

Supporting Information-

C(sp²)-H selenylation of substituted benzo[4,5]imidazo[2,1-*b*]thiazoles using PIFA [Bis(trifluoroacetoxy)iodobenzene] as a mediator

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b) NMR Spectra of compounds.....	S3- S64

X-ray crystal structure of compound 5h

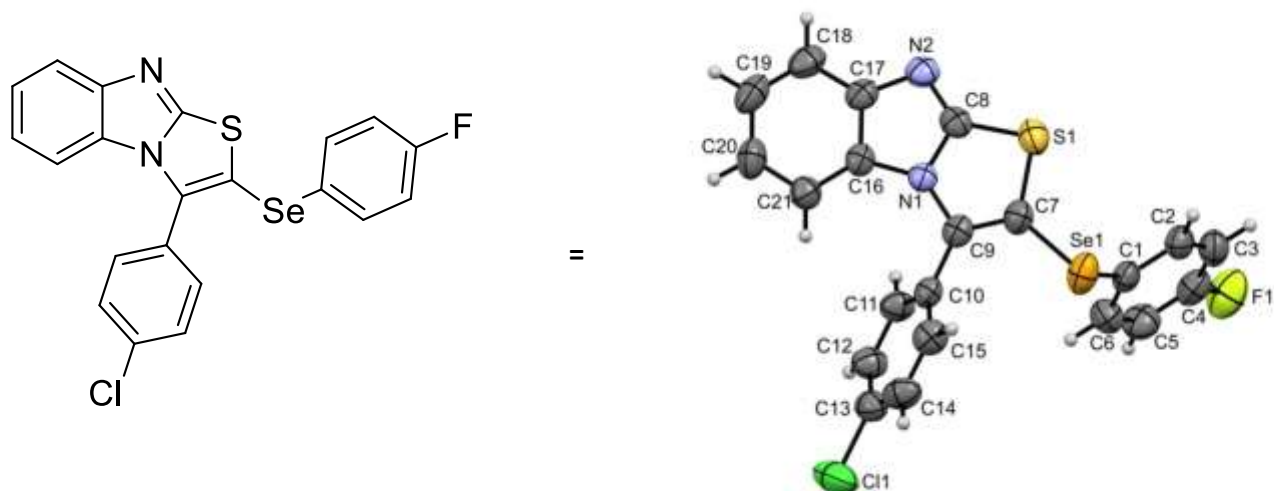
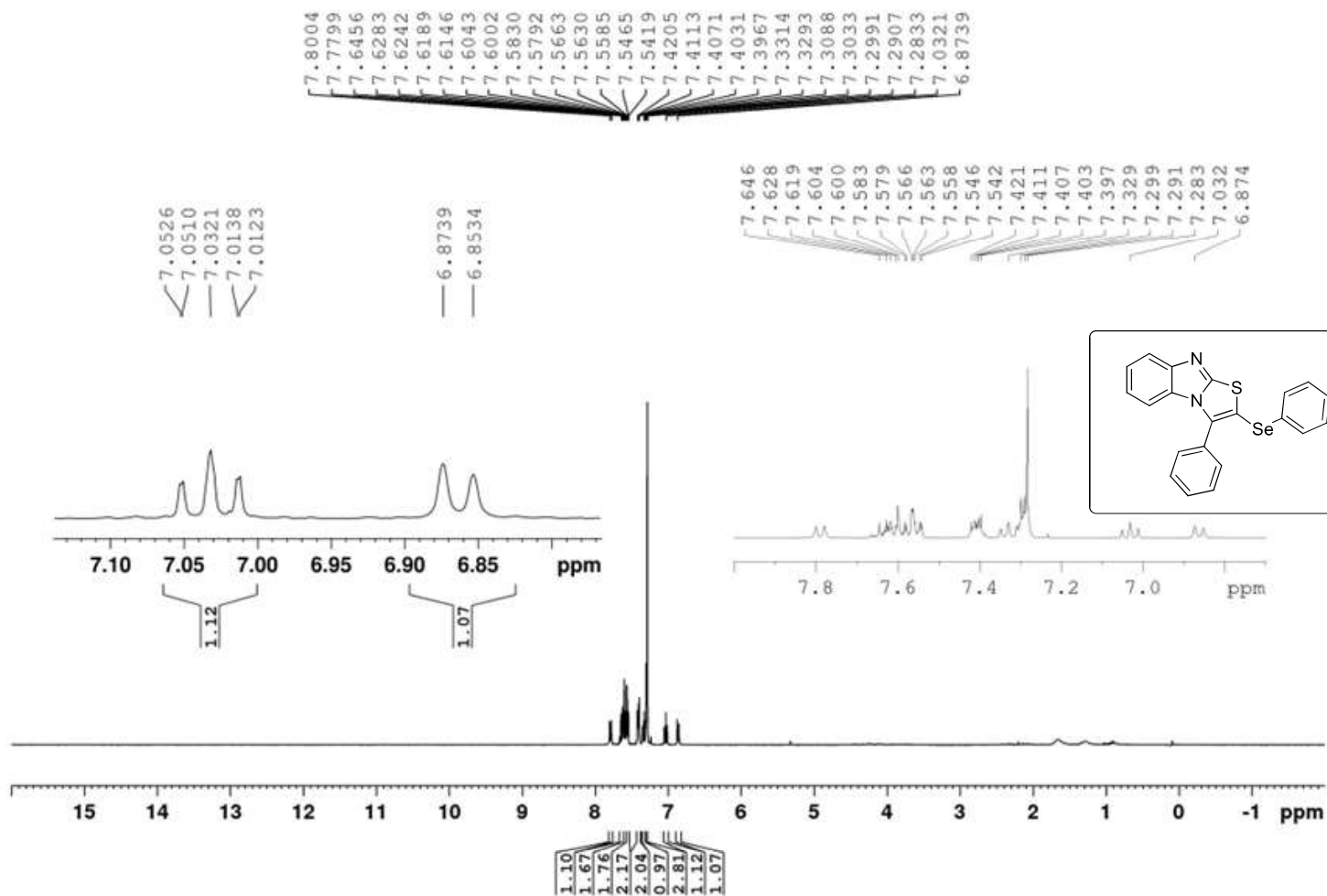


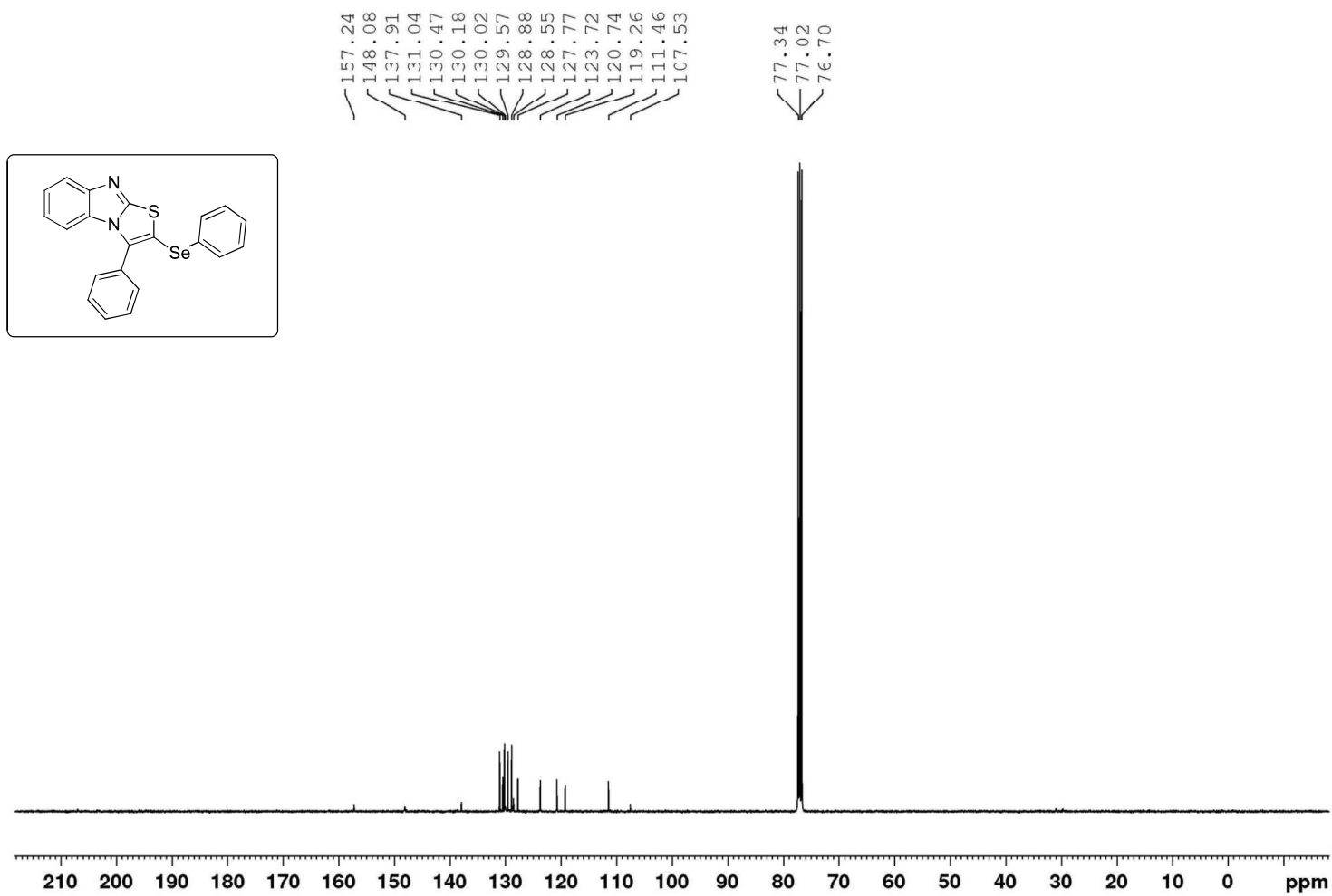
Figure : Mercury drawing of 5h.

Formula	C ₂₁ H ₁₂ ClFN ₂ SSe	
Crystal system	Triclinic	
Space group	P -1	
Volume	937(5)Å ³	
Z	2	
Density (gcm ⁻³)	1.623	
Theta range for data collection	2.42° to 22.97°	
Reflection collected/unique	10528/4102	
Observed reflection[>2sigma(I)]	2580	
Final R indices [I>2sigma(I)]	R ₁ = 0.0637	wR ₂ = 0.0782
R indices (all data)	R ₁ = 0.0332	wR ₂ = 0.0713
Unit cell dimension	a = 9.2475(173)Å	α = 70.528(22)°
	b = 9.9092(187)Å	β = 67.961(21)°
	c = 11.8955(222)Å	γ = 73.477(23)°

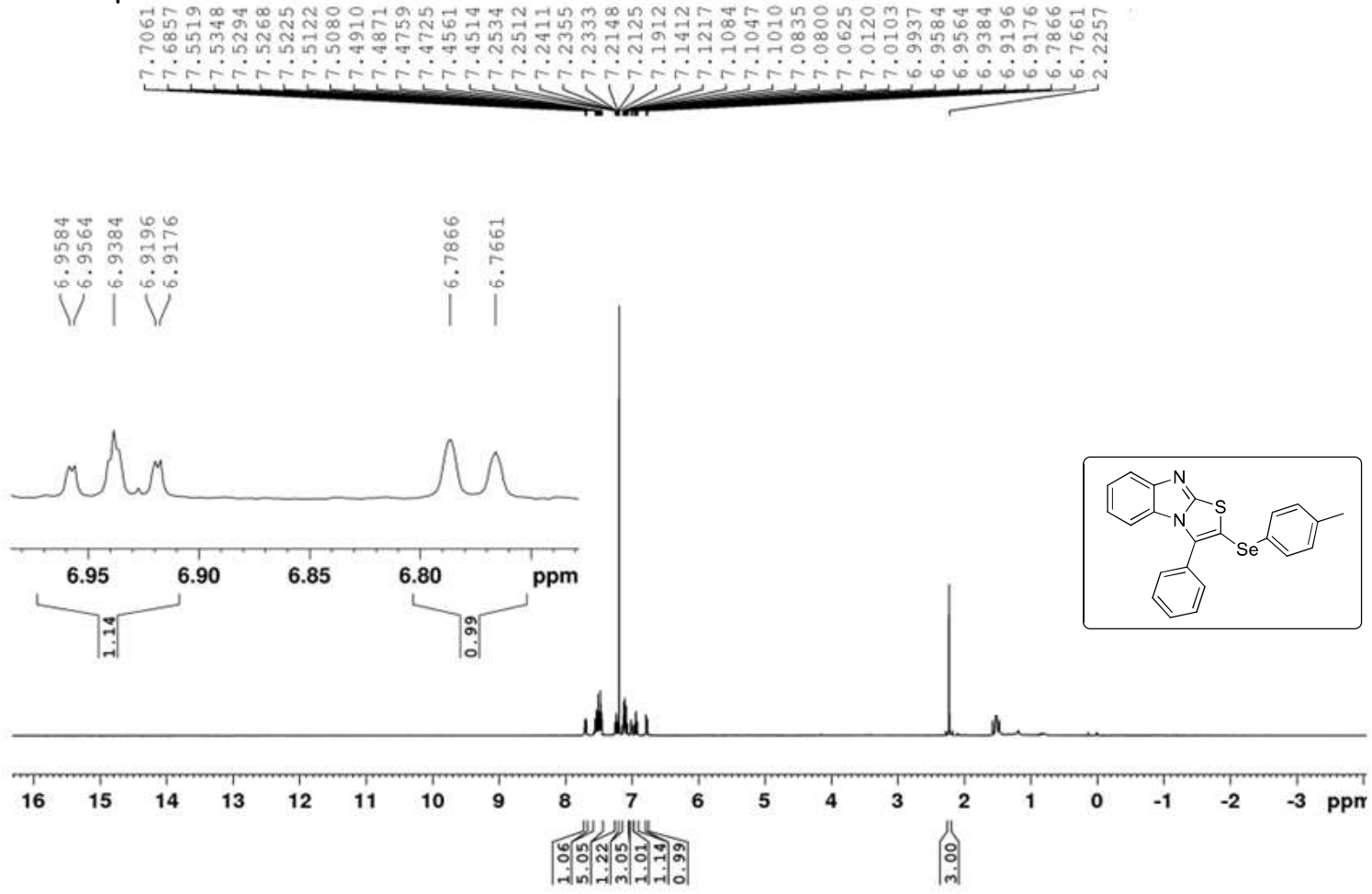
¹H NMR spectra of 3a



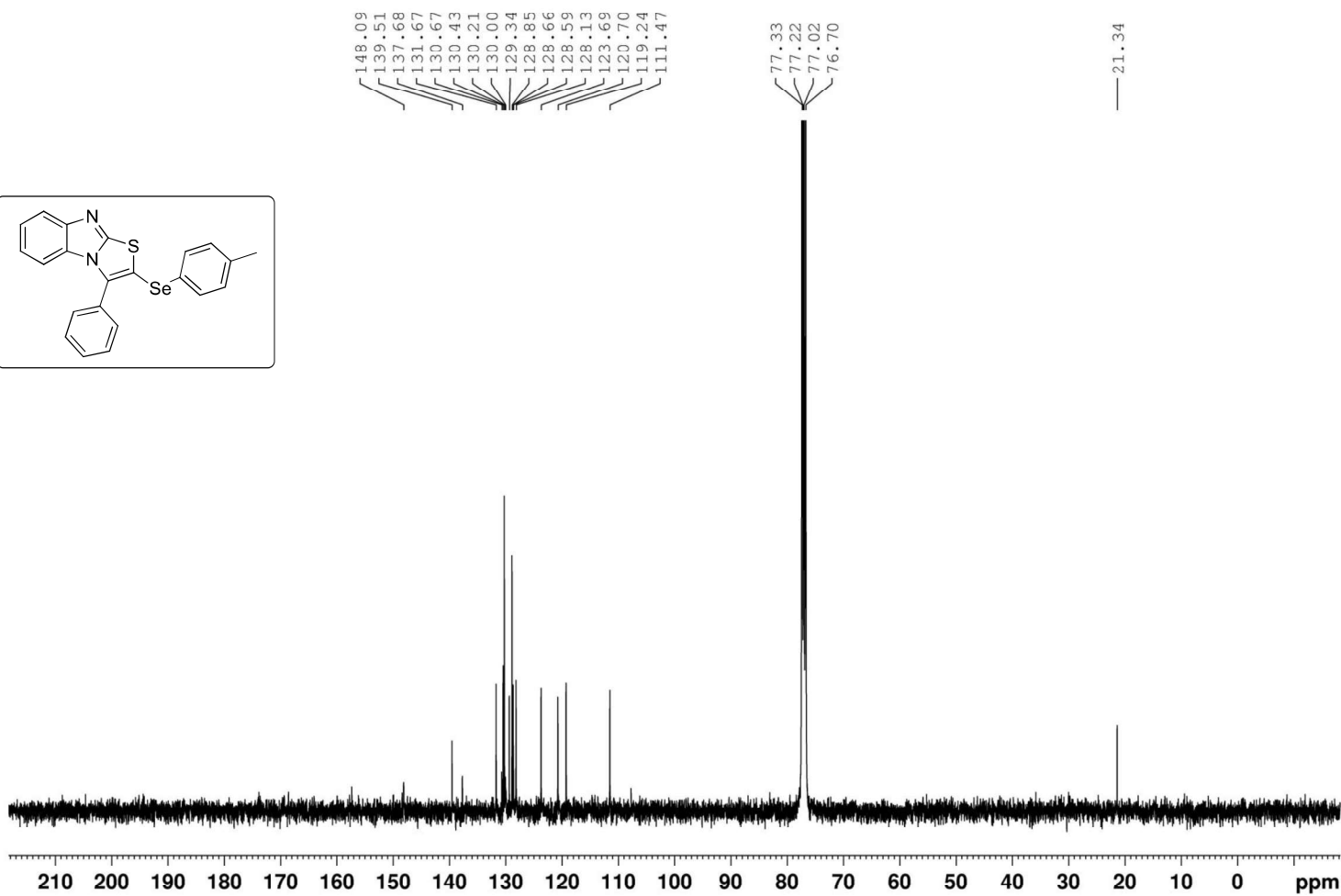
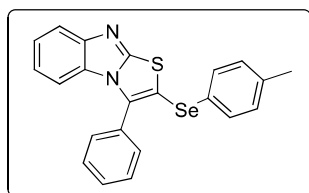
¹³C NMR spectra of 3a



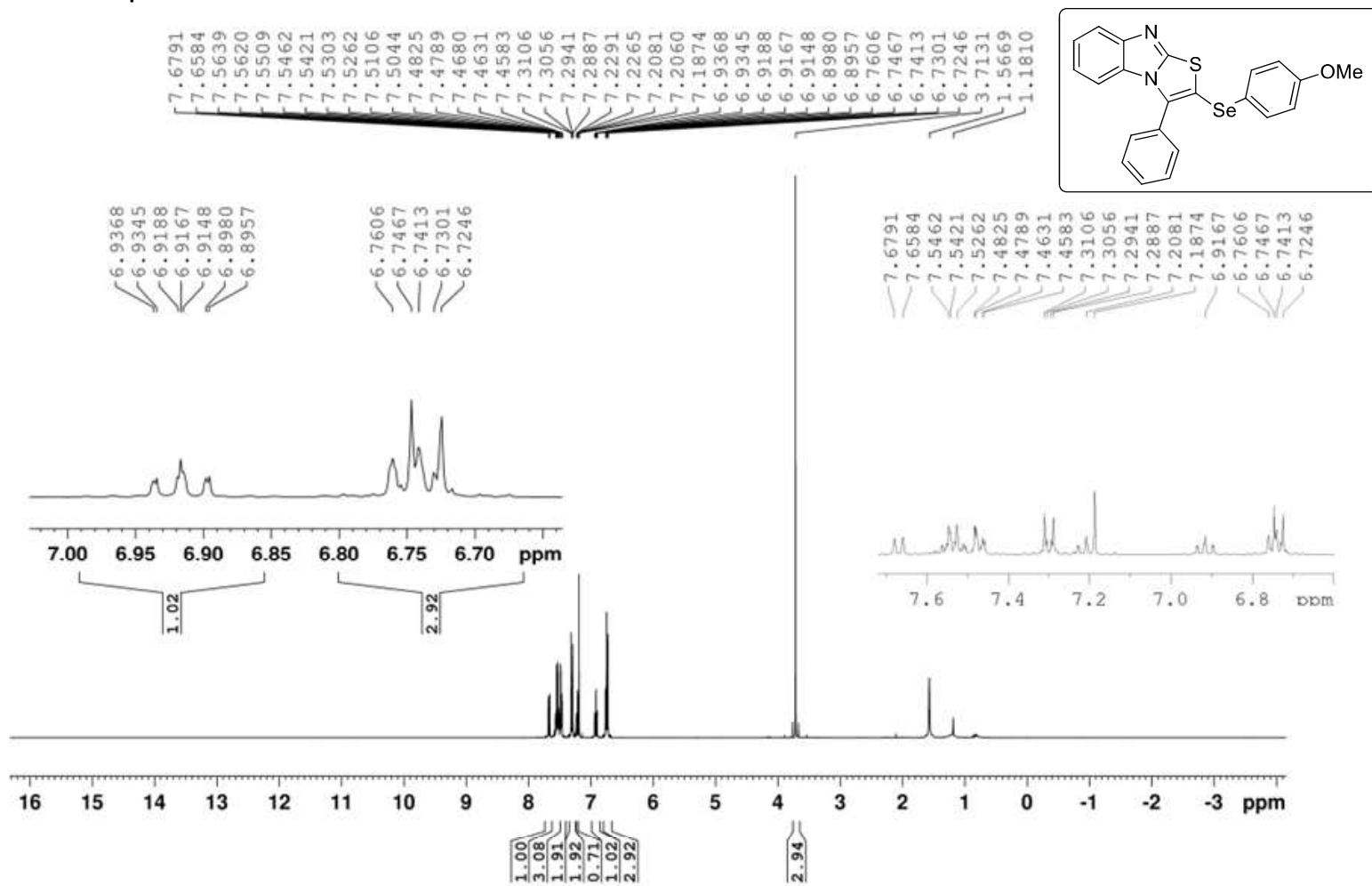
¹H NMR spectra of 3b



^{13}C NMR spectra of 3b



¹H NMR spectra of 3c

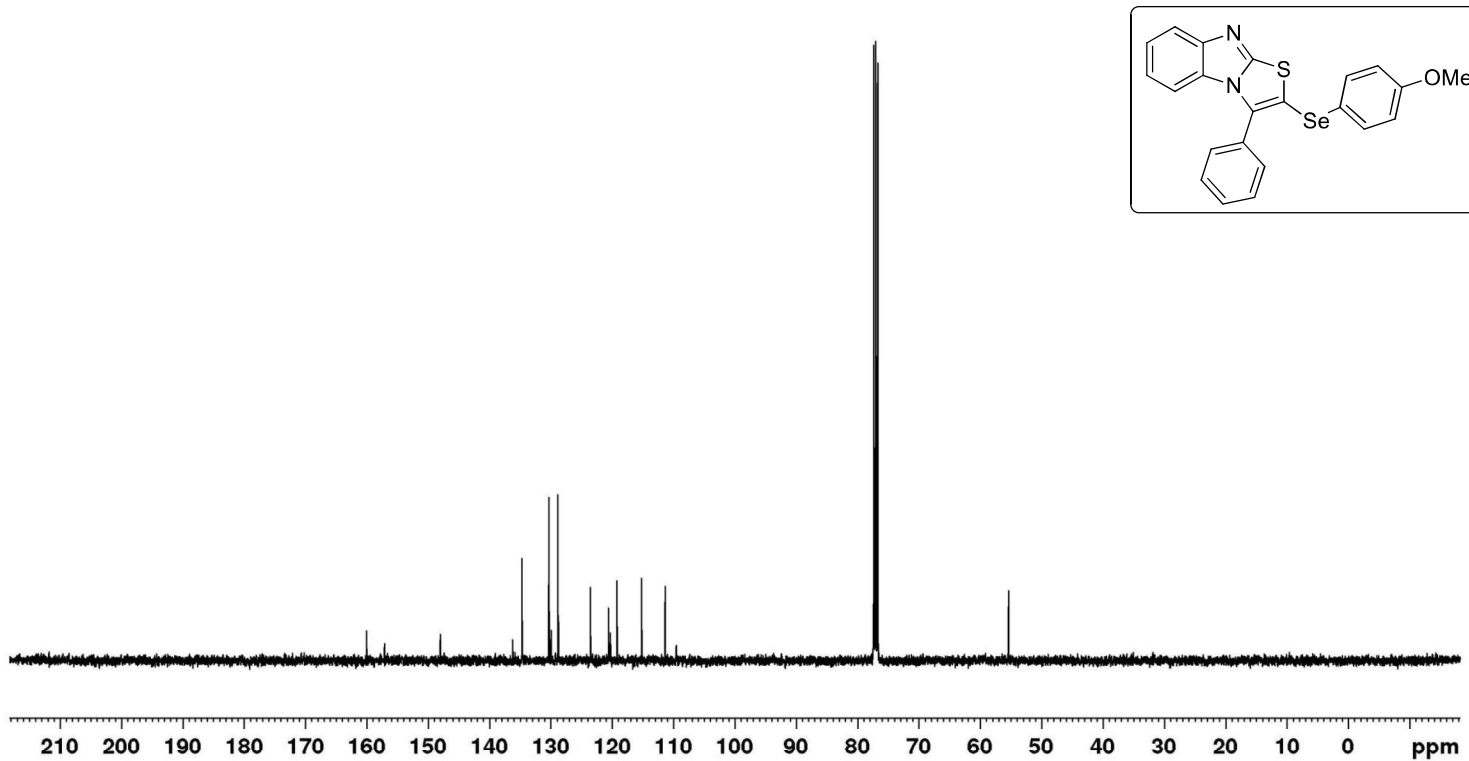


¹³C NMR spectra of 3c

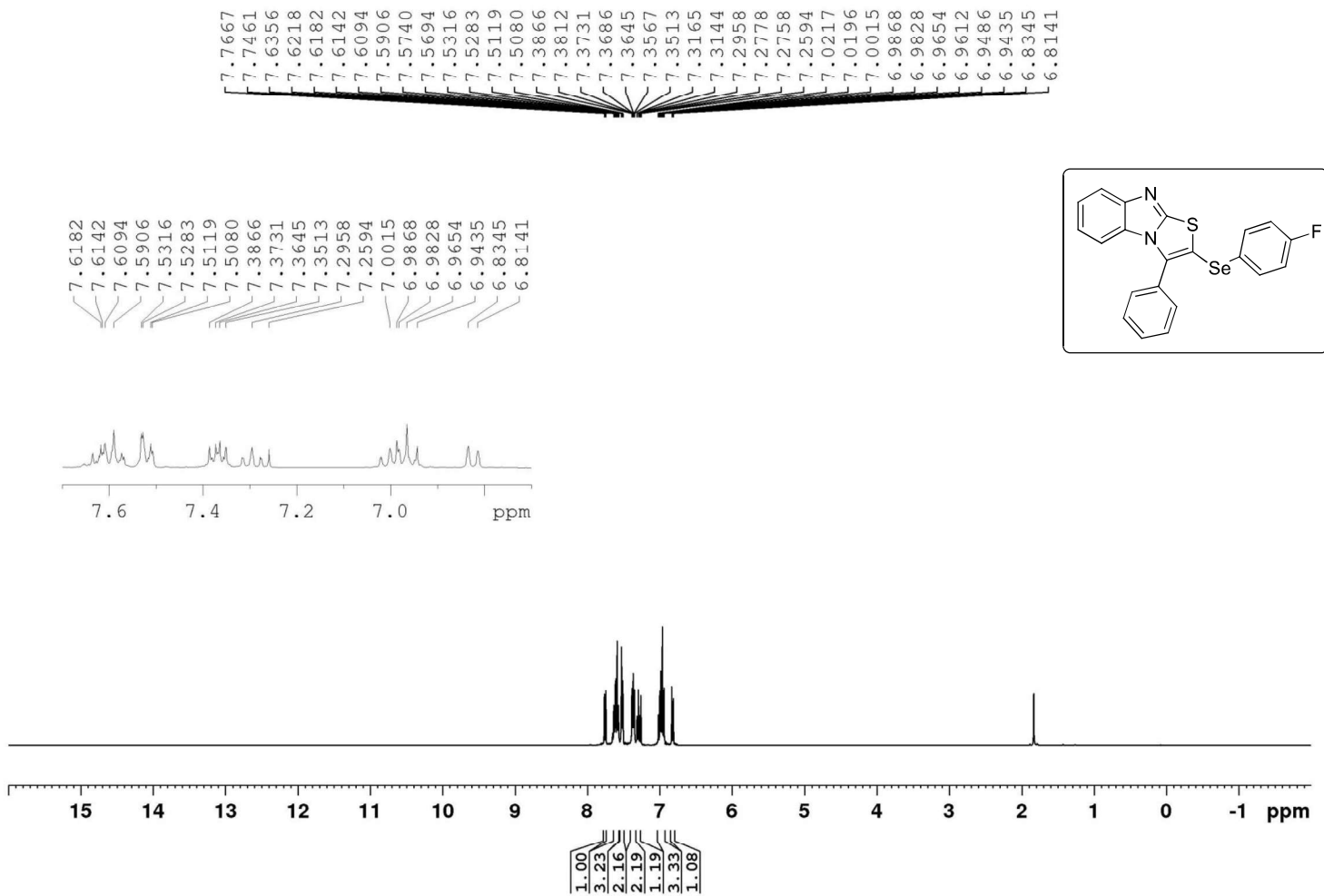
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55.36

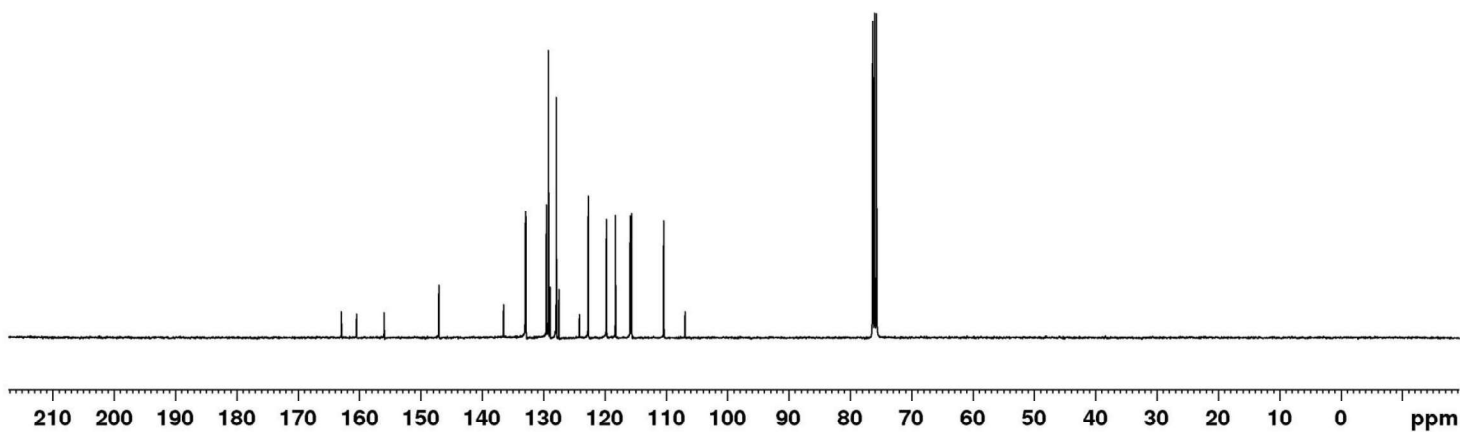
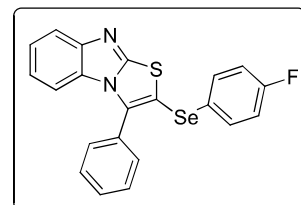


¹H NMR spectra of 3d

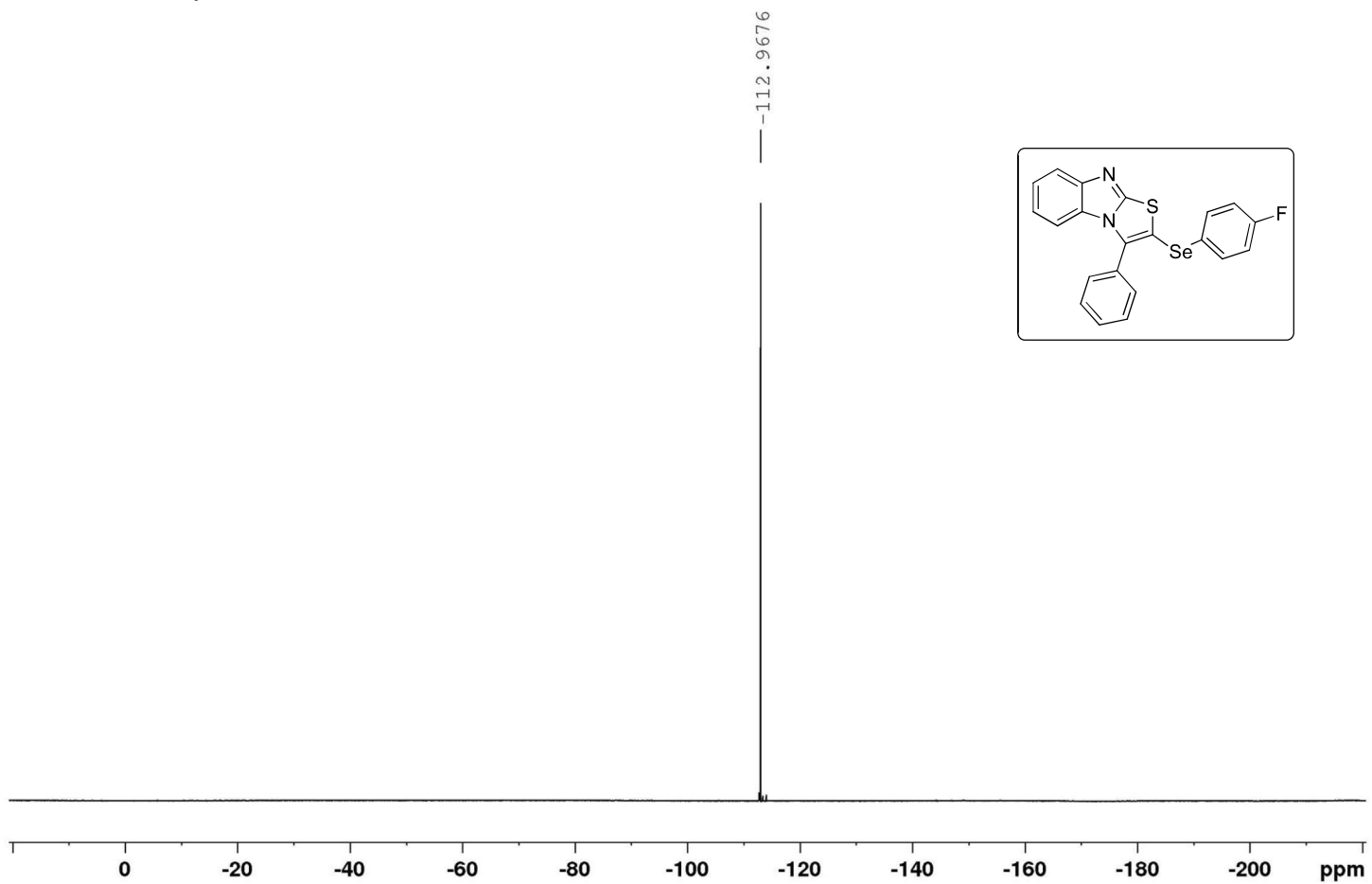


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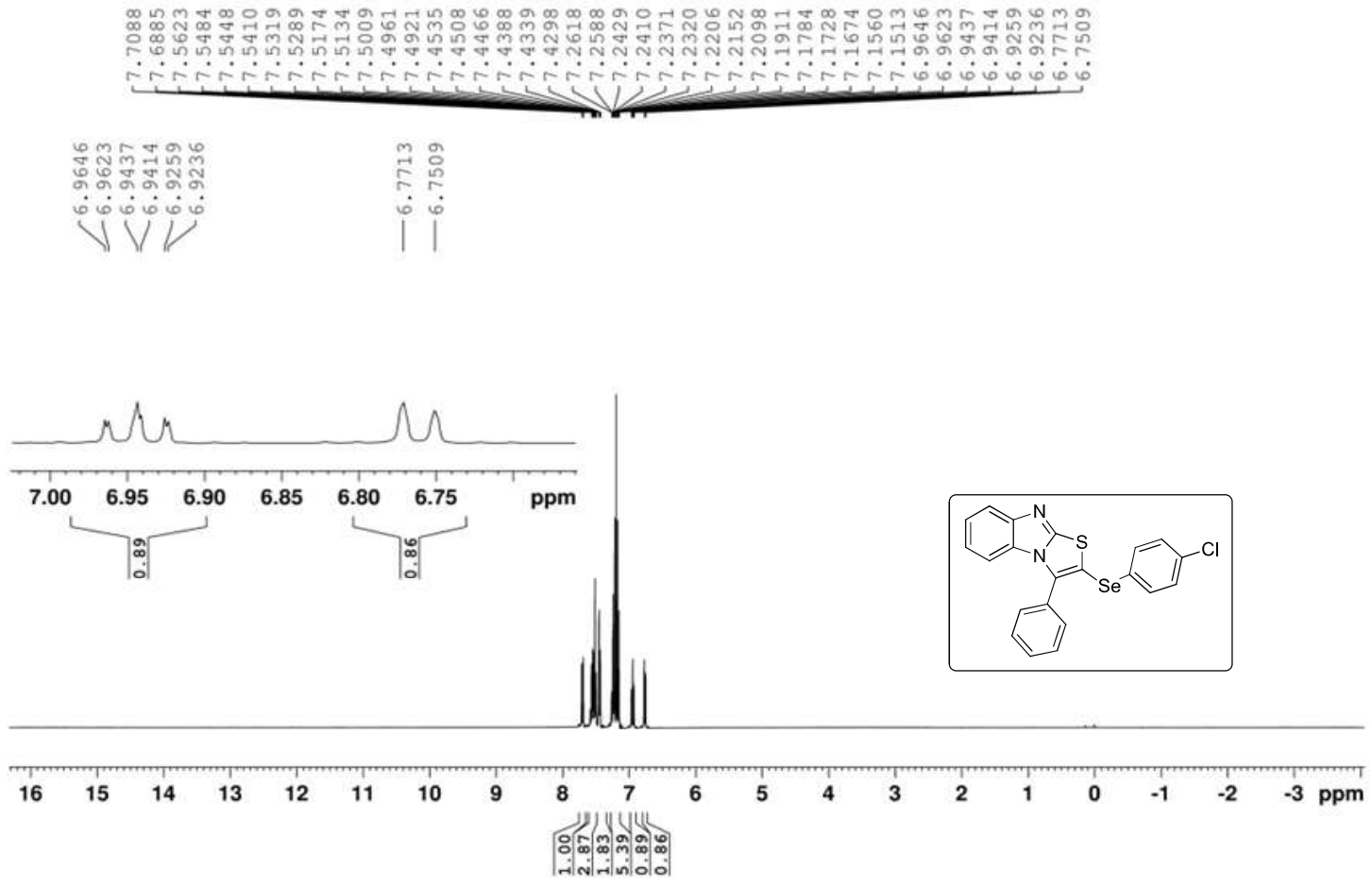
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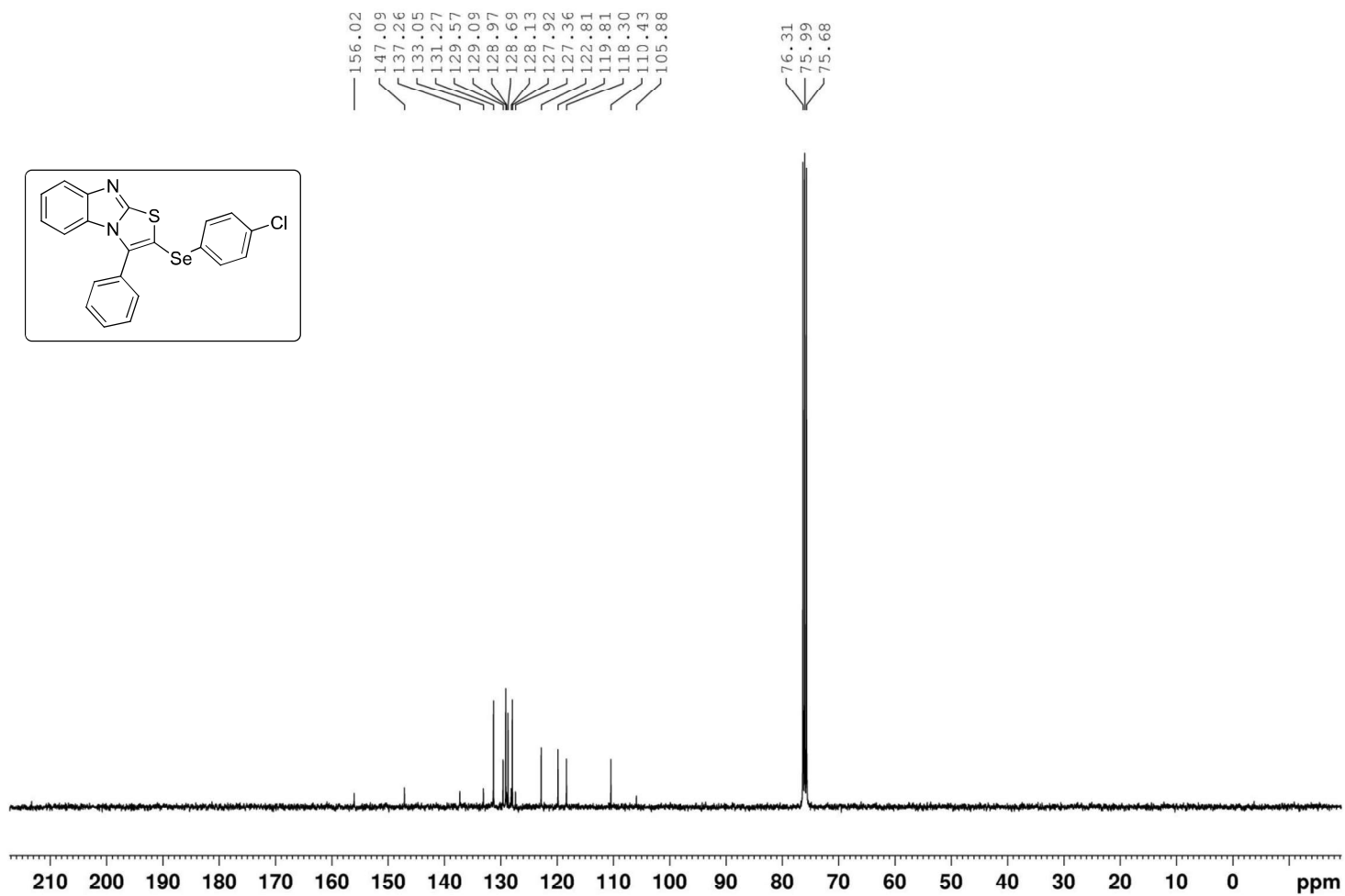
¹⁹F NMR spectra of 3d



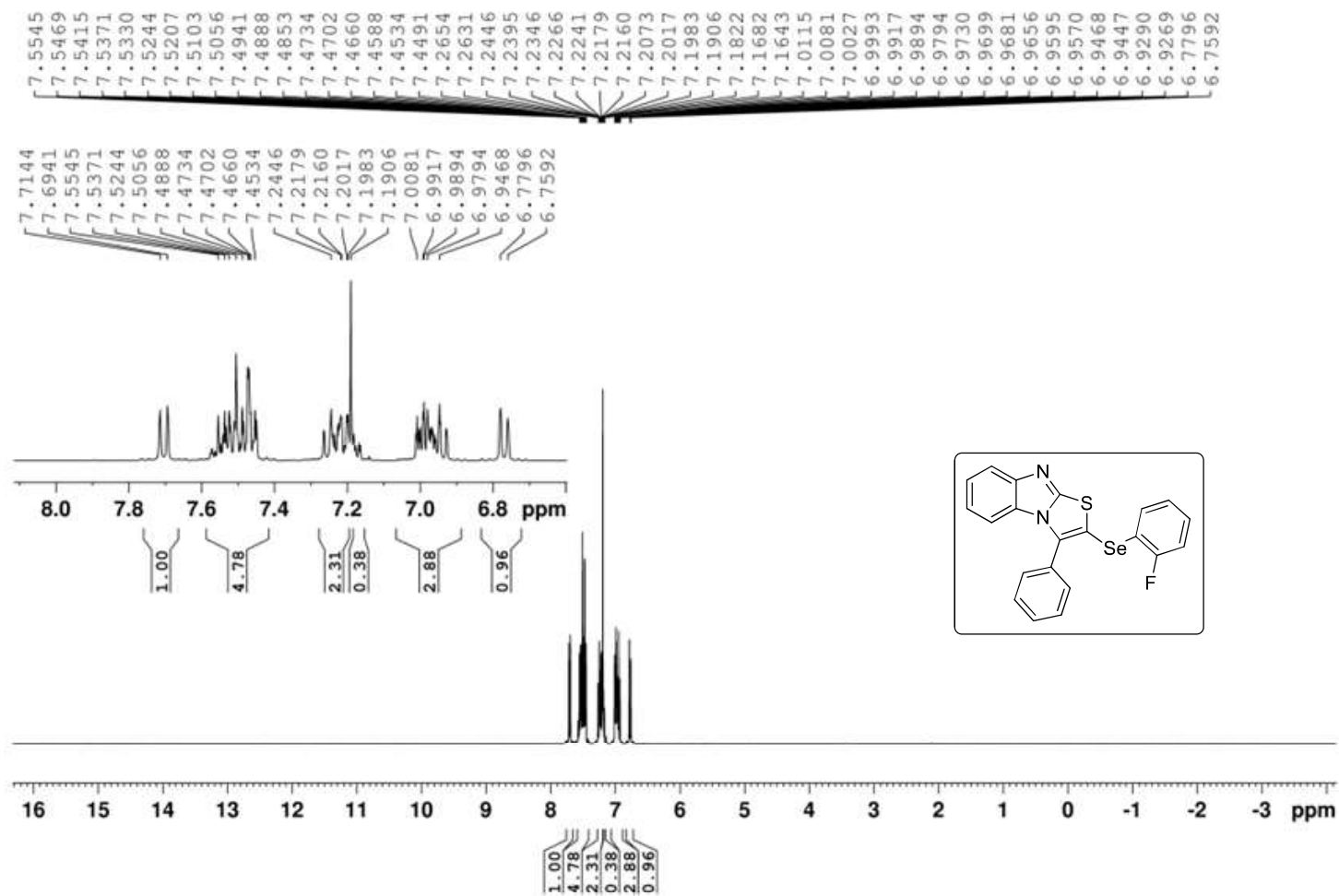
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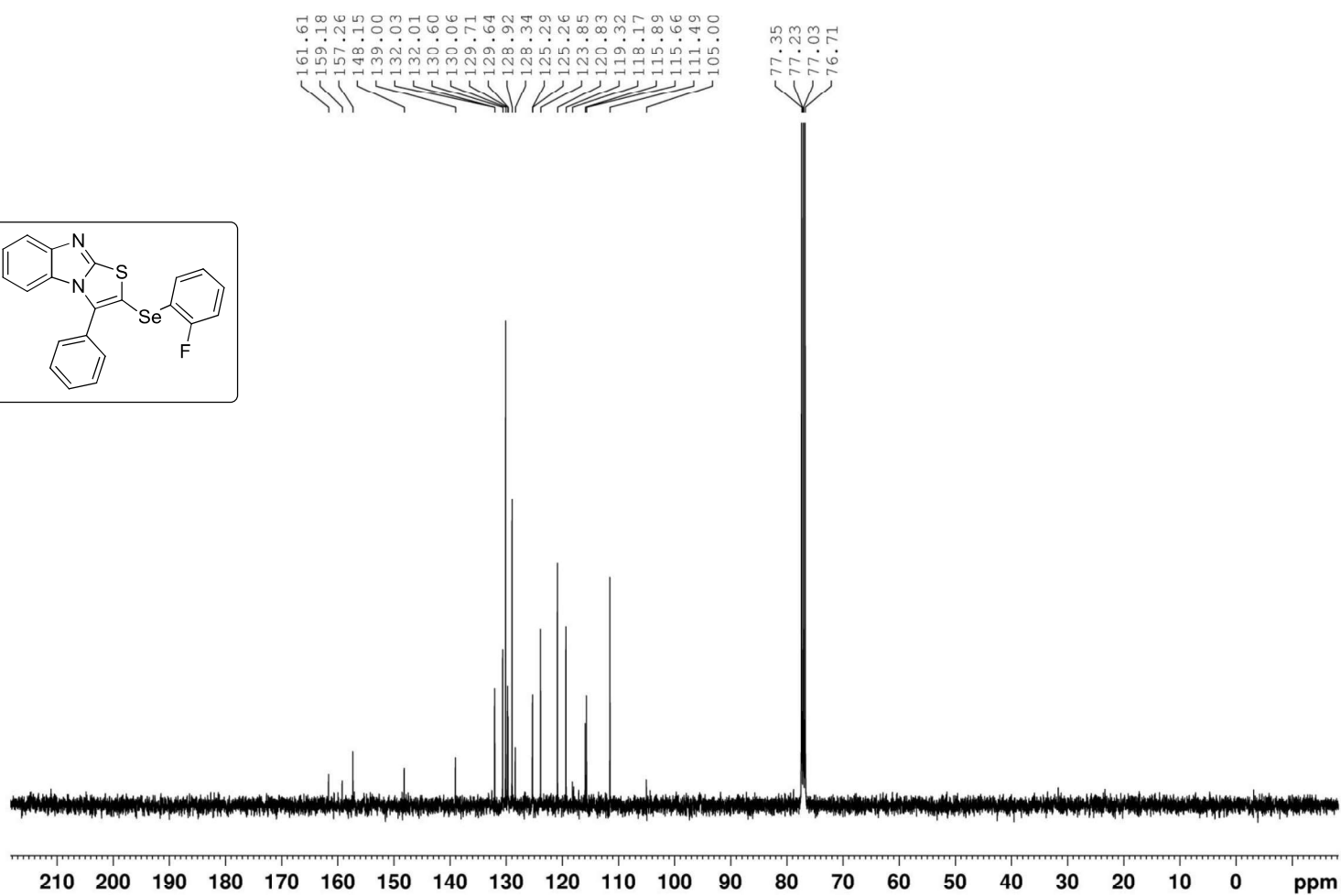
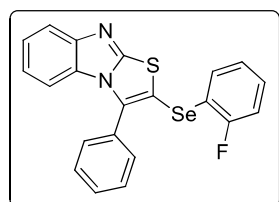
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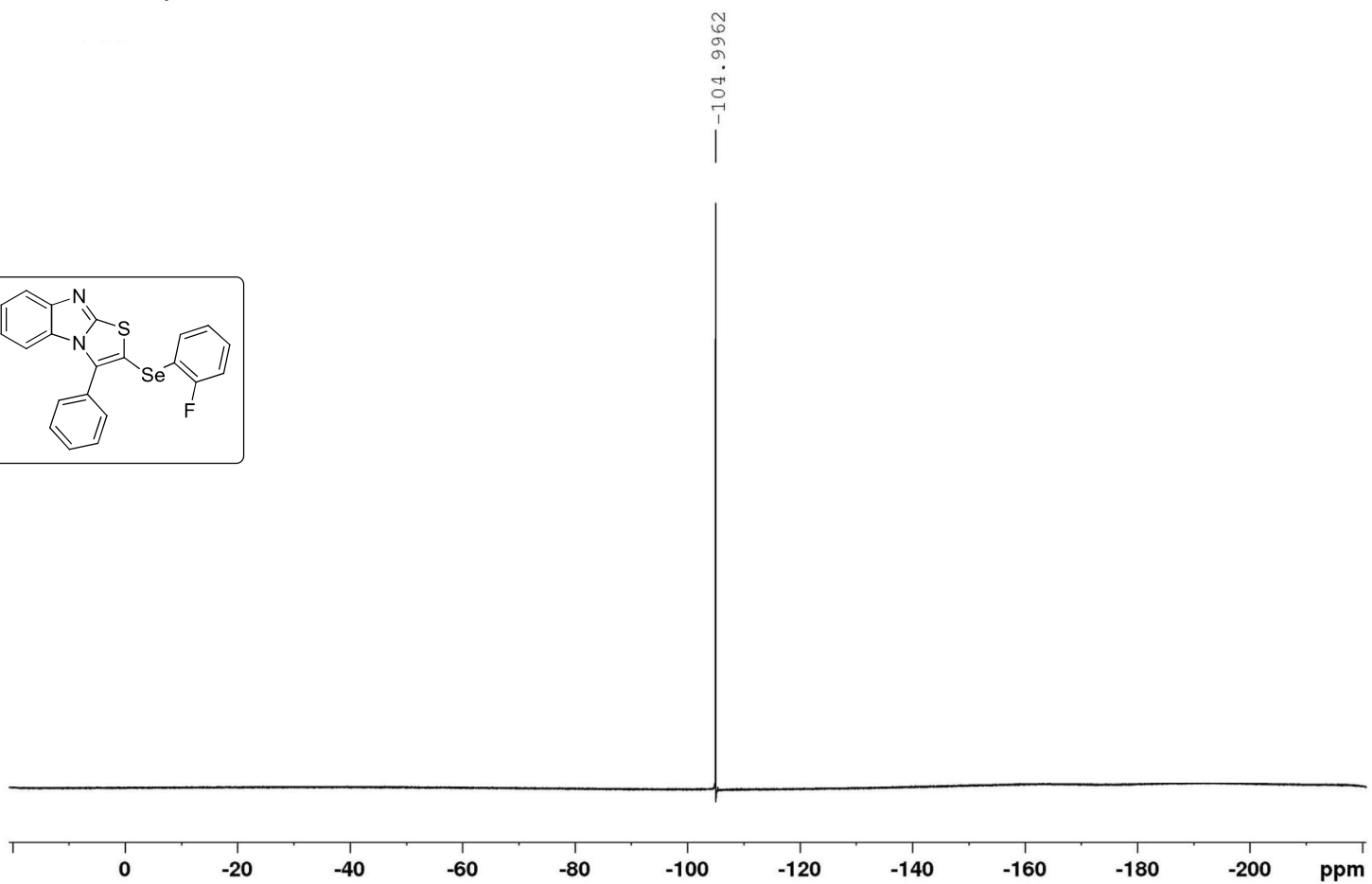
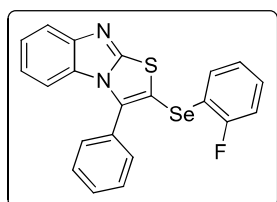
¹H NMR spectra of 3f



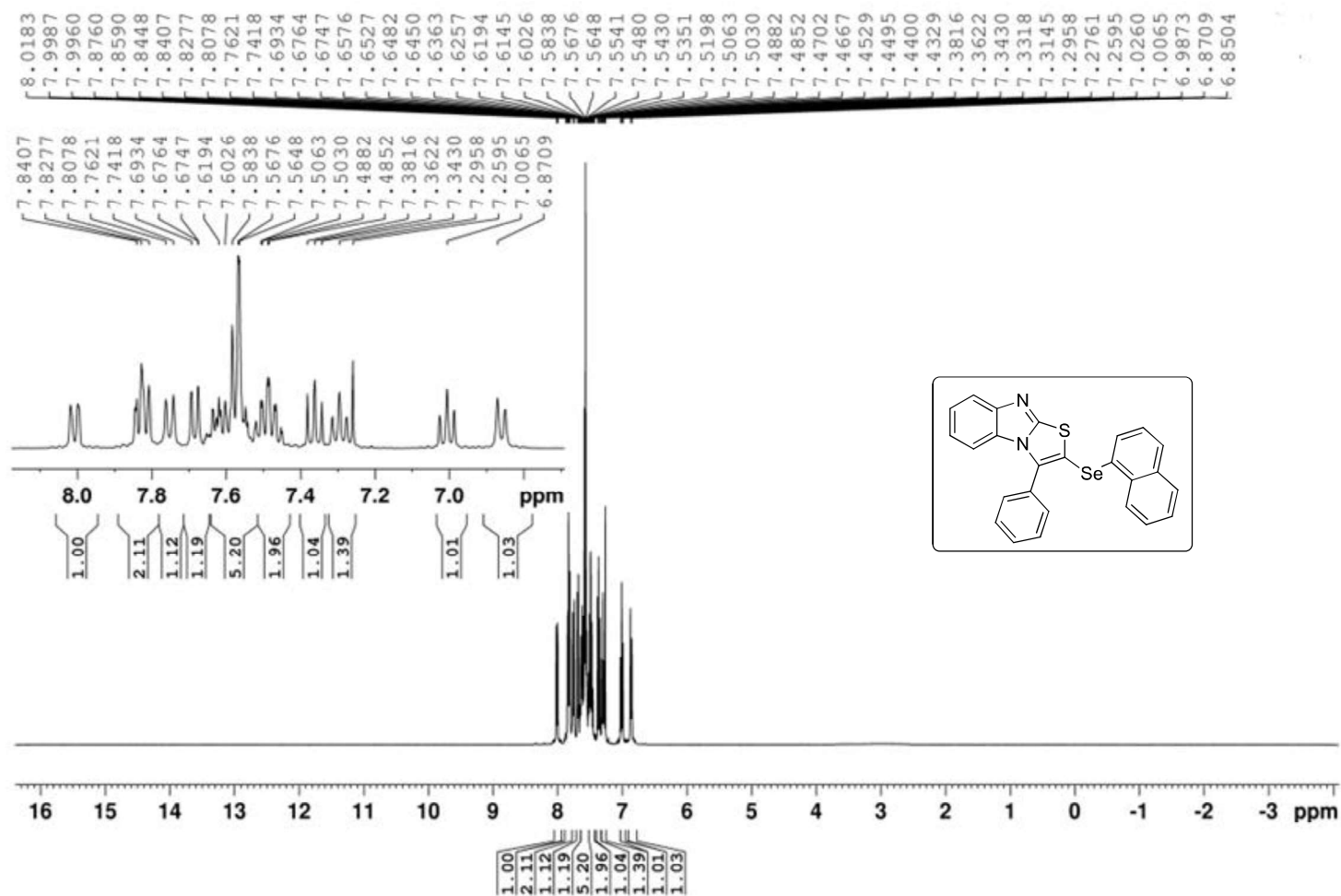
¹³C NMR spectra of 3f



¹⁹F NMR spectra of 3f

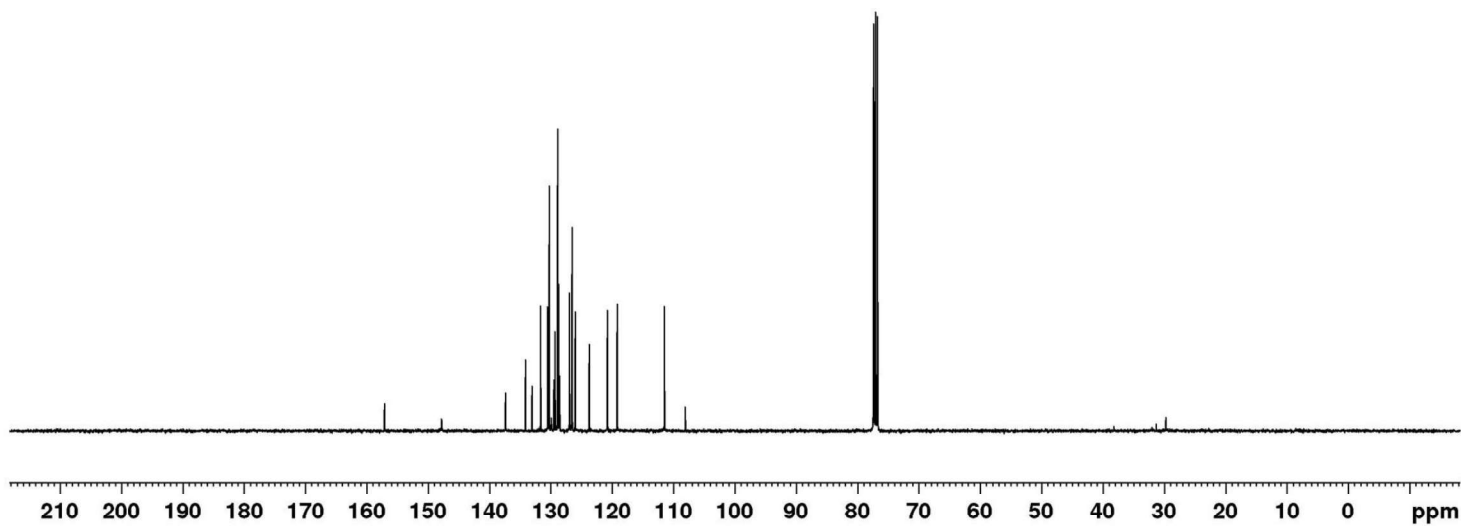
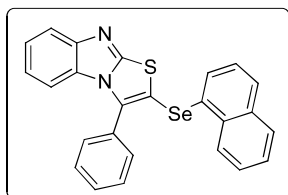


¹H NMR spectra of 3h

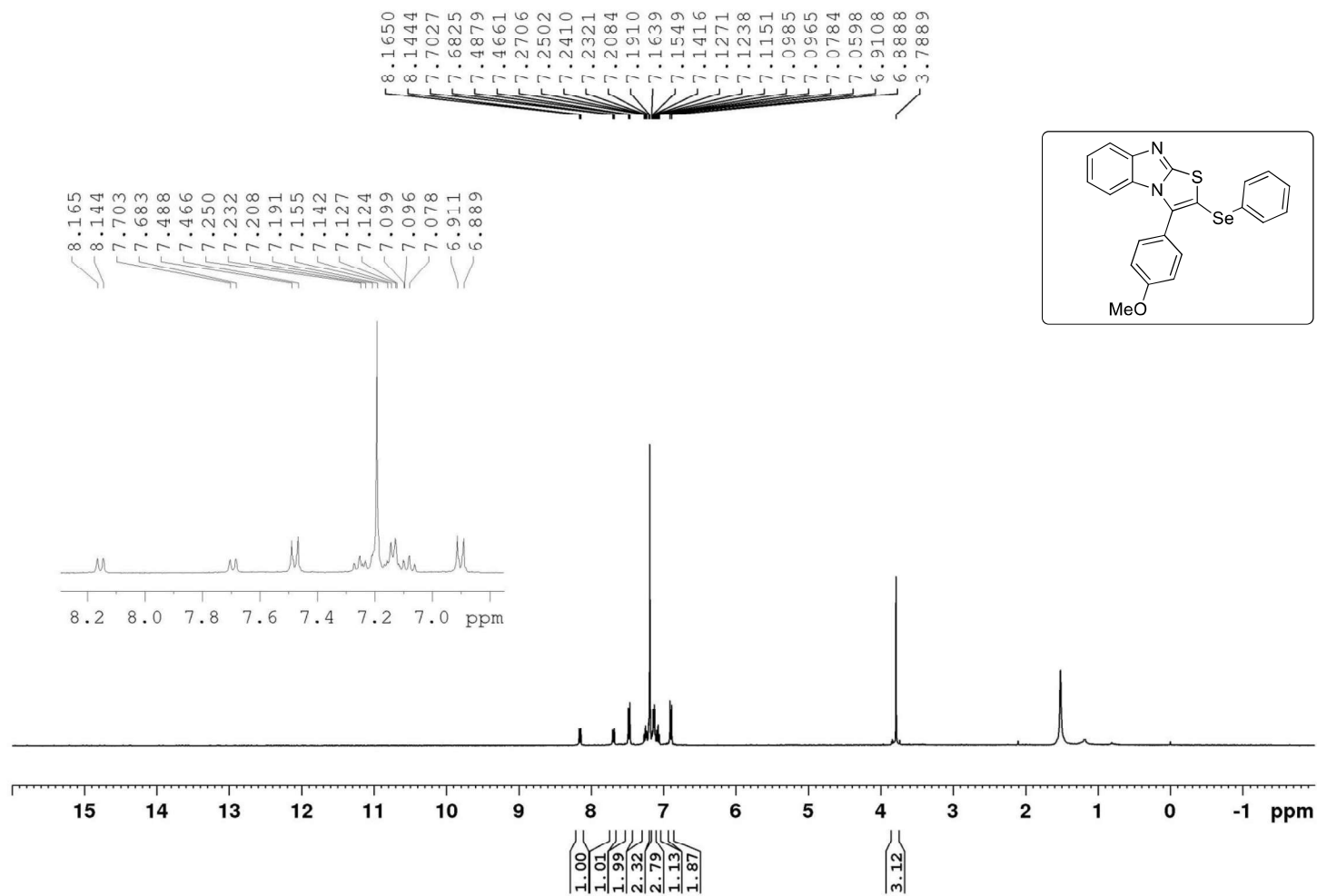


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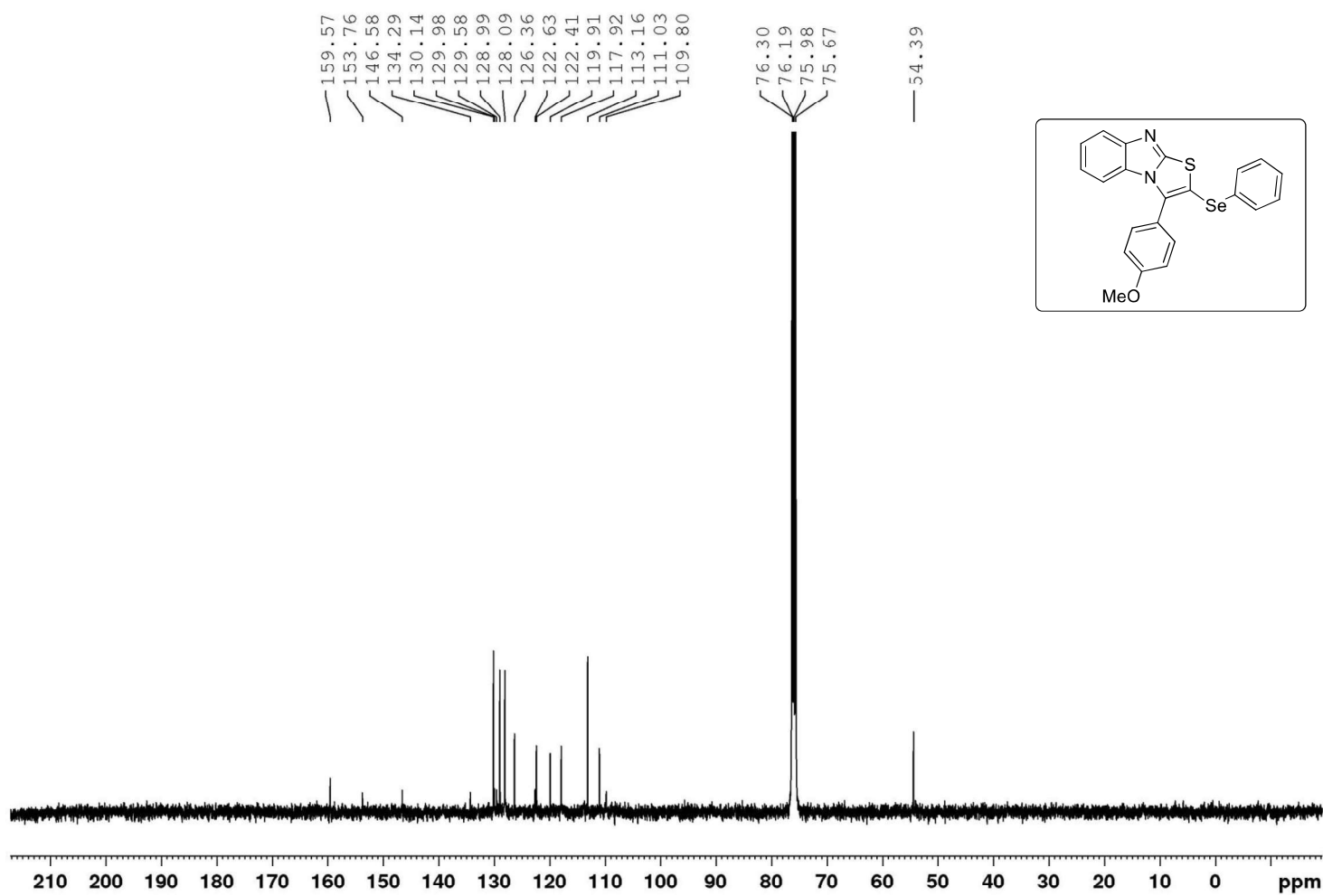
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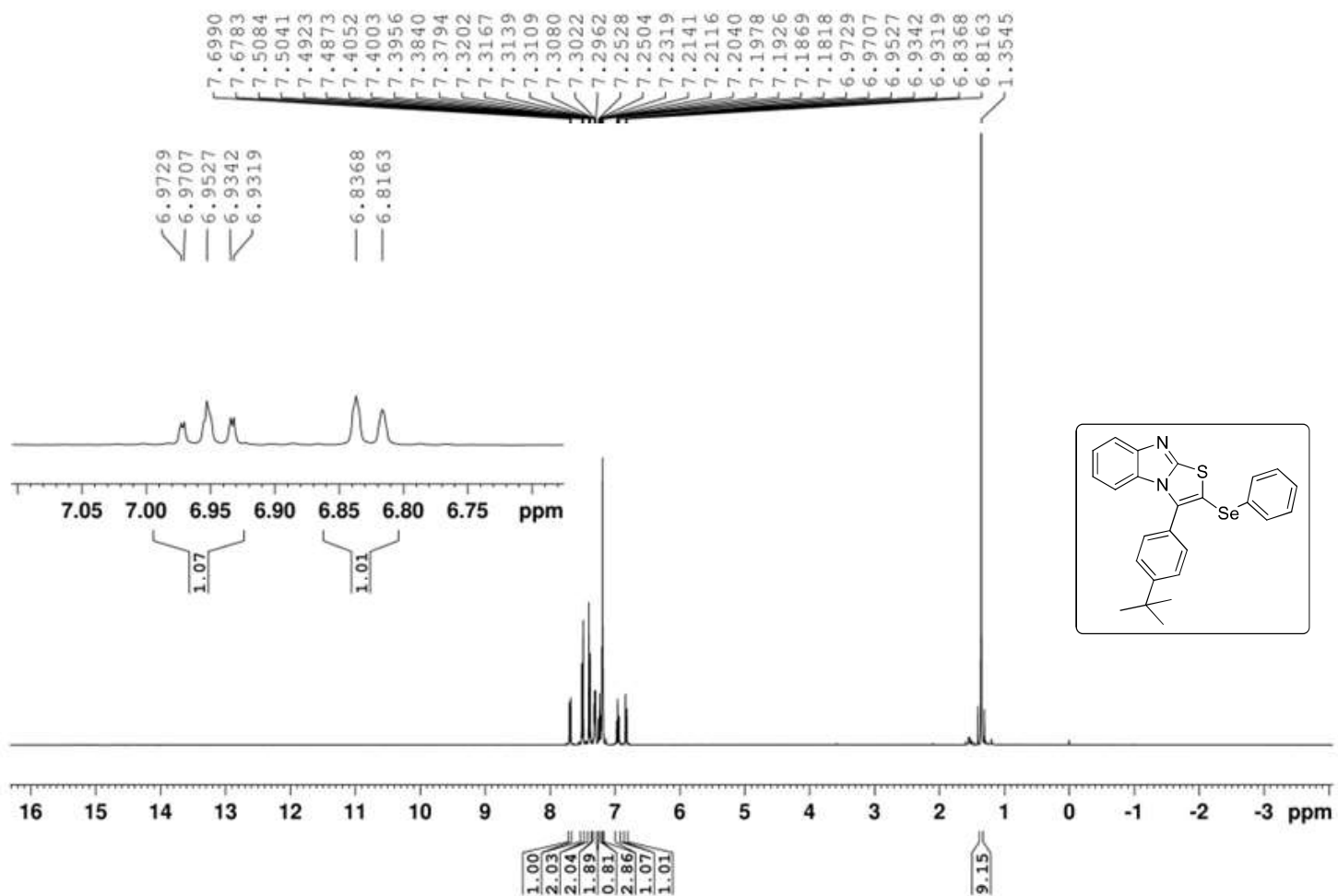
¹H NMR spectra of 4a



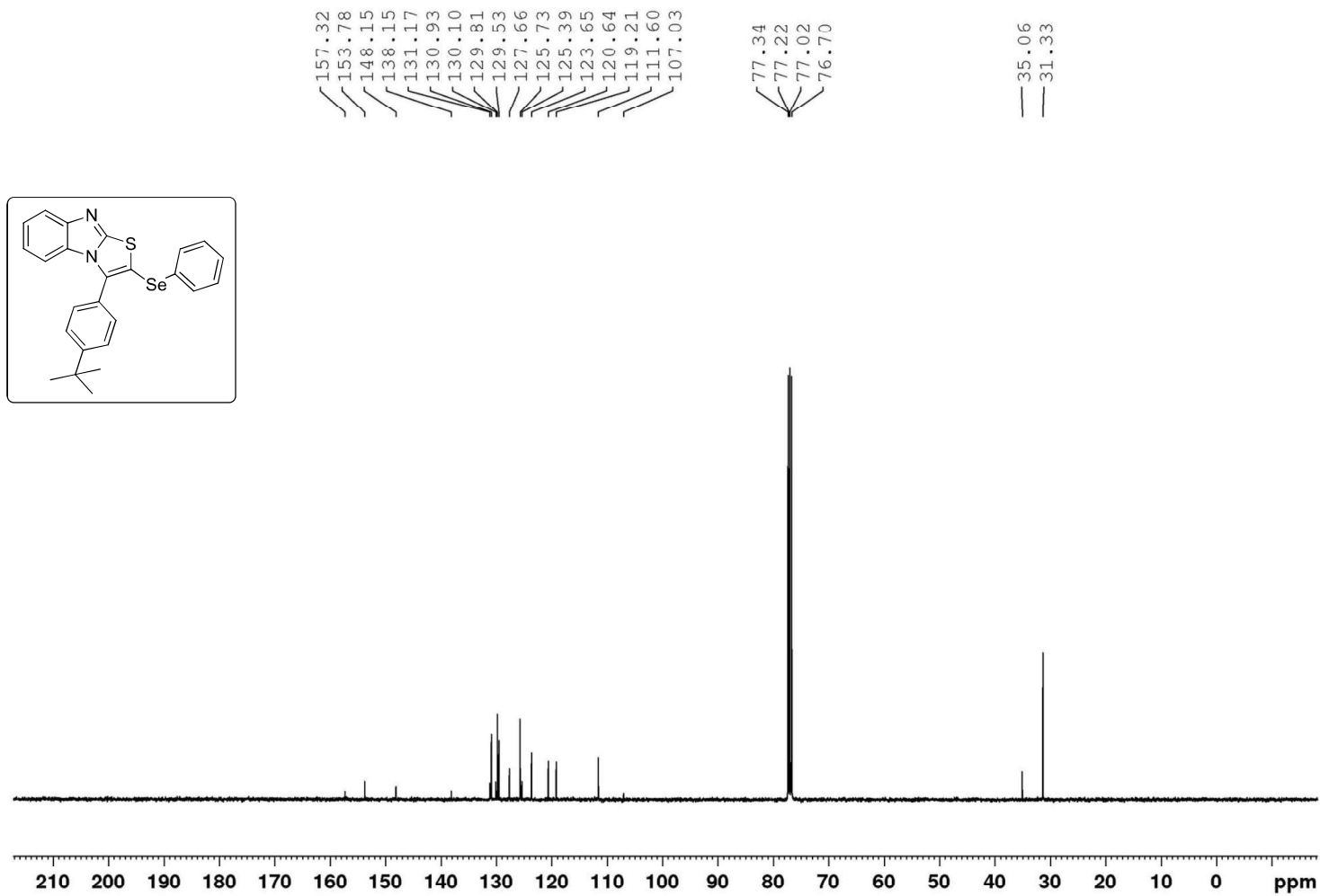
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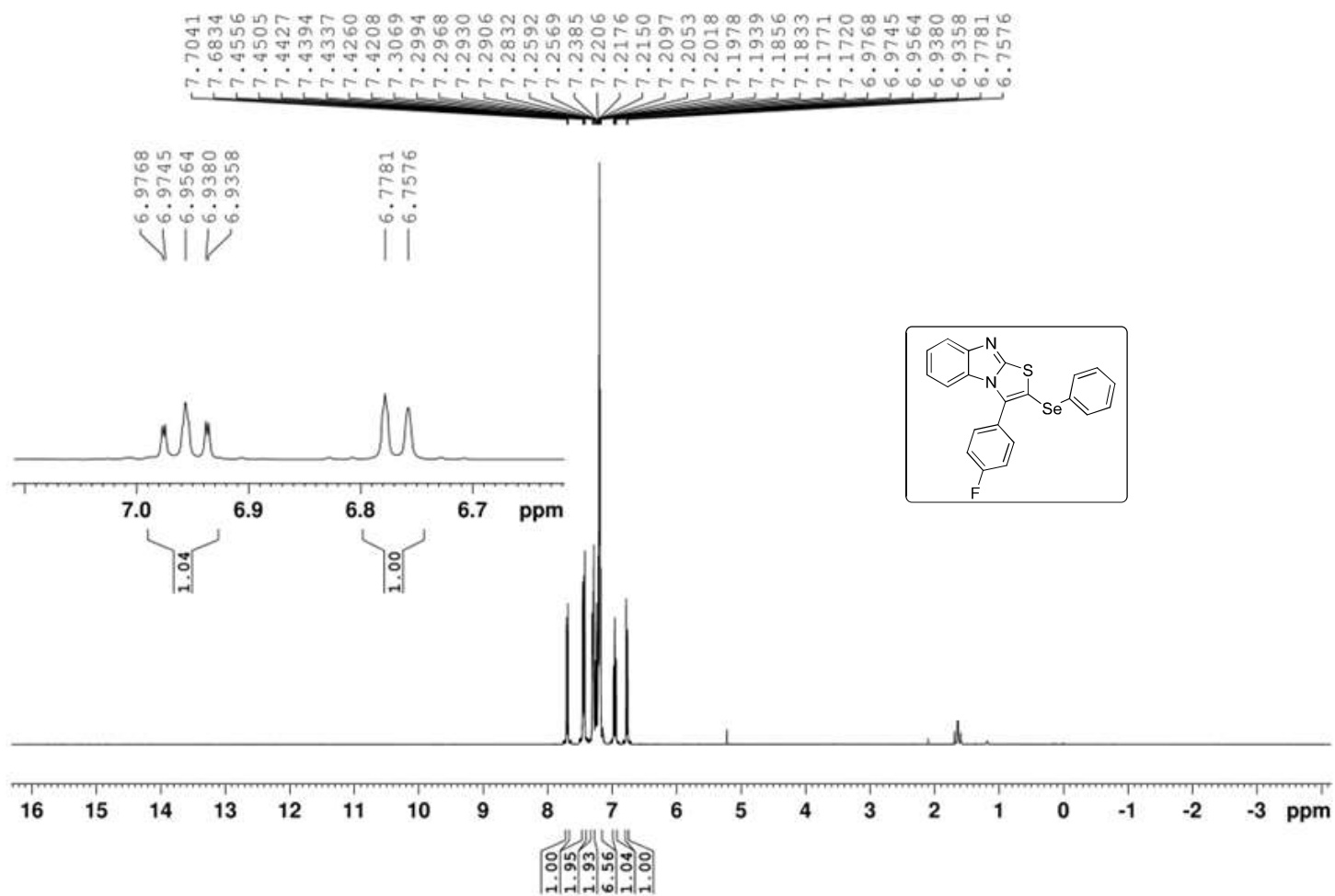
¹H NMR spectra of 4b



¹³C NMR spectra of 4b

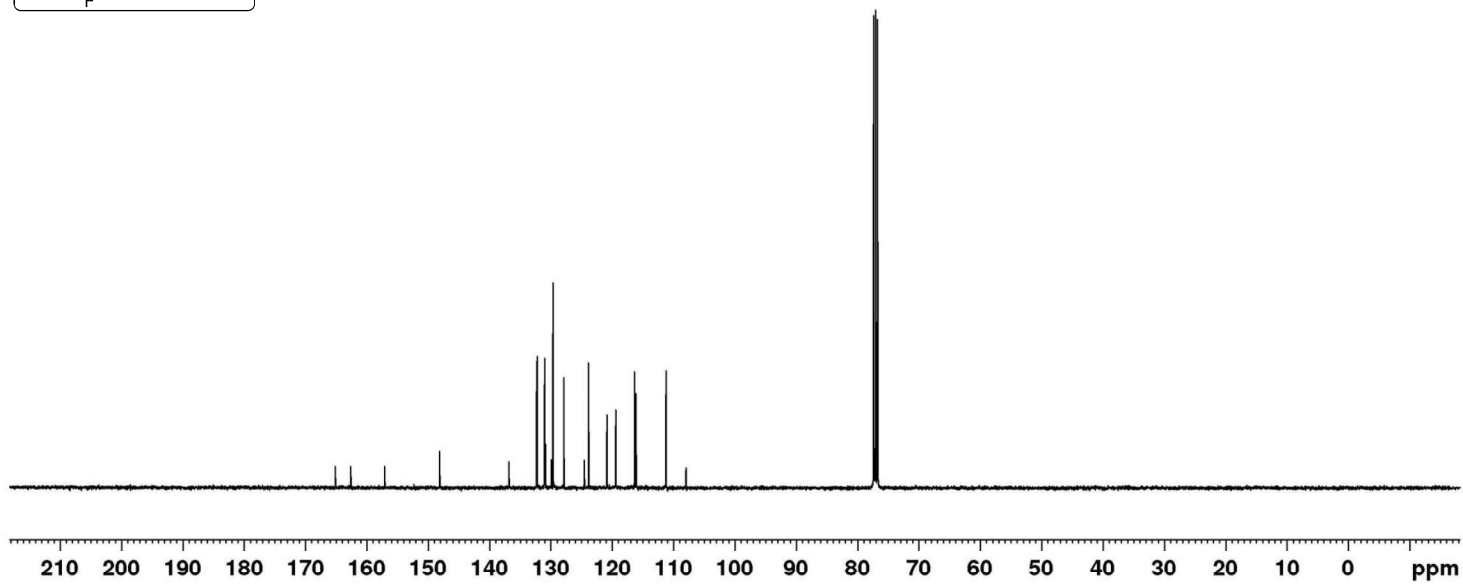
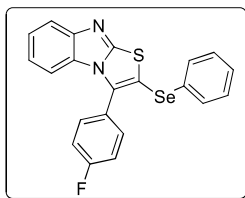


¹H NMR spectra of 4c

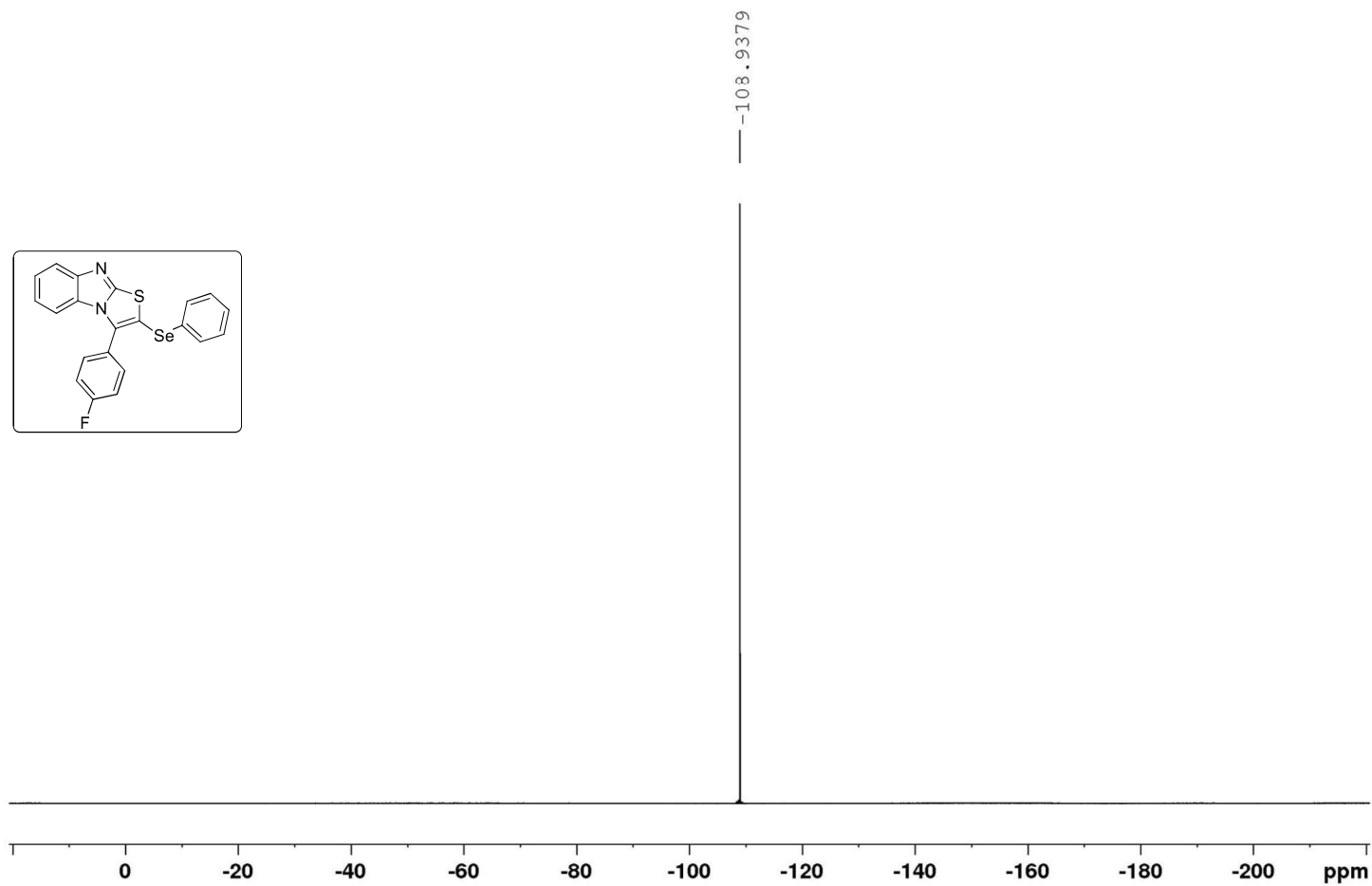
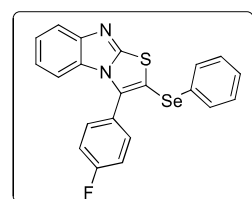


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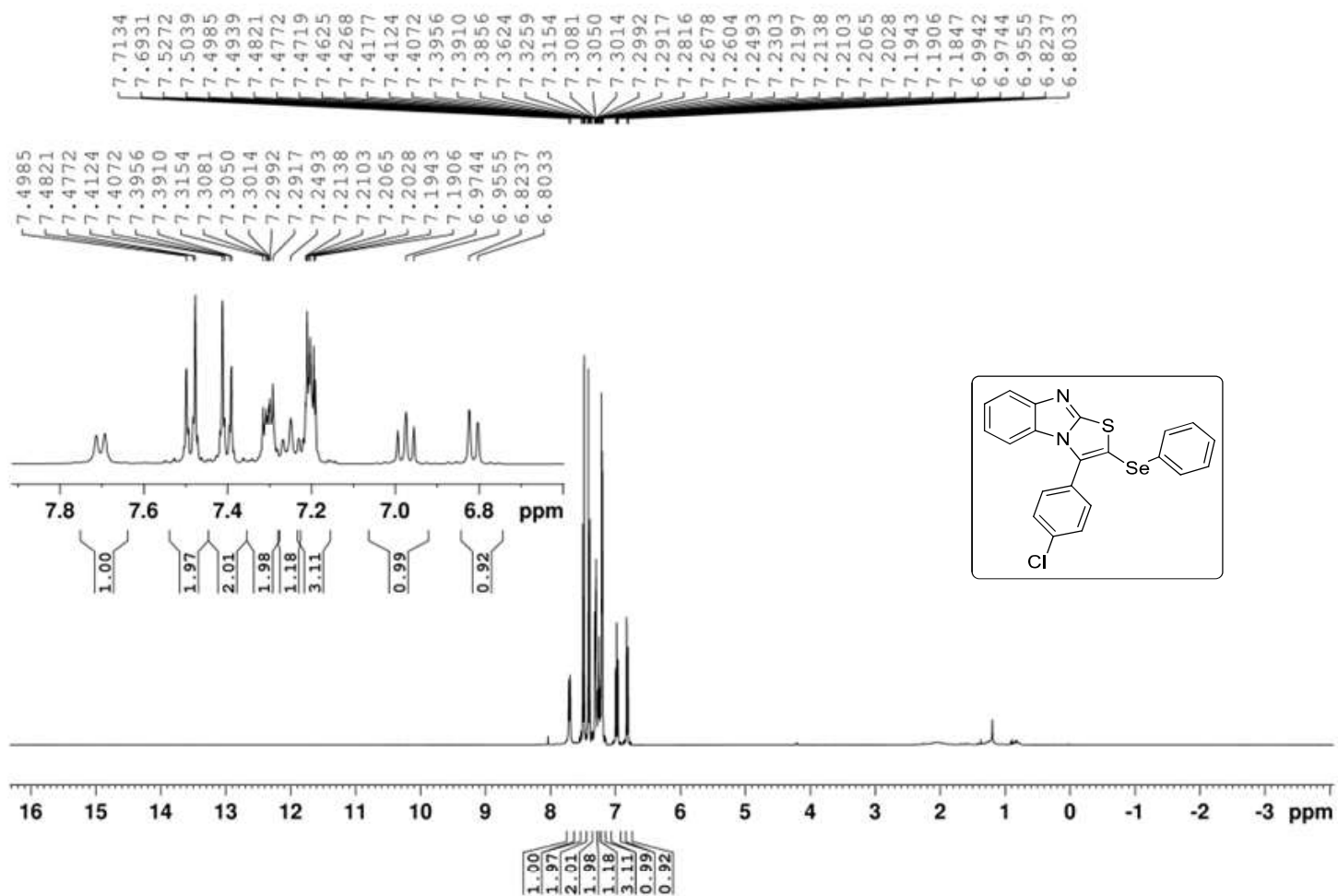
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76.72



^{19}F NMR spectra of 4c



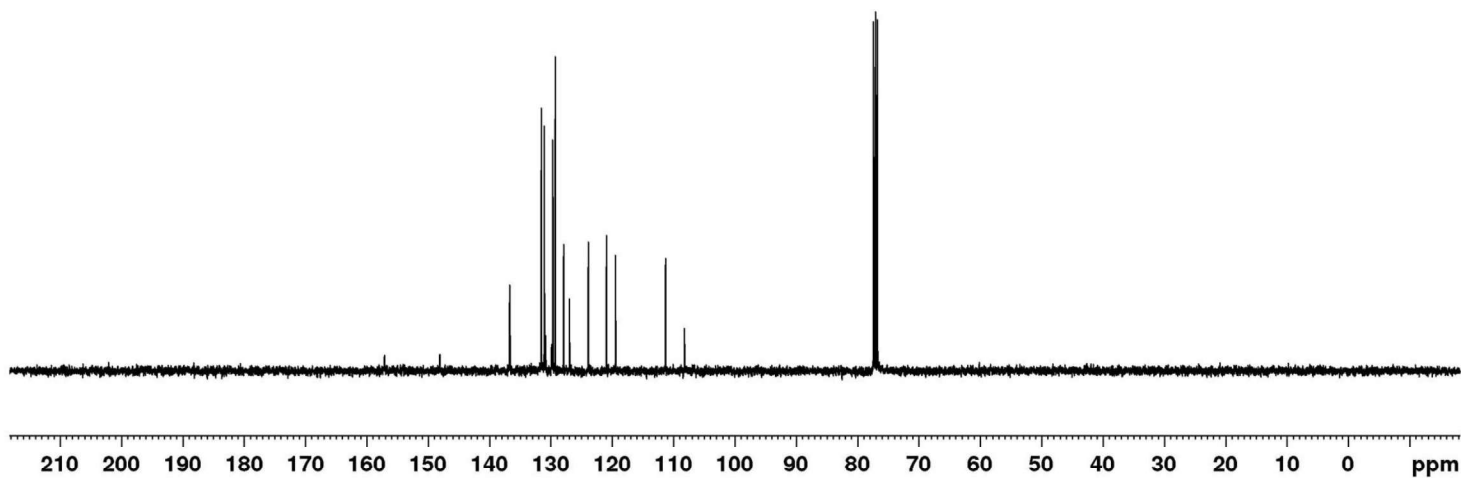
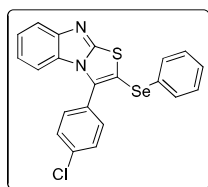
¹H NMR spectra of 4d



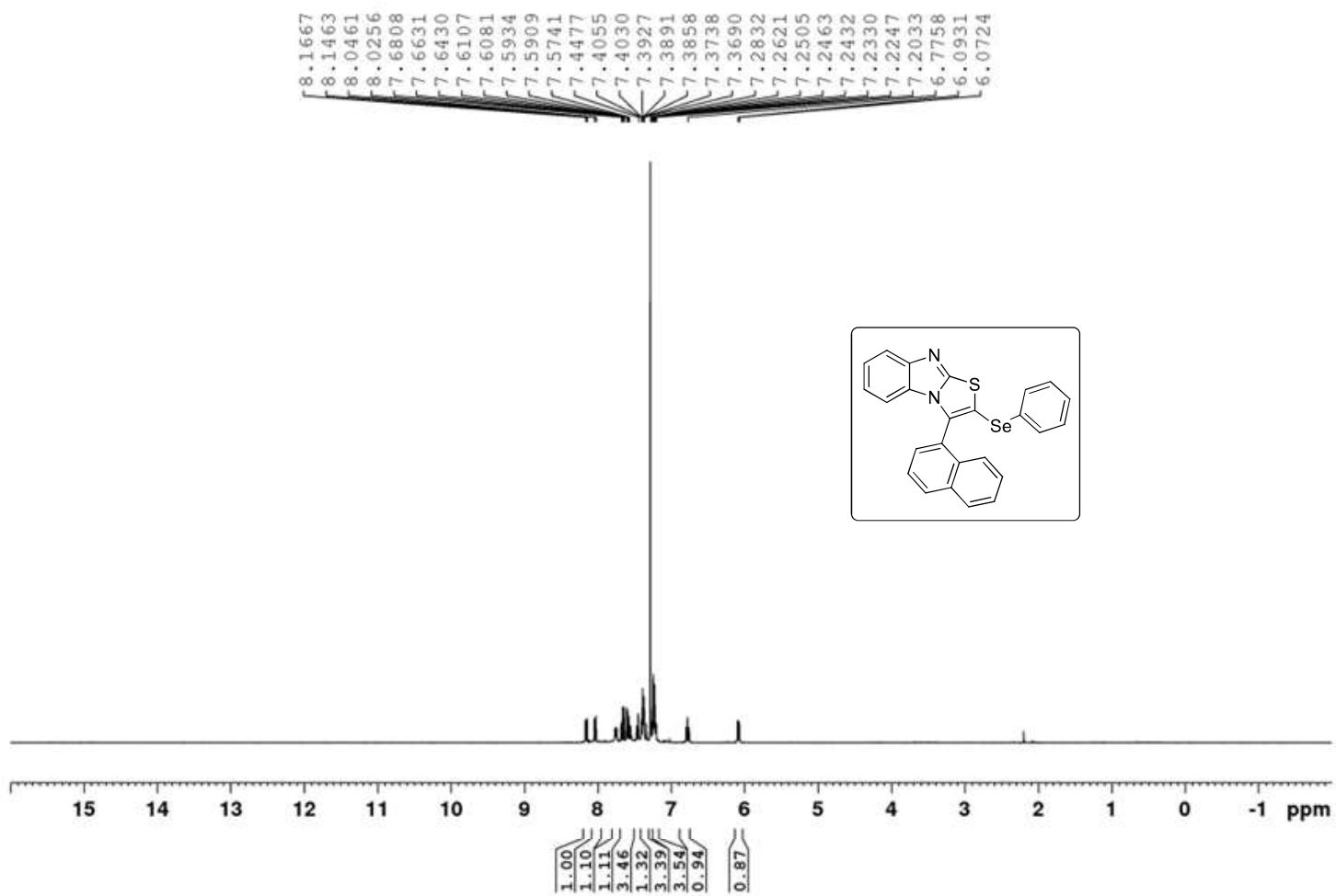
¹³C NMR spectra of 4d

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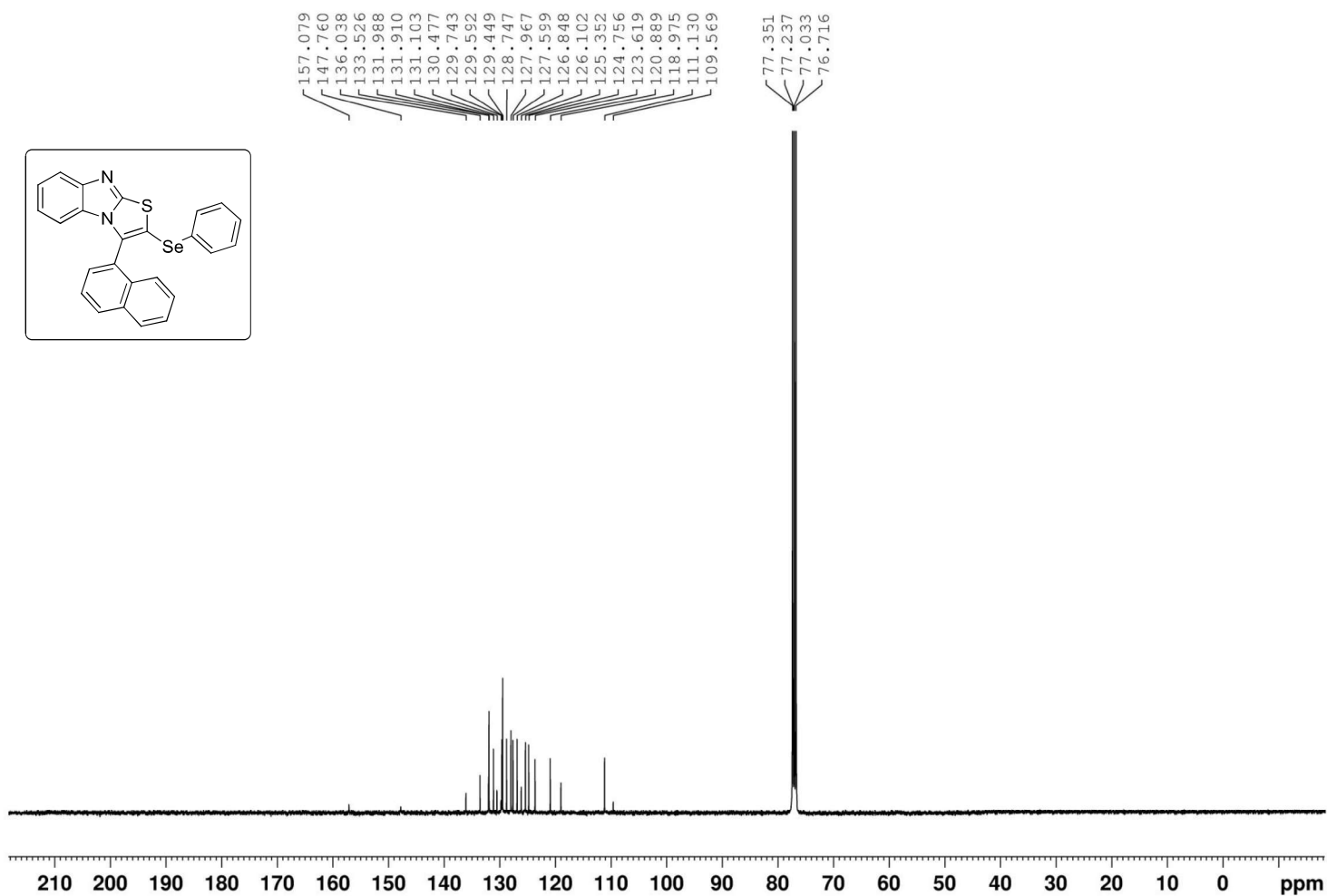
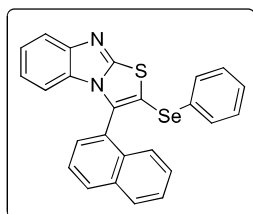
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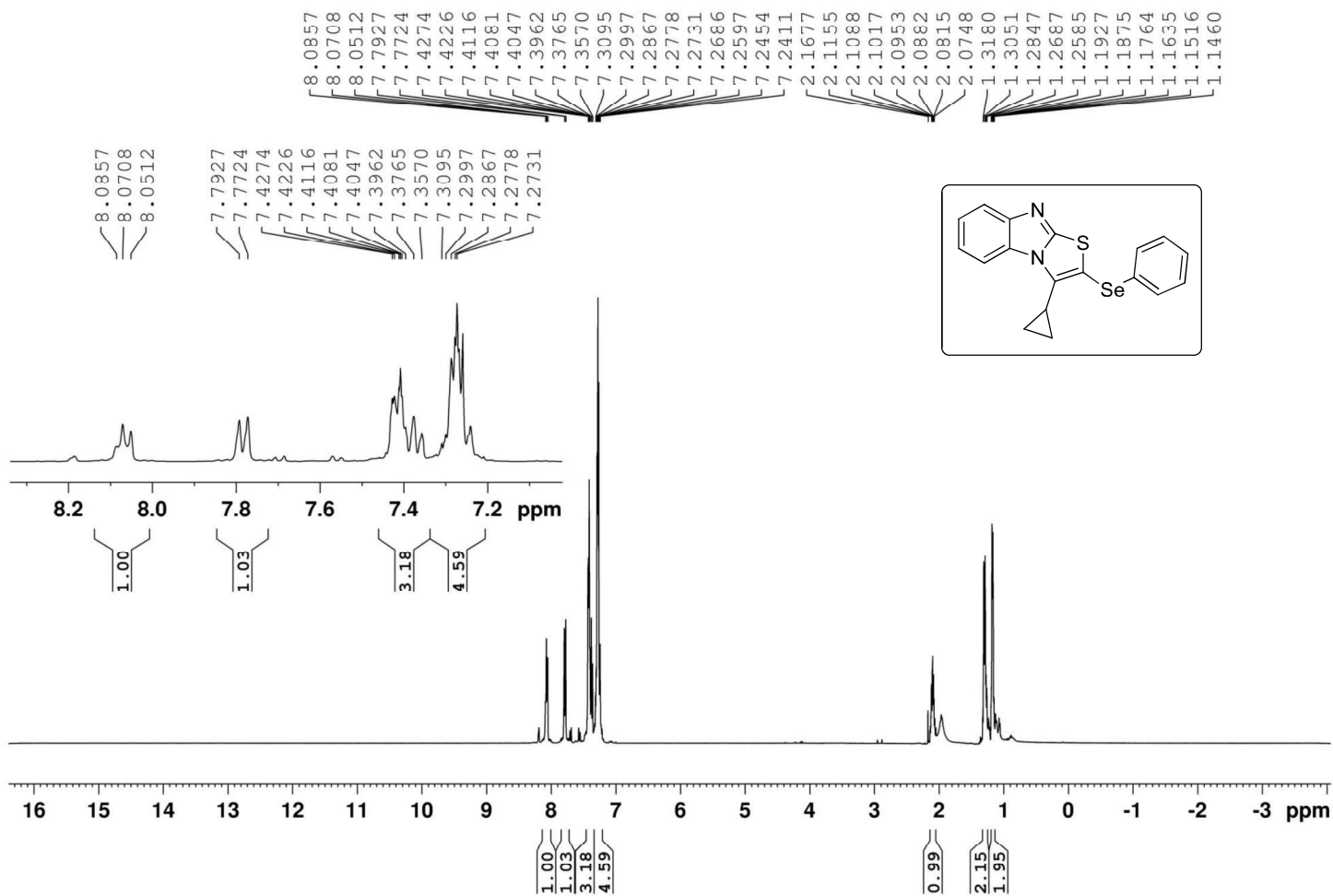
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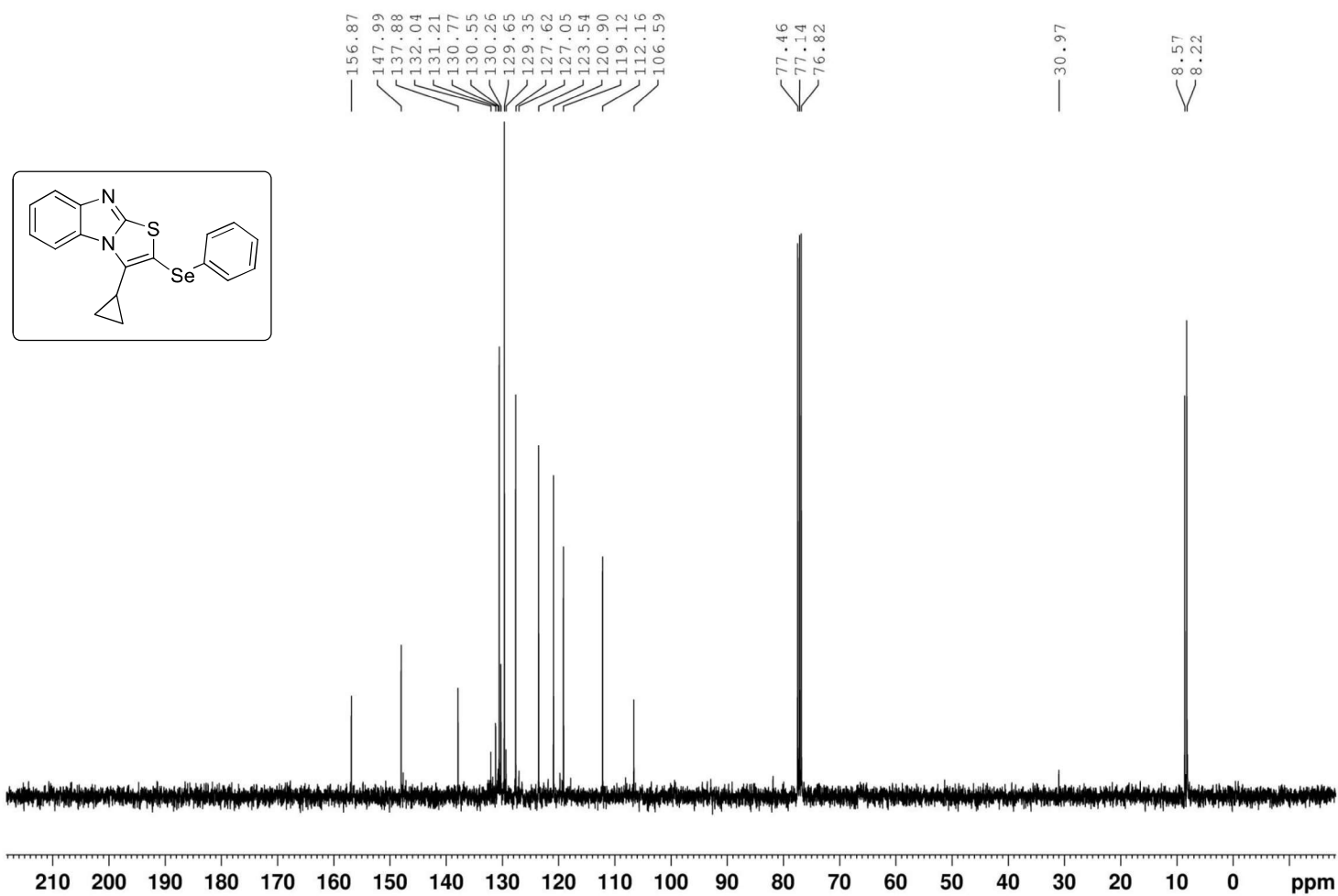
¹³C NMR spectra of 4e



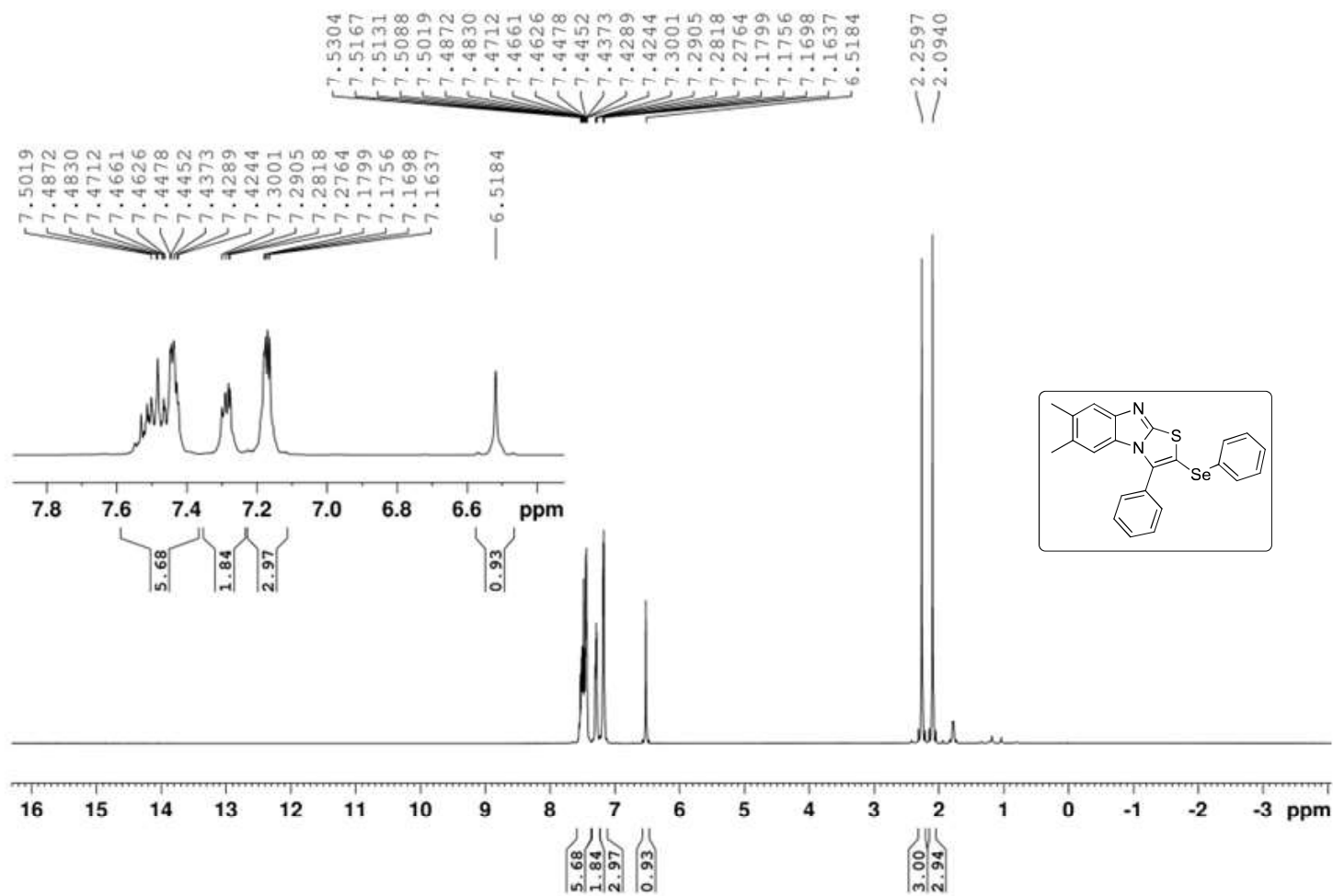
¹H NMR spectra of 4f



¹³C NMR spectra of 4f



¹H NMR spectra of 4g

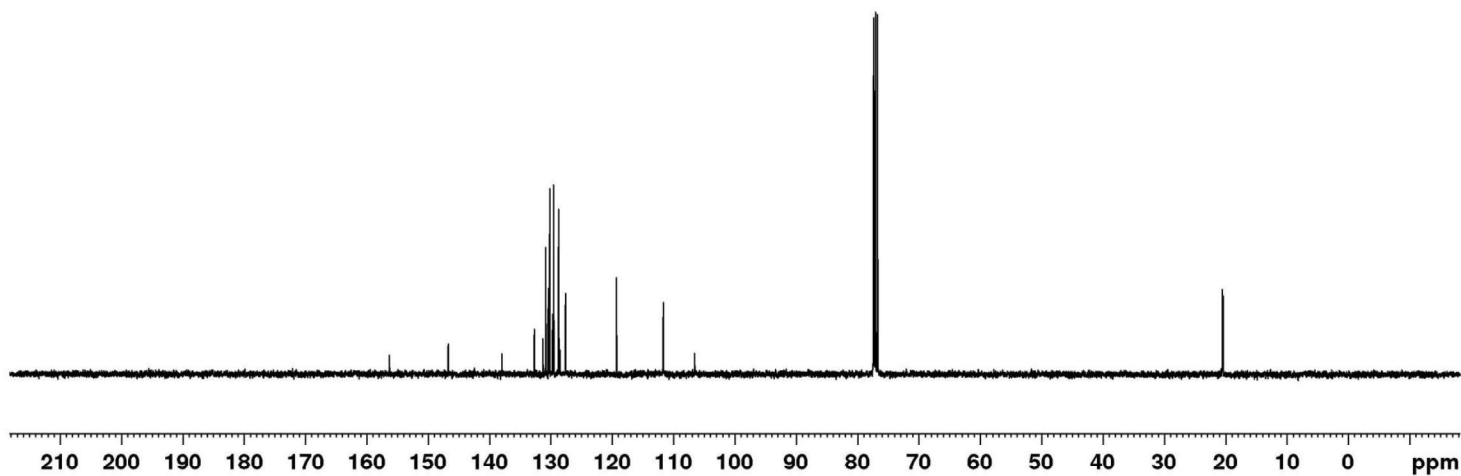
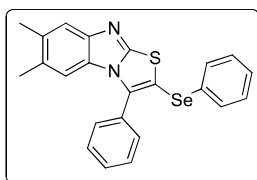


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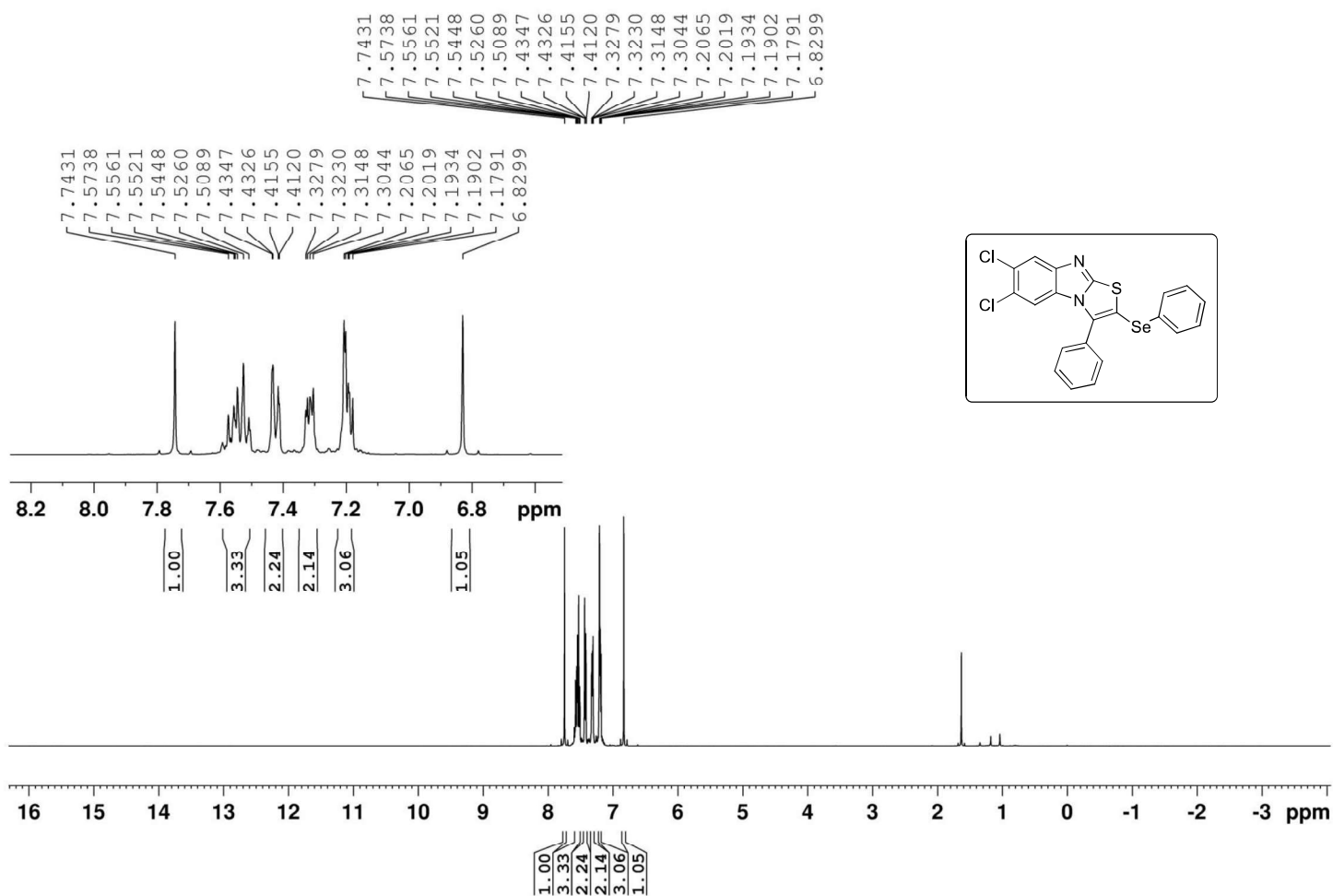
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77.38
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76.74

20.49
20.39



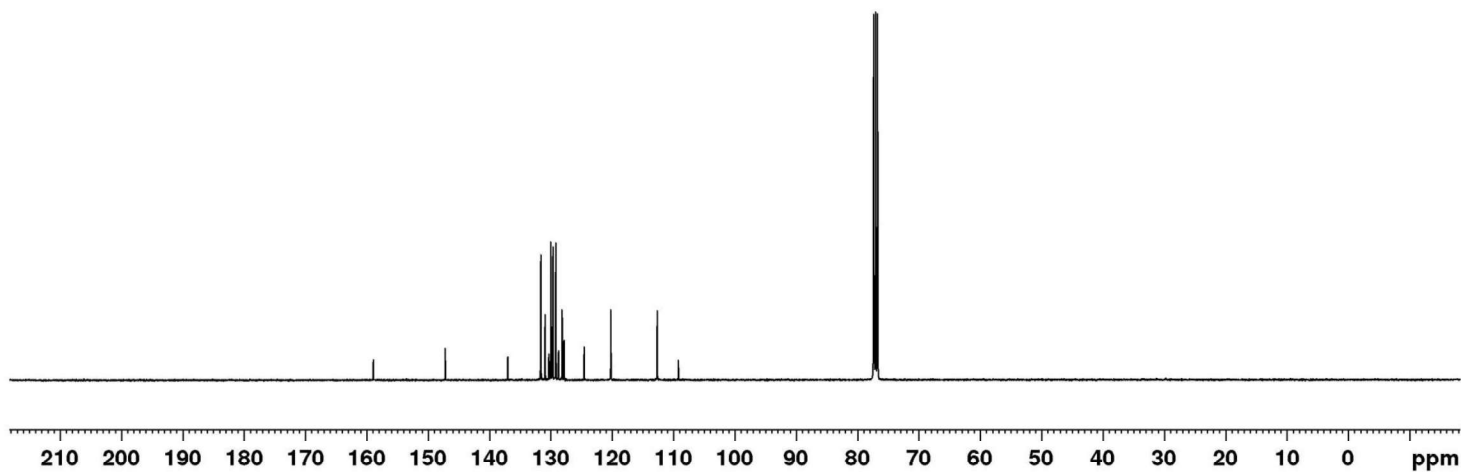
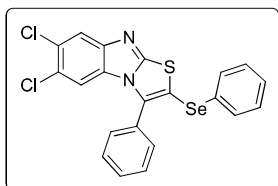
¹H NMR spectra of 4h



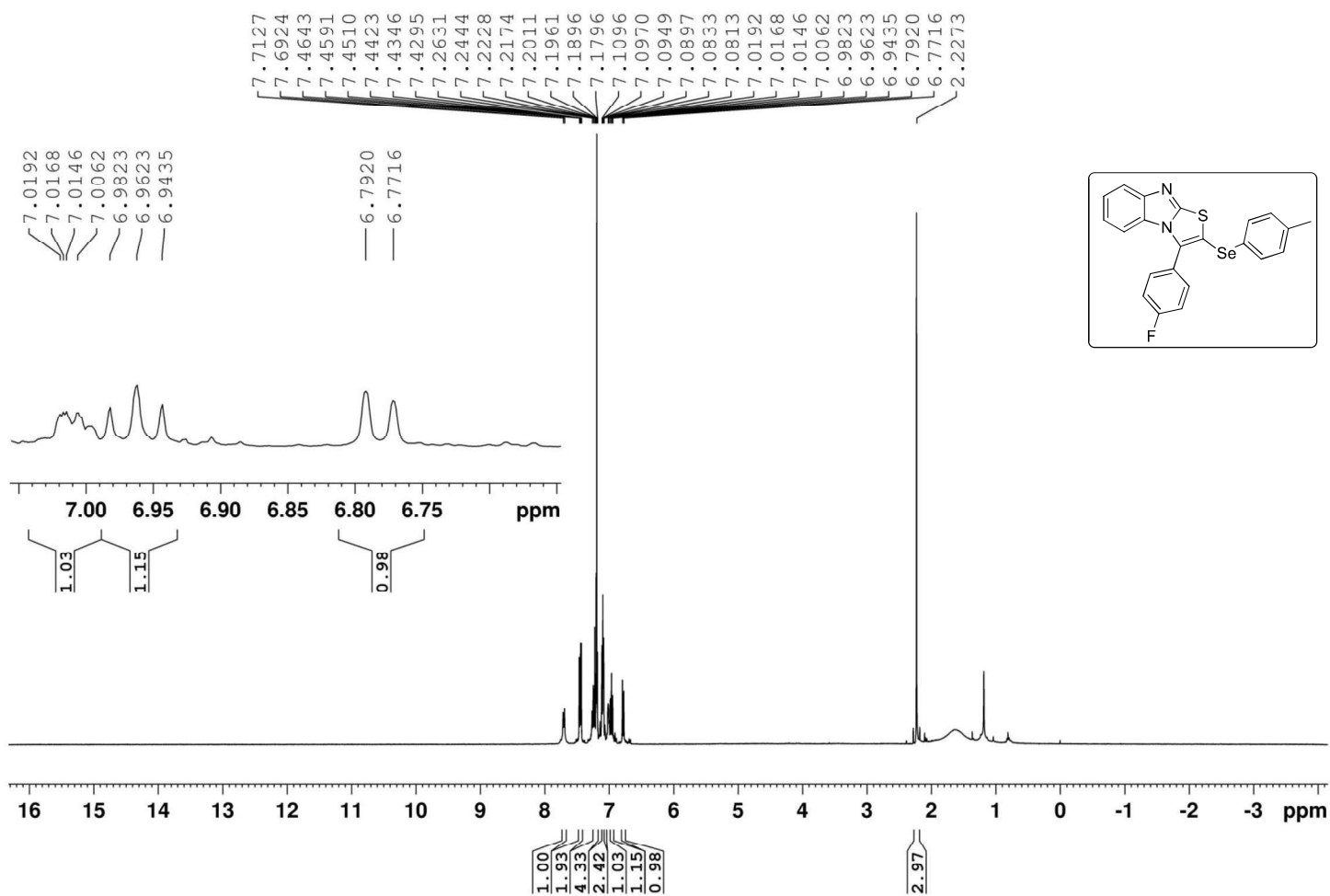
¹³C NMR spectra of 4h

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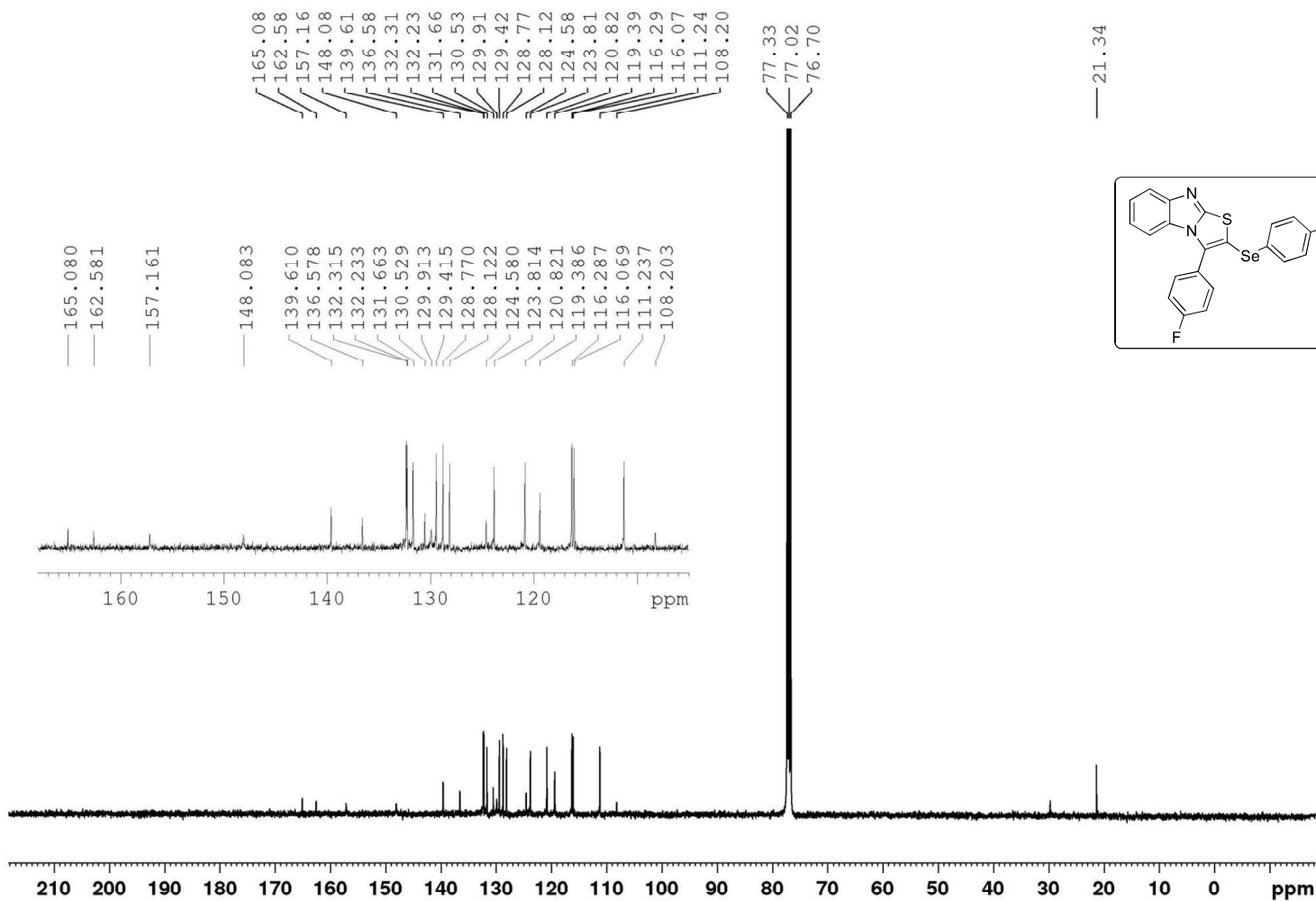
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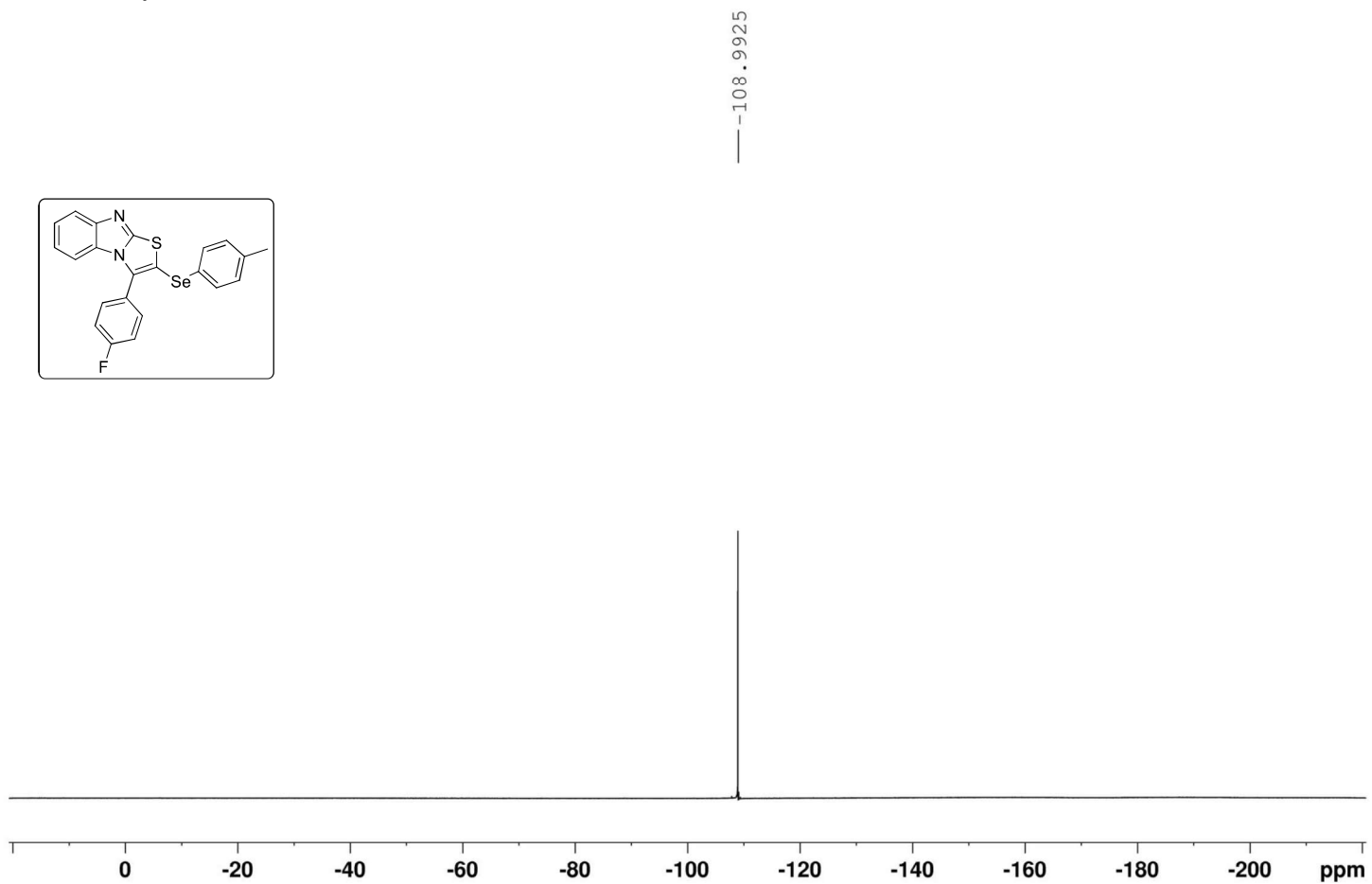
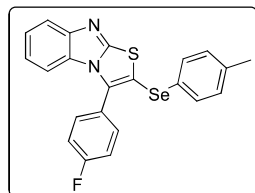
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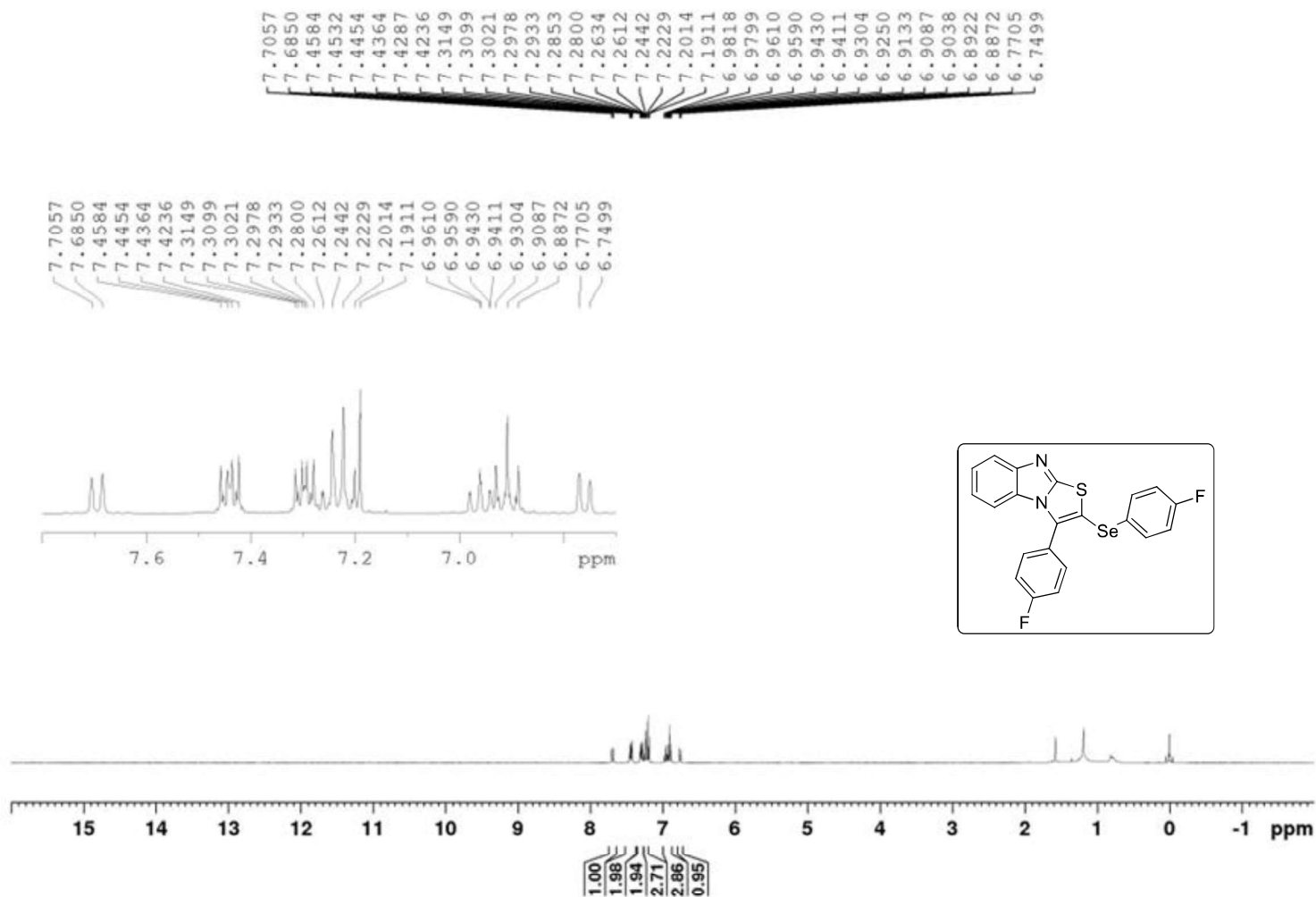
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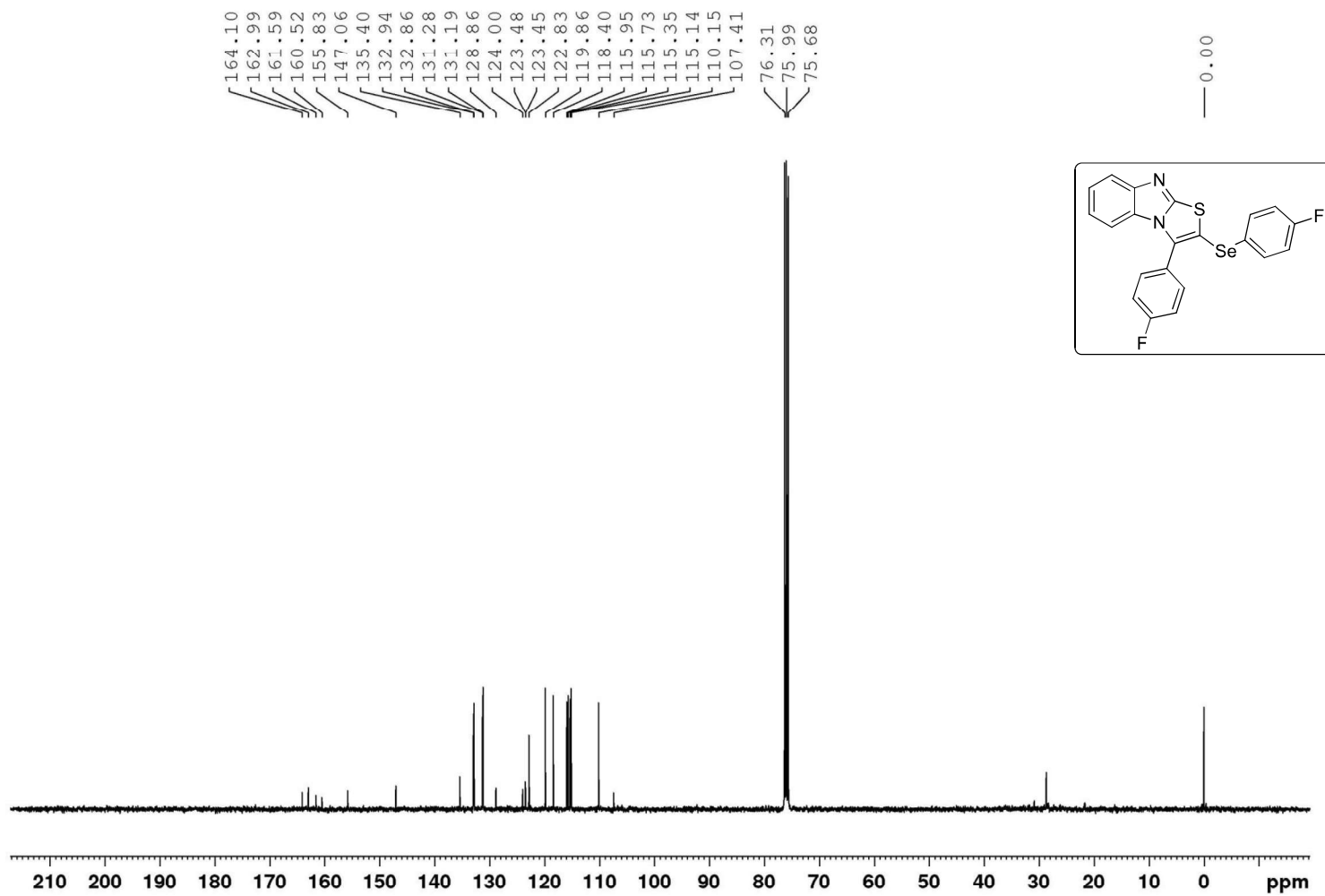
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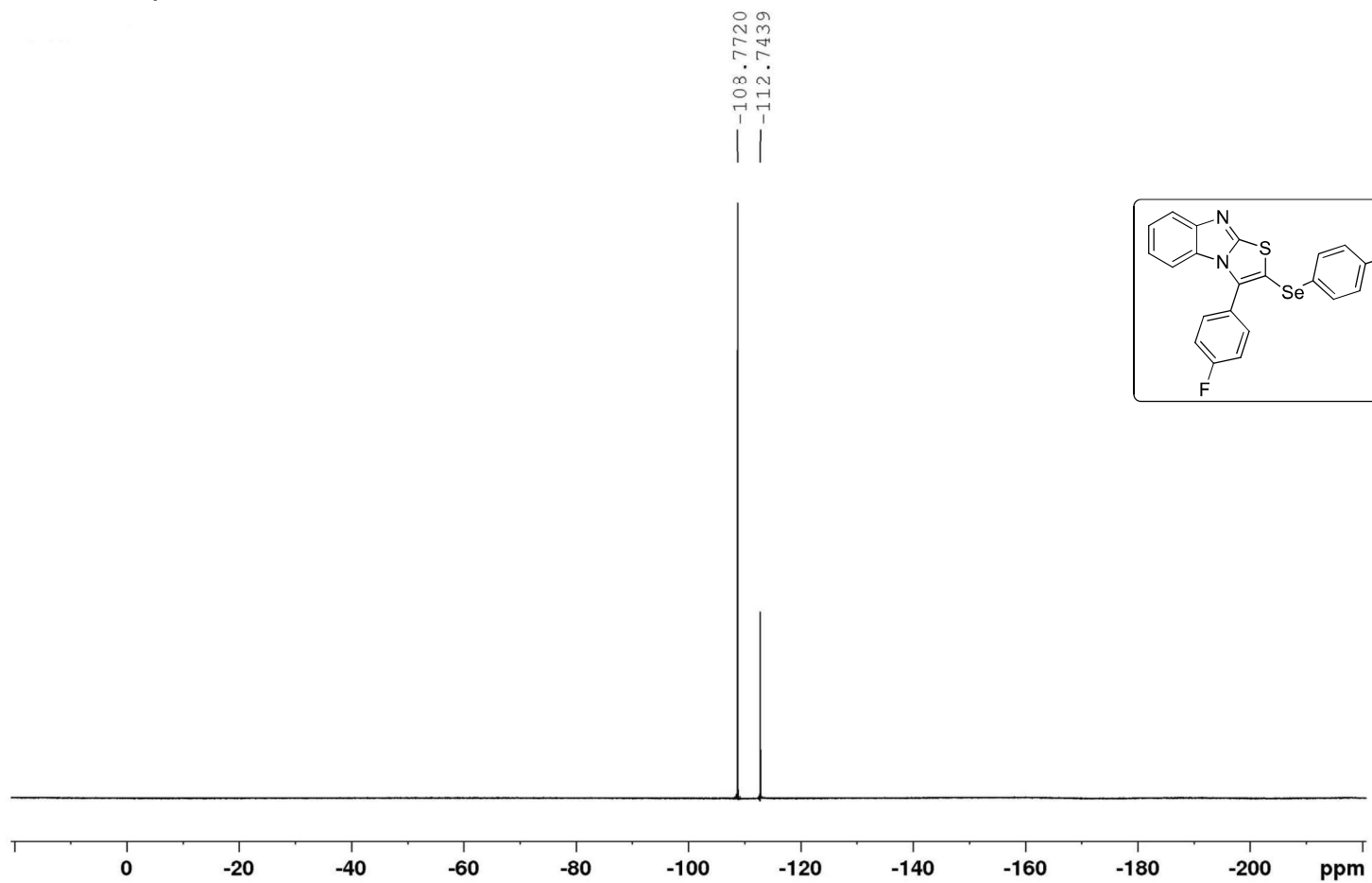
¹H NMR spectra of 5b



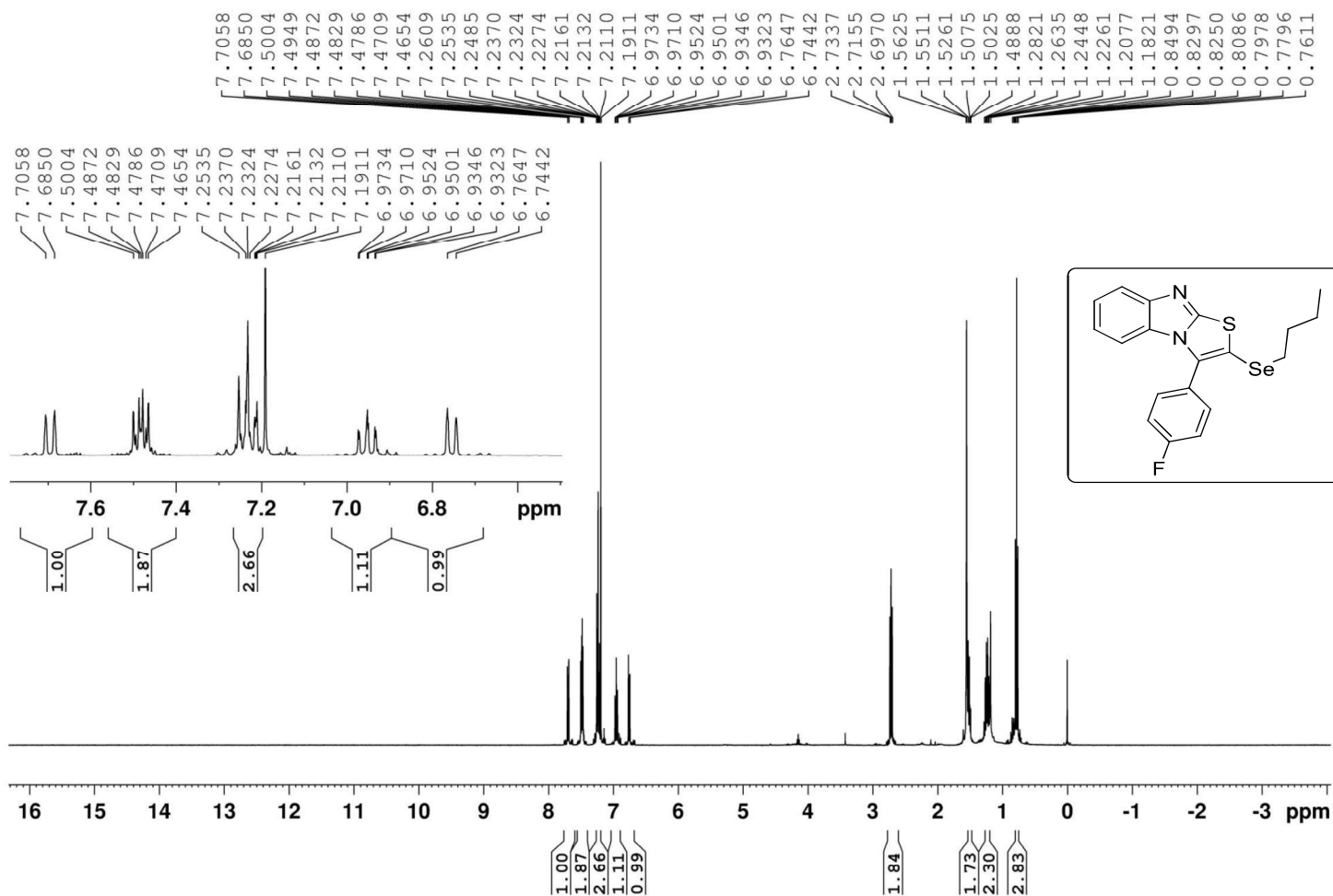
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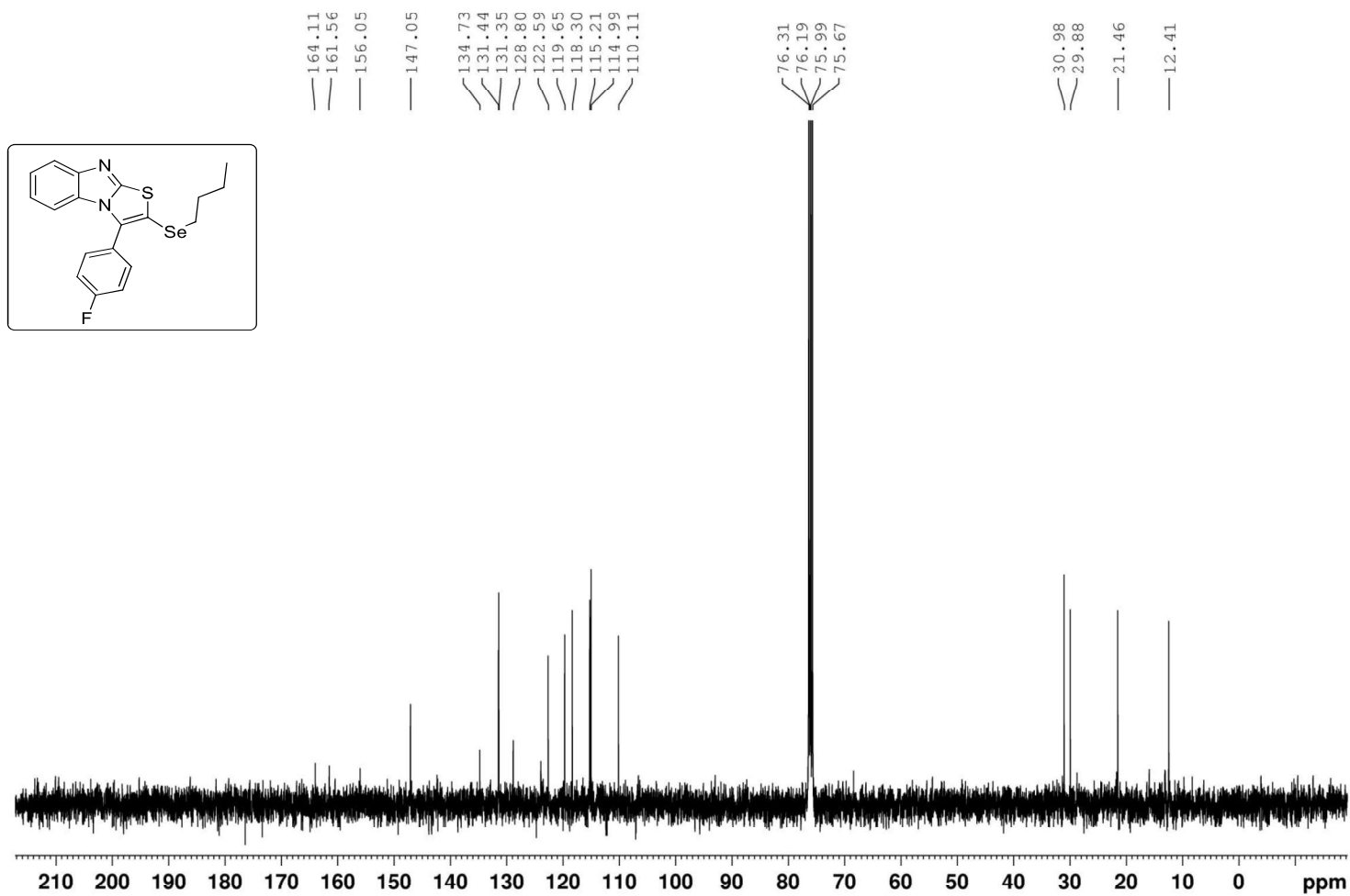
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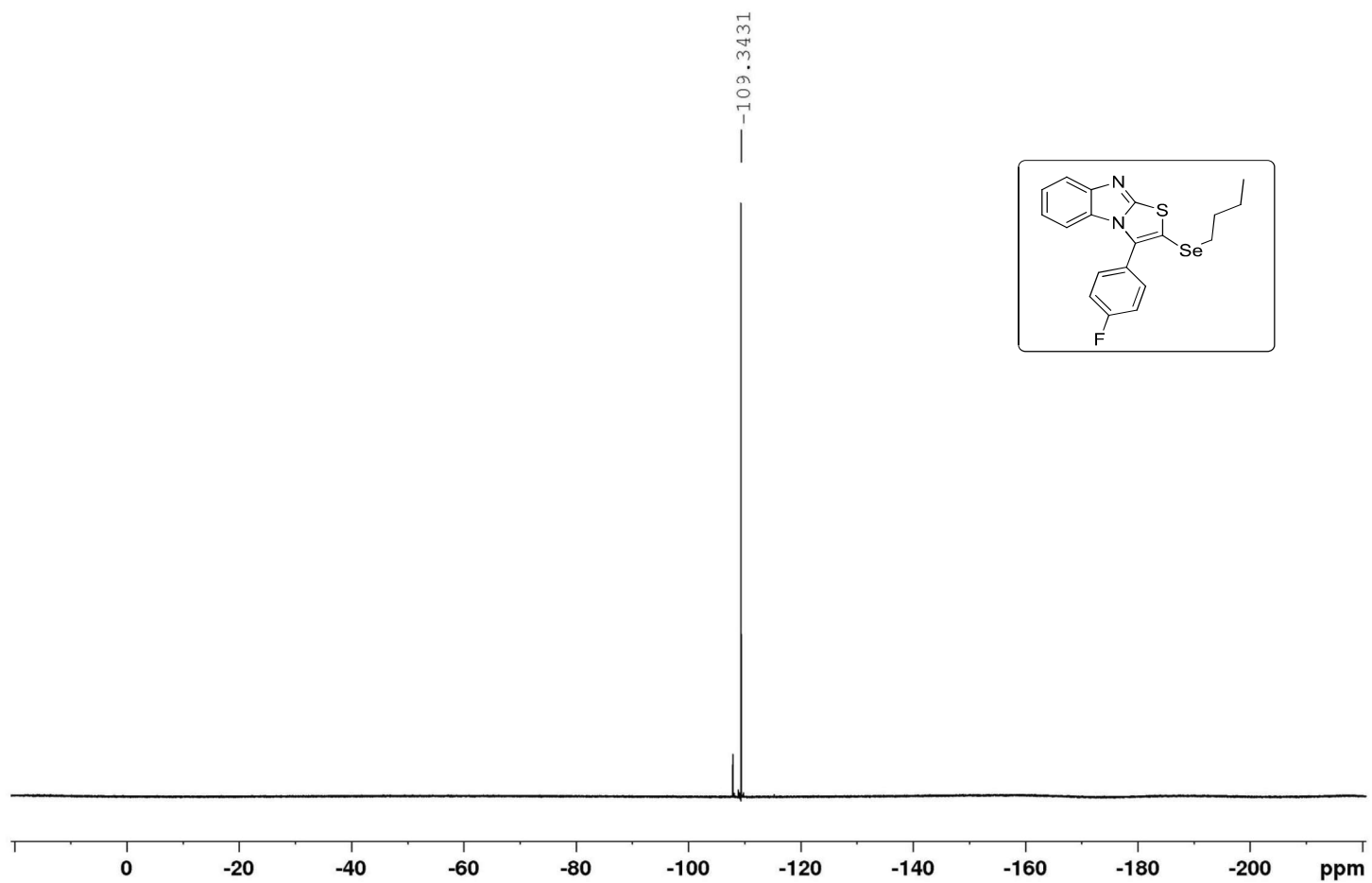
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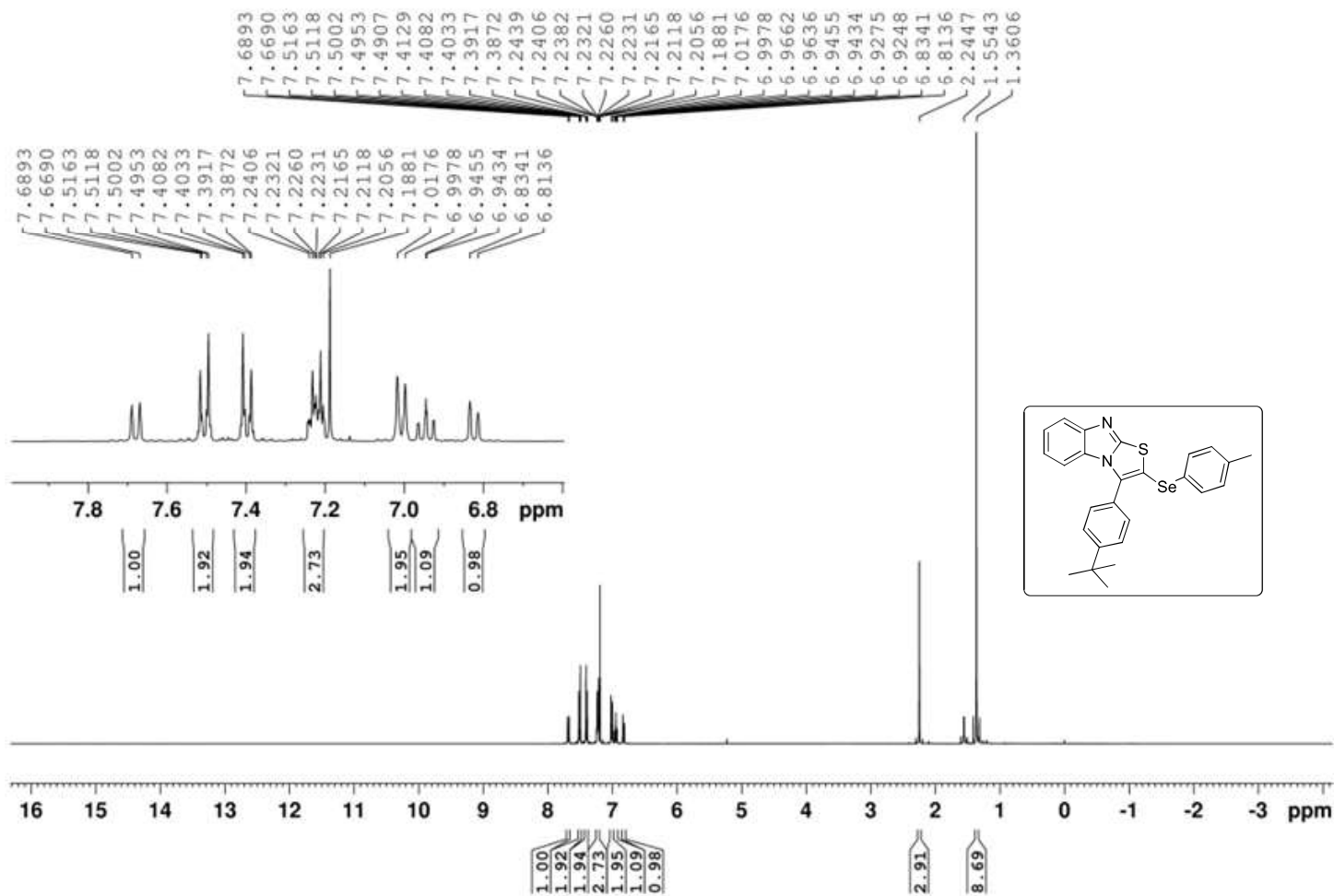
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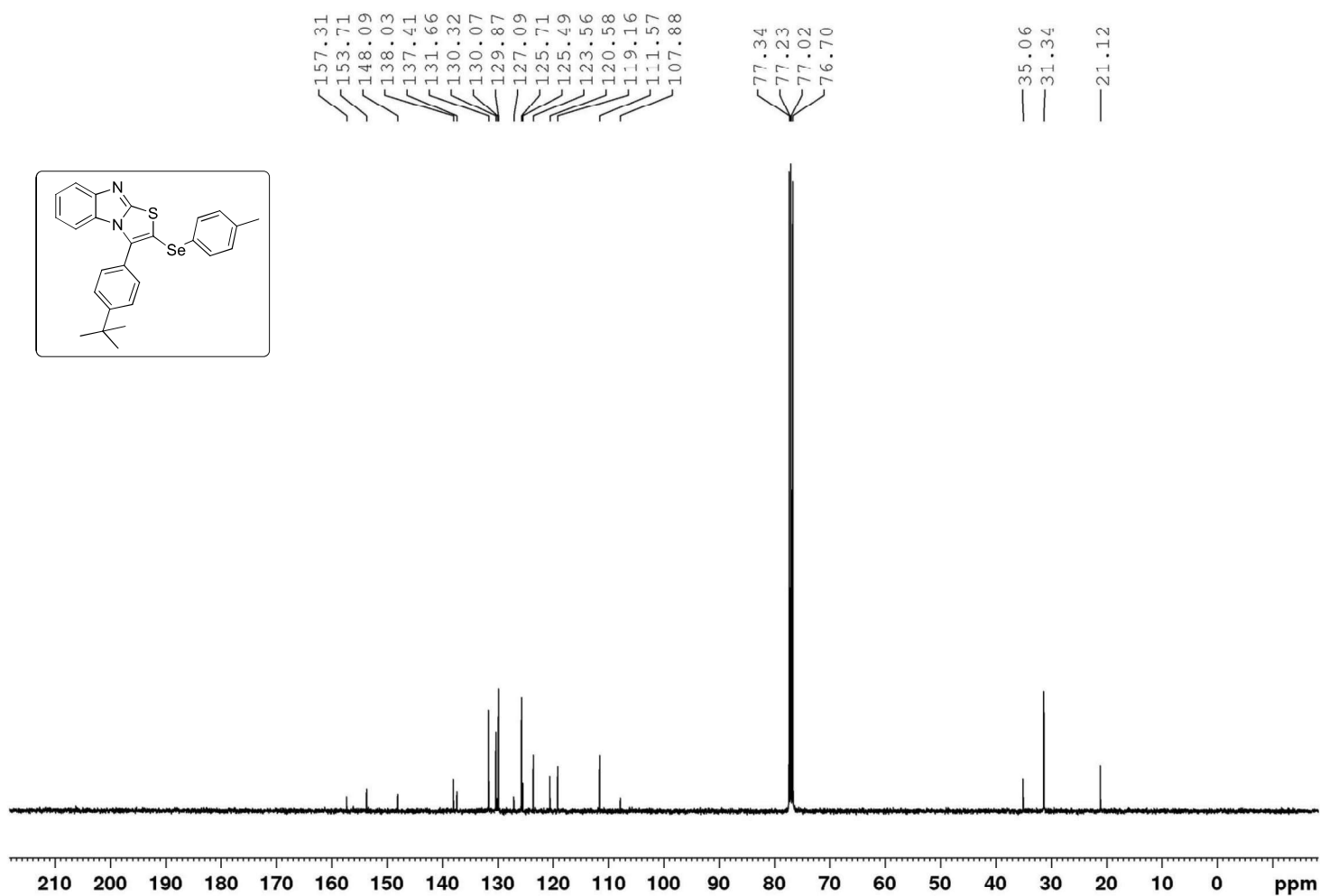
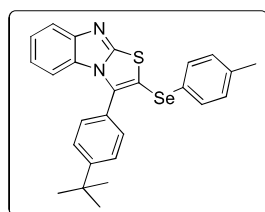
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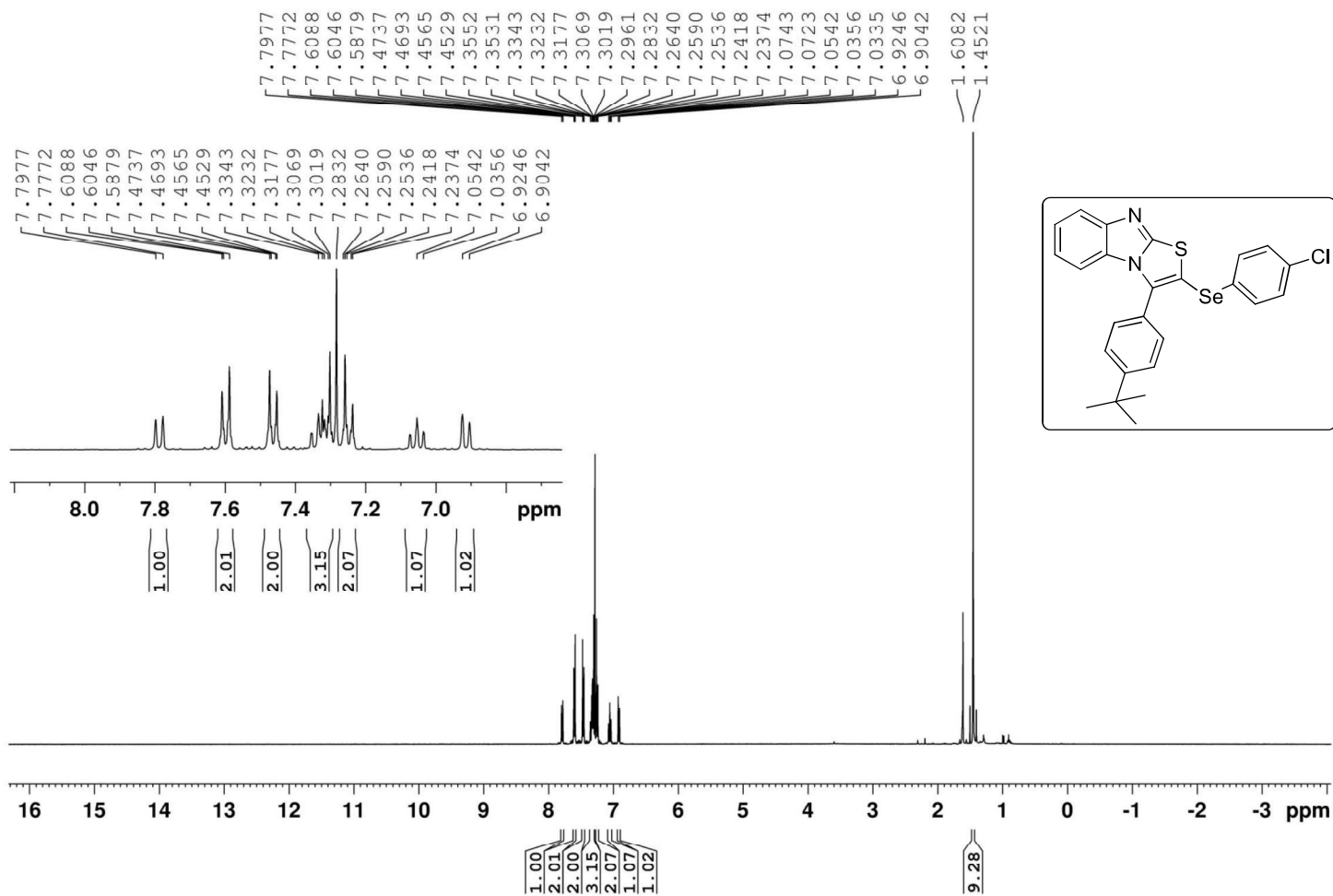
¹H NMR spectra of 5d



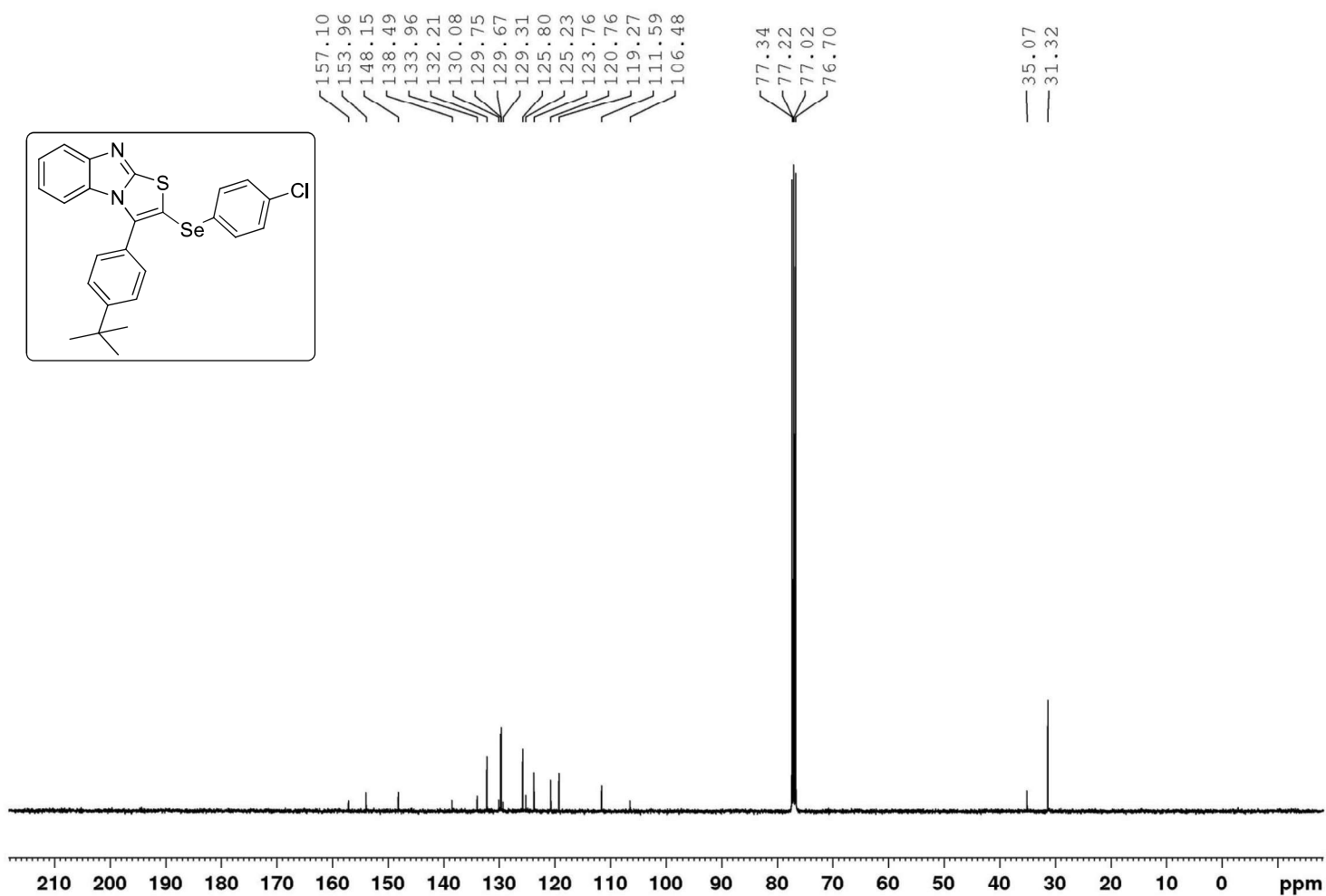
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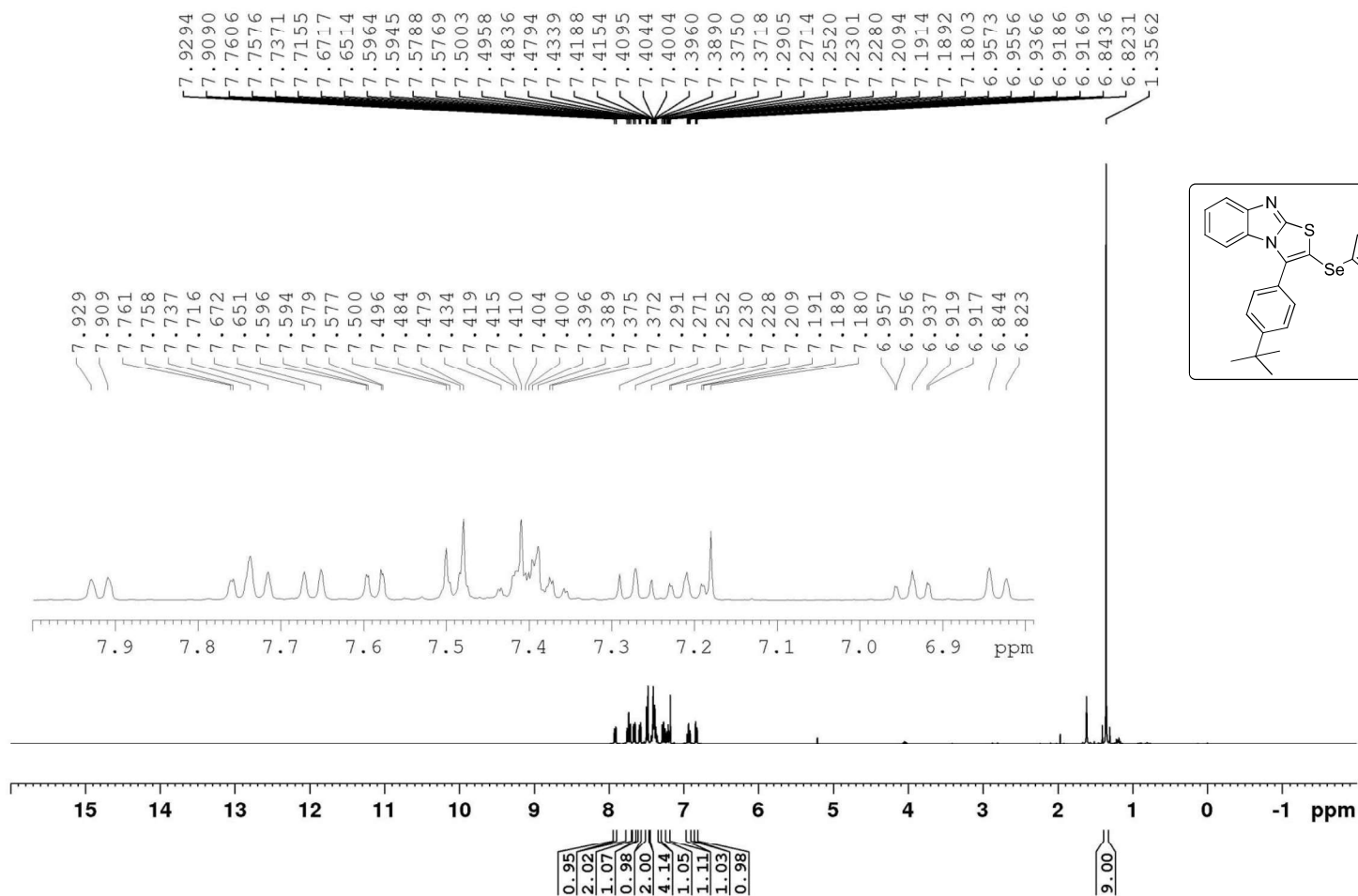
¹H NMR spectra of 5e



¹³C NMR spectra of 5e



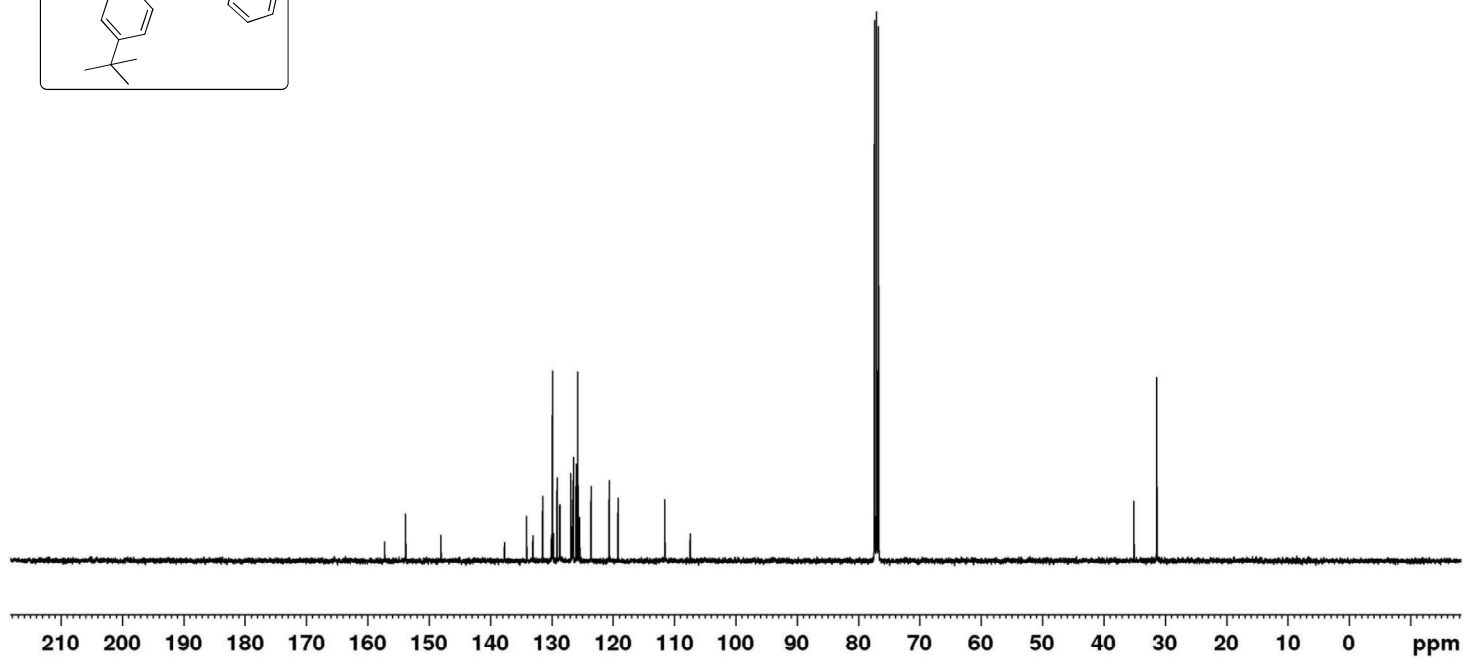
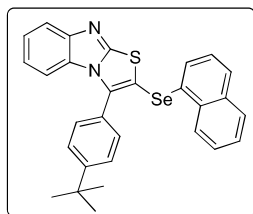
¹H NMR spectra of 5f



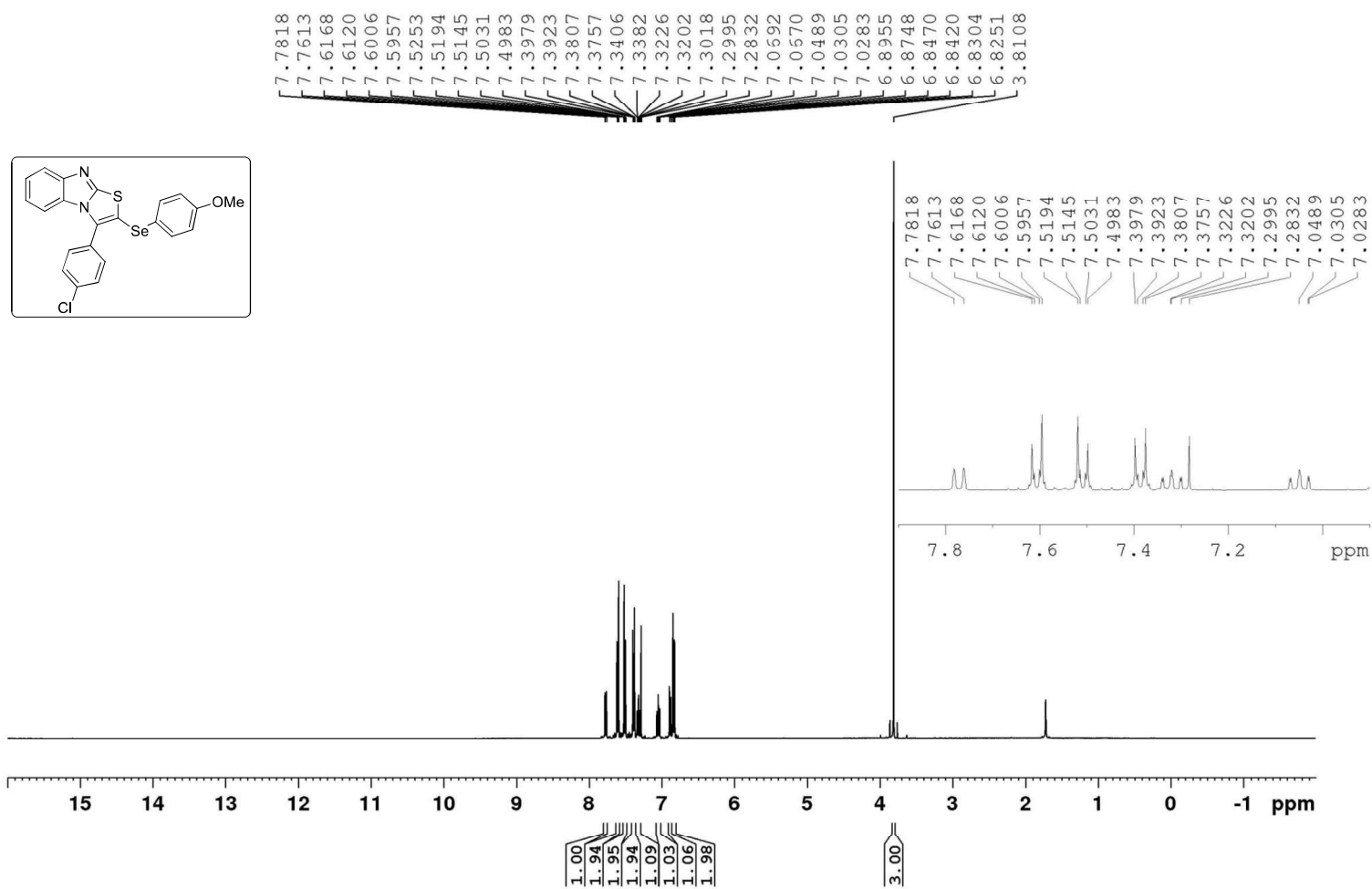
¹³C NMR spectra of 5f

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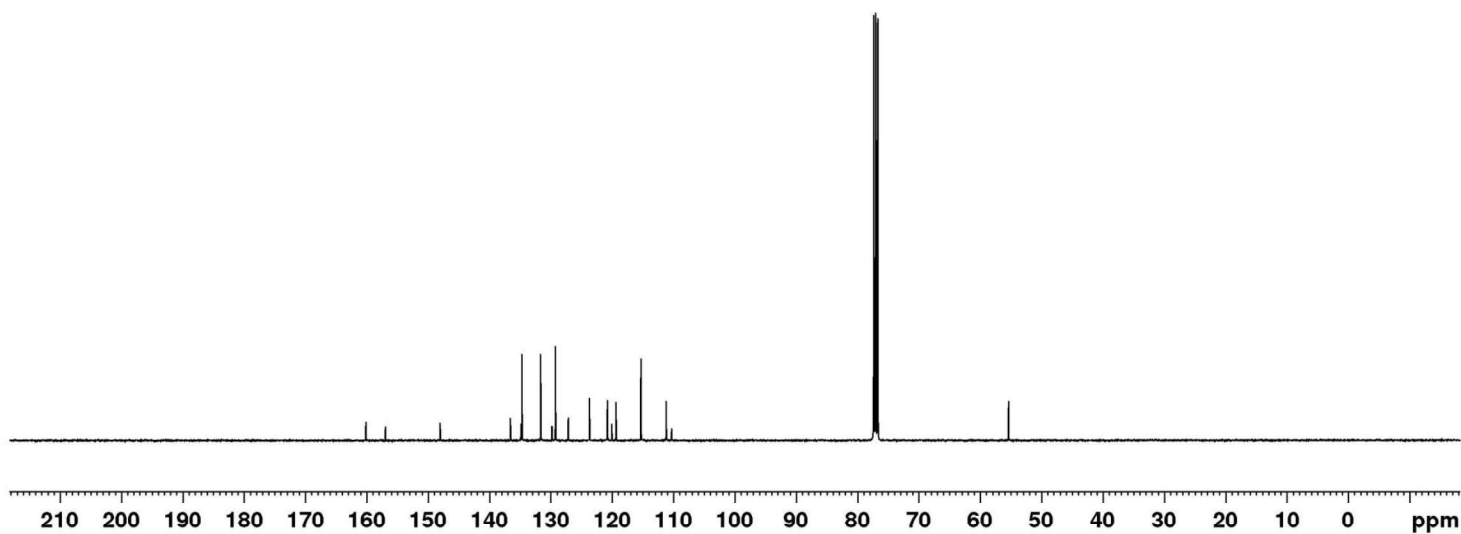
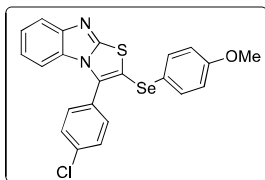


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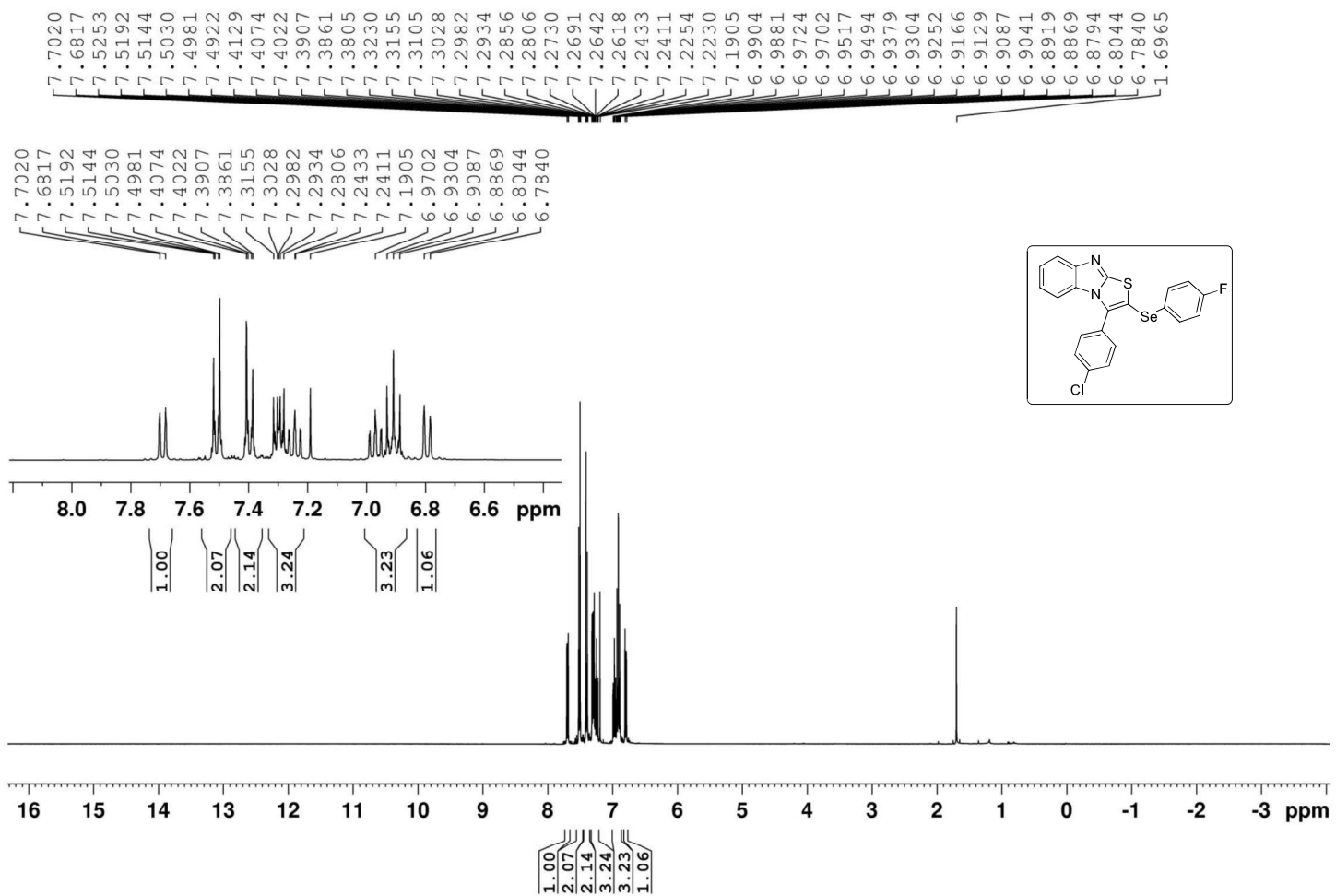


¹³C NMR spectra of 5g

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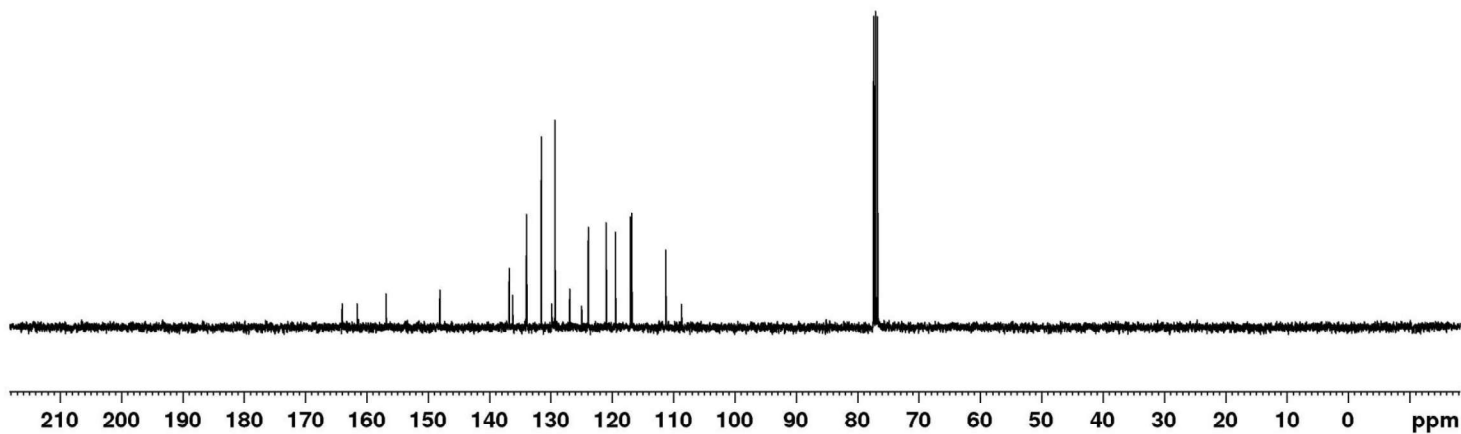
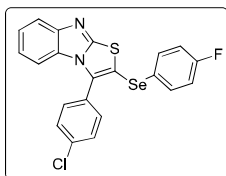


¹H NMR spectra of 5h

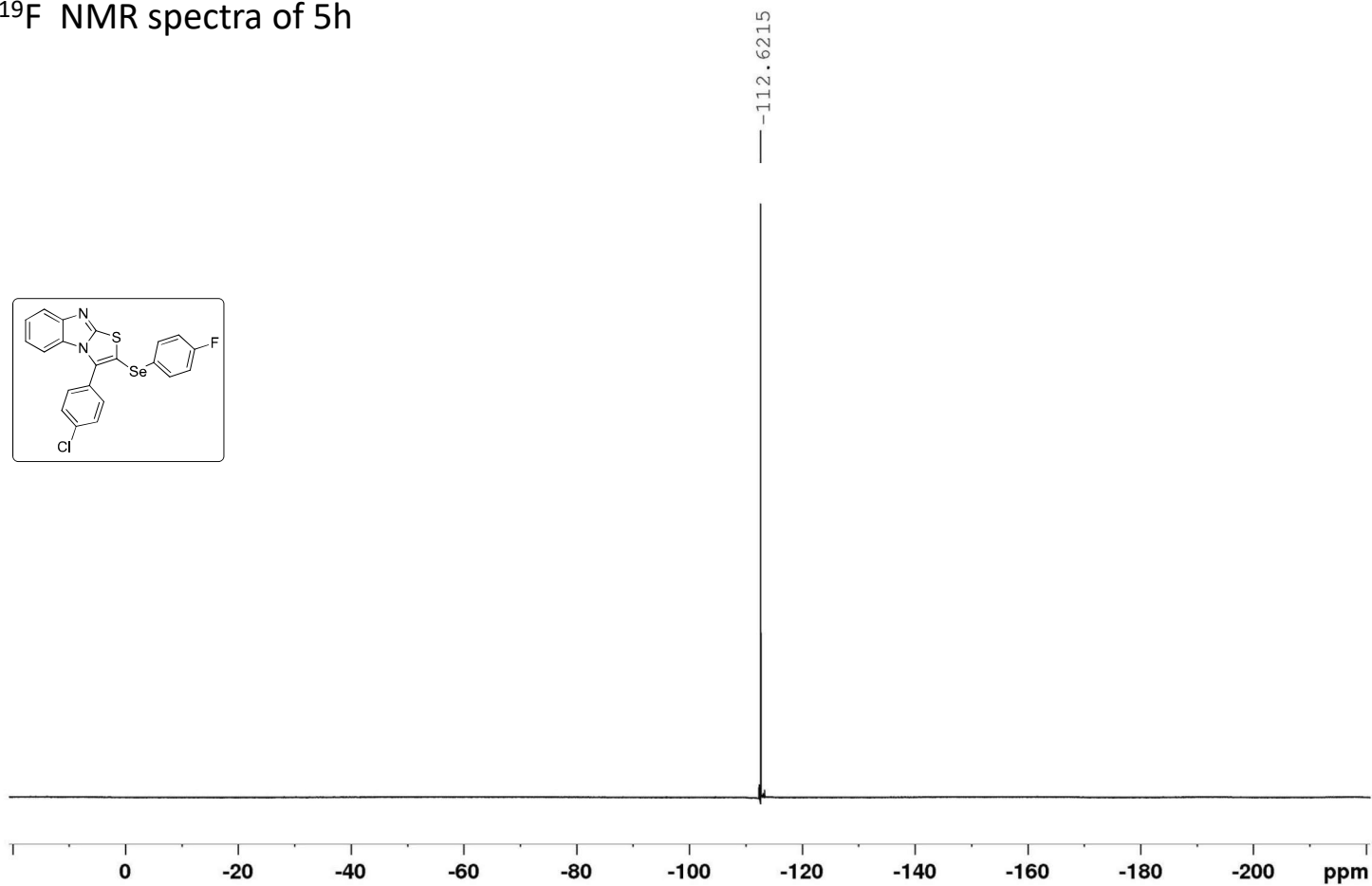
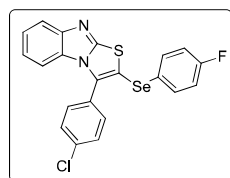


¹³C NMR spectra of 5h

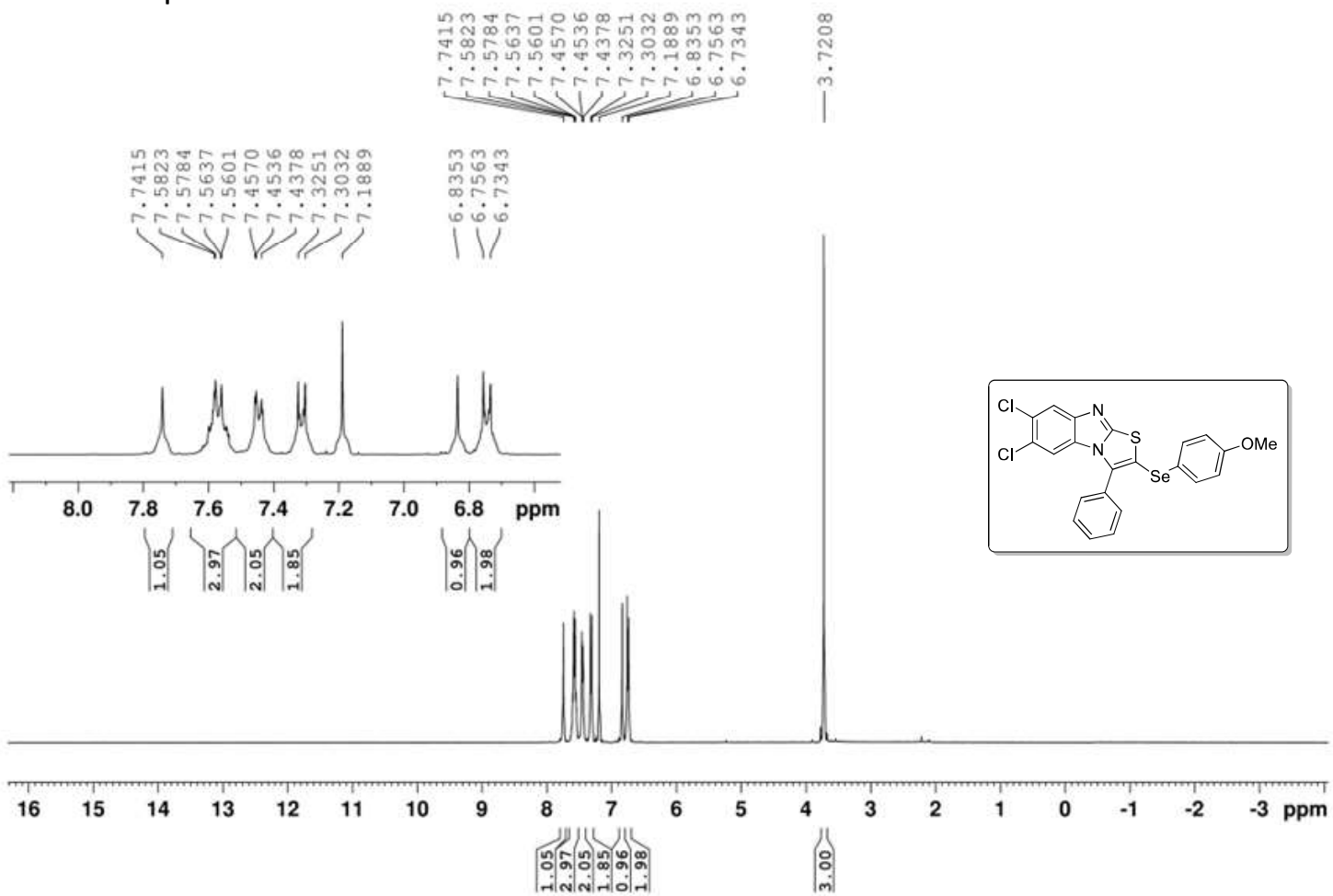
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129.32
126.89
124.97
124.94
123.89
120.94
119.46
117.00
116.79
111.25
108.66
77.37
77.05
76.73



¹⁹F NMR spectra of 5h

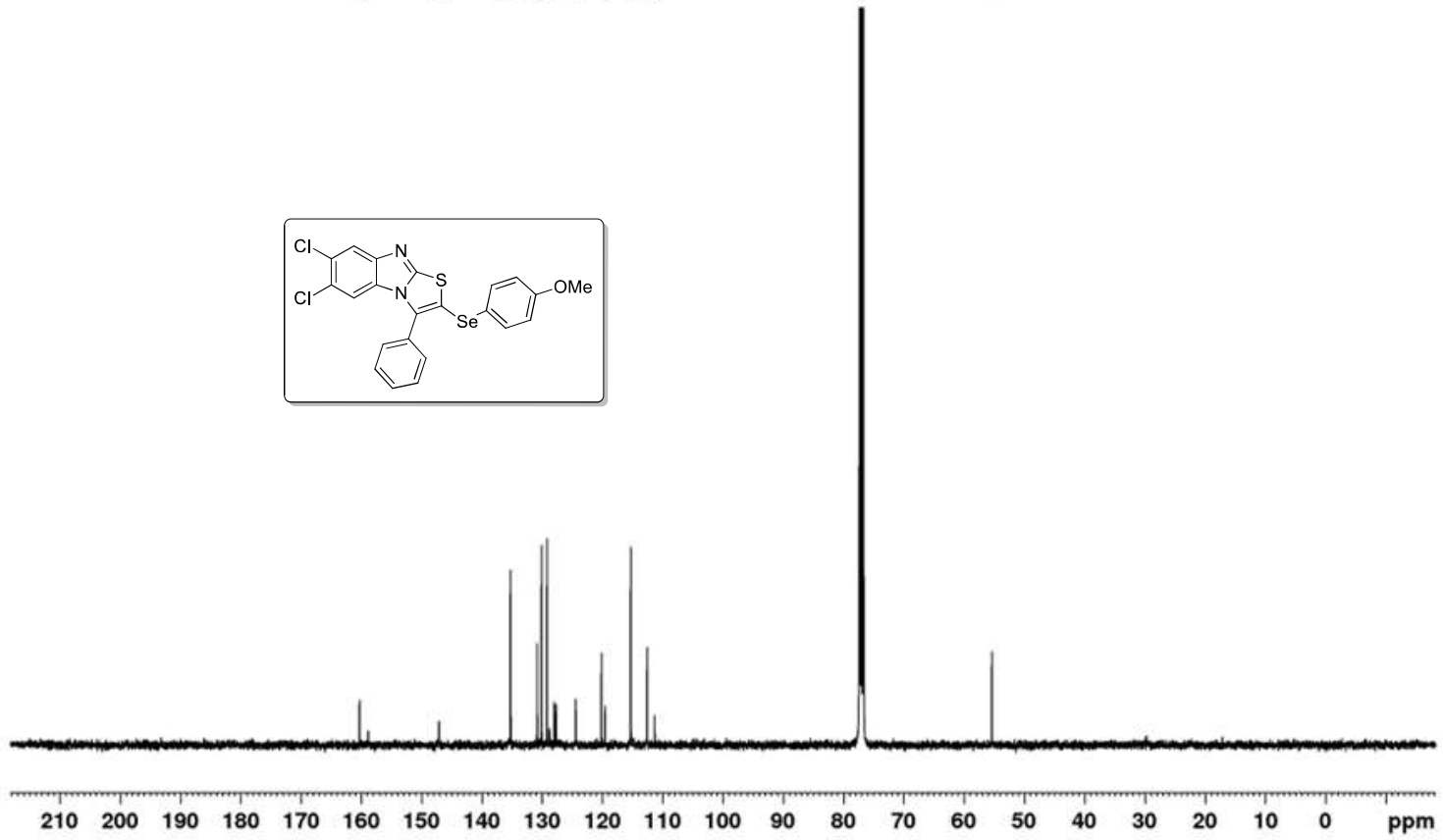
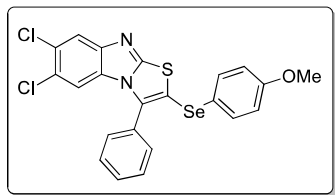


¹H NMR spectra of 5i

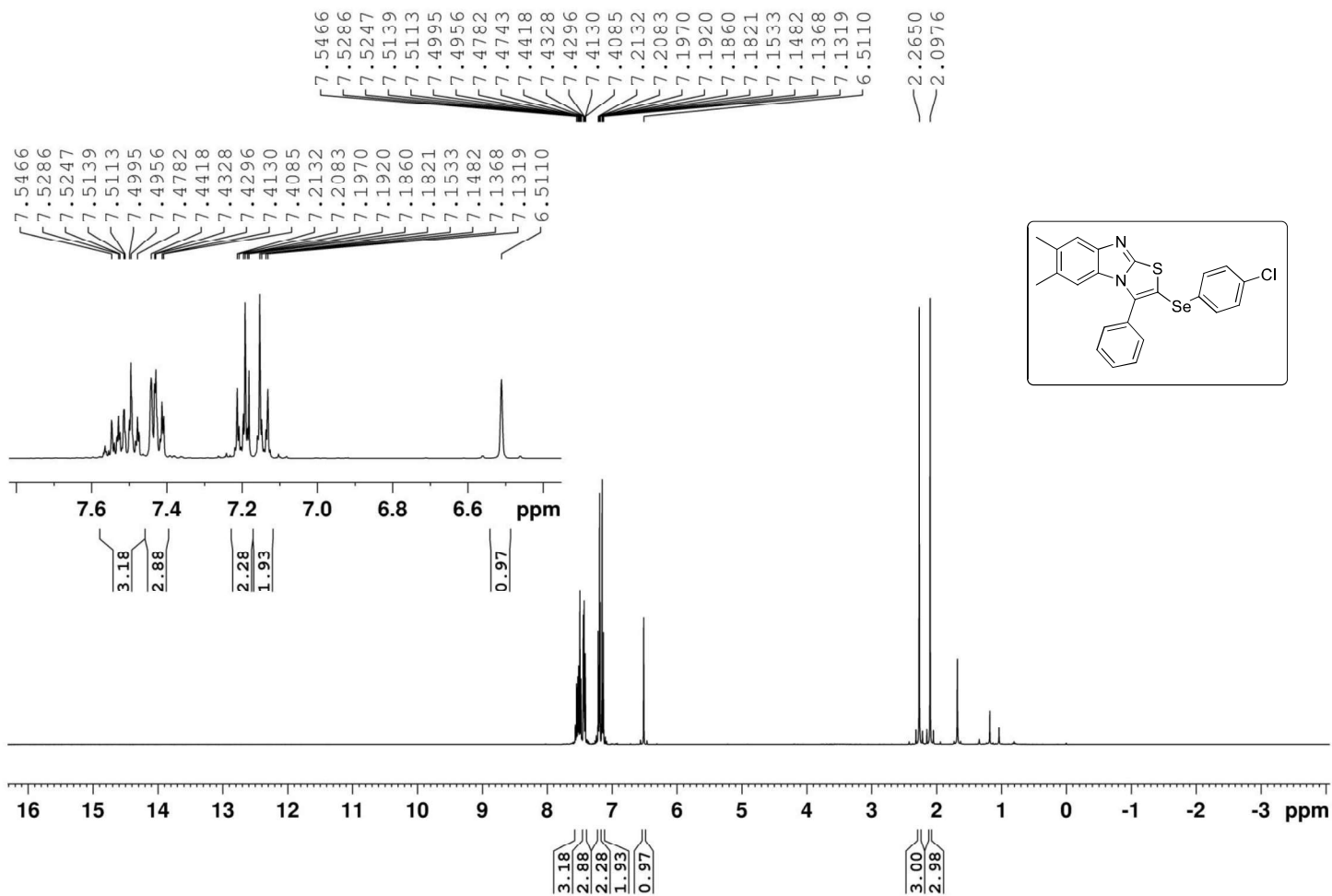


¹³C NMR spectra of 5i

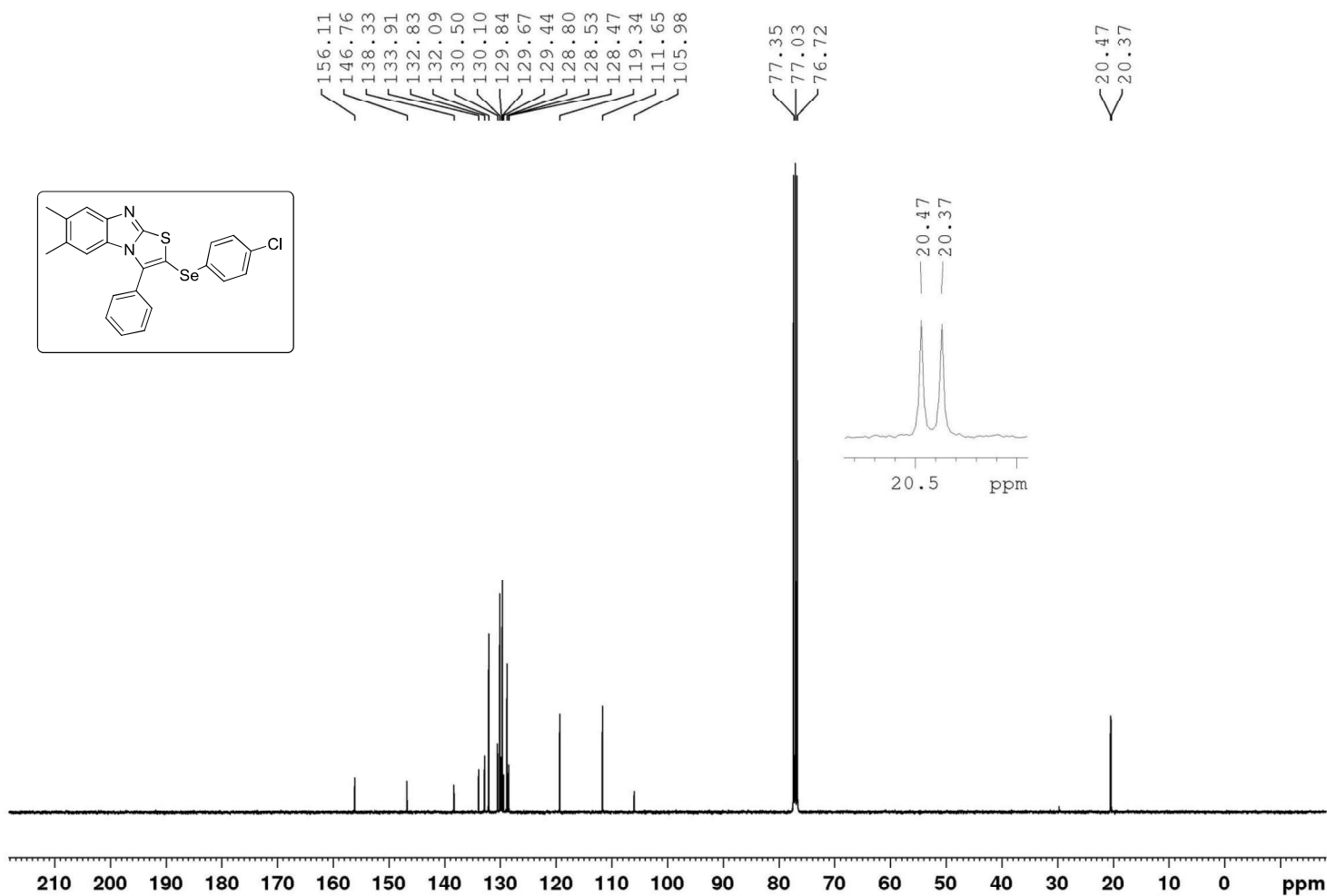
- 160.31
- 158.87
- 147.11
- 135.26
- 130.83
- 130.10
- 129.18
- 128.73
- 127.99
- 127.67
- 124.44
- 120.15
- 119.56
- 115.30
- 112.56
- 111.33
- 77.33
- 77.01
- 76.70
- 55.37



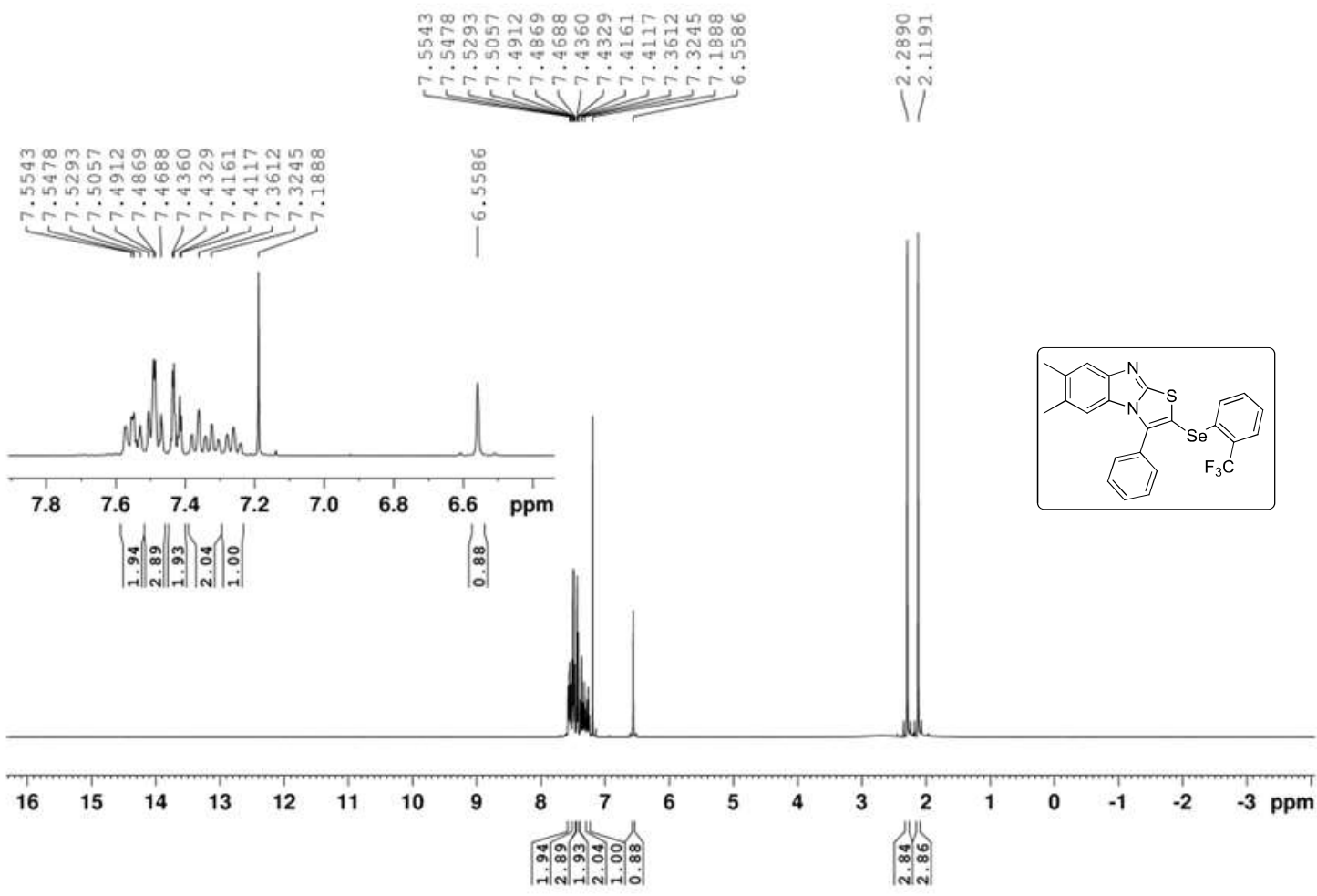
¹H NMR spectra of 5j



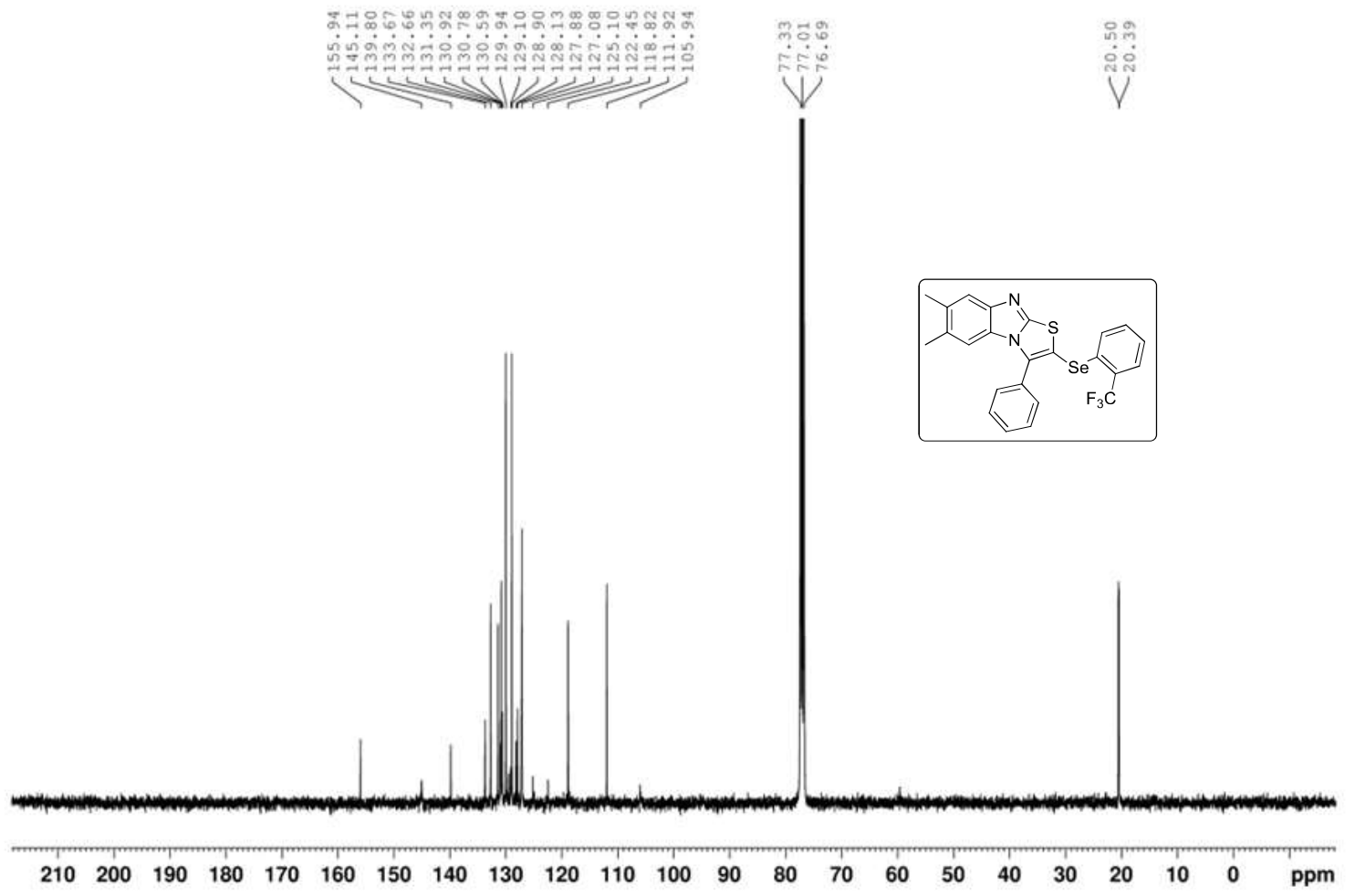
¹³C NMR spectra of 5j



¹H NMR spectra of 5k

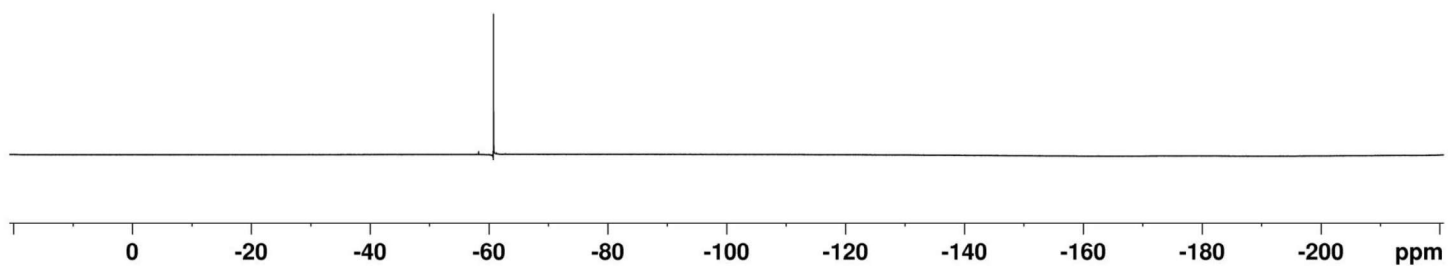
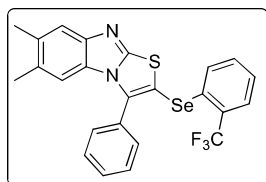


¹³C NMR spectra of 5k

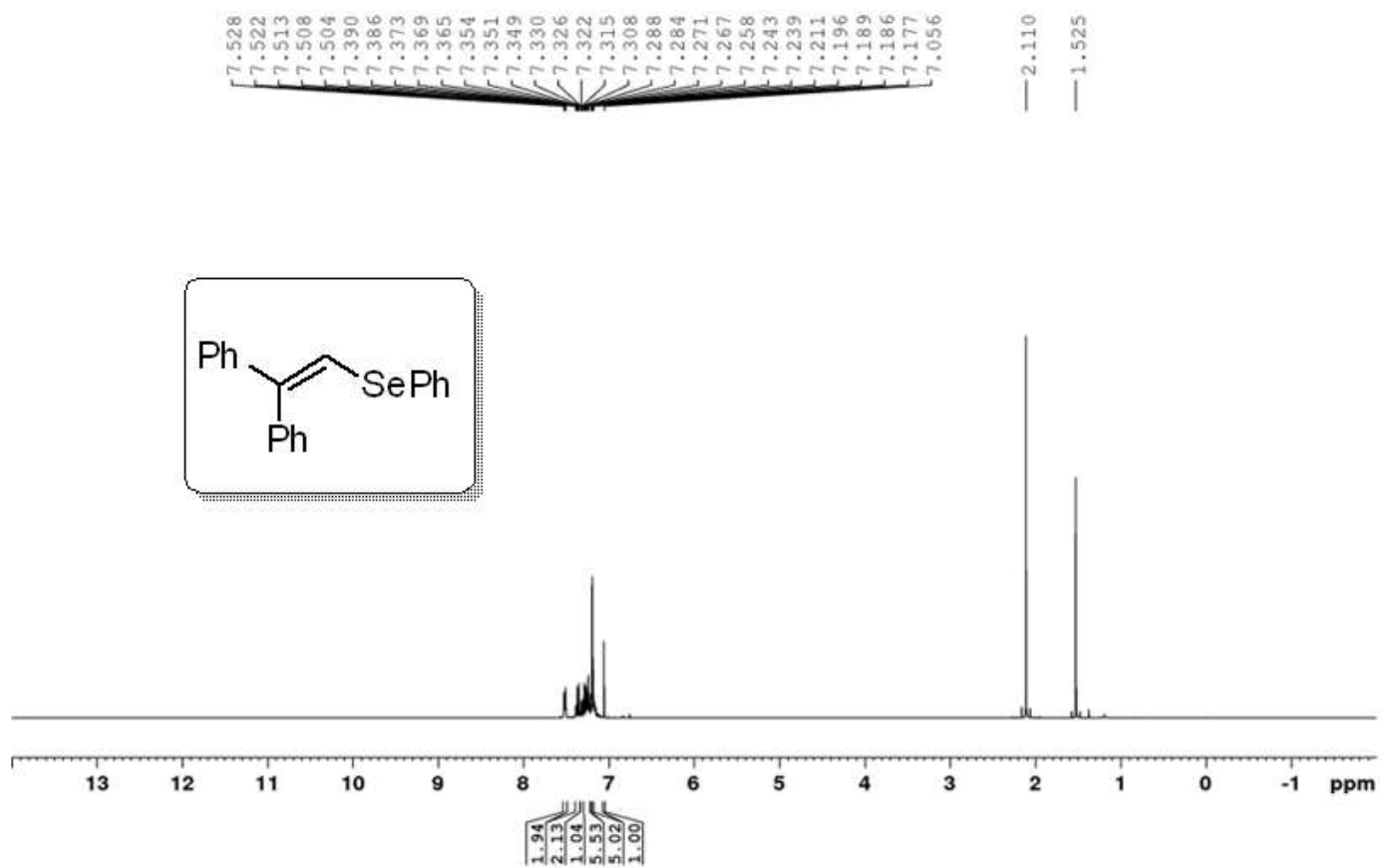


¹⁹F NMR spectra of 5k

— -60.7915



¹H NMR spectra of 6



^{13}C NMR spectra of 6

