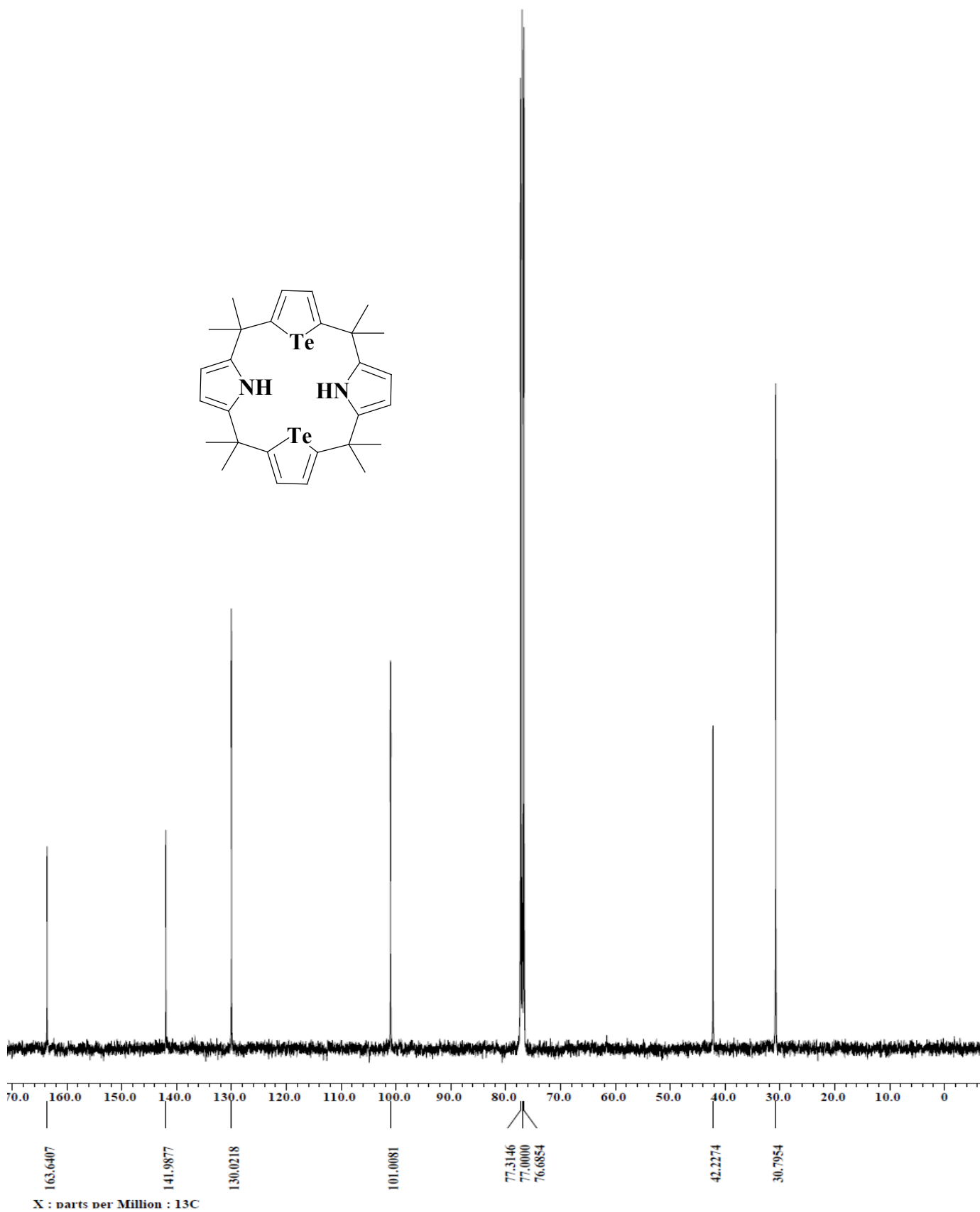
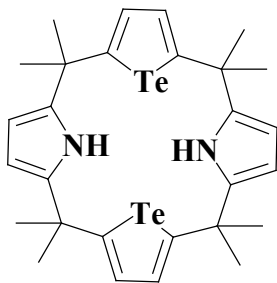


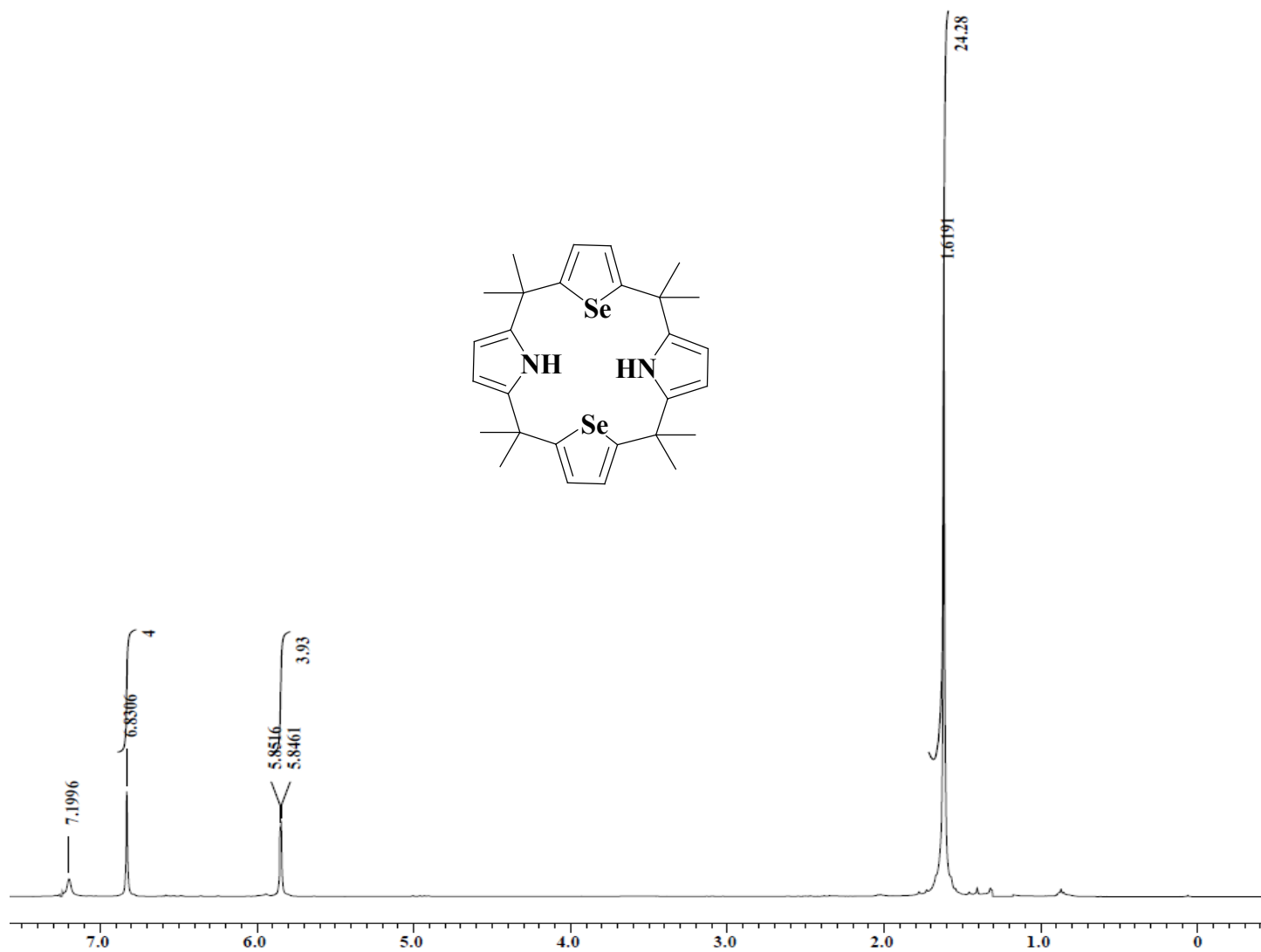


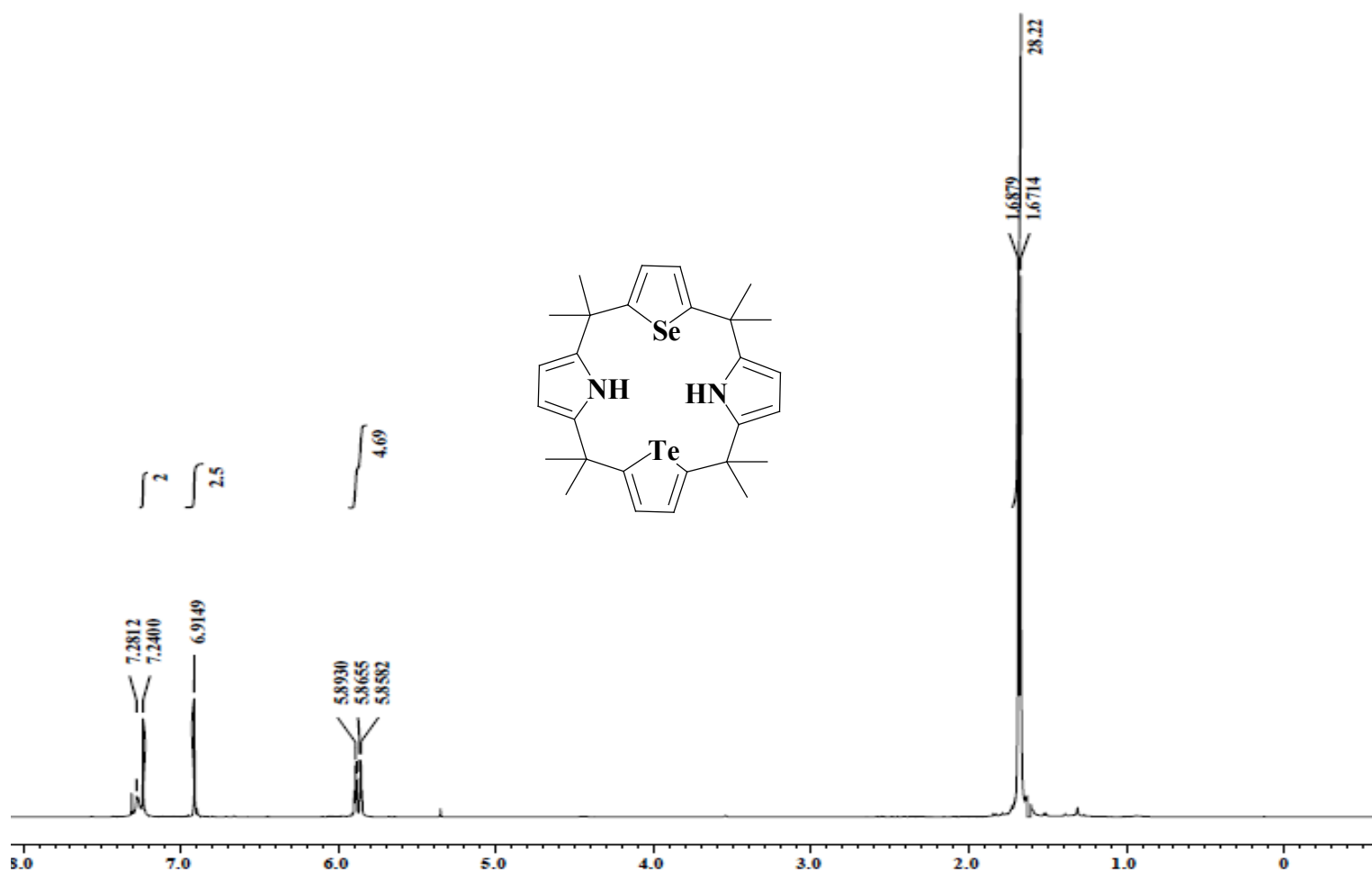


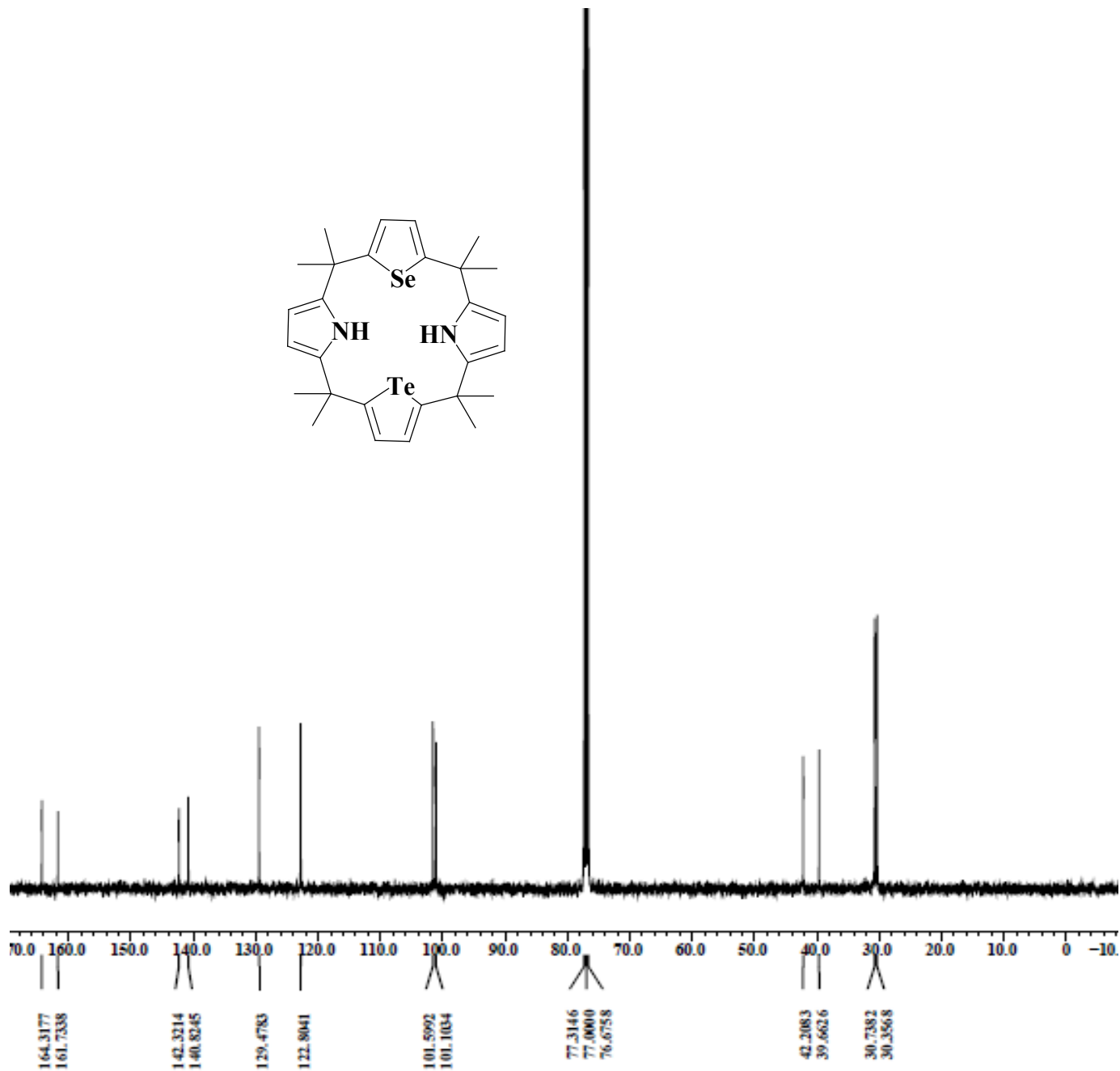
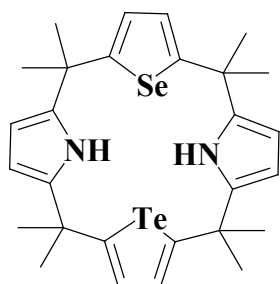


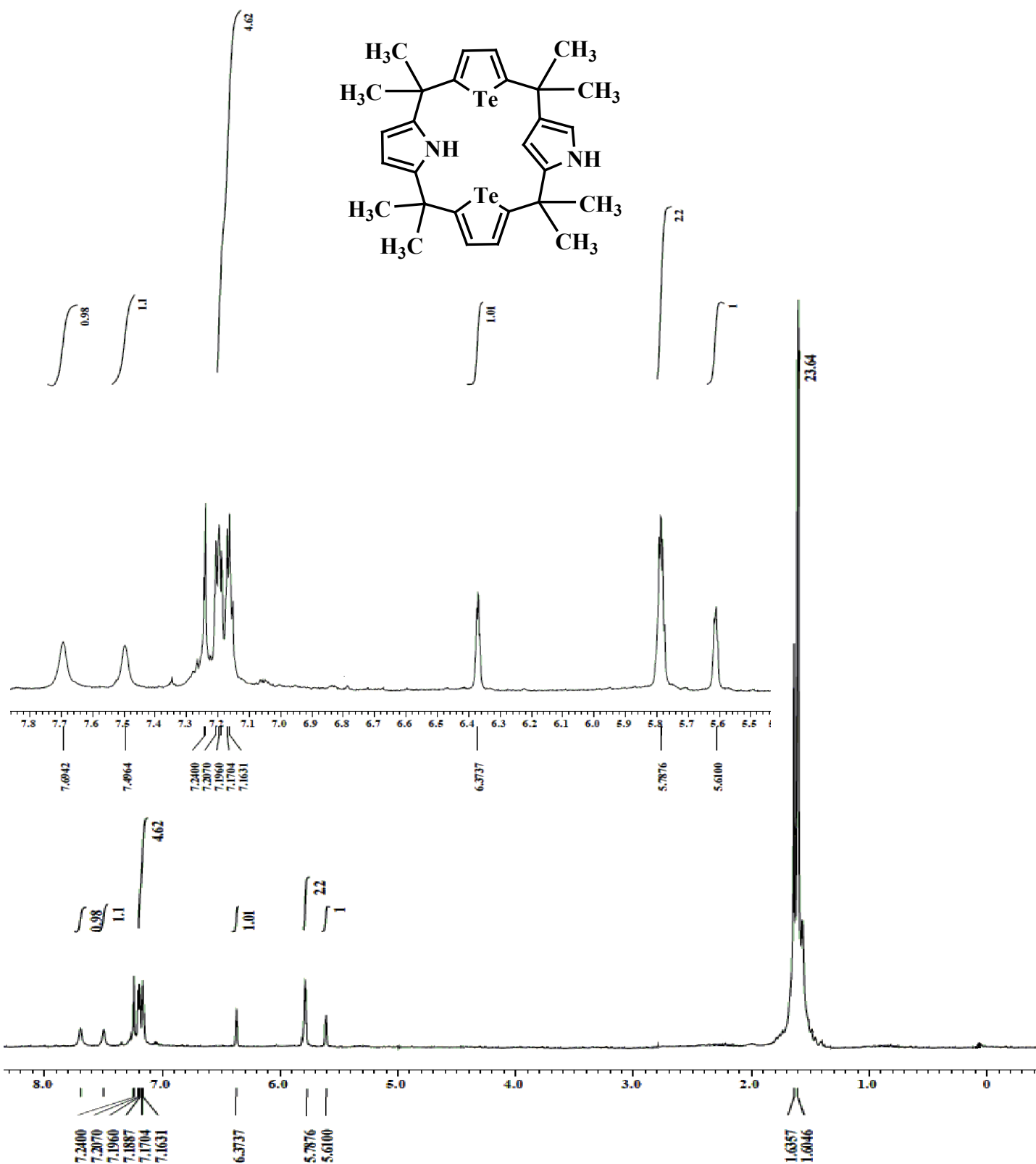


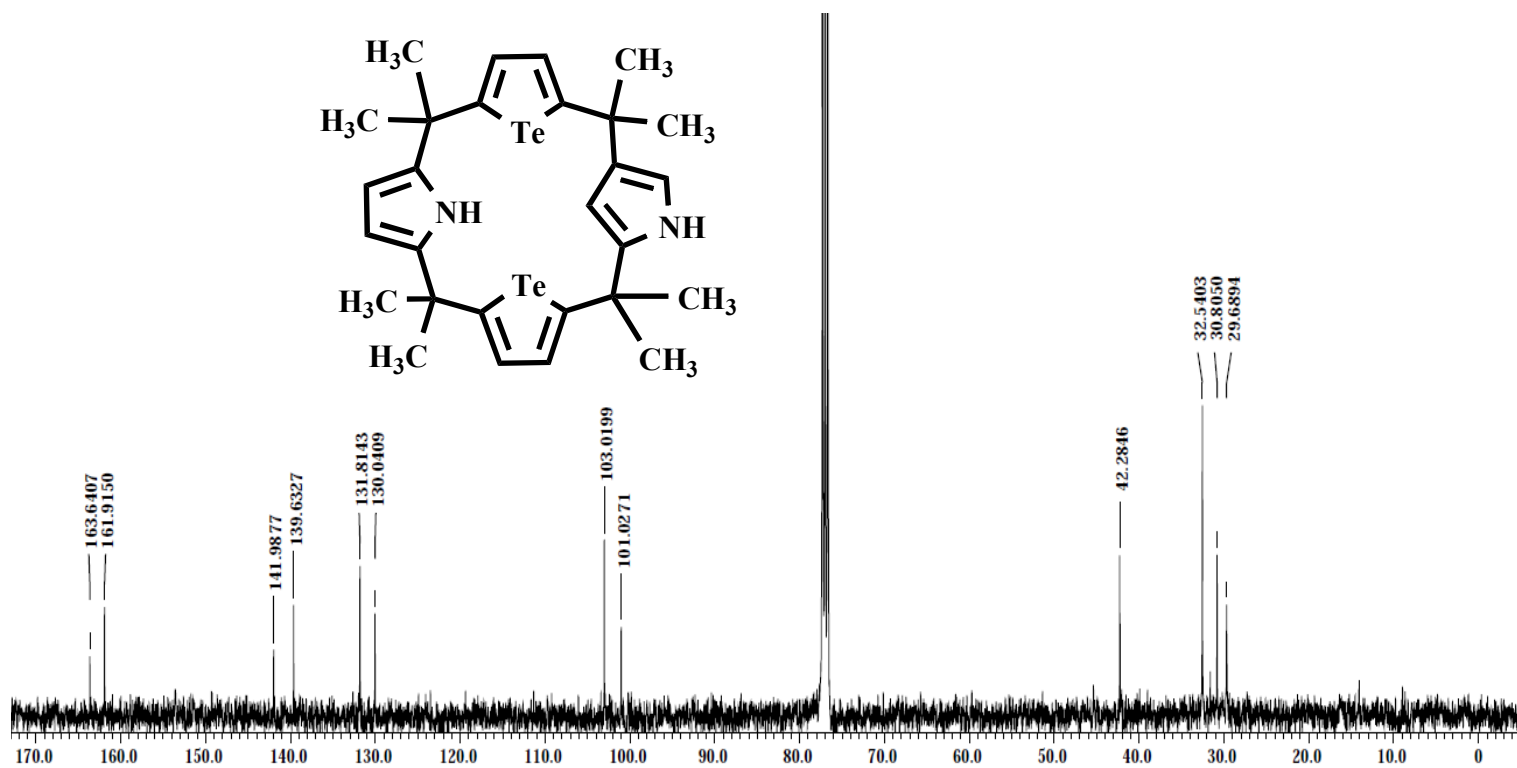


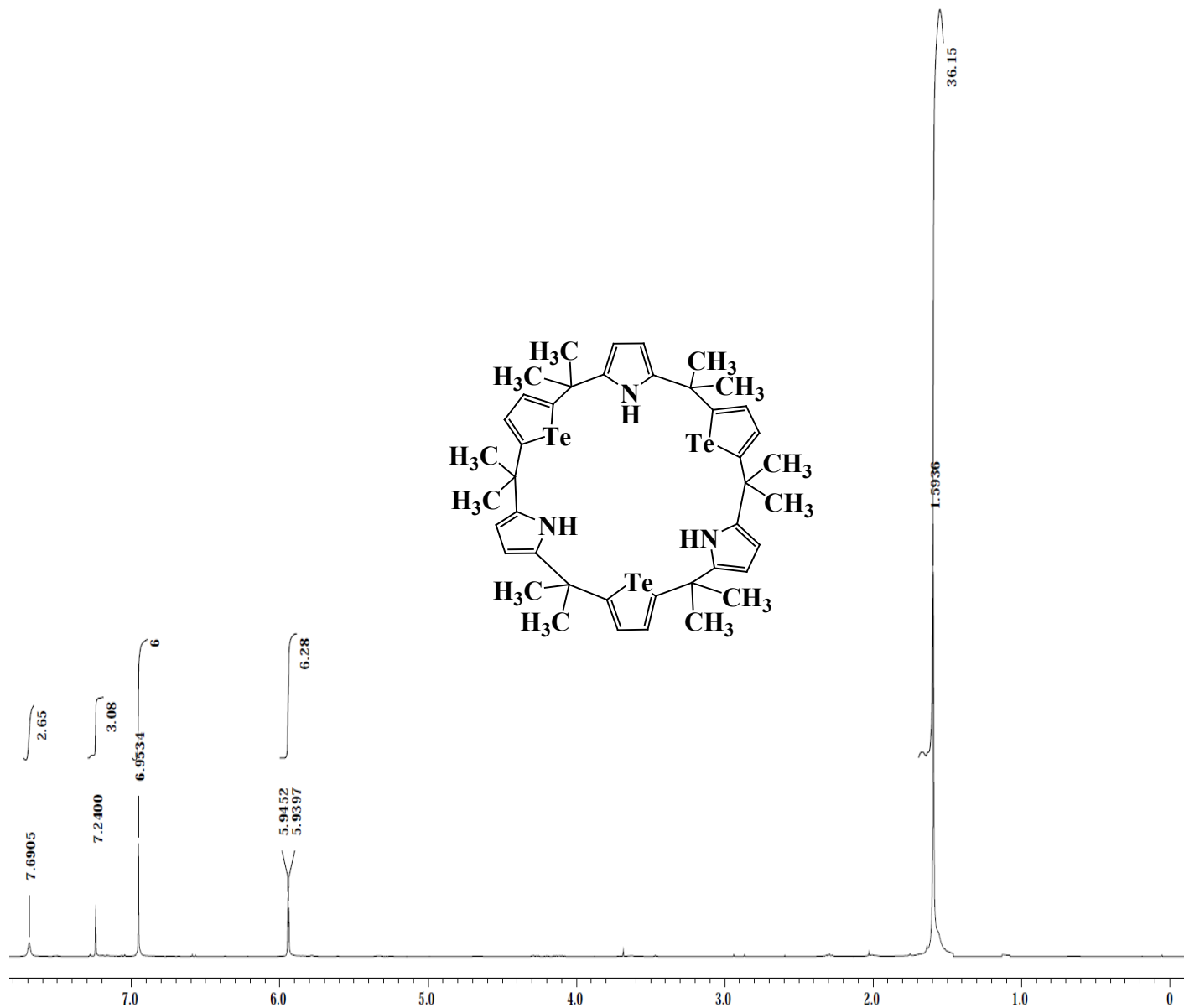


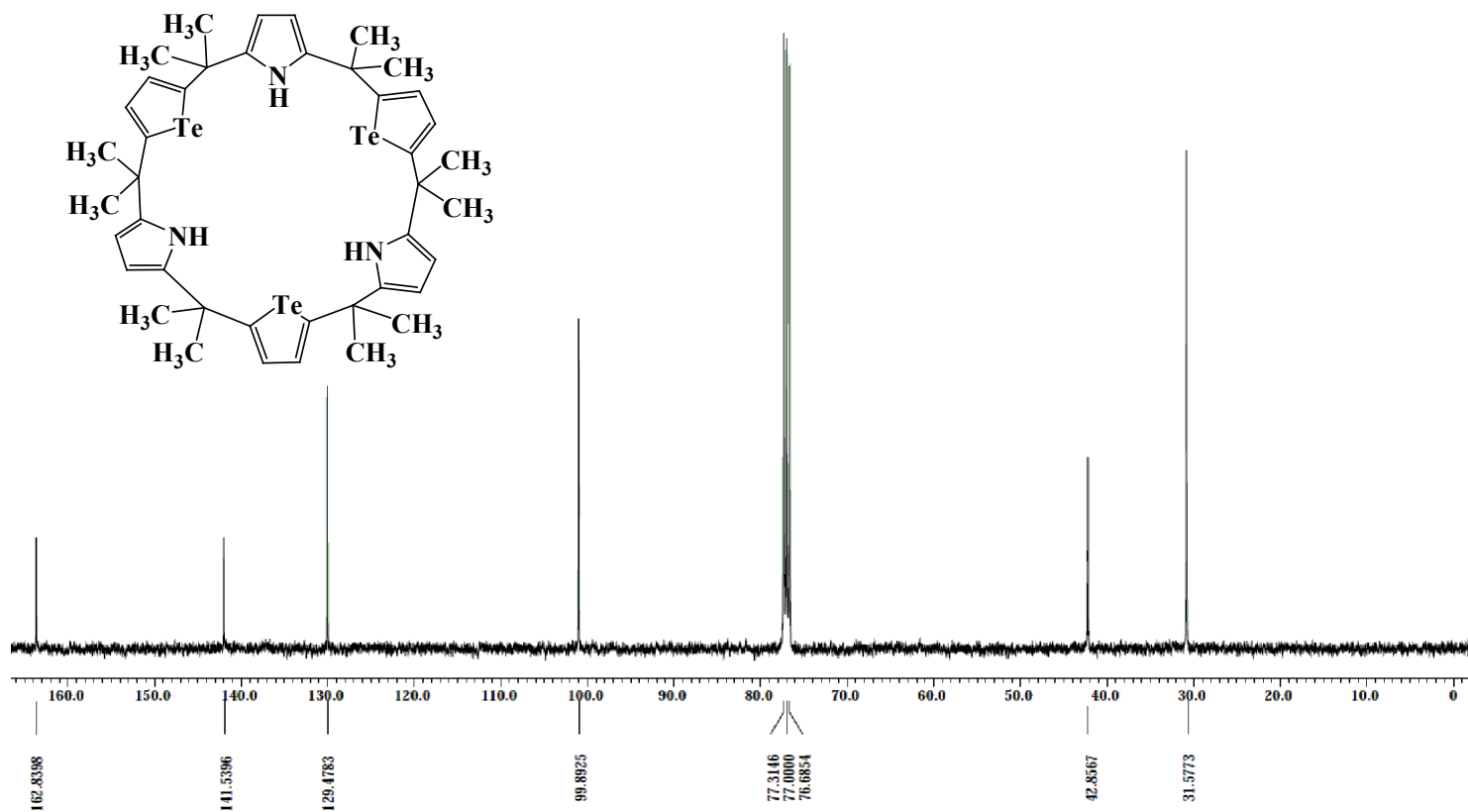




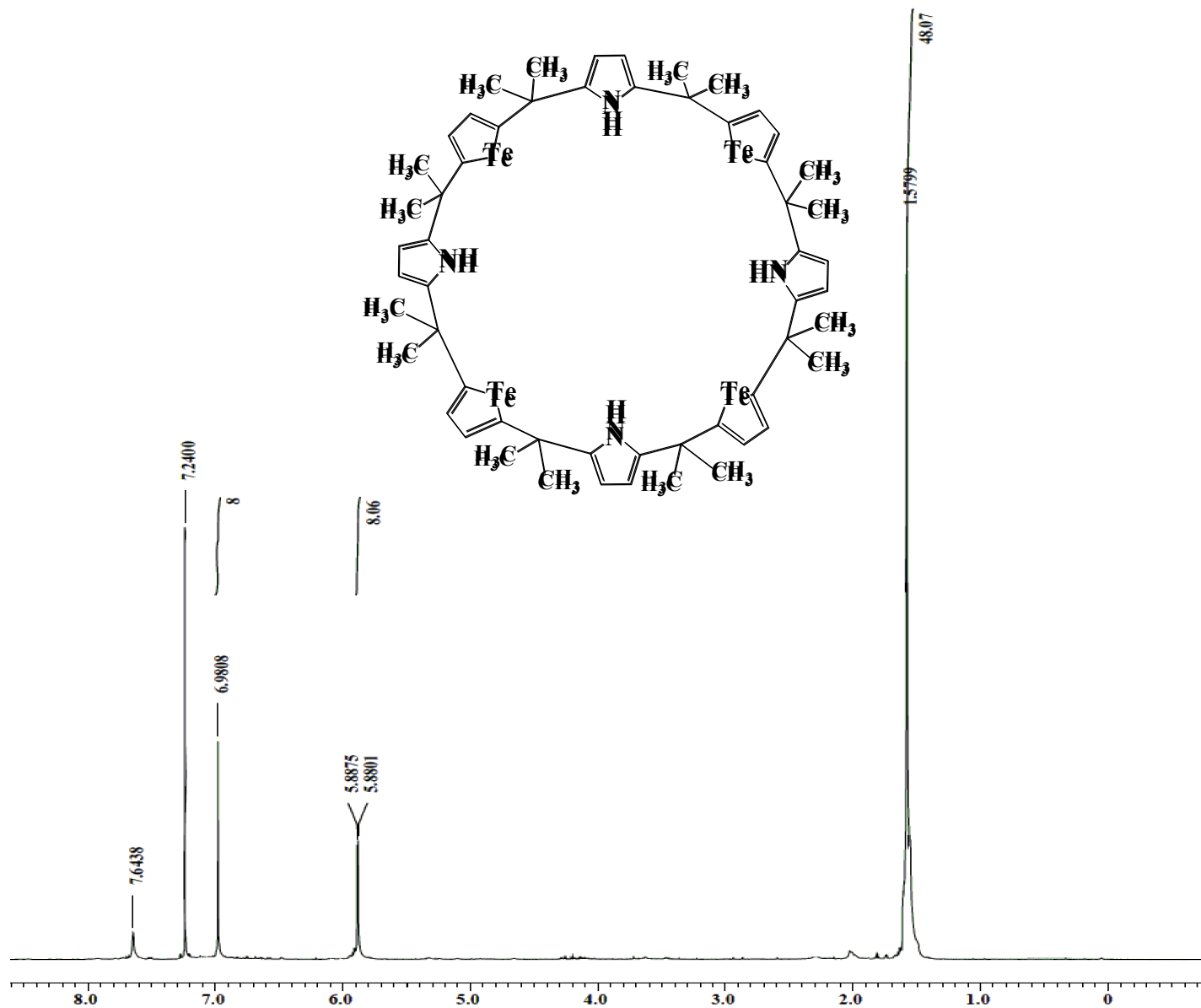


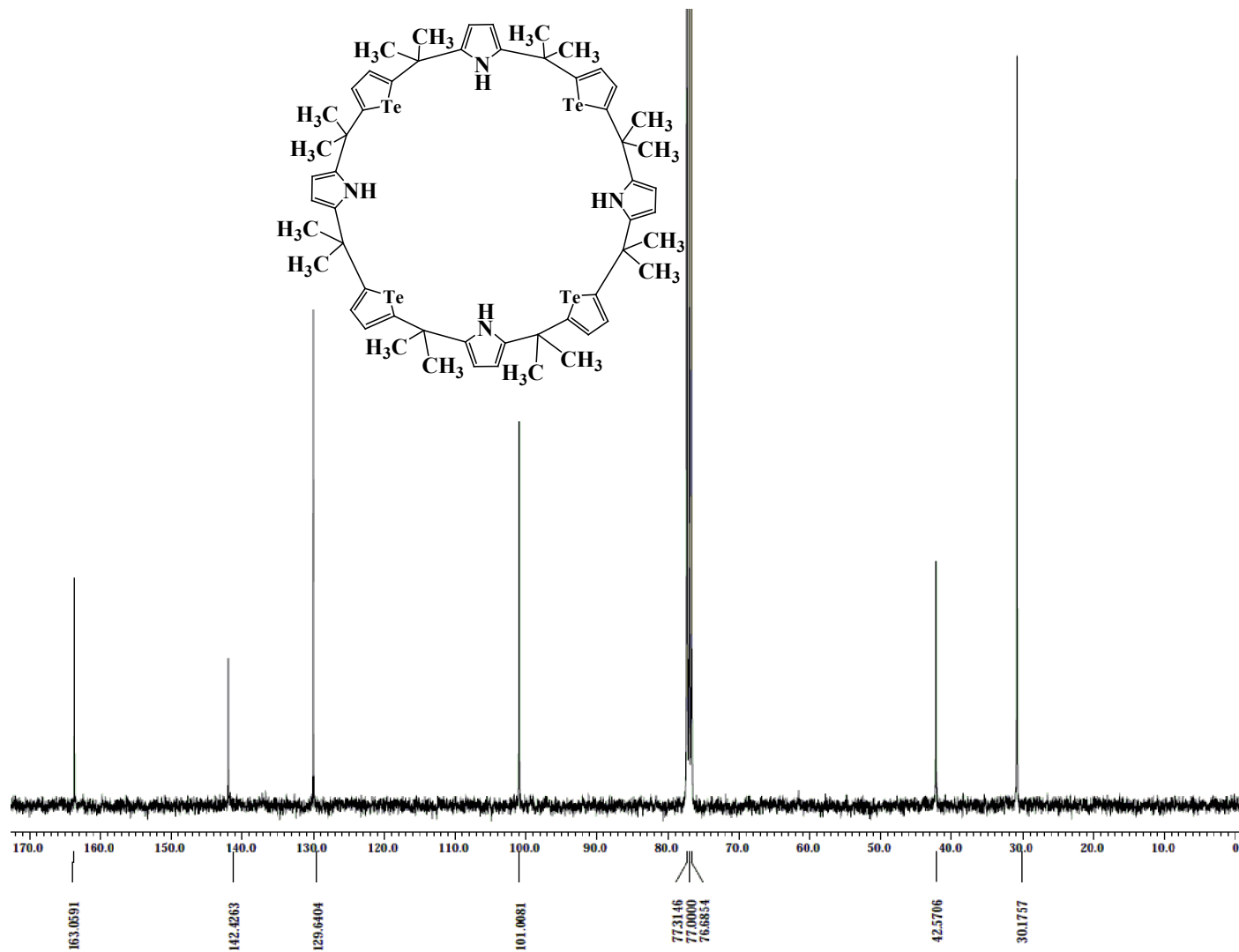


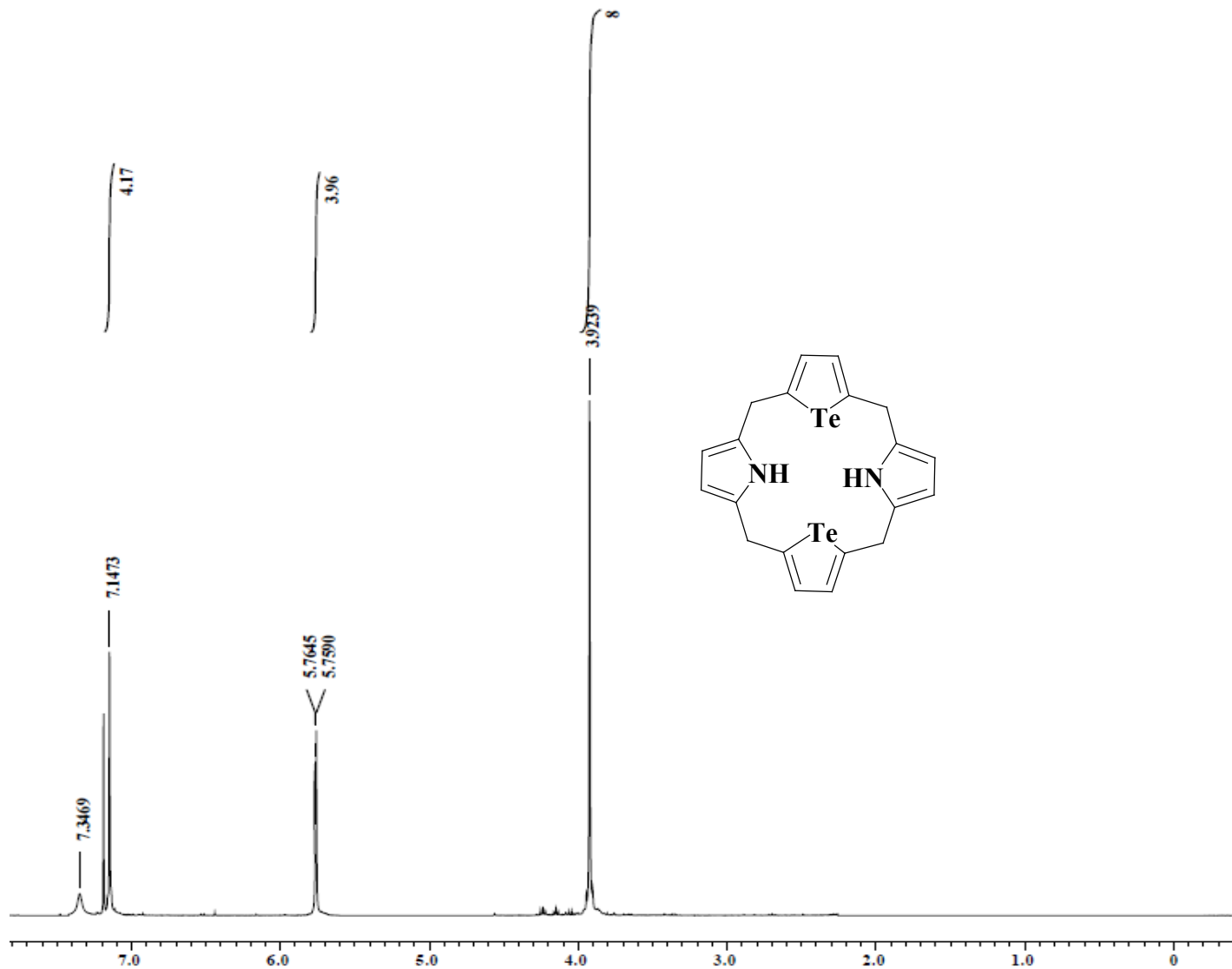


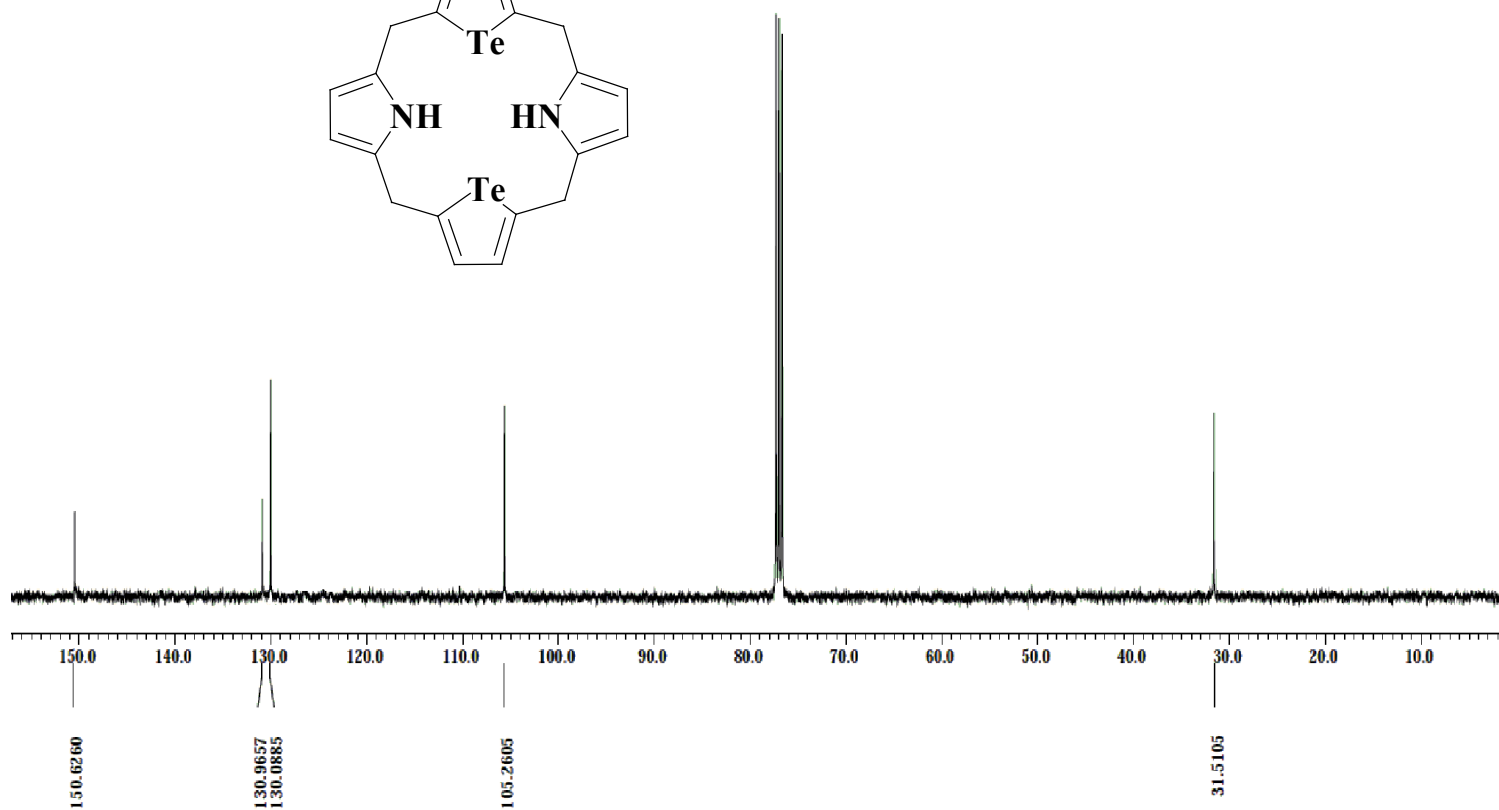
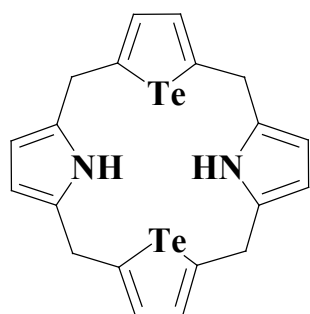


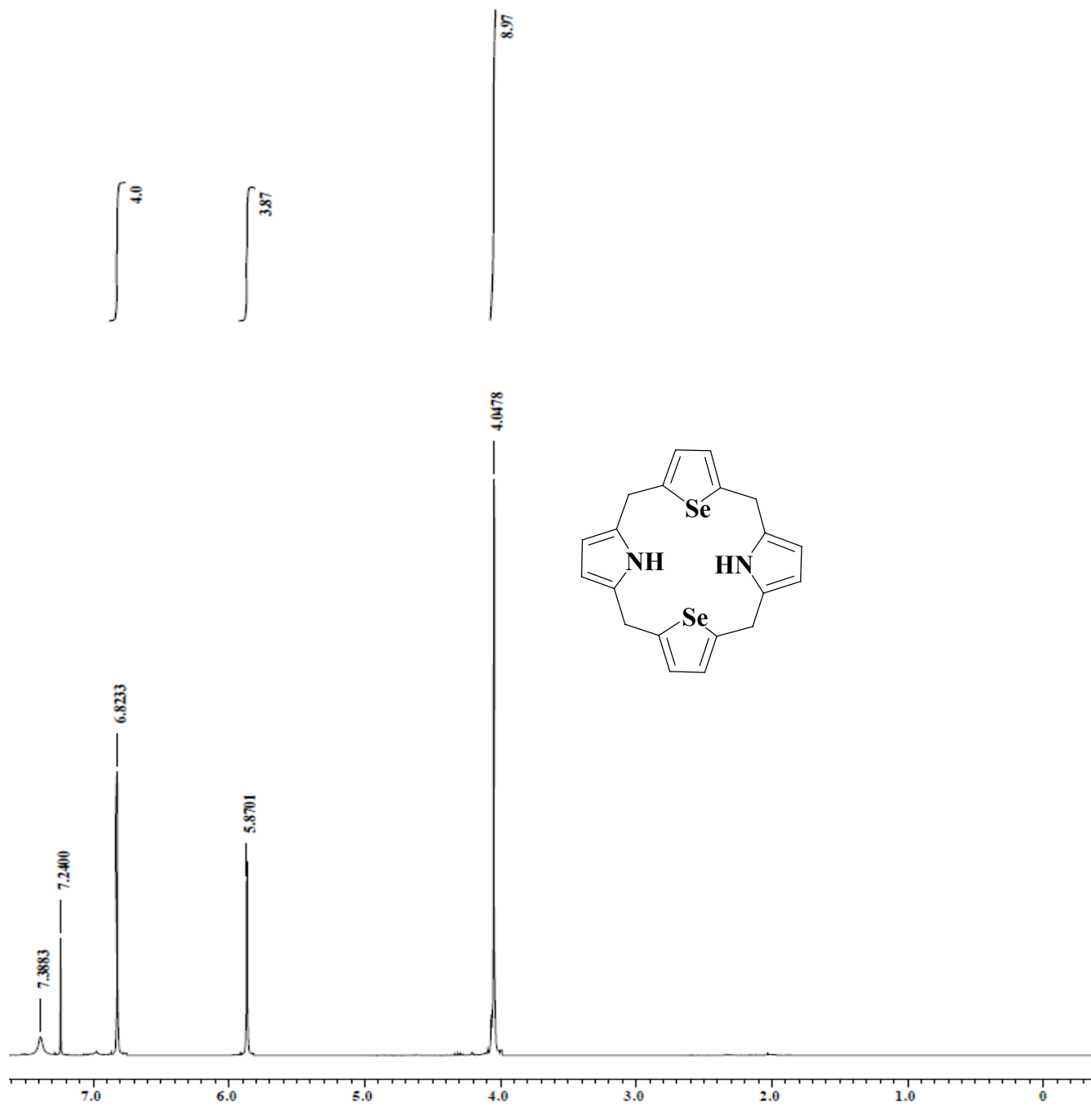


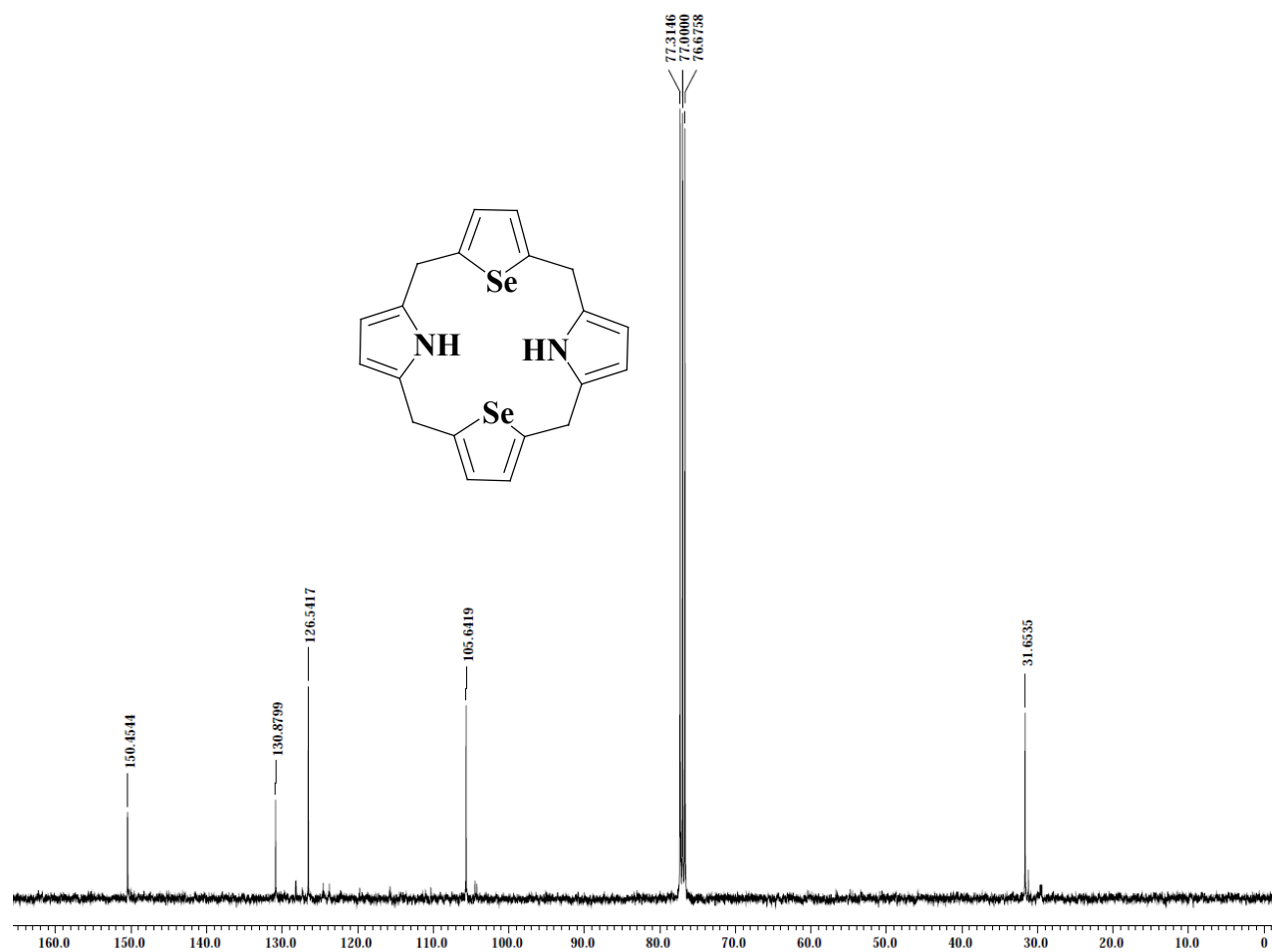


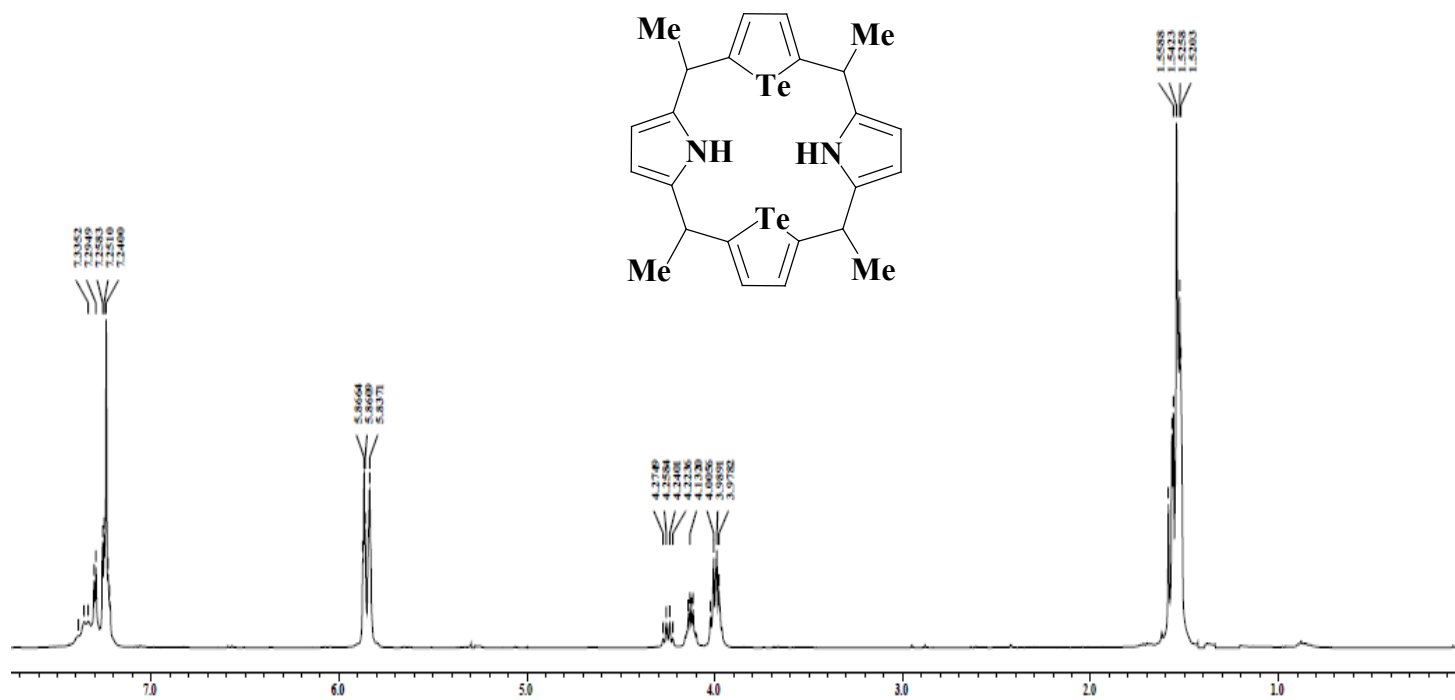


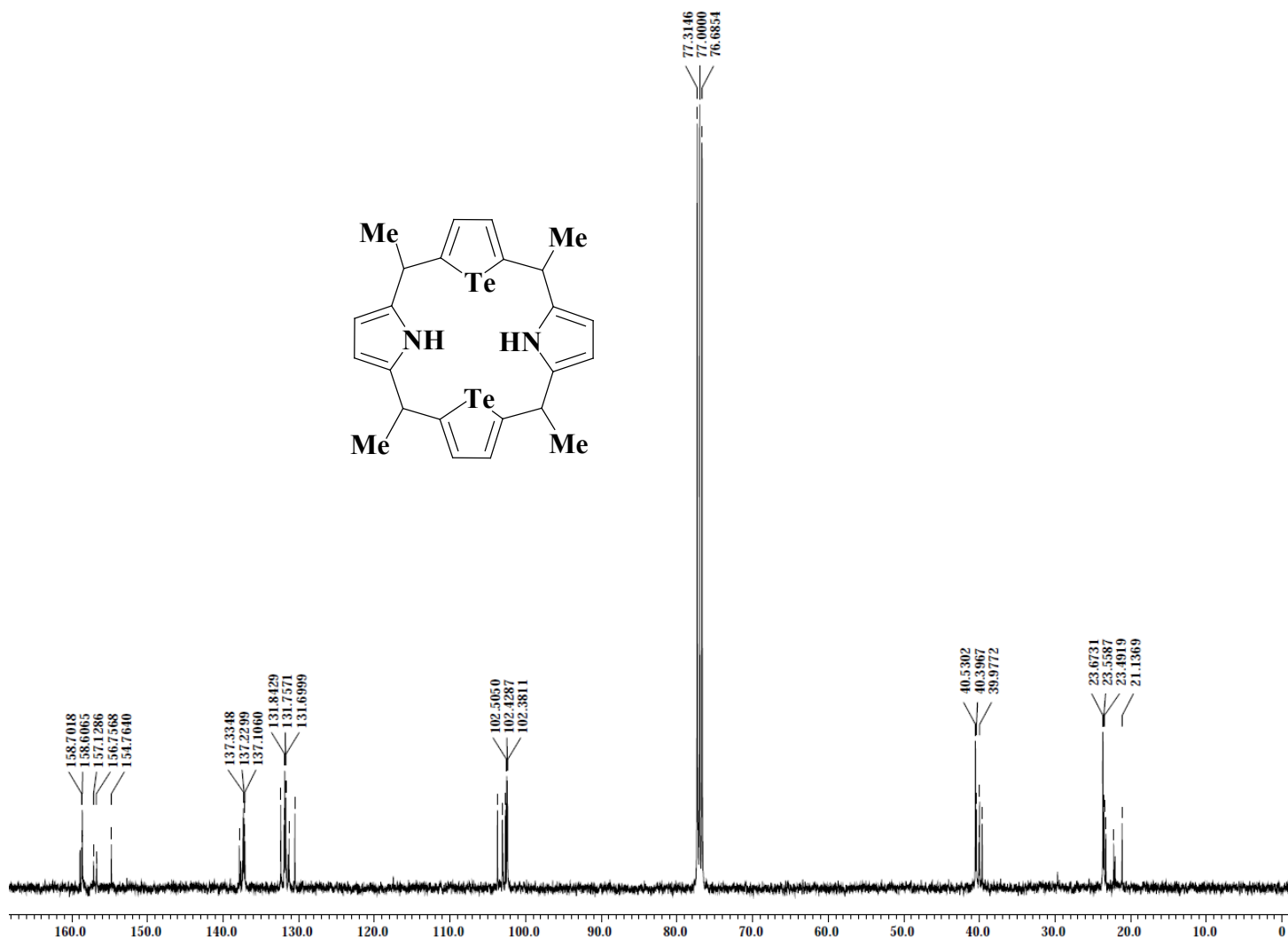




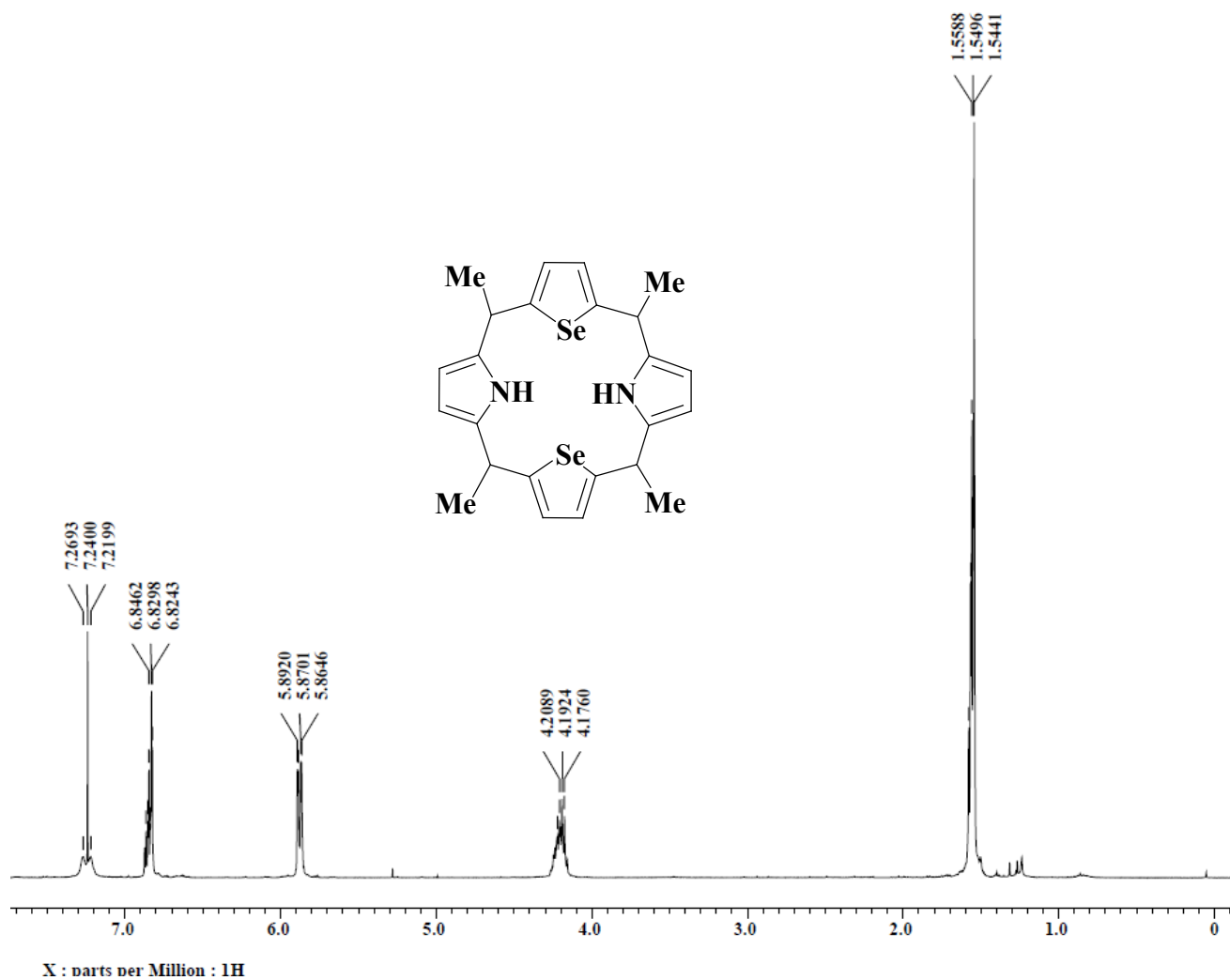


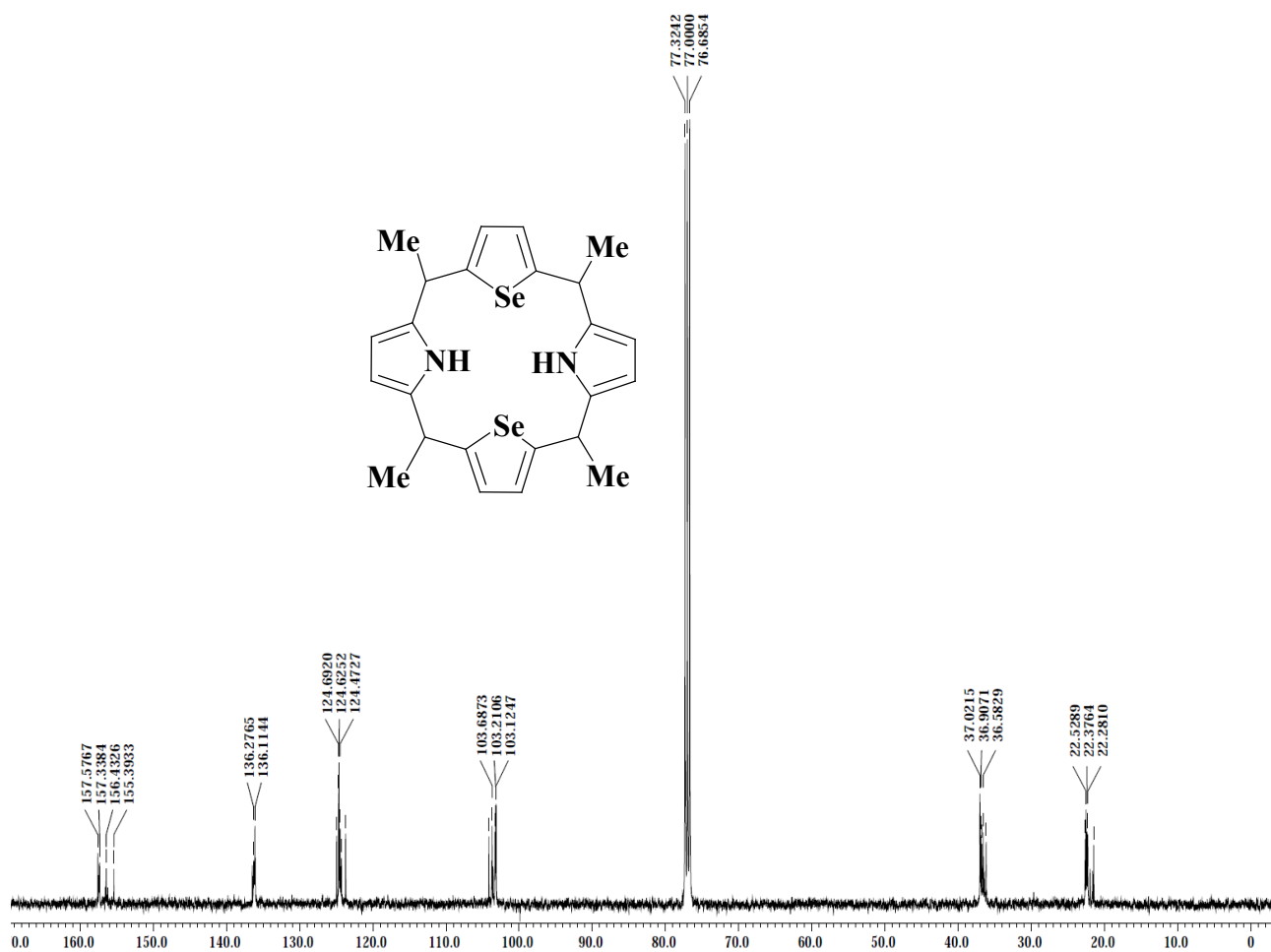


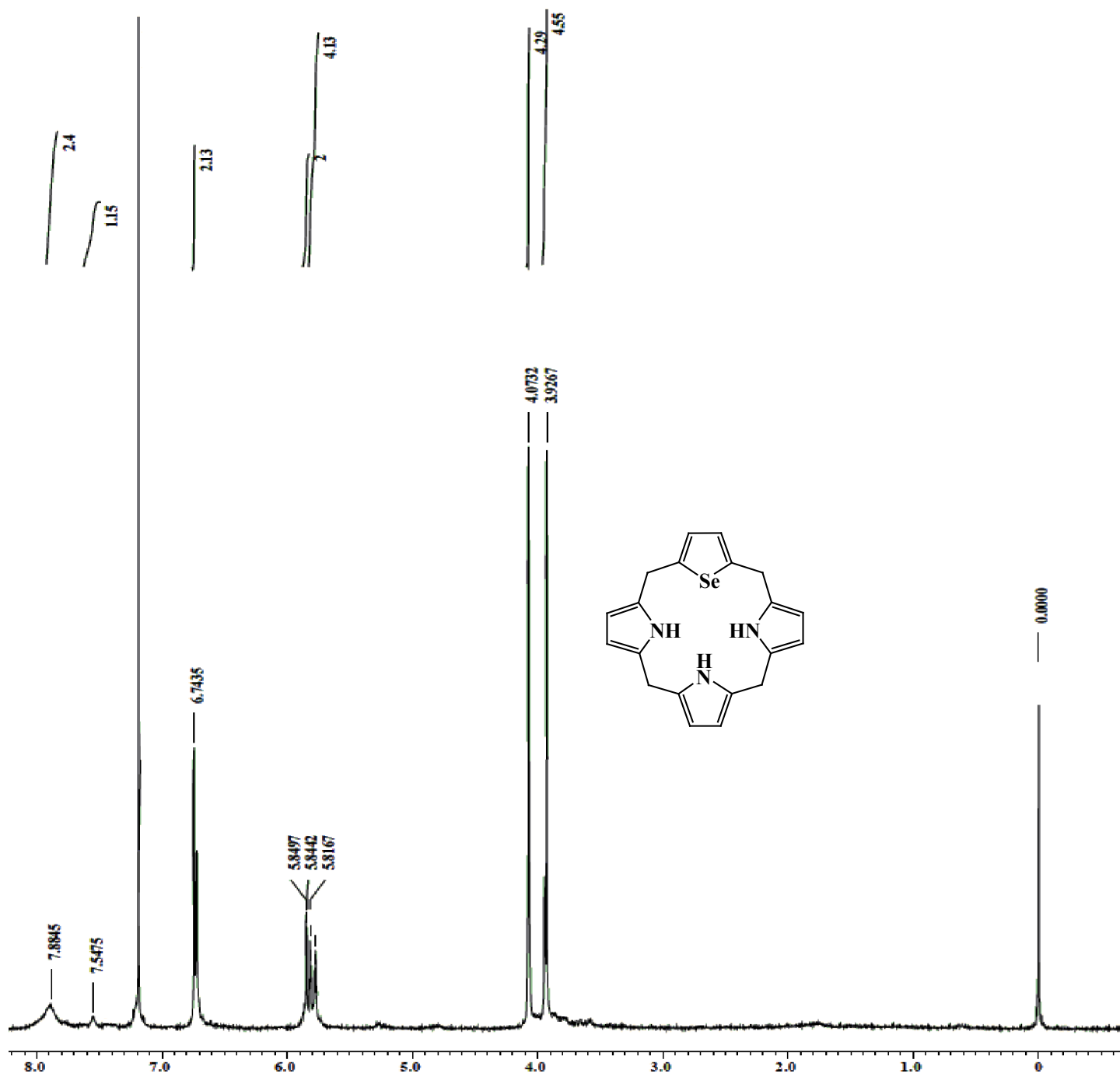


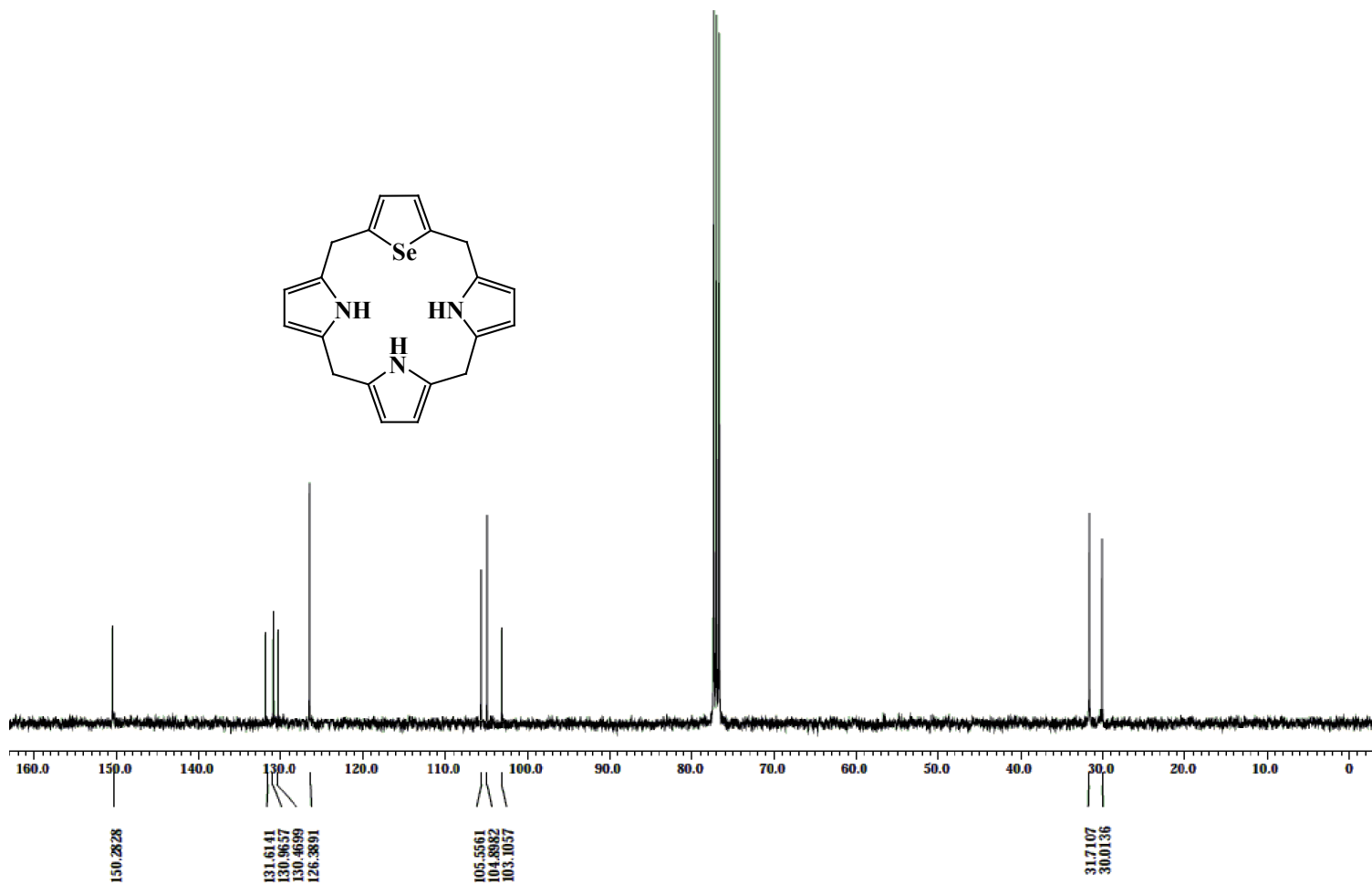
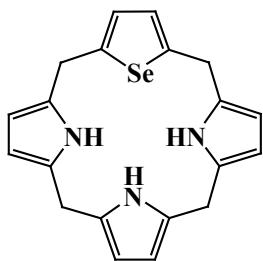


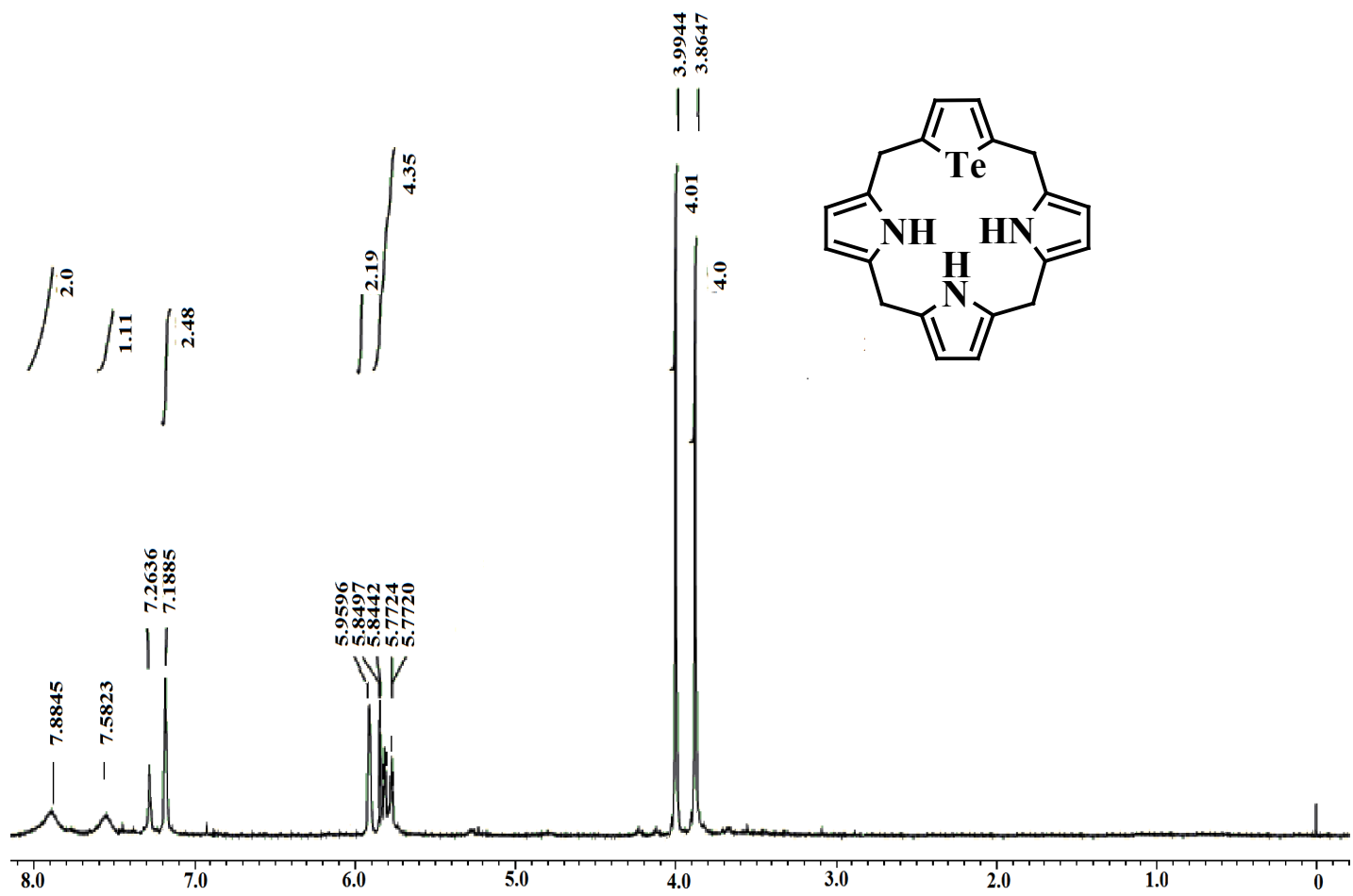


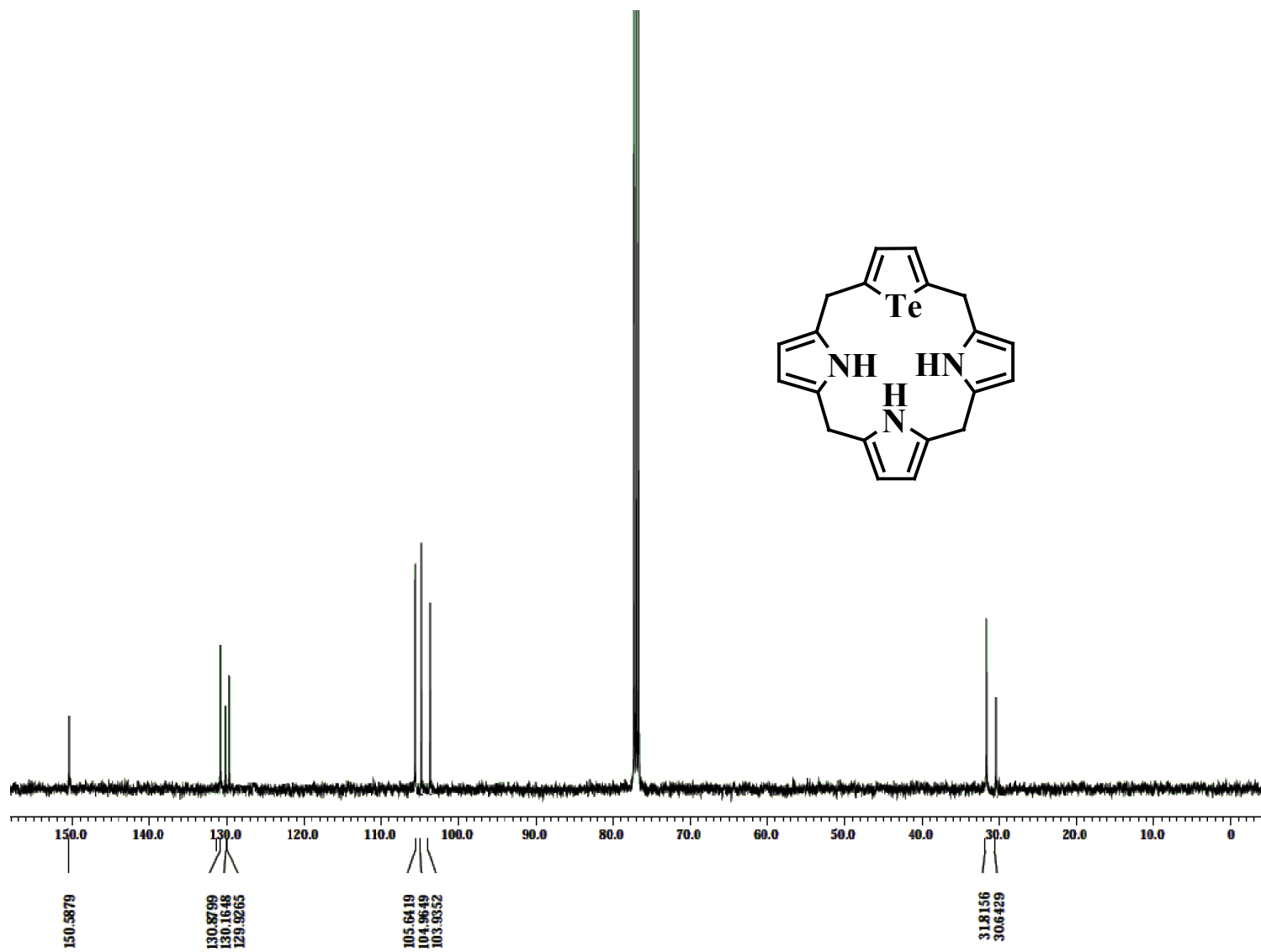


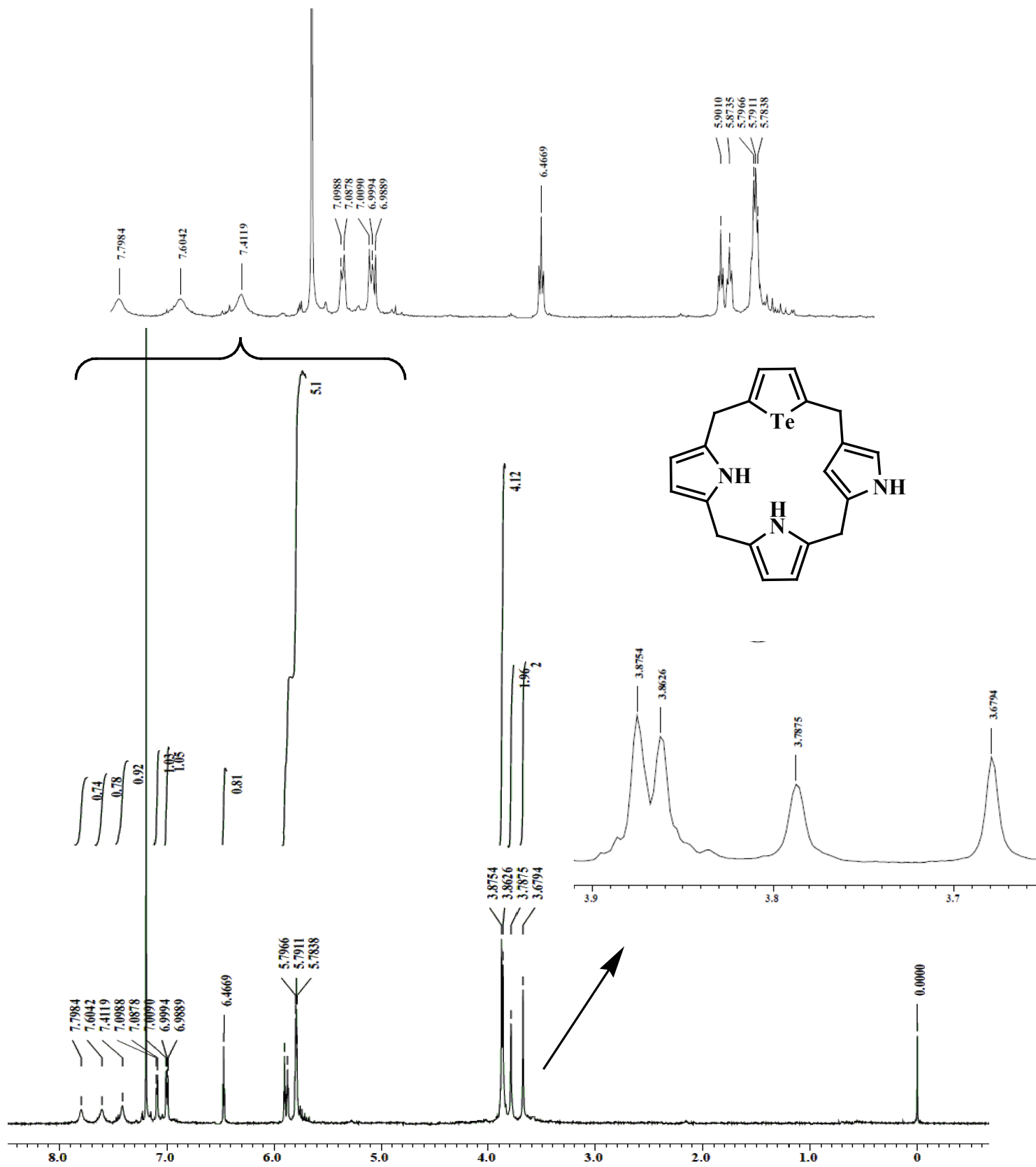


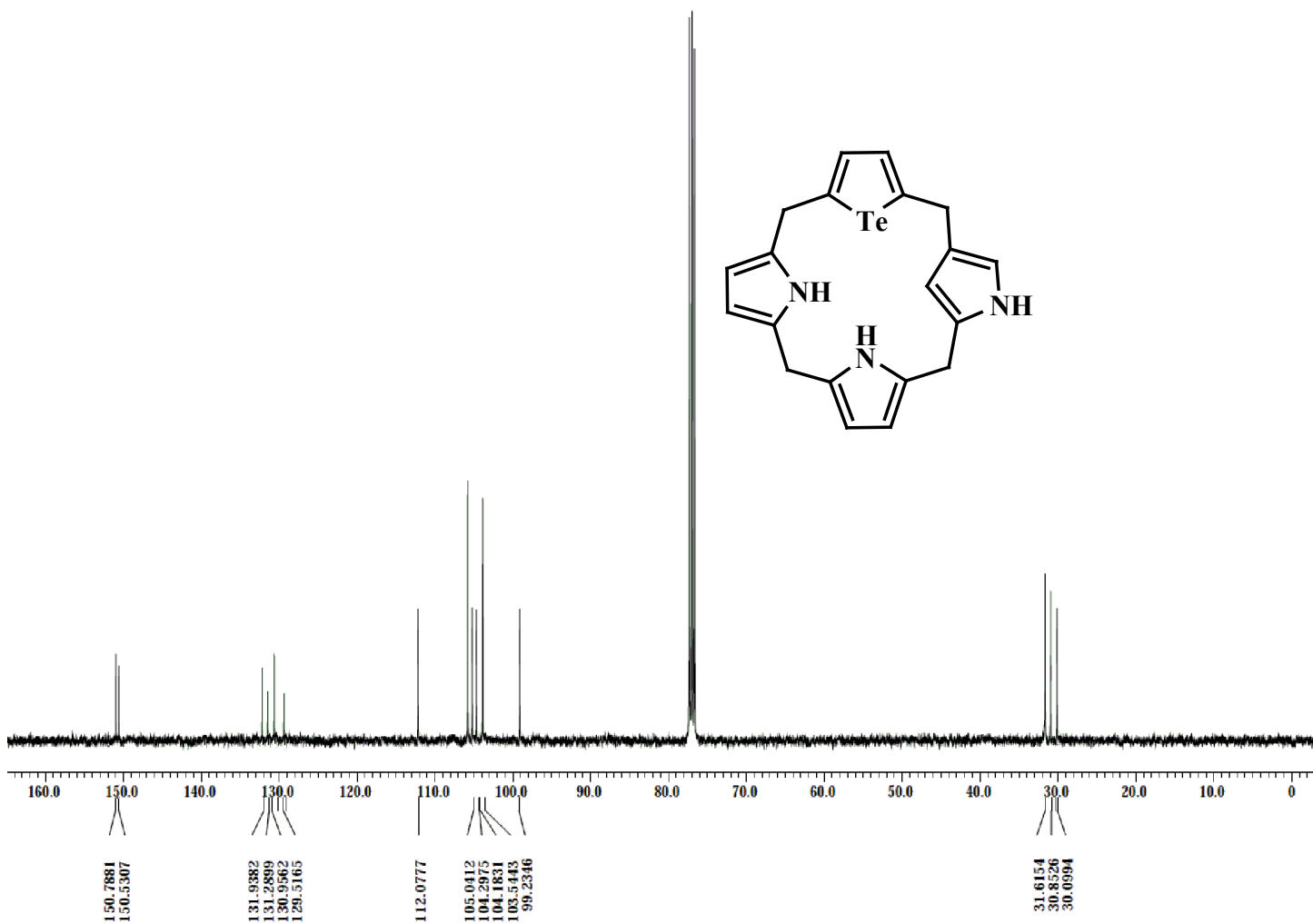




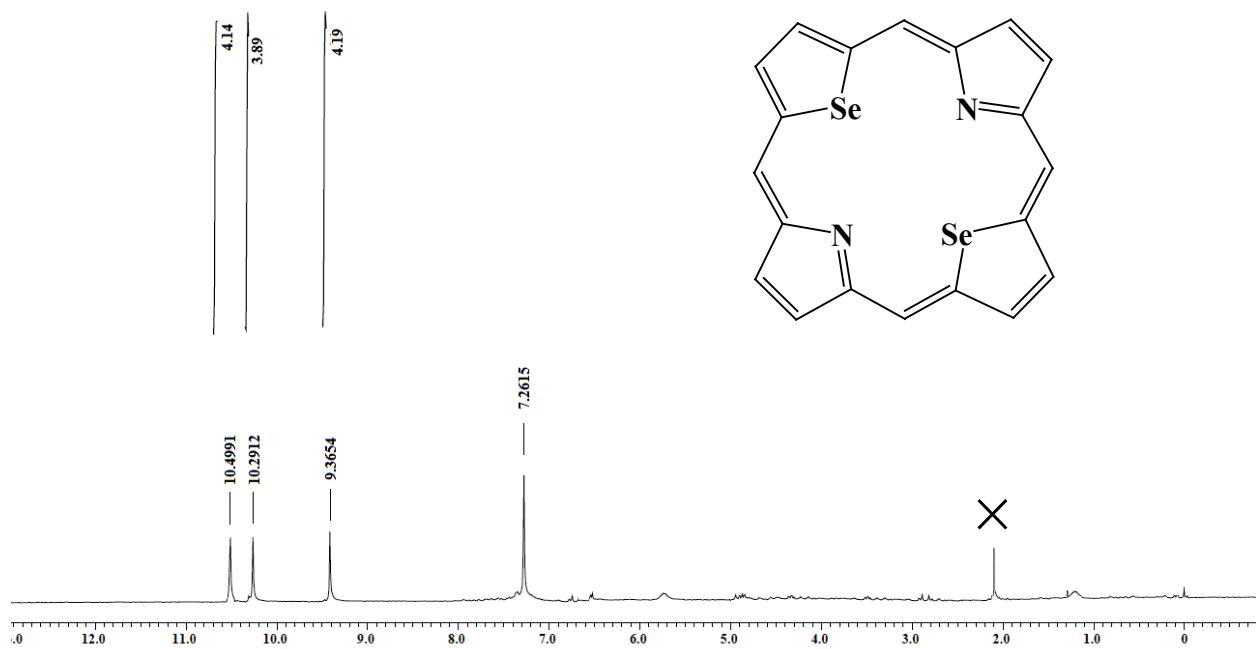


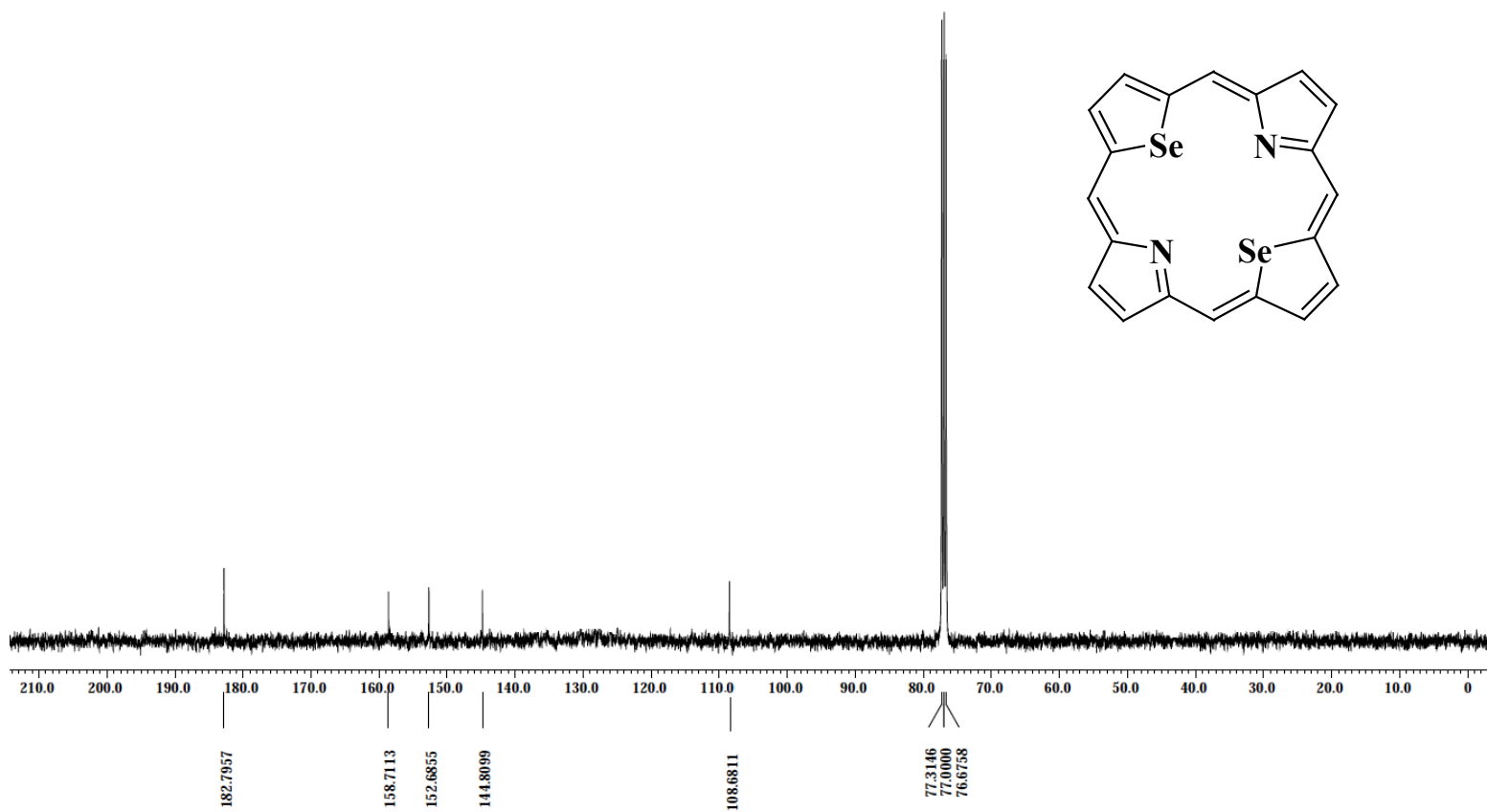


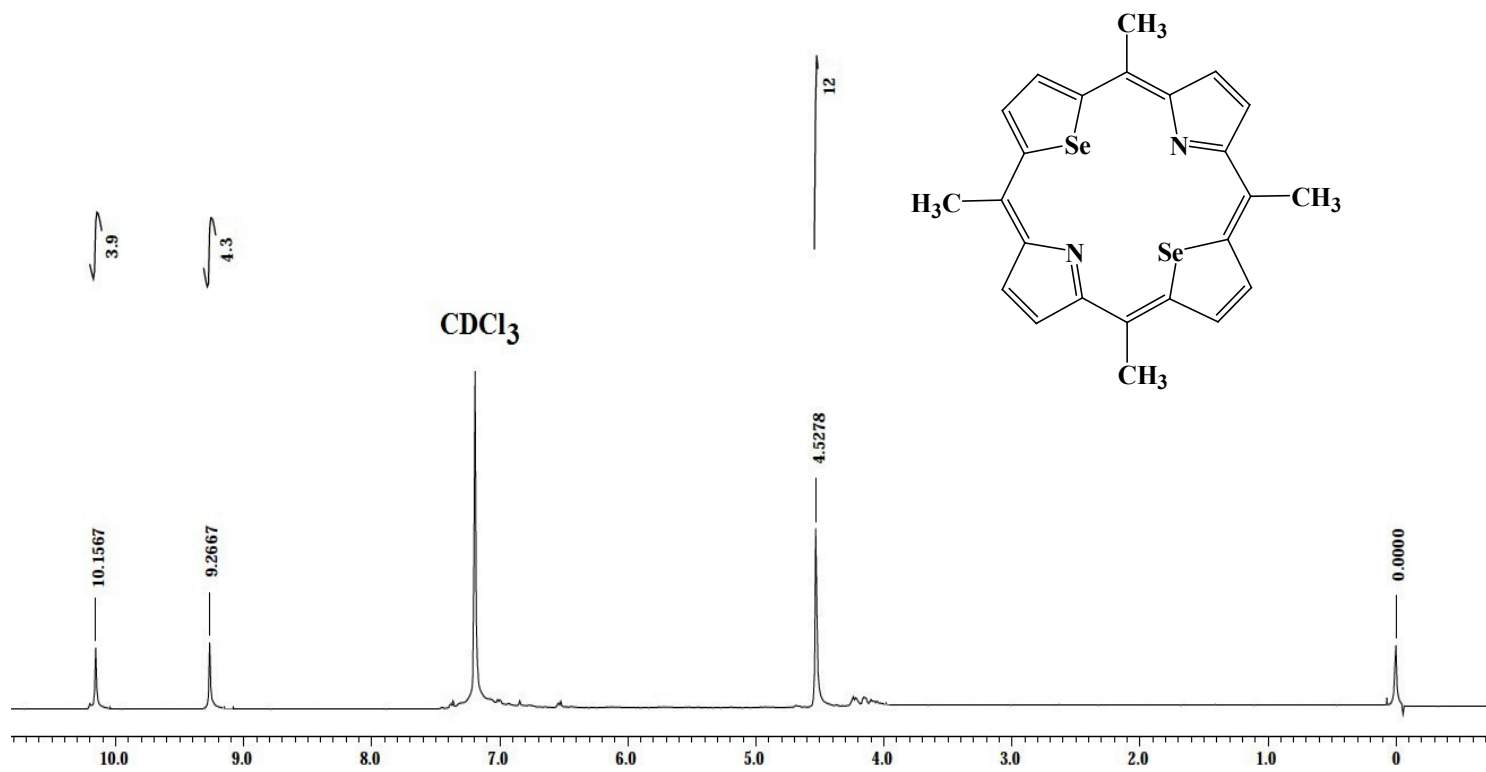


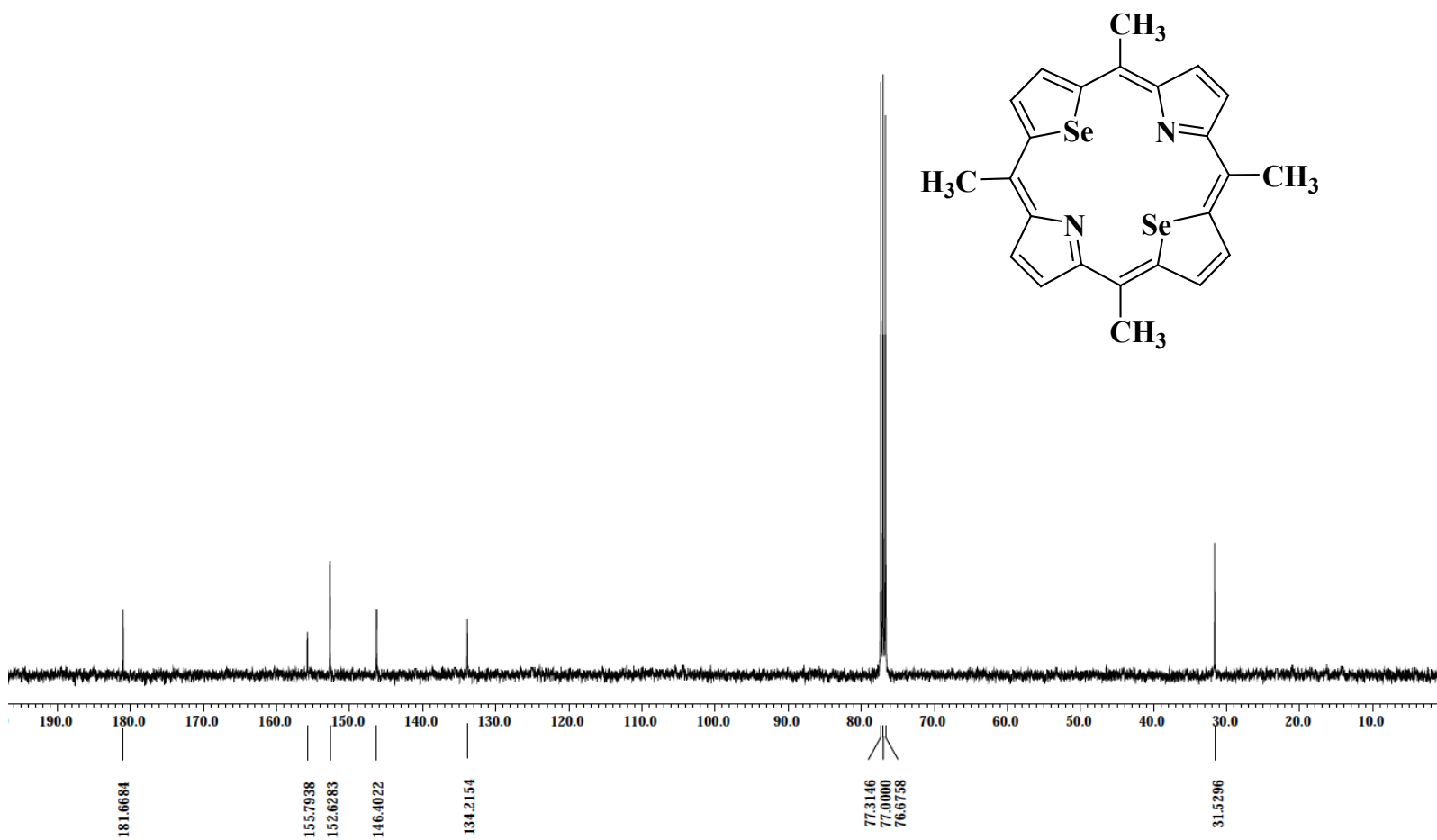


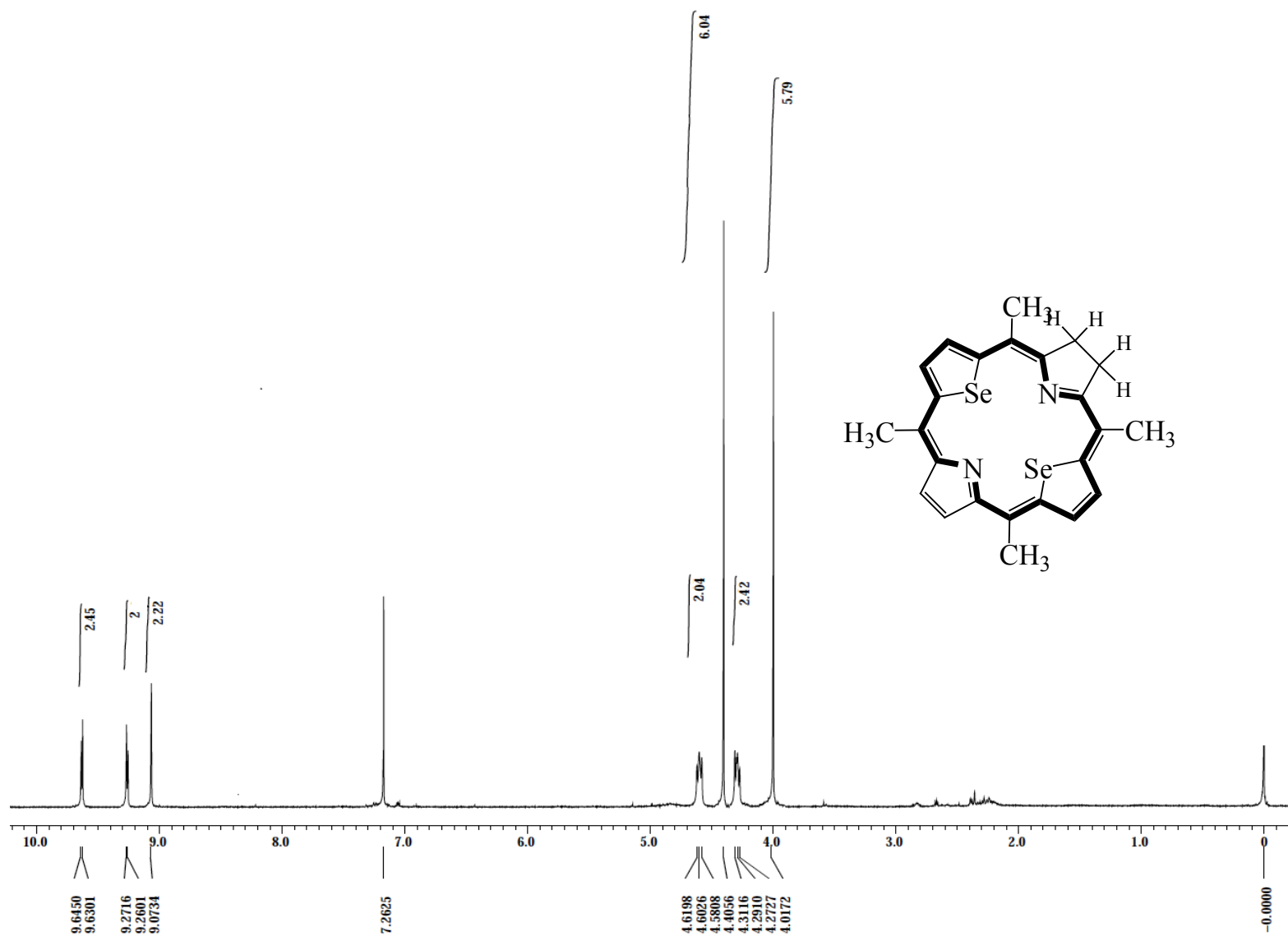


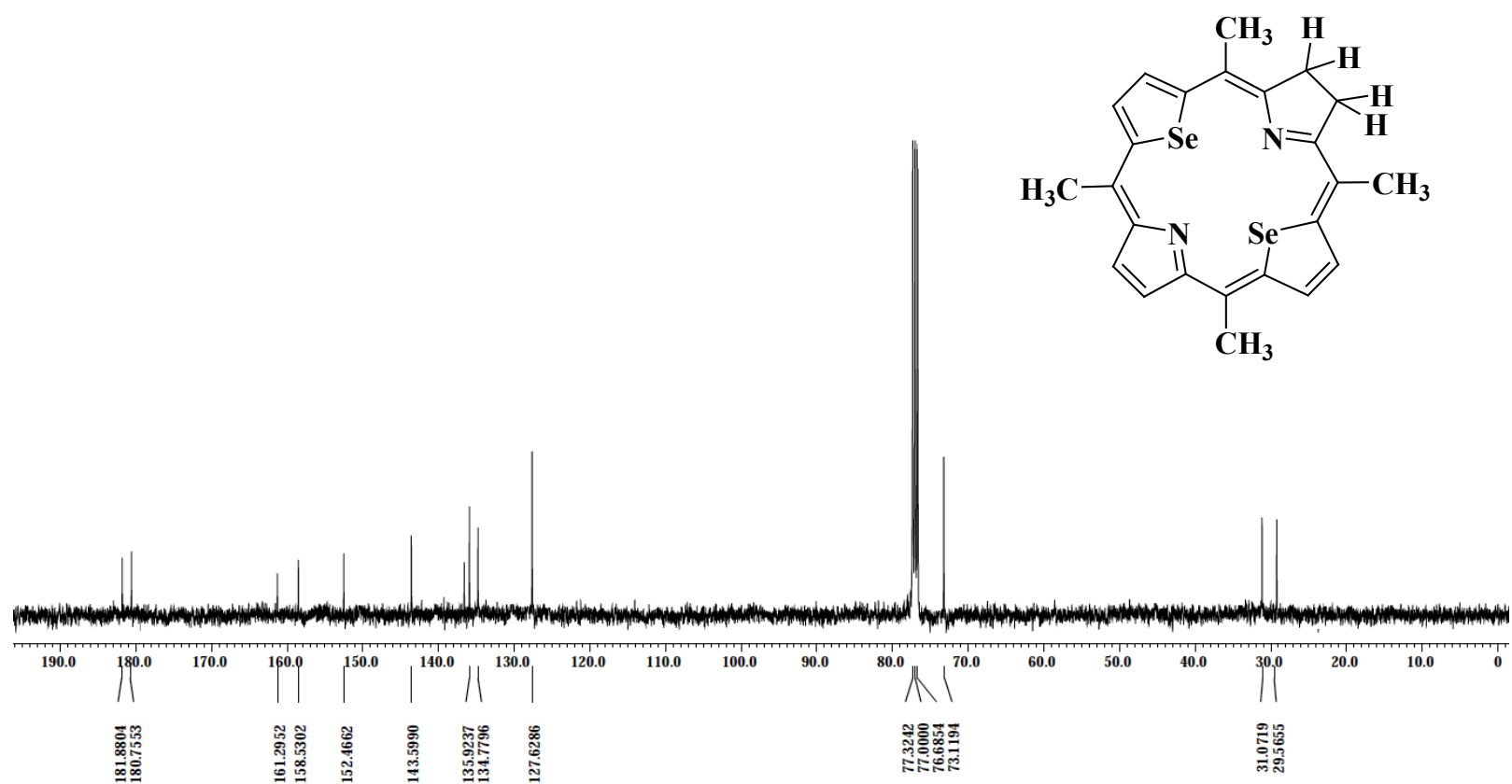


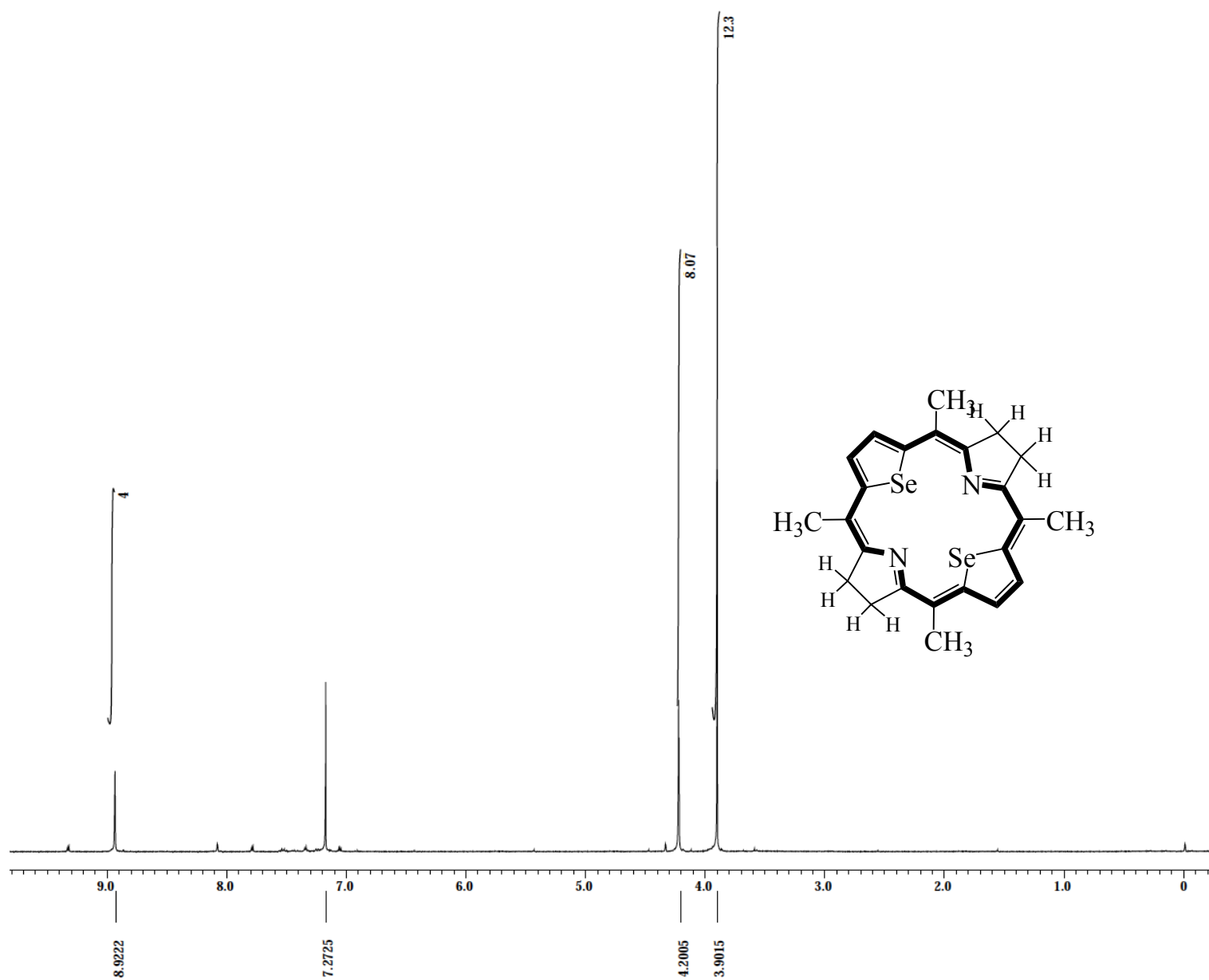


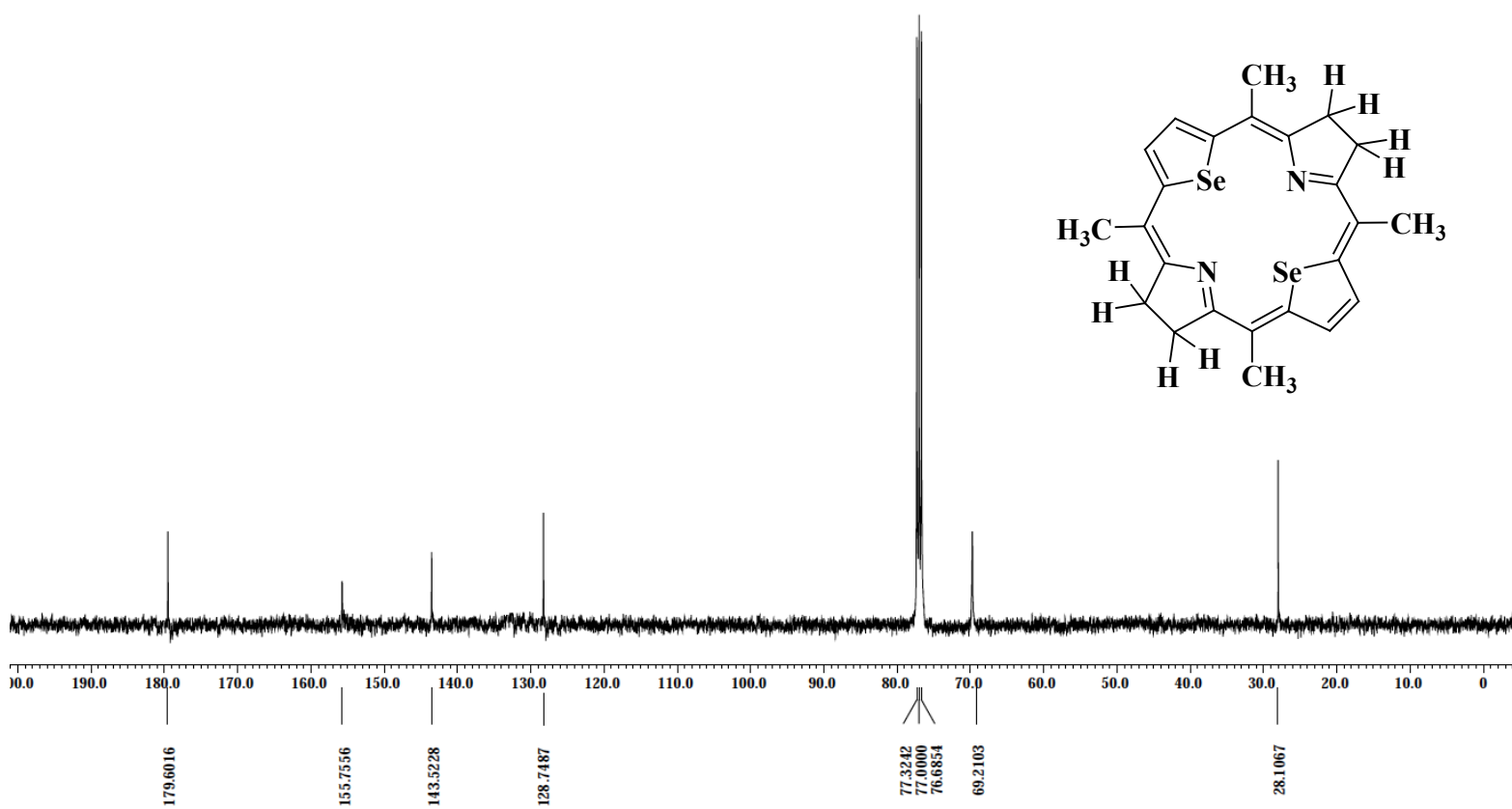




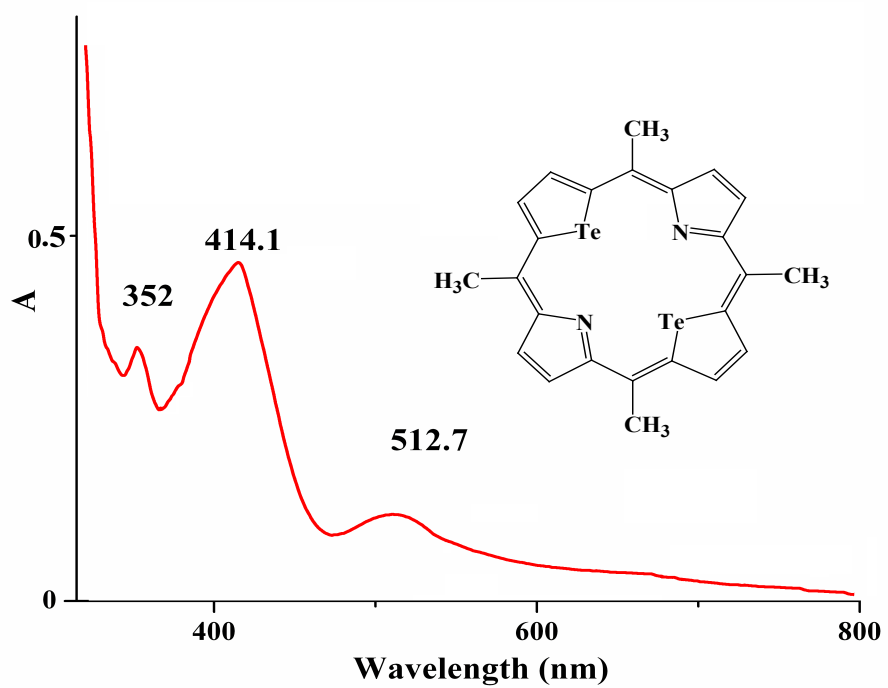
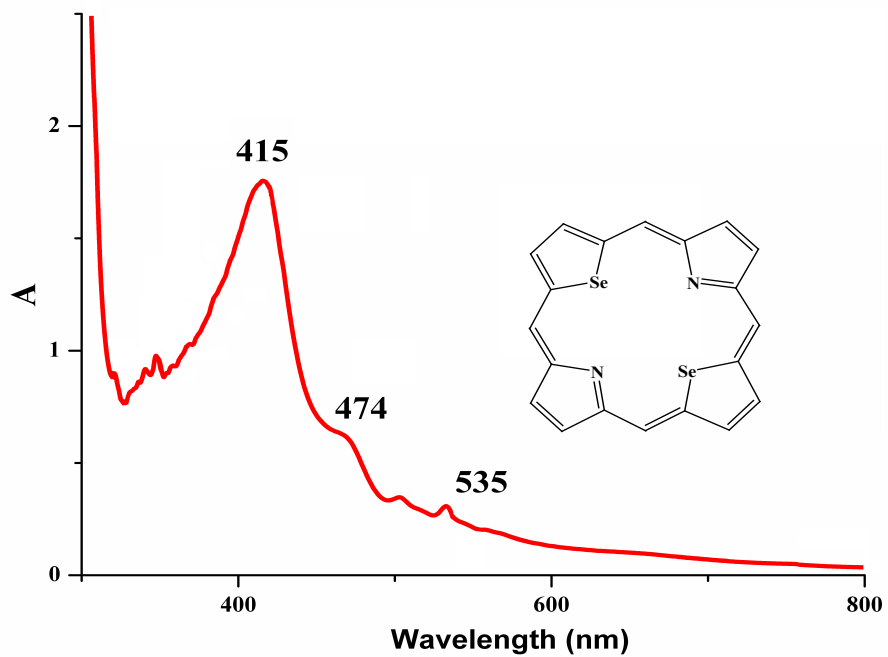


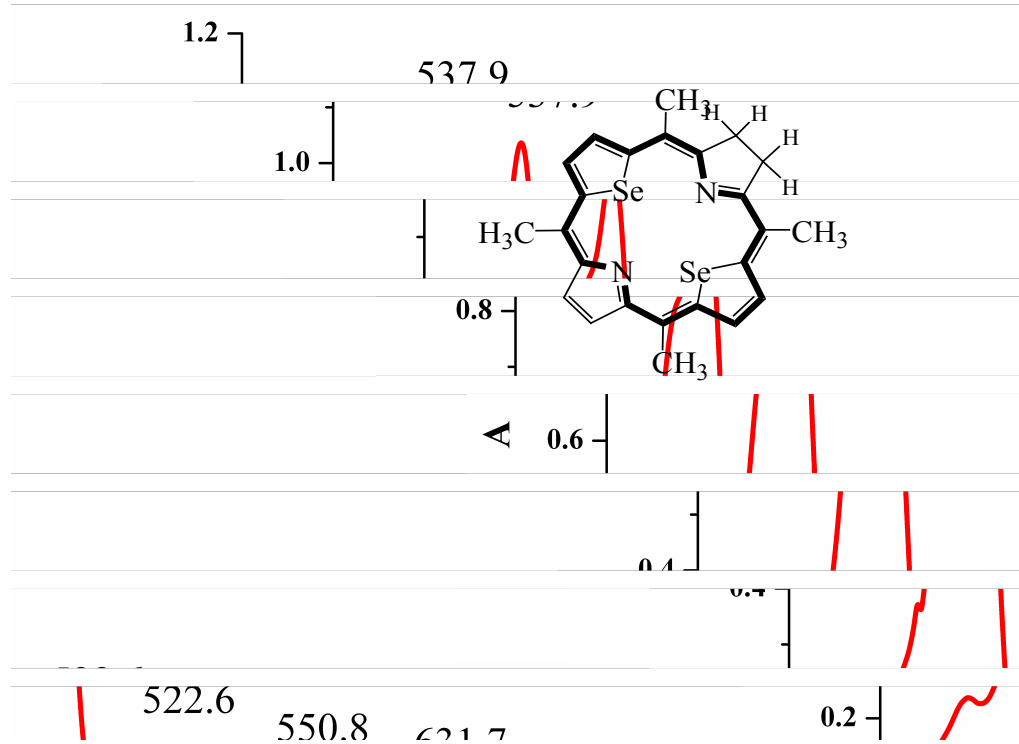
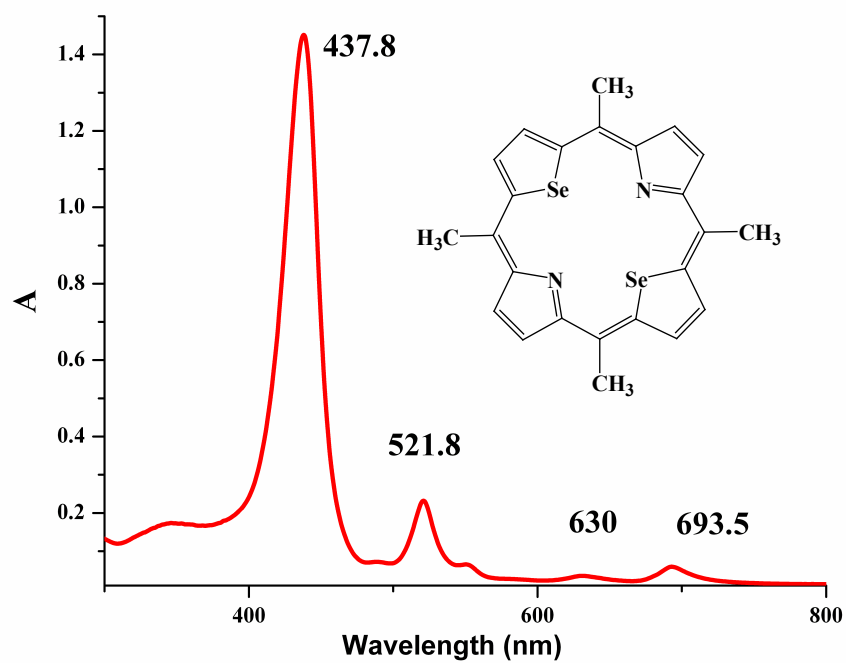


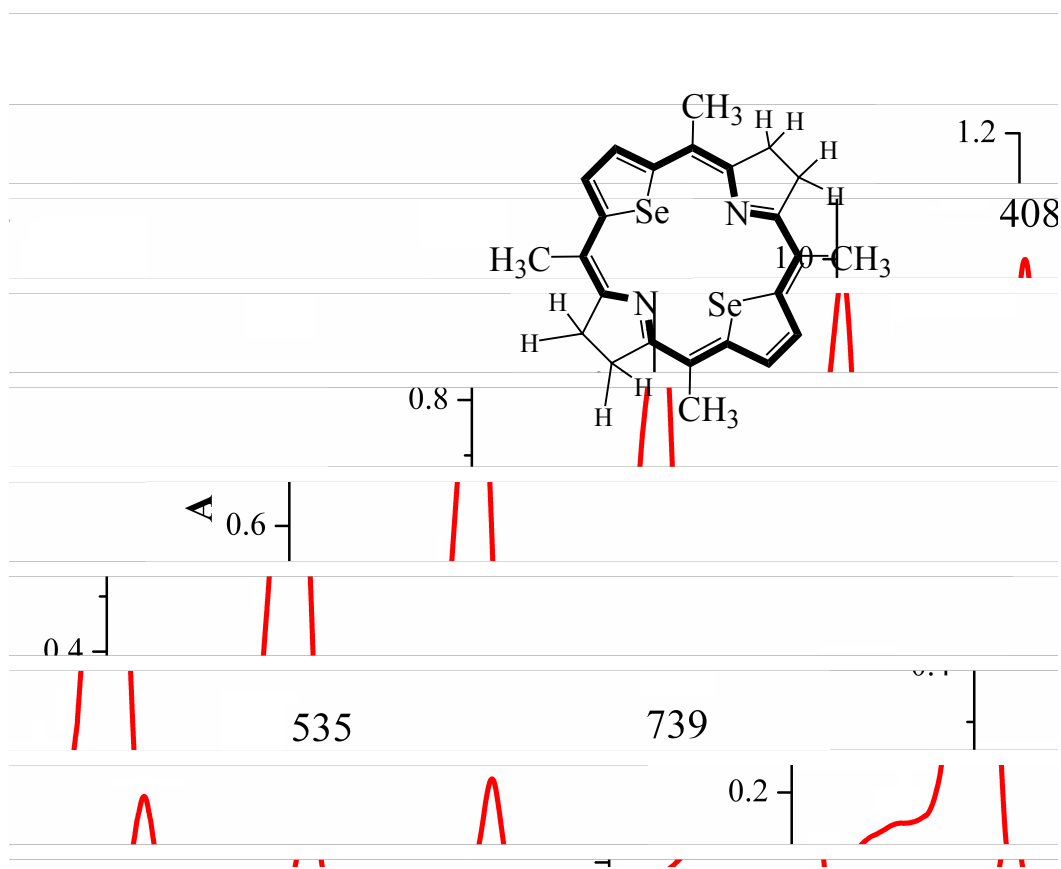


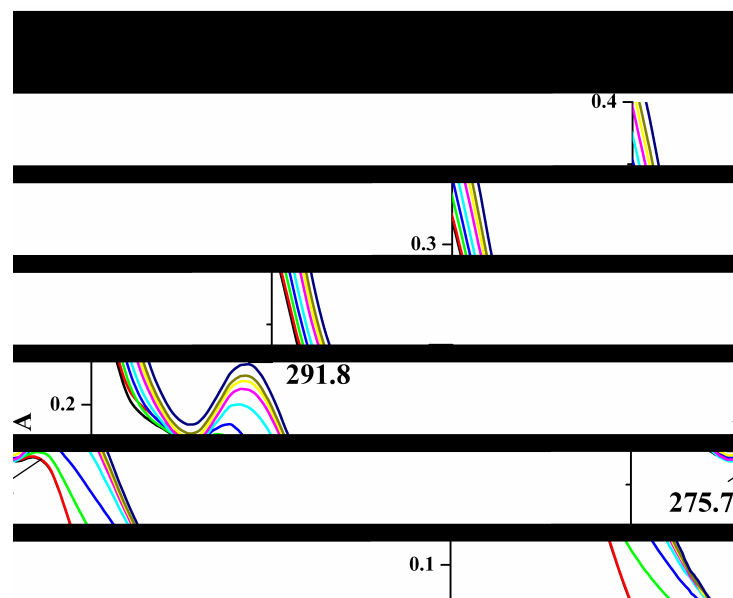




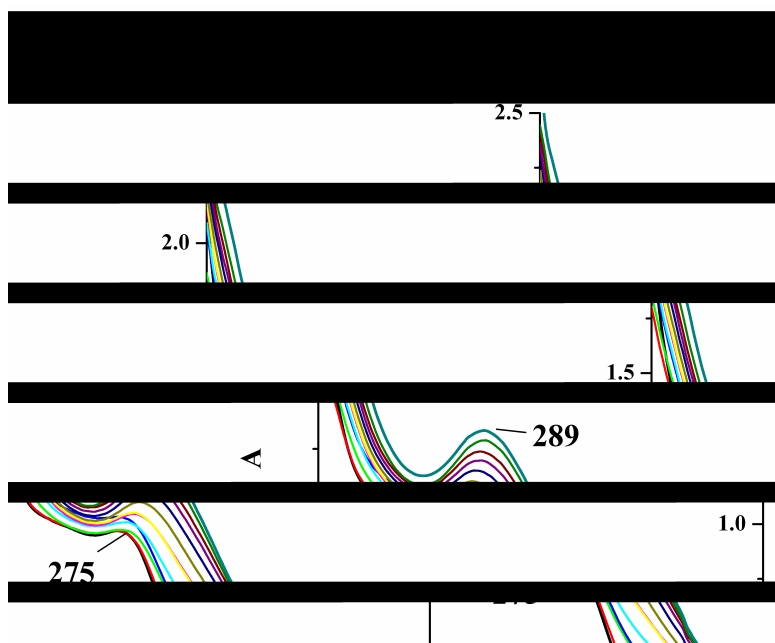




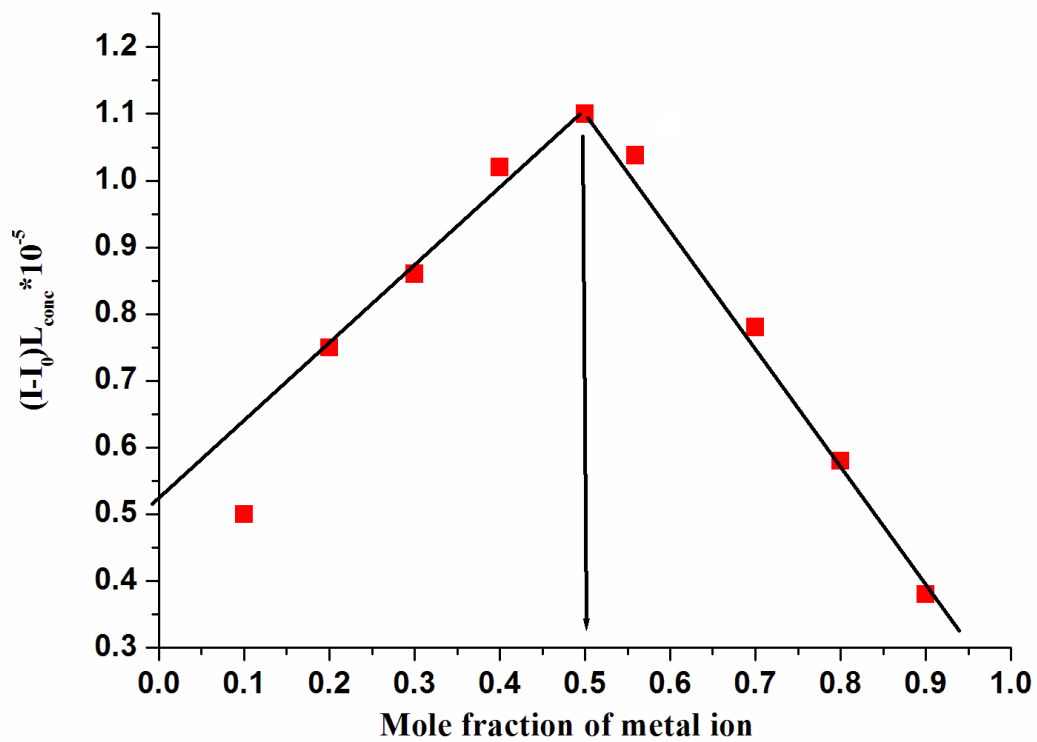




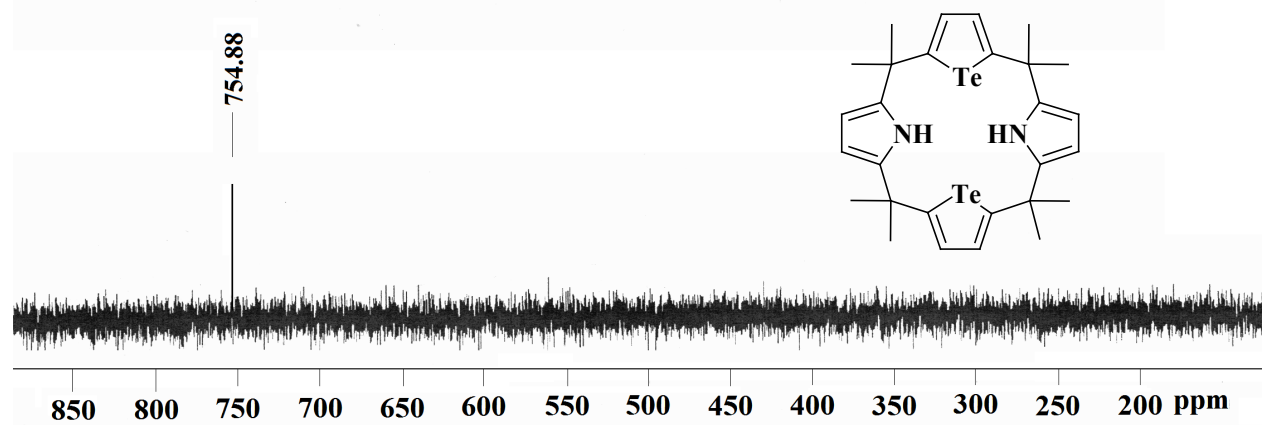
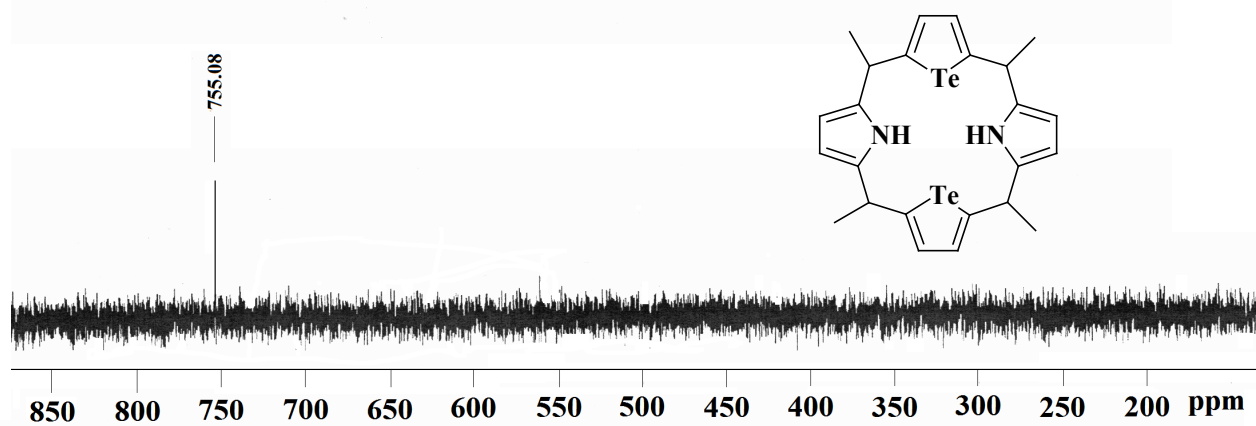
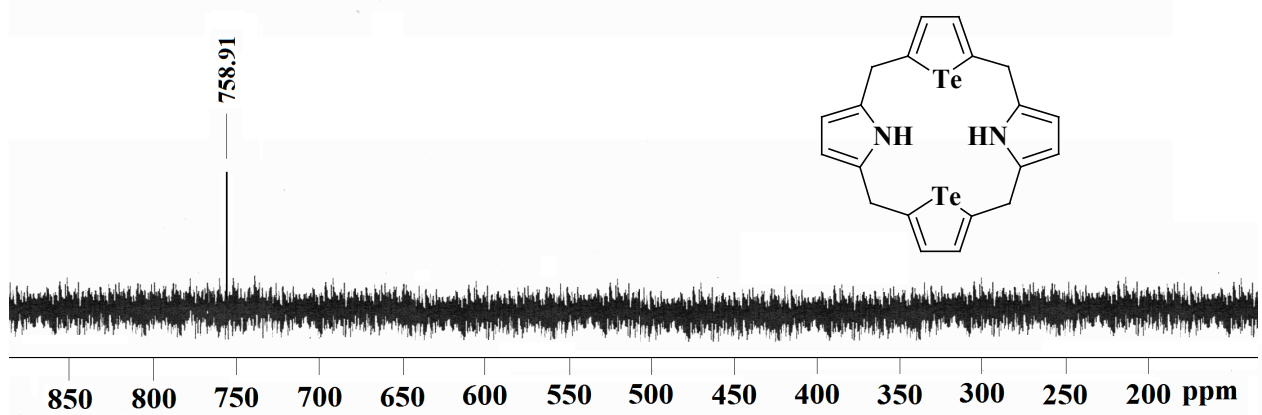
The absorption spectra of **7g** ( $2.0 \times 10^{-3}$ ) in acetonitrile upon the addition of 20  $\mu\text{l}$  stock solution ( $2 \times 10^{-3}$ ) of mercuric perchlorate.



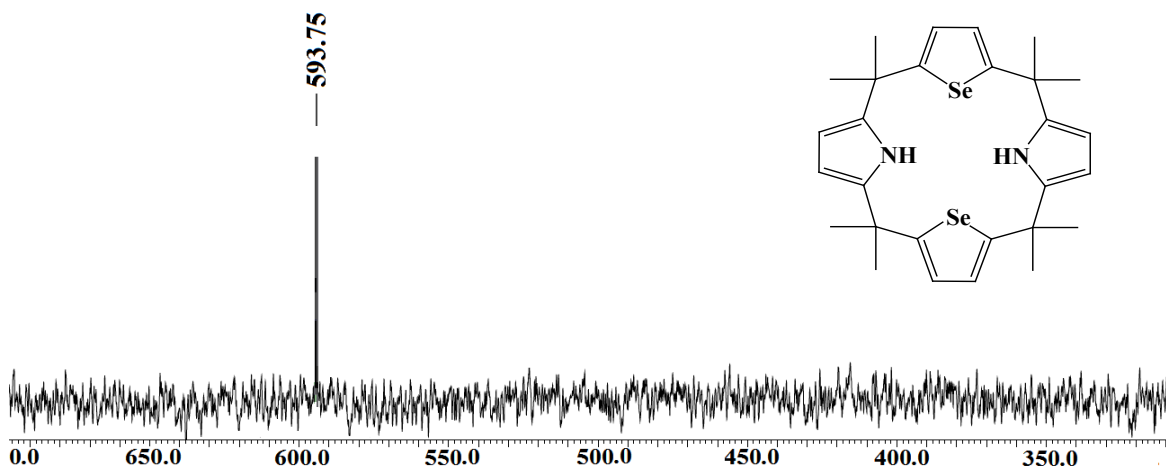
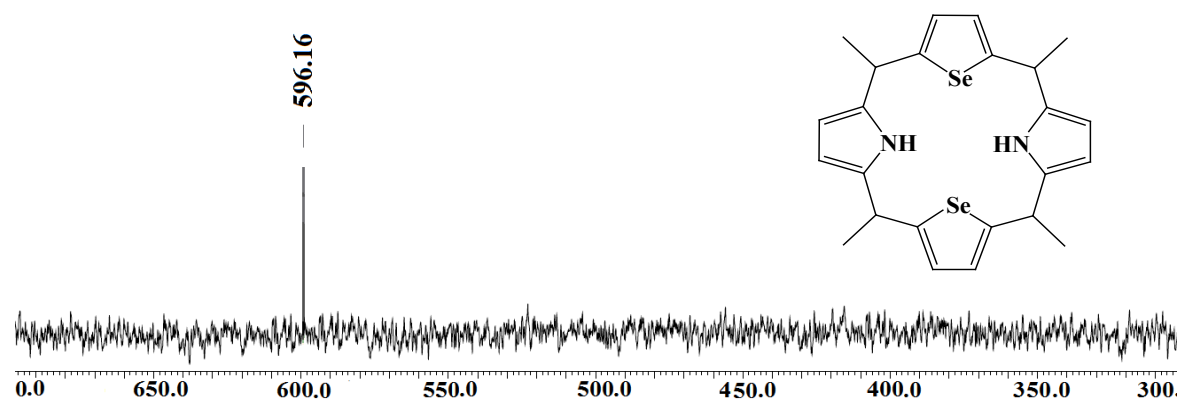
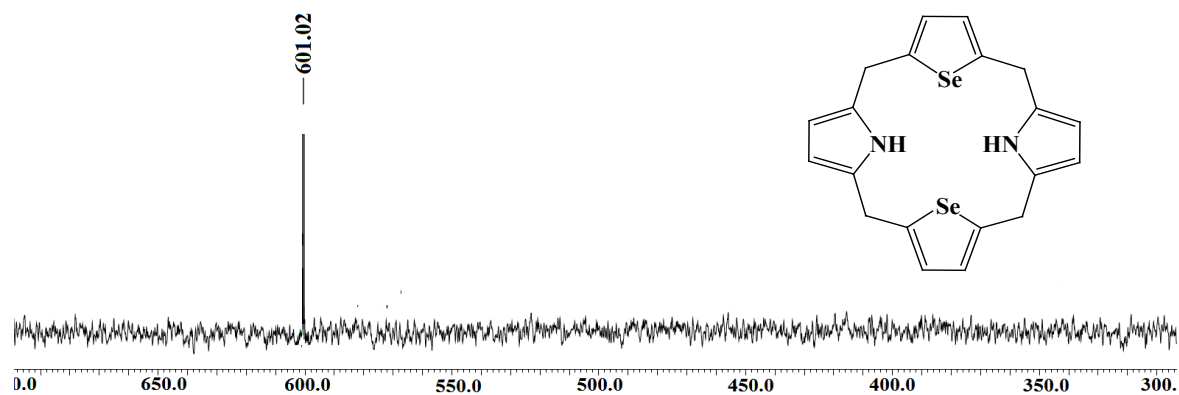
The absorption spectra of **8g** ( $1.8 \times 10^{-3}$ ) in acetonitrile upon the addition of 20  $\mu\text{l}$  stock solution ( $1.8 \times 10^{-3}$ ) of mercuric perchlorate.



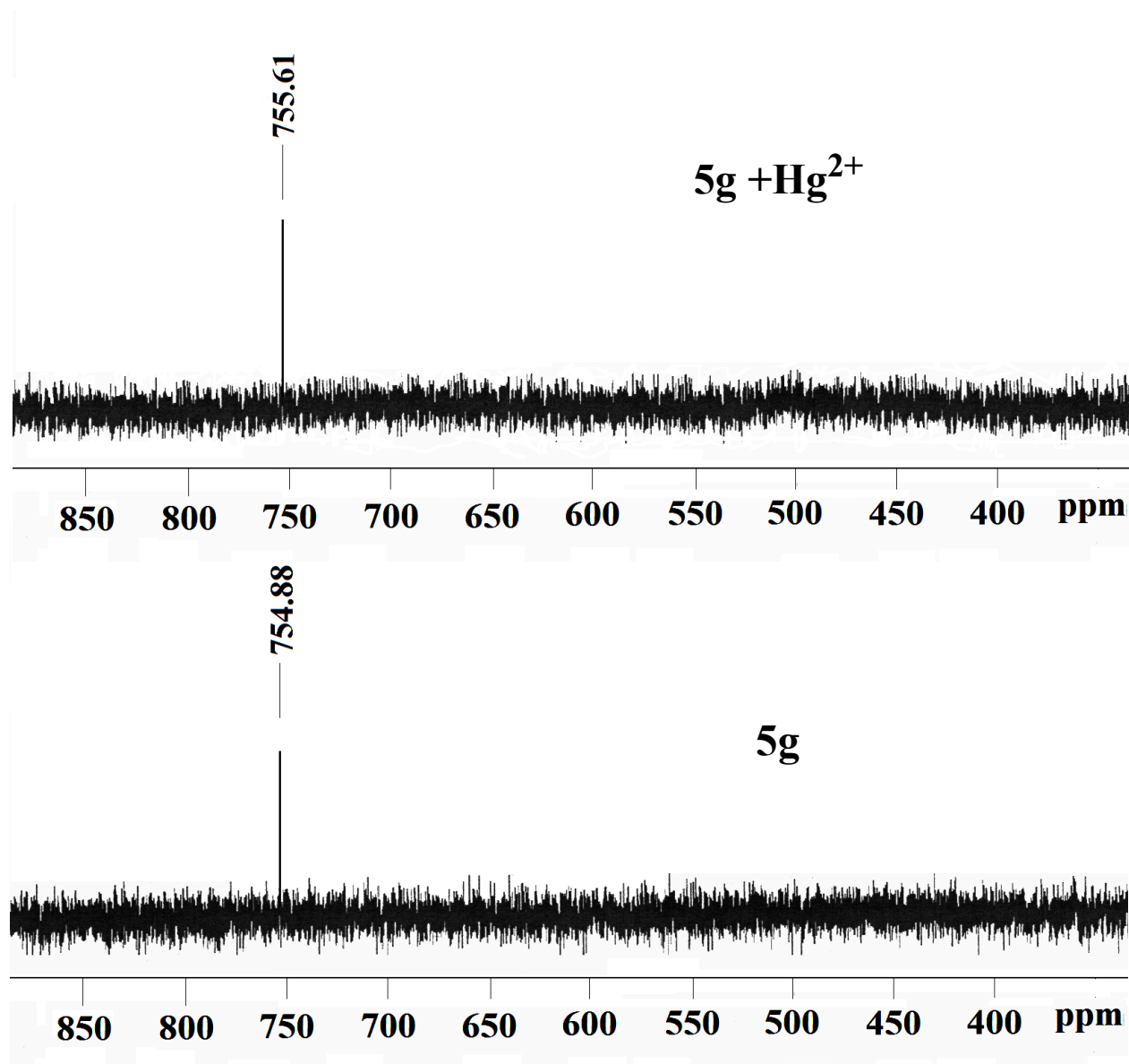
Job's plot for determining the stoichiometry (1:1) of **5g** and Hg<sup>2+</sup> ions in acetonitrile



$^{125}\text{Te}$  NMR spectra in  $\text{CDCl}_3$ , relative to  $^{125}\text{TeMe}_2$  ( $\delta$  0.0 ppm).



$^{77}\text{Se}$  NMR spectra in  $\text{CDCl}_3$ .



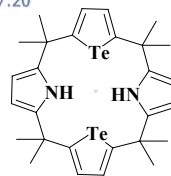
$^{125}\text{Te}$  NMR spectra of **5g** with and without  $\text{Hg}^{2+}$  in  $\text{CDCl}_3$ , relative to  $^{125}\text{TeMe}_2$  ( $\delta$  0.0 ppm).



# Mass

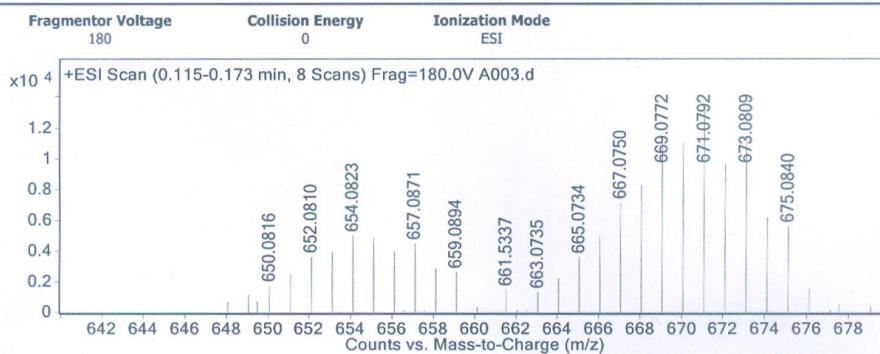
## Qualitative Analysis Report

<b>Data Filename</b>	A003.d	<b>Sample Name</b>	A <i>C<sub>28</sub>H<sub>34</sub>N<sub>2</sub>Te<sub>2</sub></i>
<b>Sample Type</b>	Sample	<b>Position</b>	P1-F1 <i>Te-Te Dimethyl</i>
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	SANJAY PANDEY
<b>Acq Method</b>	DAILY MS.m	<b>Acquired Time</b>	15-04-2013 12:57:20
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	default.m
<b>Comment</b>			
<b>Sample Group</b>		<b>Info.</b>	
<b>Acquisition SW</b>	6200 series TOF/6500 series		
<b>Version</b>	Q-TOF B.05.01 (B5125)		



**C<sub>28</sub>H<sub>34</sub>N<sub>2</sub>Te<sub>2</sub>**  
**Exact Mass: 658.08466**

### User Spectra



### Peak List

m/z	z	Abund
536.1635	1	3088.93
610.1819	1	4848.05
611.1816	1	3044.42
612.1798	1	2233.32
651.084		2480.09
652.081		3628.41
653.0844		3899.03
654.0823		5010.23
655.0858		4874.52
656.0836		4003.2
657.0871	1	4492.68
658.0865	1	2874.93
659.0894	1	2624.35
664.0719		2195.83
665.0734		3598.56
666.0734		4973.82
667.075		7113.13
668.0756		8263.29
669.0772		11380.85
670.0768		11029.67
671.0792	1	13070.51
672.0782	1	9577.67
673.0809	1	11303.08
674.0816		6222.97
675.084	1	5601.15
683.0716		2703.74

*M<sup>+</sup>*  
*M+1*

684.0722		2575.16
684.1999	1	2409.44
685.0733	1	4603.34
686.0724	1	2886.61
687.0745	1	5855.21
688.0754	1	2427.34
689.0762	1	5058.53
691.075		2652.42
699.0696		3451.99
700.0693		2937.63
701.0694	1	5713.9
702.0696	1	3540.52
703.0698	1	8013.71
704.0694	1	3144.64
705.0687	1	7200.31
706.0709	1	2412.91
707.066	1	4535.3
715.0623	1	2058.69
717.0619	1	3024.07
719.0607	1	3054.84
721.0583	1	2207.92
733.0588	1	2448.3
735.0585	1	2614.2
737.0577		2234.56

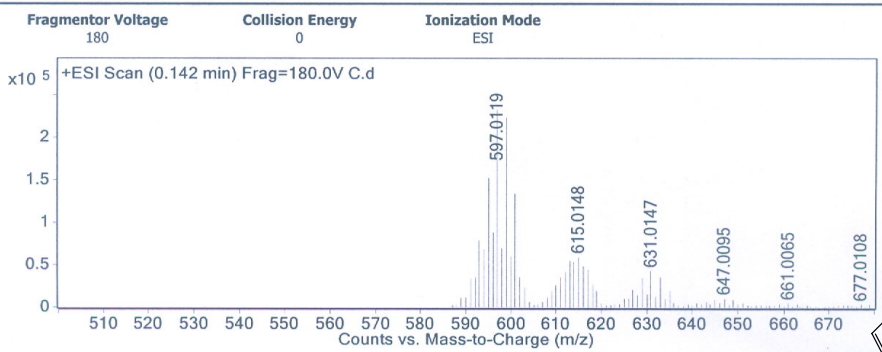
## Qualitative Analysis Report

<b>Data Filename</b>	C.d	<b>Sample Name</b>	C
<b>Sample Type</b>	Sample	<b>Position</b>	P1-F3
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	SANJAY PANDEY
<b>Acq Method</b>	DAILY MS.m	<b>Acquired Time</b>	15-04-2013 11:57:12
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	default.m

C<sub>24</sub>H<sub>26</sub>N<sub>2</sub>Te<sub>2</sub>  
 Te-Te (Me, H)

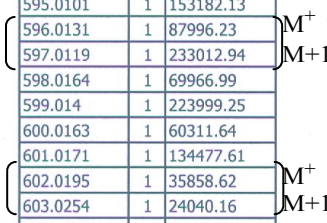
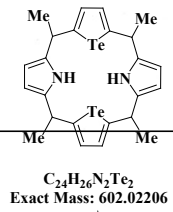
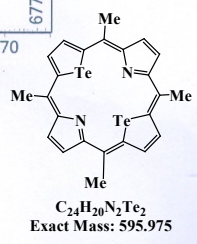
<b>Sample Group</b>	<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series
<b>Version</b>	Q-TOF B.05.01 (B5125)

### User Spectra



m/z	z	Abund
106.0043		20135.74
217.1036	1	25098.11
591.0078		33688.94
592.0097		35354.34
593.0088		79388.07
594.011		67978.62
595.0101	1	153182.13
596.0131	1	87996.23
597.0119	1	233012.94
598.0164	1	69966.99
599.014	1	223999.25
600.0163	1	60311.64
601.0171	1	134477.61
602.0195	1	35858.62
603.0254	1	24040.16
609.0076		20202.92
610.01		26369.15
611.0103		35743.45
612.0111		41574.18
613.0118		55425.52
614.0137		54205.99
615.0148		59501.16
616.015		48483.43
617.0178	1	45436.3
618.0165	1	27364.58
619.021	1	19989.58

627.0111	1	20526.82
629.0126	1	34530.49
631.0147	1	43055.51
633.0154	1	35449.29

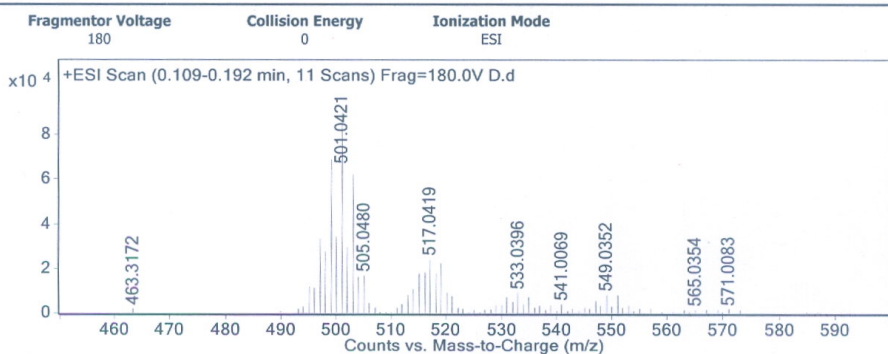


## Qualitative Analysis Report

<b>Data Filename</b>	D.d	<b>Sample Name</b>	D
<b>Sample Type</b>	Sample	<b>Position</b>	P1-F4
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	SANJAY PANDEY
<b>Acq Method</b>	DAILY MS.m	<b>Acquired Time</b>	15-04-2013 11:59:00
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	default.m
<b>Comment</b>			
<b>Sample Group</b>		<b>Info.</b>	
<b>Acquisition SW</b>	6200 series TOF/6500 series		
<b>Version</b>	Q-TOF B.05.01 (B5125)		

C<sub>24</sub> H<sub>26</sub> N<sub>2</sub> Se<sub>2</sub>  
 Se-Se (Me,H)

### User Spectra



### Peak List

<i>m/z</i>	<i>z</i>	Abund
104.0088		6306.67
106.0044		24938.39
108.0809		7363.07
138.0302		5316.96
495.0403		11656.38
496.0425		11011.62
497.0406		33875.86
498.0425		27775.81
499.0411	1	68723.09
500.0462	1	34105.49
501.0421	1	90280.62
502.0448	1	29364.46
503.0459	1	62468.51
504.0484	1	16582.54
505.048	1	16967.43
513.0412		8151.2
514.0399		10789.09
515.0414		18083.18
516.0409		18600.64
517.0419		24187.69
518.0392		17956.06
519.0427	1	22701.88
520.0413	1	9131.24
521.0425	1	7787.92
531.0403		7378.4
533.0396	1	9051.95

535.0376	1	7347.33
547.037	1	5445.25
549.0352	1	8203.96
551.0339	1	7944.32

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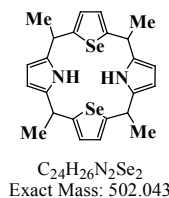
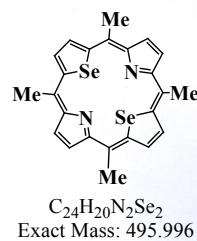
M<sup>+</sup>

M+1

{

M<sup>+</sup>

M+1



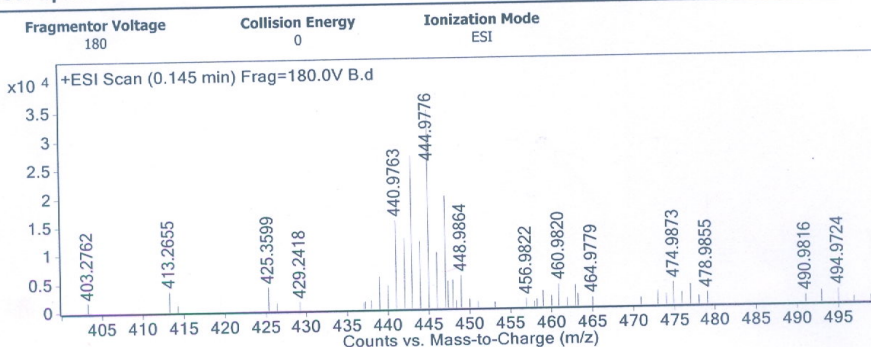
## Qualitative Analysis Report

Data Filename	B.d	Sample Name	B
Sample Type	Sample	Position	P1-F2
Instrument Name	Instrument 1	User Name	SANJAY PANDEY
Acq Method	DAILY MS.m	Acquired Time	15-04-2013 11:56:25
IRM Calibration Status	Success	DA Method	default.m

C<sub>20</sub>H<sub>18</sub>N<sub>2</sub>Se<sub>2</sub>  
 Se-Se Prop Calix

**Sample Group** Info.  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

### User Spectra

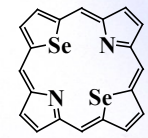


#### Peak List

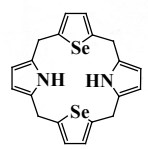
m/z	z	Abund
100.0762		5234.97
104.0088		5499.56
106.0043		23878.04
108.0809		12102.1
122.9643		5098.26
132.0034		4959.11
138.0304		6057.64
149.0227		7768.87
217.1036	1	17430.88
261.1297		6203.27
376.0703	1	21439.15
438.9777		5805.08
440.9763		15559.27
441.9784		12402.97
442.9763	1	26860.93
443.982	1	11874.24
444.9776	1	34947.79
445.9799	1	9883.26
446.9817	1	19789.09
448.9864	1	5724.04

M+1

M<sup>+</sup>  
M+1



**C<sub>20</sub>H<sub>12</sub>N<sub>2</sub>Se<sub>2</sub>**  
 Exact Mass: 439.933



**C<sub>20</sub>H<sub>18</sub>N<sub>2</sub>Se<sub>2</sub>**  
 Exact Mass: 445.980

--- End Of Report ---

## Crystal data of 5g

Table 1. Crystal data and structure refinement for 1.

Identification code	shelxl	
Empirical formula	C <sub>28</sub> H <sub>32</sub> N <sub>2</sub> Te <sub>2</sub>	
Formula weight		
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, P-1	
Unit cell dimensions		a = 10.361(2) Å    alpha = 101.396(15) deg. b = 11.572(3) Å    beta = 90.972(13) deg. c = 11.8258(15) Å    gamma = 104.51(2) deg.
Volume	1342.3(5) Å <sup>3</sup>	
Z, Calculated density	2, 1.613 Mg/m <sup>3</sup>	
Absorption coefficient	2.191 mm <sup>-1</sup>	
F(000)	636	
Crystal size	x x mm	
Theta range for data collection	3.52 to 29.04 deg.	
Limiting indices	-14<=h<=13, -15<=k<=15, -15<=l<=16	
Reflections collected / unique	13052 / 6096 [R(int) = 0.0748]	
Completeness to theta = 29.04	85.1 %	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	6096 / 0 / 290	
Goodness-of-fit on F <sup>2</sup>	0.656	
Final R indices [I>2sigma(I)]	R1 = 0.0713, wR2 = 0.1865	
R indices (all data)	R1 = 0.0848, wR2 = 0.2017	
Extinction coefficient	0.0069(9)	
Largest diff. peak and hole	2.490 and -2.417 e.Å <sup>-3</sup>	

Table 2. Atomic coordinates (x 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup> x 10<sup>3</sup>) for 1. U(eq) is defined as one third of the trace of the orthogonalized U<sub>ij</sub> tensor.

	x	y	z	U(eq)
Te(1)	1005(1)	6023(1)	1687(1)	44(1)
Te(2)	-3599(1)	4740(1)	1379(1)	39(1)
C(6)	2131(10)	3411(9)	1096(15)	85(5)
C(21)	-4761(9)	7342(8)	1838(10)	50(2)
N(1)	-1301(6)	2904(5)	2247(6)	30(1)
C(15)	-3845(6)	3532(6)	2503(6)	26(1)
C(18)	-3873(6)	5952(6)	2830(6)	26(1)
C(25)	-175(7)	8554(6)	2963(7)	31(1)
C(8)	-214(7)	2742(7)	1636(7)	35(2)
C(24)	-526(8)	9249(7)	2262(8)	40(2)
N(2)	-1338(6)	7811(5)	3221(5)	29(1)
C(22)	-2426(7)	7990(6)	2665(6)	26(1)
C(11)	-2466(7)	2179(6)	1638(6)	28(1)
C(12)	-3803(7)	2205(6)	2110(6)	29(1)
C(10)	-2104(9)	1549(9)	655(8)	47(2)
C(4)	1221(7)	4764(7)	2681(9)	42(2)
C(19)	-3834(7)	7286(6)	2827(7)	31(1)
C(9)	-697(10)	1880(9)	660(9)	51(2)
C(23)	-1929(8)	8907(7)	2079(7)	37(2)
C(1)	1183(7)	7165(7)	3296(8)	36(2)
C(17)	-4024(10)	5381(8)	3742(7)	45(2)
C(14)	-4940(8)	1512(8)	1170(9)	48(2)
C(5)	1207(7)	3440(7)	2114(9)	44(2)
C(27)	2294(9)	9230(9)	2826(12)	64(3)
C(7)	1666(11)	2820(10)	3036(13)	76(4)
C(26)	1163(7)	8516(7)	3462(8)	39(2)
C(16)	-4002(10)	4138(8)	3577(7)	43(2)
C(3)	1360(10)	5379(12)	3805(9)	58(3)
C(13)	-4016(9)	1539(8)	3131(8)	43(2)
C(20)	-4296(10)	7896(8)	3976(9)	50(2)

C(2)	1340(10)	6465(12)	4096(8)	57(3)
C(28)	1336(10)	9127(9)	4757(10)	62(3)

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Table 3. Selected bond lengths [Å] and angles [deg] for 1.

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Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [Å] and angles [deg] for 1.

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Te(1)-C(1)	2.067(9)
Te(1)-C(4)	2.095(8)
Te(2)-C(18)	2.064(7)
Te(2)-C(15)	2.086(7)
C(6)-C(5)	1.551(15)
C(21)-C(19)	1.522(11)
N(1)-C(8)	1.380(9)
N(1)-C(11)	1.380(9)
C(15)-C(16)	1.358(10)
C(15)-C(12)	1.525(9)
C(18)-C(17)	1.364(11)
C(18)-C(19)	1.535(9)
C(25)-C(24)	1.367(11)
C(25)-N(2)	1.371(9)
C(25)-C(26)	1.511(10)
C(8)-C(9)	1.362(13)
C(8)-C(5)	1.528(11)
C(24)-C(23)	1.408(11)
N(2)-C(22)	1.375(9)
C(22)-C(23)	1.379(10)
C(22)-C(19)	1.518(9)
C(11)-C(10)	1.356(11)
C(11)-C(12)	1.507(9)
C(12)-C(13)	1.547(11)
C(12)-C(14)	1.548(10)
C(10)-C(9)	1.412(13)
C(4)-C(3)	1.365(14)
C(4)-C(5)	1.543(11)
C(19)-C(20)	1.545(11)
C(1)-C(2)	1.393(13)
C(1)-C(26)	1.543(10)
C(17)-C(16)	1.419(12)
C(5)-C(7)	1.547(15)
C(27)-C(26)	1.552(12)
C(26)-C(28)	1.542(14)
C(3)-C(2)	1.241(16)
C(1)-Te(1)-C(4)	82.3(4)
C(18)-Te(2)-C(15)	83.3(3)
C(8)-N(1)-C(11)	109.9(6)
C(16)-C(15)-C(12)	128.7(7)
C(16)-C(15)-Te(2)	108.8(5)
C(12)-C(15)-Te(2)	122.4(5)
C(17)-C(18)-C(19)	128.2(7)
C(17)-C(18)-Te(2)	108.9(5)
C(19)-C(18)-Te(2)	122.9(5)
C(24)-C(25)-N(2)	107.0(6)
C(24)-C(25)-C(26)	132.2(7)
N(2)-C(25)-C(26)	120.8(7)
C(9)-C(8)-N(1)	106.9(7)
C(9)-C(8)-C(5)	132.1(7)
N(1)-C(8)-C(5)	120.9(7)
C(25)-C(24)-C(23)	108.0(7)

C(25)-N(2)-C(22)	110.7(6)
N(2)-C(22)-C(23)	106.1(6)
N(2)-C(22)-C(19)	120.8(6)
C(23)-C(22)-C(19)	132.9(6)
C(10)-C(11)-N(1)	106.7(7)
C(10)-C(11)-C(12)	132.8(7)
N(1)-C(11)-C(12)	120.4(6)
C(11)-C(12)-C(15)	108.7(6)
C(11)-C(12)-C(13)	110.0(6)
C(15)-C(12)-C(13)	110.6(6)
C(11)-C(12)-C(14)	110.0(6)
C(15)-C(12)-C(14)	110.7(6)
C(13)-C(12)-C(14)	106.8(7)
C(11)-C(10)-C(9)	108.5(8)
C(3)-C(4)-C(5)	132.7(9)
C(3)-C(4)-Te(1)	105.8(7)
C(5)-C(4)-Te(1)	121.5(7)
C(22)-C(19)-C(21)	108.6(7)
C(22)-C(19)-C(18)	110.2(5)
C(21)-C(19)-C(18)	109.9(6)
C(22)-C(19)-C(20)	109.2(6)
C(21)-C(19)-C(20)	108.5(7)
C(18)-C(19)-C(20)	110.5(7)
C(8)-C(9)-C(10)	107.8(7)
C(22)-C(23)-C(24)	108.2(7)
C(2)-C(1)-C(26)	131.1(9)
C(2)-C(1)-Te(1)	106.0(7)
C(26)-C(1)-Te(1)	122.9(6)
C(18)-C(17)-C(16)	119.9(7)
C(8)-C(5)-C(4)	109.2(6)
C(8)-C(5)-C(7)	109.3(7)
C(4)-C(5)-C(7)	109.1(9)
C(8)-C(5)-C(6)	108.1(9)
C(4)-C(5)-C(6)	110.9(7)
C(7)-C(5)-C(6)	110.3(9)
C(25)-C(26)-C(28)	109.3(7)
C(25)-C(26)-C(1)	107.7(6)
C(28)-C(26)-C(1)	110.5(8)
C(25)-C(26)-C(27)	109.3(8)
C(28)-C(26)-C(27)	108.9(8)
C(1)-C(26)-C(27)	111.1(7)
C(15)-C(16)-C(17)	119.1(7)
C(2)-C(3)-C(4)	123.2(10)
C(3)-C(2)-C(1)	122.6(10)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.

The anisotropic displacement factor exponent takes the form:

$-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	U11	U22	U33	U23	U13	U12
Te(1)	46(1)	34(1)	53(1)	11(1)	3(1)	10(1)
Te(2)	55(1)	32(1)	30(1)	10(1)	12(1)	8(1)
C(6)	38(5)	36(5)	171(15)	4(7)	49(7)	2(4)
C(21)	33(4)	36(4)	77(7)	8(4)	-20(4)	5(3)
N(1)	20(3)	26(3)	40(3)	6(2)	10(2)	-3(2)
C(15)	18(3)	24(3)	34(3)	8(3)	4(2)	-2(2)
C(18)	15(3)	20(3)	39(4)	10(3)	6(2)	-6(2)
C(25)	20(3)	23(3)	43(4)	3(3)	5(3)	-2(3)
C(8)	21(3)	27(3)	58(5)	16(3)	19(3)	3(3)
C(24)	37(4)	27(4)	53(5)	18(3)	11(3)	-5(3)
N(2)	23(3)	29(3)	38(3)	16(3)	4(2)	3(2)
C(22)	22(3)	23(3)	30(3)	6(3)	2(2)	2(3)
C(11)	26(3)	23(3)	34(3)	9(3)	7(3)	1(3)
C(12)	22(3)	24(3)	36(4)	6(3)	5(3)	-2(3)
C(10)	46(5)	48(5)	40(4)	-3(4)	4(4)	11(4)
C(4)	12(3)	28(4)	87(7)	27(4)	5(3)	-4(3)

C(19)	24(3)	26(3)	43(4)	9(3)	6(3)	5(3)
C(9)	51(5)	51(5)	52(5)	1(4)	19(4)	20(4)
C(23)	34(4)	32(4)	45(4)	15(3)	-2(3)	3(3)
C(1)	14(3)	29(3)	61(5)	10(3)	6(3)	-1(3)
C(17)	62(6)	45(5)	32(4)	9(3)	16(4)	20(4)
C(14)	32(4)	36(4)	60(6)	-7(4)	-7(4)	-6(3)
C(5)	18(3)	23(3)	93(7)	16(4)	12(4)	1(3)
C(27)	25(4)	39(5)	123(10)	24(6)	19(5)	-5(4)
C(7)	48(6)	43(5)	138(12)	26(7)	-20(7)	14(5)
C(26)	19(3)	27(3)	64(5)	5(4)	0(3)	0(3)
C(16)	62(5)	39(4)	30(4)	13(3)	18(4)	15(4)
C(3)	41(5)	80(8)	43(5)	25(5)	0(4)	-12(5)
C(13)	41(4)	33(4)	56(5)	23(4)	16(4)	0(3)
C(20)	52(5)	40(5)	62(6)	9(4)	22(4)	18(4)
C(2)	39(5)	92(8)	39(5)	30(5)	-3(4)	2(5)
C(28)	51(6)	47(5)	72(7)	-14(5)	-31(5)	10(4)

Table 6. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{Å}^2 \times 10^3$ ) for 1.

	x	y	z	U(eq)
H(6A)	3030	3846	1378	127
H(6B)	1830	3790	526	127
H(6C)	2103	2580	754	127
H(21A)	-5656	6900	1930	75
H(21B)	-4472	6984	1116	75
H(21C)	-4738	8178	1845	75
H(1)	-1258	3385	2909	36
H(24)	59	9843	1958	48
H(2)	-1381	7303	3670	35
H(10)	-2686	992	75	56
H(9)	-189	1564	97	61
H(23)	-2433	9242	1639	44
H(17)	-4141	5806	4471	54
H(14A)	-5788	1525	1480	72
H(14B)	-4893	682	930	72
H(14C)	-4844	1898	518	72
H(27A)	3146	9208	3141	95
H(27B)	2248	10062	2927	95
H(27C)	2188	8861	2017	95
H(7A)	2559	3256	3337	113
H(7B)	1647	1992	2691	113
H(7C)	1076	2828	3654	113
H(16)	-4094	3744	4195	51
H(3)	1475	4964	4382	70
H(13A)	-4869	1559	3425	64
H(13B)	-3322	1938	3732	64
H(13C)	-3987	706	2868	64
H(20A)	-5184	7450	4085	75
H(20B)	-4292	8721	3952	75
H(20C)	-3699	7895	4606	75
H(2)	1433	6826	4879	68
H(28A)	2186	9105	5076	92
H(28B)	635	8696	5156	92
H(28C)	1295	9960	4846	92

Table 7. Selected torsion angles [deg] for 1.


Symmetry transformations used to generate equivalent atoms:

Table 8. Torsion angles [deg] for 1.

C(18)-Te(2)-C(15)-C(16)	-2.2(6)
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C(18)-Te(2)-C(15)-C(12)	179.3(5)
C(15)-Te(2)-C(18)-C(17)	1.8(6)
C(15)-Te(2)-C(18)-C(19)	179.3(5)
C(11)-N(1)-C(8)-C(9)	-2.2(9)
C(11)-N(1)-C(8)-C(5)	179.9(7)
N(2)-C(25)-C(24)-C(23)	-0.8(9)
C(26)-C(25)-C(24)-C(23)	-179.2(8)
C(24)-C(25)-N(2)-C(22)	2.1(8)
C(26)-C(25)-N(2)-C(22)	-179.4(6)
C(25)-N(2)-C(22)-C(23)	-2.4(8)
C(25)-N(2)-C(22)-C(19)	-179.1(6)
C(8)-N(1)-C(11)-C(10)	1.1(9)
C(8)-N(1)-C(11)-C(12)	-178.8(6)
C(10)-C(11)-C(12)-C(15)	-131.9(9)
N(1)-C(11)-C(12)-C(15)	47.9(9)
C(10)-C(11)-C(12)-C(13)	106.8(10)
N(1)-C(11)-C(12)-C(13)	-73.4(8)
C(10)-C(11)-C(12)-C(14)	-10.6(12)
N(1)-C(11)-C(12)-C(14)	169.2(7)
C(16)-C(15)-C(12)-C(11)	-119.1(9)
Te(2)-C(15)-C(12)-C(11)	59.1(7)
C(16)-C(15)-C(12)-C(13)	1.8(11)
Te(2)-C(15)-C(12)-C(13)	180.0(5)
C(16)-C(15)-C(12)-C(14)	120.0(9)
Te(2)-C(15)-C(12)-C(14)	-61.8(8)
N(1)-C(11)-C(10)-C(9)	0.5(10)
C(12)-C(11)-C(10)-C(9)	-179.7(8)
C(1)-Te(1)-C(4)-C(3)	-0.2(6)
C(1)-Te(1)-C(4)-C(5)	179.9(6)
N(2)-C(22)-C(19)-C(21)	-161.4(7)
C(23)-C(22)-C(19)-C(21)	23.0(11)
N(2)-C(22)-C(19)-C(18)	-41.0(9)
C(23)-C(22)-C(19)-C(18)	143.4(8)
N(2)-C(22)-C(19)-C(20)	80.5(8)
C(23)-C(22)-C(19)-C(20)	-95.1(10)
C(17)-C(18)-C(19)-C(22)	108.5(9)
Te(2)-C(18)-C(19)-C(22)	-68.4(7)
C(17)-C(18)-C(19)-C(21)	-132.0(9)
Te(2)-C(18)-C(19)-C(21)	51.1(8)
C(17)-C(18)-C(19)-C(20)	-12.2(11)
Te(2)-C(18)-C(19)-C(20)	170.8(5)
N(1)-C(8)-C(9)-C(10)	2.4(10)
C(5)-C(8)-C(9)-C(10)	180.0(9)
C(11)-C(10)-C(9)-C(8)	-1.9(11)
N(2)-C(22)-C(23)-C(24)	1.8(9)
C(19)-C(22)-C(23)-C(24)	177.9(8)
C(25)-C(24)-C(23)-C(22)	-0.6(10)
C(4)-Te(1)-C(1)-C(2)	0.0(6)
C(4)-Te(1)-C(1)-C(26)	178.7(6)
C(19)-C(18)-C(17)-C(16)	-178.5(8)
Te(2)-C(18)-C(17)-C(16)	-1.2(11)
C(9)-C(8)-C(5)-C(4)	142.4(10)
N(1)-C(8)-C(5)-C(4)	-40.4(11)
C(9)-C(8)-C(5)-C(7)	-98.4(12)
N(1)-C(8)-C(5)-C(7)	78.9(10)
C(9)-C(8)-C(5)-C(6)	21.7(13)
N(1)-C(8)-C(5)-C(6)	-161.1(8)
C(3)-C(4)-C(5)-C(8)	108.4(10)
Te(1)-C(4)-C(5)-C(8)	-71.8(8)
C(3)-C(4)-C(5)-C(7)	-11.0(12)
Te(1)-C(4)-C(5)-C(7)	168.8(6)
C(3)-C(4)-C(5)-C(6)	-132.6(11)
Te(1)-C(4)-C(5)-C(6)	47.2(10)
C(24)-C(25)-C(26)-C(28)	105.2(11)
N(2)-C(25)-C(26)-C(28)	-73.0(9)
C(24)-C(25)-C(26)-C(1)	-134.7(9)
N(2)-C(25)-C(26)-C(1)	47.2(10)

C(24)-C(25)-C(26)-C(27)	-13.9(12)
N(2)-C(25)-C(26)-C(27)	167.9(7)
C(2)-C(1)-C(26)-C(25)	-120.2(9)
Te(1)-C(1)-C(26)-C(25)	61.5(8)
C(2)-C(1)-C(26)-C(28)	-0.8(11)
Te(1)-C(1)-C(26)-C(28)	-179.2(6)
C(2)-C(1)-C(26)-C(27)	120.2(10)
Te(1)-C(1)-C(26)-C(27)	-58.2(9)
C(12)-C(15)-C(16)-C(17)	-179.3(8)
Te(2)-C(15)-C(16)-C(17)	2.2(10)
C(18)-C(17)-C(16)-C(15)	-0.8(14)
C(5)-C(4)-C(3)-C(2)	-179.7(9)
Te(1)-C(4)-C(3)-C(2)	0.4(12)
C(4)-C(3)-C(2)-C(1)	-0.5(16)
C(26)-C(1)-C(2)-C(3)	-178.3(9)
Te(1)-C(1)-C(2)-C(3)	0.3(12)

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Symmetry transformations used to generate equivalent atoms:

Table 9. Hydrogen bonds for 1 [A and deg.].

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D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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