Supporting Information

Synthesis of 21,23-Selenium and Tellurium substituted 5-Porphomethenes, 5,10-Porphodimethenes, 5,15-Porphodimethenes, and Porphotrimethenes and their interactions with mercury

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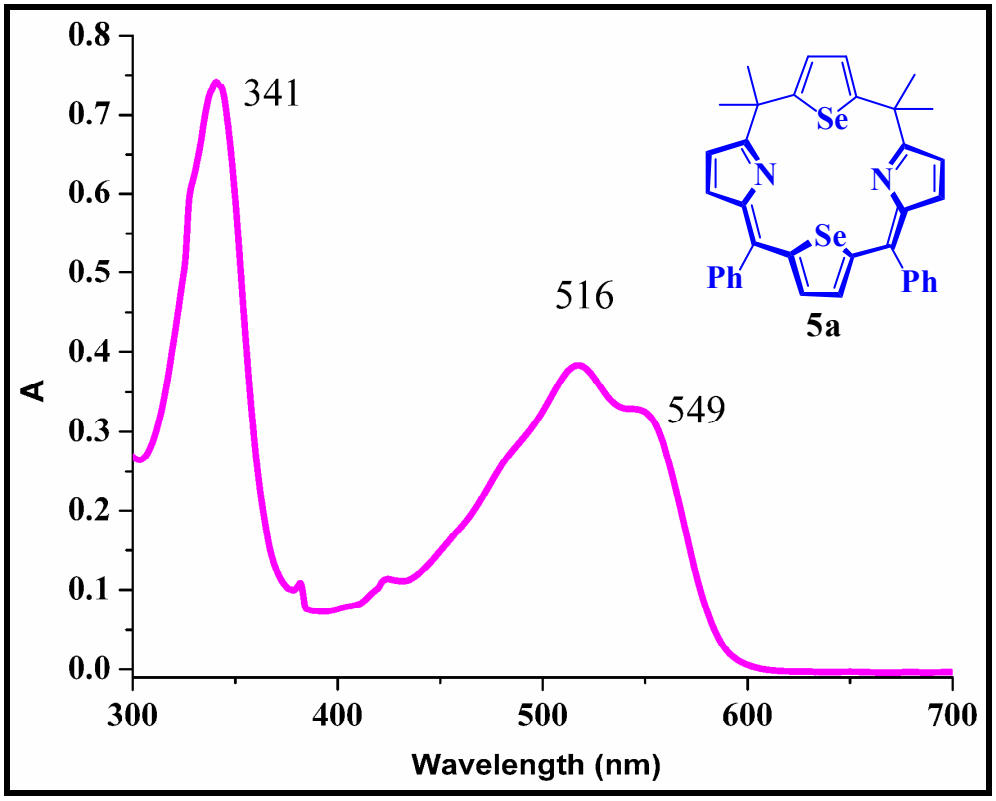
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0.5
0.4
0.3
0.2
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A
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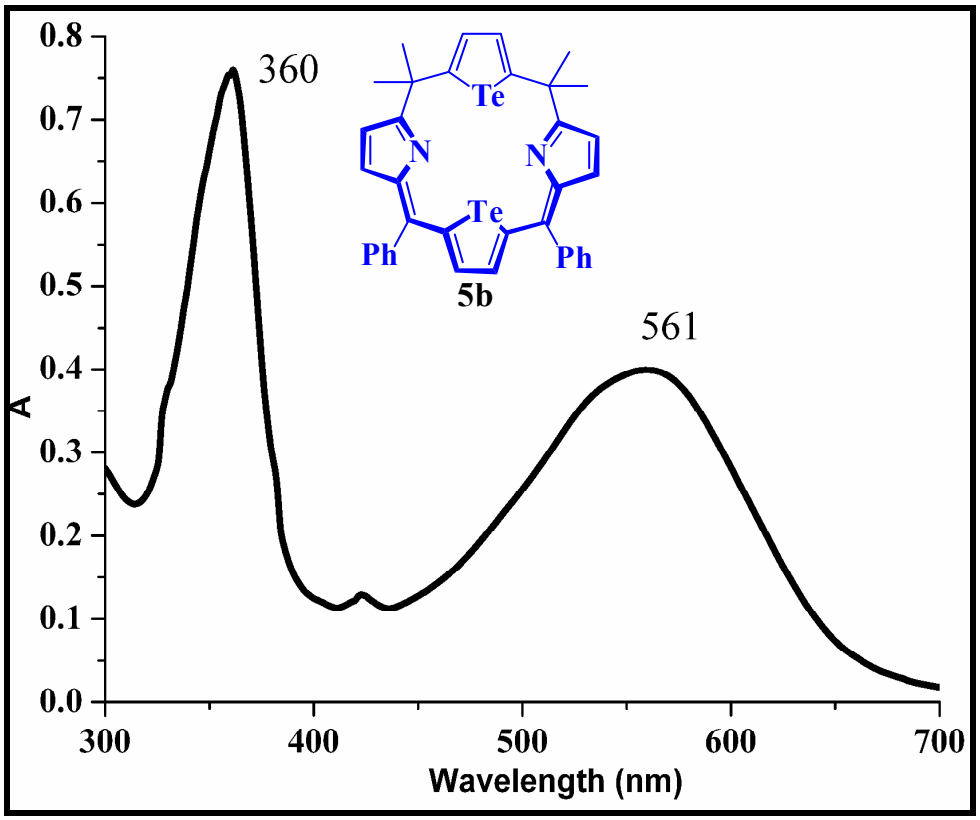
516
549
300
400
500
600
700
Wavelength (nm)
Se
N
N
Se
Ph
Ph
5a

Figure S1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0.5
0.4
0.3
0.2
0.1
0.0
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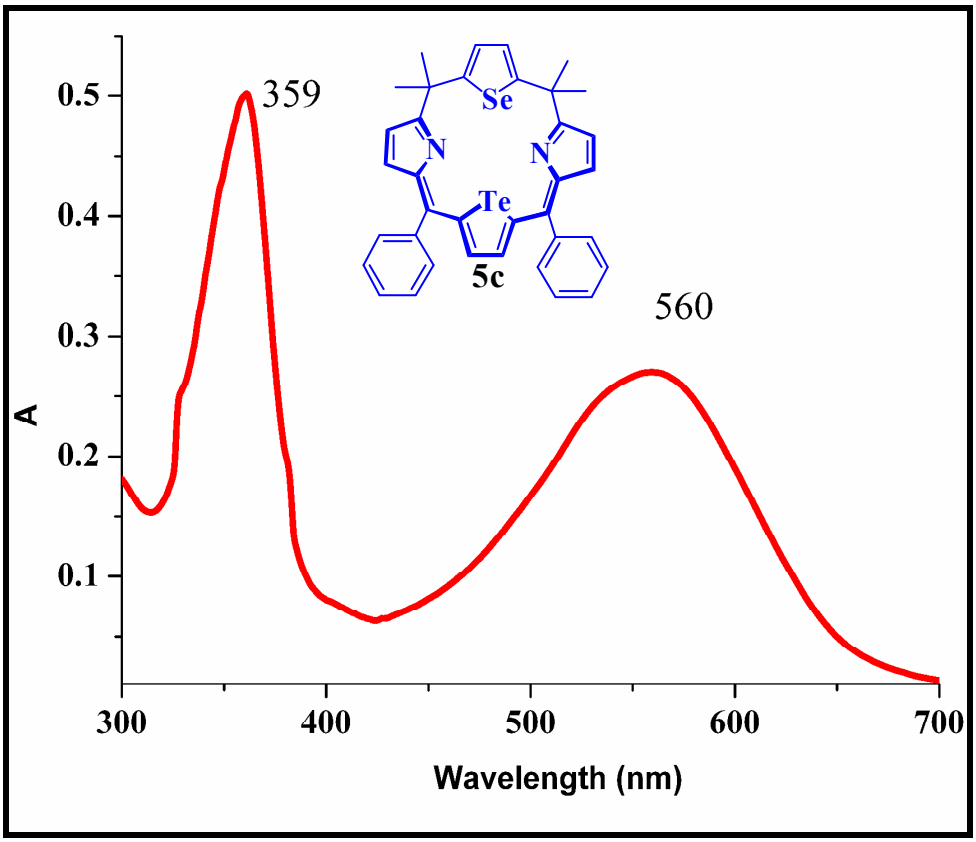
Te
N
N
Te
Ph
Ph
5b
300
400
500
600
700
Wavelength (nm)

Figure S2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560
Se
N
N
Te
5c
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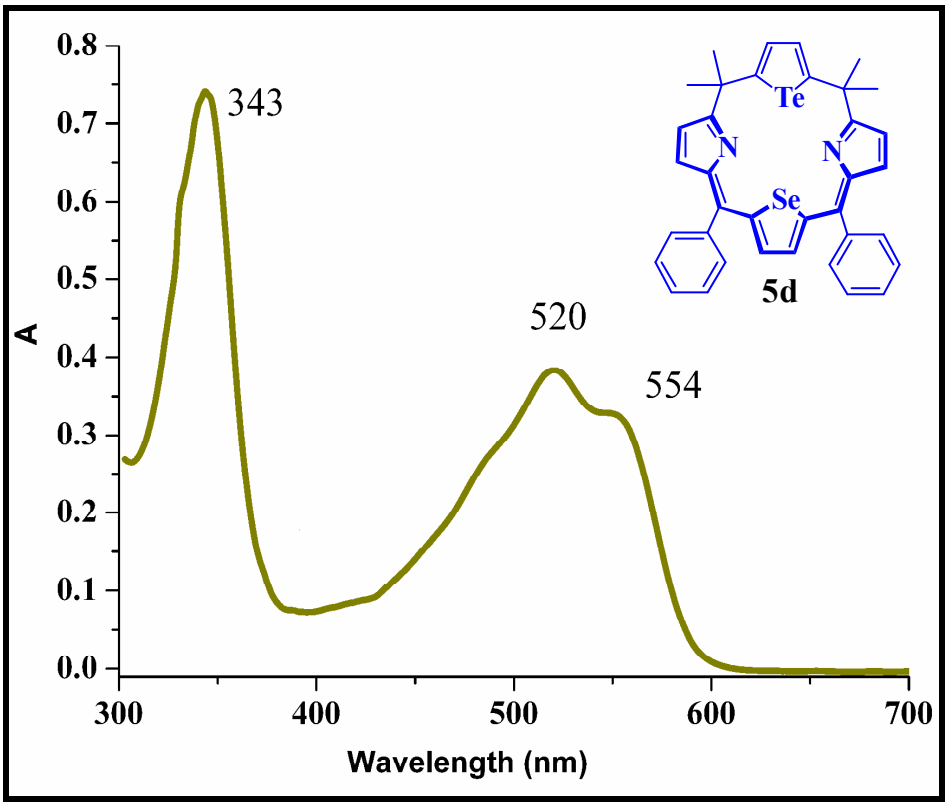
0.4
0.3
0.2
0.1
300
400
500
600
700
Wavelength (nm)

Figure S3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0.1
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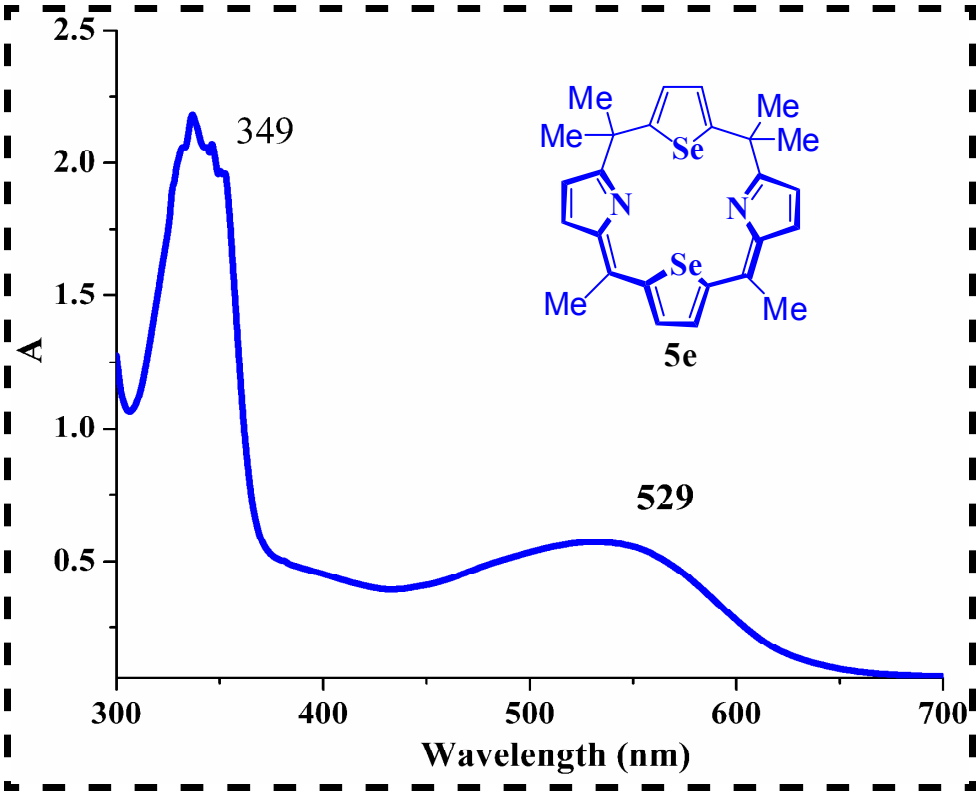
520
554
300
400
500
600
700
Wavelength (nm)
Te
N
N
Se
5d

Figure S4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1.5
1.0
0.5
A
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529
300
400
500
600
700
Wavelength (nm)
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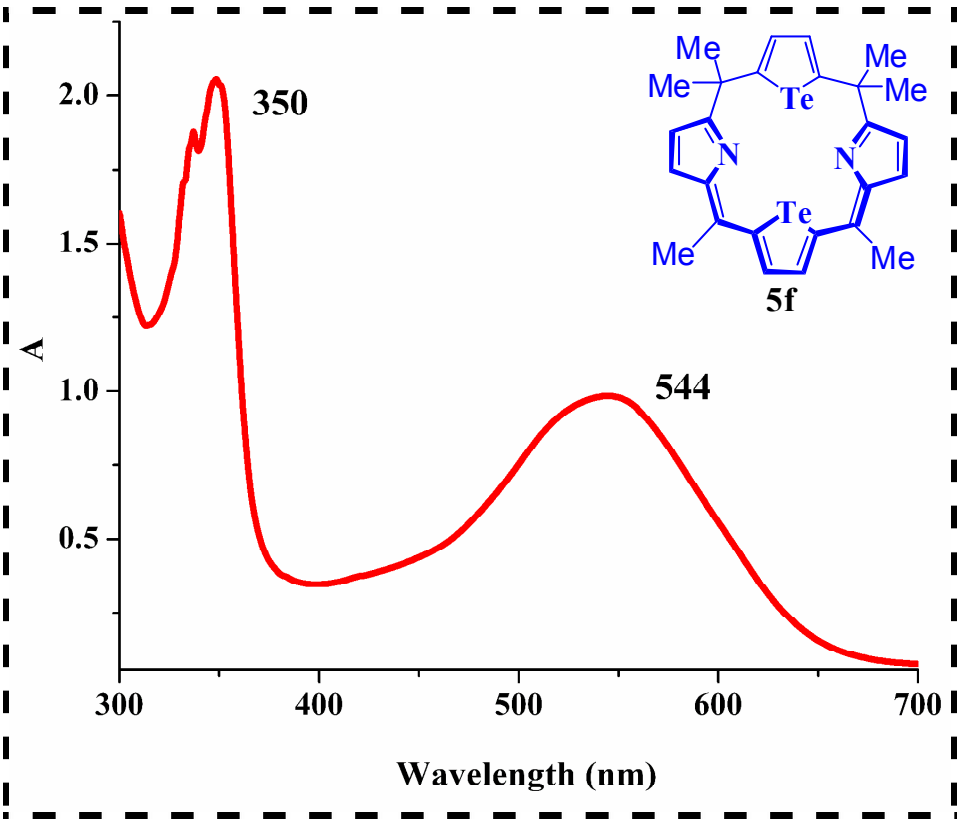
Me
Se
N
N
Se
Me
Me
5e

Figure S5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1.0
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A
350
544
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400
500
600
700
Wavelength (nm)
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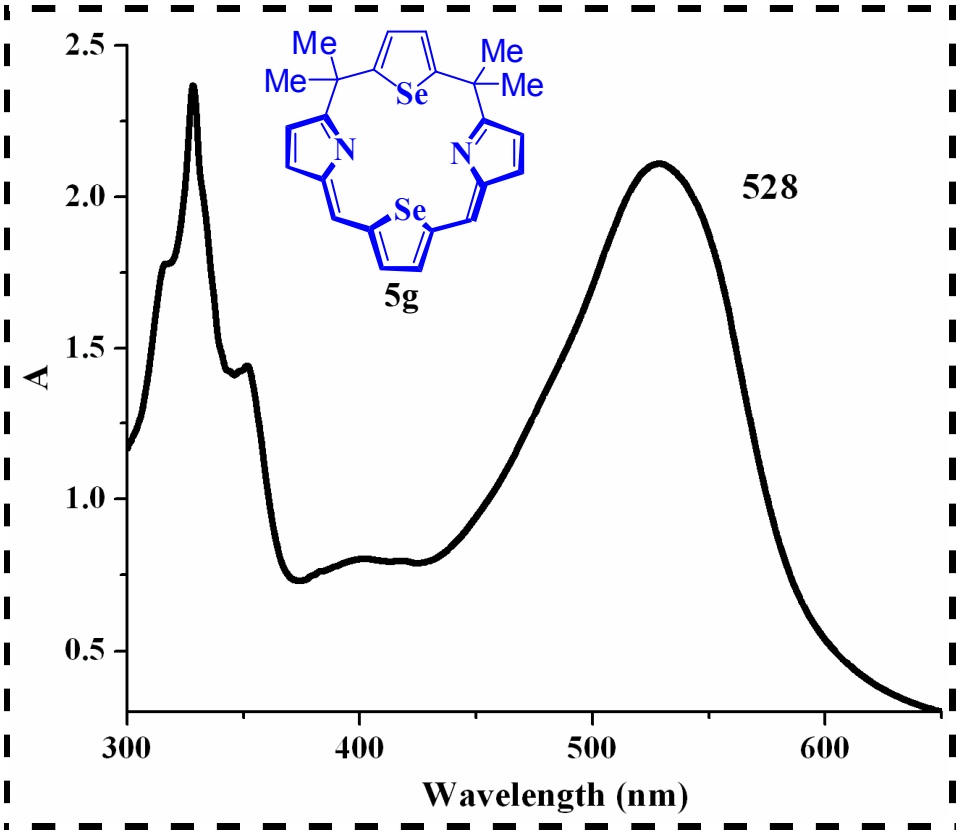
Me
Me
Me
Te
N
N
Te
Me
Me
5f

Figure S6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Me
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Me
Se
N
N
Se
5g
528
A
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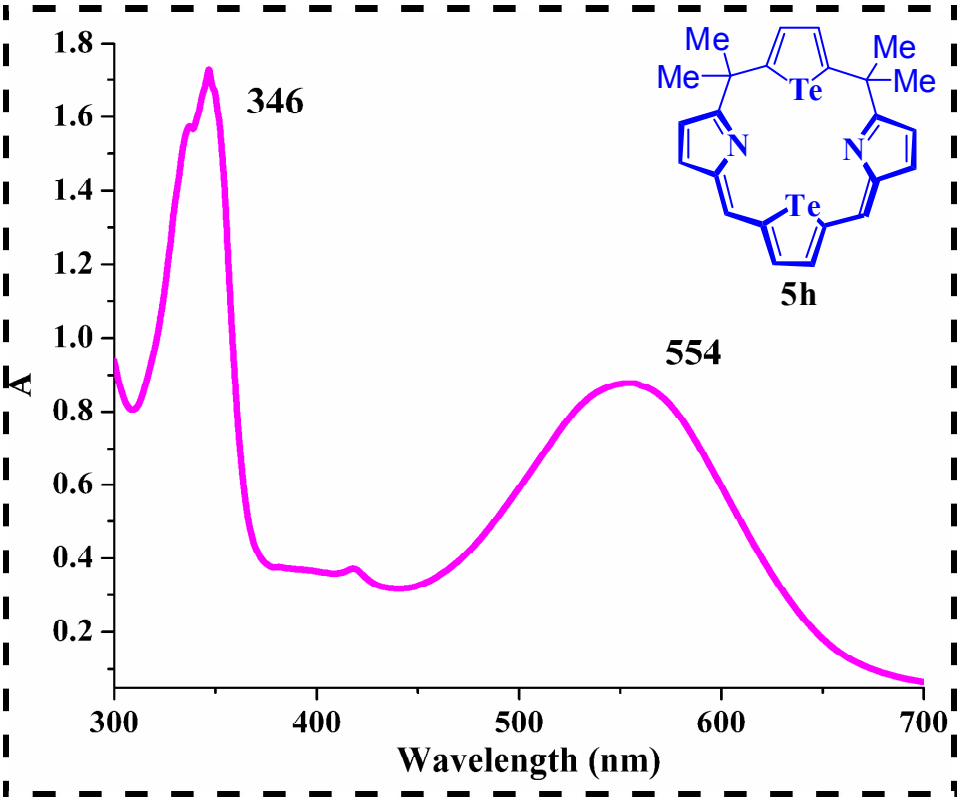
1.5
1.0
0.5
300
400
500
600
Wavelength (nm)

Figure S7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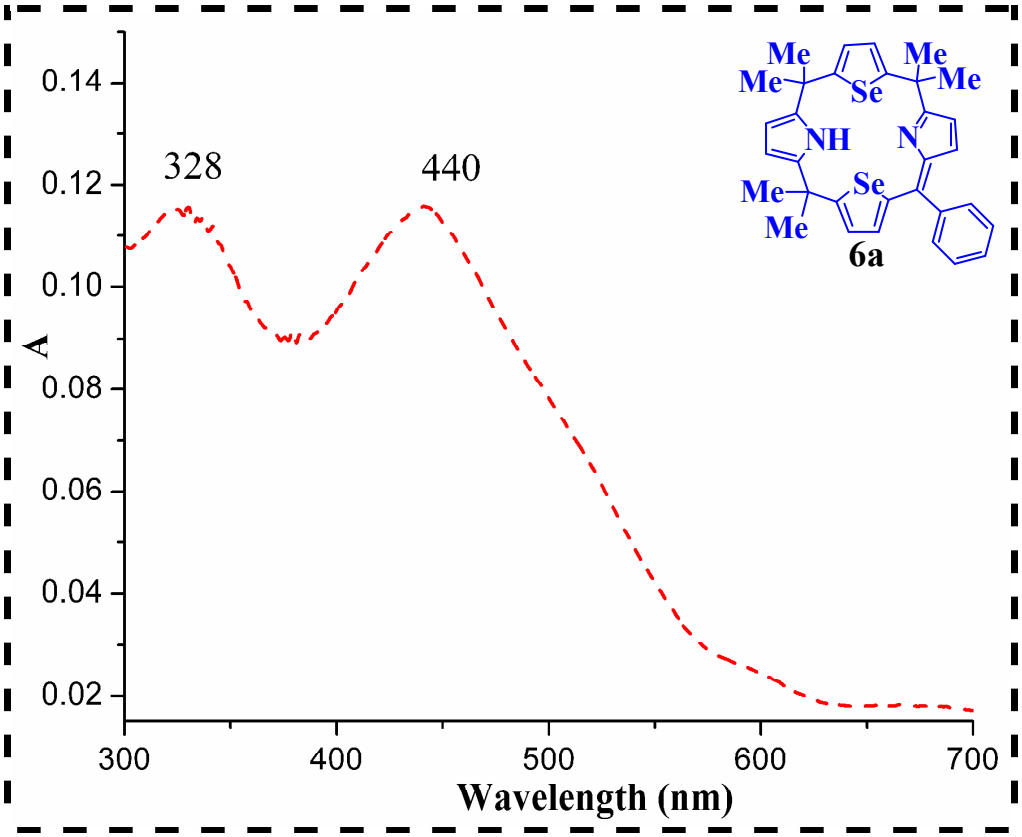
1.4
1.2
1.0
0.8
0.6
0.4
0.2
A
346
554
300
400
500
600
700
Wavelength (nm)
Me
Me
Me
Me
Te
N
N
Te
5h

Figure S8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0.10
0.08
0.06
0.04
0.02
A
328
440
300
400
500
600
700
Wavelength (nm)
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Me
Me
Me
Se
NH
N
Me
Me
Se
6a

Figure S9

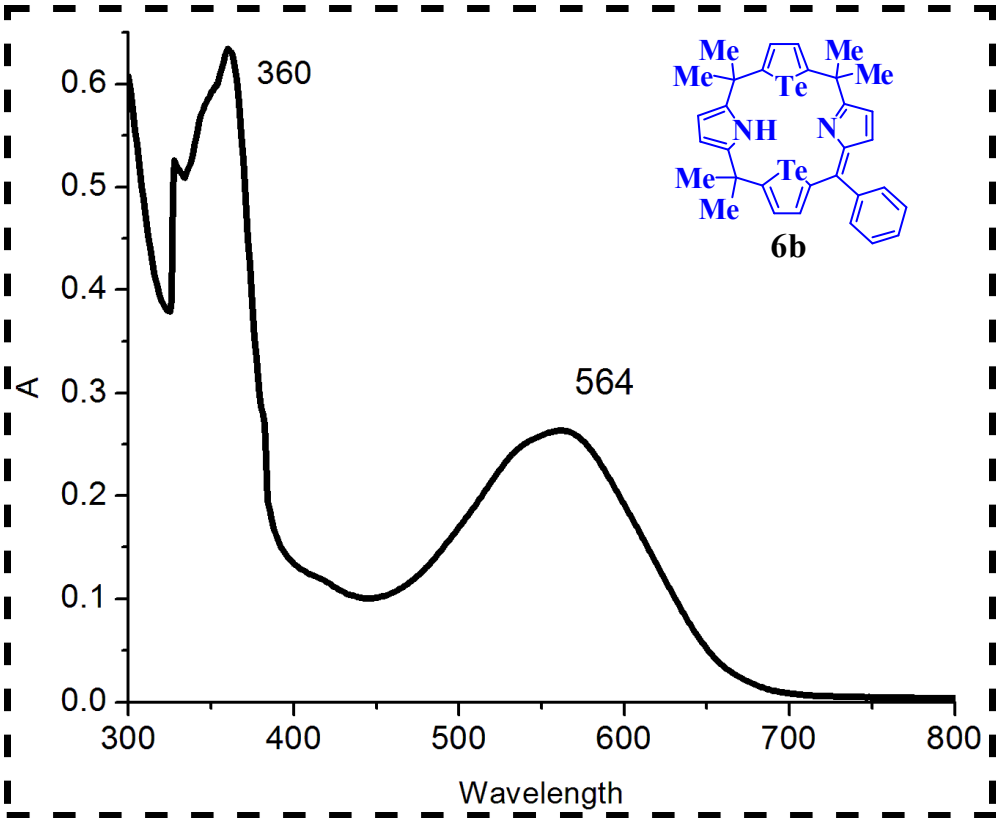
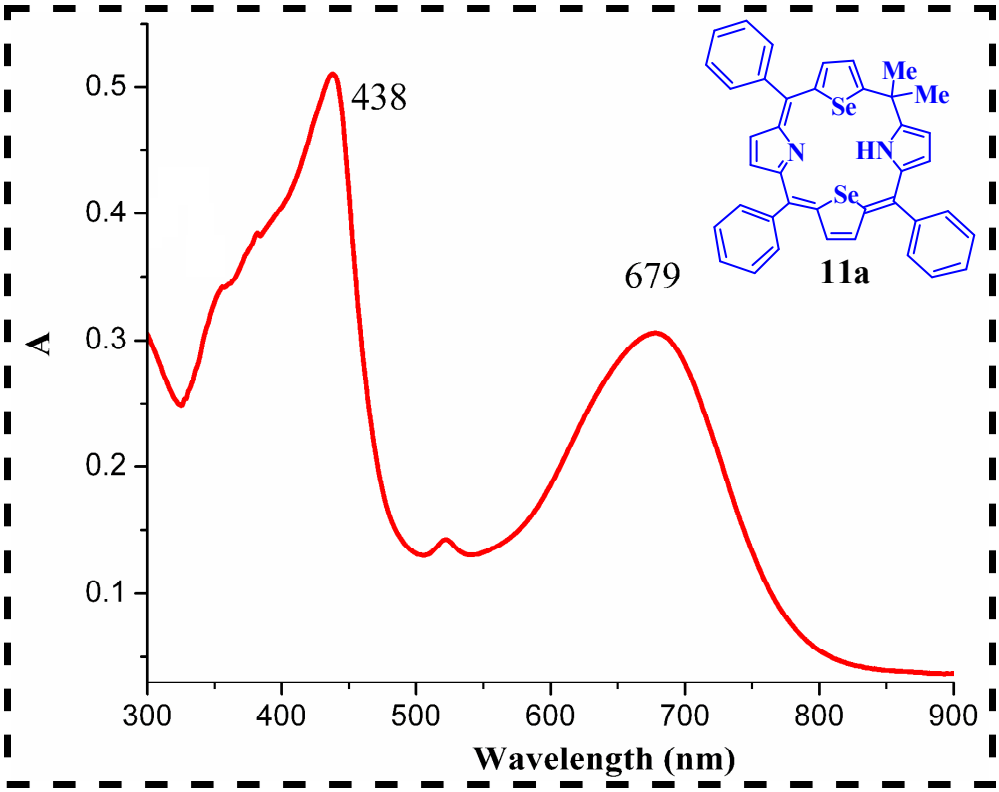

360
564
A
Wavelength
0.0
0.1
0.2
0.3
0.4
0.5
0.6
300
400
500
600
700
800
Me
Me
Me
Me
Te
NH
N
Te
Me
Me
6b

Figure S10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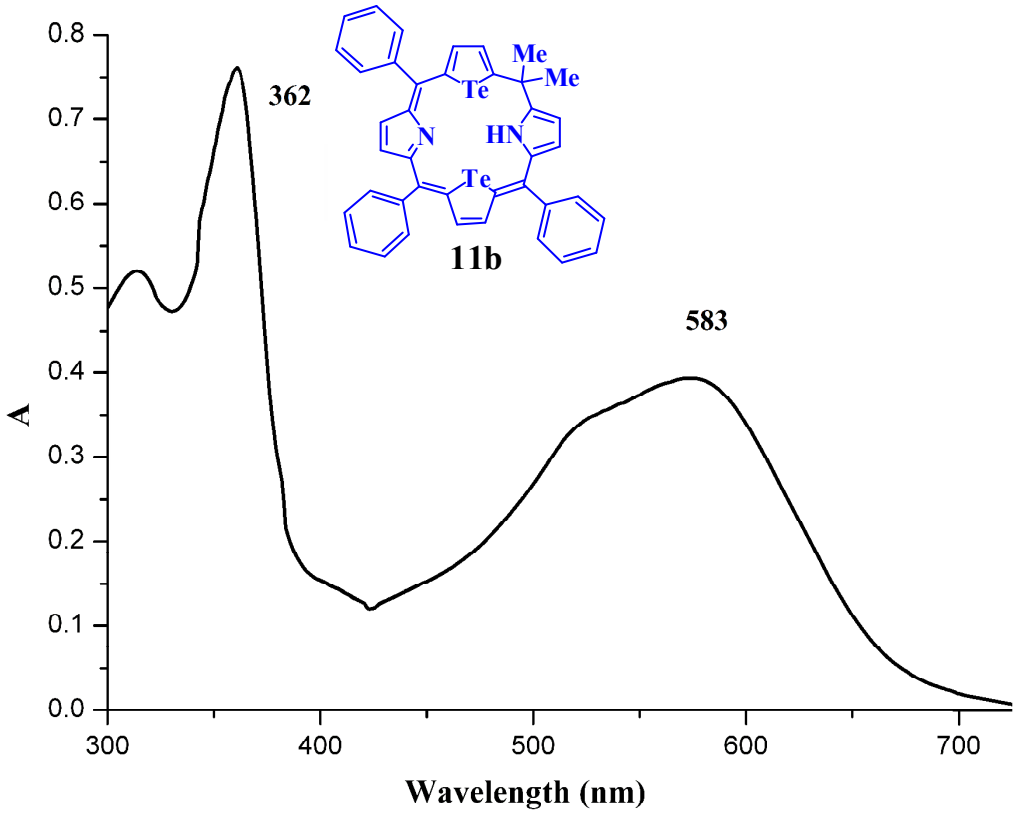
679
11a
Me
Me
Se
N
HN
Se
A
0.5
0.4
0.3
0.2
0.1
300
400
500
600
700
800
900
Wavelength (nm)

Figure S11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0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
A
362
583
Me
Me
Te
N
HN
Te
11b
300
400
500
600
700
Wavelength (nm)

Figure S12

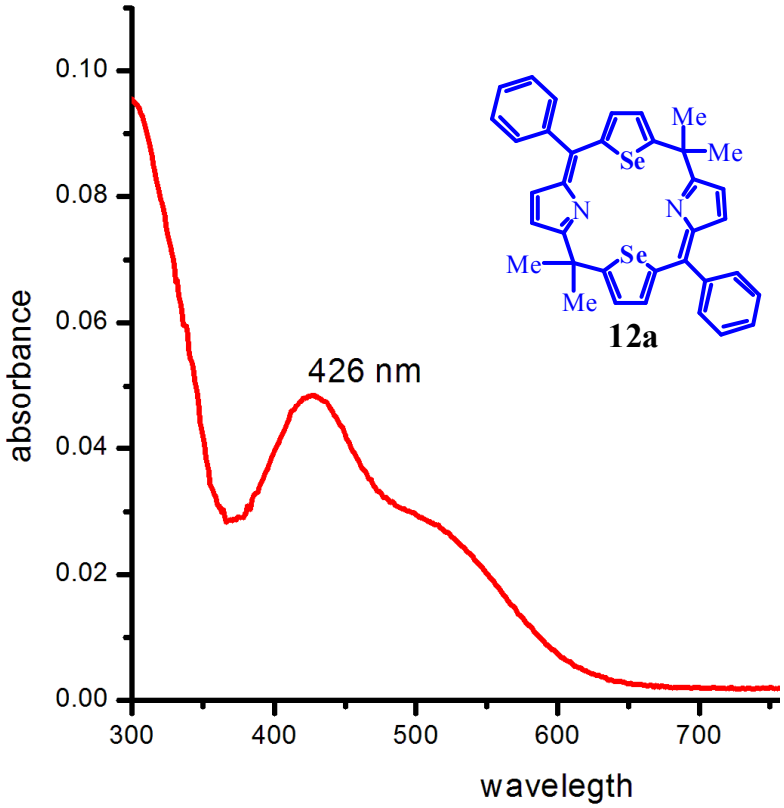

0.10
0.08
0.06
0.04
0.02
0.00
absorbance
426 nm
300
400
500
600
700
wavelegth
Me
Me
Se
N
N
Se
Me
Me
12a

Figure S13

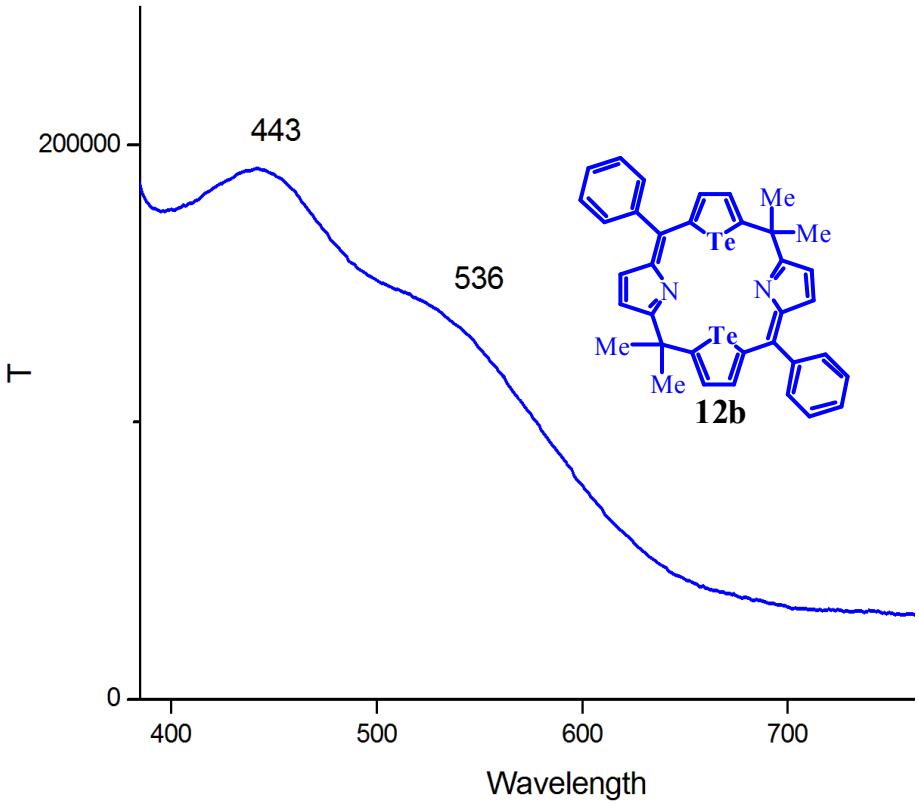

200000
0
T
443
536
400
500
600
700
Wavelength
Me
Me
Te
N
N
Te
Me
Me
12b

Figure S14

The electronic absorption spectroscopic titration of Se_2,N_2-hybrid 5,10-bis(phenyl)-15,20-tetramethyl-21-23-diselenaporphodimethene (5a) with different metal ions.

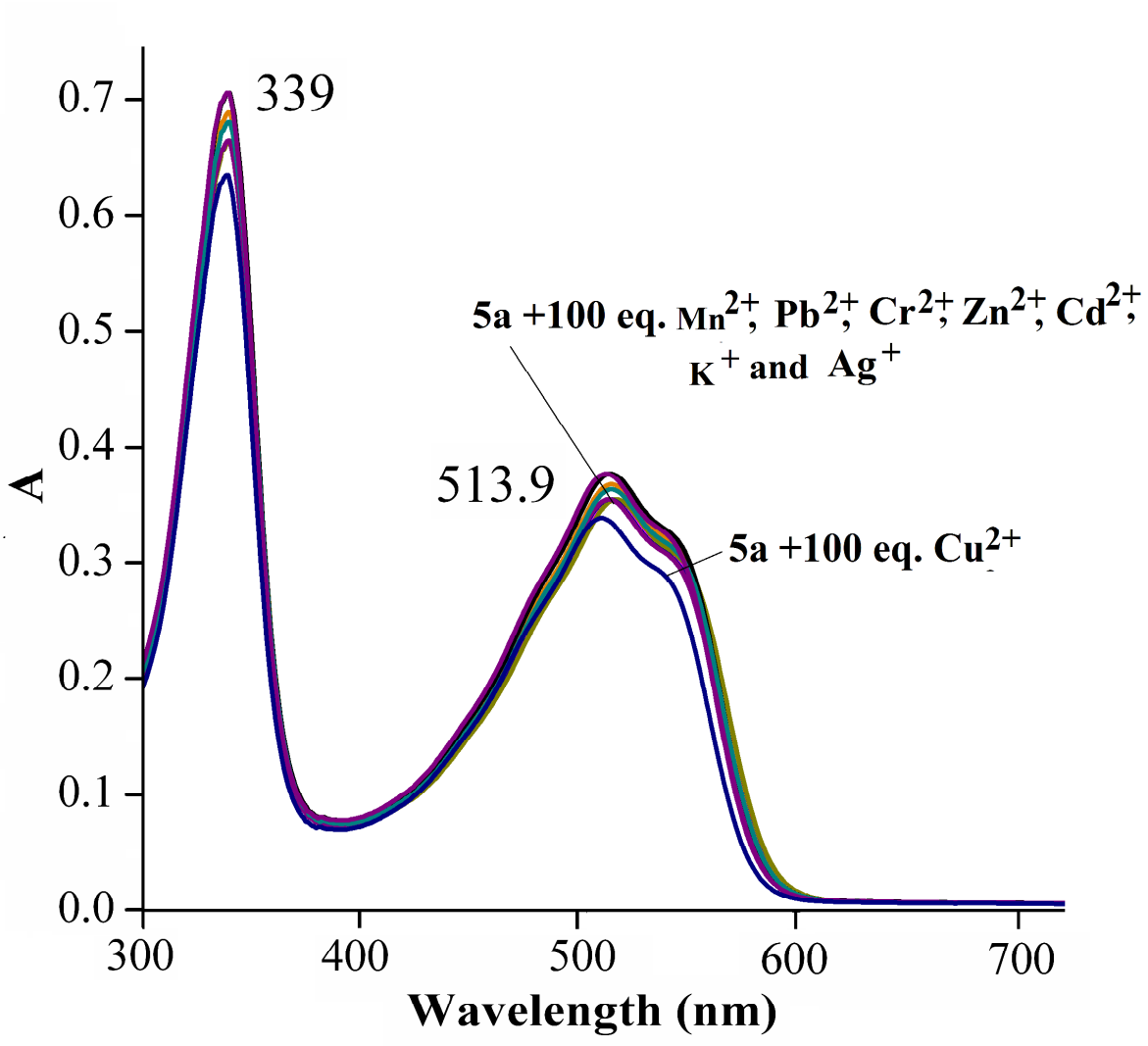


Figure S15

The fluorescence titration of Se_2,N_2-hybrid 5,10-bis(phenyl)-15,20-tetramethyl-21-23-diselenaporphodimethene (5a) with different metal ions.

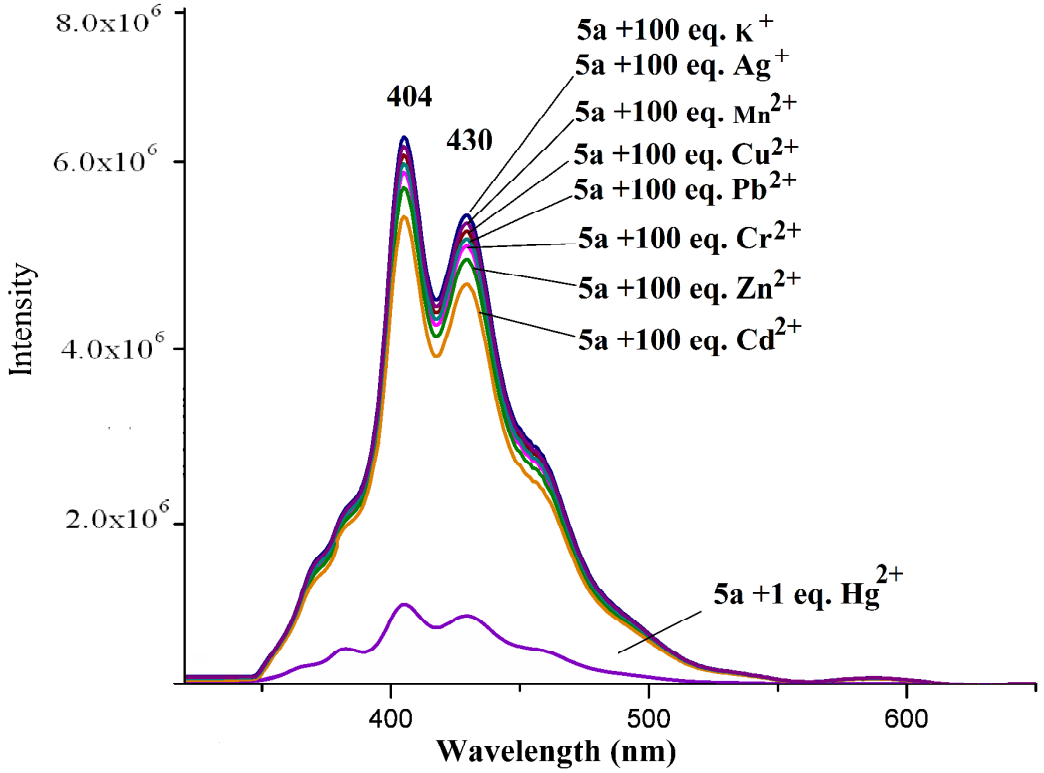


Figure S16

The fluorescence spectroscopic titration of Te_2,N_2-hybrid 5,10-bis(phenyl)-15,20-tetramethyl-21-23-ditelluraporphodimethene (5b) with Hg^{2+}

The fluorescence spectroscopic titration of Te_2,N_2-hybrid calixphyrin (**5b**) with $Hg(ClO_4)_2$ was performed in ACN/H_2O (6:4, v/v) at room temperature. Te_2,N_2-hybrid calixphyrin (**5b**, 2 µm) showed characteristic emission peak at 406 and 429 nm on excitation at 350 nm. The addition of Hg^{2+} (from 0.5 to 5.0 µm) to ACN/H_2O (6:4, v/v) solution of Te_2,N_2-hybrid calixphyrin (**5b**), leads to the quenching in characteristic emission peaks (**Figure S18**).

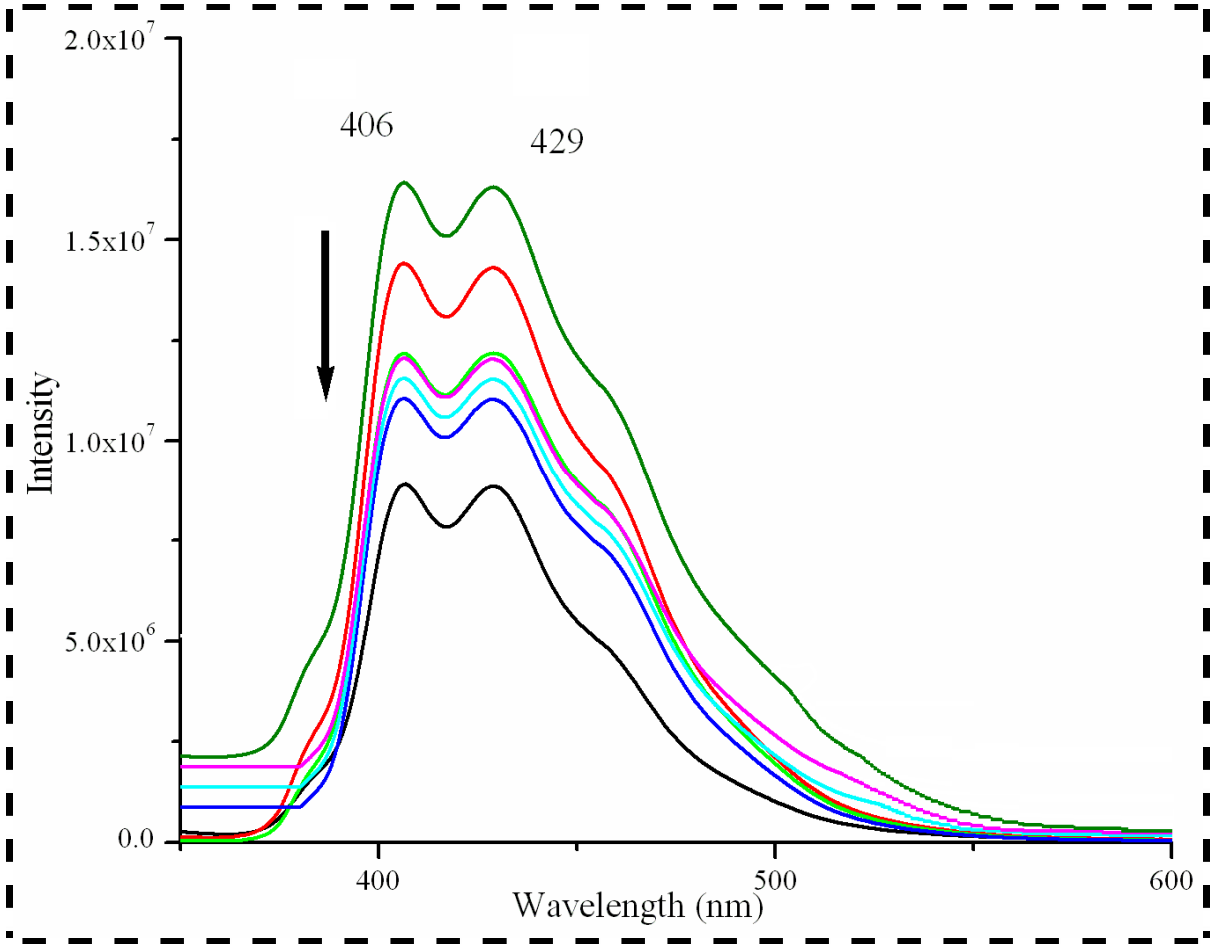


Figure S17: Change in fluorescence spectra (λ_{ex} = 350 nm) of **5b** measured upon addition of Hg^{2+}.

^{1}H NMR data of 5a and 5b with Hg^{2+}

Table S1 Changes in the ^{1}H NMR chemical shifts (δ in ppm) for **5a** and **5b** complexes with Hg^{2+} in $CDCl_3$ at 298 K

Porphodimethane	Conjugated		Unconjugated
	$H_{Pyrrole}$	$H_{Telluro/Seleno}$	$H_{Telluro/Seleno}$
5a	6.71-6.67	7.07	6.91
5a + Hg^2	+0.03	+0.38	+0.35
5b	6.69	7.6	7.59
5b + Hg^{2+}	+0.04	+0.29	+0.24

Calculation of detection limit:

The detection limit of **5a** was carried out by plotting fluorescence intensity as a function of Hg^{2+} ions added. Aliquots of mercury solution of minimum concentration were added to record the fluorescence spectrum of **5a**. From this graph the equivalents for which there was a sharp change in the fluorescence intensity multiplied with the concentration of compound **5a** gave the detection limit. The detection limit was calculated by following equation:[S1]

Detection limit = Conc. of Ligand × Equiv. of Titrant at which change was observed

Detection limit of 5a = $1 \times 10^{-6} \times 0.11 = 1.1 \times 10^{-7}$ molar

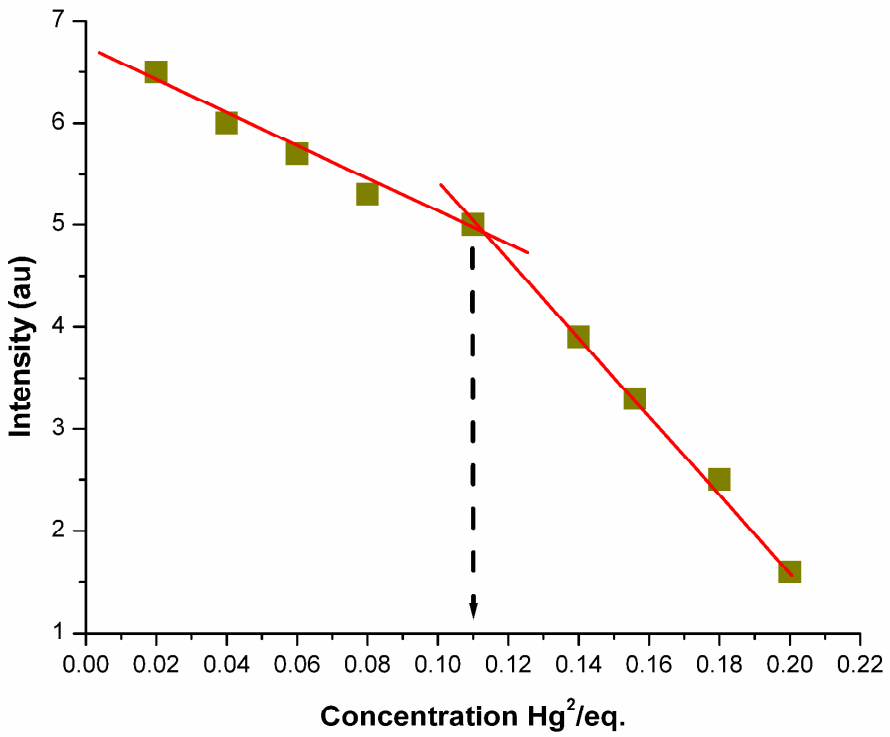


Figure S18: Figure showing the fluorescence intensity (**5a**) at 404 nm as a function of Hg^{2+} ions concentration.

S1. Kumar, M.; Reja, S. I.; Bhalla, V. *Org. Lett*. **2012**, 14, 6084.

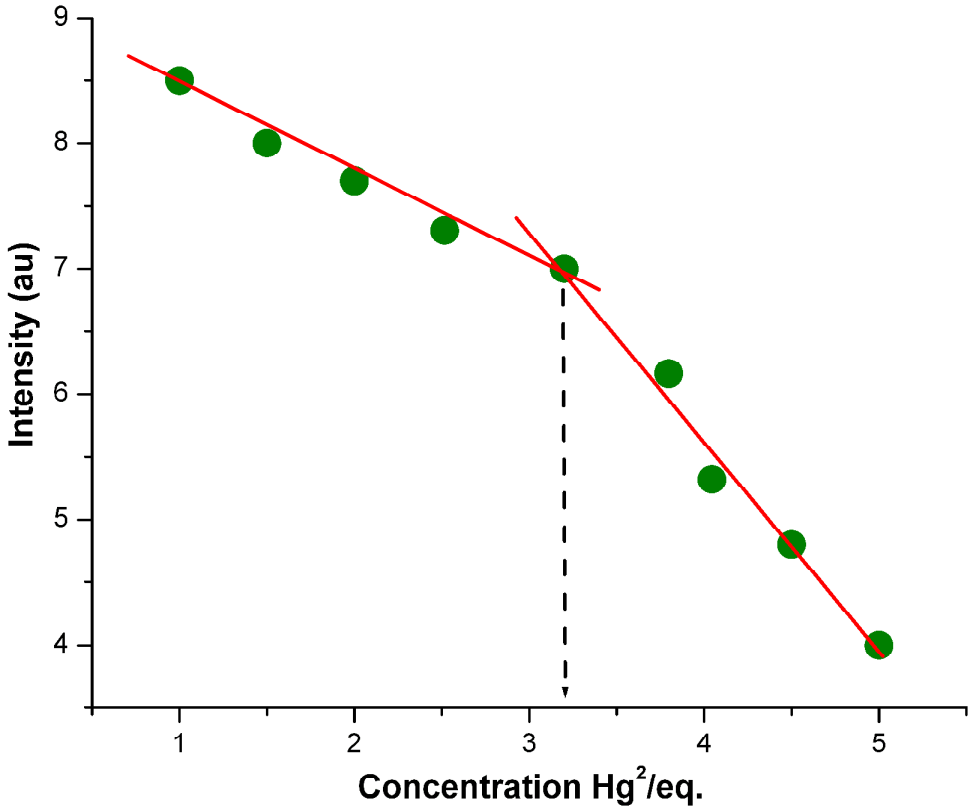


Figure S19: Figure showing the fluorescence intensity (**5b**) at 406 nm as a function of Hg^{2+} ions concentration.

Detection limit = Conc. of Ligand × Equiv. of Titrant at which change observed.

Detection limit of 5b = $1 \times 10^{-6} \times 3.2 = 3.2 \times 10^{-6}$ molar

The electronic absorption spectroscopic titration of 5,15-porphodimethene (12a-b) with Hg^{2+}

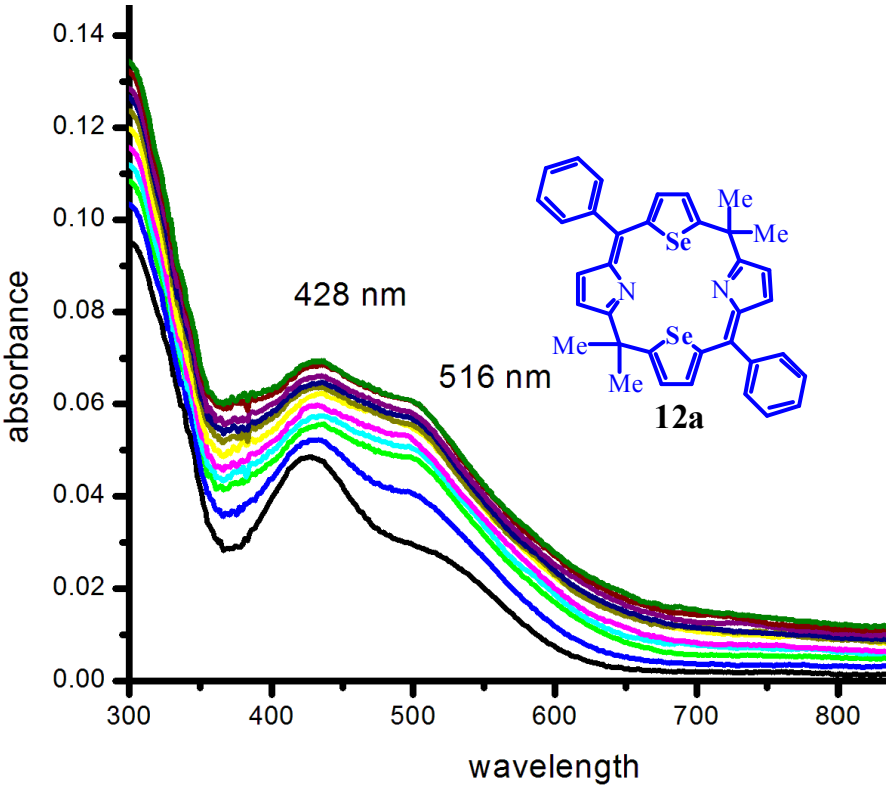


Figure S20

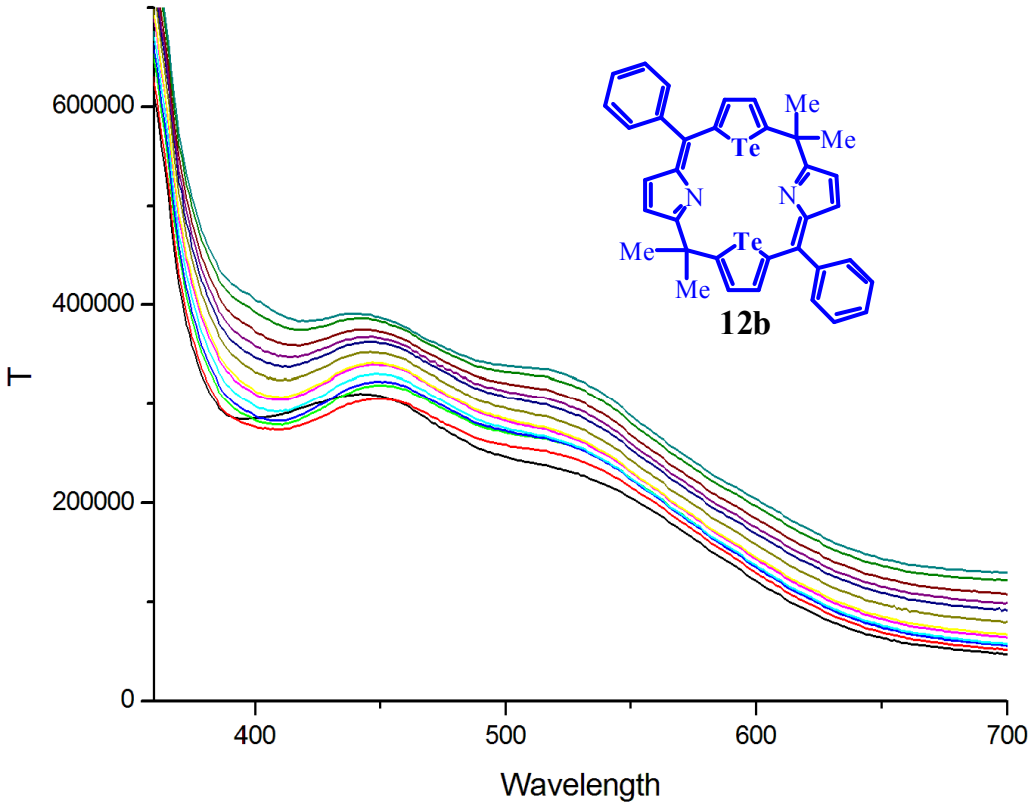

600000
400000
200000
0
T
400
500
600
700
Wavelength
Me
Me
Te
N
N
Te
Me
Me
12b

Figure S21

Selected ^{1}H NMR and ^{13}C NMR Spectra

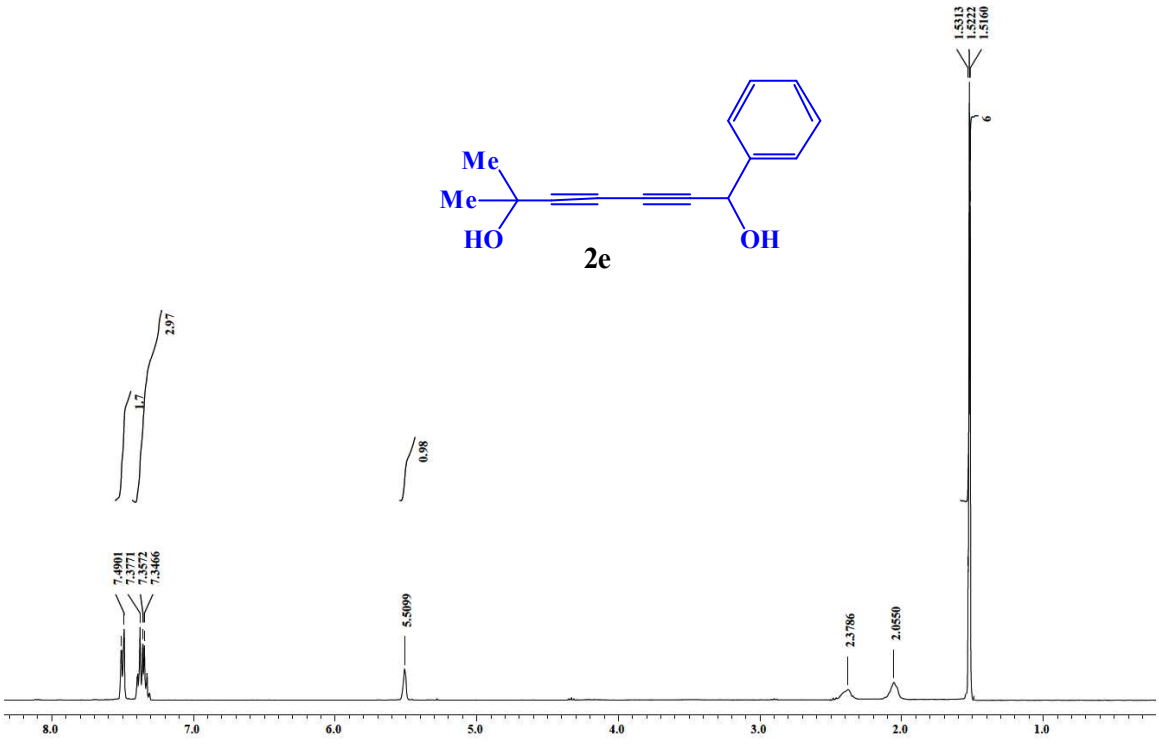


Figure S22

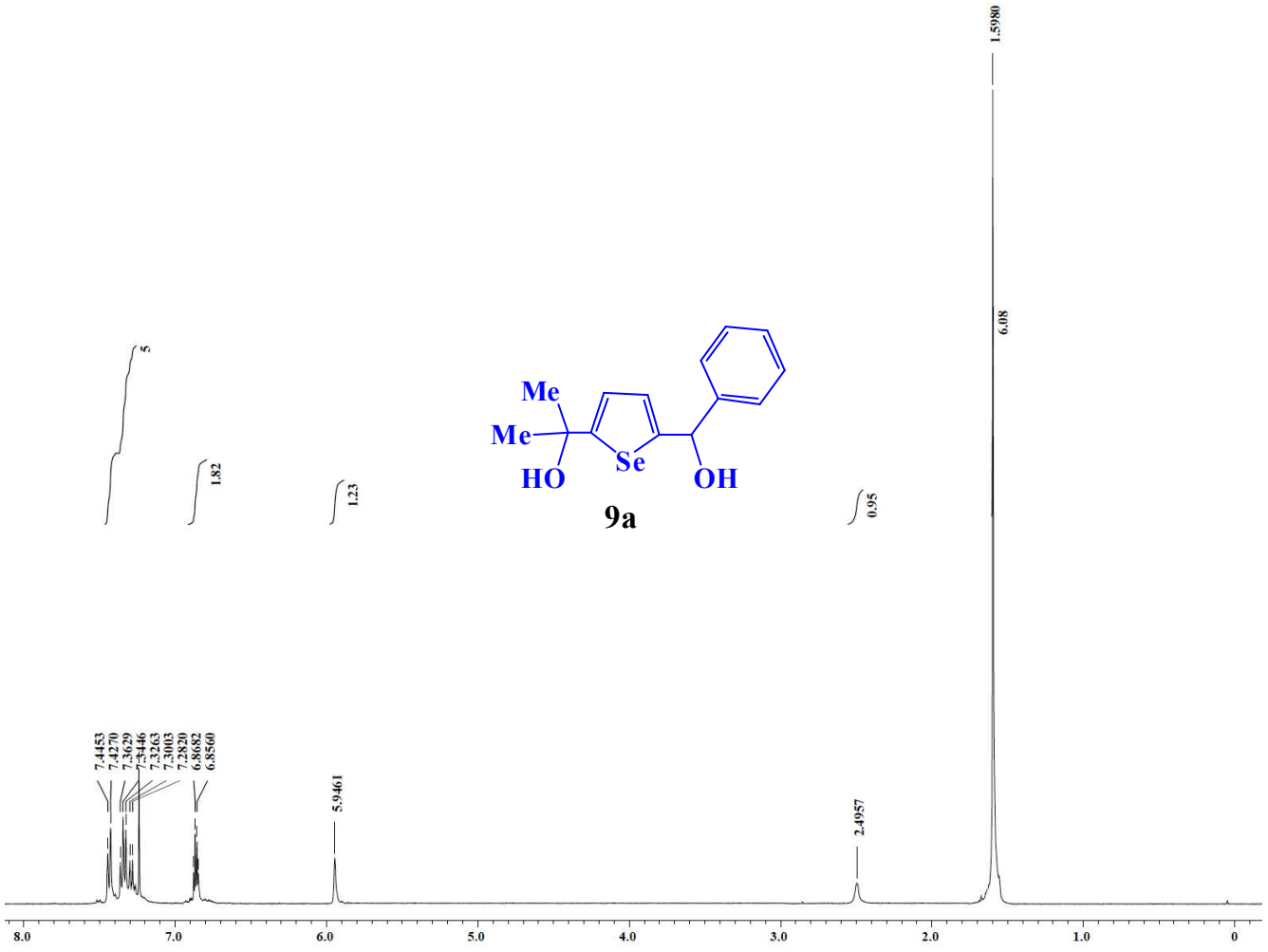

1.5980
6.08
Me
Me
HO
Se
OH
9a
1.82
1.23
0.95
7.4453
7.4270
7.3629
7.3446
7.3263
7.3003
7.2820
6.8682
6.8560
5.9461
2.4957
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S23

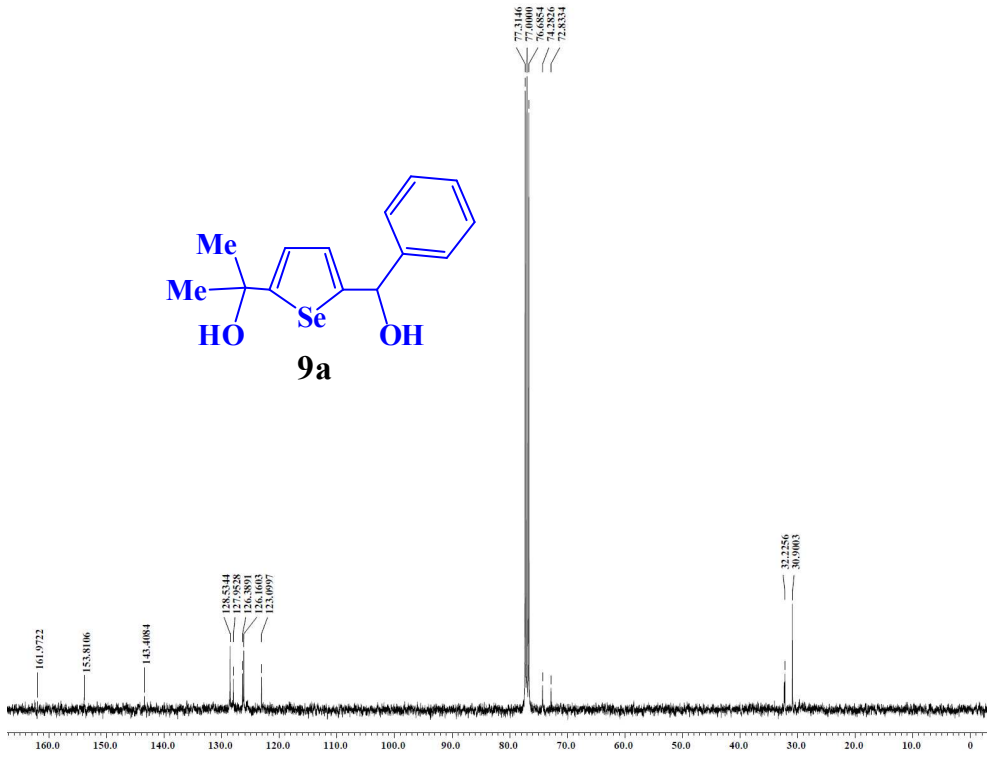

Me
Me
HO
Se
OH
9a
77.3146
77.0000
76.6854
74.2826
72.6534
161.9722
153.8106
143.4084
128.5344
127.9528
126.3891
126.1603
123.0997
32.2256
30.9003
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Figure S24

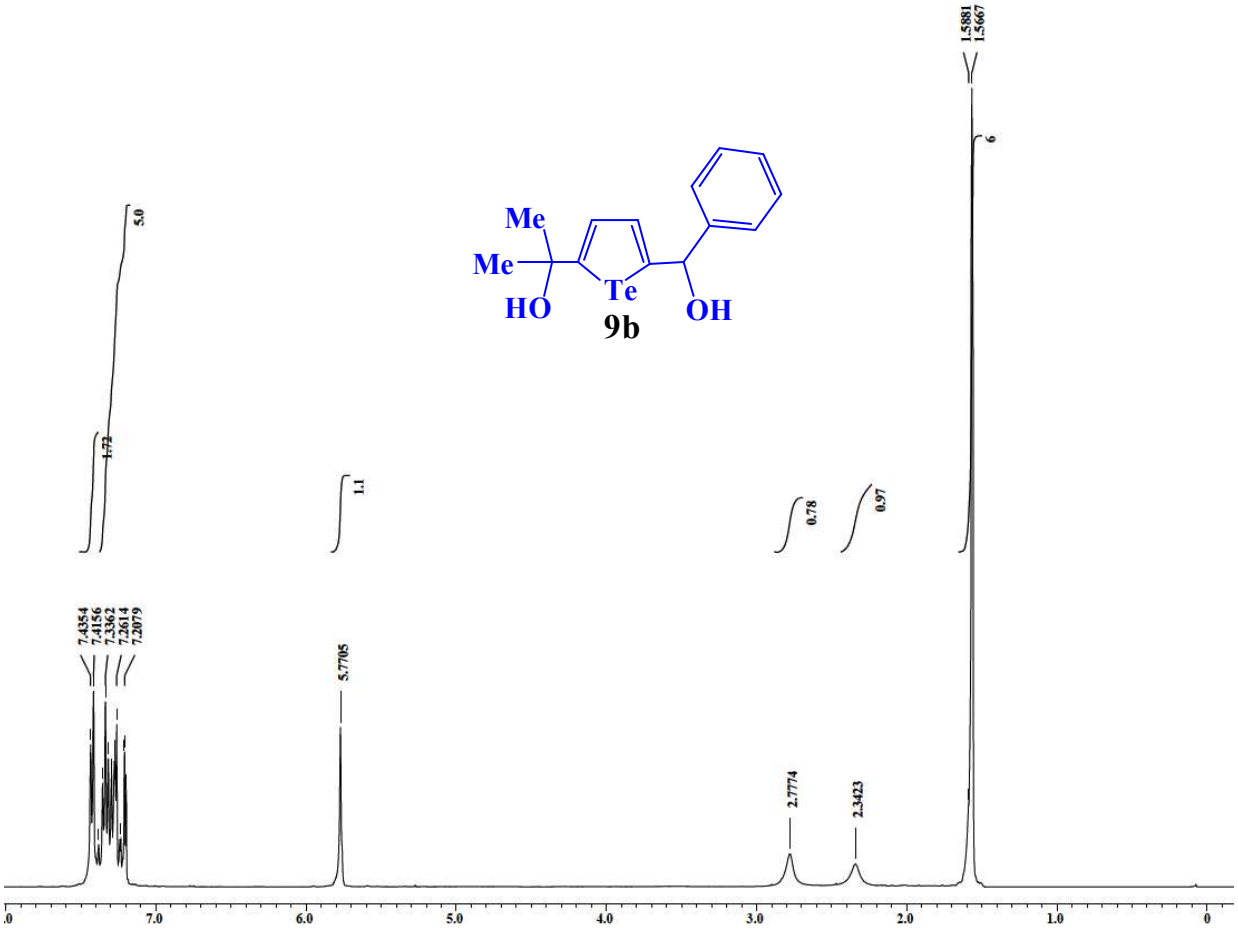

Me
Me
HO
Te
OH
9b
1.5881
1.5667
6
5.0
1.72
1.1
0.78
0.97
7.4354
7.4156
7.3362
7.2614
7.2079
5.7705
2.7774
2.3423
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S25

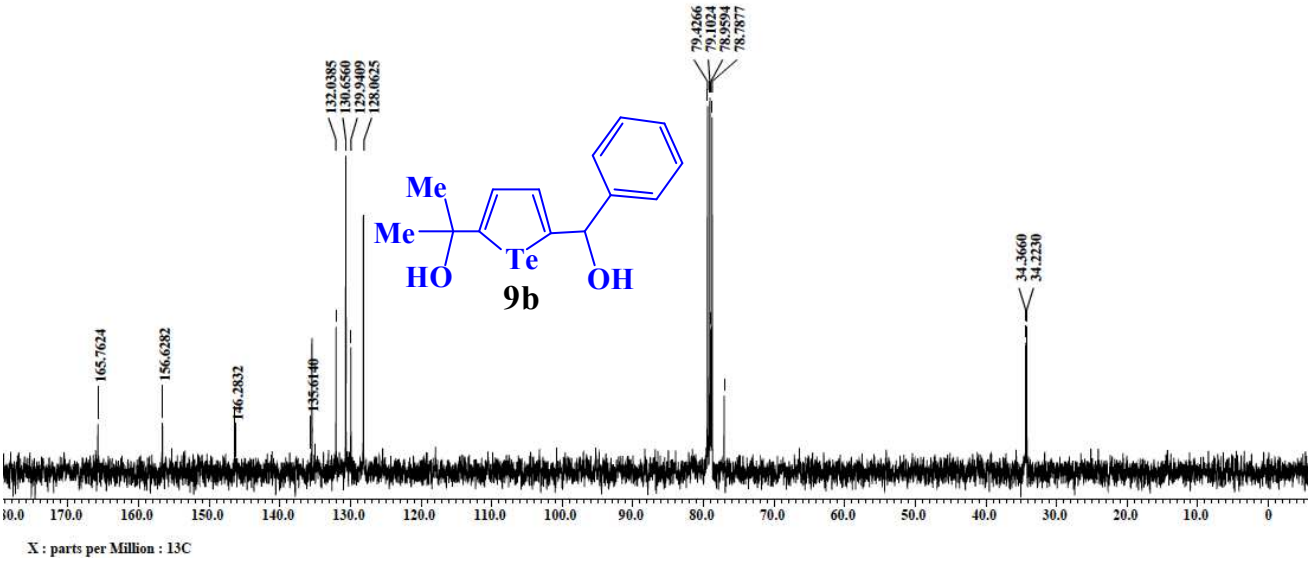

79.4266
79.1024
78.9594
78.7877
132.0385
130.6560
129.9409
128.0625
Me
Me
HO
Te
OH
9b
34.3660
34.2230
165.7624
156.6282
146.2832
135.6140
X : parts per Million : 13C

Figure S26

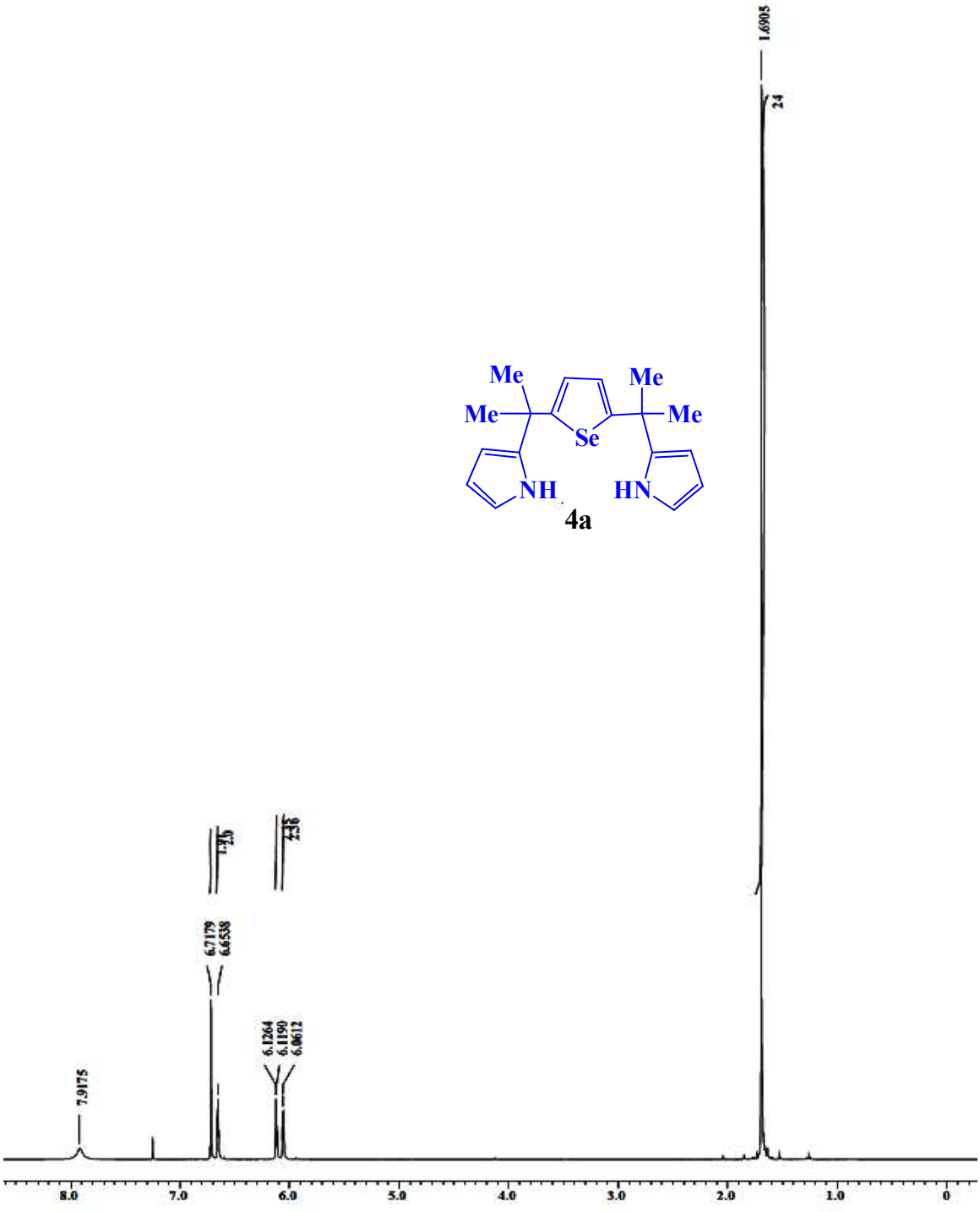

Me
Me
Me
Me
Se
NH
HN
4a
1.6905
2.4
7.9175
6.7179
6.6538
6.1264
6.1190
6.0612
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S27

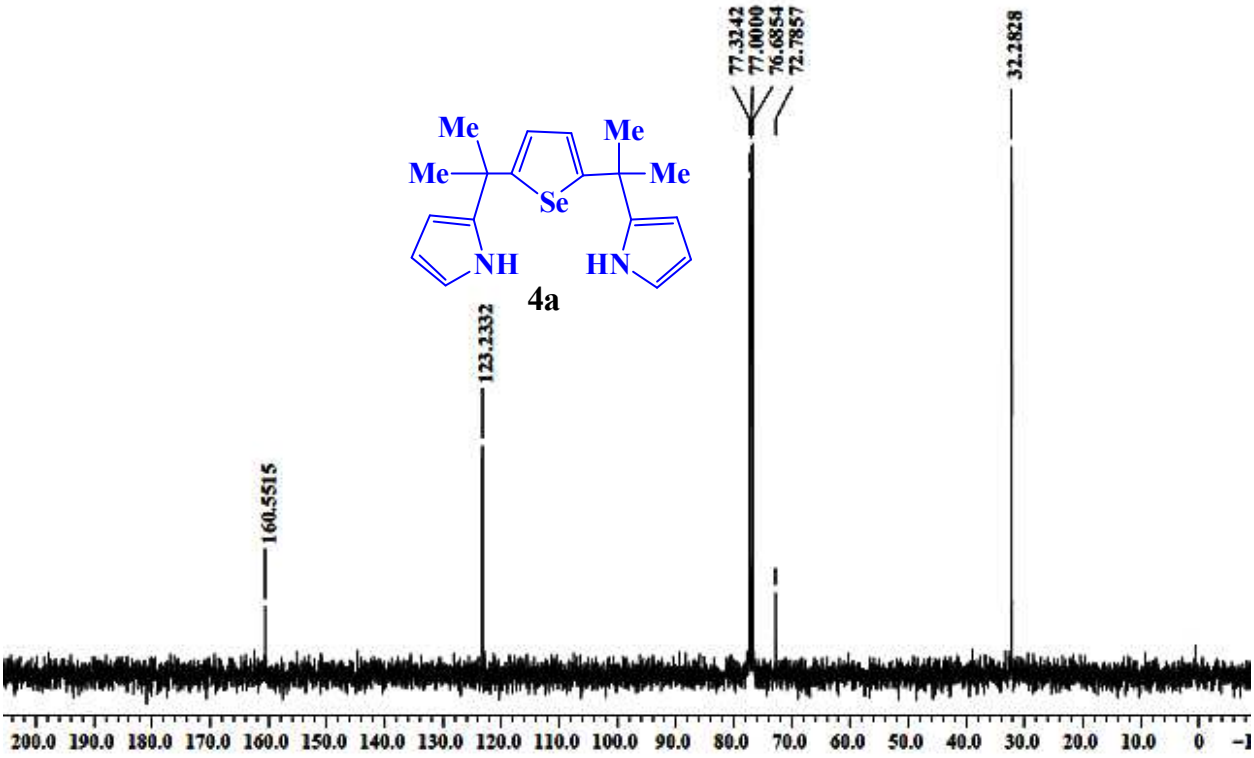

77.3242
77.0000
76.6854
72.7857
32.2828
Me
Me
Me
Me
Se
NH
HN
4a
123.2332
160.5515
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0

Figure S28

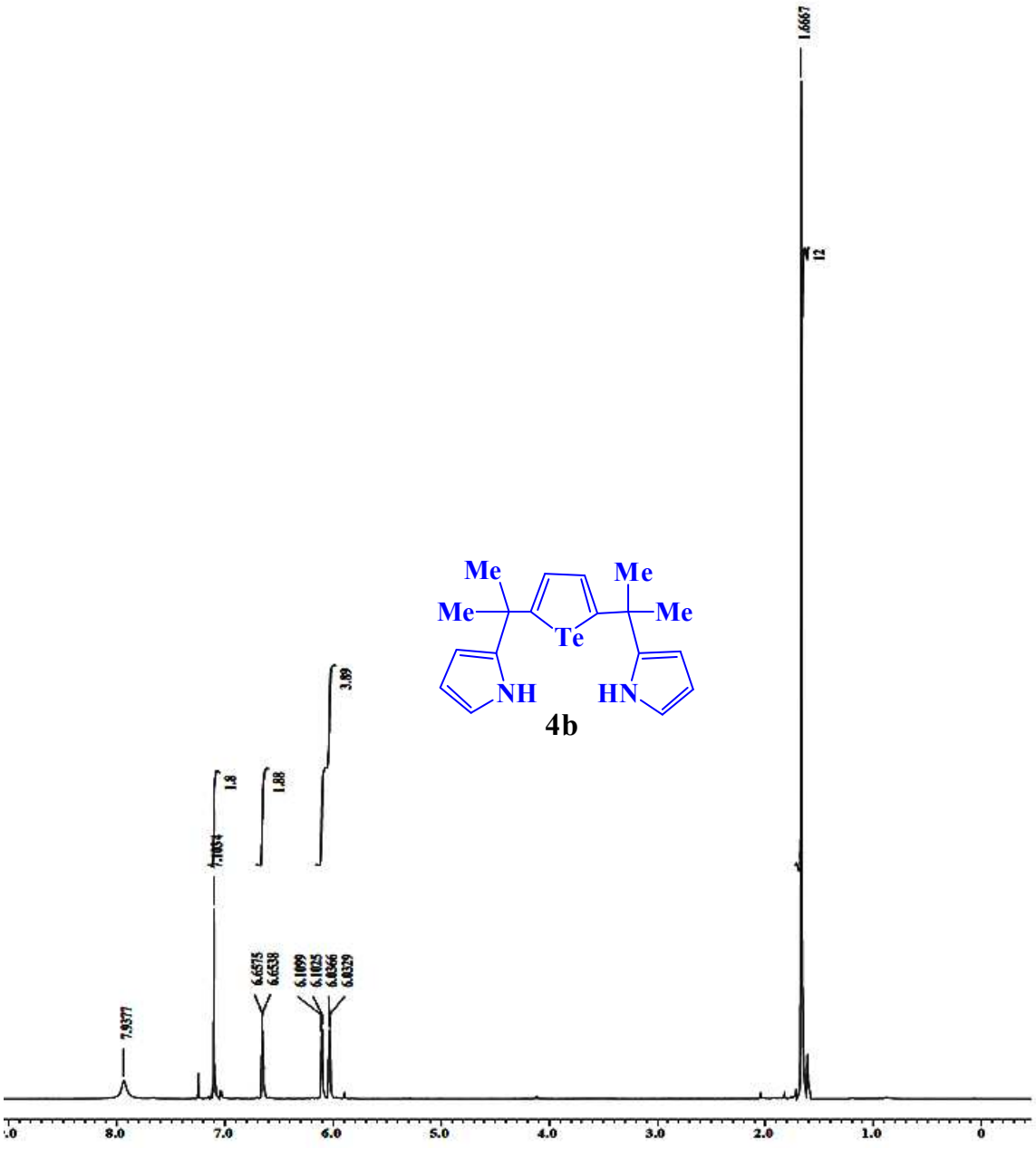

Me
Me
Me
Me
Te
NH
HN
4b
1.6667
12
3.89
1.88
1.8
7.9377
6.6515
6.6338
6.1099
6.1025
6.0566
6.0329
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S29

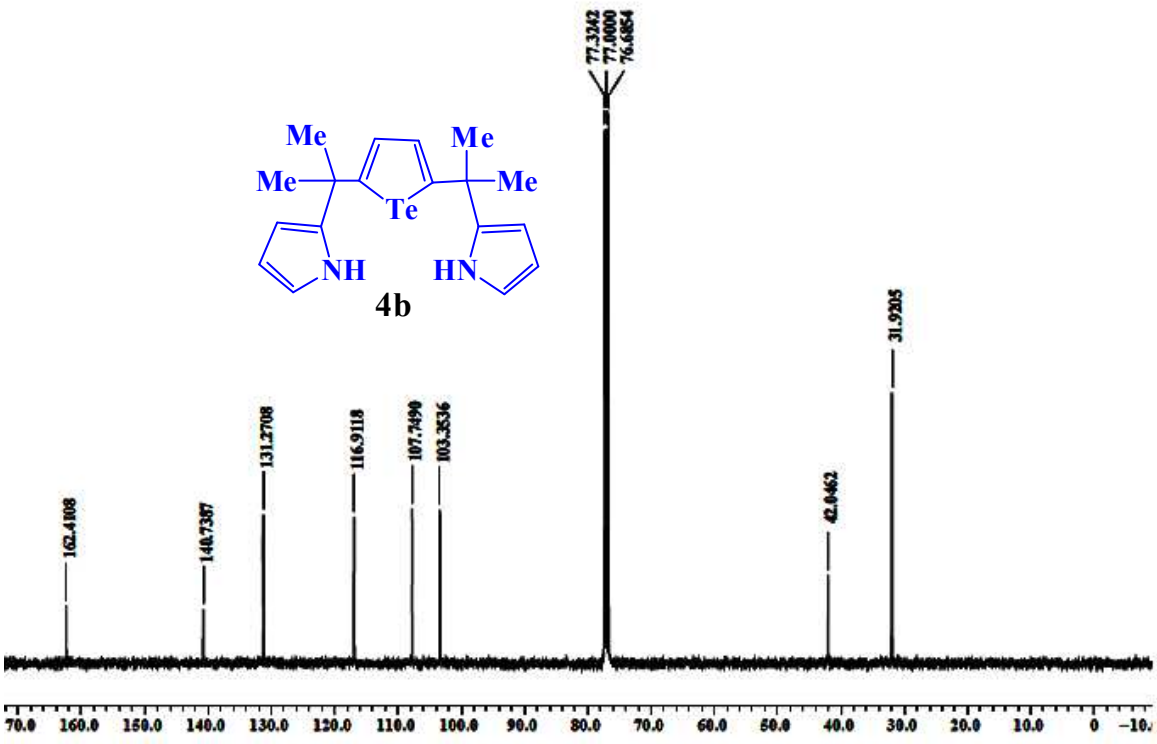
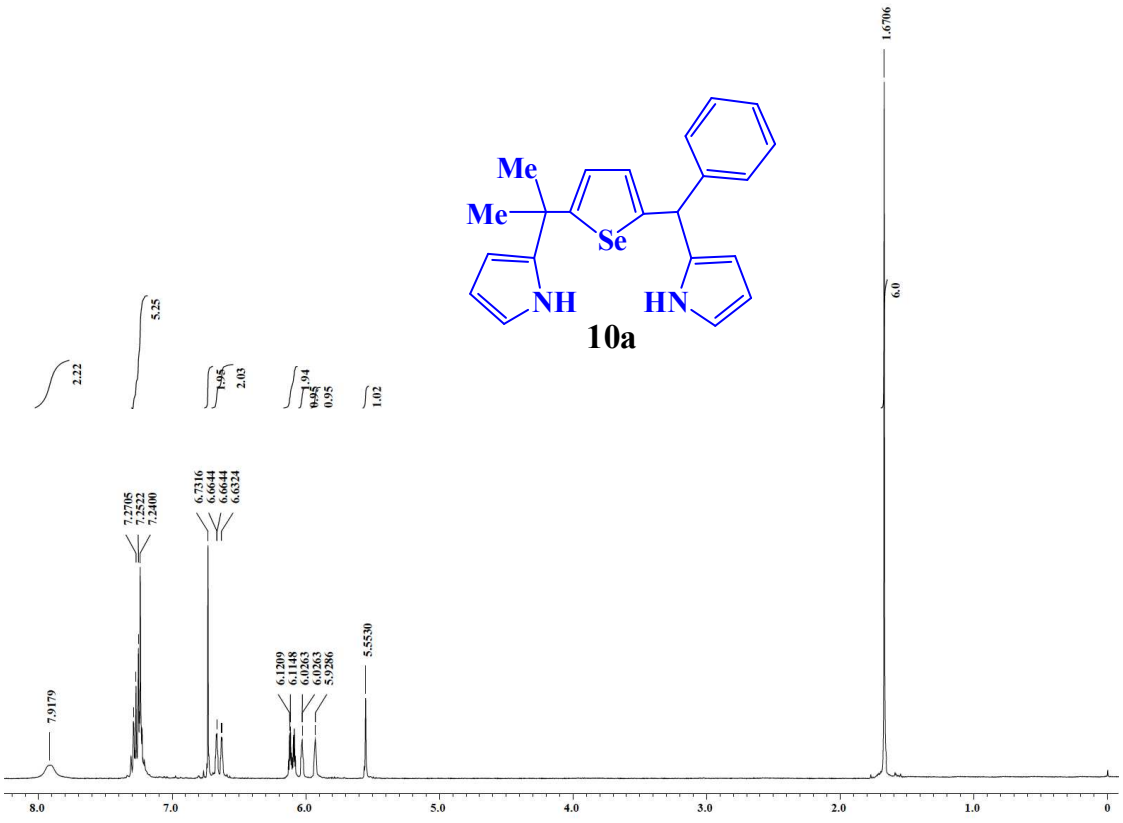

Me
Me
Me
Me
Te
NH
HN
4b
77.3242
77.0000
76.6854
162.4108
148.7387
131.2708
116.9118
107.7490
103.3536
42.0462
31.9205
70.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Figure S30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Me
Se
NH
HN
10a
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6.0
5.25
2.22
2.03
1.94
0.95
1.02
7.9179
7.2705
7.2522
7.2400
6.7316
6.6644
6.6644
6.6324
6.1209
6.1148
6.0263
5.9286
5.5530
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S31

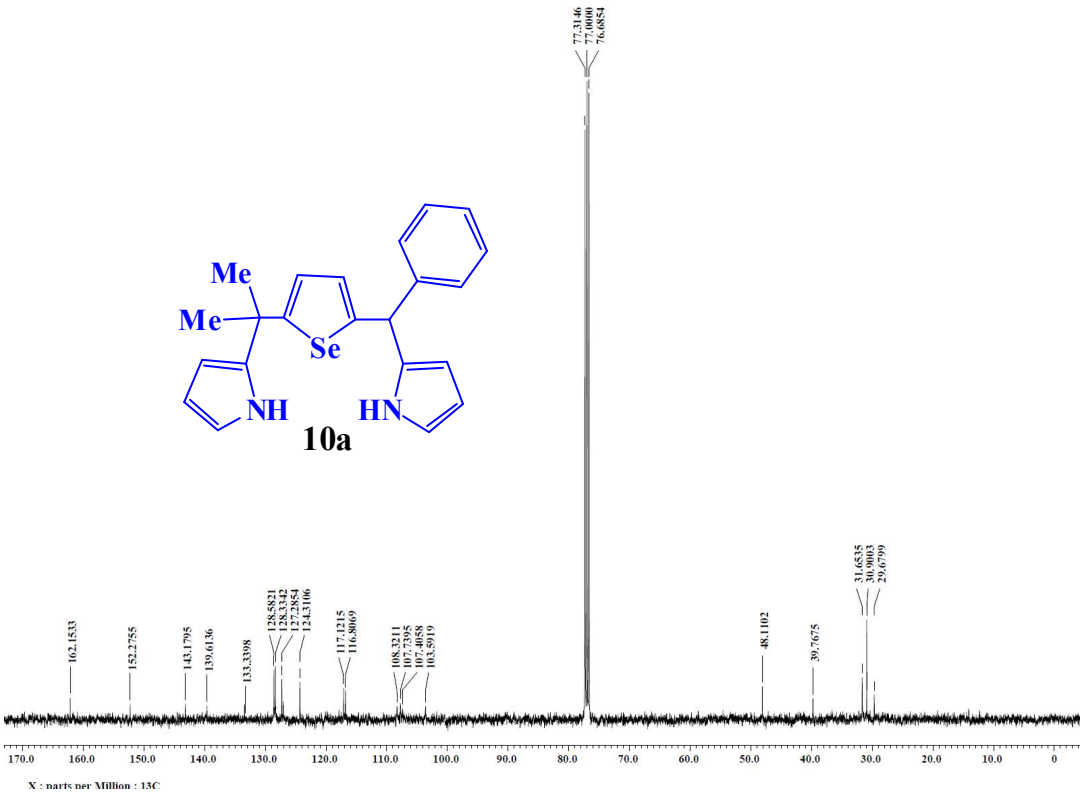

Me
Me
Se
NH
HN
10a
77.3146
77.0000
76.6854
162.1533
152.2755
143.1795
139.6136
133.3398
128.5821
128.3342
127.2854
124.3106
117.1215
116.8069
108.3211
107.7395
107.4058
103.5919
48.1102
39.7675
31.6535
30.9003
29.6799
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
X : parts per Million : 13C

Figure S32

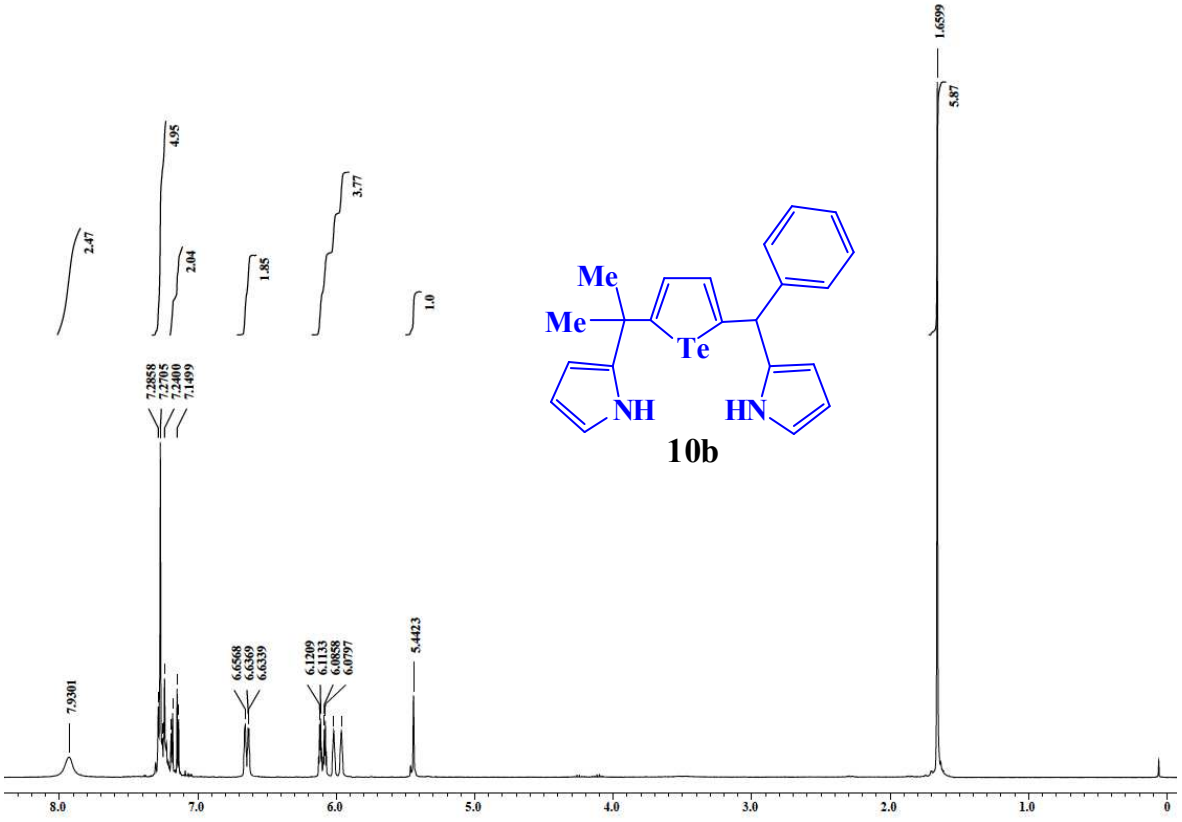

1.6599
5.87
4.95
3.77
2.47
2.04
1.85
1.0
7.2858
7.2705
7.2400
7.1499
6.6568
6.6369
6.6339
6.1209
6.1133
6.0858
6.0797
5.4423
7.9301
Me
Me
Te
NH
HN
10b
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S33

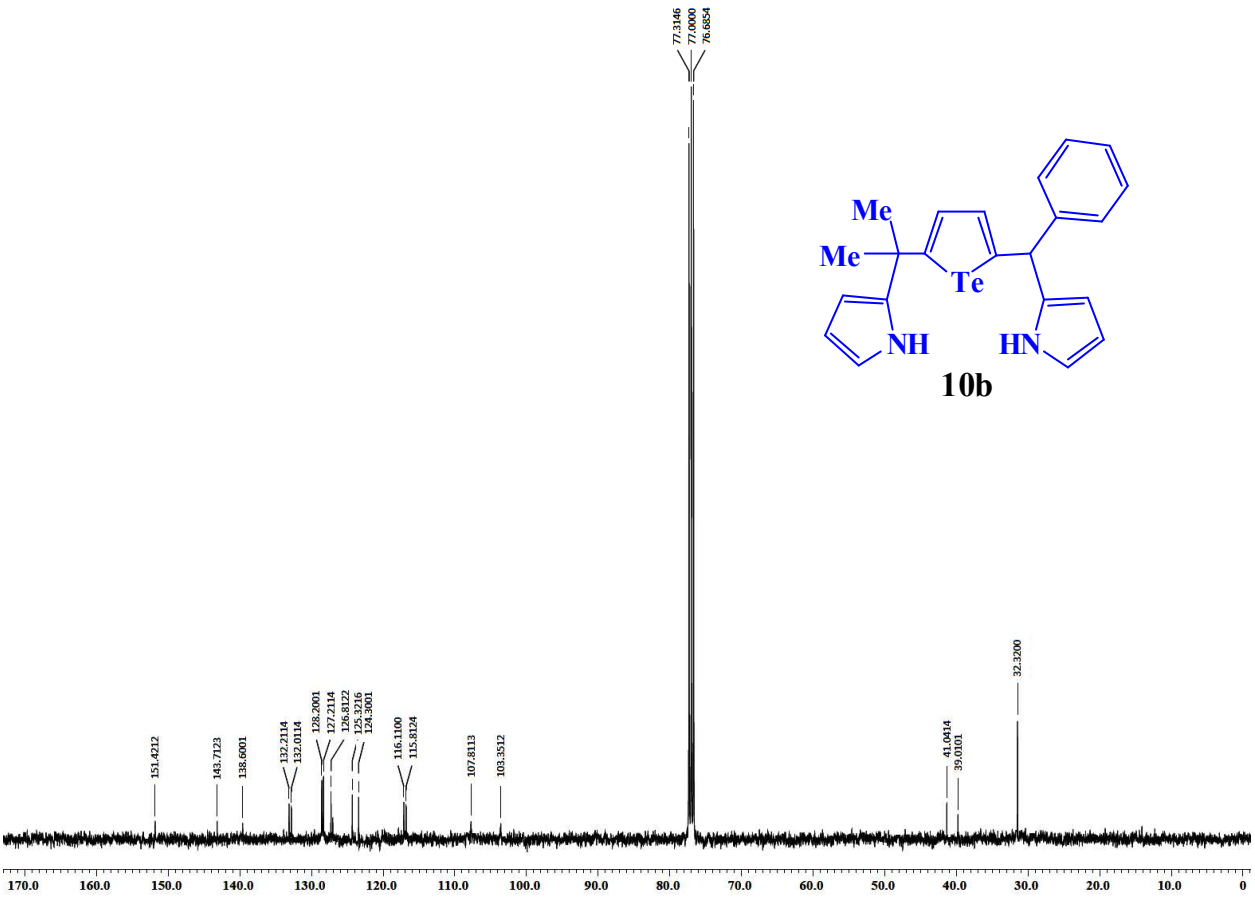

77.3146
77.0000
76.6854
Me
Me
Te
NH
HN
10b
151.4212
143.7123
138.6001
132.2114
132.0114
128.2001
127.2114
126.8122
125.3216
124.3001
116.1100
115.8124
107.8113
103.3512
41.0414
39.0101
32.3200
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Figure S34

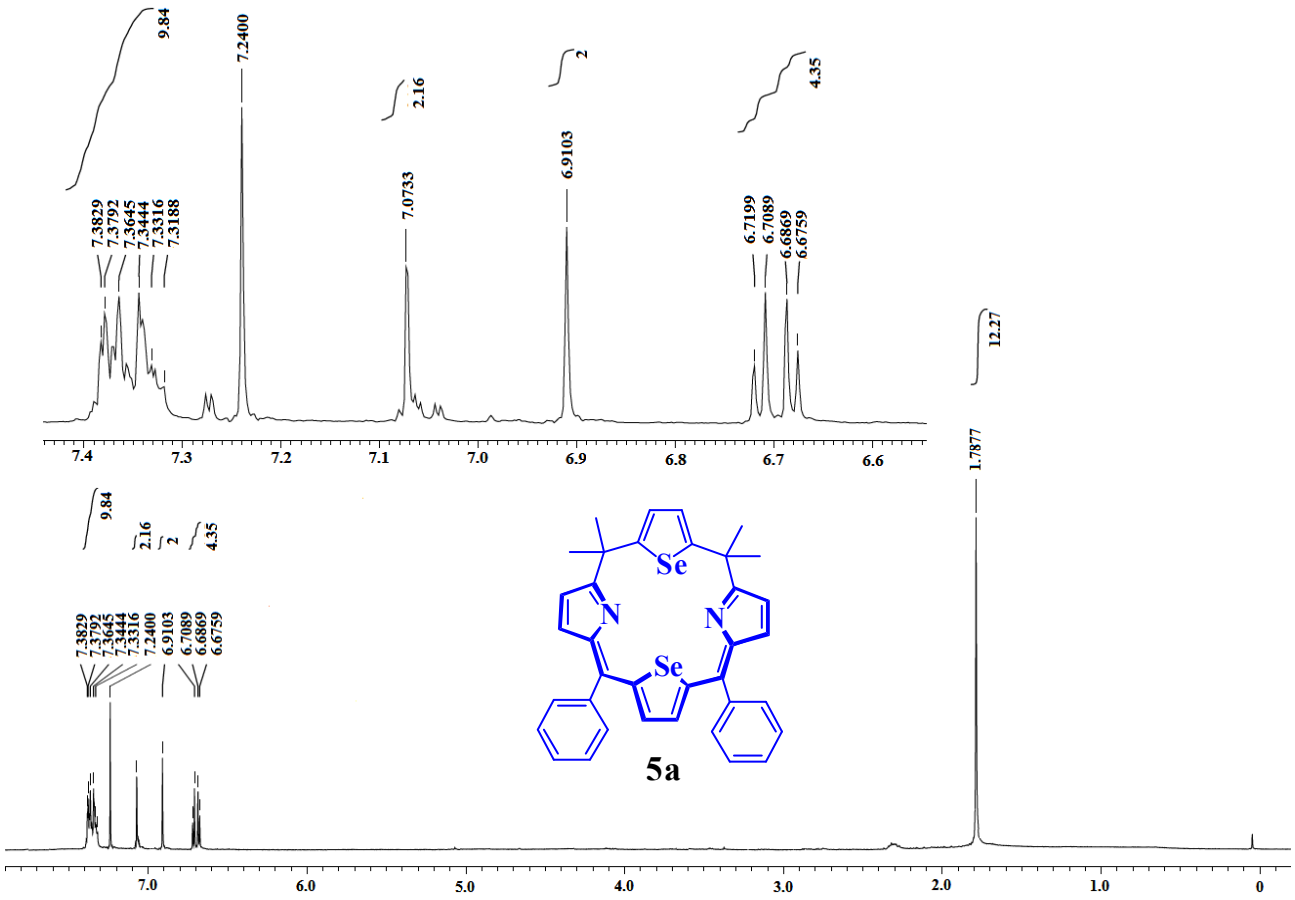

9.84
7.2400
2.16
2
4.35
7.3829
7.3792
7.3645
7.3444
7.3316
7.3188
7.0733
6.9103
6.7199
6.7089
6.6869
6.6759
12.27
1.7877
Se
N
N
Se
5a

Figure S35

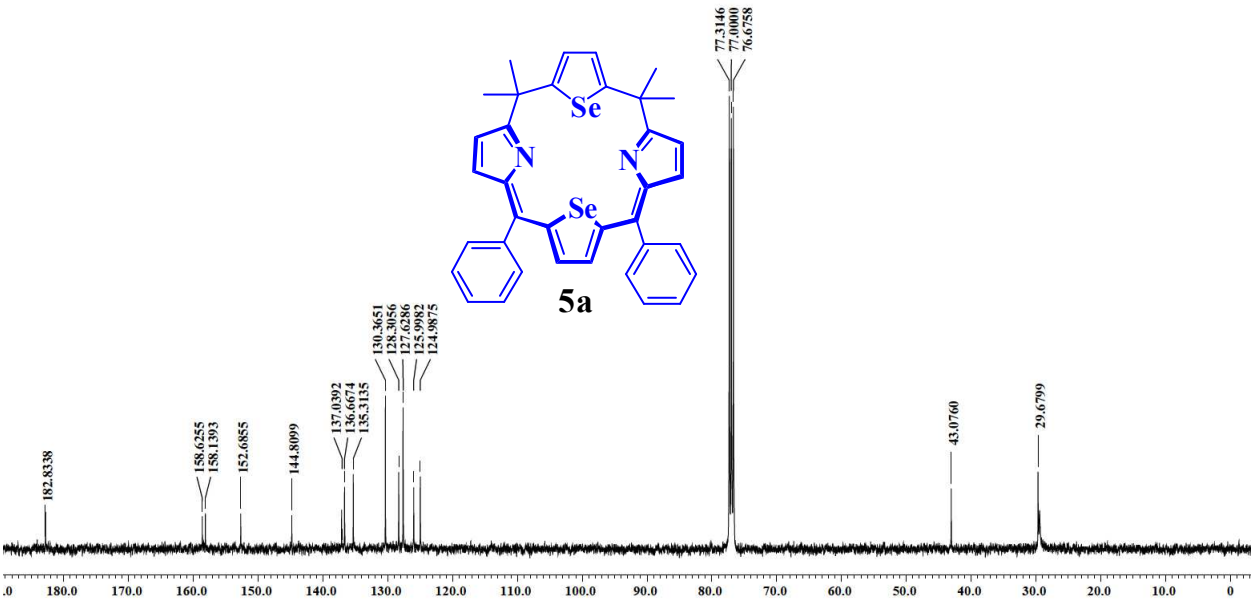

77.3146
77.0000
76.6758
Se
N
N
Se
5a
130.3651
128.3056
127.6286
125.9982
124.9875
137.0392
136.6674
135.3135
158.6255
158.1393
152.6855
144.8099
182.8338
43.0760
29.6799
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Figure S36

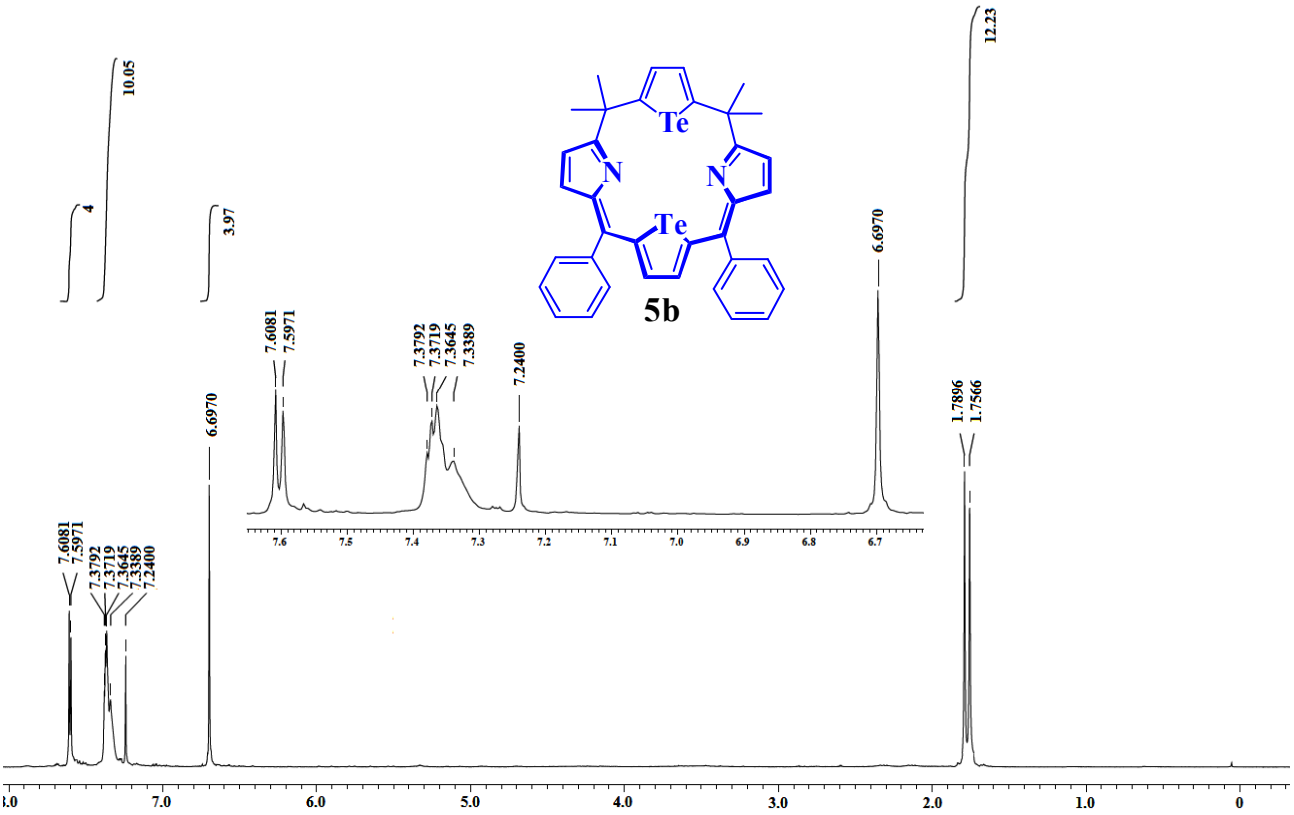

Te
N
N
Te
5b
12.23
10.05
4
3.97
6.6970
1.7896
1.7566
7.6081
7.5971
7.3792
7.3719
7.3645
7.3389
7.2400

Figure S37

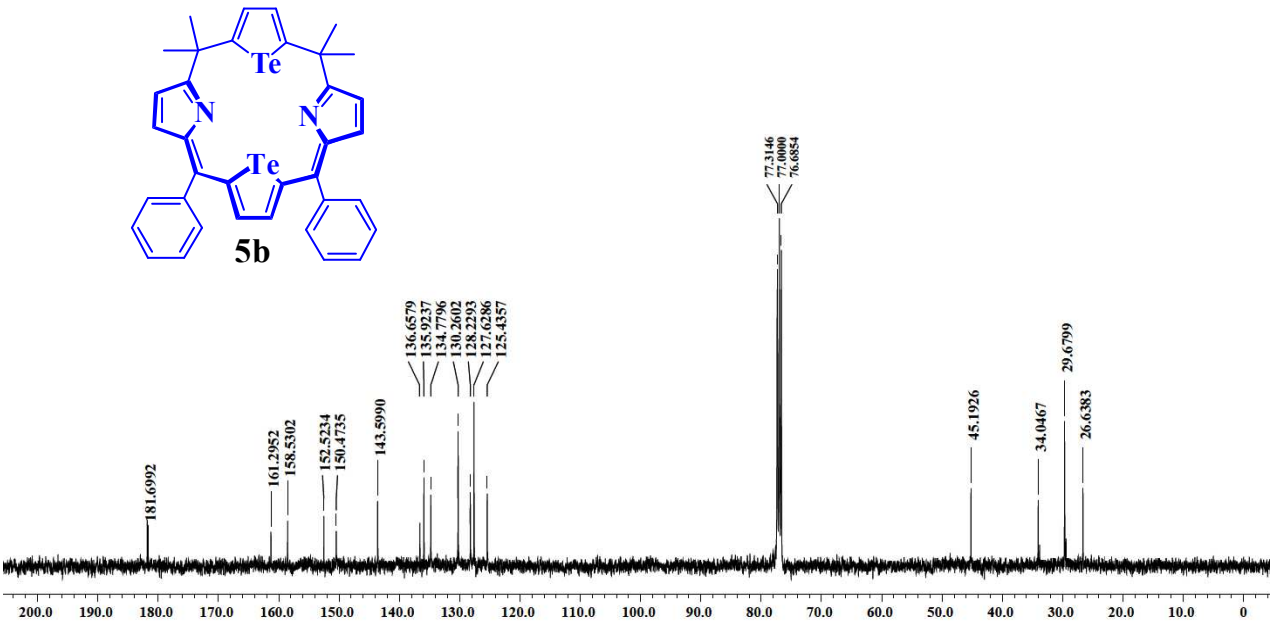

Te
N
N
Te
5b
181.6992
161.2952
158.5302
152.5234
150.4735
143.5990
136.6579
135.9237
134.7796
130.2602
128.2293
127.6286
125.4357
77.3146
77.0000
76.6854
45.1926
34.0467
29.6799
26.6383
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Figure S38

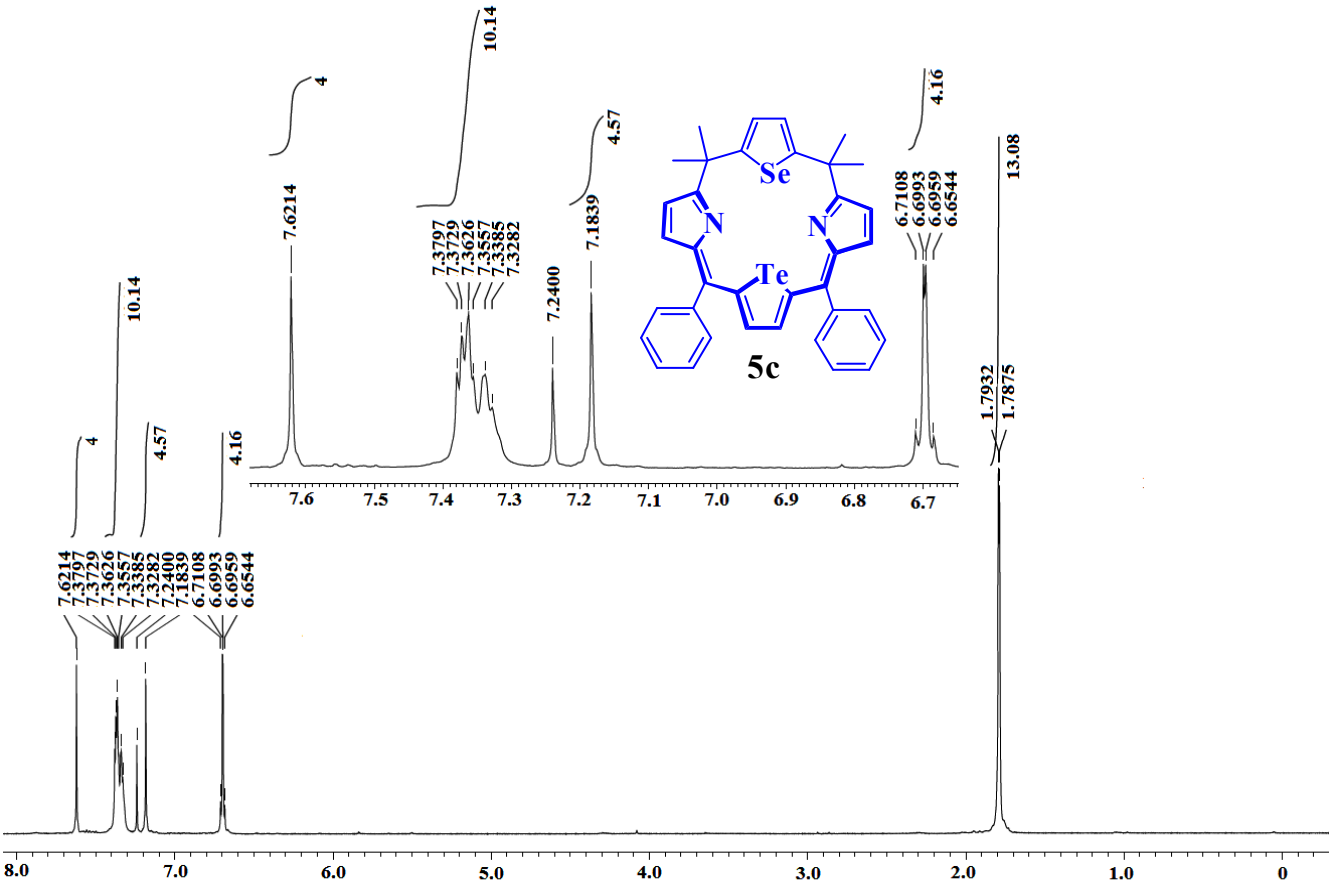


Figure S39

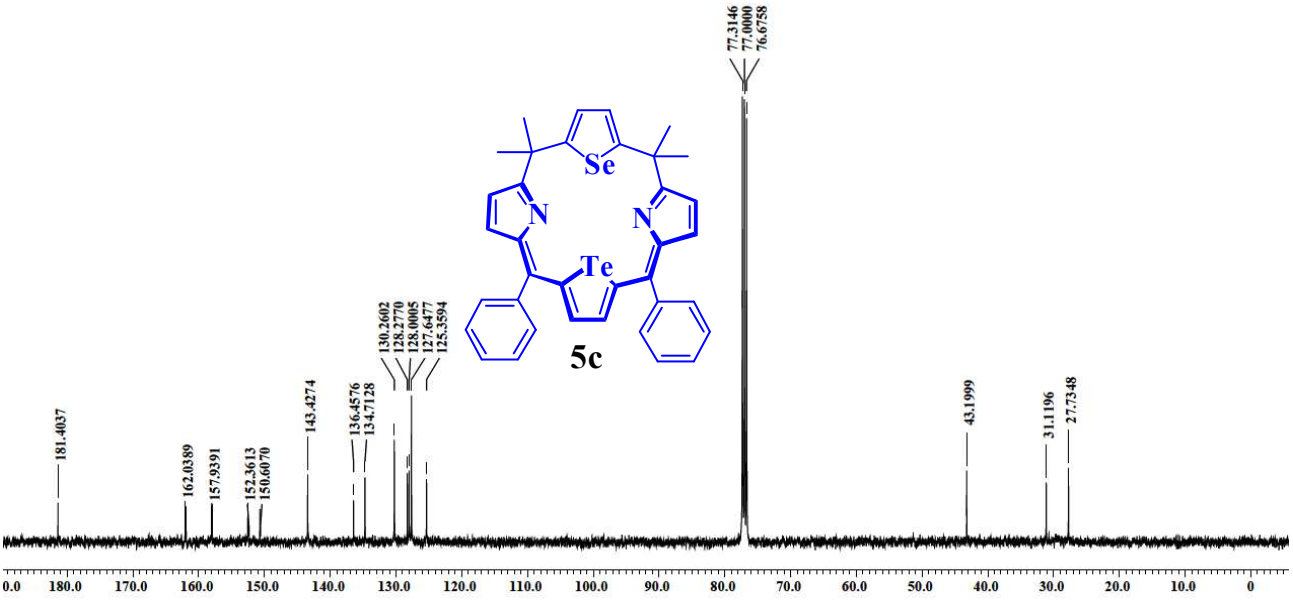

77.3146
77.0000
76.6758
Se
N
N
Te
5c
130.2602
128.2770
128.0065
127.6477
125.3594
143.4274
136.4576
134.7128
181.4037
162.0389
157.9391
152.3613
150.6070
43.1999
31.1196
27.7348
0.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Figure S40

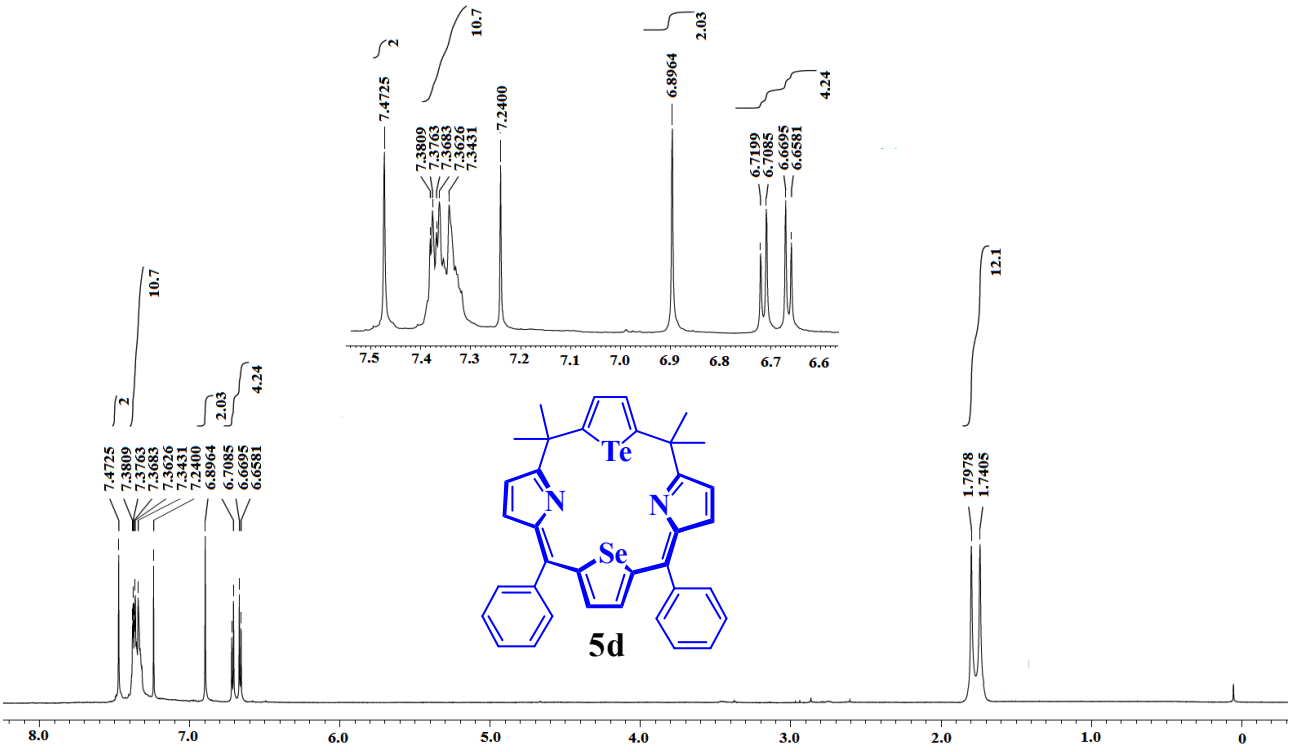

7.4725
7.3809
7.3763
7.3683
7.3626
7.3431
7.2400
6.8964
6.7199
6.7085
6.6695
6.6581
1.7978
1.7405
Te
N
N
Se
5d

Figure S41

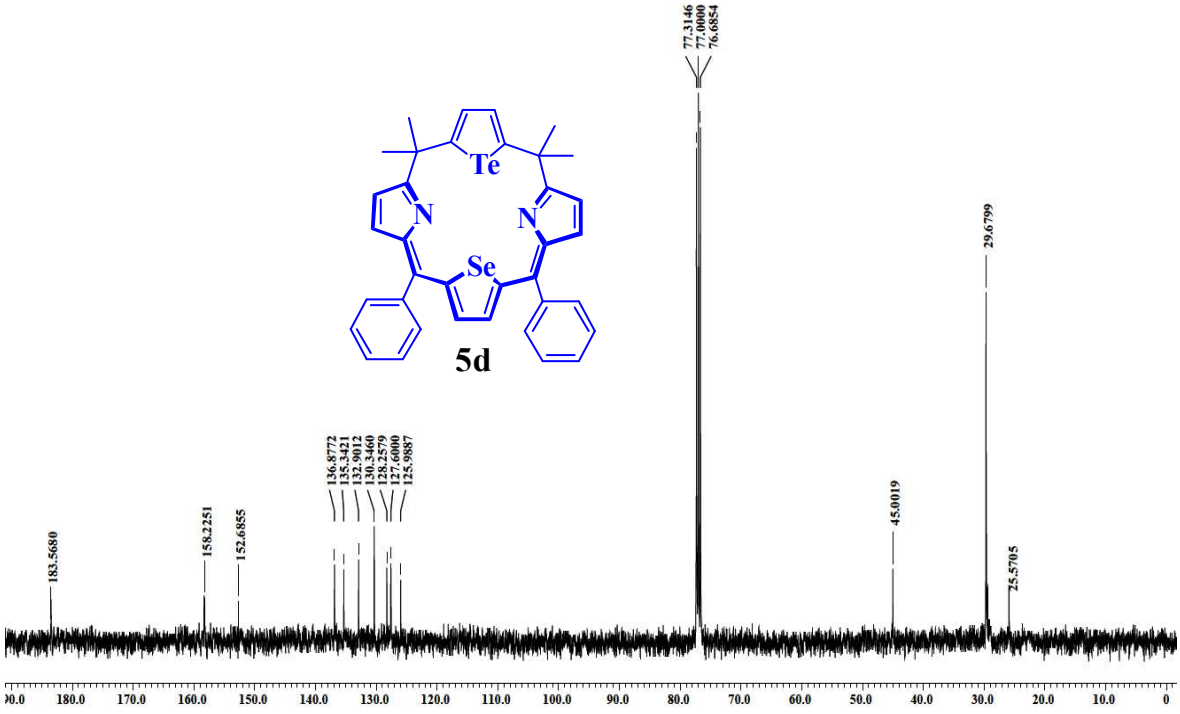

77.3146
77.0000
76.6854
Te
N
N
Se
5d
136.8772
135.3421
132.9012
130.3460
128.2579
127.6000
125.9887
183.5680
158.2251
152.6855
45.0019
29.6799
25.5705
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Figure S42

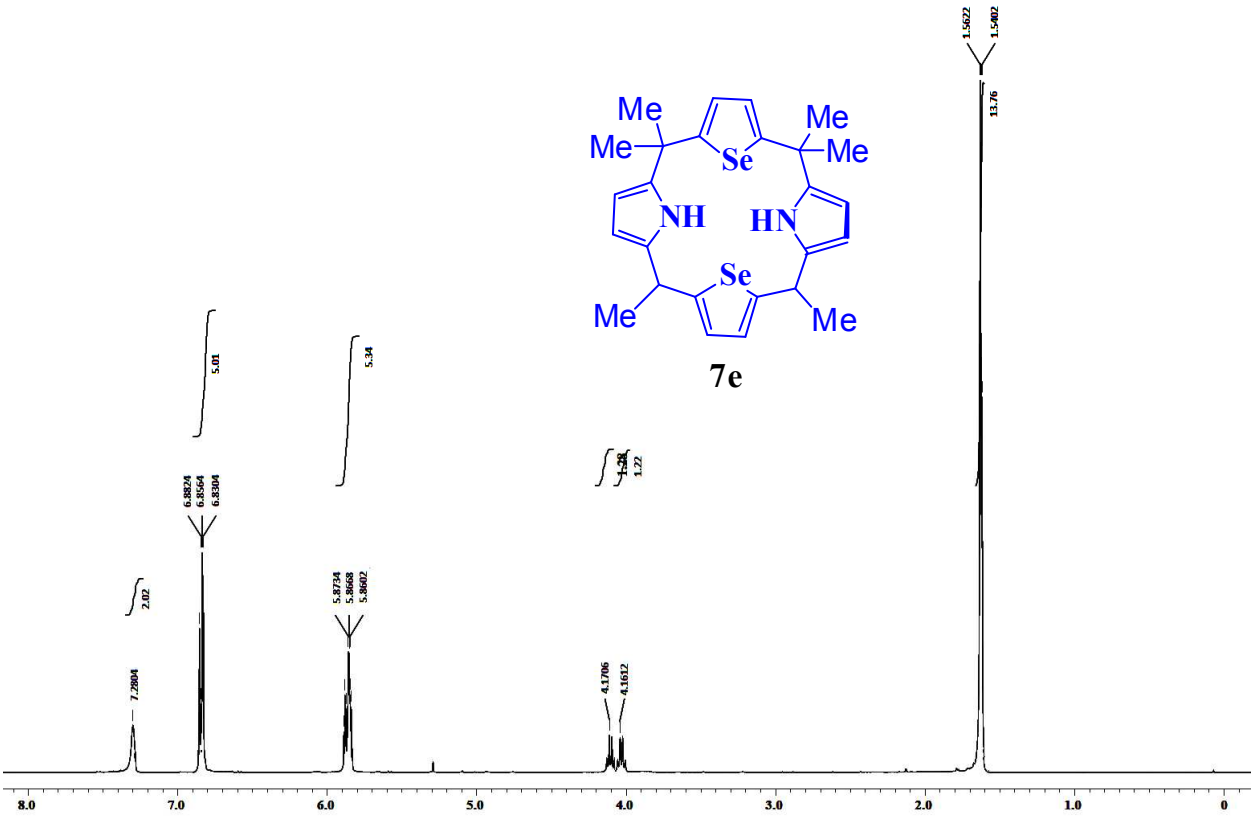

Me
Me
Me
Me
Se
NH
HN
Se
Me
Me
7e
1.5622
1.5402
13.76
5.01
5.34
1.28
1.22
6.8824
6.8564
6.8304
2.02
5.8734
5.8668
5.8602
7.2804
4.1706
4.1612
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S43

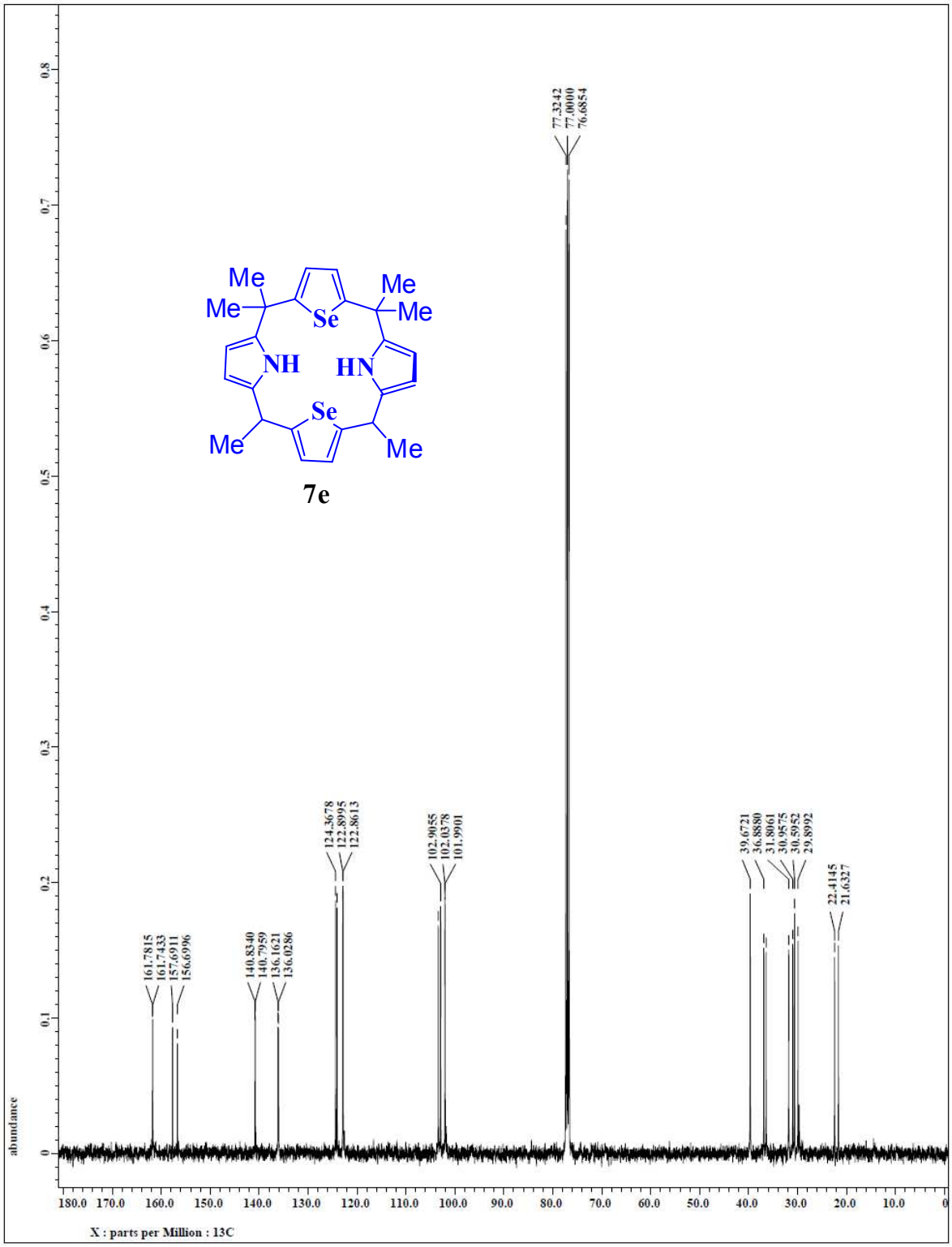

Me
Me
Me
Me
Se
NH
HN
Se
Me
Me
7e
77.3242
77.0000
76.6854
161.7815
161.7433
157.6911
156.6996
140.8340
140.7959
136.1621
136.0286
124.3678
122.8995
122.8613
102.9055
102.0378
101.9901
39.6721
36.8880
31.8061
30.9575
30.5952
29.8992
22.4145
21.6327
abundance
X : parts per Million : 13C

Figure S44

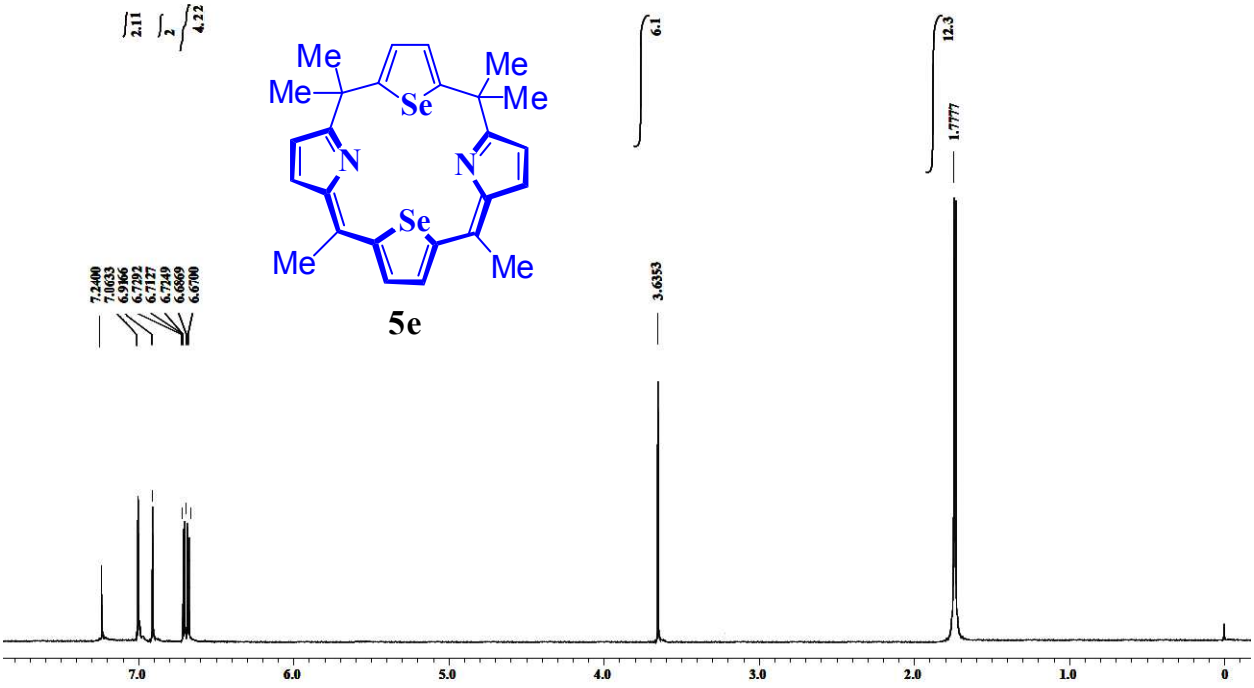

2.11
2
4.22
6.1
12.3
1.7777
3.6353
7.2400
7.1033
6.9866
6.7392
6.7127
6.7249
6.6869
6.6700
Me
Me
Me
Me
Se
N
N
Se
Me
Me
5e
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S45

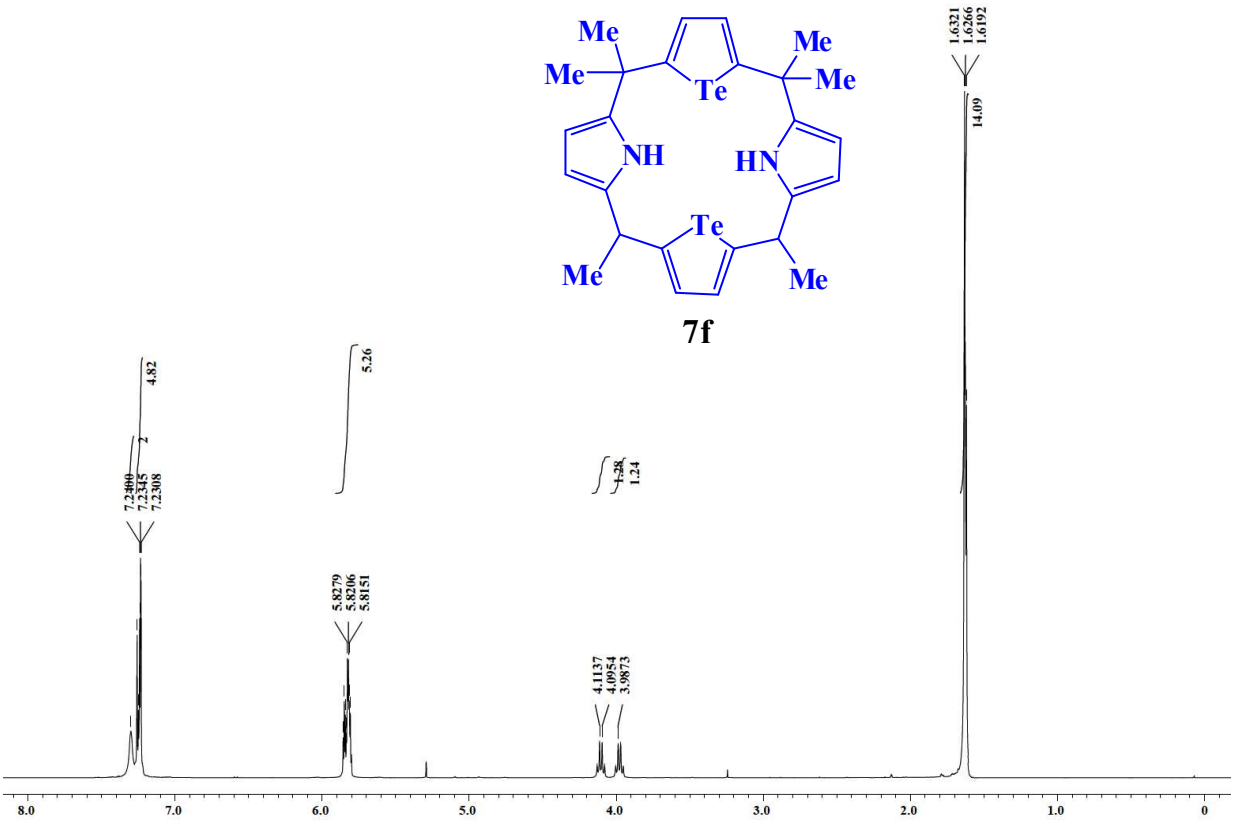

Me
Me
Te
Me
Me
NH
HN
Te
Me
Me
7f
1.6321
1.6266
1.6192
14.09
4.82
5.26
7.2400
7.2345
7.2308
1.28
1.24
5.8279
5.8206
5.8151
4.1137
4.0954
3.9873
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S46

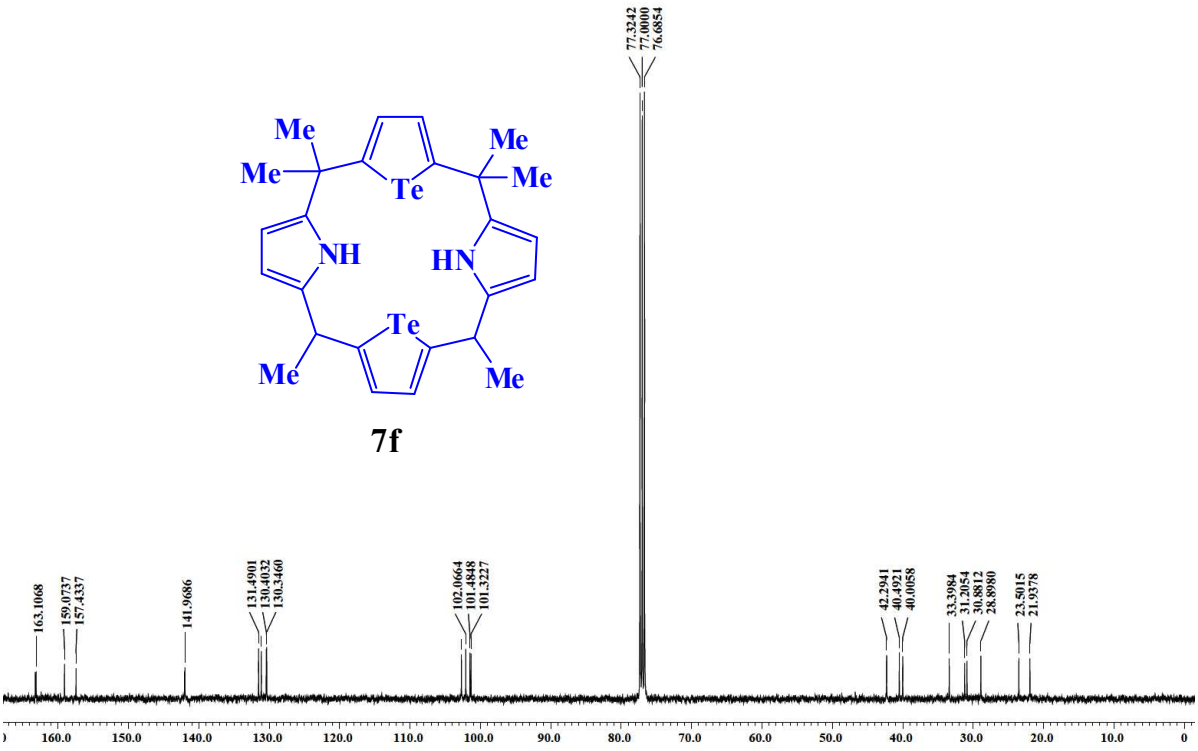

Me
Me
Me
Me
Te
NH
HN
Te
Me
Me
7f
77.3242
77.0000
76.6854
163.1068
159.0737
157.4337
141.9686
131.4901
130.4032
130.3460
102.0664
101.4848
101.3227
42.2941
40.4921
40.0058
33.3984
31.2054
30.8812
28.8980
23.5015
21.9378
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Figure S47

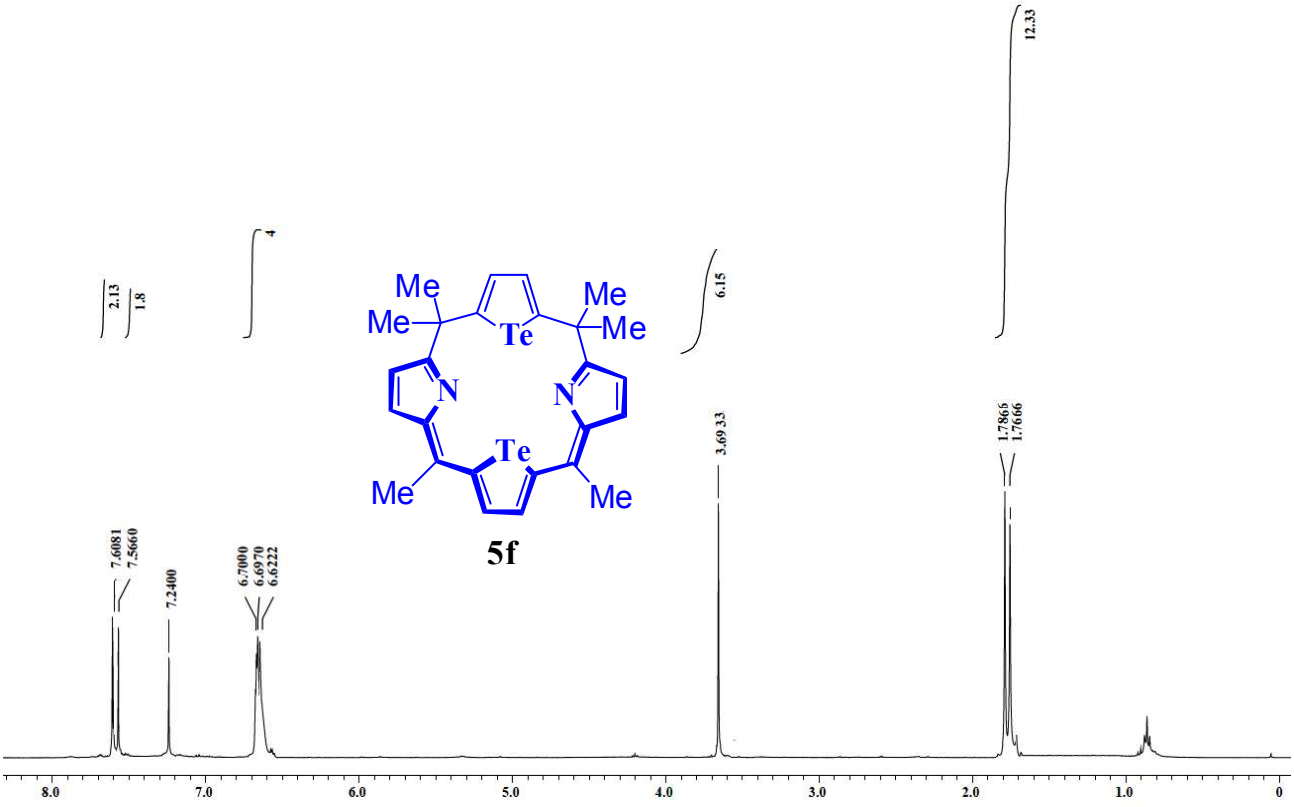

2.13
1.8
4
6.15
12.33
7.6081
7.5660
7.2400
6.7000
6.6970
6.6222
3.6933
1.7866
1.7666
Me
Me
Me
Me
Te
N
N
Te
Me
Me
5f
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S48

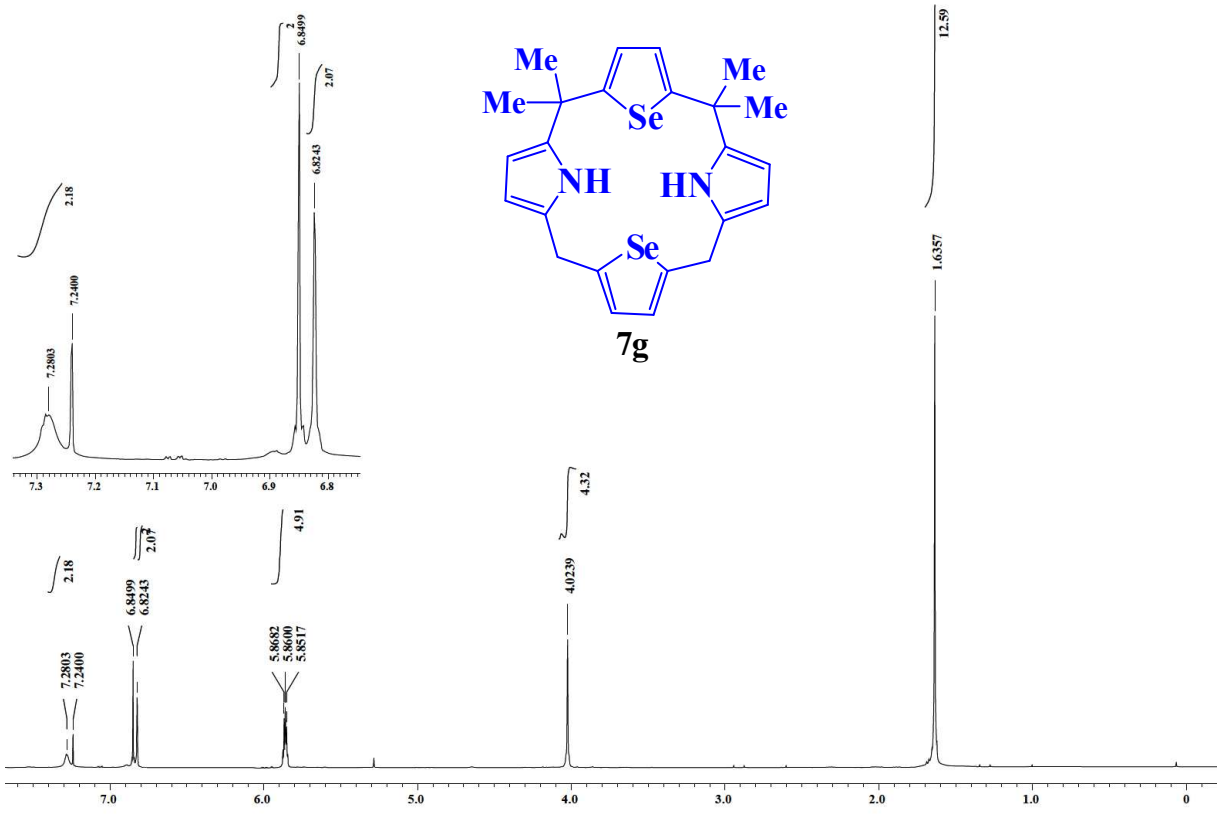

Me
Me
Me
Me
Se
NH
HN
Se
7g
12.59
1.6357
4.32
4.0239
4.91
2.18
2.07
6.8499
6.8243
5.8682
5.8600
5.8517
7.2803
7.2400
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S49

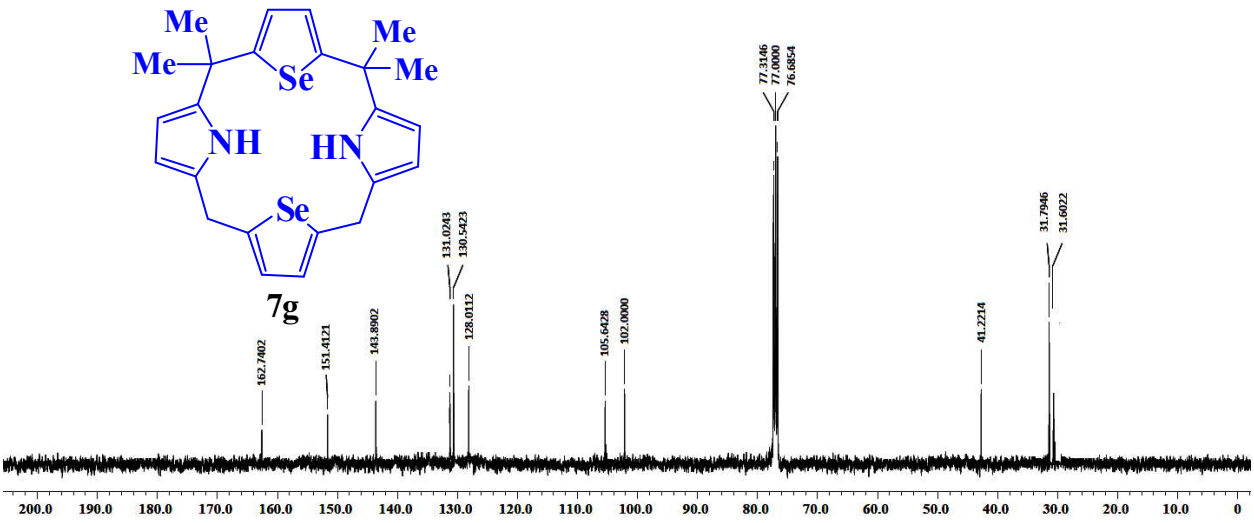
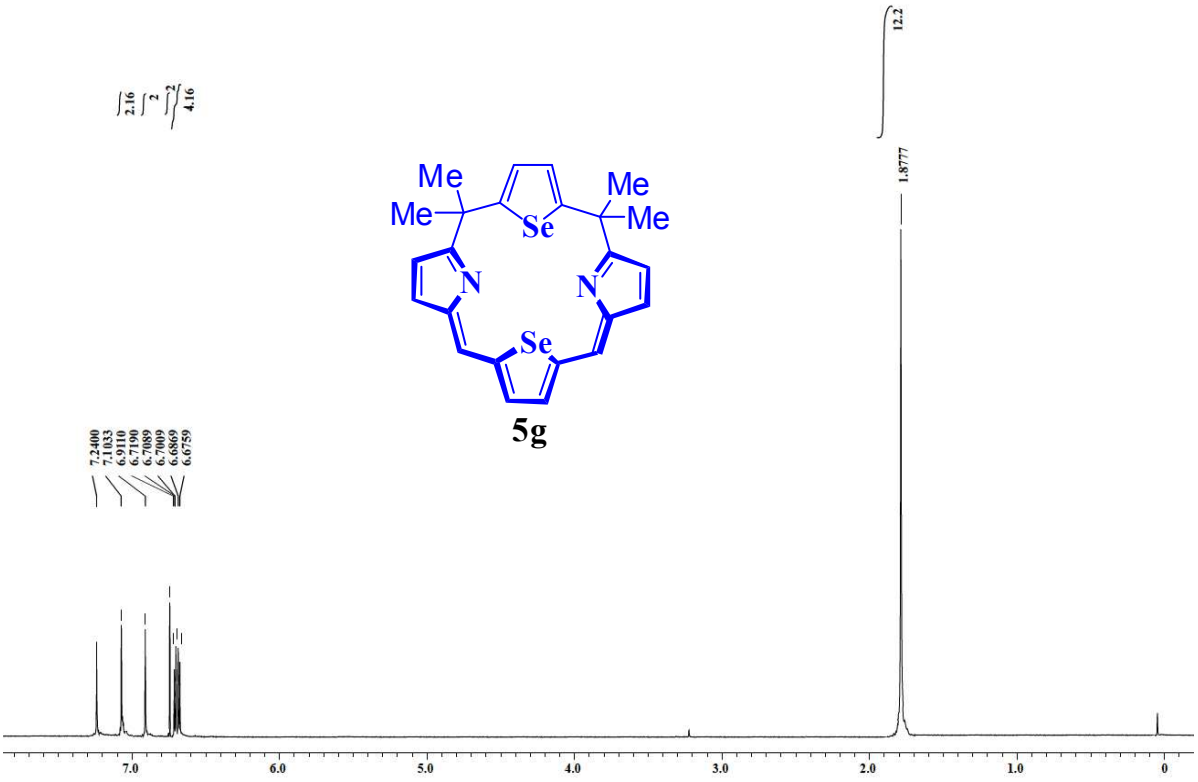

Me
Me
Me
Me
Se
NH
HN
Se
7g
162.7402
151.4121
143.8902
131.0243
130.5423
128.0112
105.6428
102.0000
77.3146
77.0000
76.6854
41.2214
31.7946
31.6022
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Figure S50



5g

Figure S51

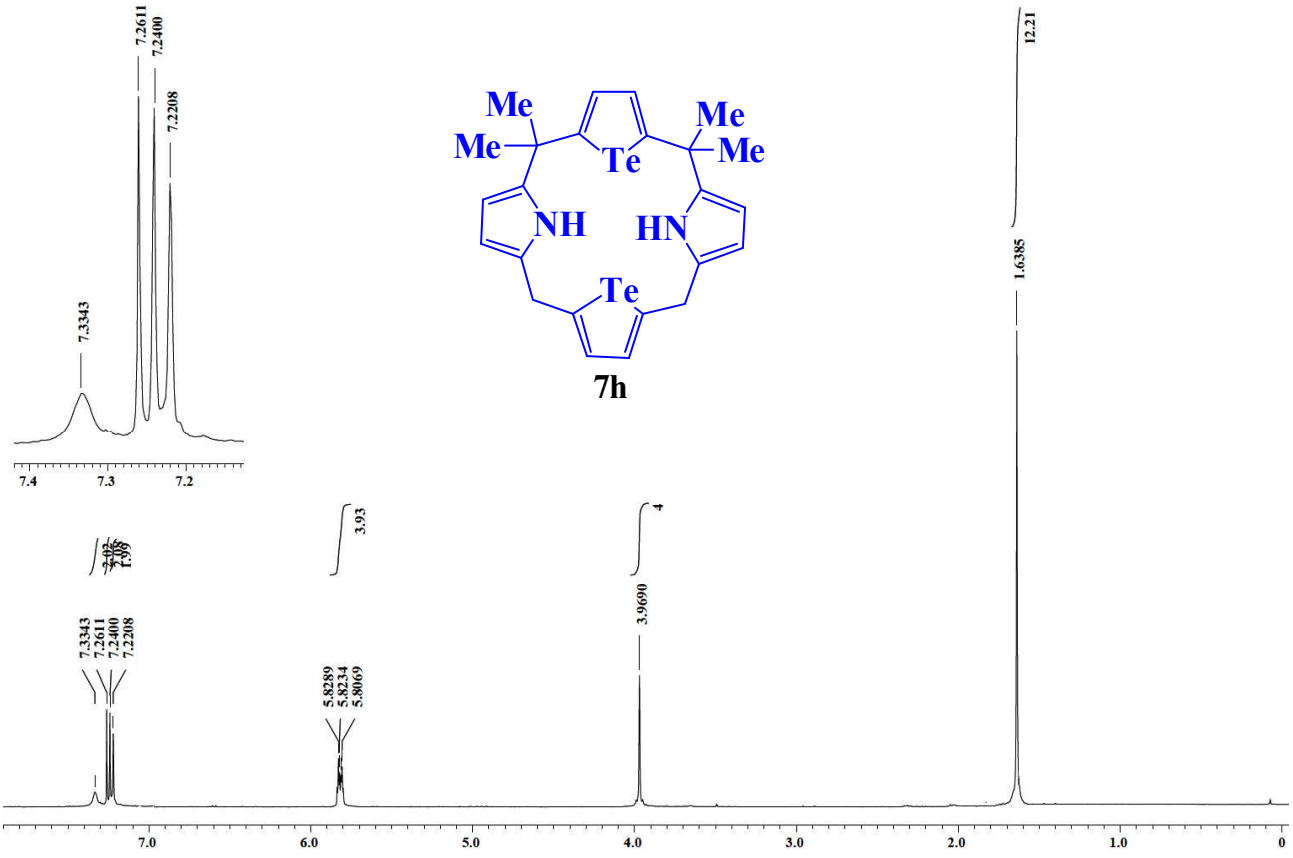

Me
Me
Me
Me
Te
NH
HN
Te
7h
7.2611
7.2400
7.2208
7.3343
12.21
1.6385
3.93
3.9690
5.8289
5.8234
5.8069
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S52

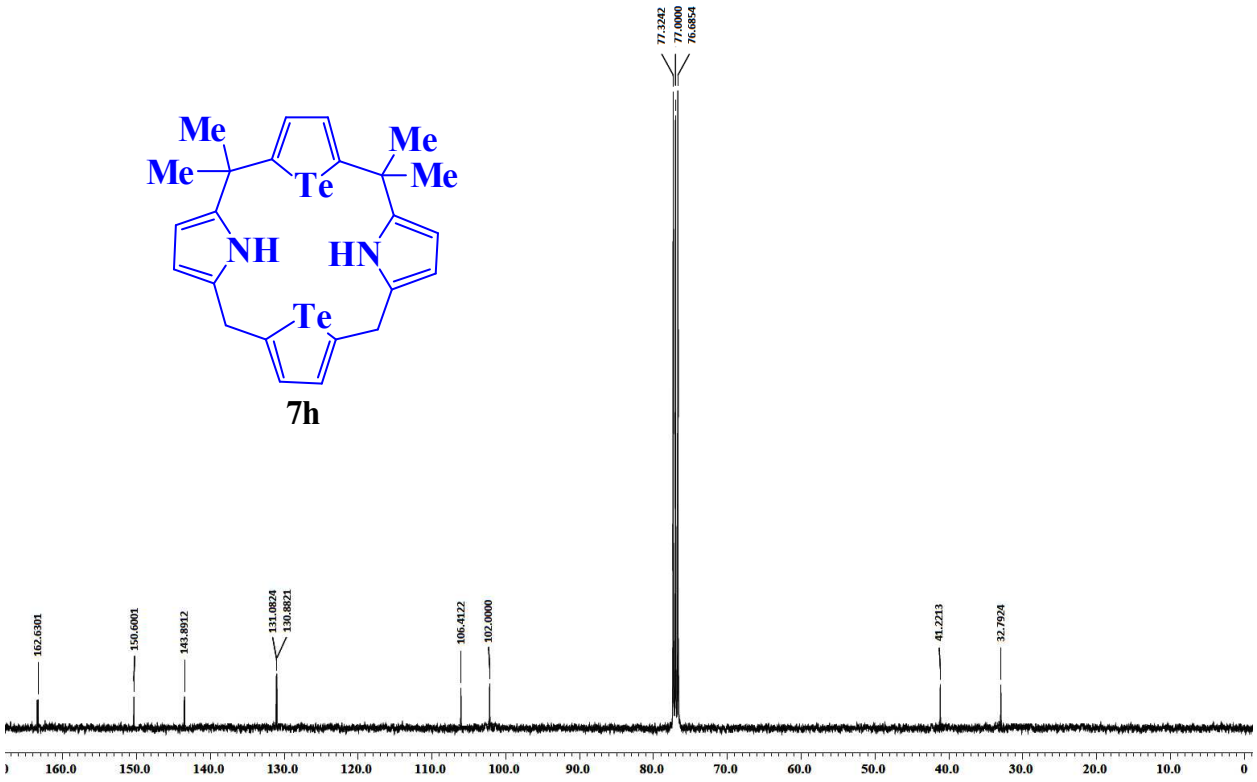

Me
Me
Me
Me
Te
NH
HN
Te
7h
77.3242
77.0000
76.6854
162.6301
150.6001
143.8912
131.0824
130.8821
106.4122
102.0000
41.2213
32.7924
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Figure S53

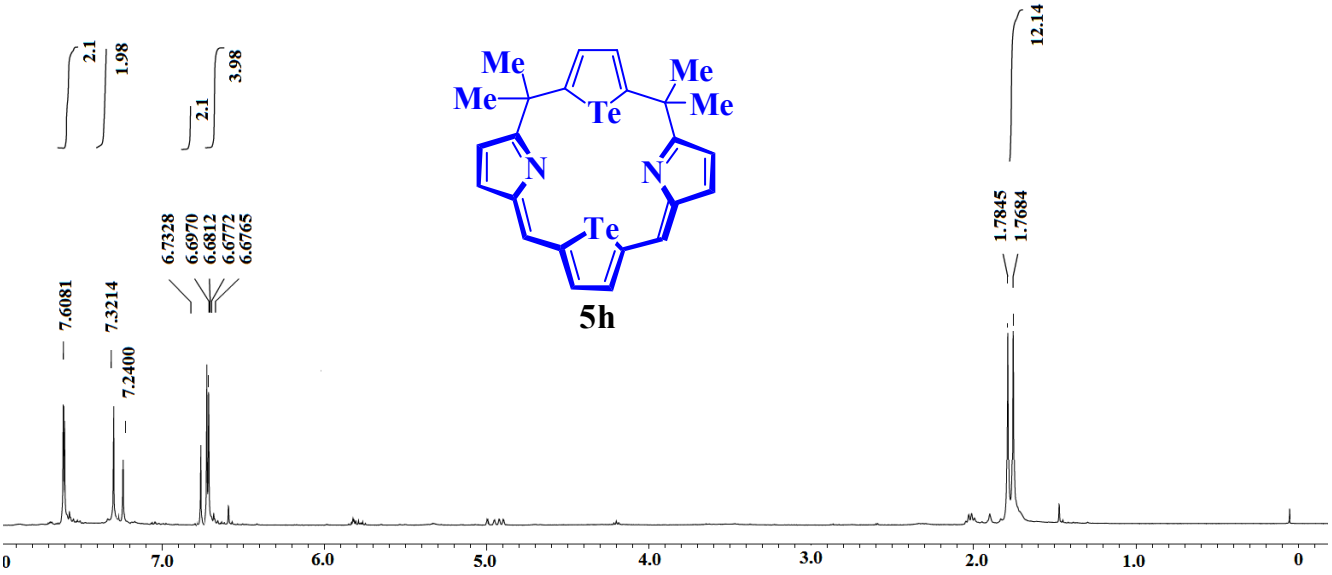

2.1
1.98
2.1
3.98
12.14
Me
Me
Me
Me
Te
N
N
Te
5h
7.6081
7.3214
7.2400
6.7328
6.6970
6.6812
6.6772
6.6765
1.7845
1.7684
0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S54

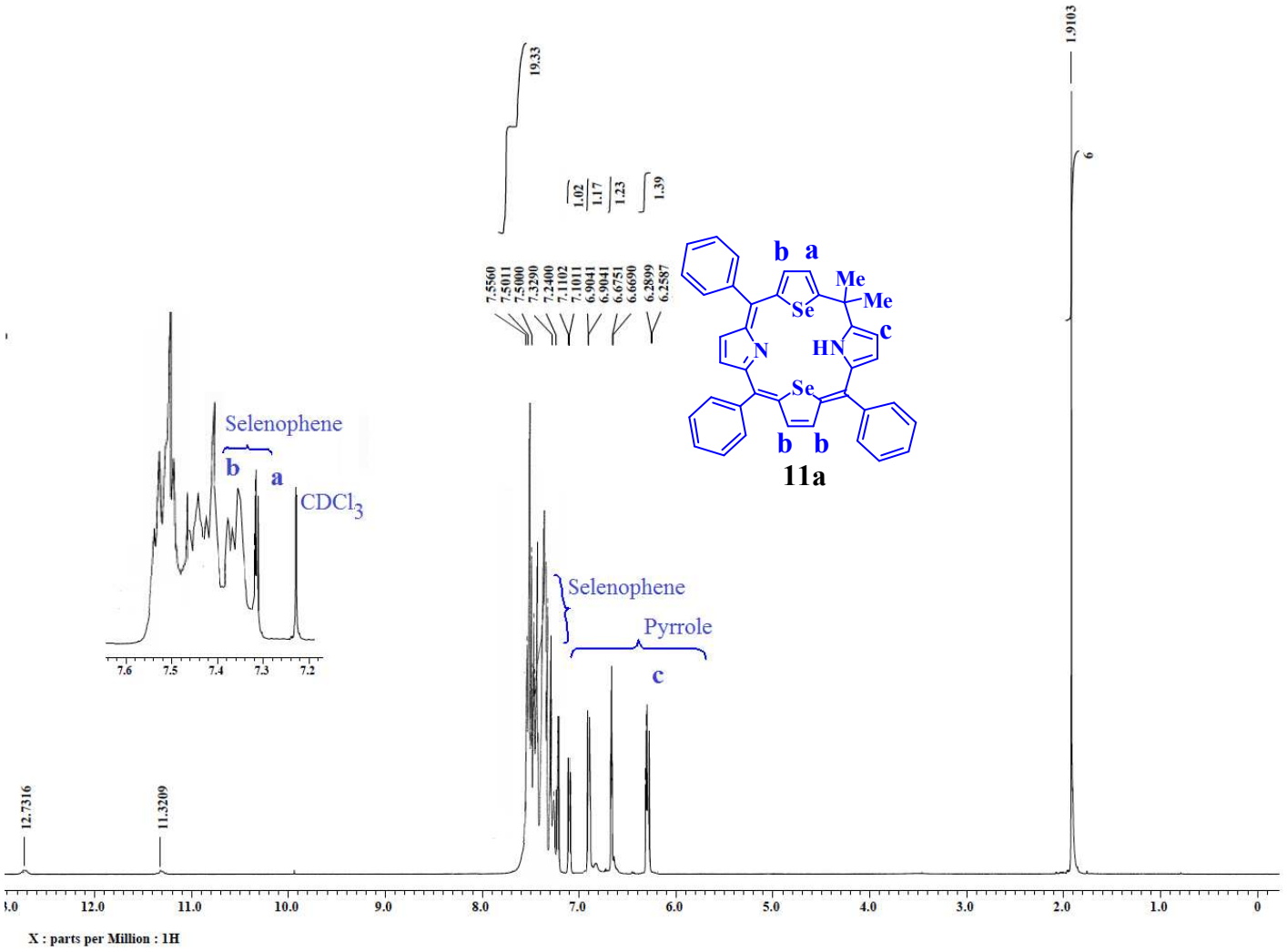

19.33
1.02
1.17
1.23
1.39
1.9103
6
7.5560
7.5011
7.5000
7.3290
7.2400
7.1102
7.1011
6.9041
6.9041
6.6751
6.6690
6.2899
6.2587
b a
Me
Me
Se
c
N
HN
Se
b b
11a
Selenophene
b
a
CDCl3
Selenophene
Pyrrole
c
12.7316
11.3209
X : parts per Million : 1H

Figure S55

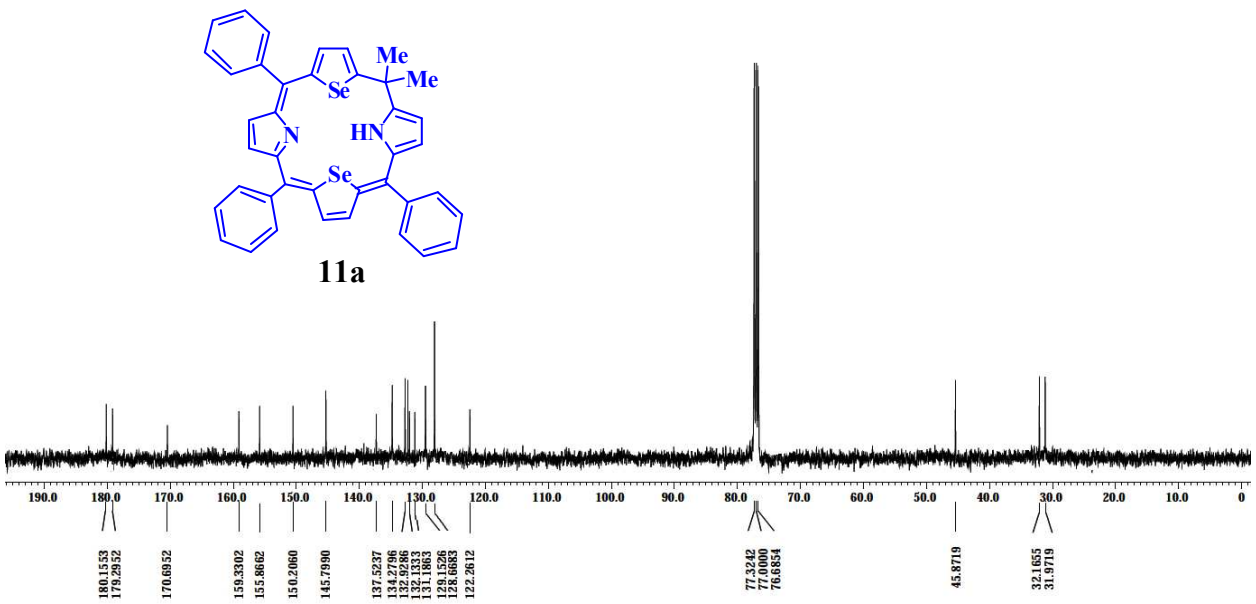

Me
Me
Se
N
HN
Se
11a
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
180.1553
179.2952
170.6952
159.3302
155.8662
150.2060
145.7990
137.5237
134.2796
132.9286
131.1373
131.1063
129.1526
128.6683
122.2612
77.3242
77.0000
76.6854
45.8719
32.1655
31.9719

Figure S56

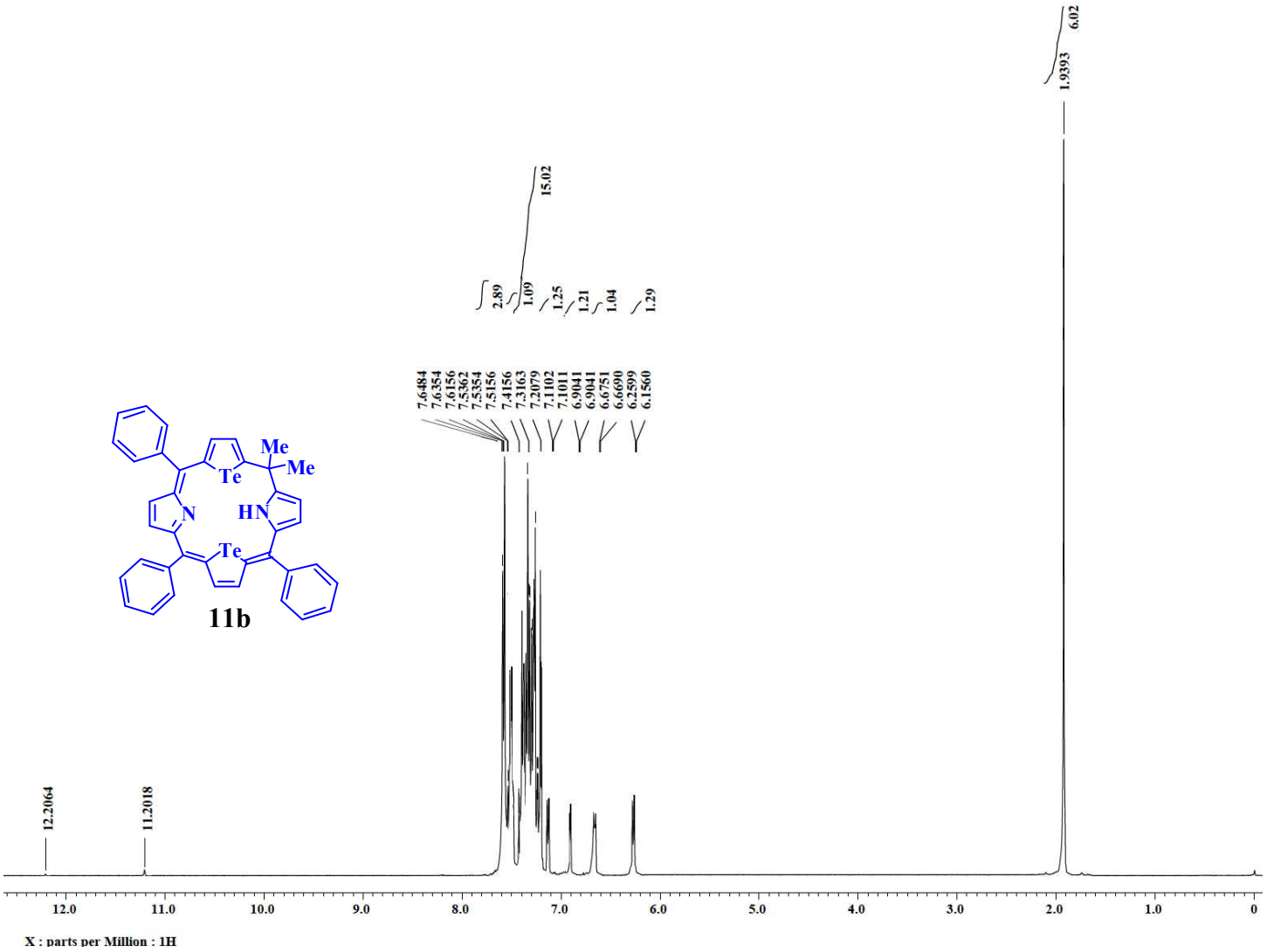

Me
Me
Te
N
HN
Te
11b
12.2064
11.2018
2.89
15.02
1.09
1.25
1.21
1.04
1.29
1.9393
6.02
7.6484
7.6354
7.6156
7.5362
7.5354
7.5156
7.4156
7.3163
7.2079
7.1102
7.1011
6.9041
6.9041
6.6751
6.6690
6.2599
6.1560
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : 1H

Figure S57

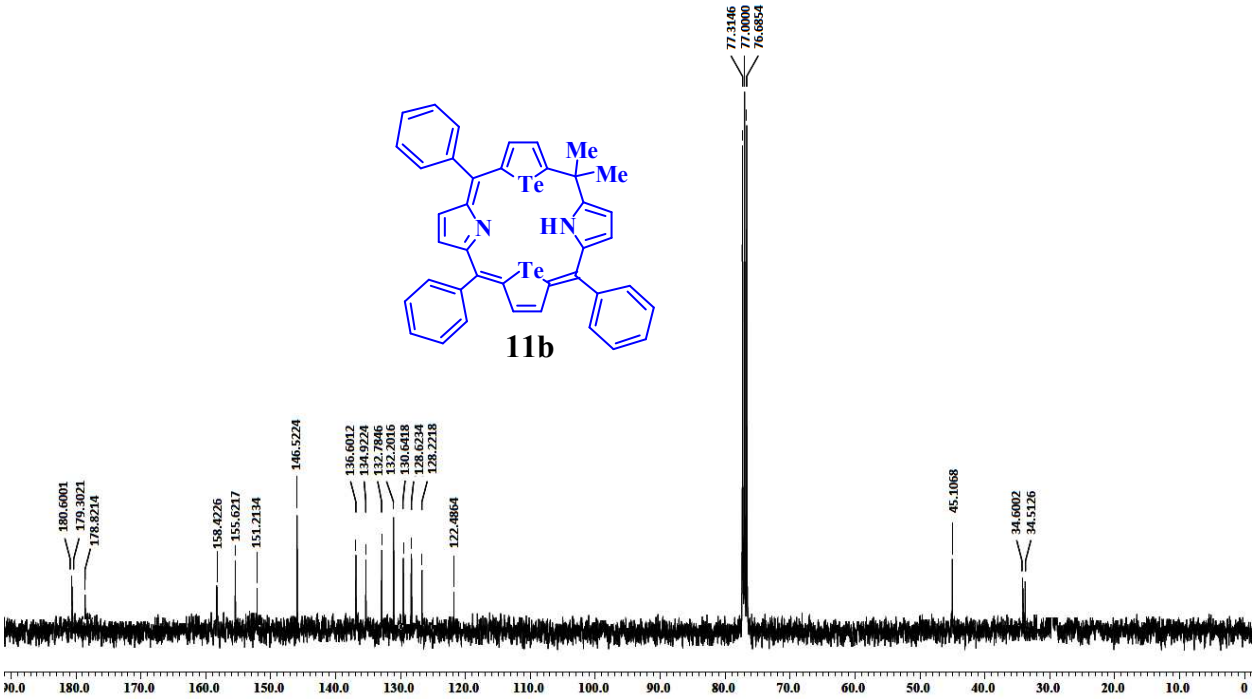

Me
Me
Te
N
HN
Te
11b
77.3146
77.0000
76.6854
180.6001
179.3021
178.8214
158.4226
155.6217
151.2134
146.5224
136.6012
134.9224
132.7846
132.2016
130.6418
128.6234
128.2218
122.4864
45.1068
34.6002
34.5126
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Figure S58

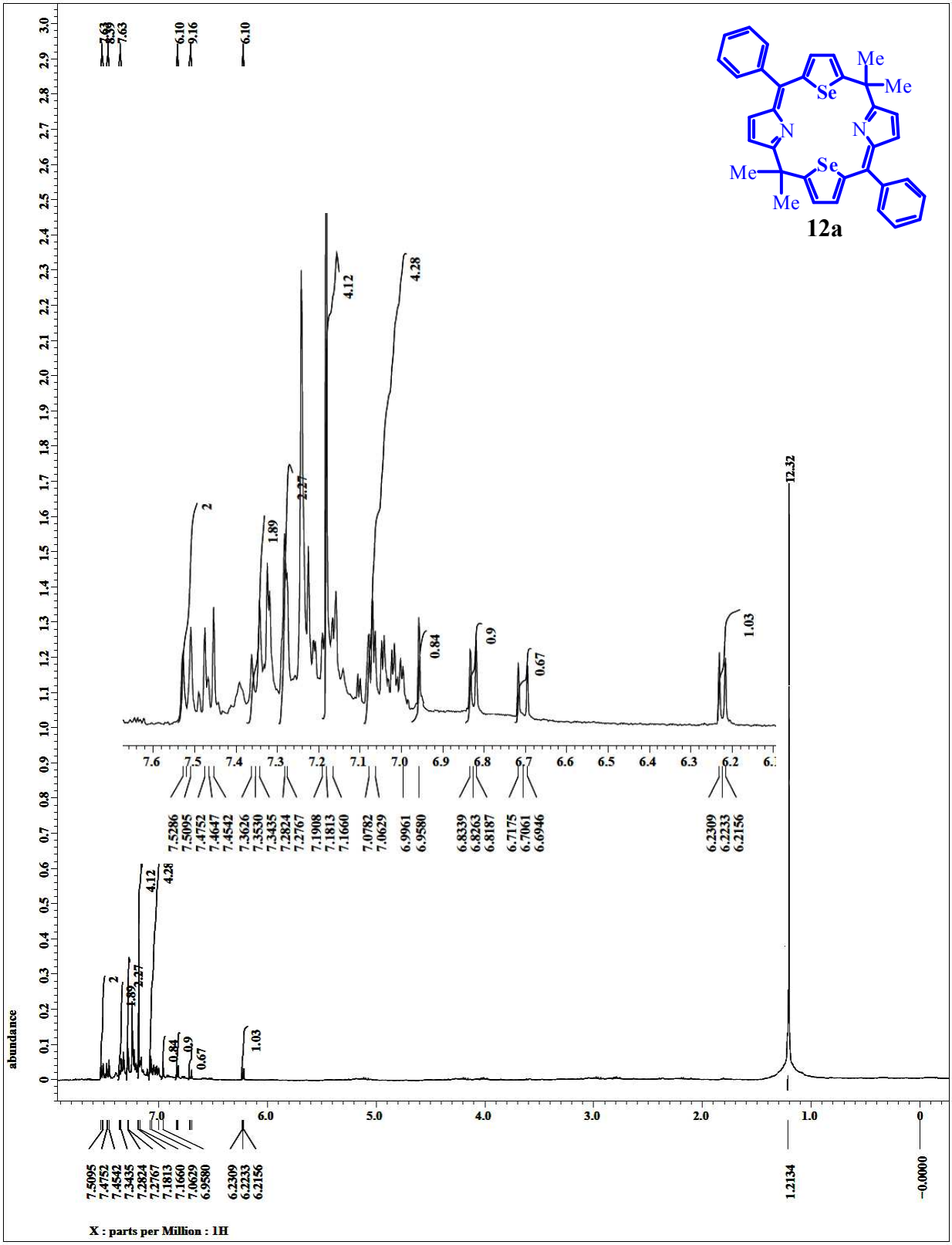


Figure S59

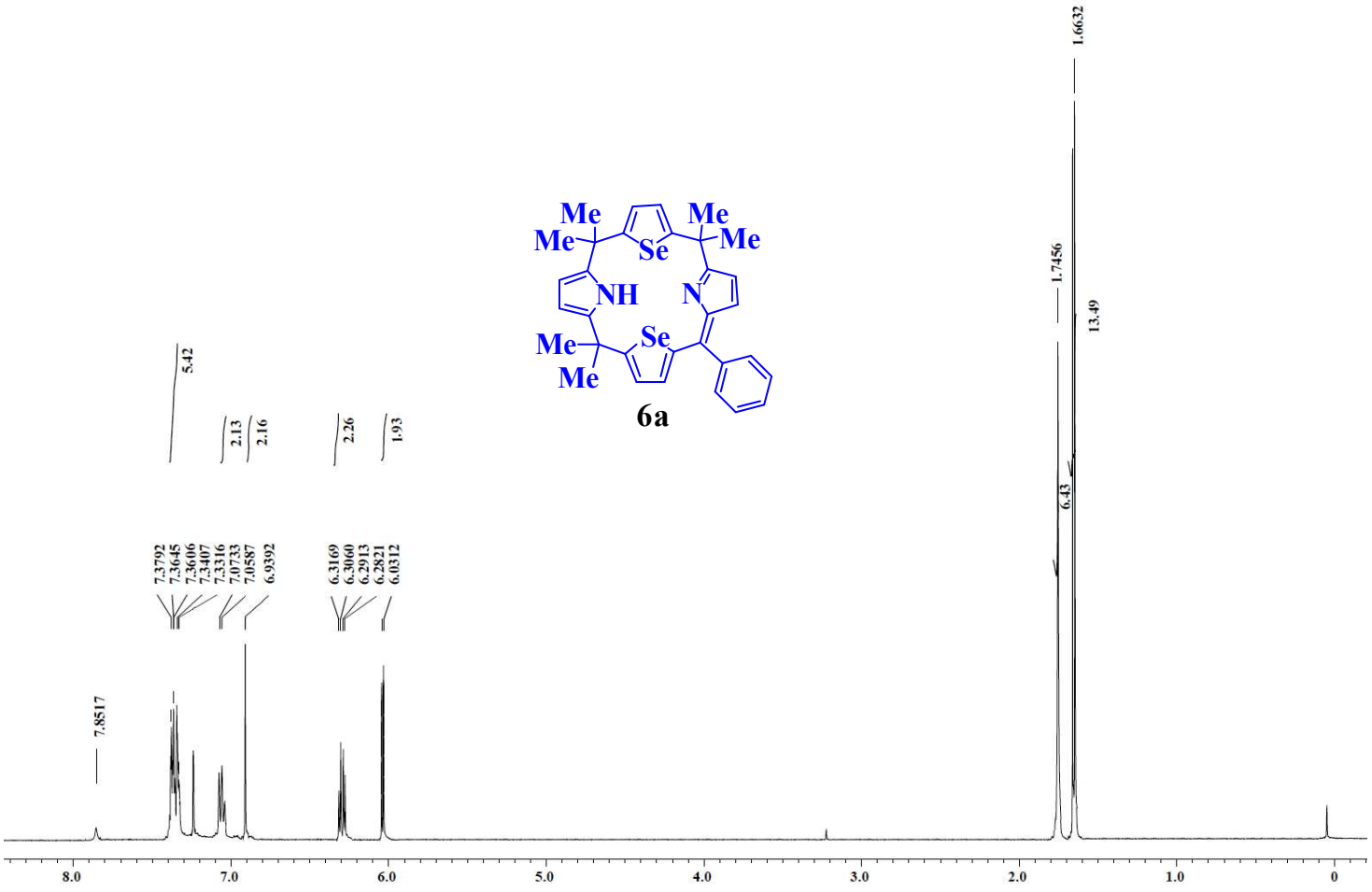

Me
Me
Me
Me
Se
NH
N
Se
Me
Me
6a
1.6632
1.7456
13.49
6.43
5.42
2.13
2.16
2.26
1.93
7.3792
7.3645
7.3606
7.3407
7.3316
7.0733
7.0587
6.9392
6.3169
6.3060
6.2913
6.2821
6.0312
7.8517
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S60

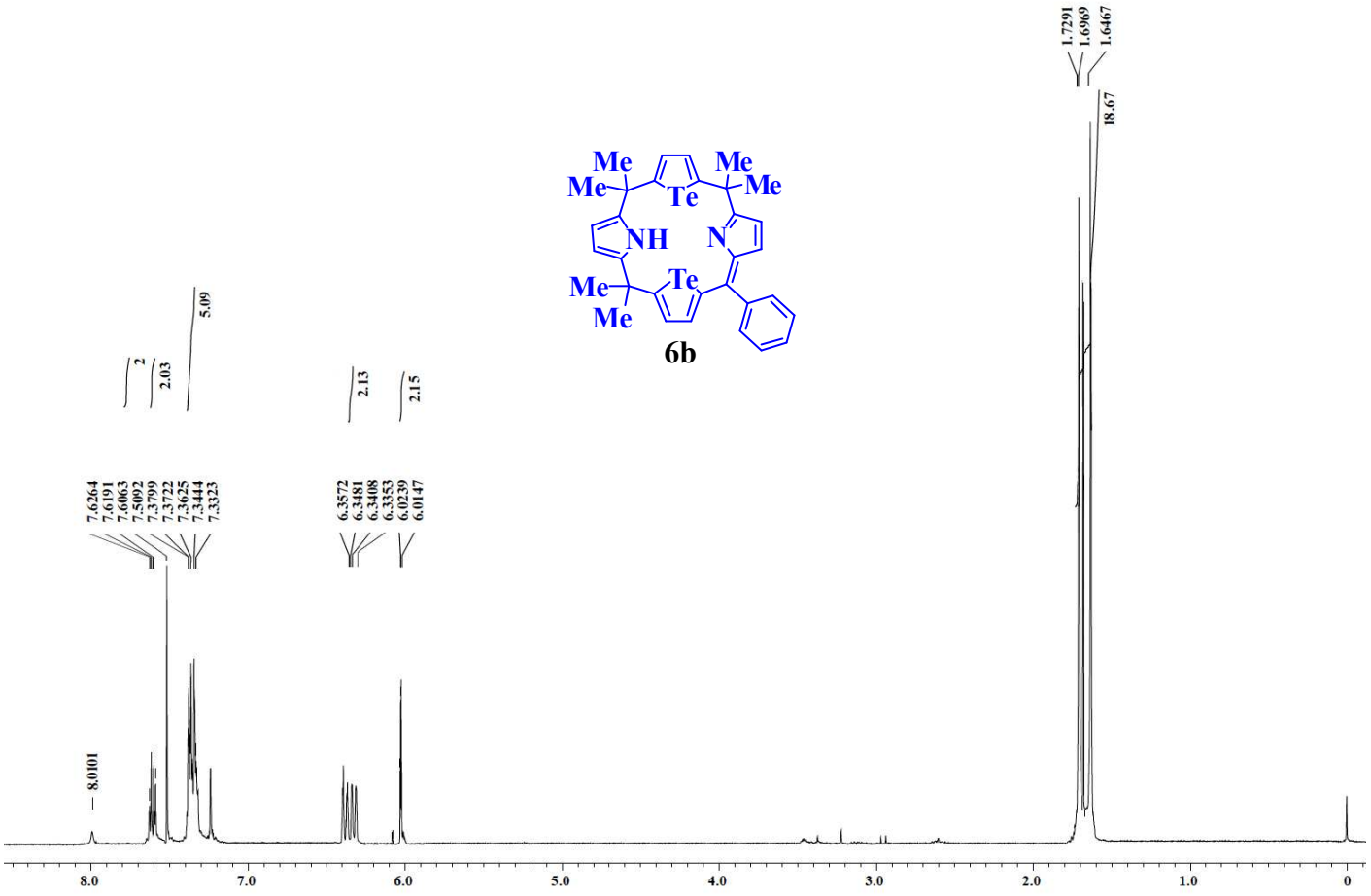

Me
Me
Me
Me
Te
NH
N
Te
Me
Me
6b
1.7291
1.6969
1.6467
18.67
5.09
2
2.03
2.13
2.15
7.6264
7.6191
7.6063
7.5092
7.3799
7.3722
7.3625
7.3444
7.3323
6.3572
6.3481
6.3408
6.3353
6.0239
6.0147
8.0101
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

Figure S61

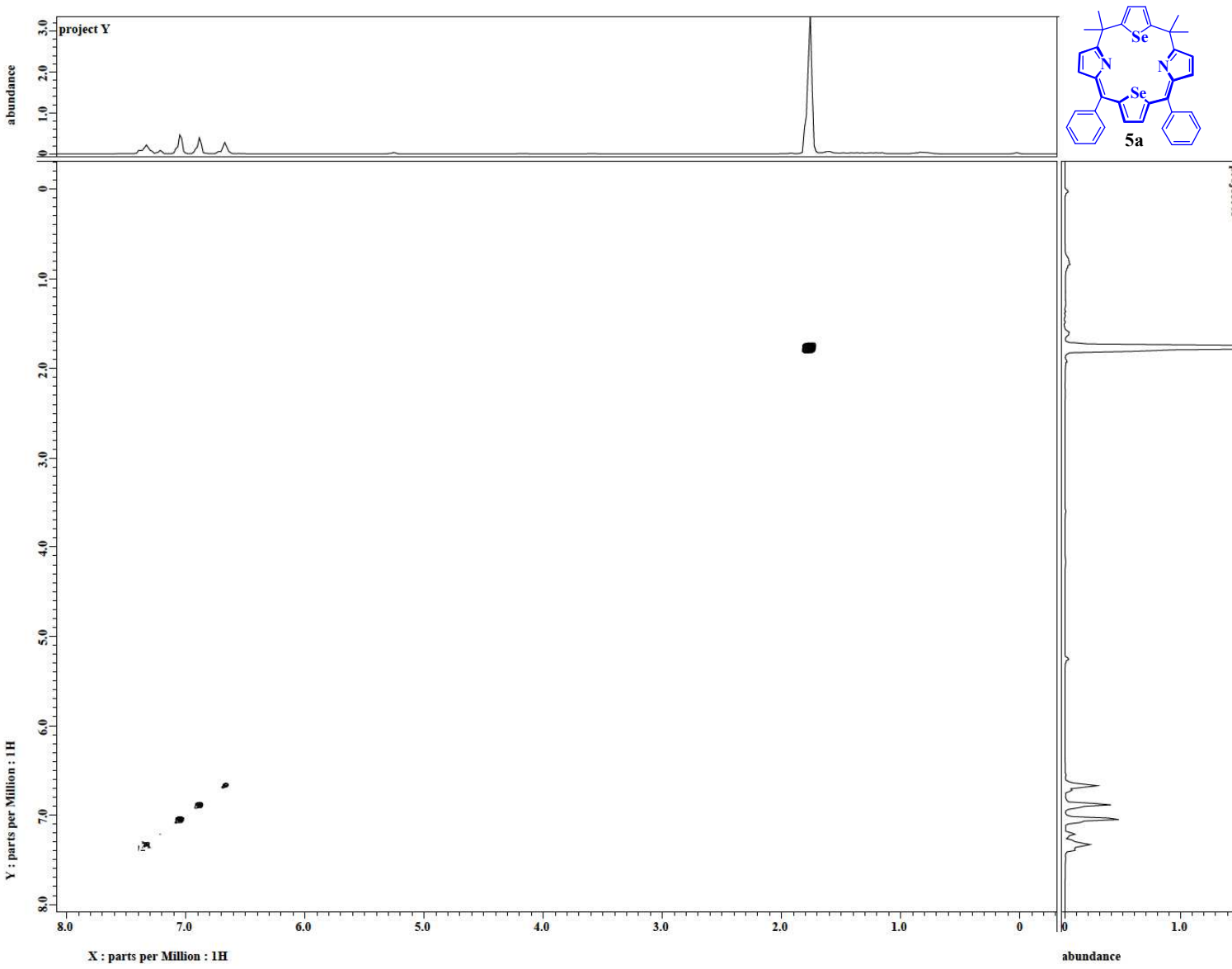

project Y
abundance
Se
N
N
Se
5a
Y : parts per Million : 1H
X : parts per Million : 1H
abundance

Figure S62

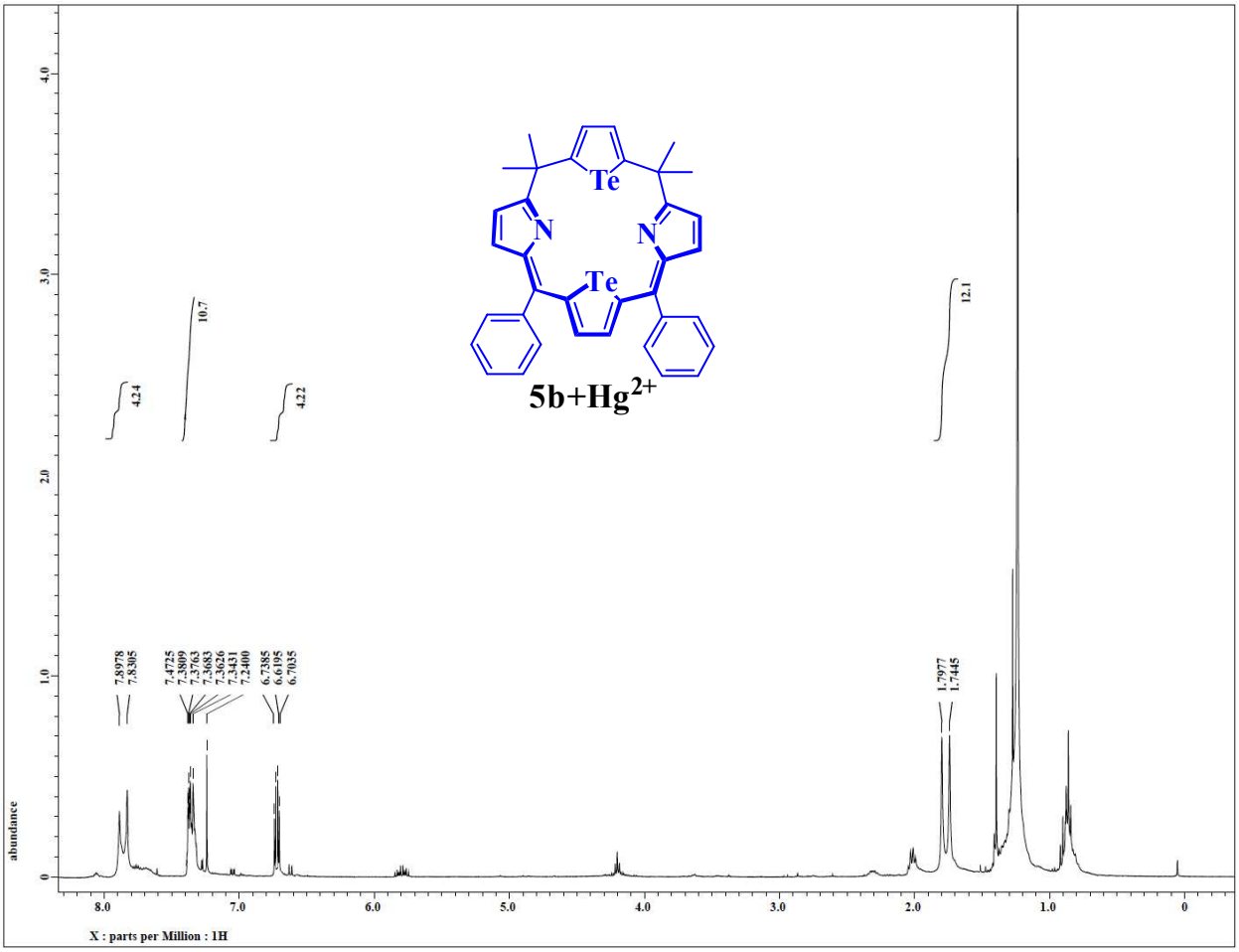

Te
N
N
Te
5b+Hg2+
4.24
10.7
4.22
12.1
7.8978
7.8305
7.4725
7.3809
7.3763
7.3683
7.3626
7.3431
7.2400
6.7385
6.6195
6.7035
1.7977
1.7445
abundance
X : parts per Million : 1H

Figure S63

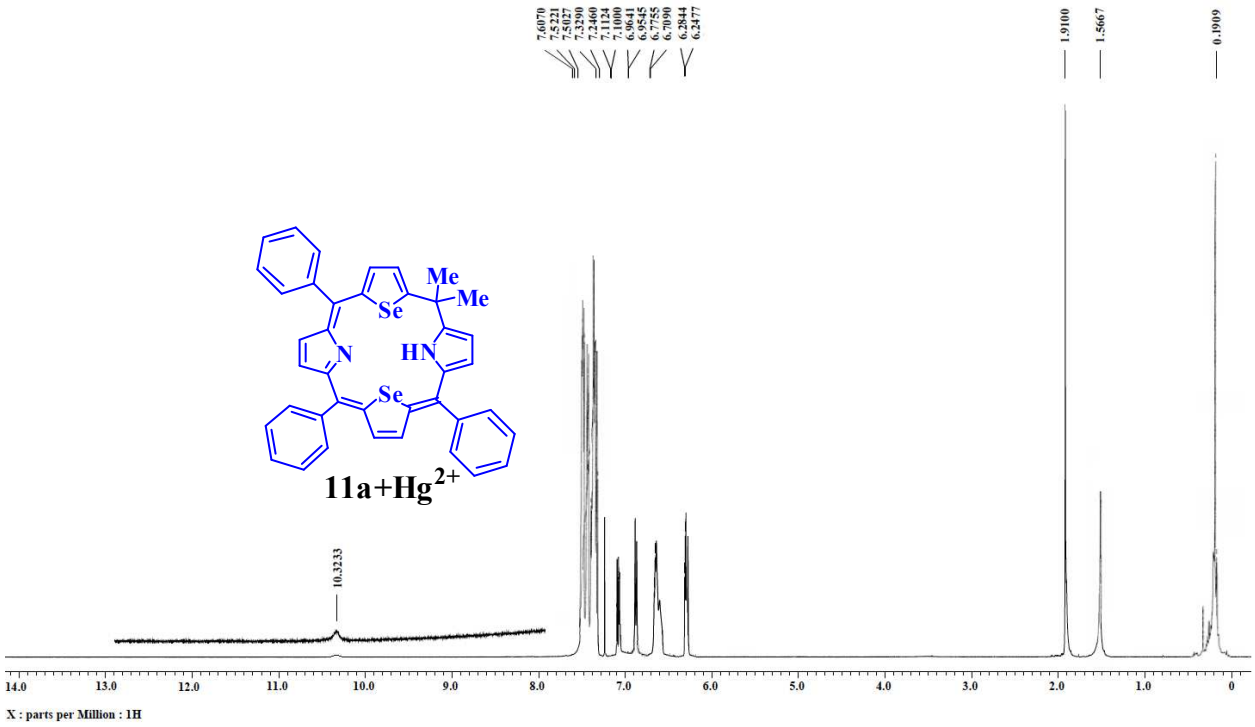
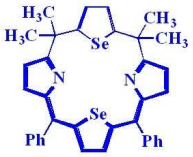

7.6070
7.5221
7.5027
7.3290
7.2460
7.1124
7.1000
6.9641
6.9545
6.7755
6.7090
6.2844
6.2477
1.9100
1.5667
0.1909
10.3233
Me
Me
Se
N
HN
Se
11a+Hg2+
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : 1H

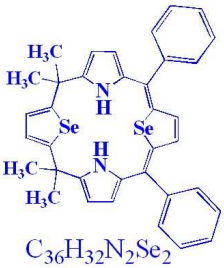
Figure S64

Qualitative Analysis Report

Data Filename	E.d	**Sample Name**	E
Sample Type	Sample	**Position**	P1-F5
Instrument Name	Instrument 1	**User Name**	SANJAY PANDEY
Acq Method	DAILY MS.m	**Acquired Time**	15-04-2013 12:01:49
IRM Calibration Status	Success	**DA Method**	
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		



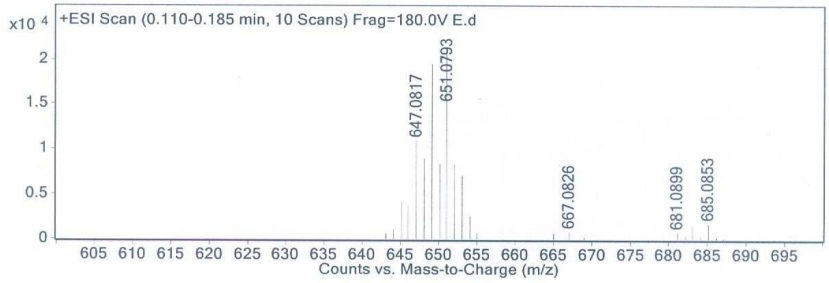
5a $C_{36}H_{30}N_2Se_2$
650.07



$C_{36}H_{32}N_2Se_2$
652.09
8a

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
180	0	ESI



Peak List

m/z	z	Abund
100.0759		3300.52
102.1278		3923.1
104.0087		6162.19
106.0043		24142.43
108.0807		6548.74
110.0084		4065.95
121.9664		4052.55
122.9638		5325.55
132.0033		4772.56
138.03		4848.99
140.9609	1	3574.59
149.0226		6062.15
217.1038		6581.52
301.14		4661.89
338.3402		3283.43
391.2824	1	4311.51
413.2645	1	9578.1
425.361	1	4369.58
429.2388	1	4013.46
447.3426	1	8522.79
463.3163	1	4098.19
645.0824		4187.88
646.0841		3798.07
647.0817		10926.78
648.0828		9029.21
649.0807	1	19472.7

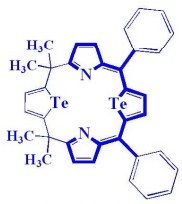
650.0834	1	8360.48	→ M
651.0793	1	20630.67	→ M+1
652.0927	1	8235.92	→ M
653.0797	1	7094.27	→ M+1

--- End Of Report ---

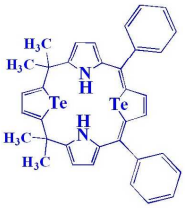
Figure S65

Qualitative Analysis Report

Data Filename	KKY216.d	**Sample Name**	KKY216
Sample Type	Sample	**Position**	P1-E6
Instrument Name	Instrument 1	**User Name**	
Acq Method	DAILY MS.m	**Acquired Time**	
IRM Calibration Status	[redacted]	**DA Method**	
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		



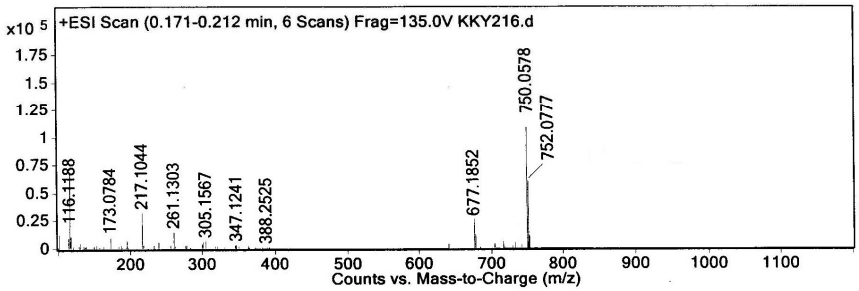
$C_{36}H_{30}N_2Te_2$
750.05
5b



$C_{36}H_{32}N_2Te_2$
752.07
8b

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund
100.0767		1017.78
100.1128		1238.98
100.5216		1228.94
101.0719	1	2385.69
102.1286	1	10690.11
115.0872		9351.56
116.1188	1	71547.54
117.1212	1	10462.11
121.5712		2107.28
129.5596		2275.71
130.1591		4968.32
135.0027		1929.94
139.0505		1471.75
151.0965		1511.26
153.1383		2934.66
157.0837		828.3
158.0967		774.06
163.1261		1694.81
173.0784		10240.74
185.1143		1652.42
187.1214		3143.39
189.0525		1262.71
194.1176		1242.02
195.1223		6785.64
198.1036		940.14
217.1044	1	32266.27
218.108	1	3072.61
233.0805		2894.07
239.1479		5497.98
256.1751		2797.83
261.1303	1	14948.37
262.1343	1	1805.28
277.1035		2937.71
278.1653		1778.87
279.1008		2164.05
279.1594		3062.73
283.1743		1155.88
300.2013		3894.6
301.1401	1	5702.34
305.1567	1	6463.43
317.1147		2137.89
321.1307		1614.55
331.0908		1386.16
344.2262		2915.47
347.1241	1	3148.3
349.182		1899.29
357.1545		2955.43
365.1552		927.24
372.2408		1113.64
388.2525		1005.6
677.3615		21187.3
684.2055		1370.29
704.2412		889.56
709.3072		3436.15
710.1847	1	4207.92
750.0578	1	113114.55 — M^+
751.0247	1	5181.31 — M+1
752.0777	1	62335.69 — M^+

--- End Of Report ---

Figure S66

Qualitative Analysis Report

Data Filename	A003.d	**Sample Name**	A
Sample Type	Sample	**Position**	P1-F1
Instrument Name	Instrument 1	**User Name**	SANJAY PANDEY
Acq Method	DAILY MS.m	**Acquired Time**	15-04-2013 12:57:20
IRM Calibration Status	Success	**DA Method**	default.m
Comment			

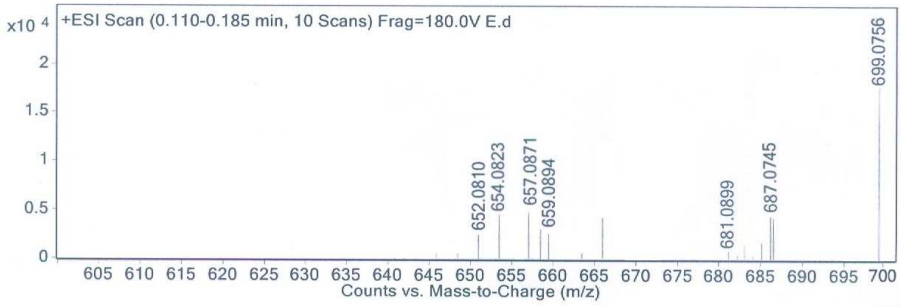
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

$C_{40}H_{30}N_2Se_2$
698.07

11a

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
180	0	ESI



Peak List

m/z	z	Abund
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
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		5058.53
698.0694	1	2652.42
699.0756		17448.3
700.0693		2937.63

] → M
] → M+1

Figure S67

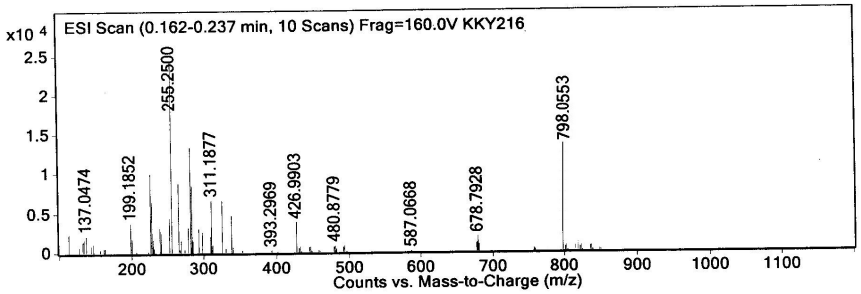
Qualitative Analysis Report

Data Filename	KKY216	**Sample Name**	KKY216
Sample Type	Sample	**Position**	P1-E6
Instrument Name	Instrument 1	**User Name**	
Acq Method	DAILY MS.m	**Acquired Time**	06-06-2013 13:52:35
IRM Calibration Status	[redacted]	**DA Method**	default.m
Comment			
Sample Group	**Info.**		
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

$C_{40}H_{30}N_2Te_2$
11b 798.05

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
160	0	ESI



Peak List

m/z	z	Abund
112.9969		2309.57
128.0468		718.47
132.8799		1357.75
134.8773		1617.14
137.0474		2113.37
143.1206		852.3
146.996		1074.9
199.1852		3667.91
201.0532		1833.98
225.9503		5133.76
226.9579	1	10015.24
227.2176	1	4159.26
227.9507	1	3672.38
228.9549	1	6489.1
229.1971		1663.7
229.9536	1	672.64
239.082		3111.9
241.2335		2412.36
253.2345		4410.73
255.25	1	24276.24
256.2535	1	4200.73
265.1655	1	8830.89
266.1688	1	939.73
269.2655		1502.59
279.2509		3189.45
281.0013		1013.18
281.2666	1	13247.54
282.27	1	2606.22
283.2819	1	8543.46
284.2865	1	1530.28
293.1979		2987.38
297.172		2655.73
309.1935		2039.22
311.1877	1	6629.14
312.1911	1	1019.77
325.2038	1	6566.65
326.2072	1	1432.3
339.2203	1	4717.06
340.2233	1	689.48
426.9903		3790.01
432.9006		717.24
444.918		719.73
446.9147		746.75
478.8805		628.65
480.8779		869.11
492.8934		619.83
494.8921		844.23
676.7955		1097.15
678.7928		1919.65
680.7909		914.06
798.0553	1	14015.24
804.4419		1461.76
816.4663	1	11857.78
817.4691	1	6380.91
818.4721	1	1758.21
846.4508		1065.28

--- End Of Report ---

Figure S68