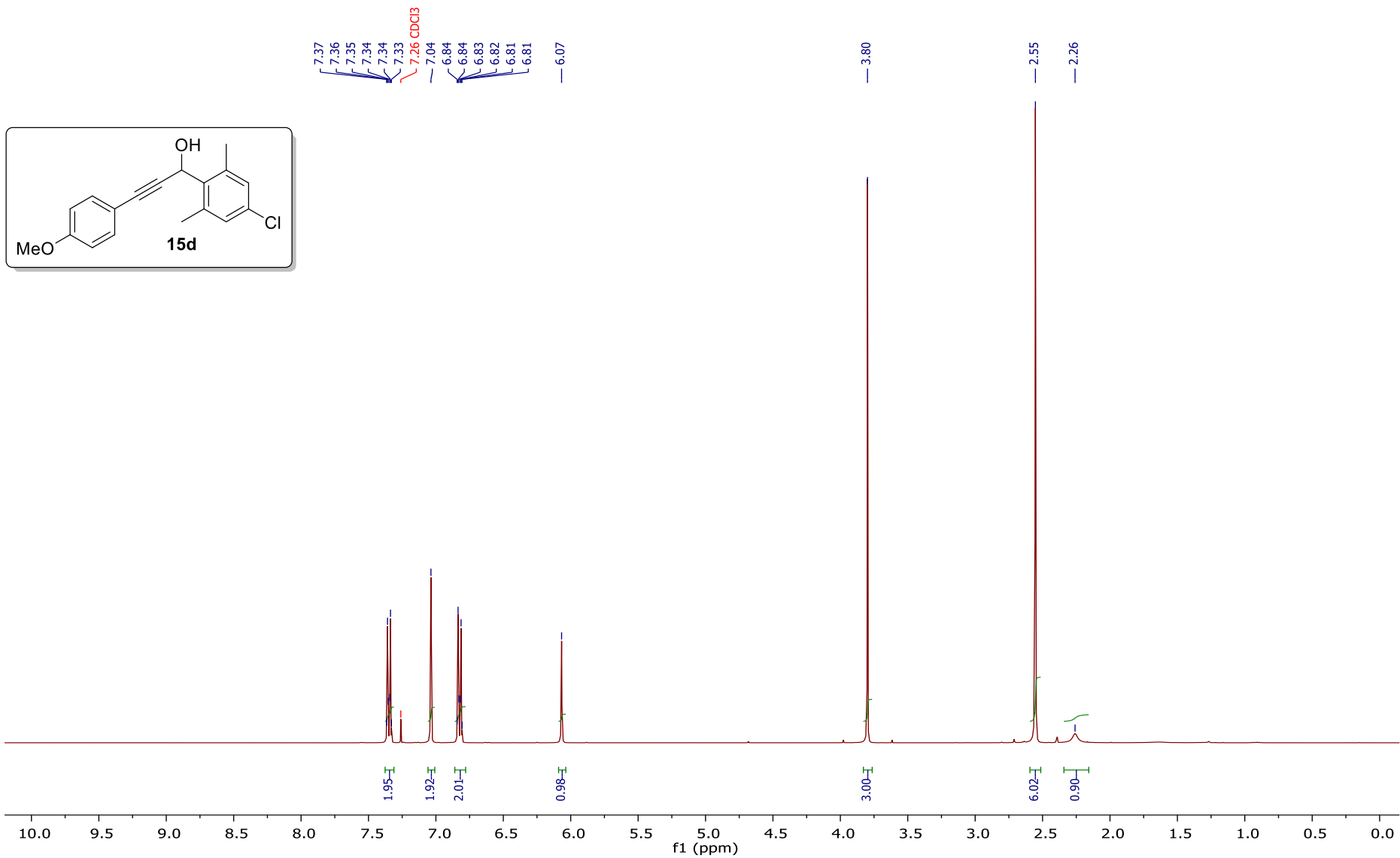


Supporting information

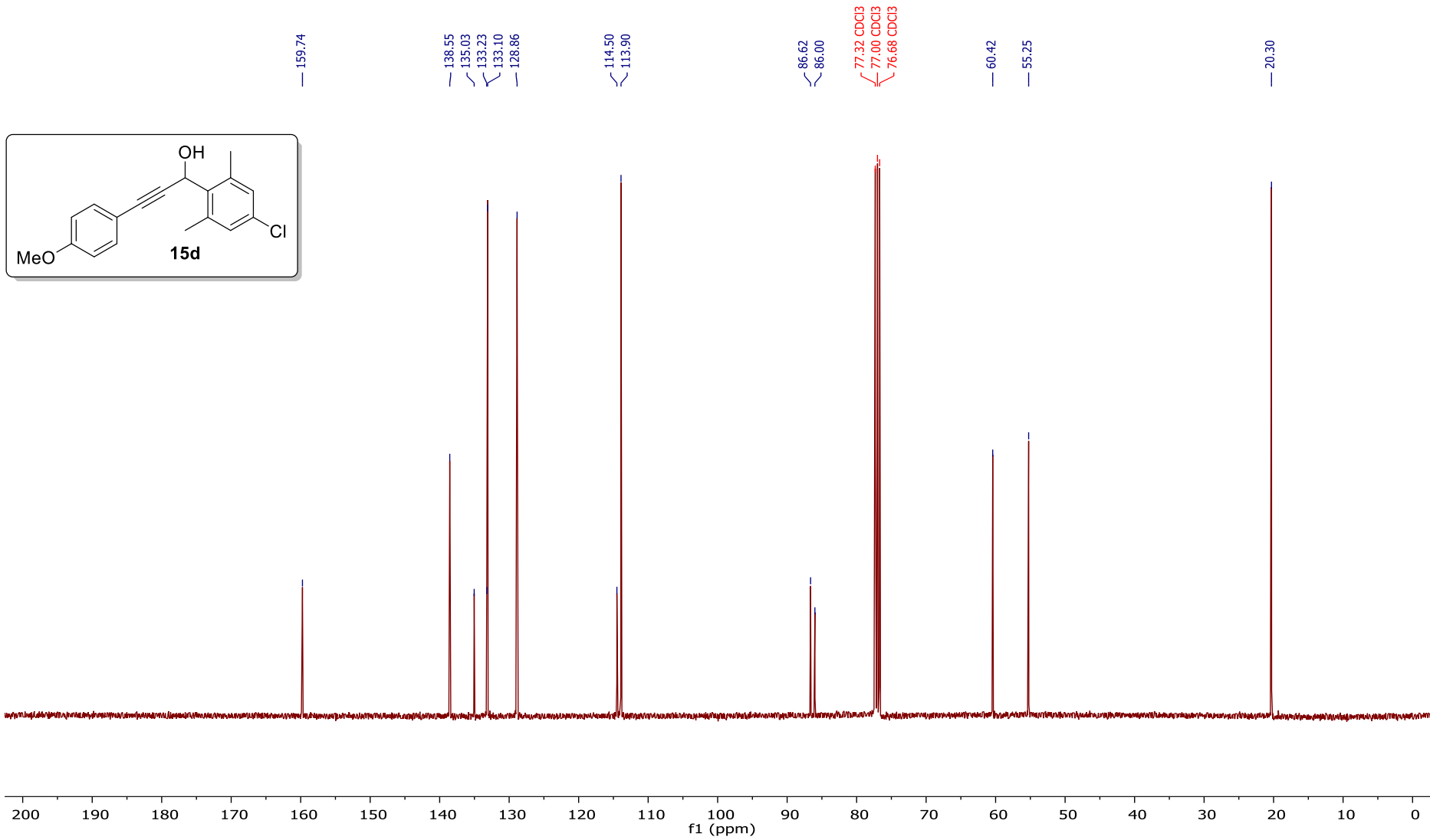
Selenium Analogues of Rintodestrant (G1T48) as Potent Estrogen Receptor Modulators and Downregulators

Edgars Paegle, Pavels Dimitrijevs, and Pavel Arsenyan*

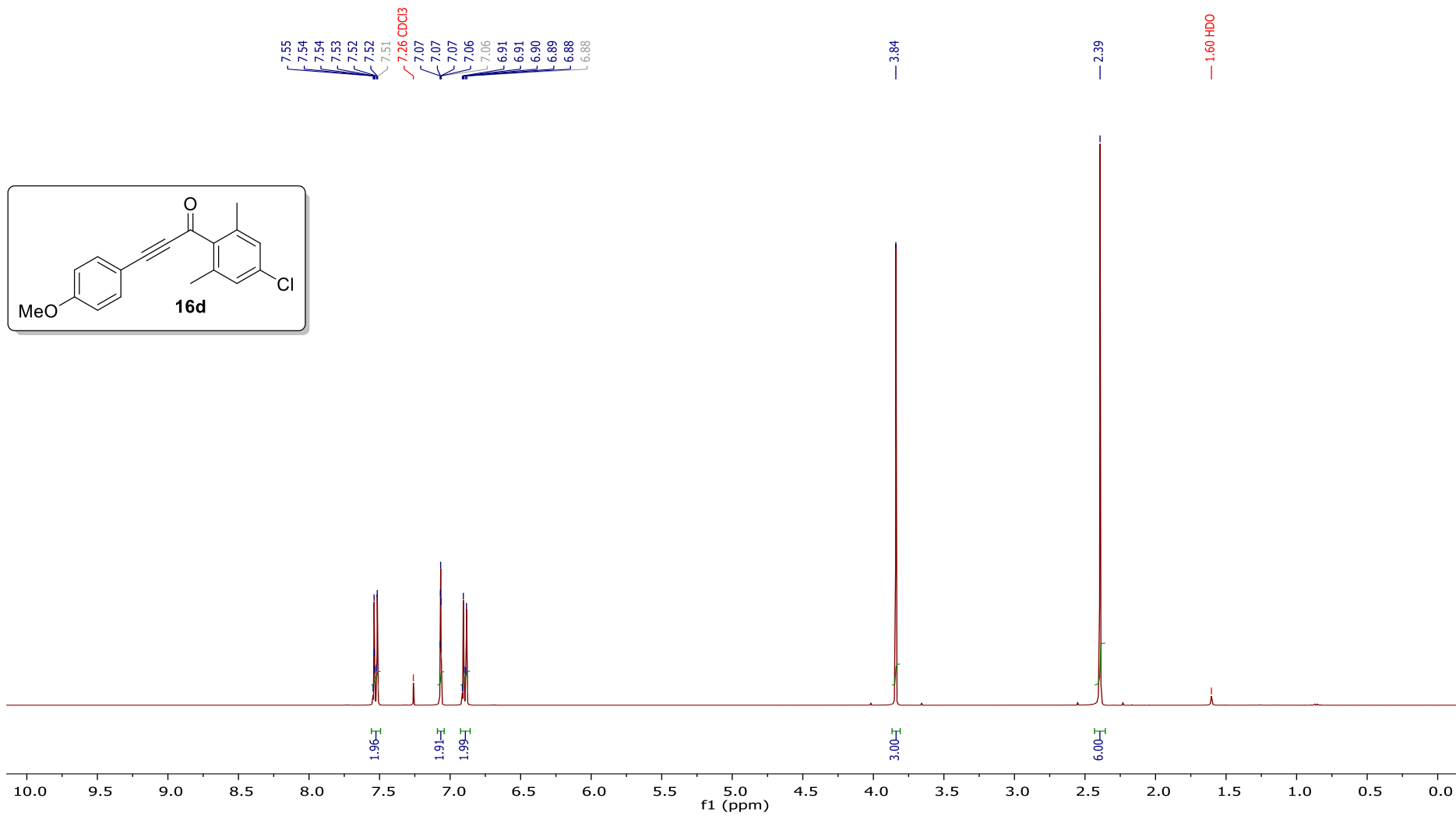
^1H NMR (400 MHz, CDCl_3):



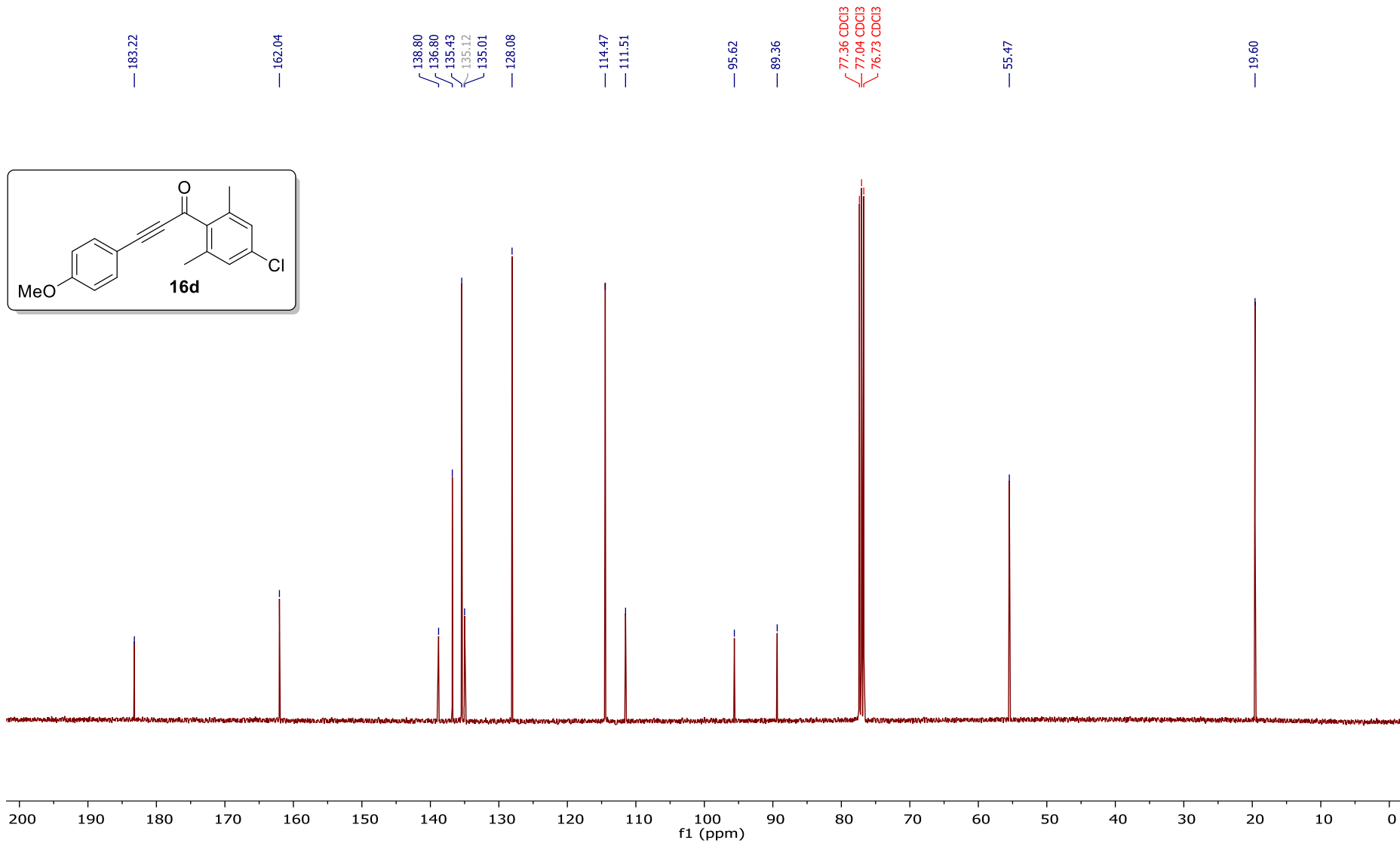
^{13}C NMR (100.6 MHz, CDCl_3):



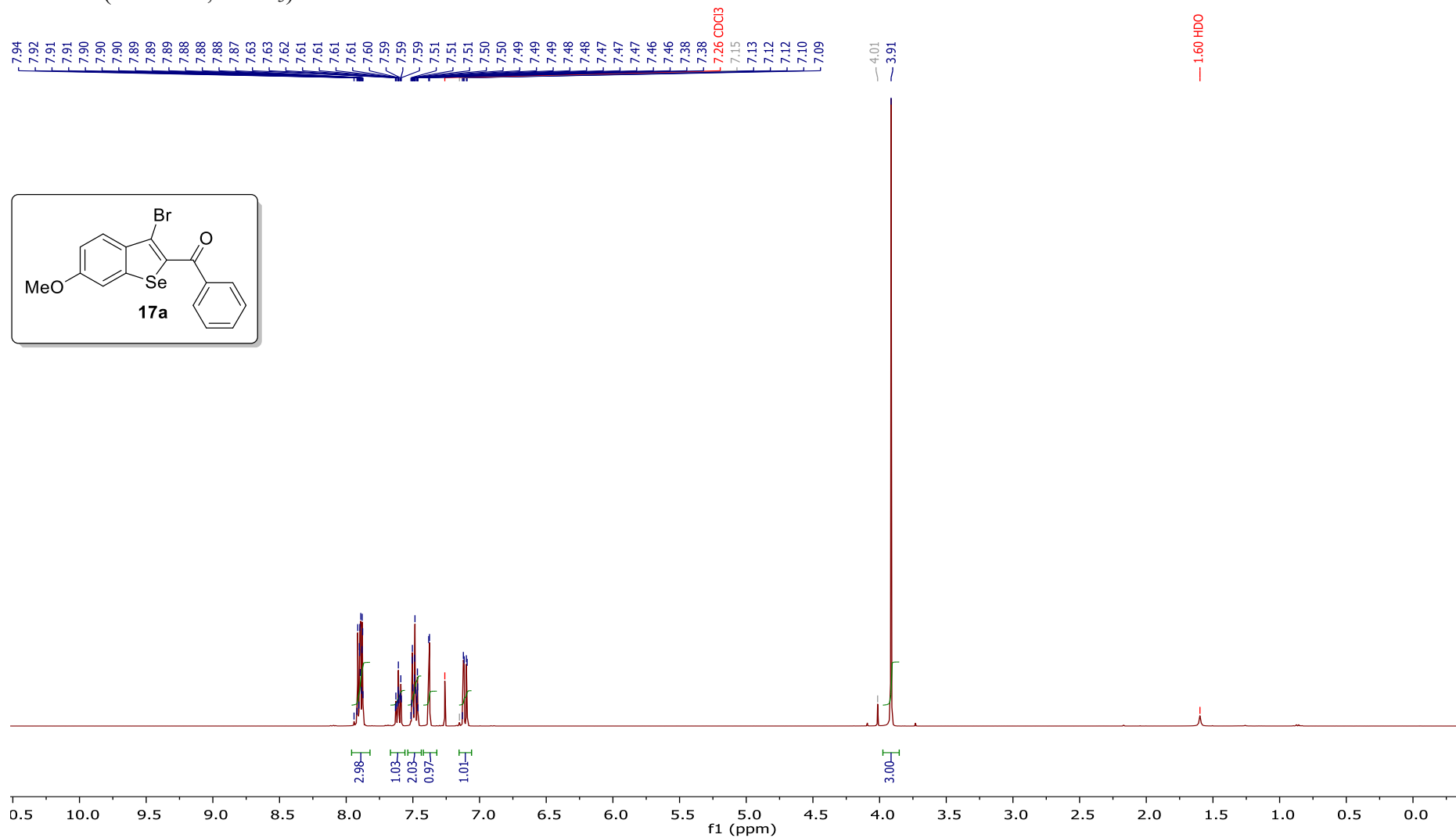
^1H NMR (400 MHz, CDCl_3):



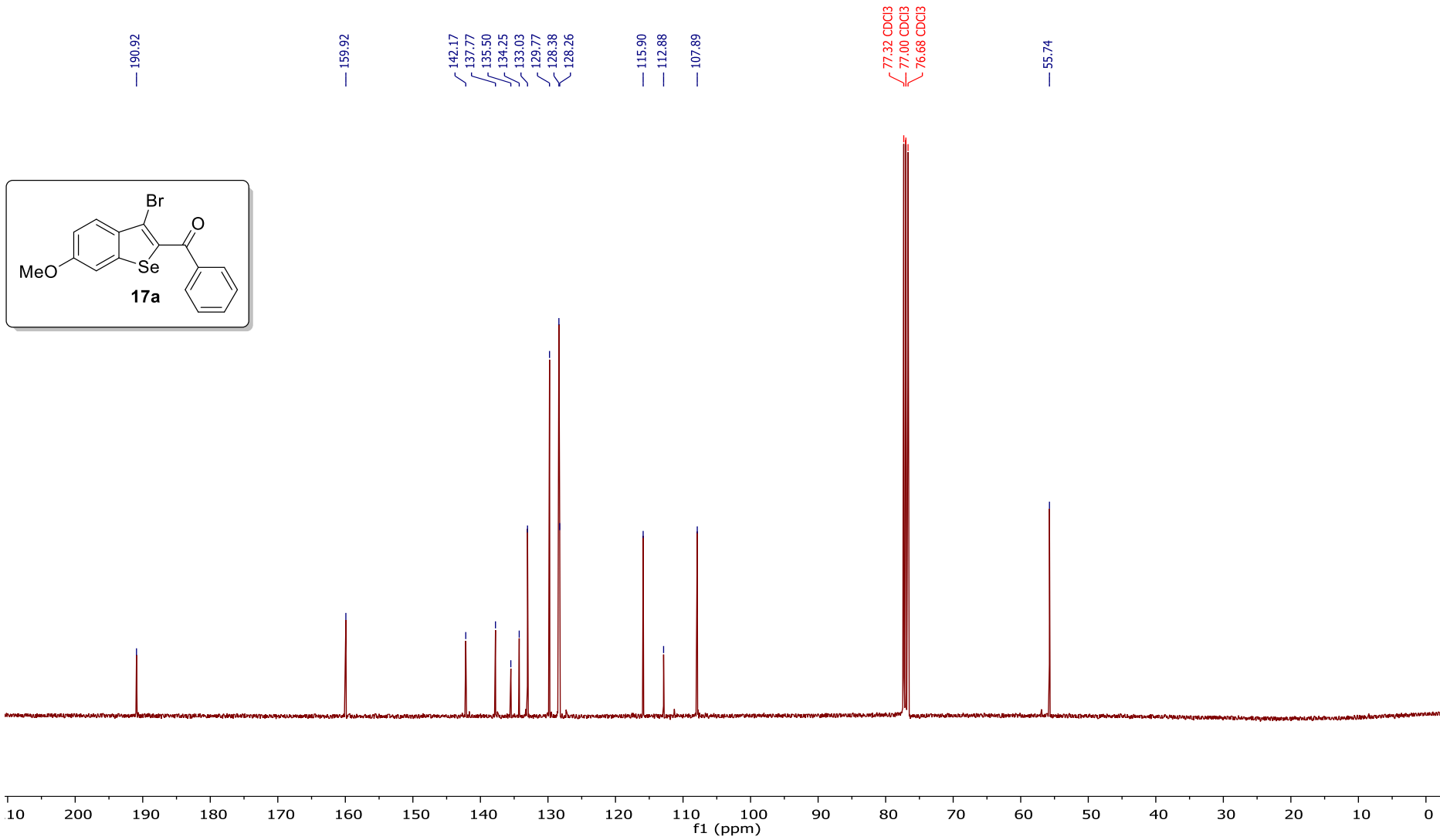
^{13}C NMR (100.6 MHz, CDCl_3):



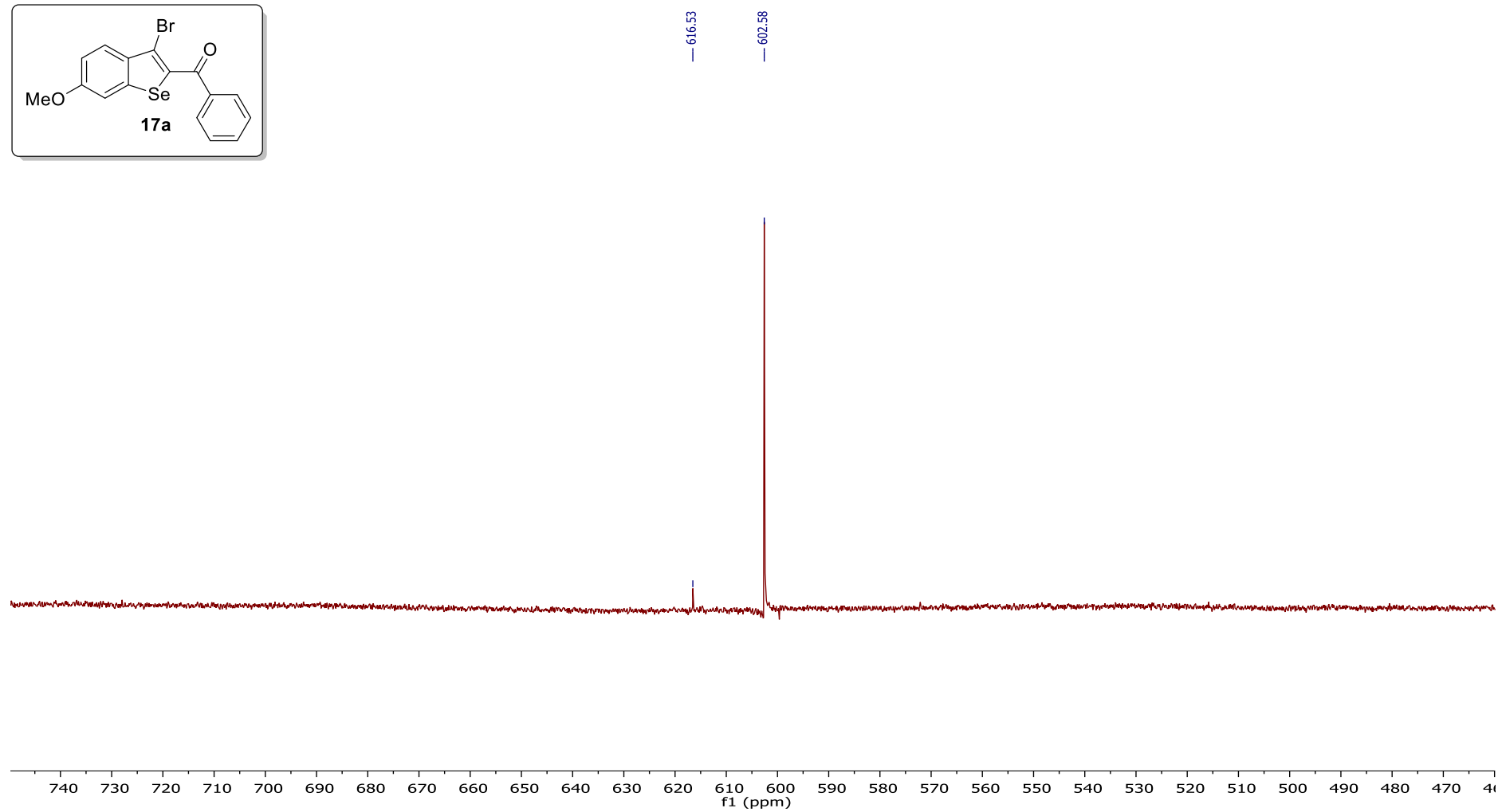
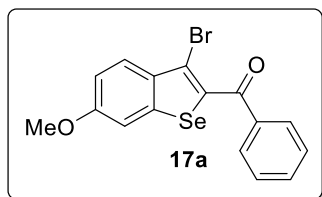
^1H NMR (400 MHz, CDCl_3):



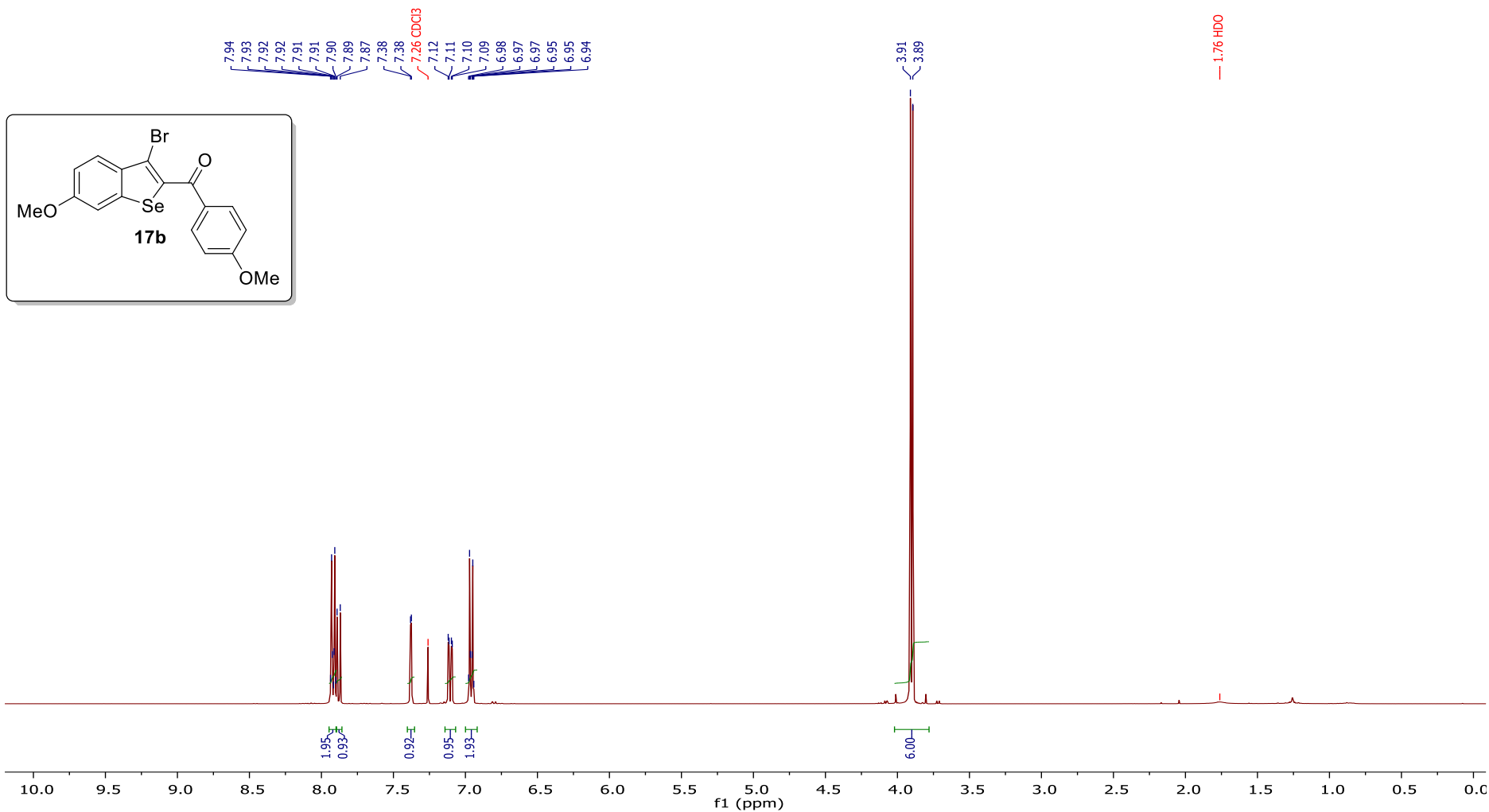
^{13}C NMR (100.6 MHz, CDCl_3):



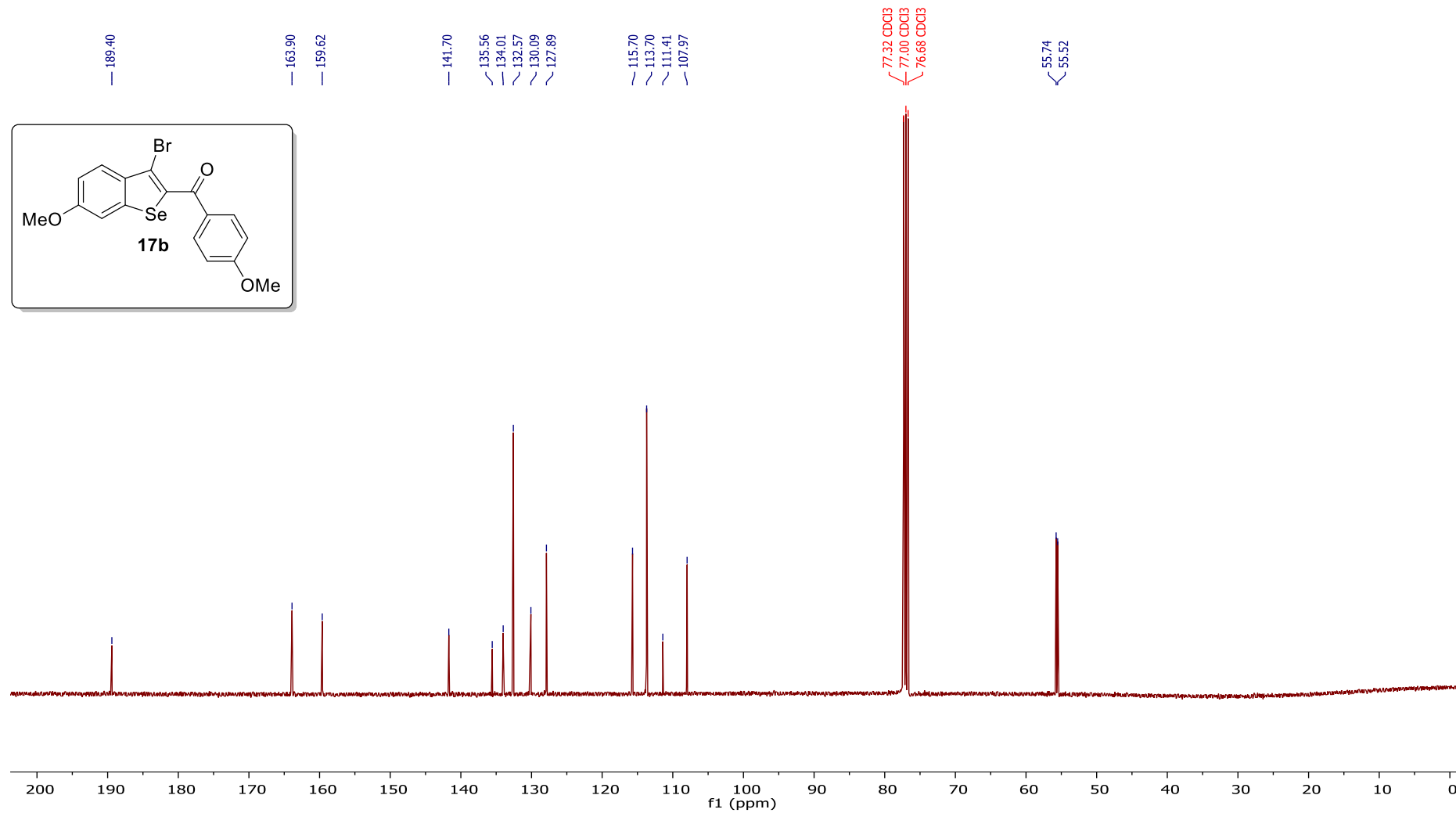
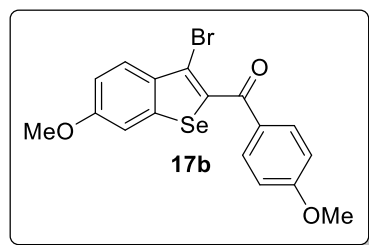
^{77}Se NMR (76.37 MHz, CDCl_3):



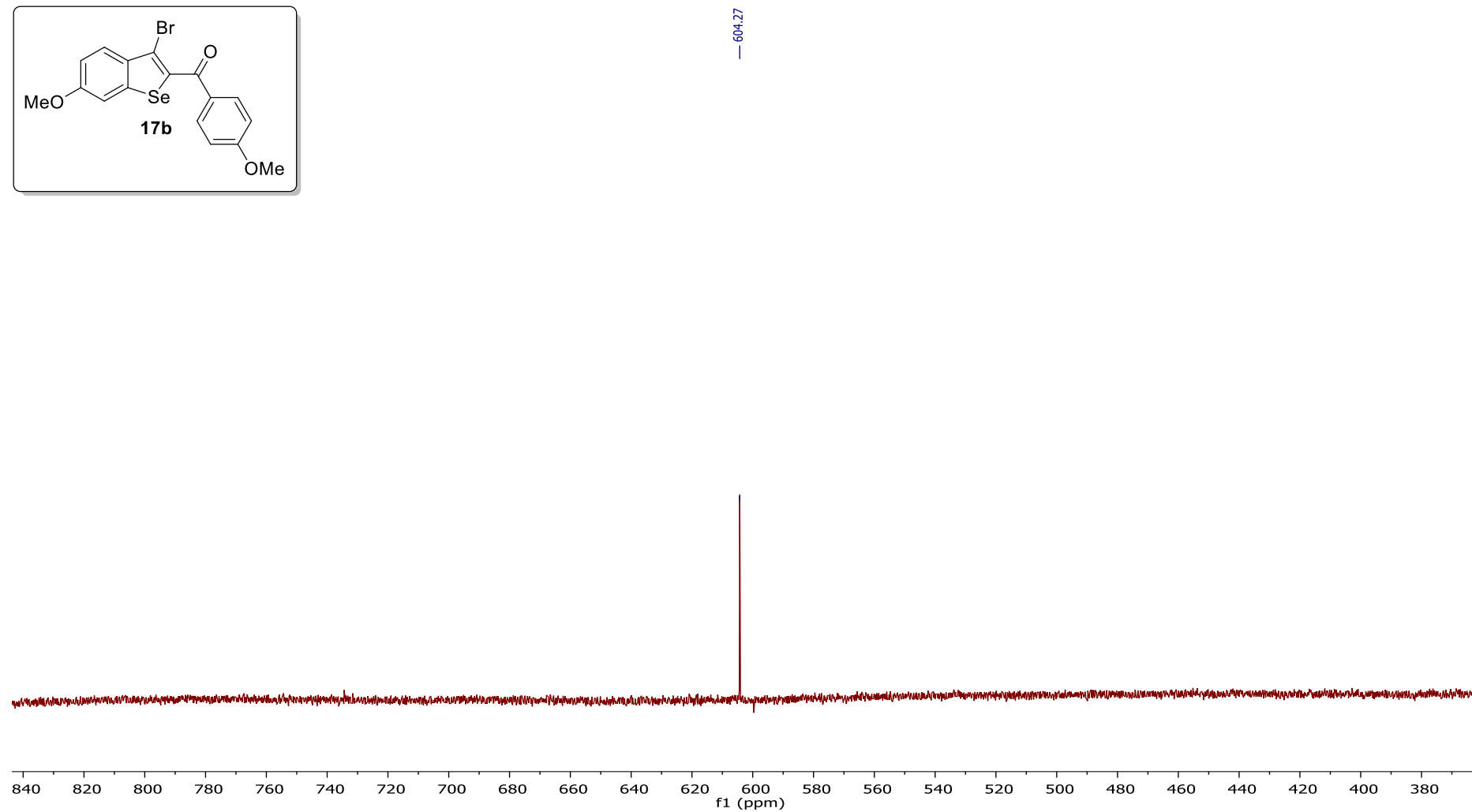
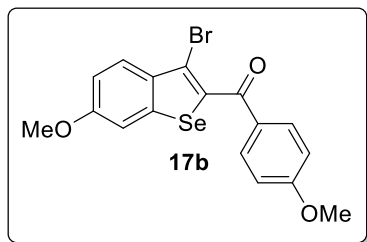
^1H NMR (400 MHz, CDCl_3):



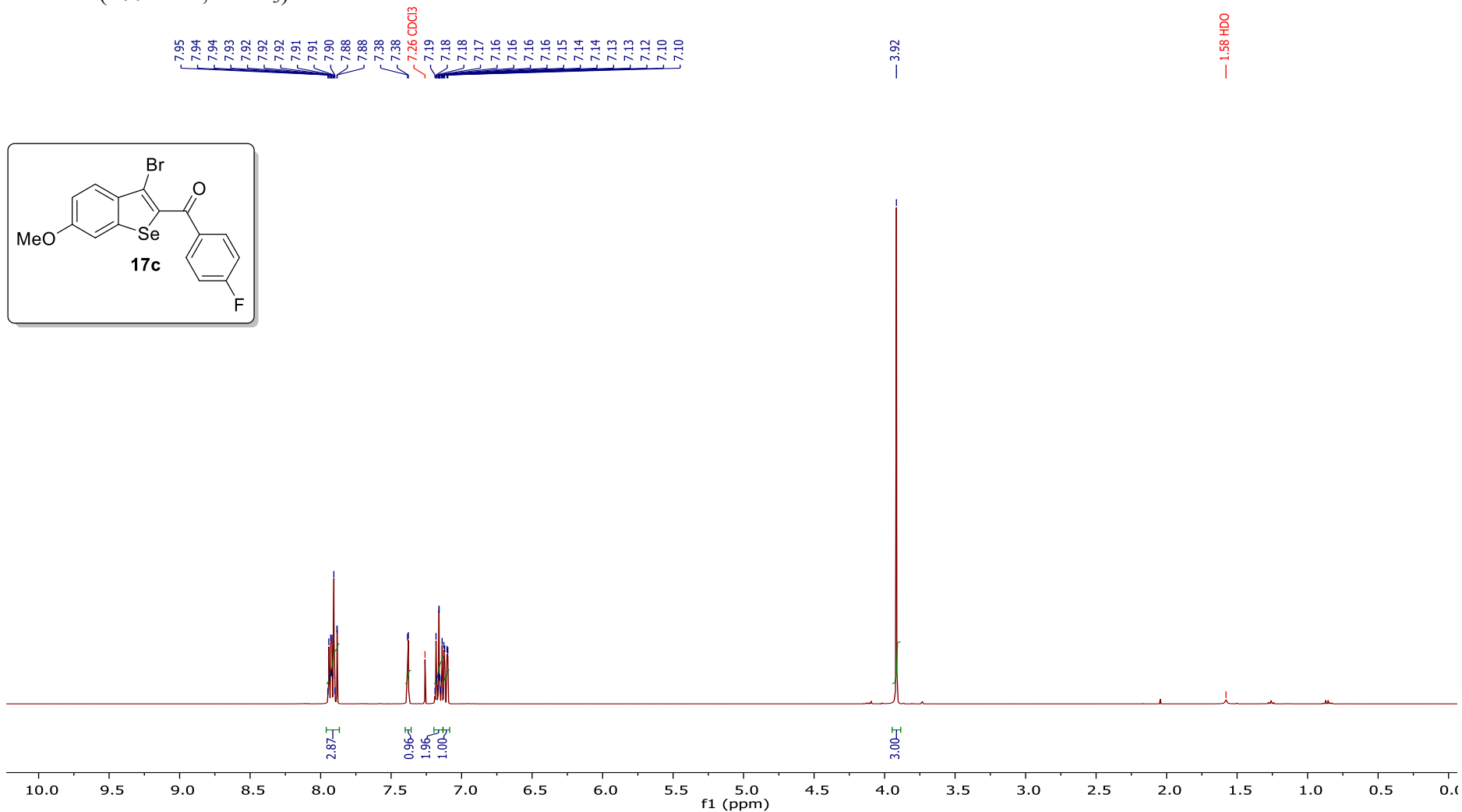
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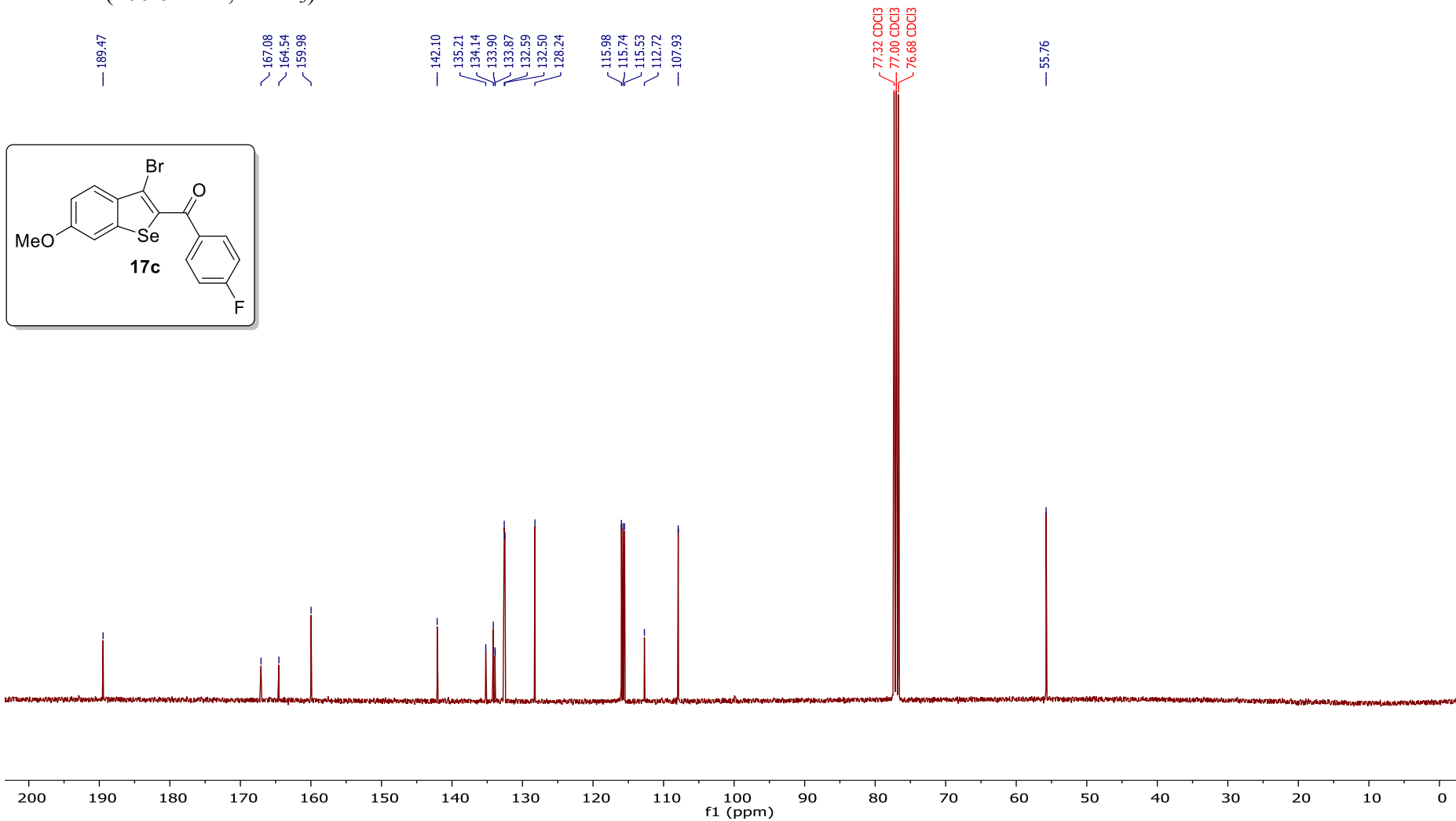
^{77}Se NMR (76.37 MHz, CDCl_3):



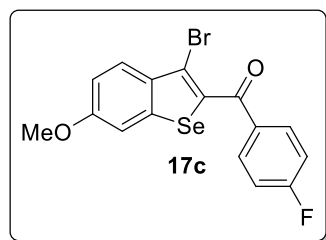
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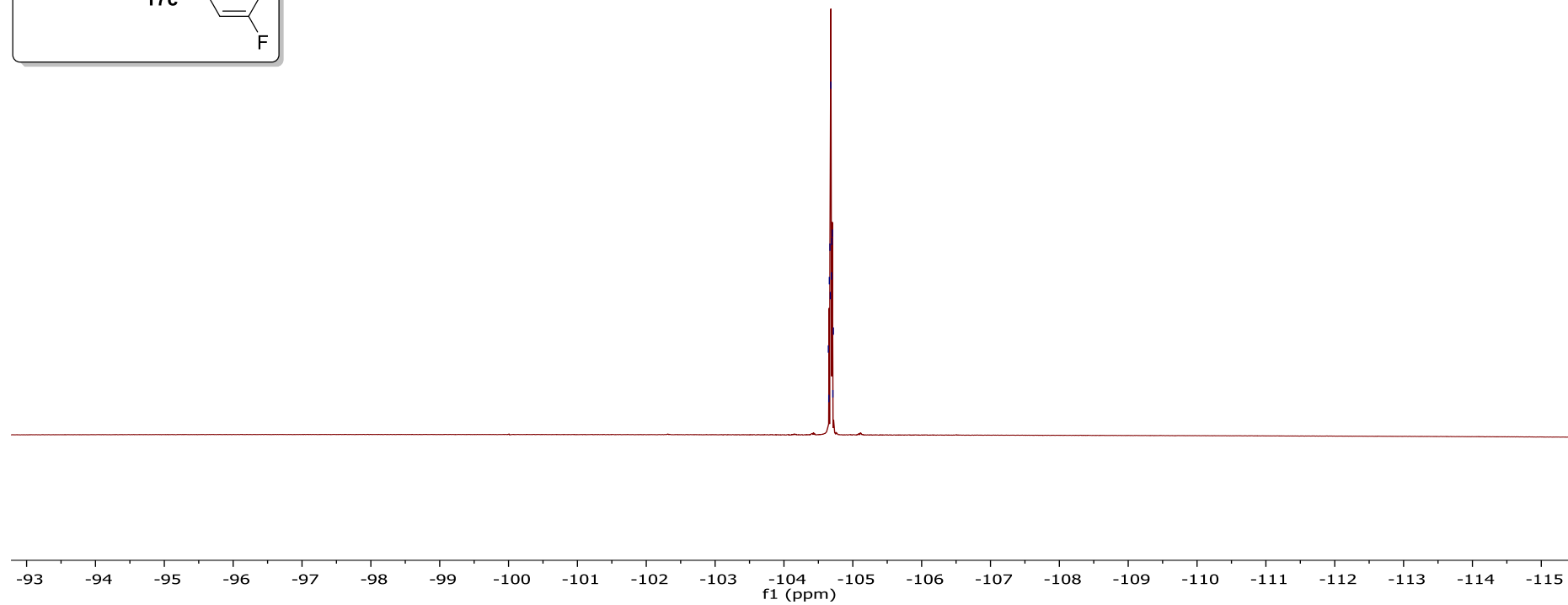
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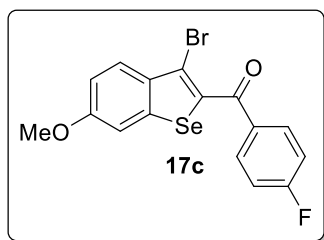
^{19}F NMR (376.21 MHz, CDCl_3):



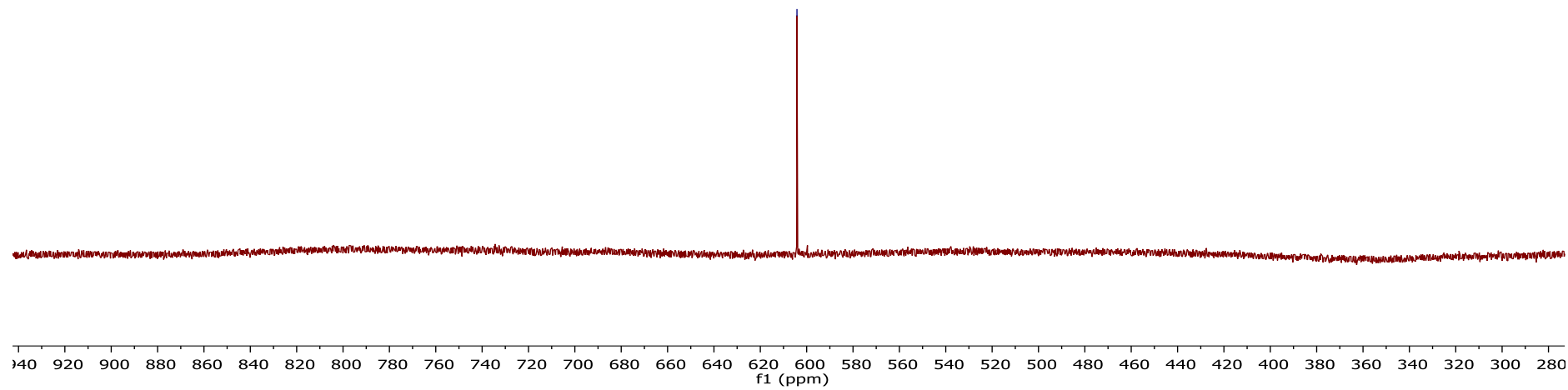
-104.64
-104.65
-104.66
-104.67
-104.68
-104.69
-104.70
-104.71
-104.72



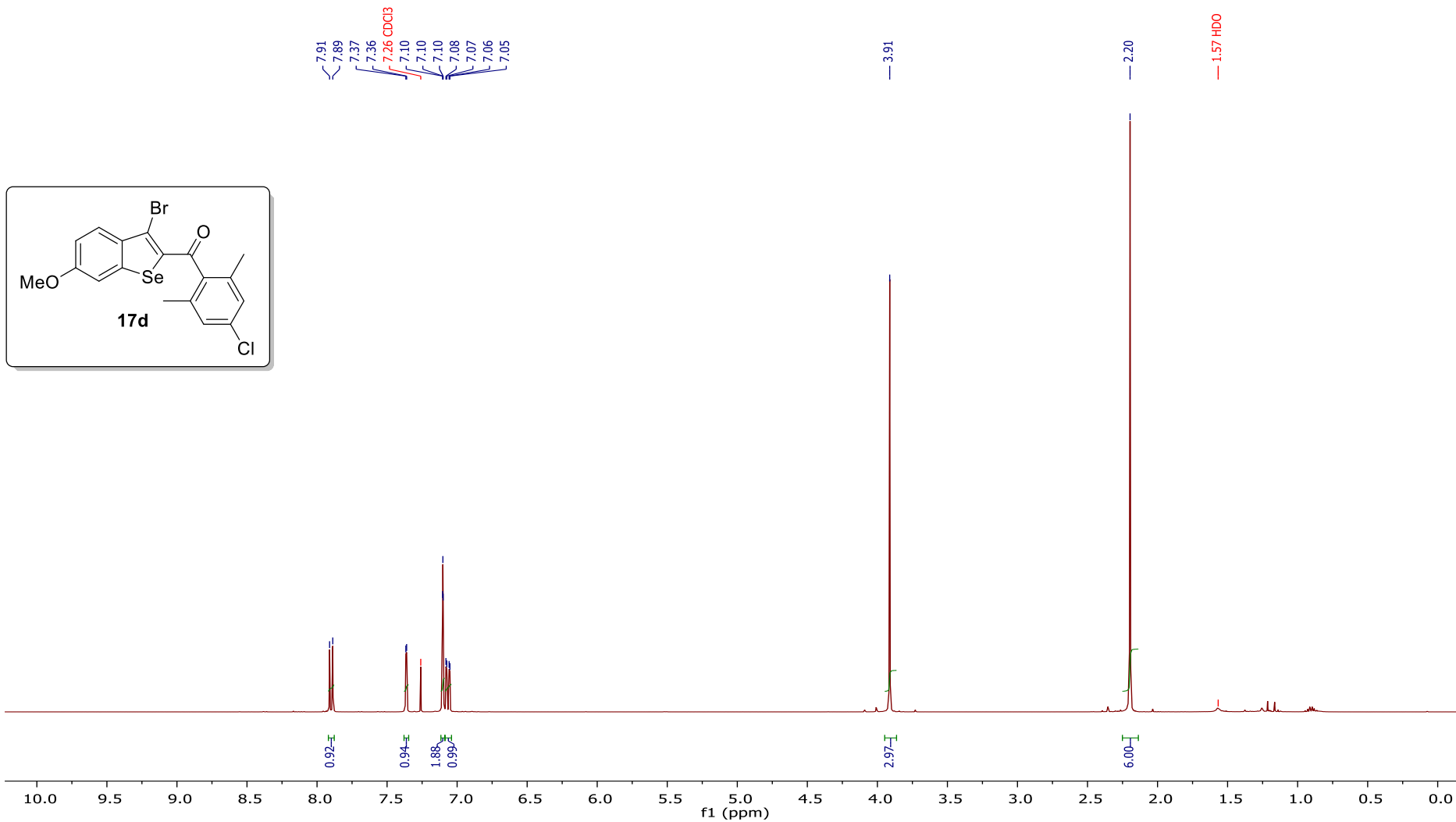
^{77}Se NMR (76.37 MHz, CDCl_3):



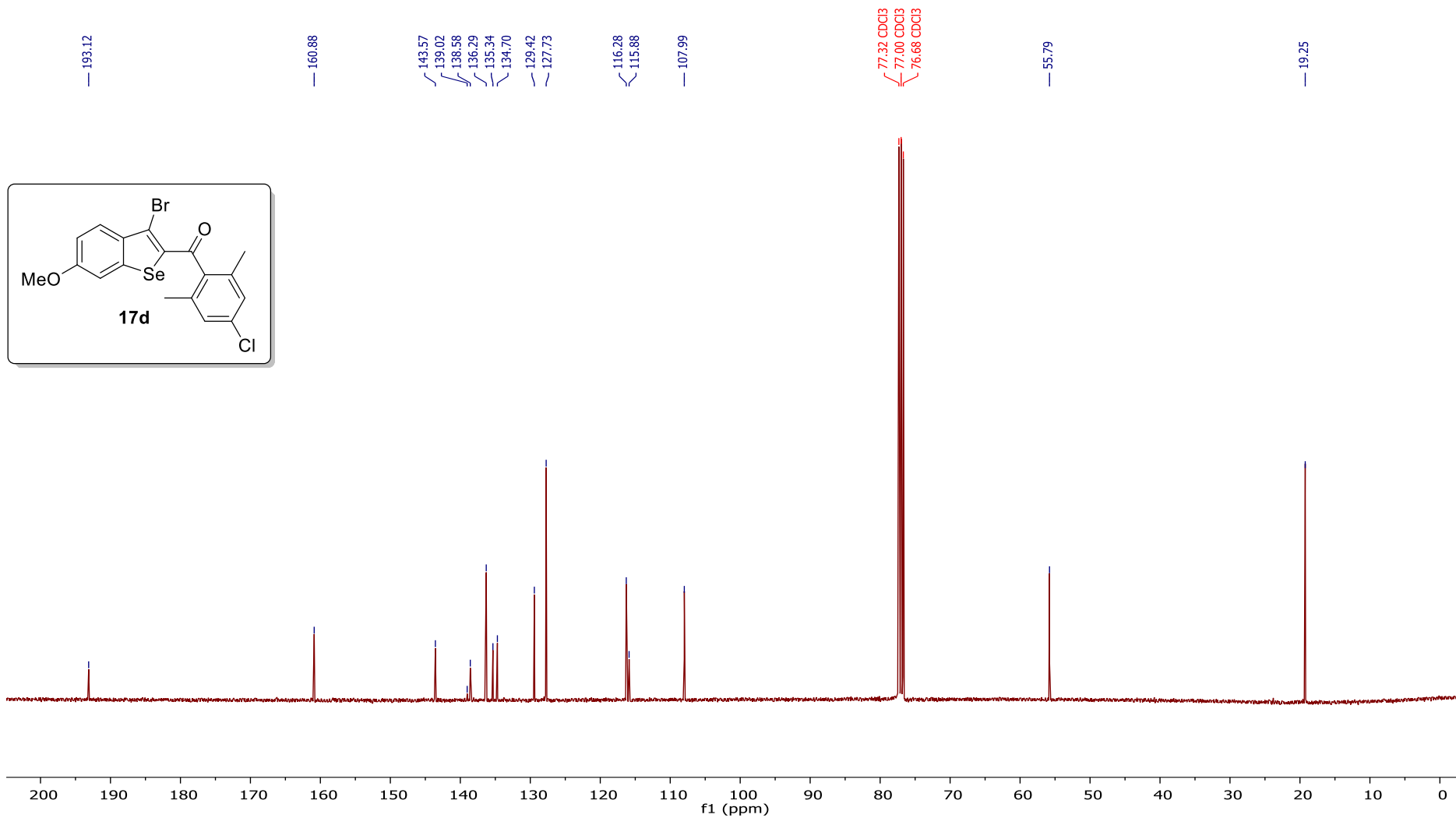
— 604.19



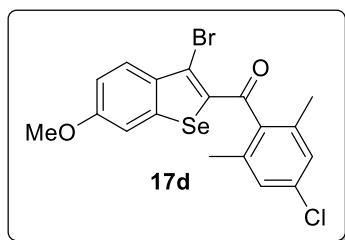
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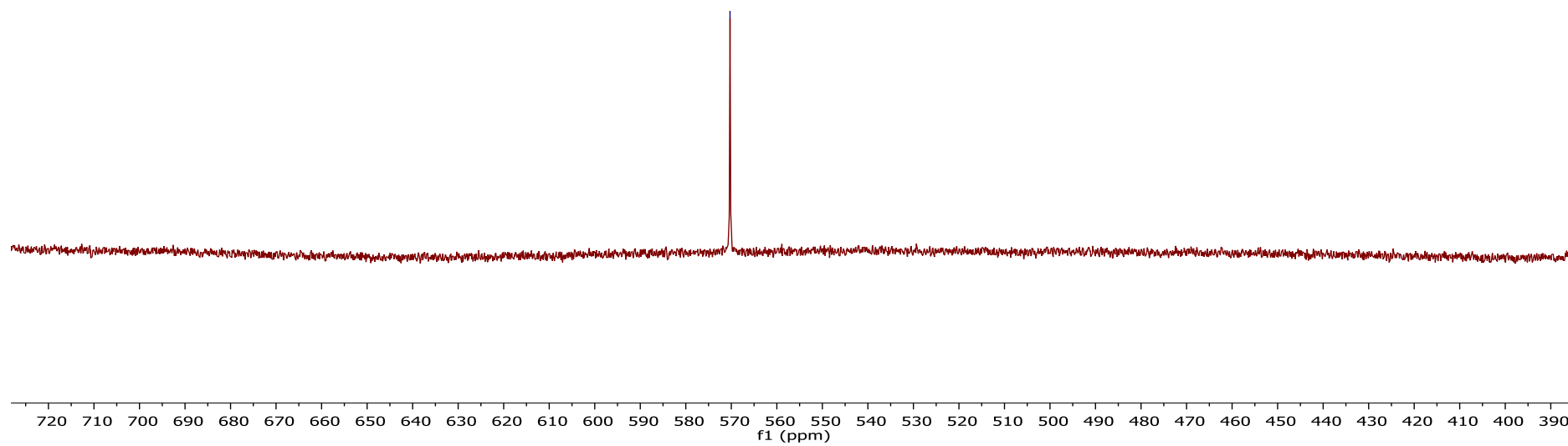
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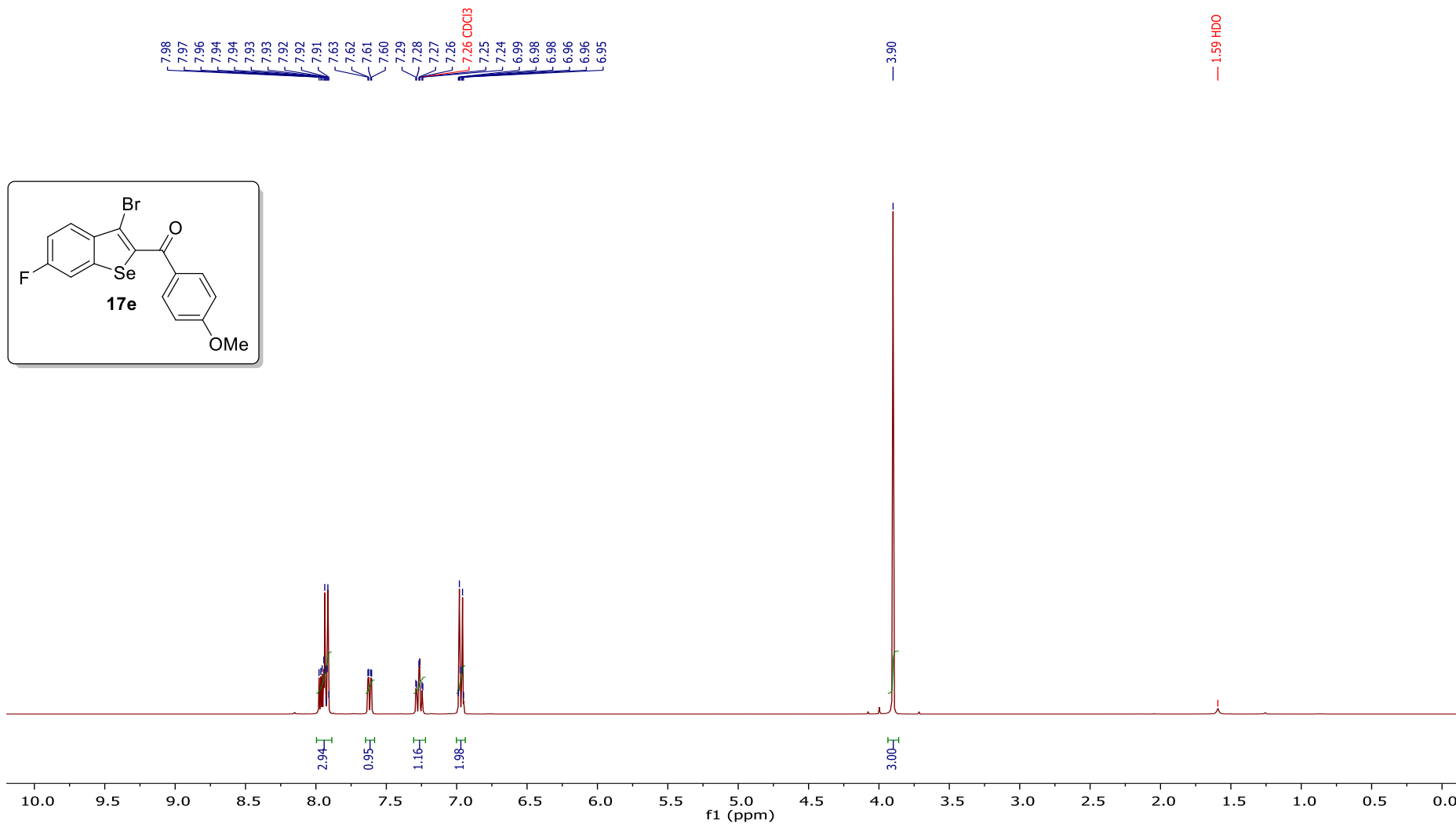
^{77}Se NMR (76.37 MHz, CDCl_3):



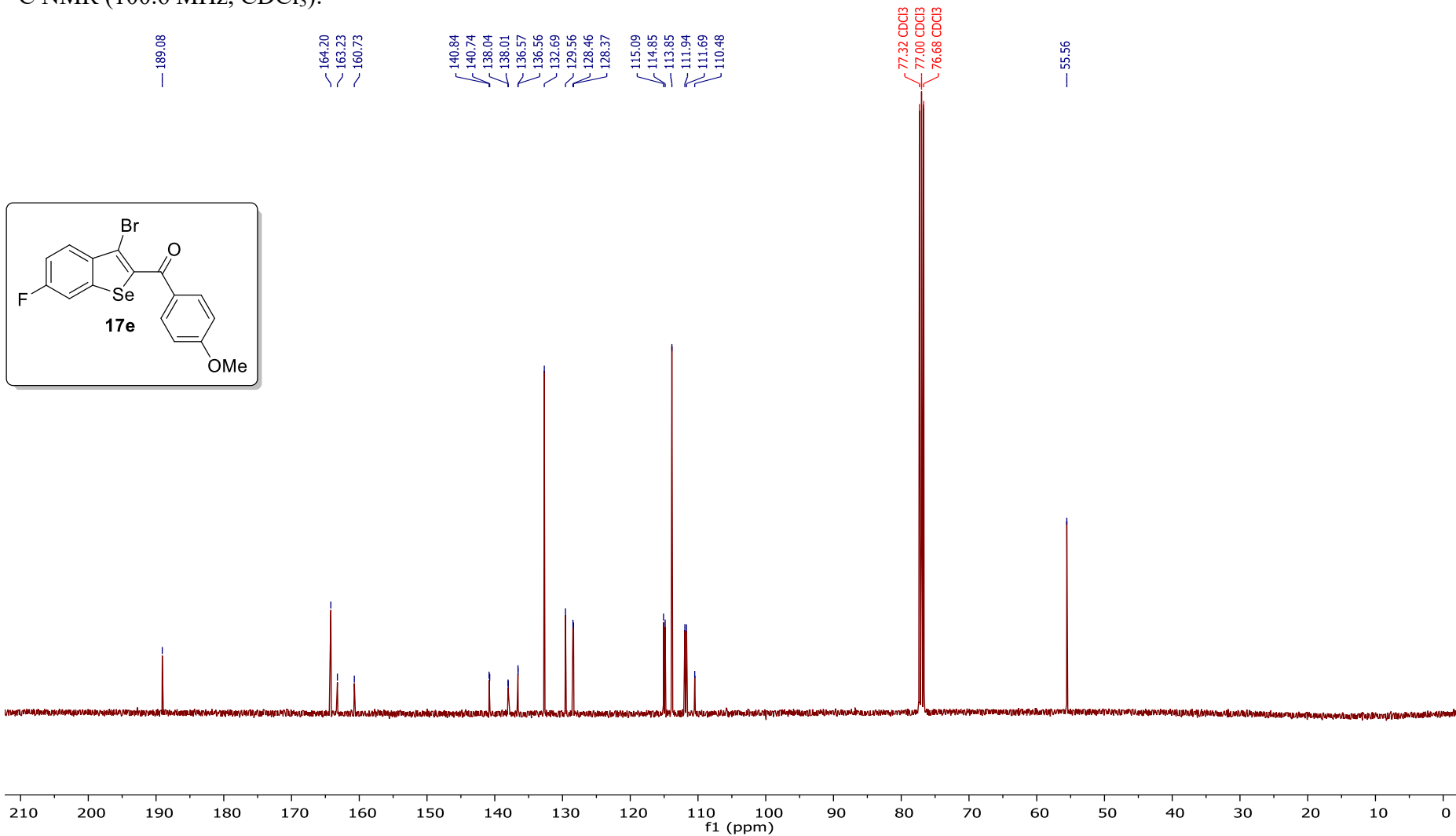
— 570.29



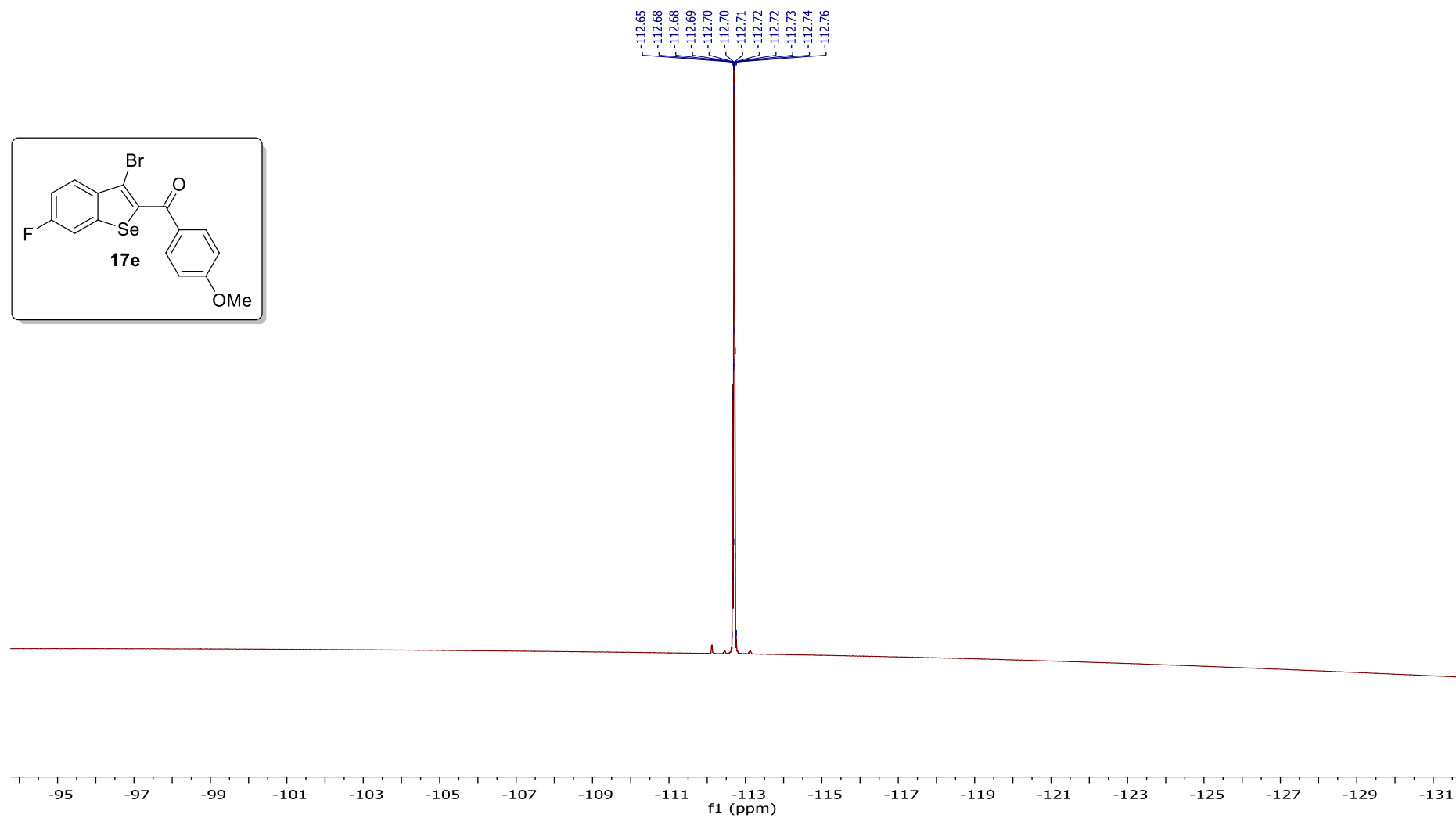
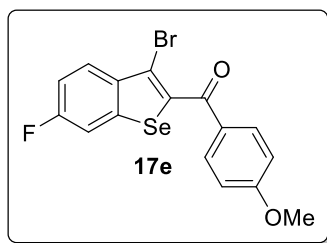
^1H NMR (400 MHz, CDCl_3):



^{13}C NMR (100.6 MHz, CDCl_3):

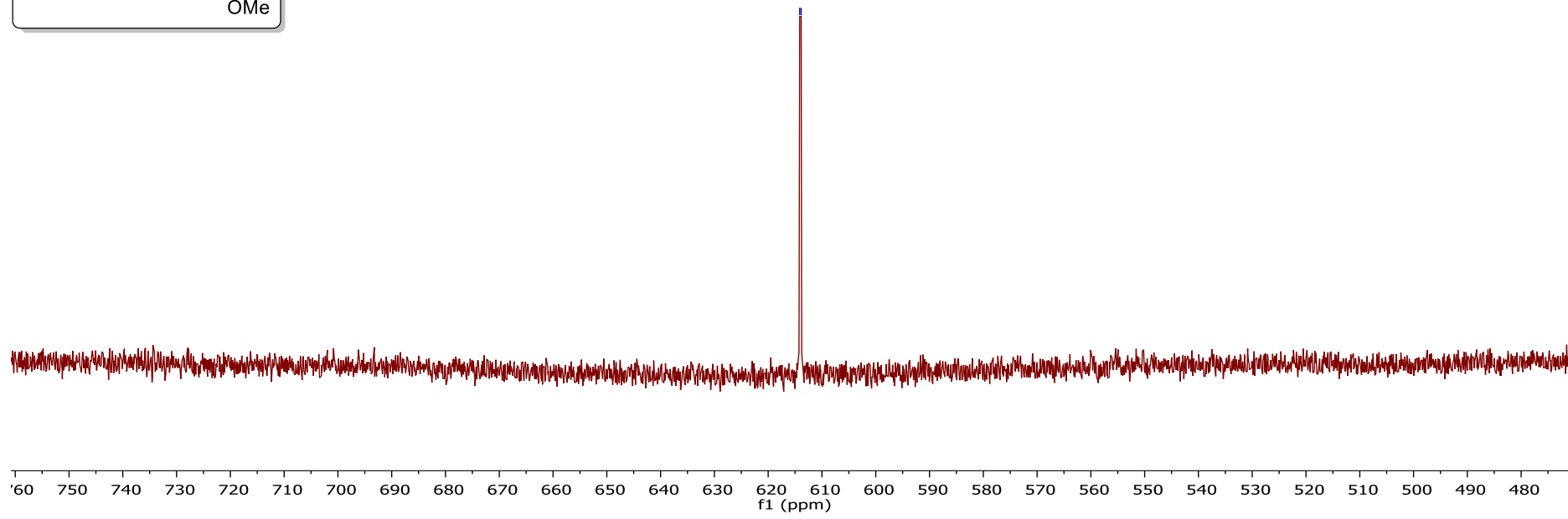
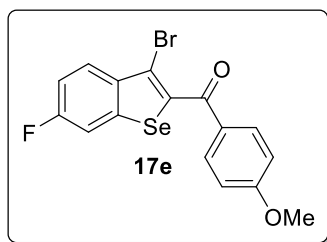


^{19}F NMR (376.21 MHz, CDCl_3):

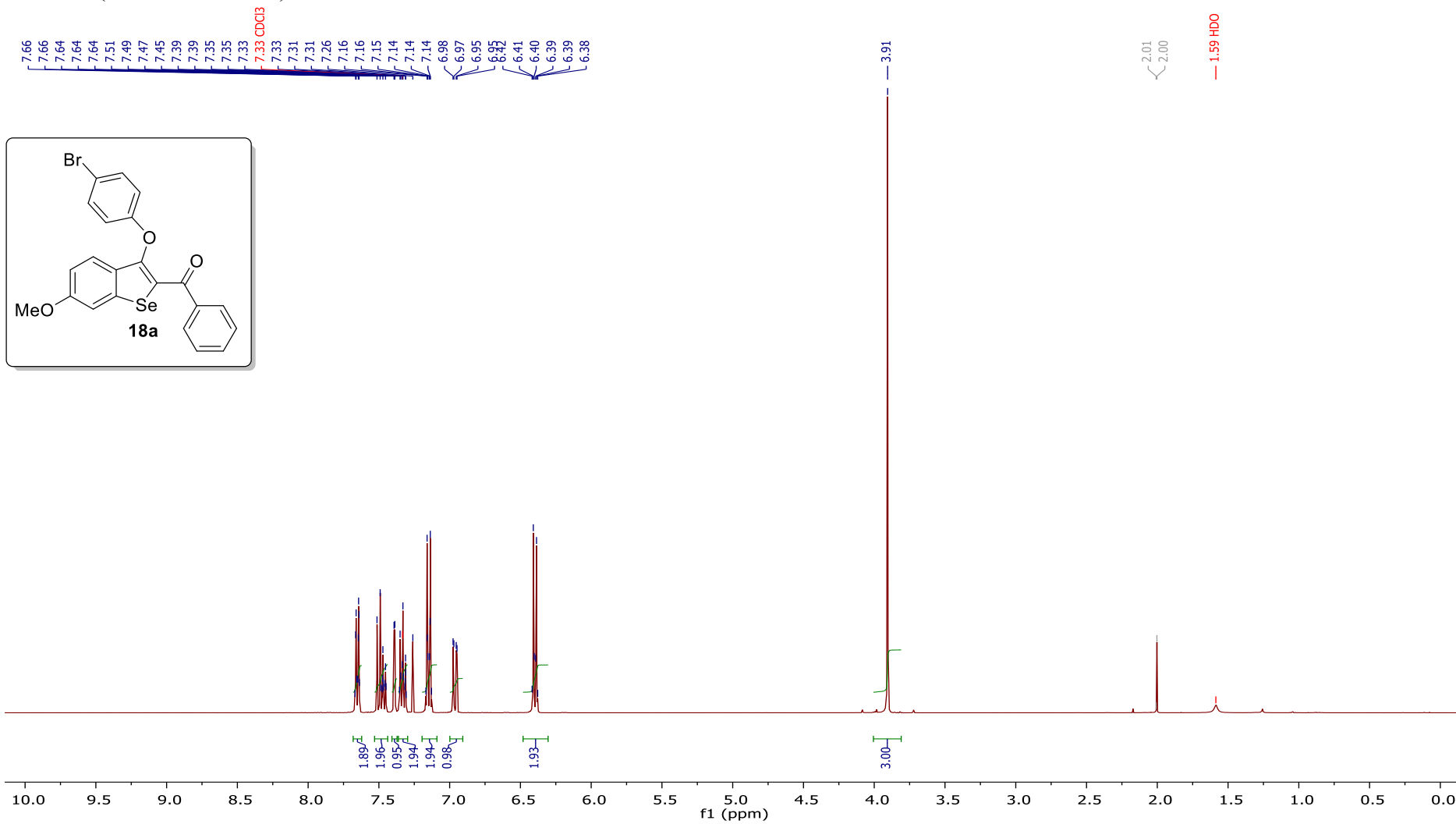


^{77}Se NMR (76.37 MHz, CDCl_3):

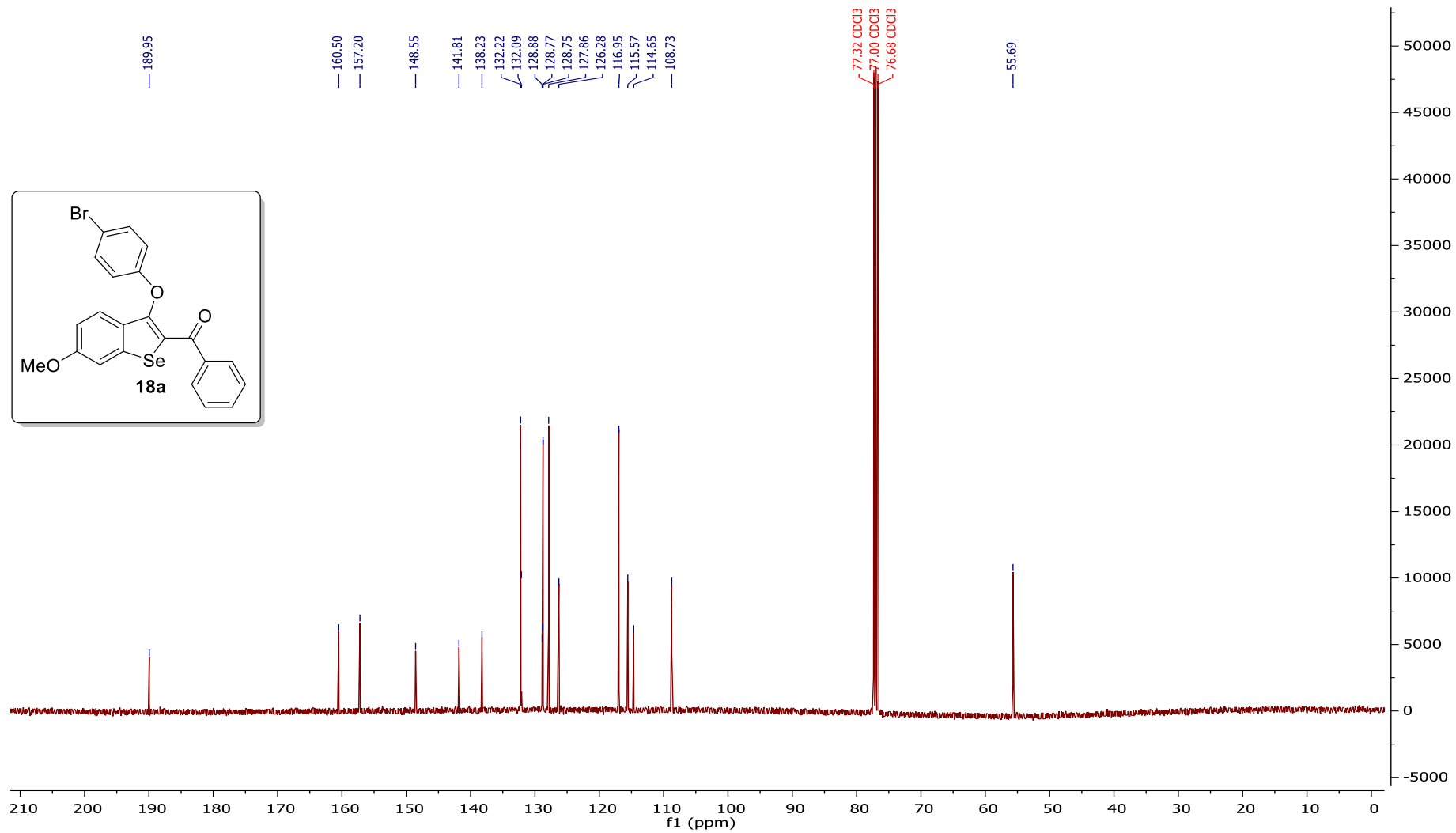
614.14
613.87



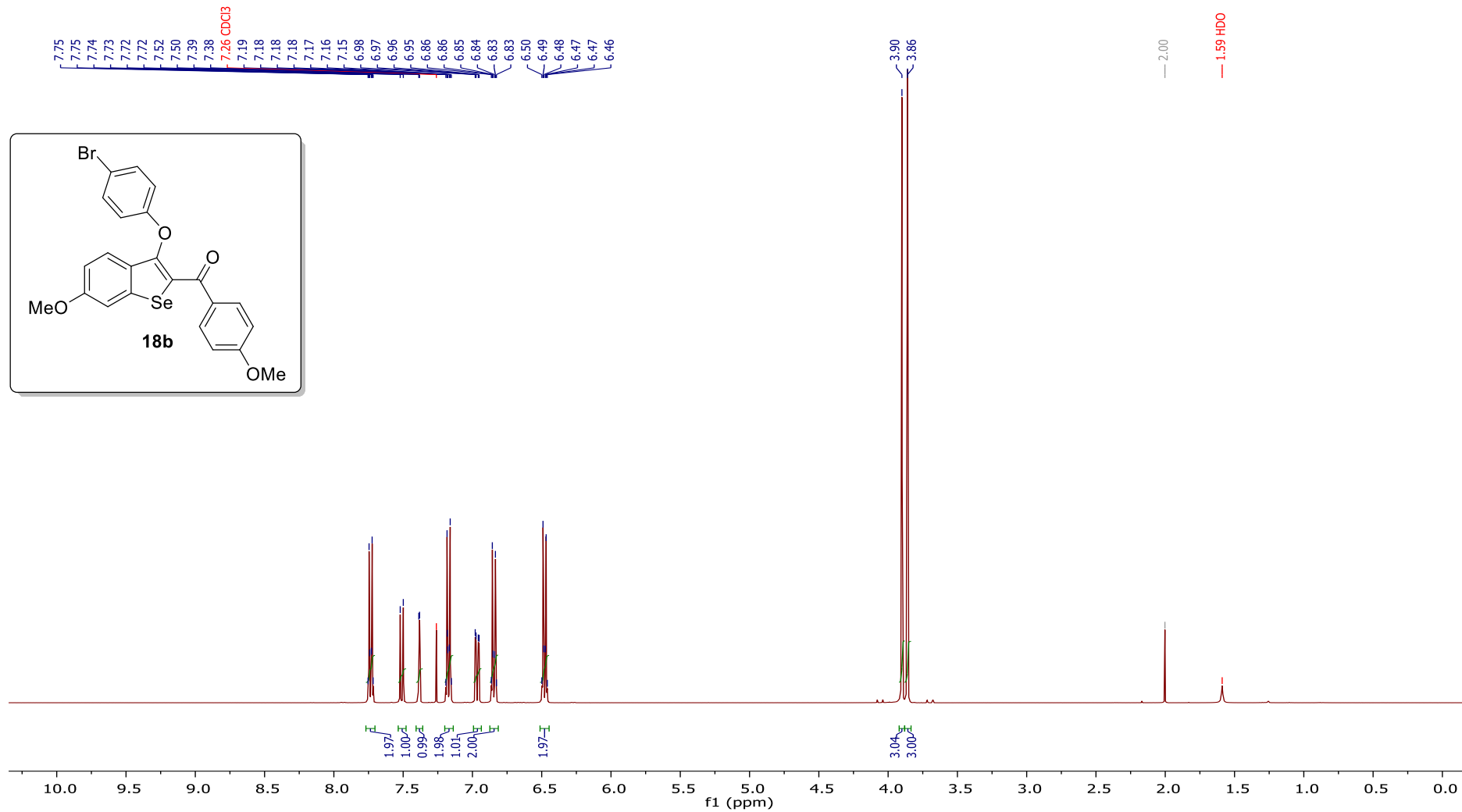
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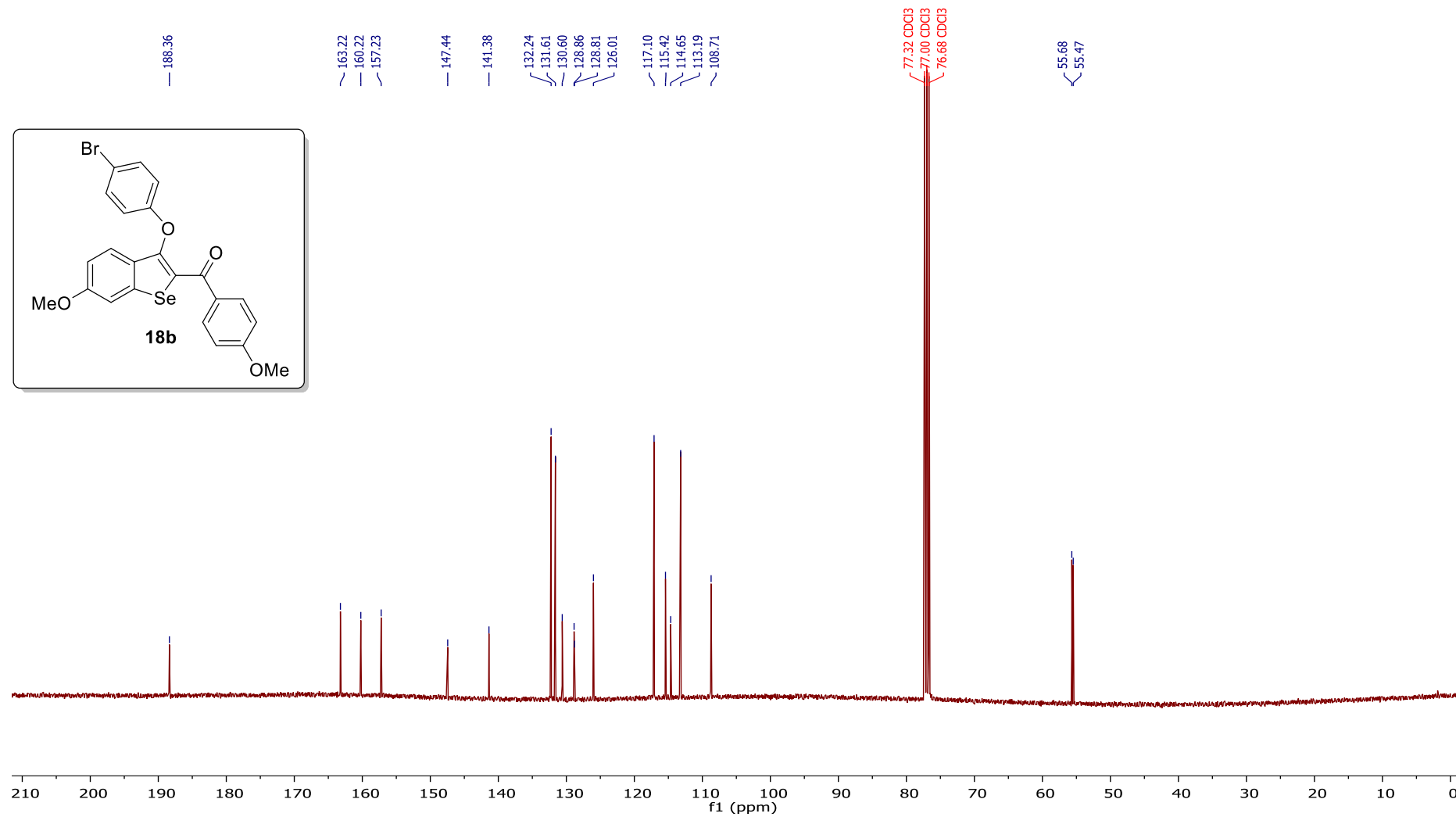
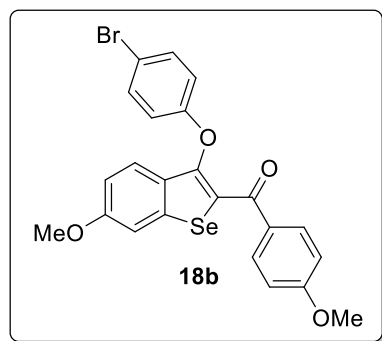
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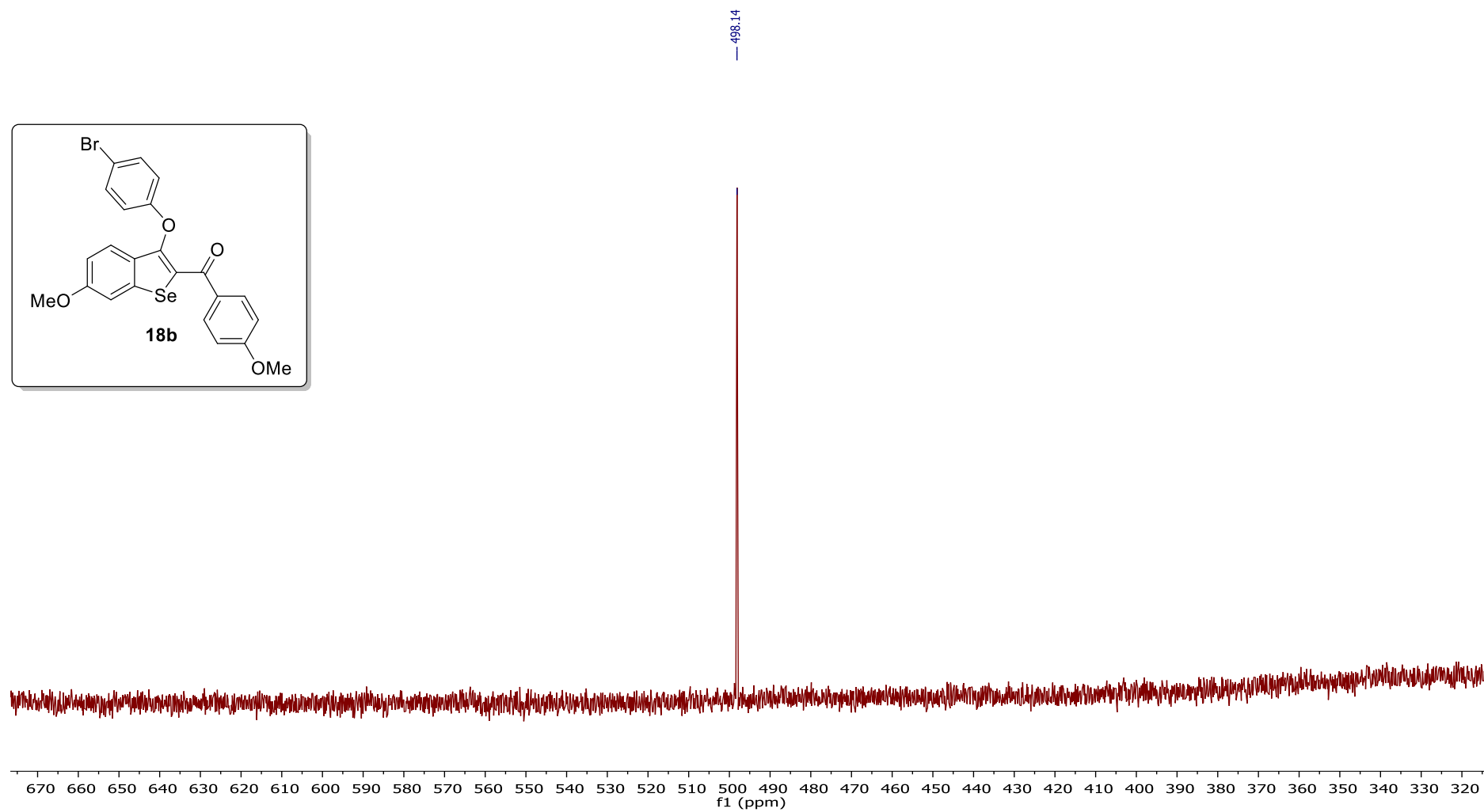
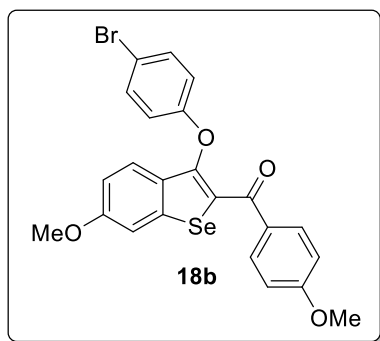
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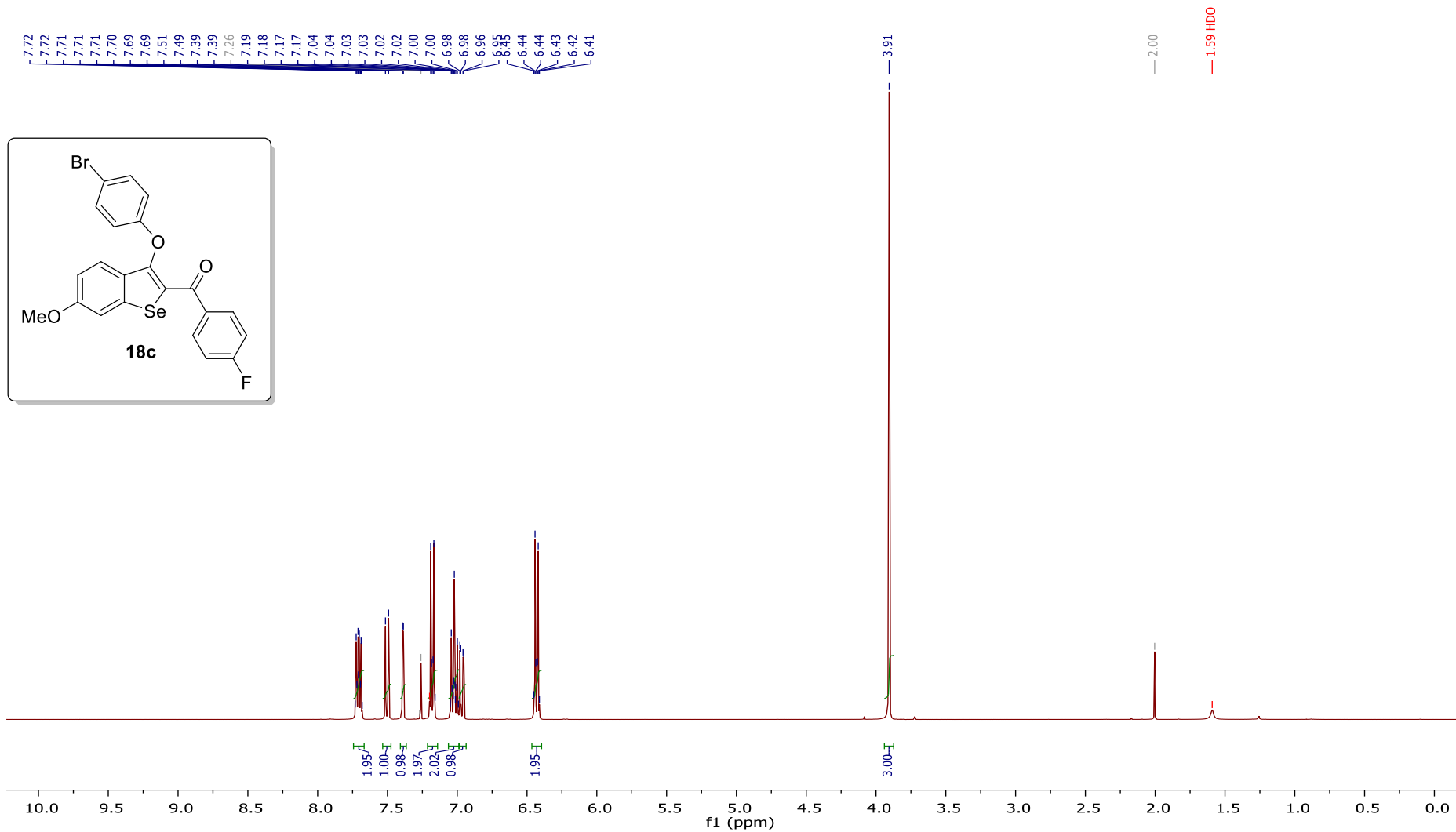
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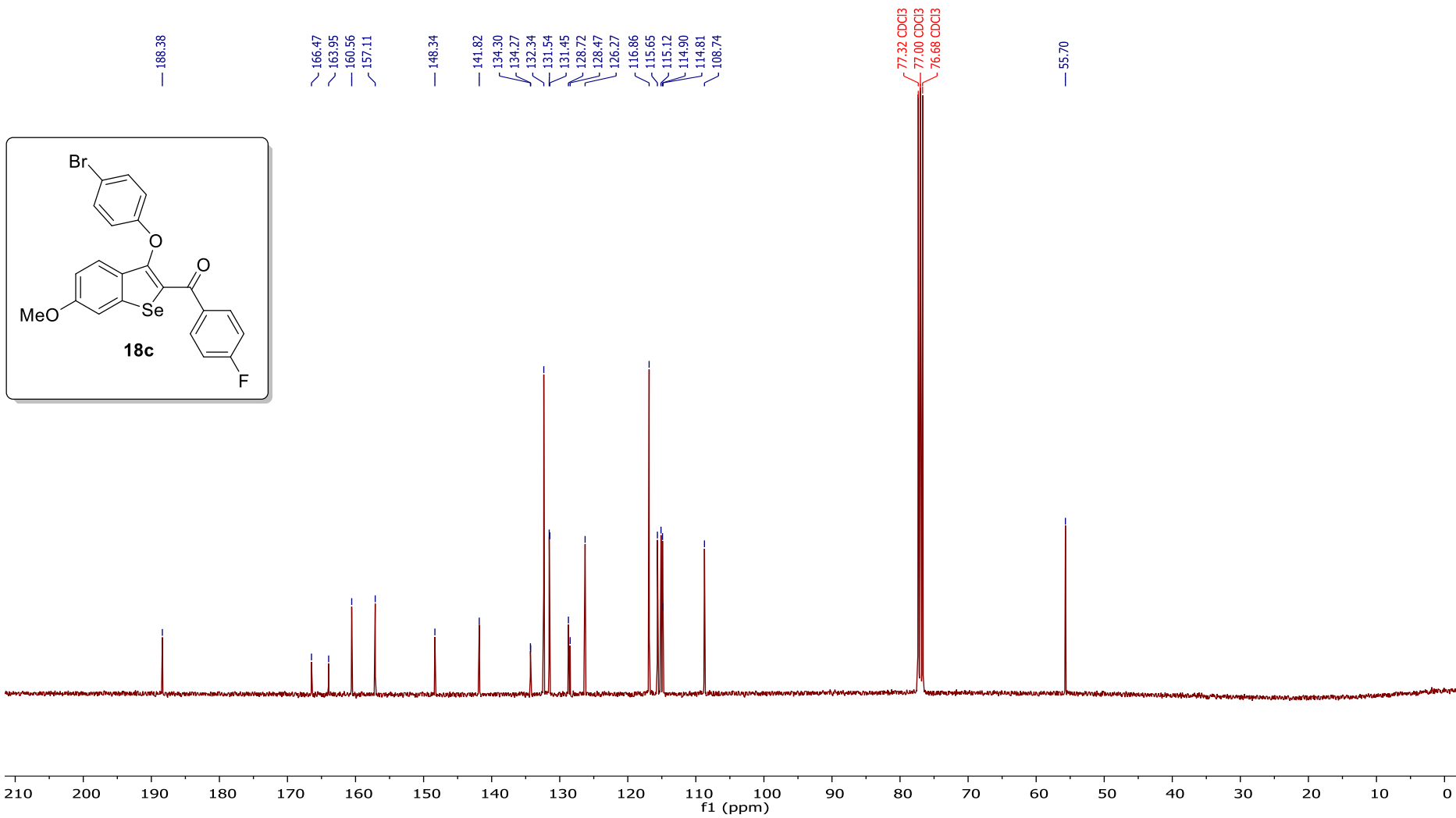
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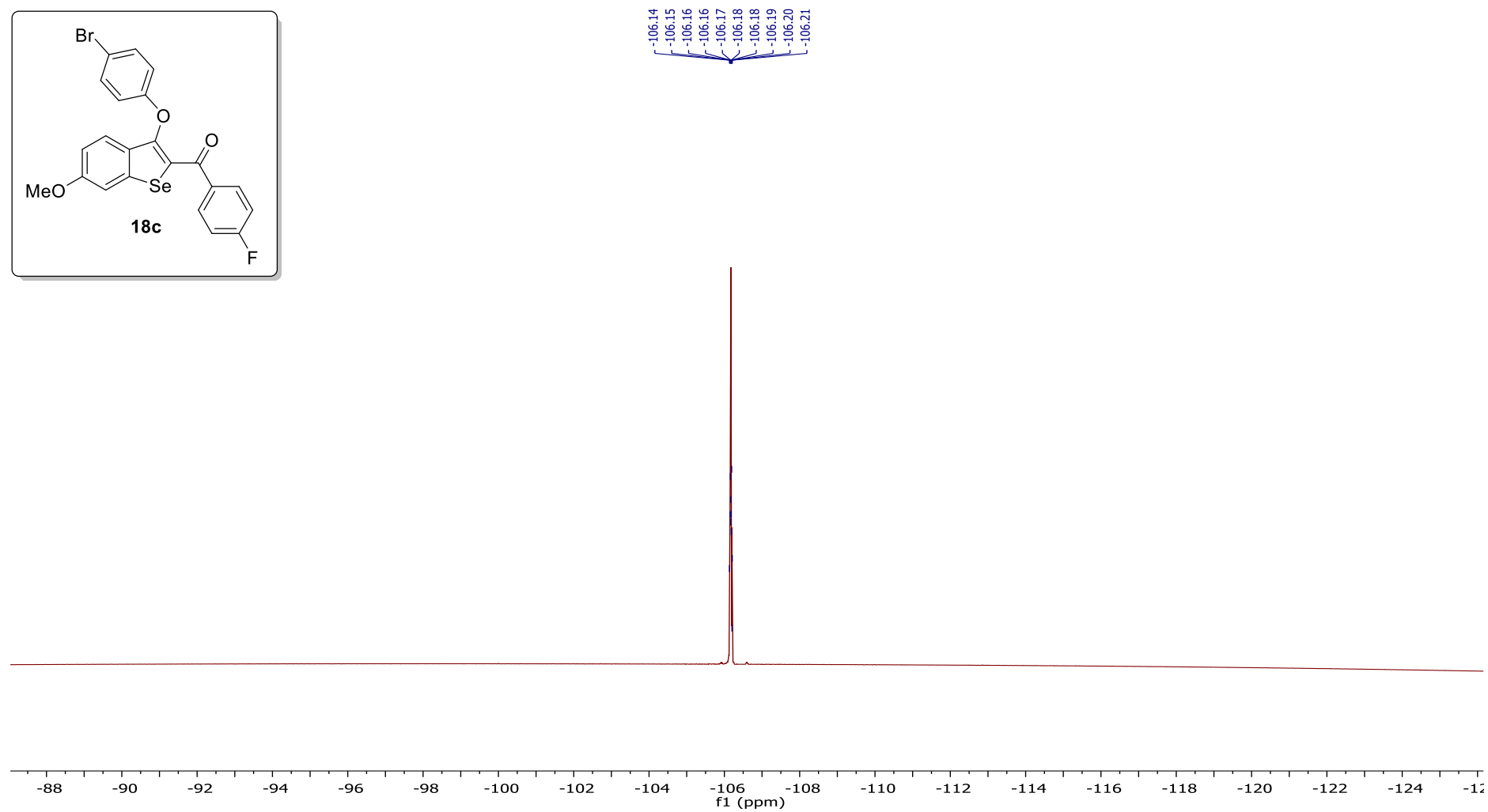
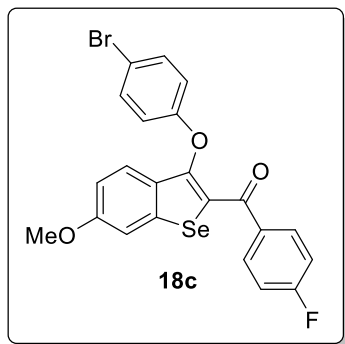
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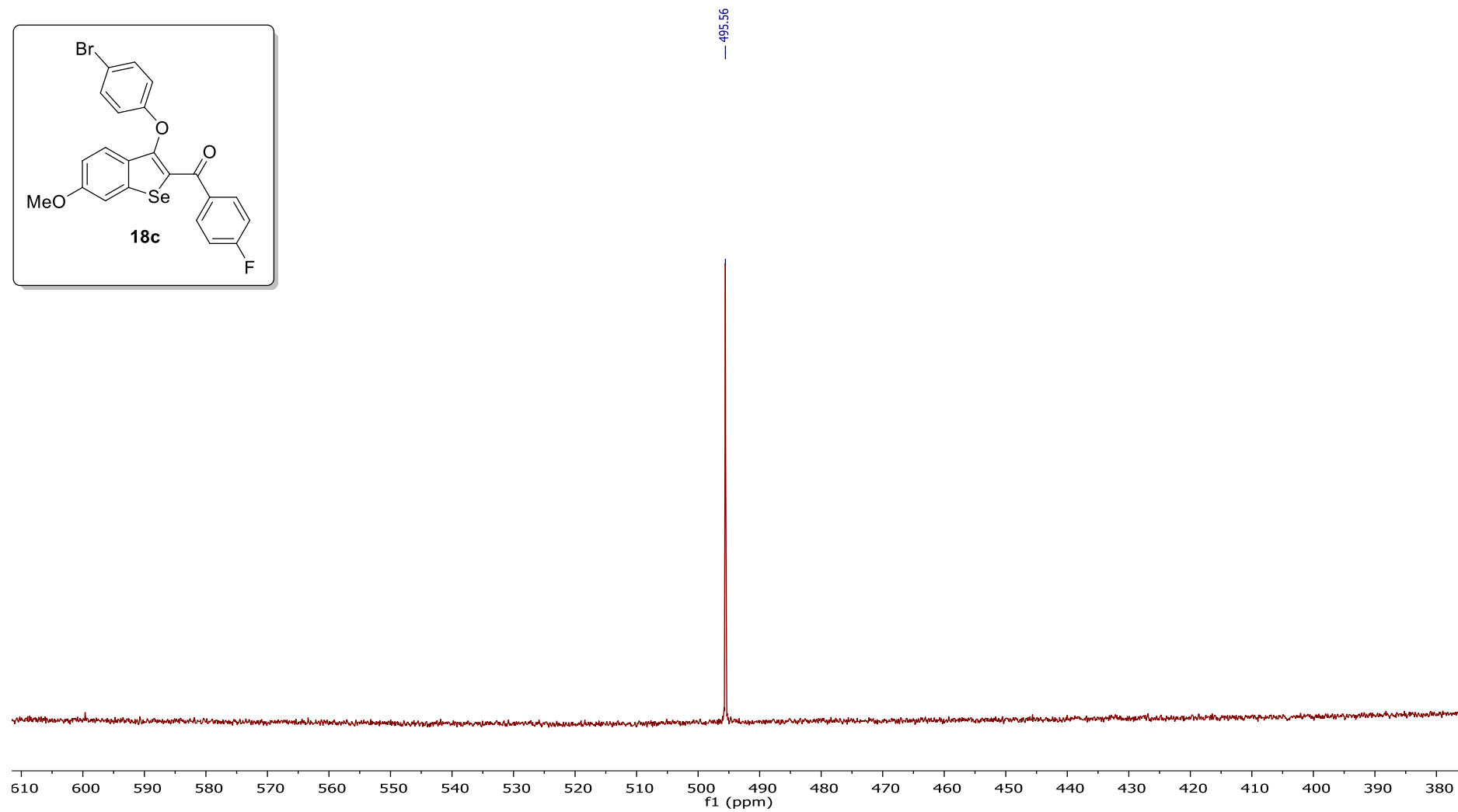
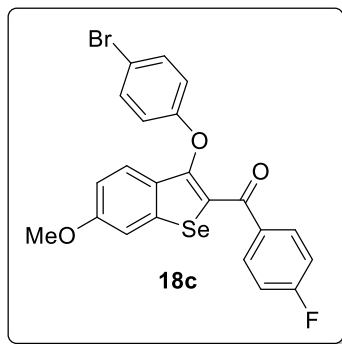
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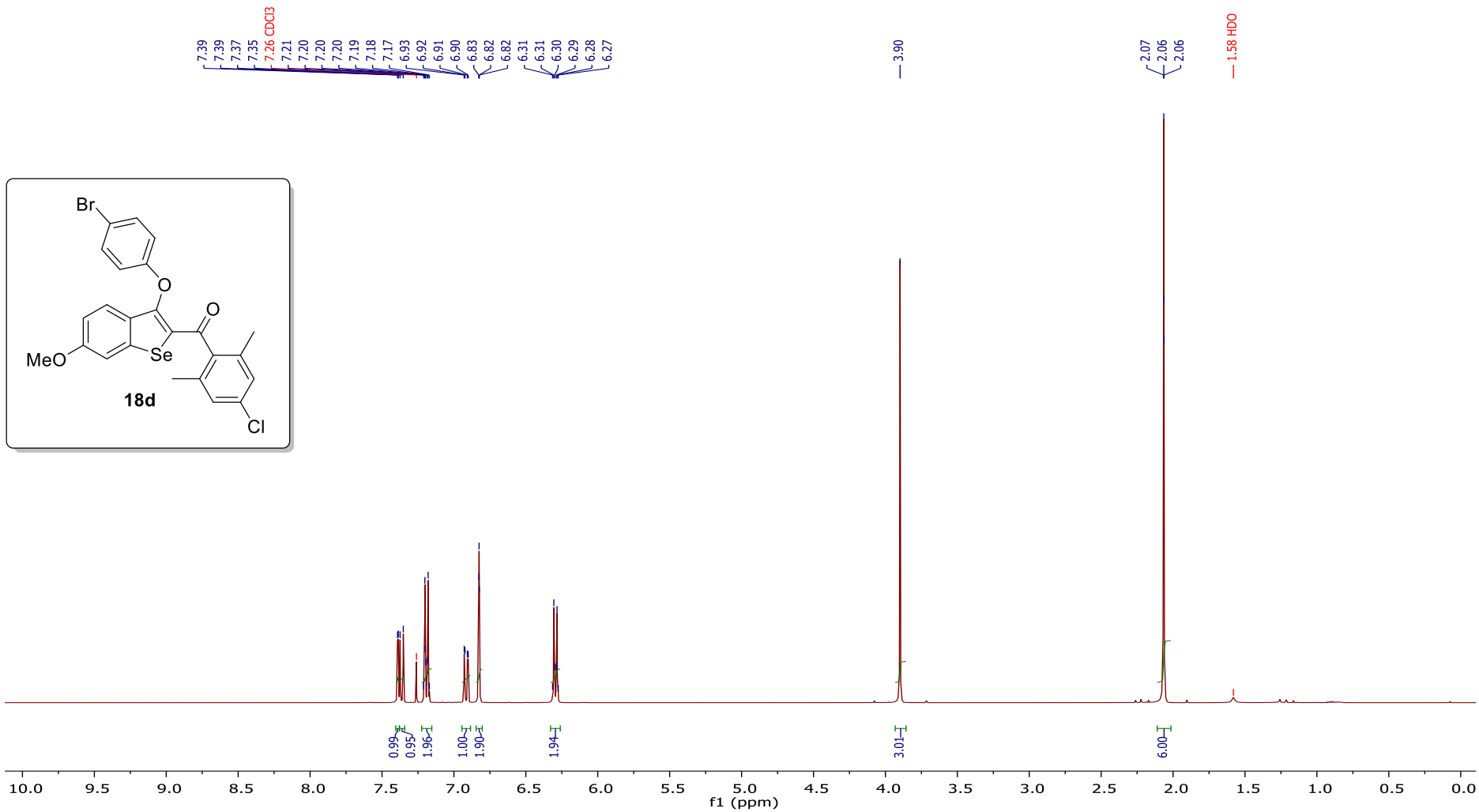
^{19}F NMR (376.21 MHz, CDCl_3):



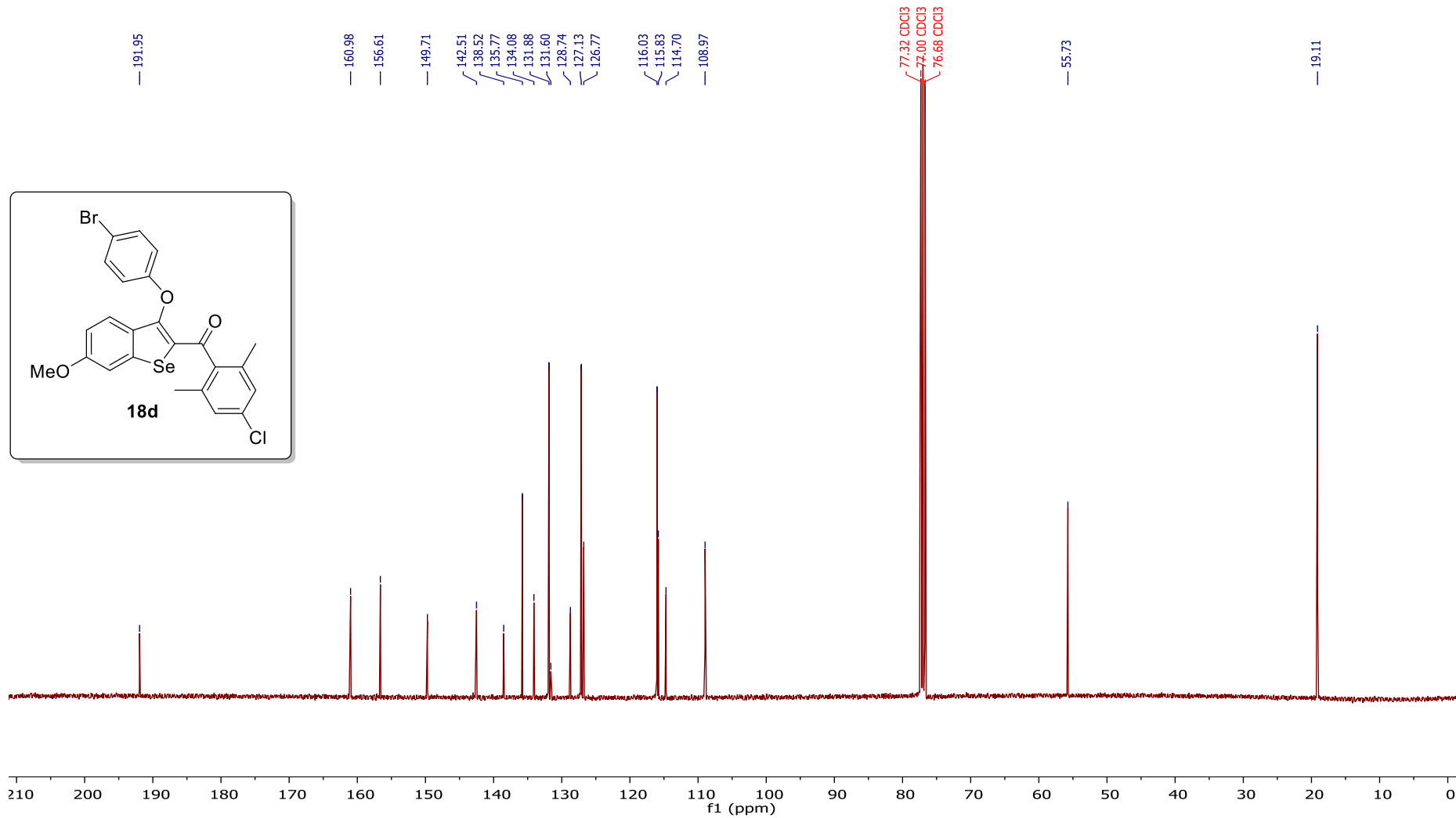
^{77}Se NMR (76.37 MHz, CDCl_3):



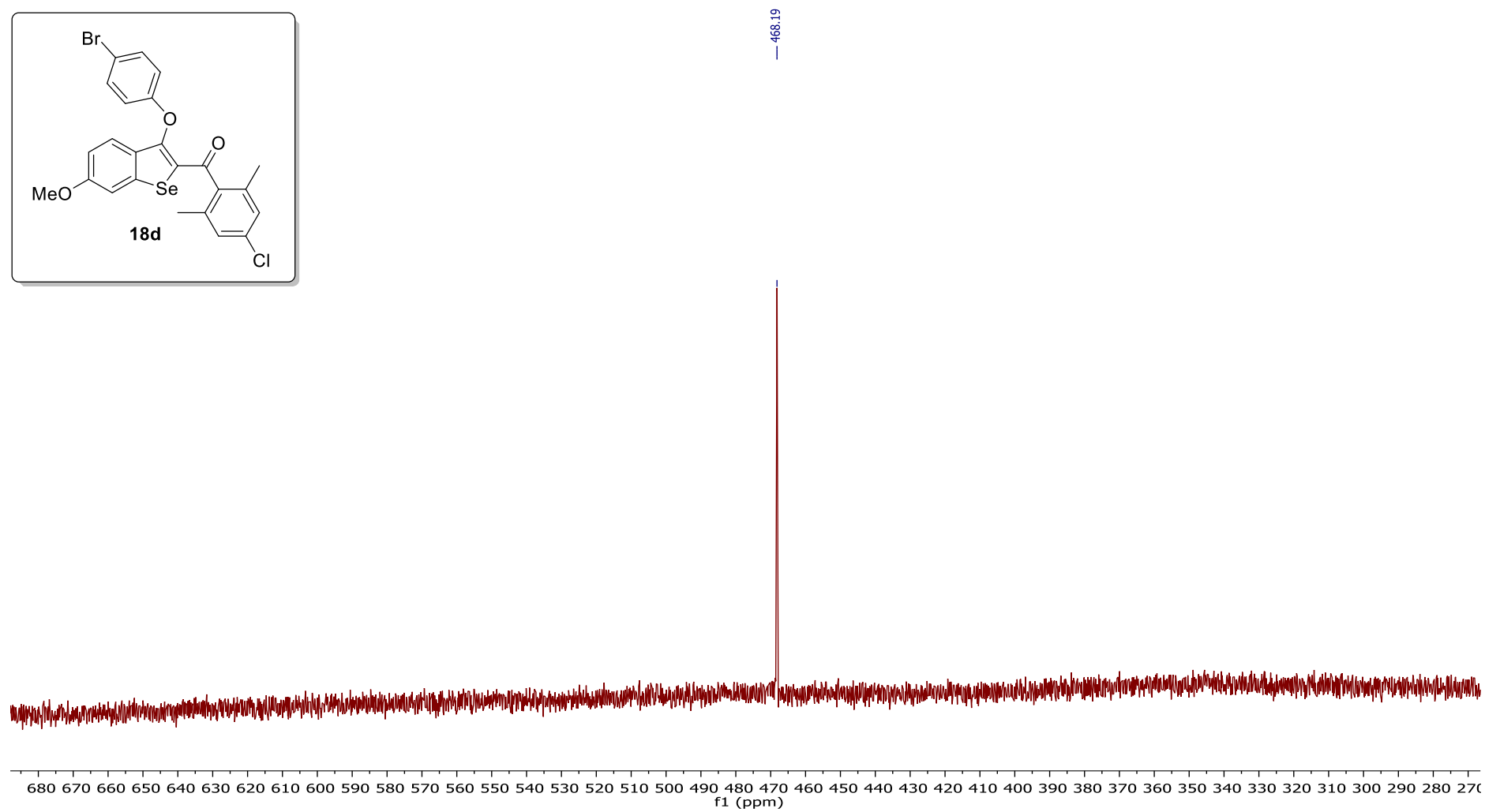
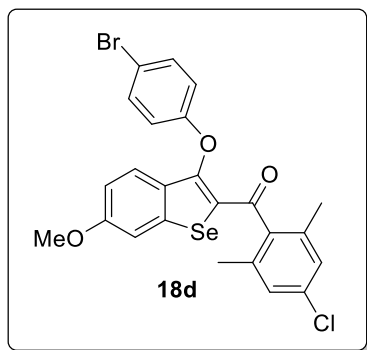
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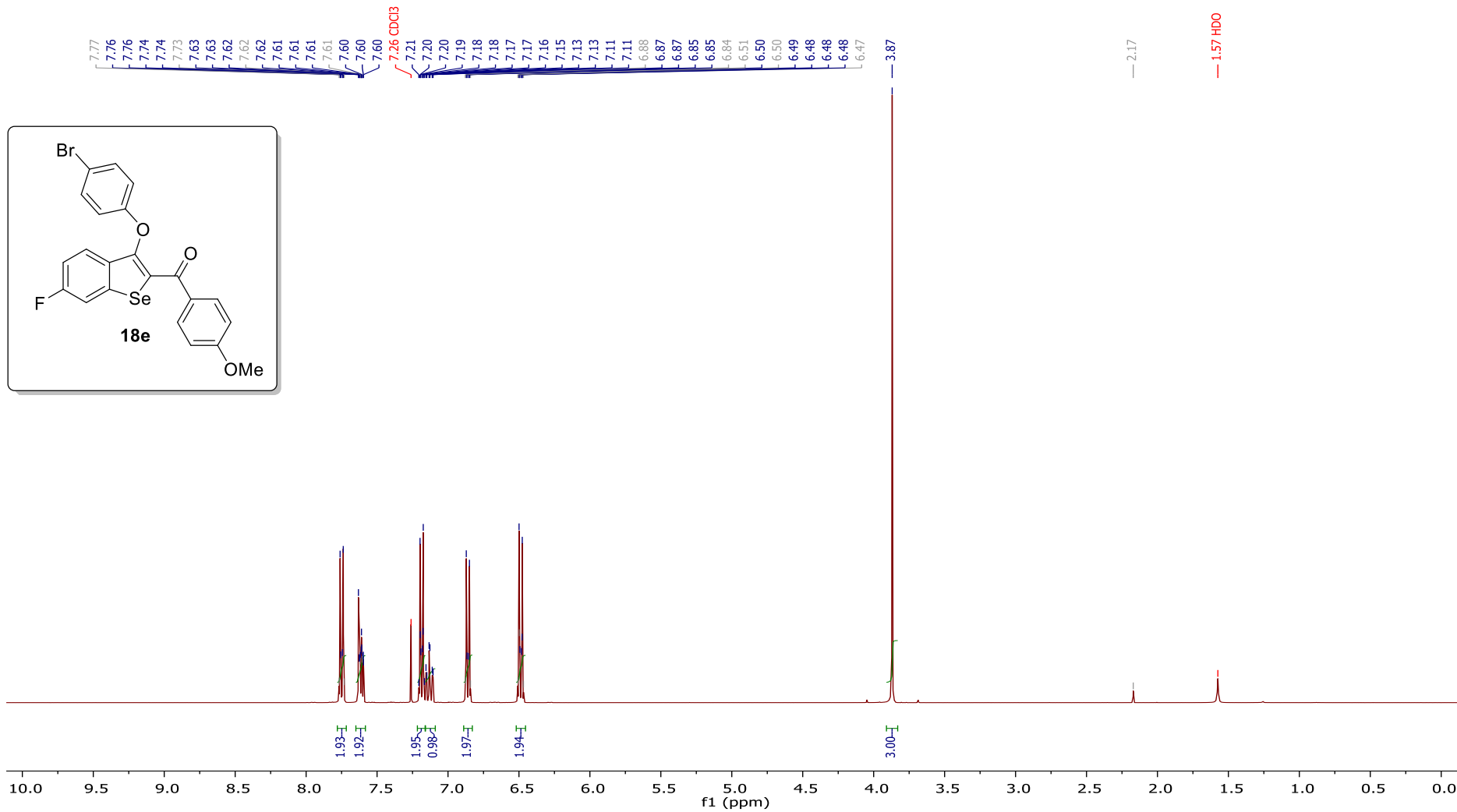
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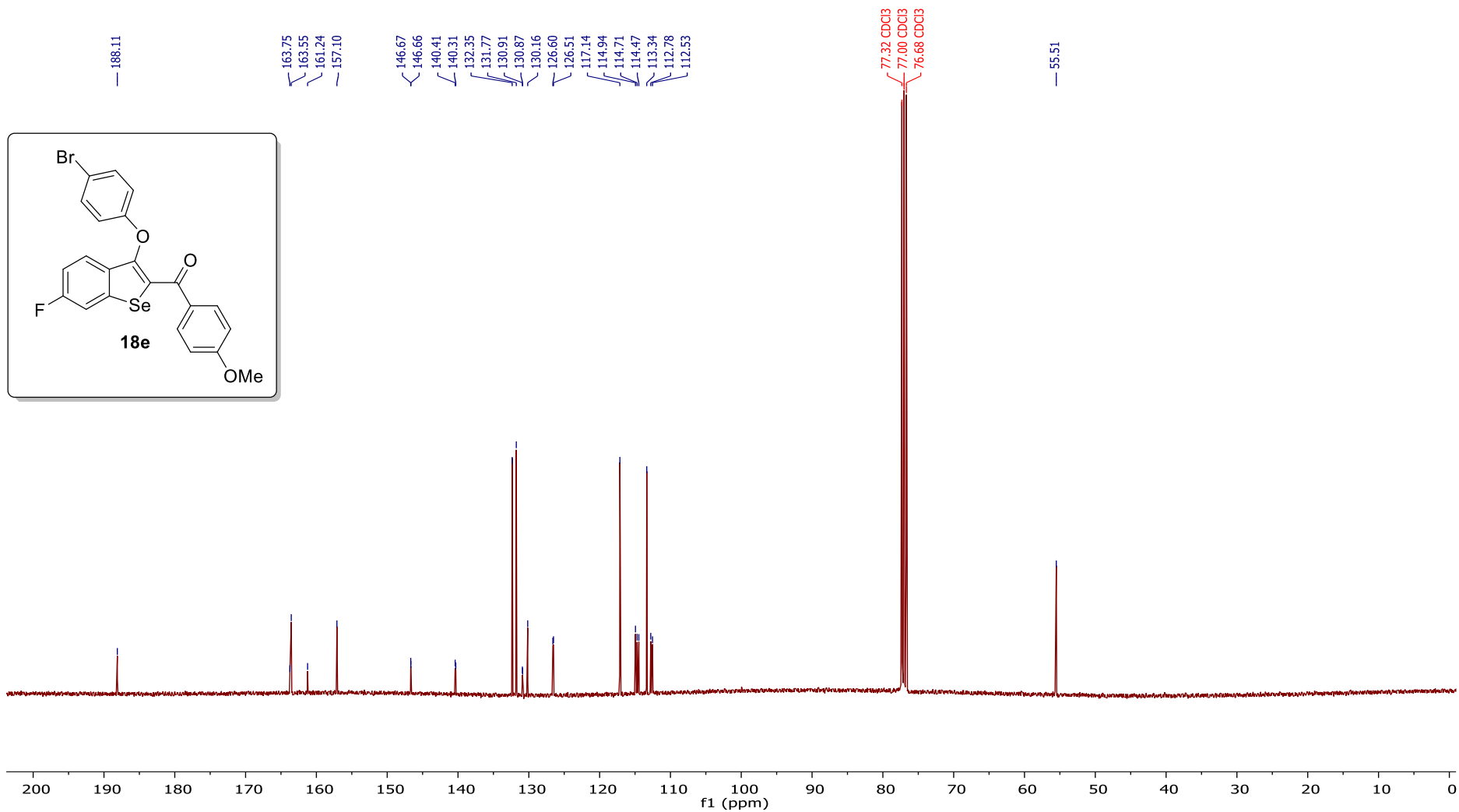
^{77}Se NMR (76.37 MHz, CDCl_3):



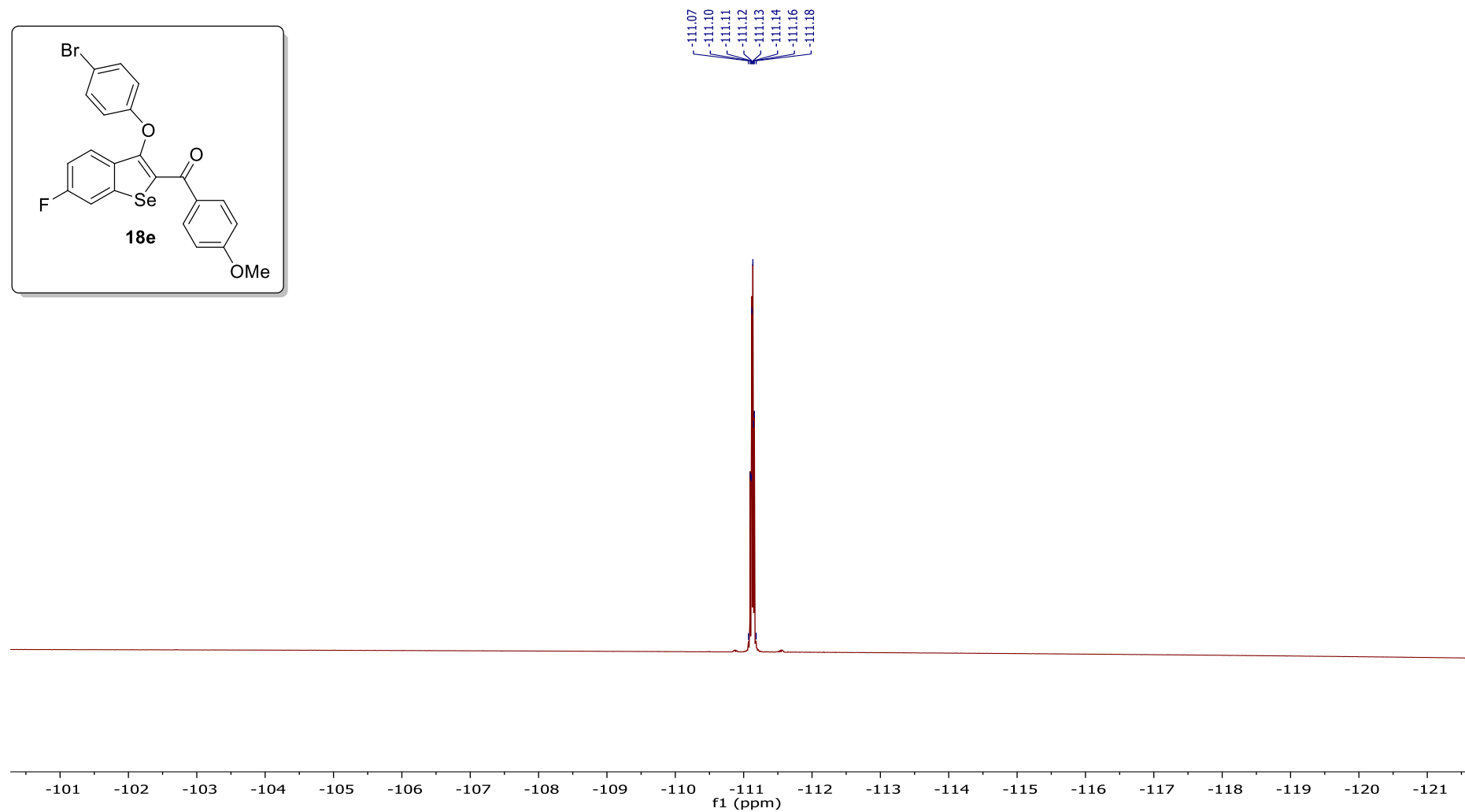
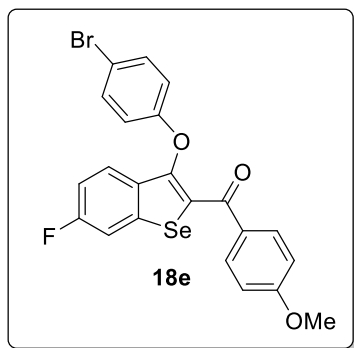
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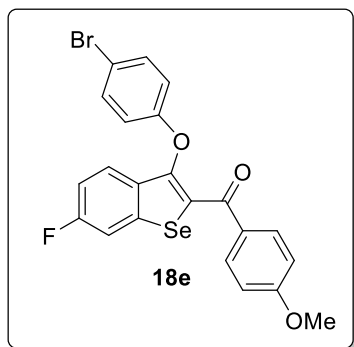
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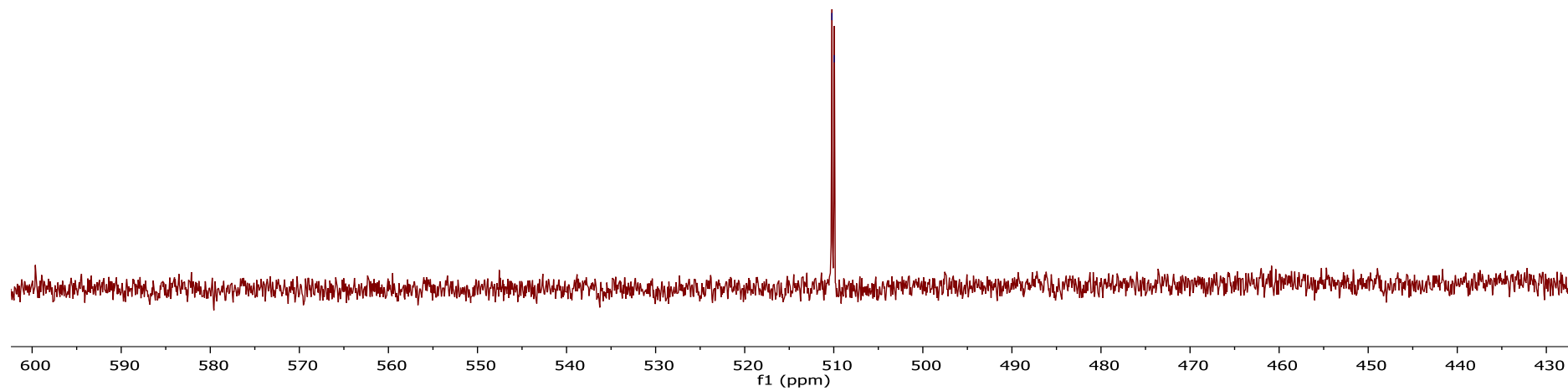
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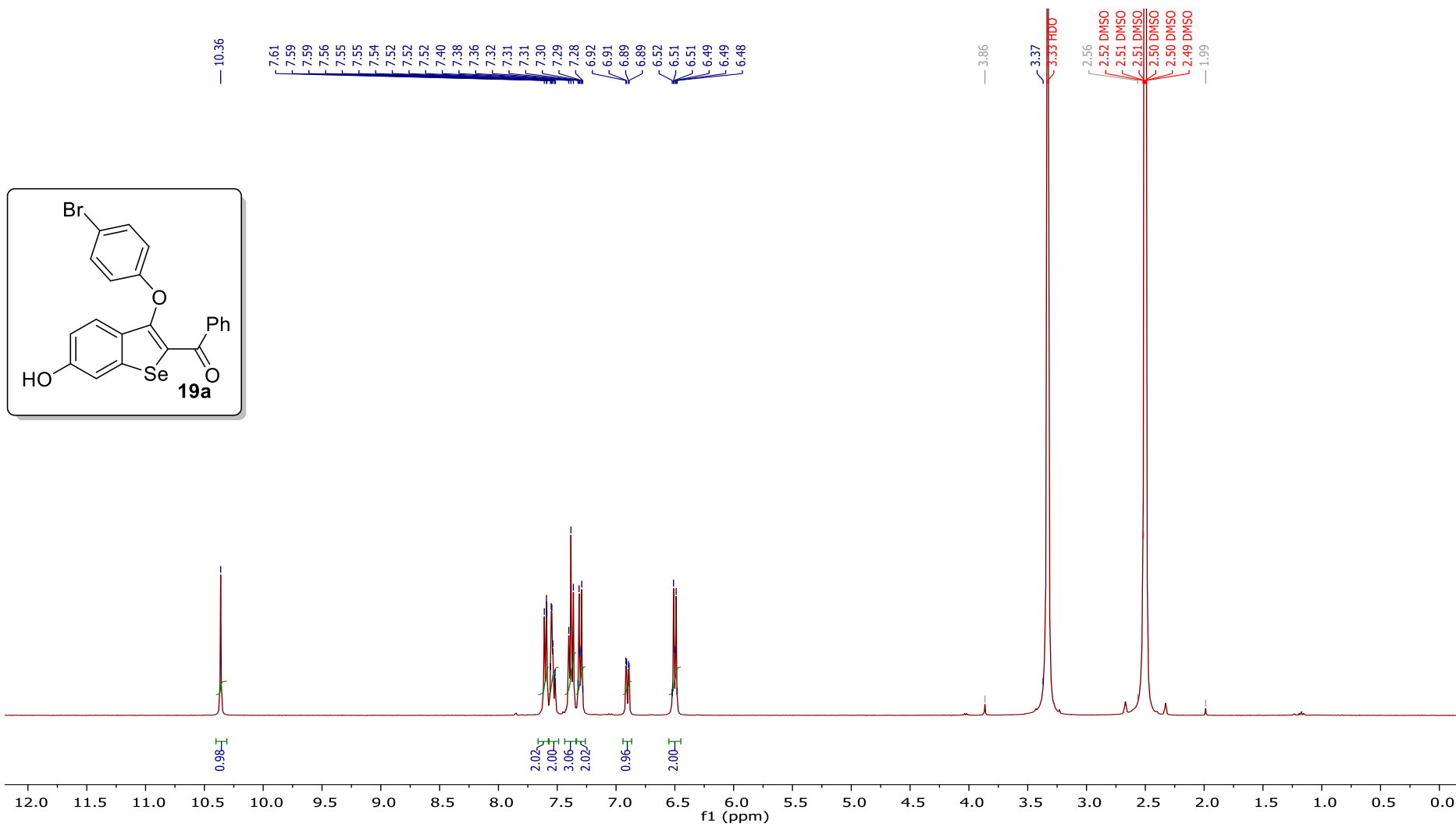
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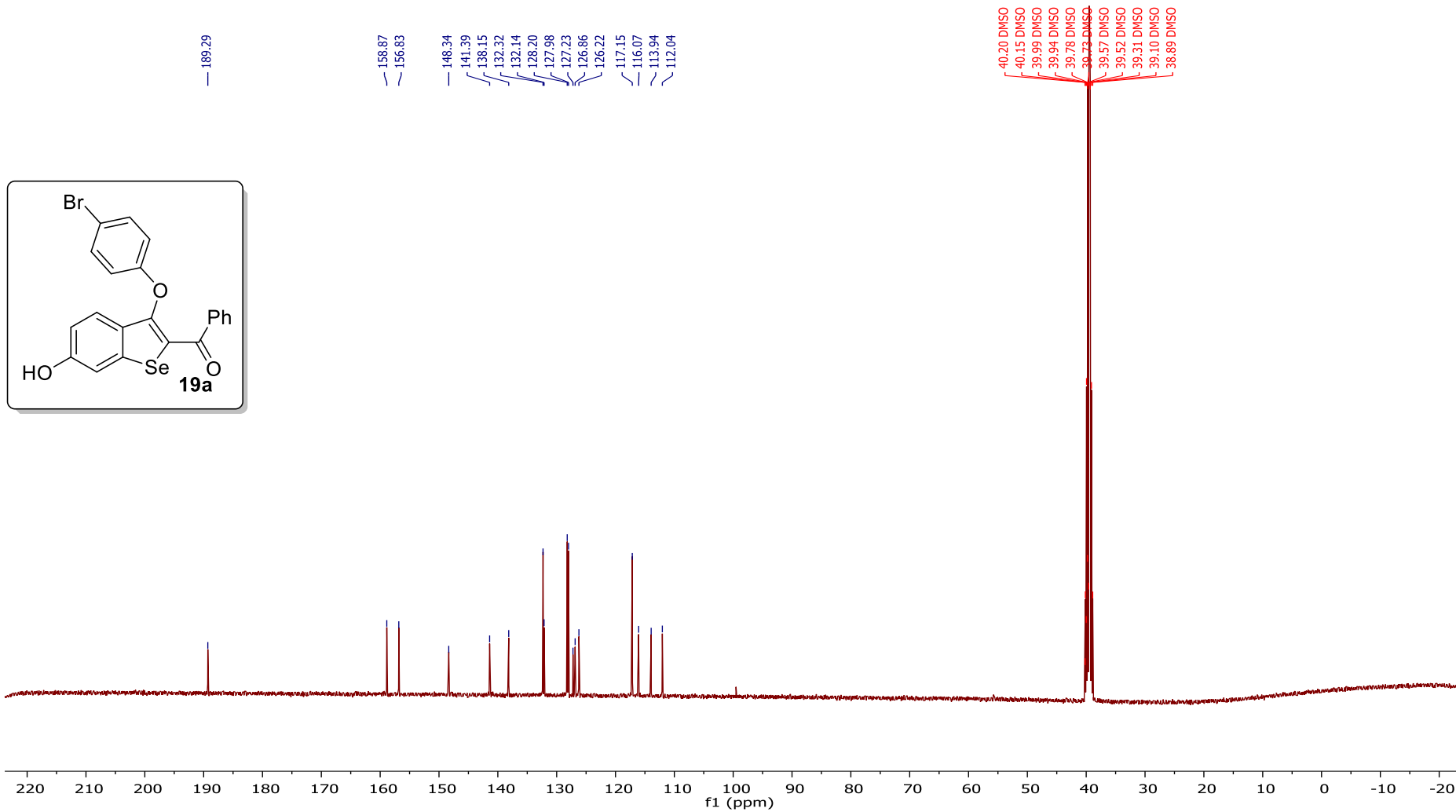
510.21
509.95



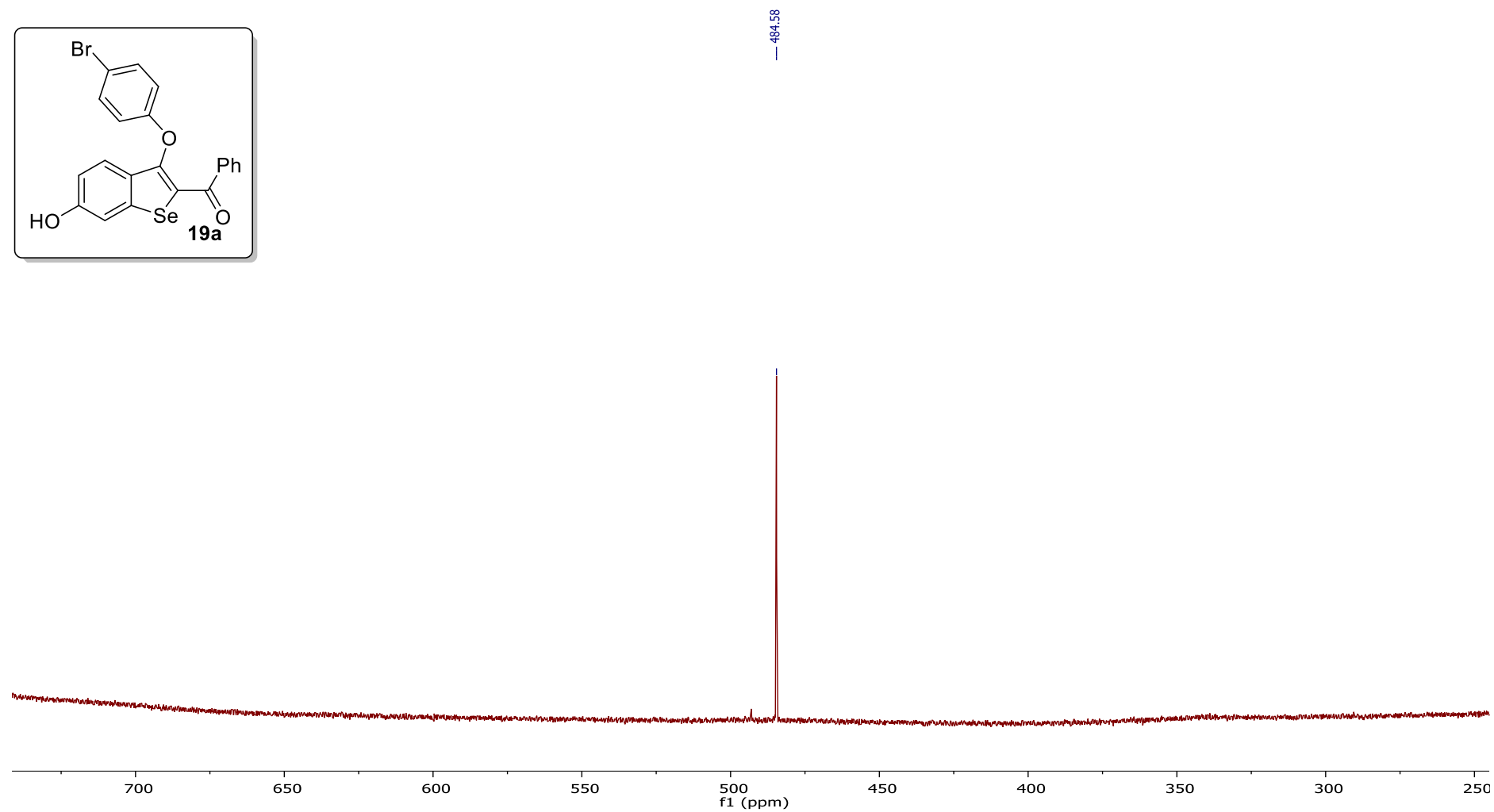
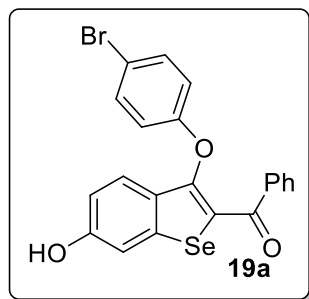
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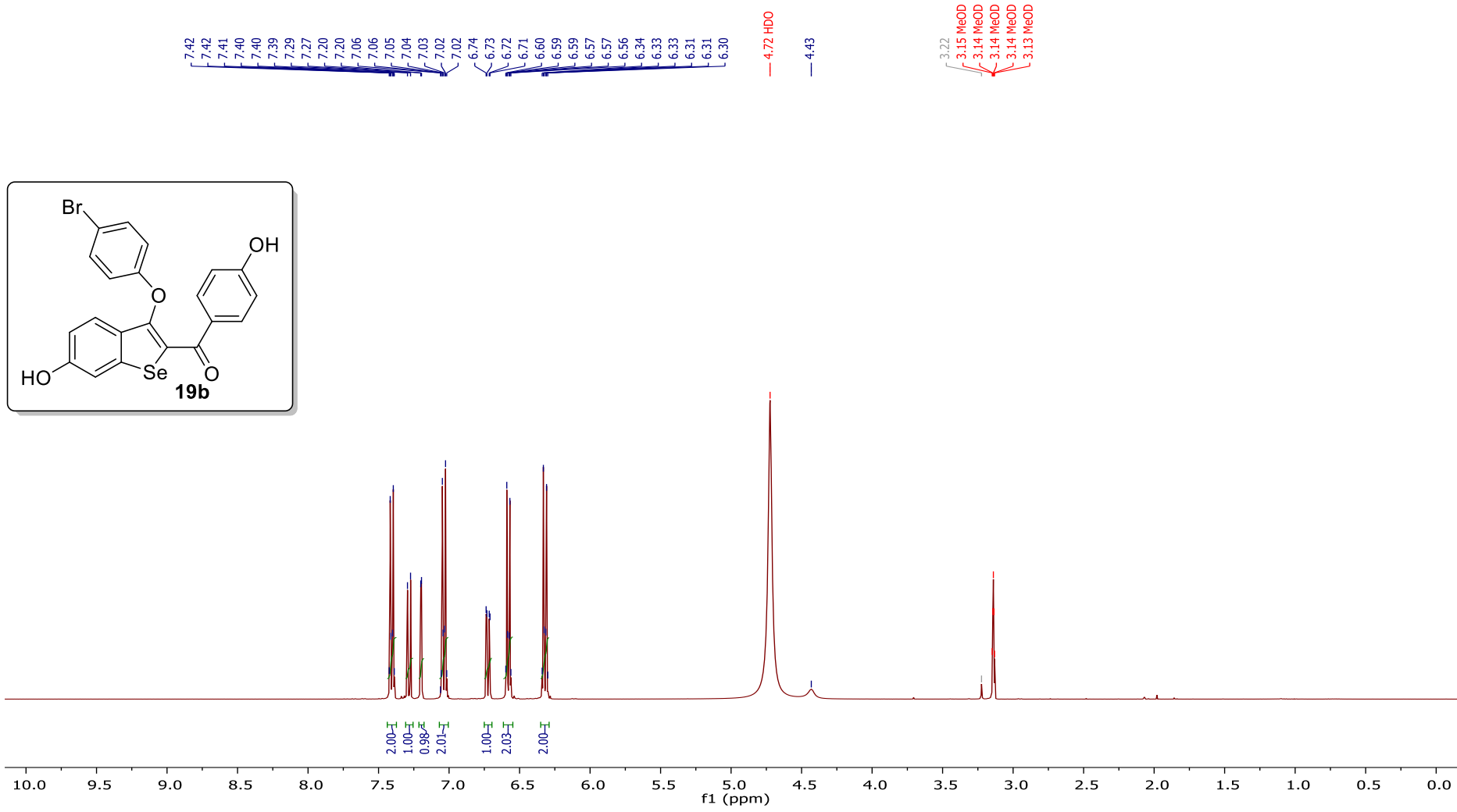
^{13}C NMR (100.6 MHz, DMSO- d_6):



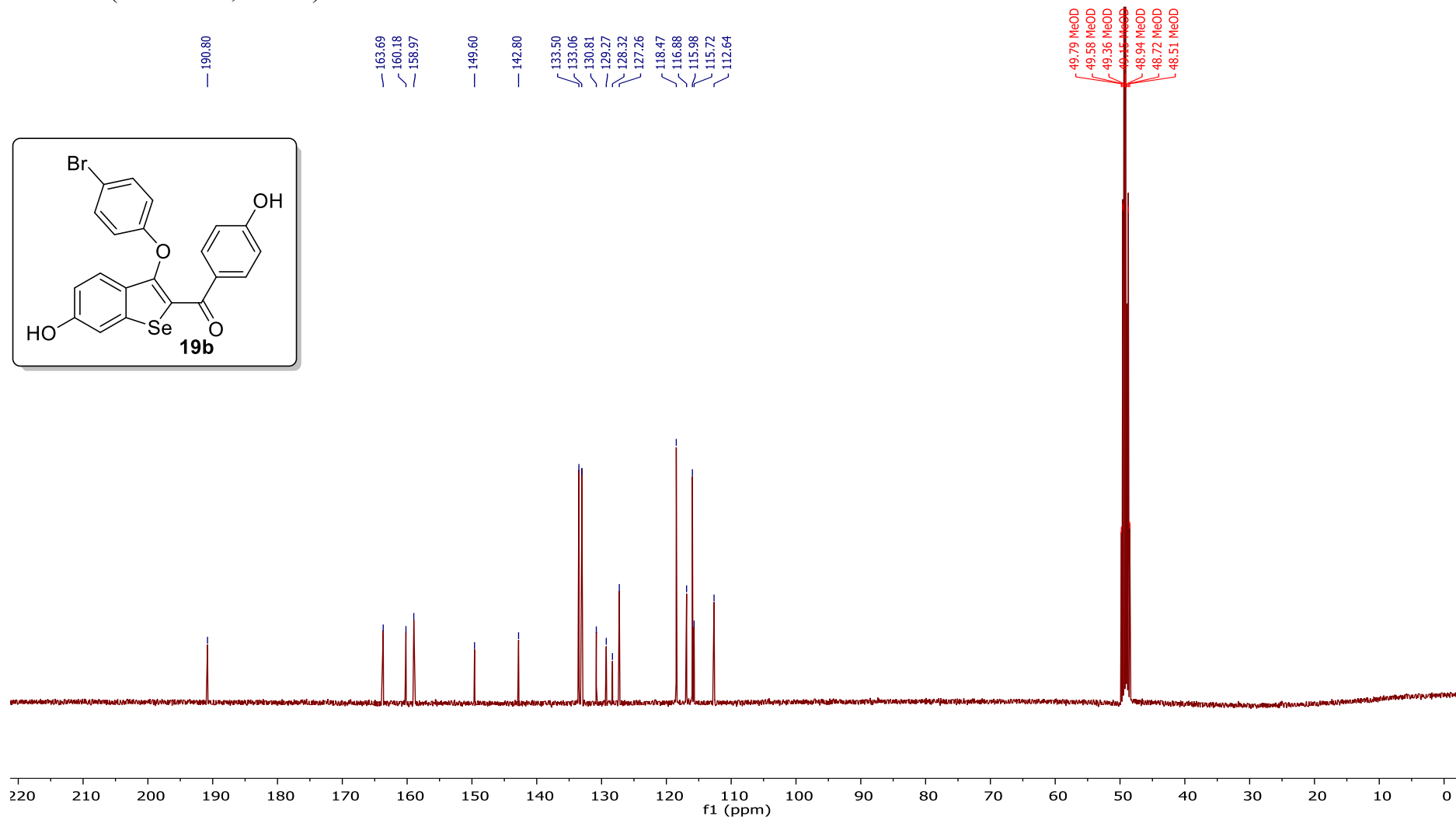
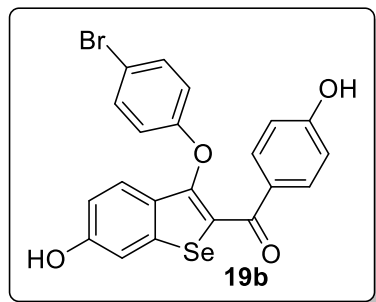
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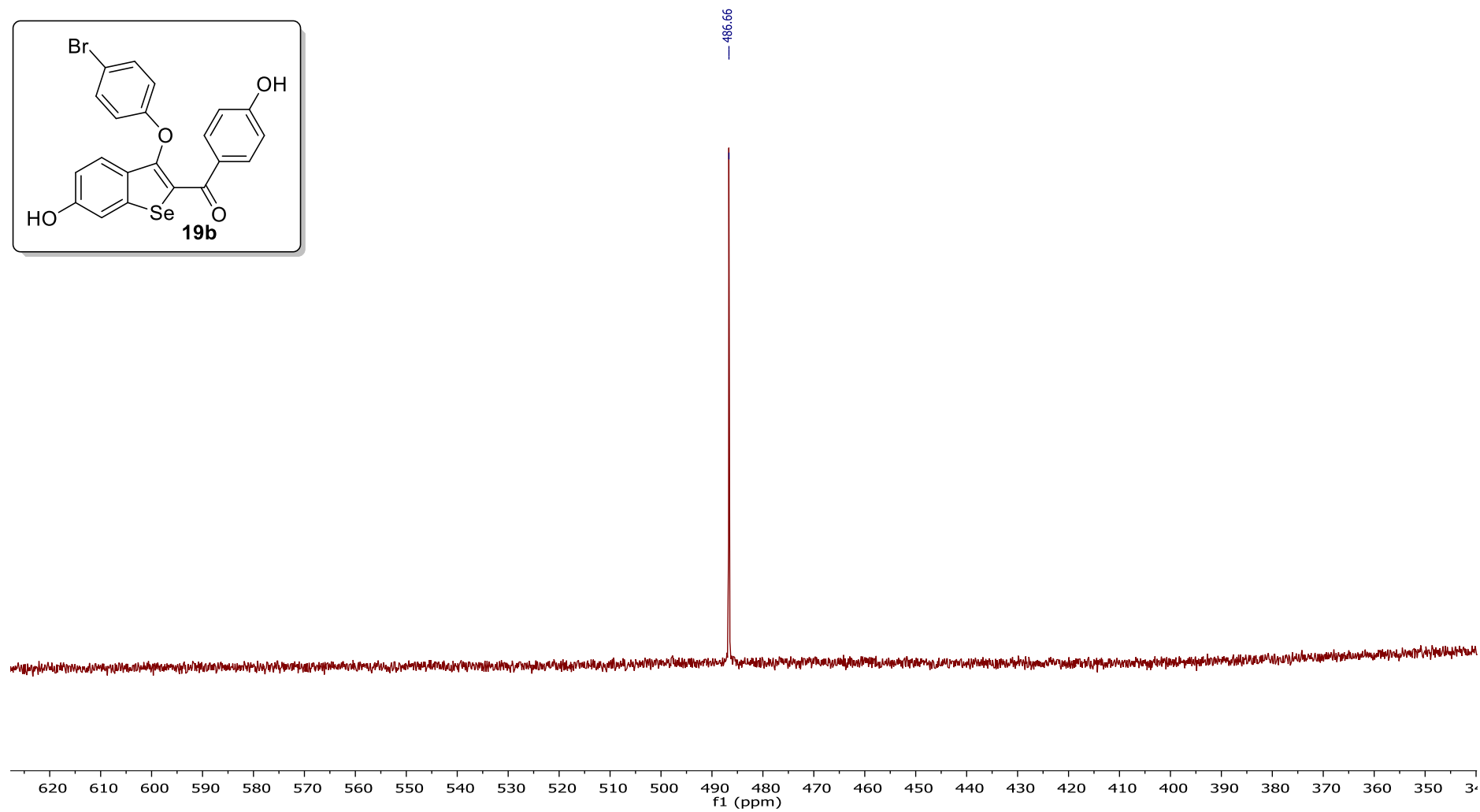
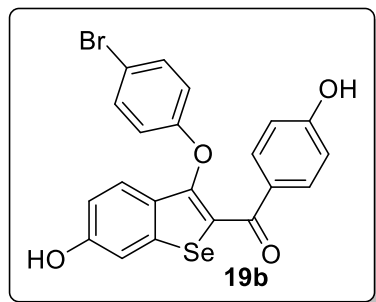
^1H NMR (400 MHz, MeOD):



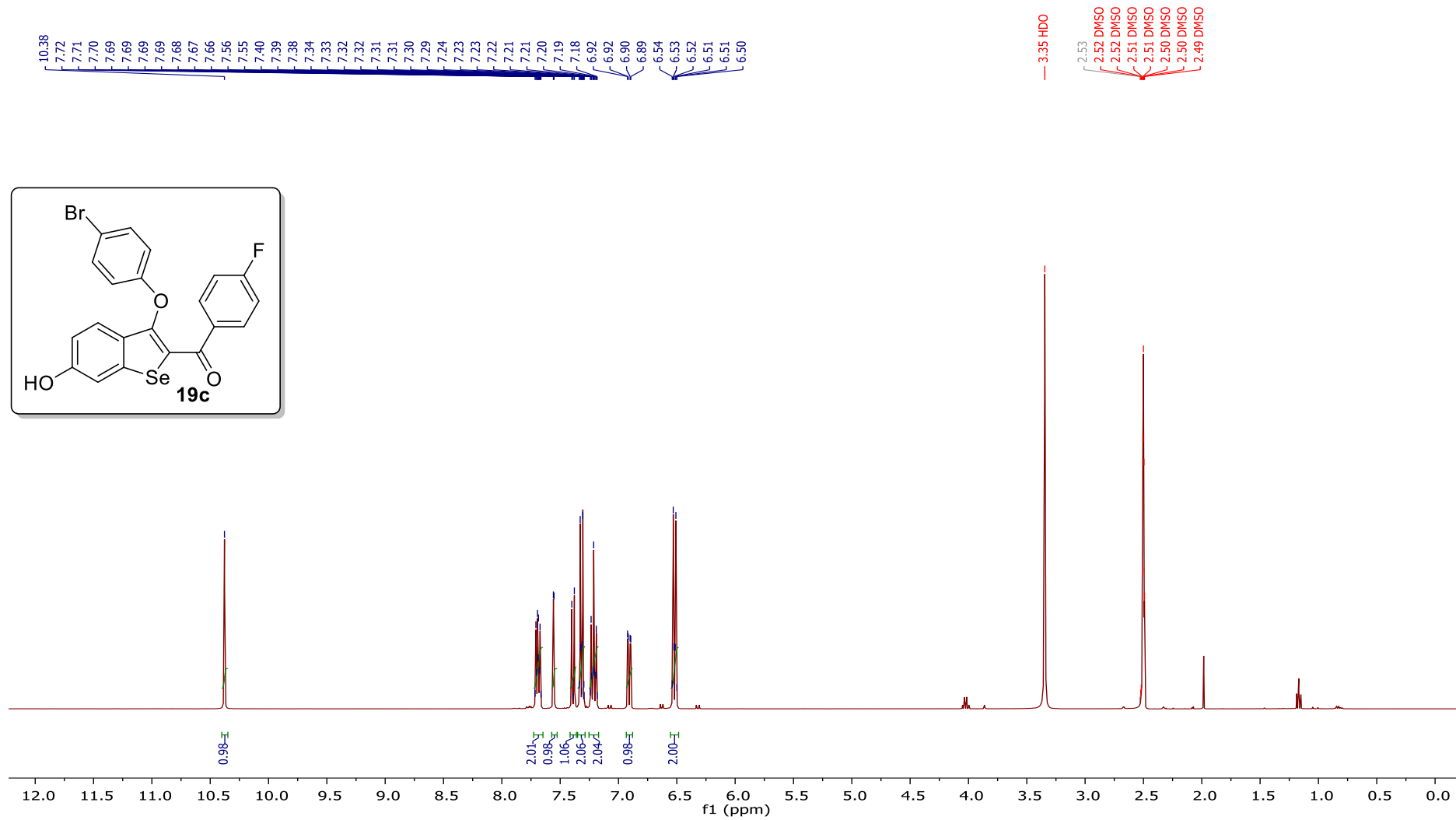
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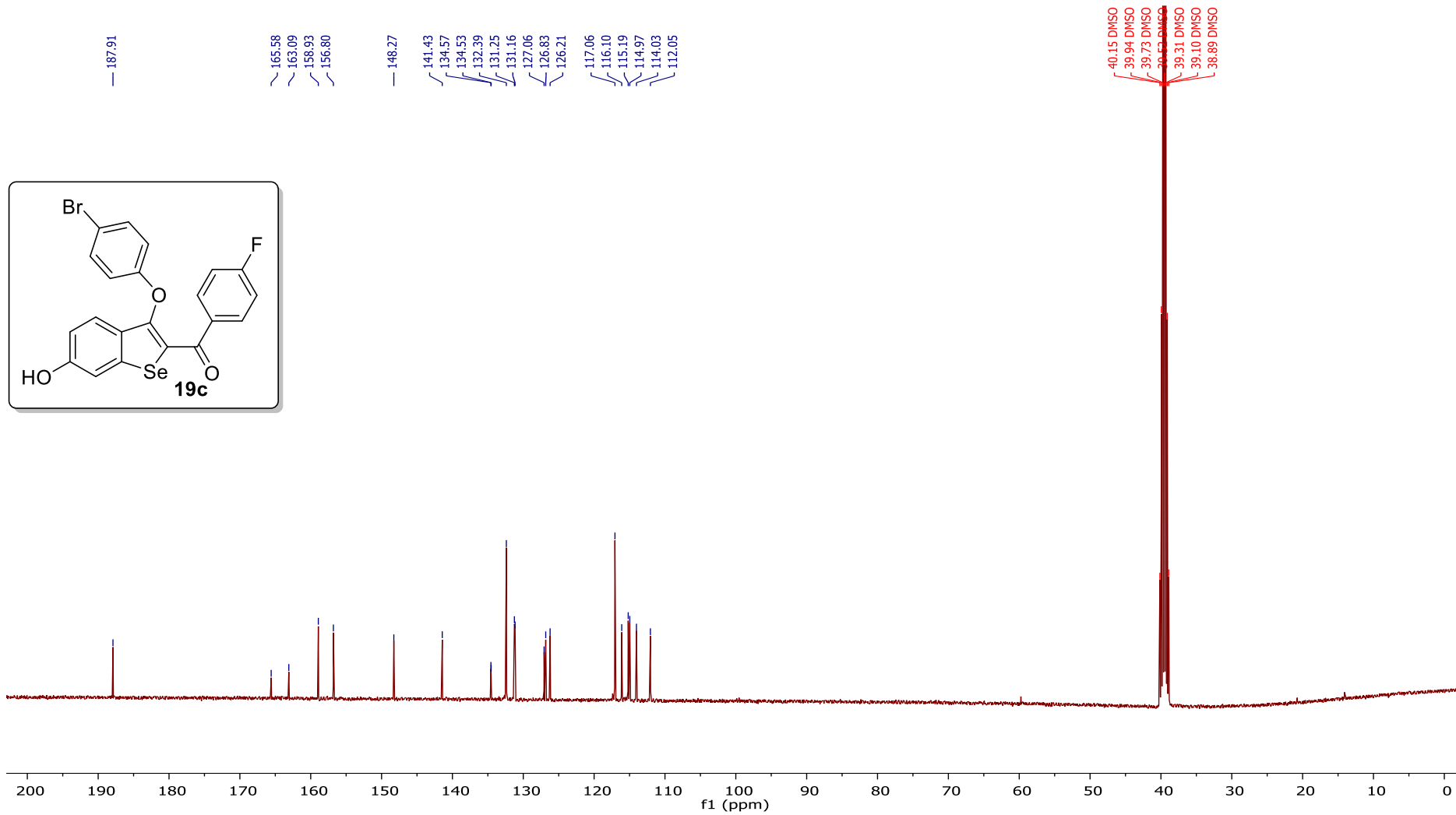
^{77}Se NMR (76.37 MHz, MeOD):



^1H NMR (400 MHz, DMSO- d_6):

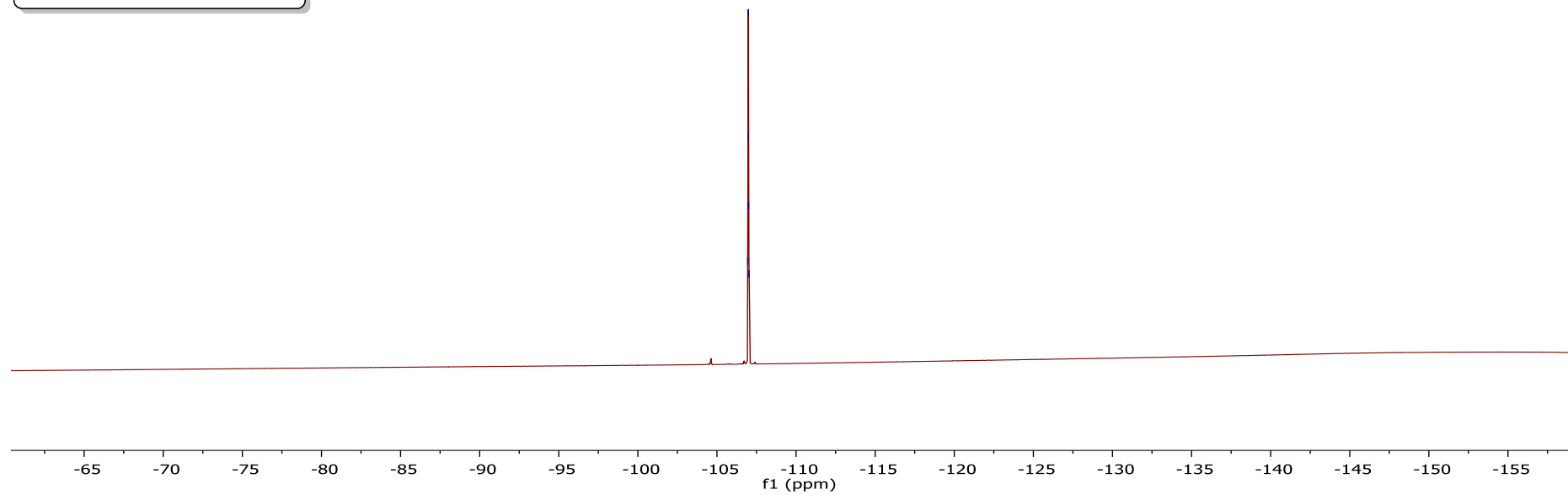
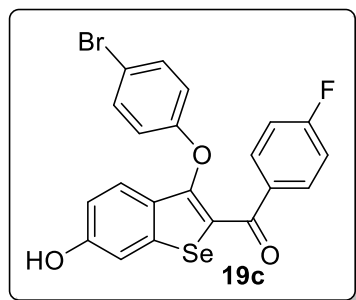


^{13}C NMR (100.6 MHz, DMSO- d_6):

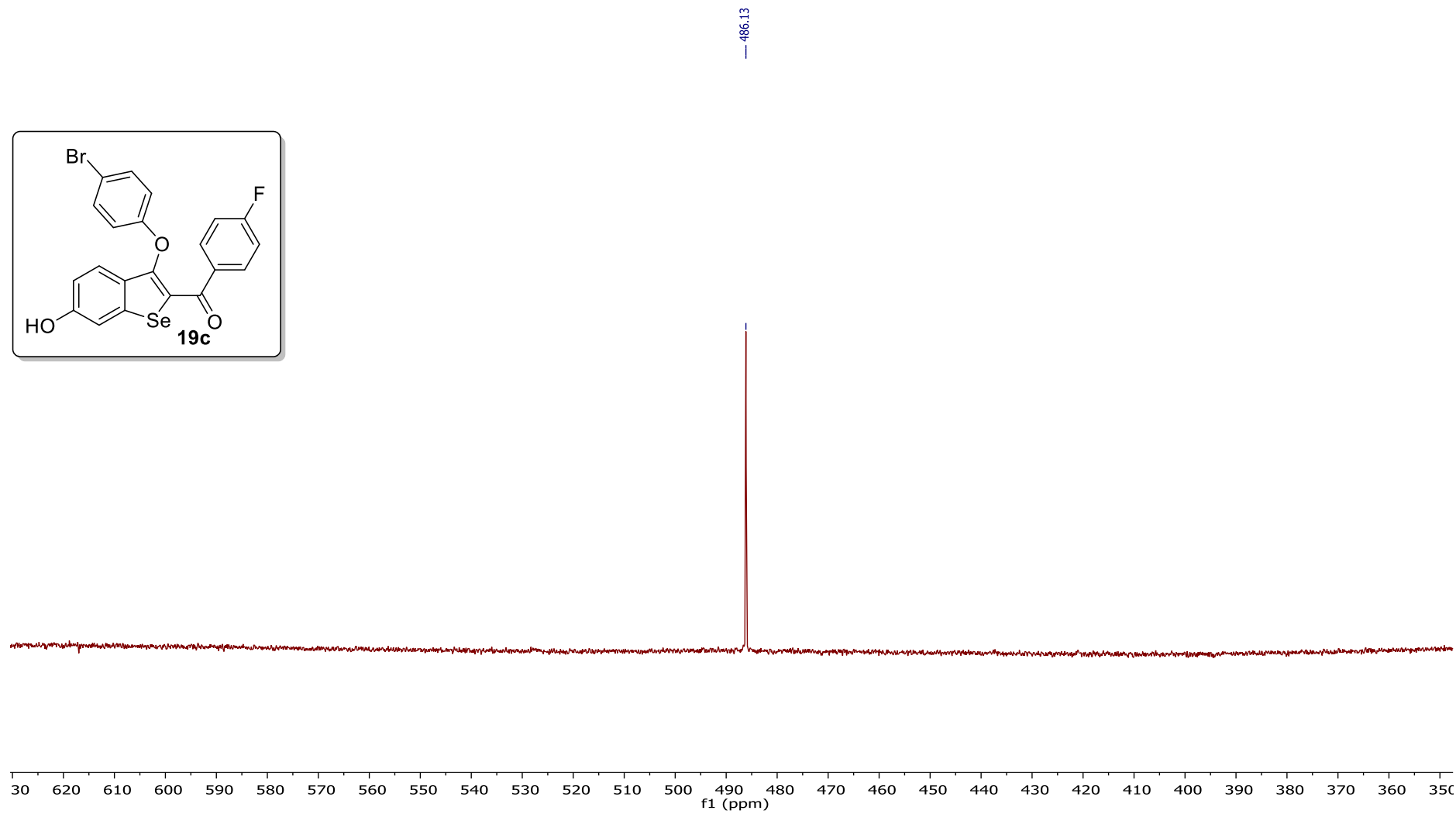
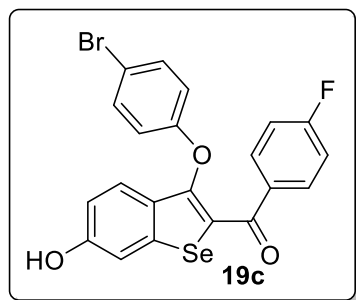


^{19}F NMR (376.21 MHz, DMSO-d_6):

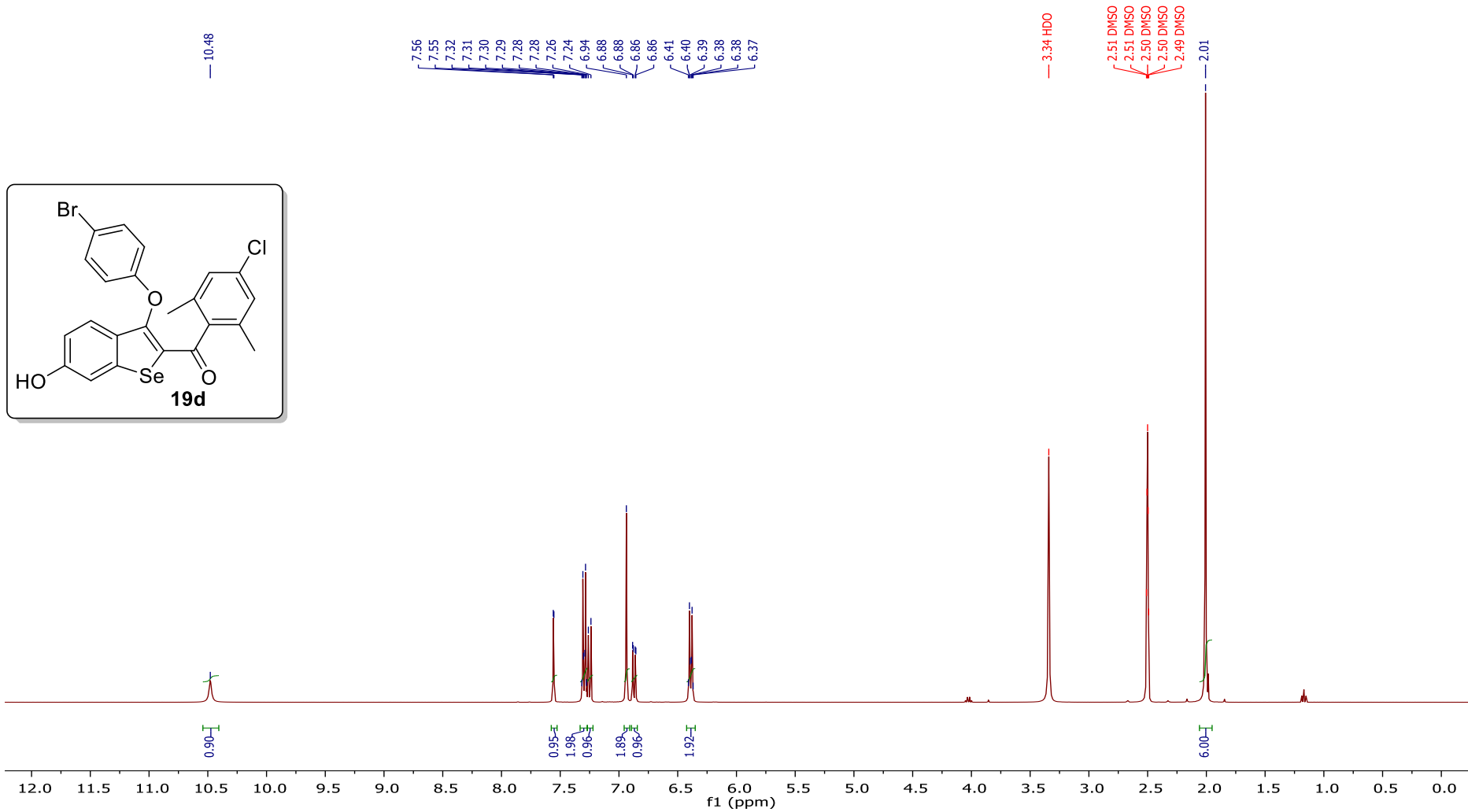
-106.94
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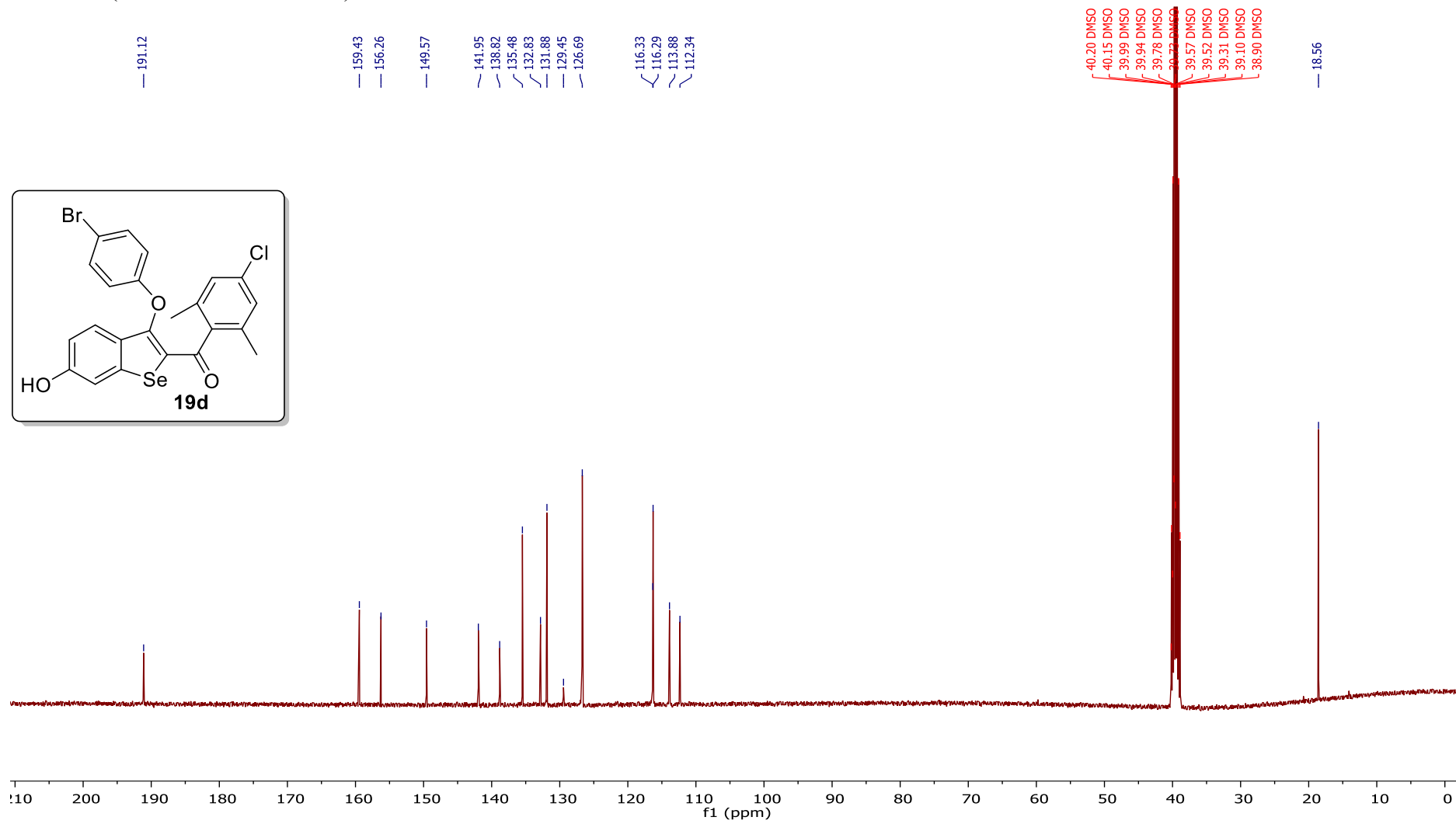
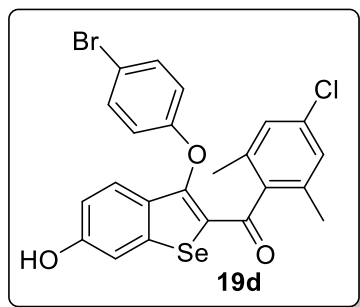
^{77}Se NMR (76.37 MHz, DMSO- d_6):



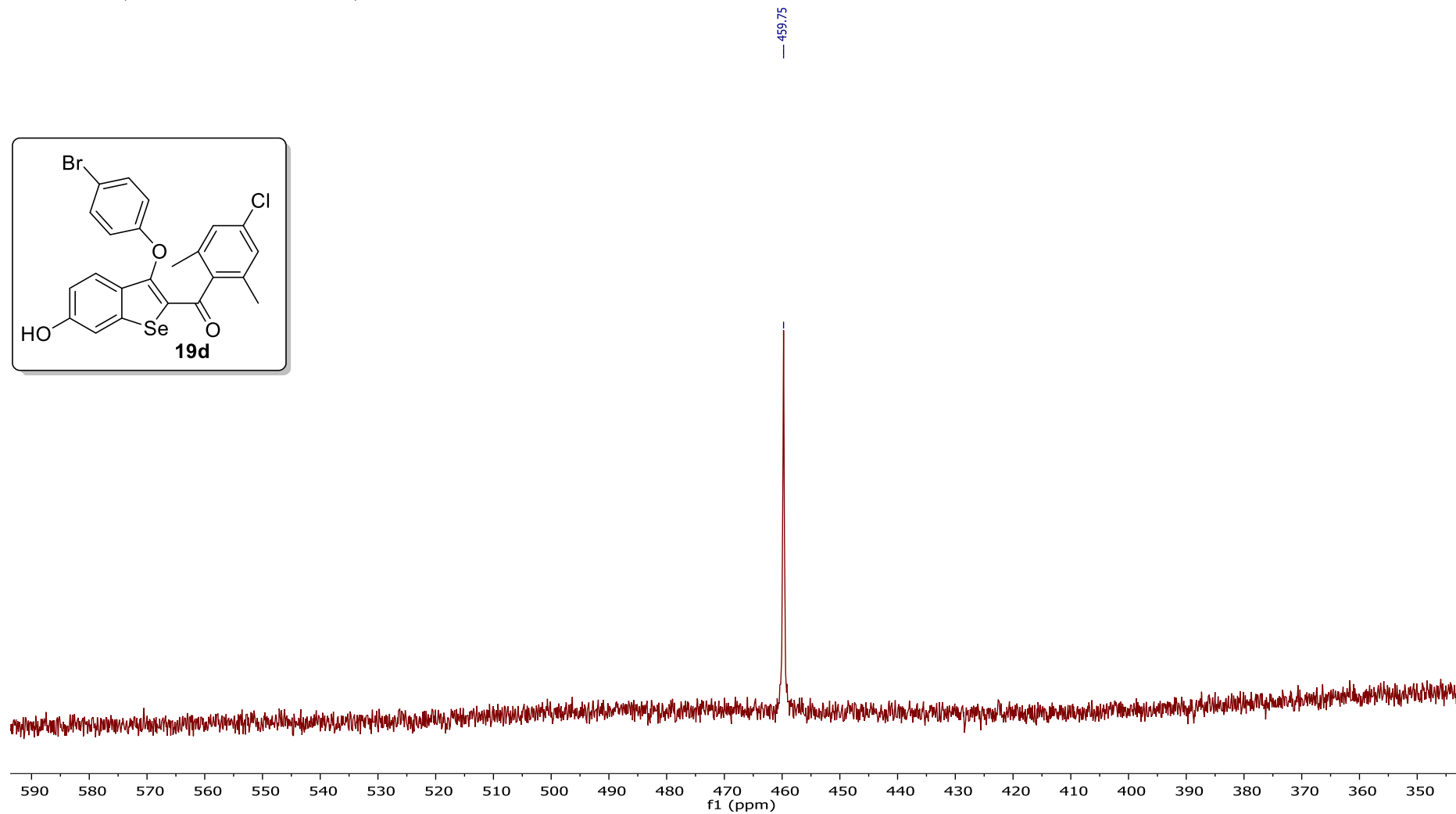
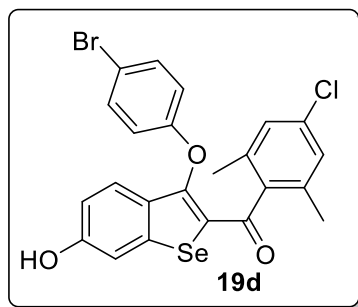
^1H NMR (400 MHz, DMSO- d_6):



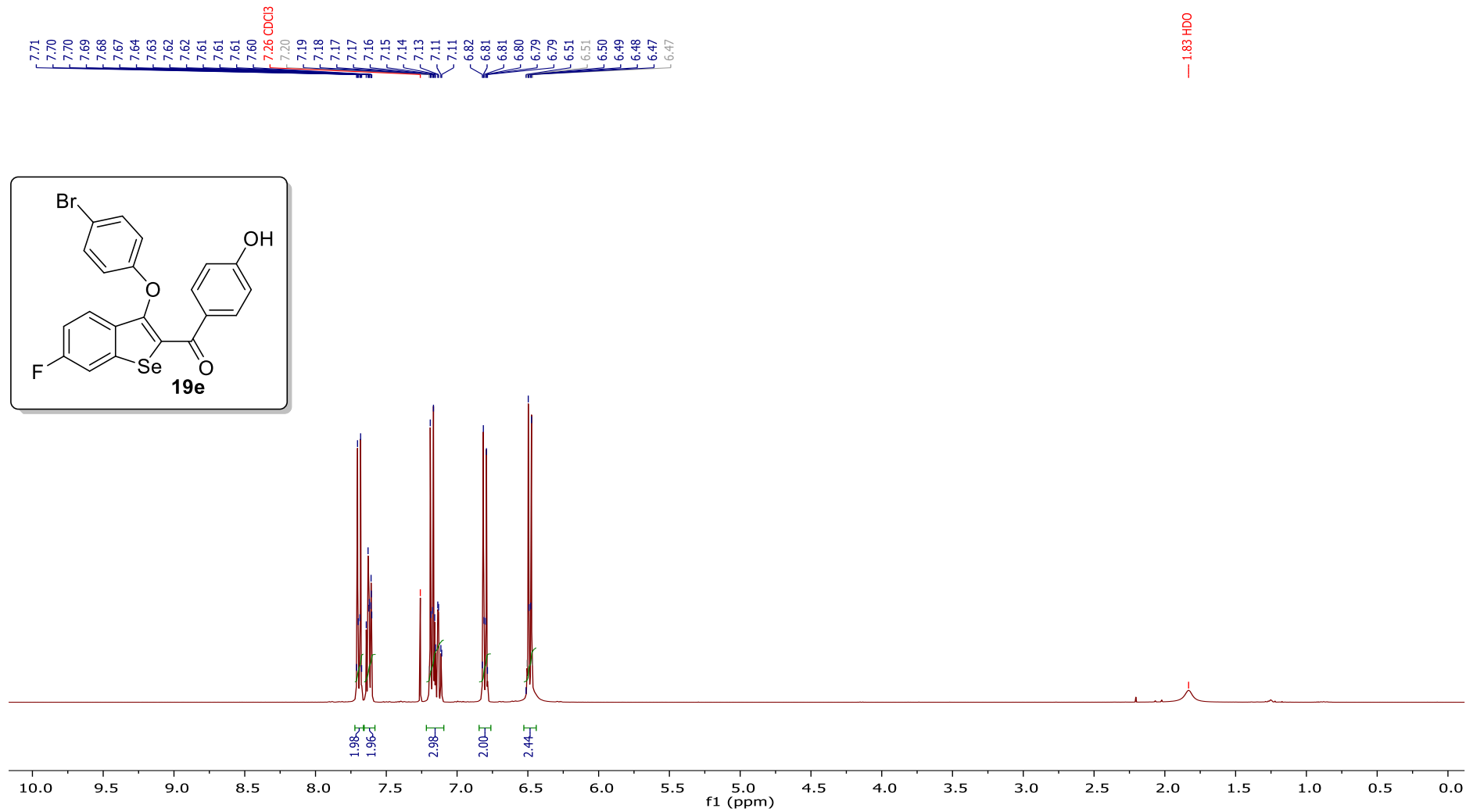
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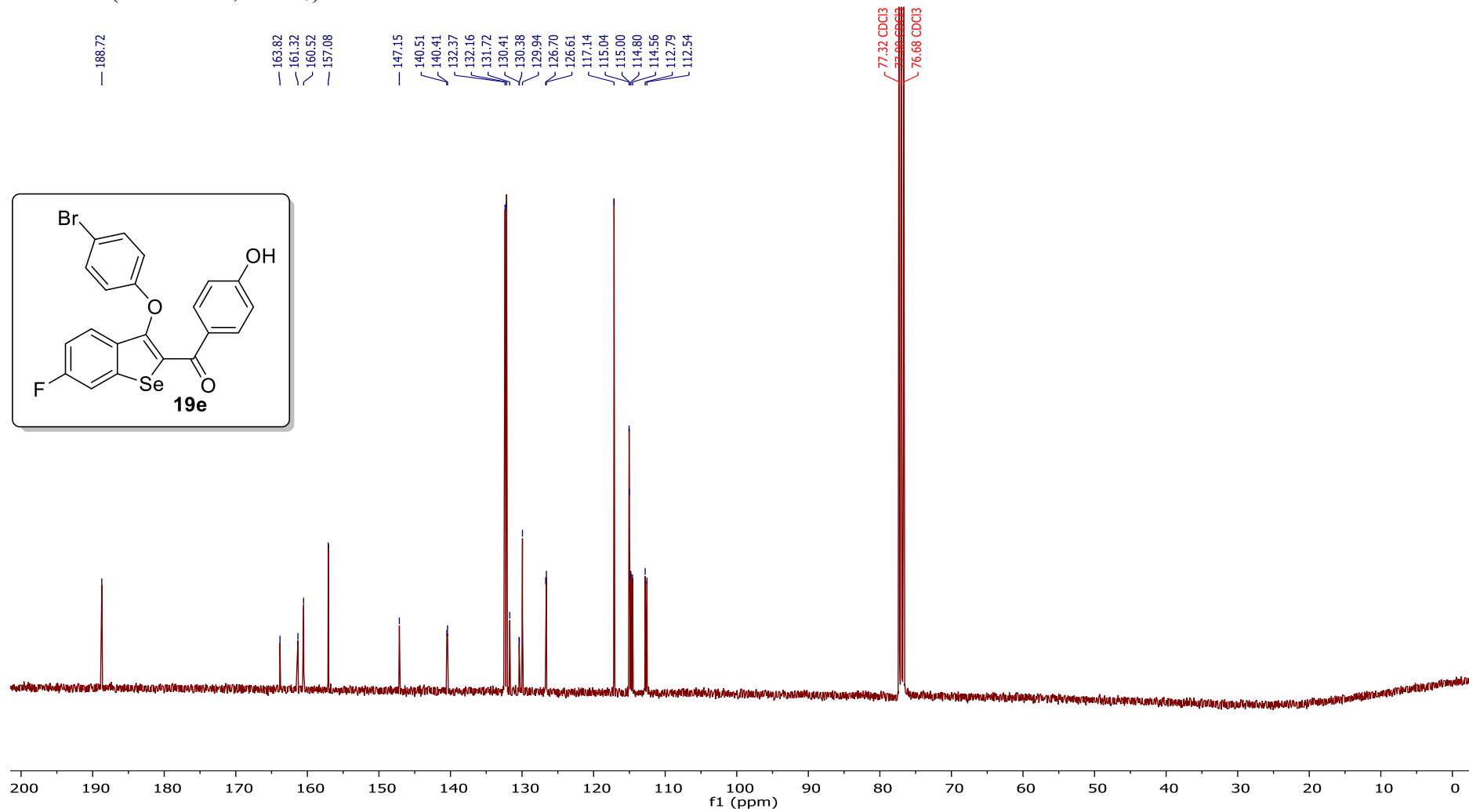
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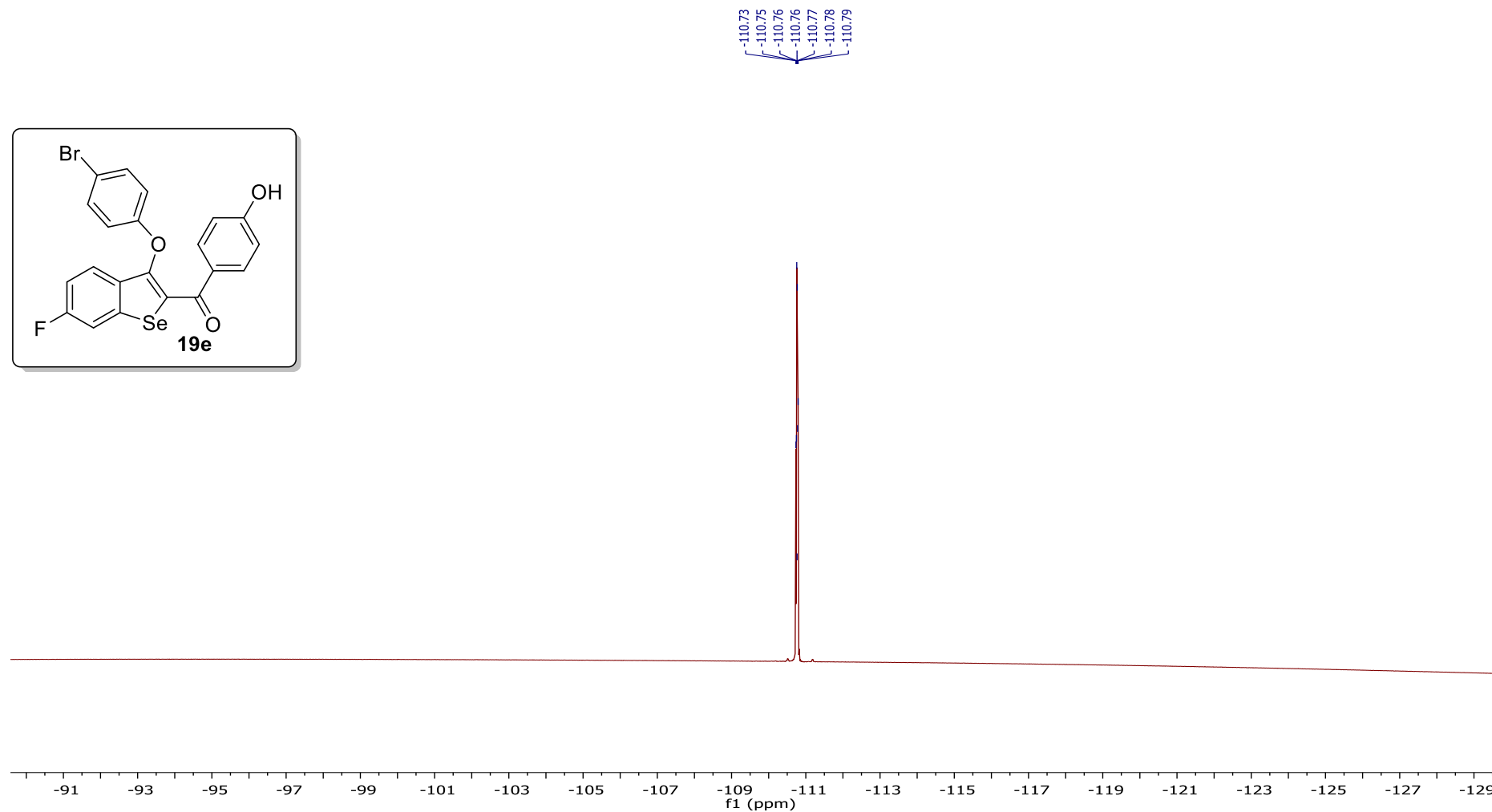
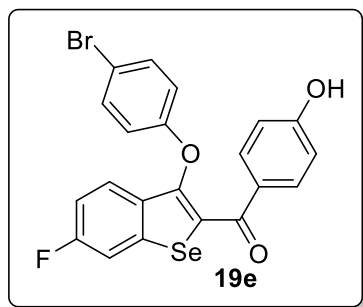
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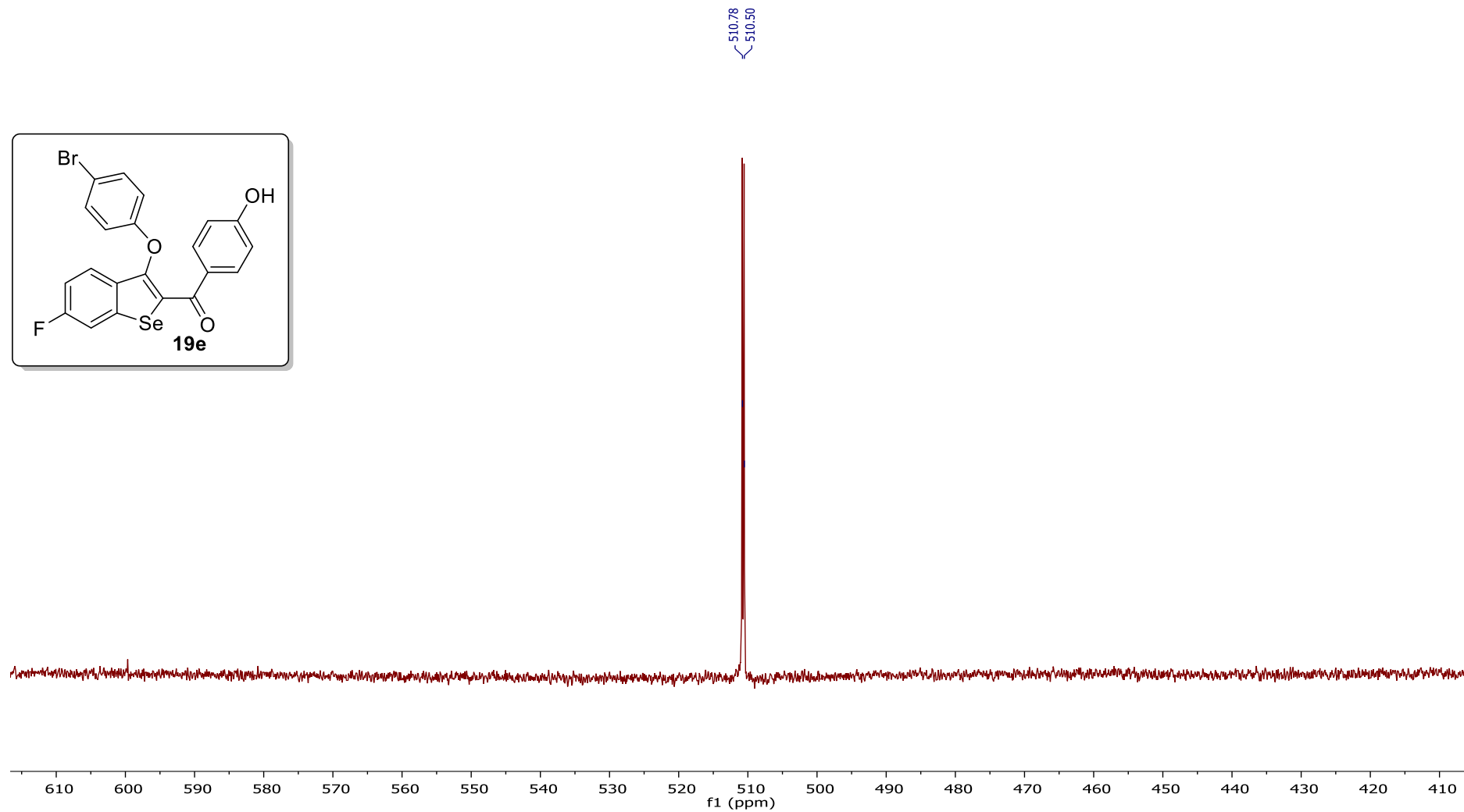
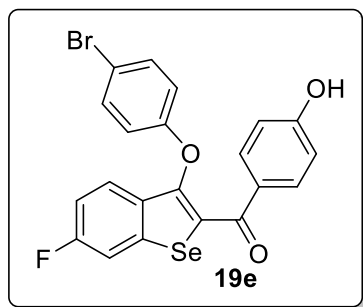
^{13}C NMR (100.6 MHz, CDCl_3):



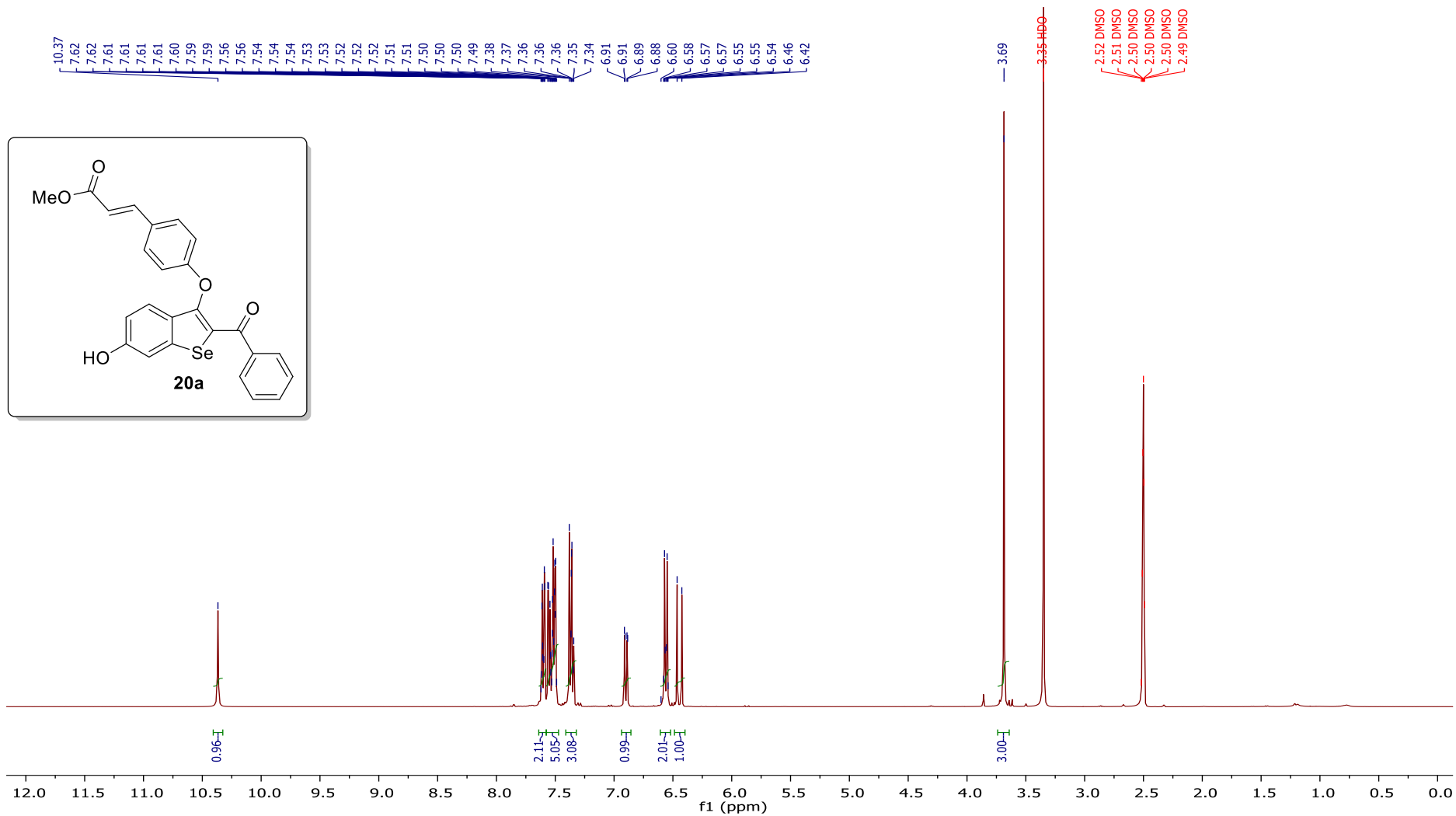
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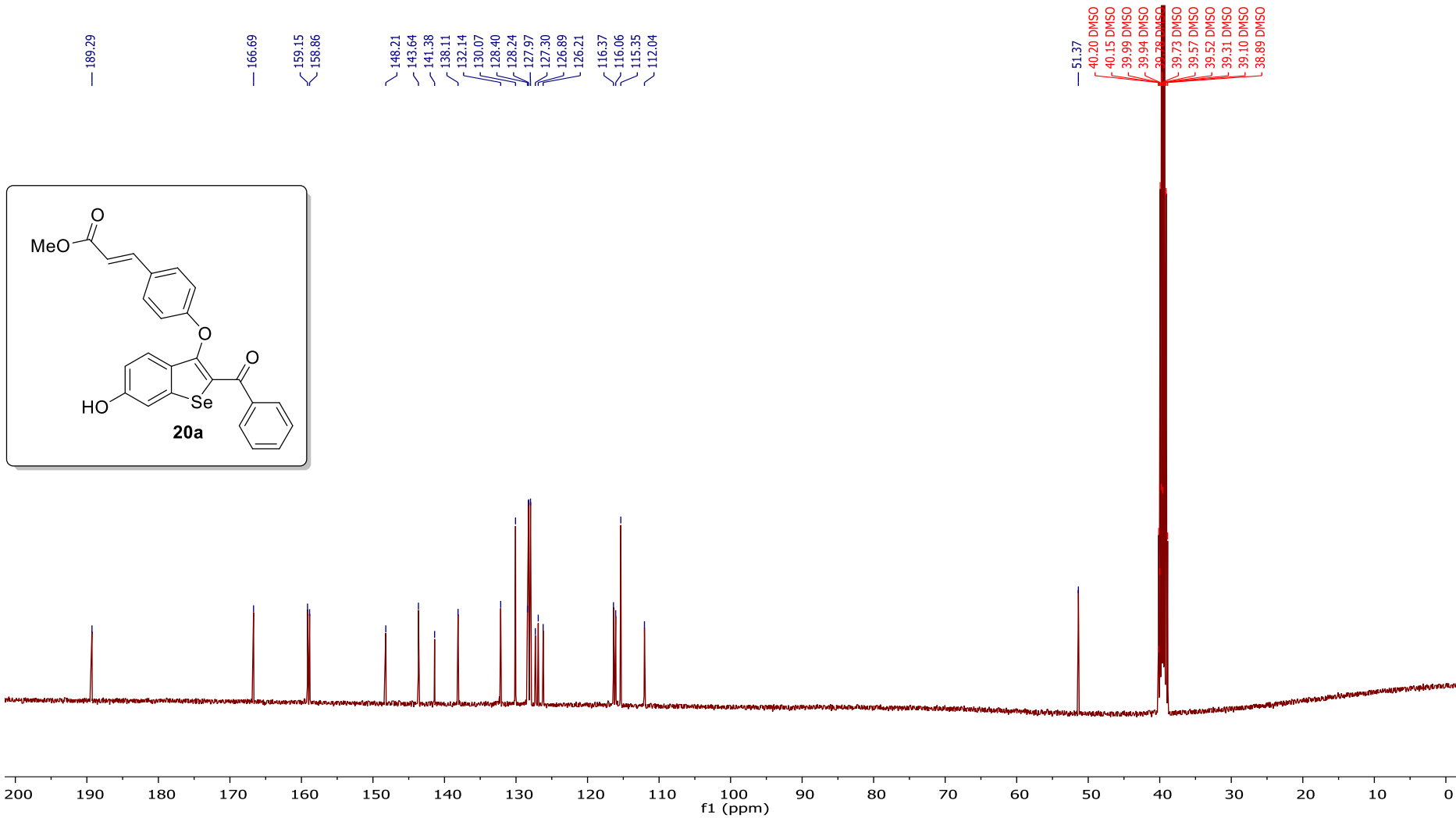
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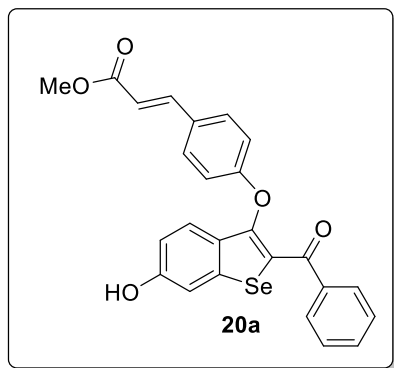
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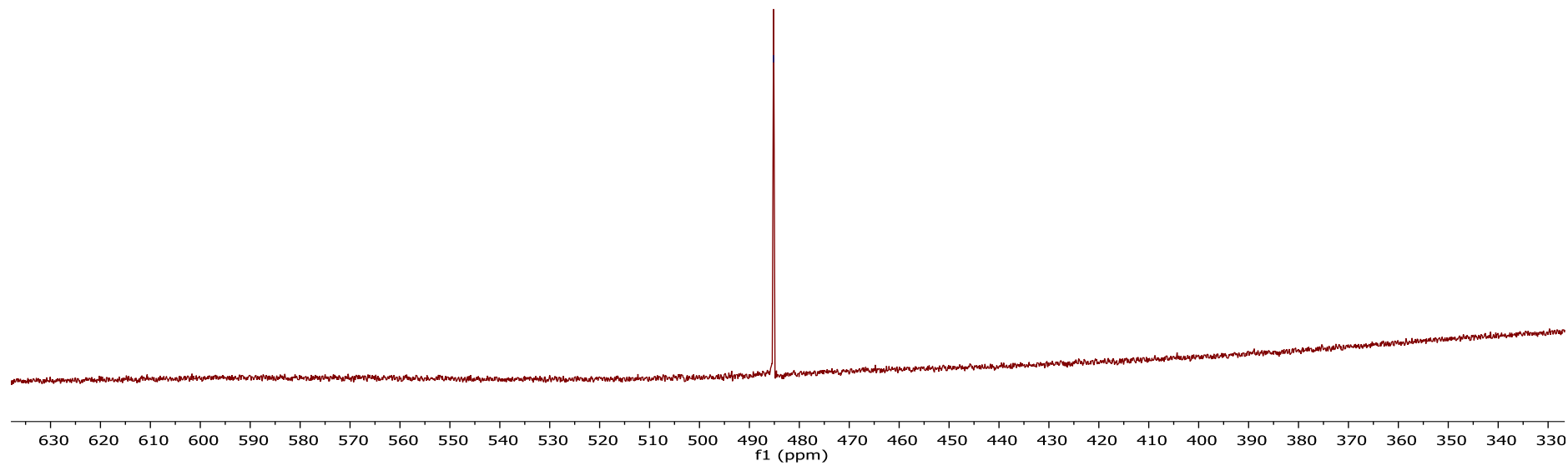
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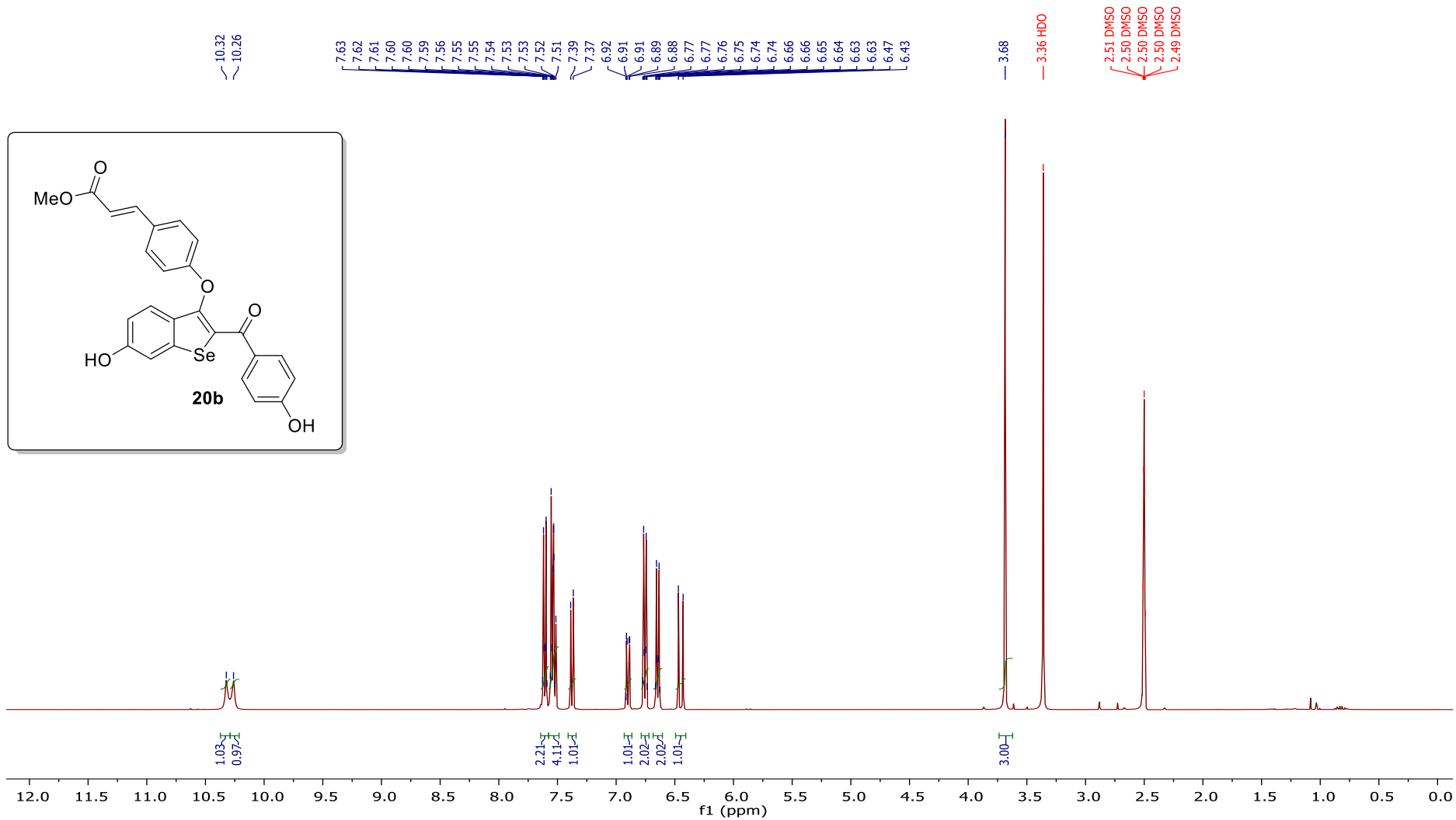
^{77}Se NMR (76.37 MHz, DMSO- d_6):



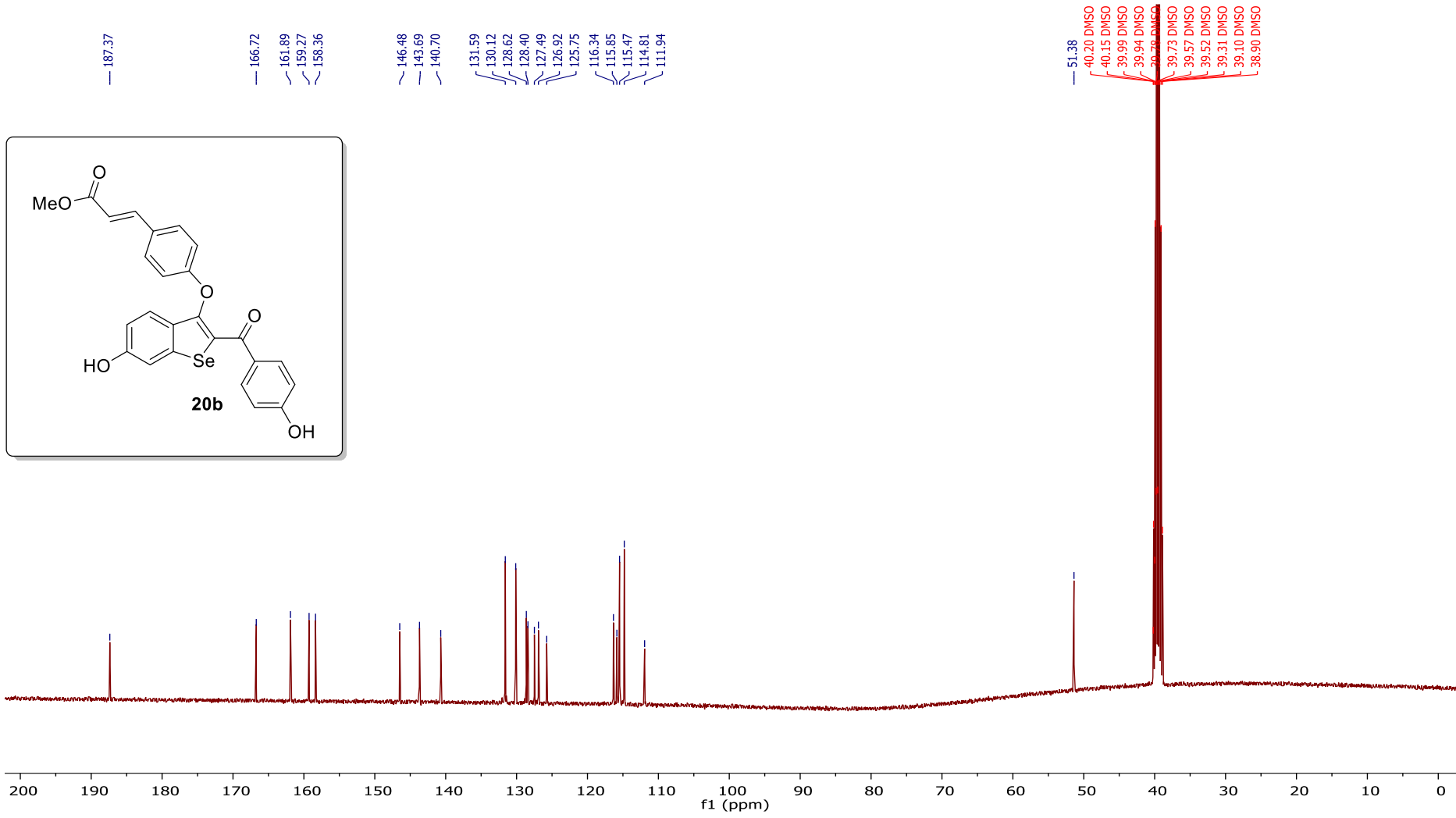
— 485.17



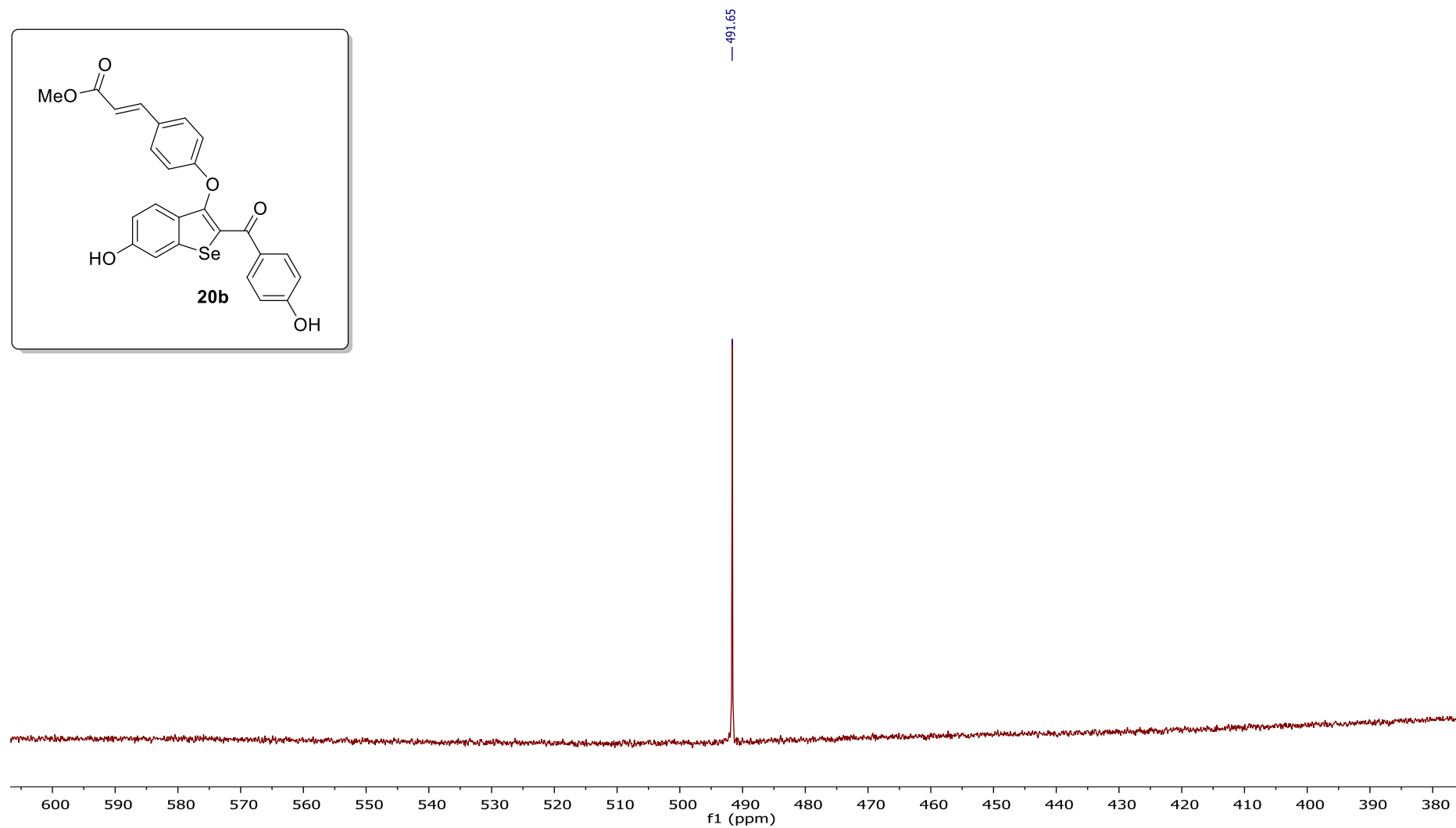
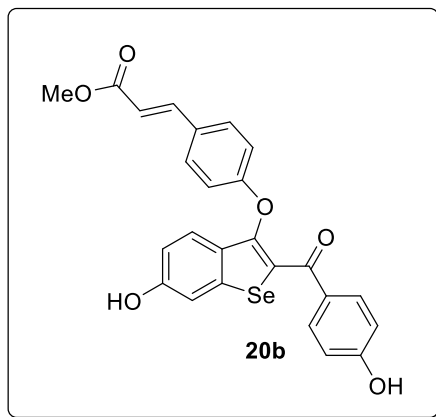
^1H NMR (400 MHz, DMSO- d_6):



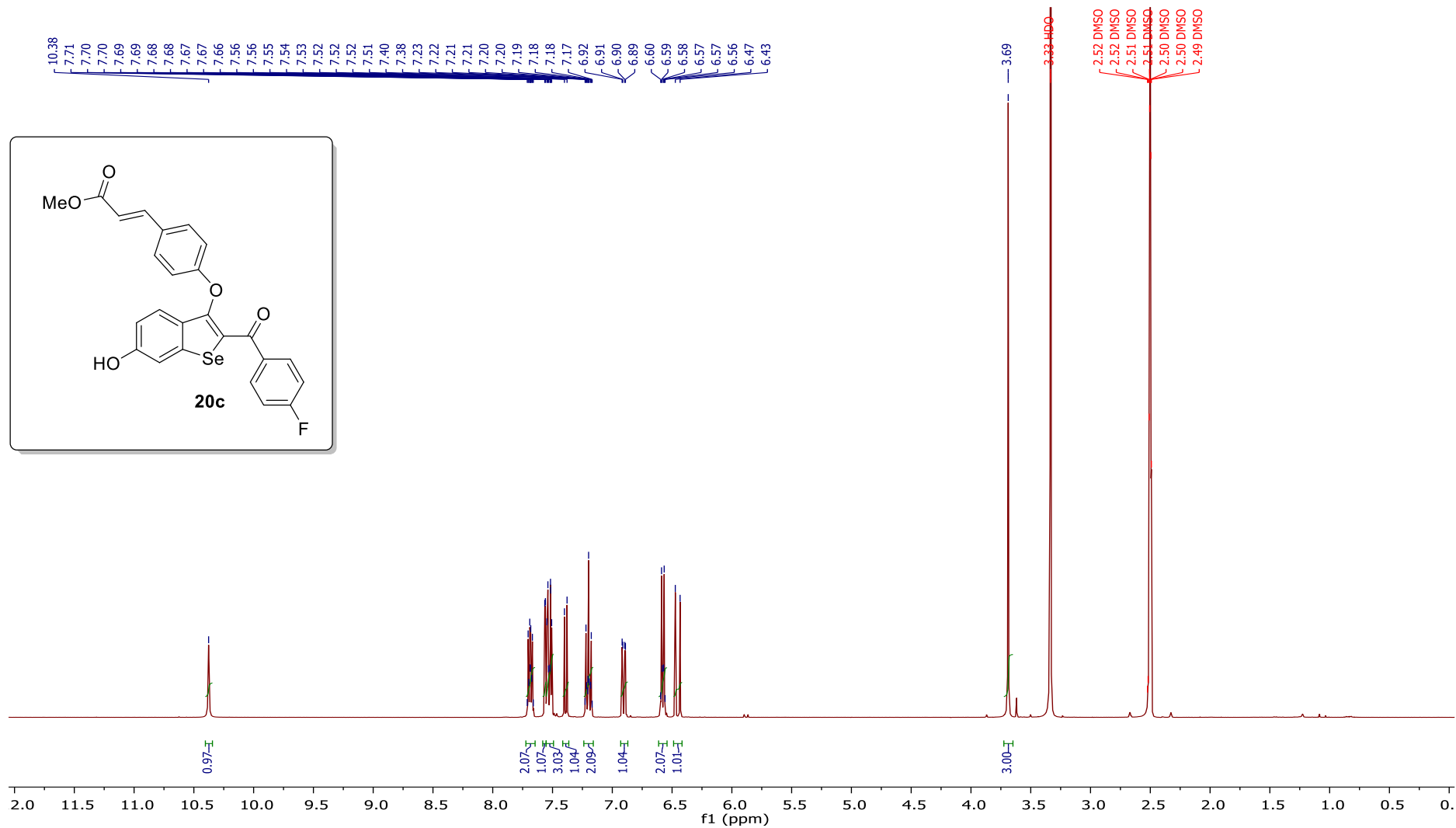
¹³C NMR (100.6 MHz, DMSO-d₆):



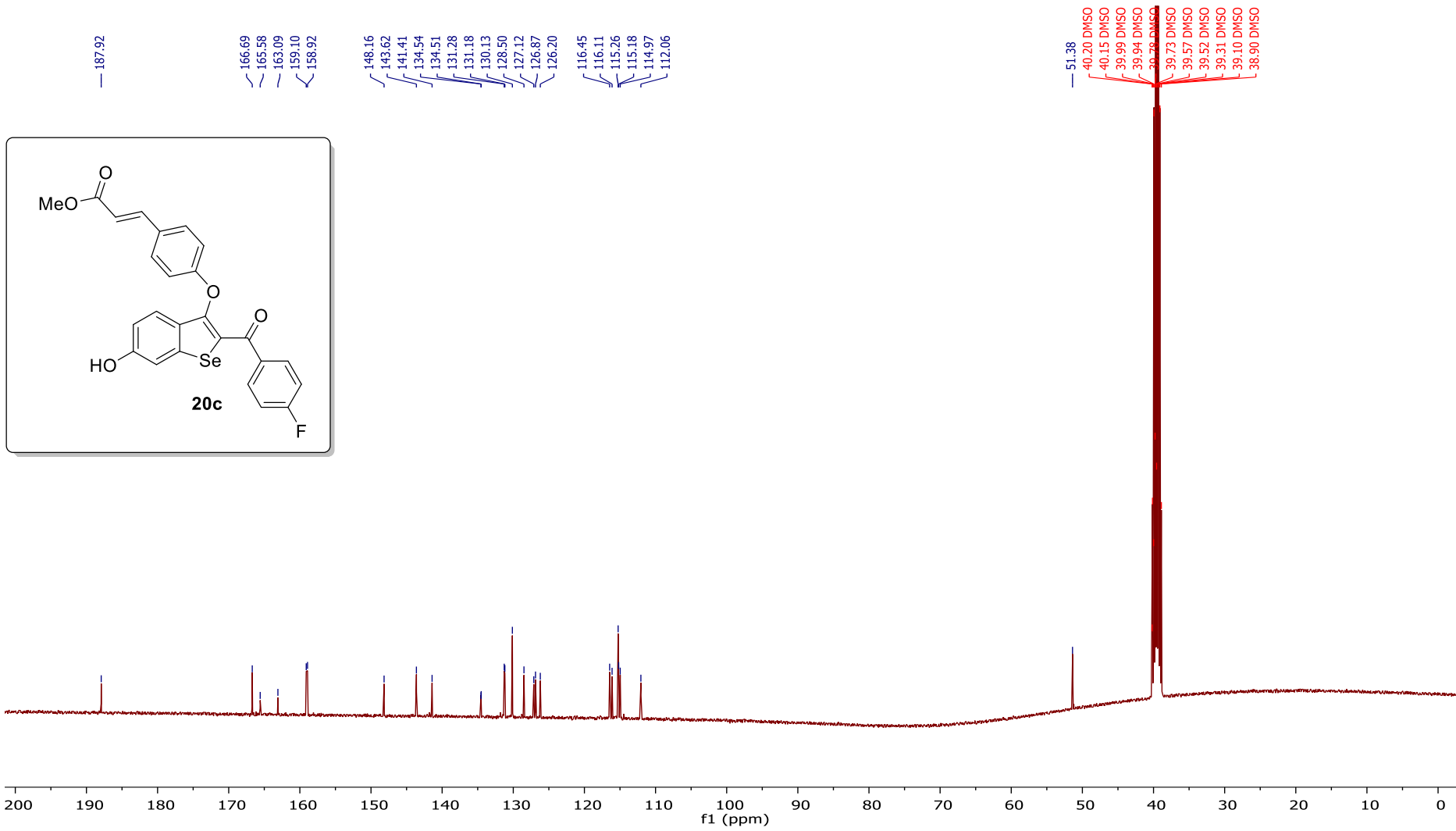
^{77}Se NMR (76.37 MHz, DMSO- d_6):



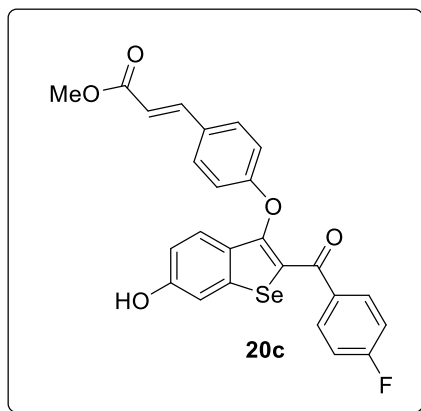
^1H NMR (400 MHz, DMSO- d_6):



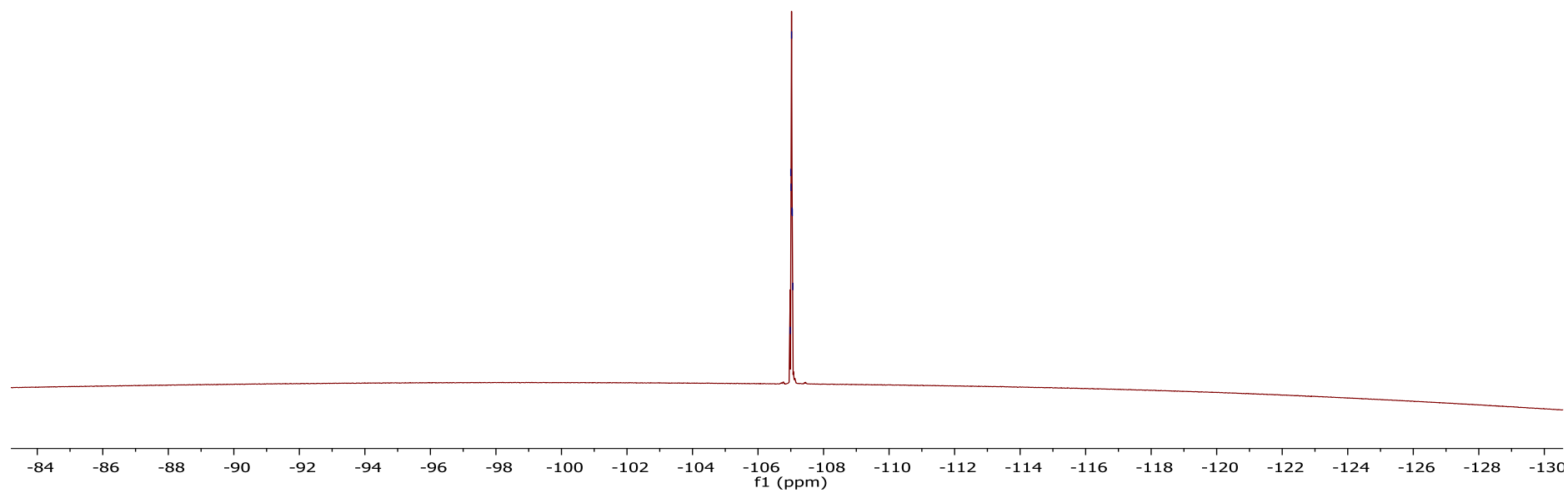
^{13}C NMR (100.6 MHz, DMSO- d_6):



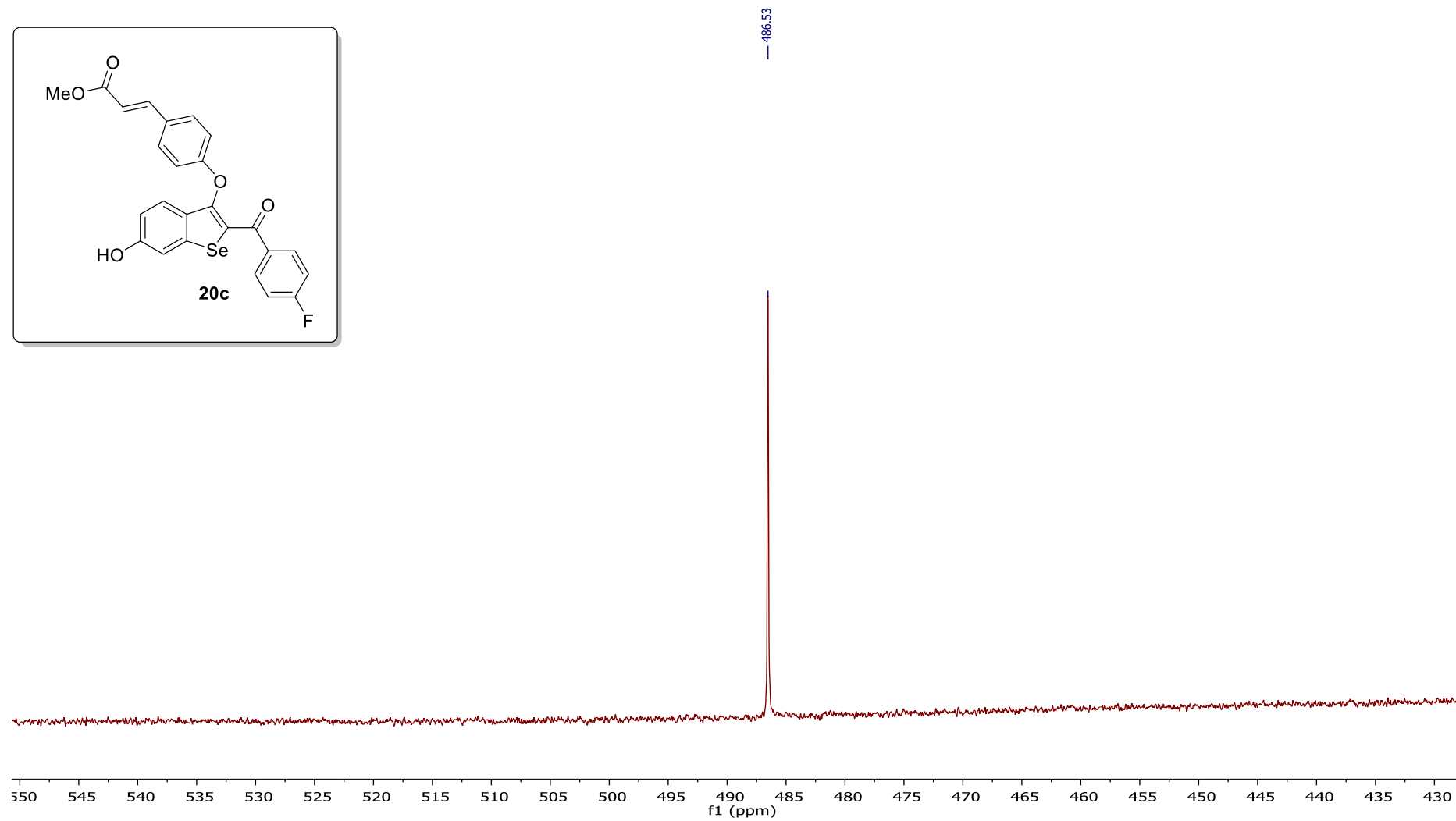
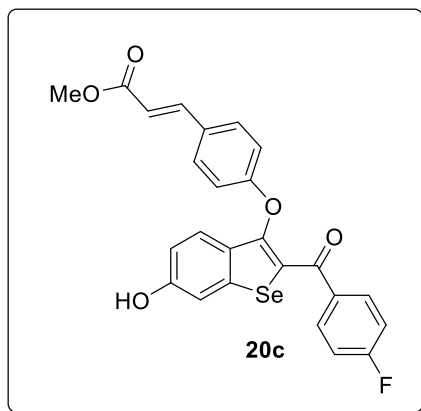
^{19}F NMR (376.21 MHz, DMSO- d_6):



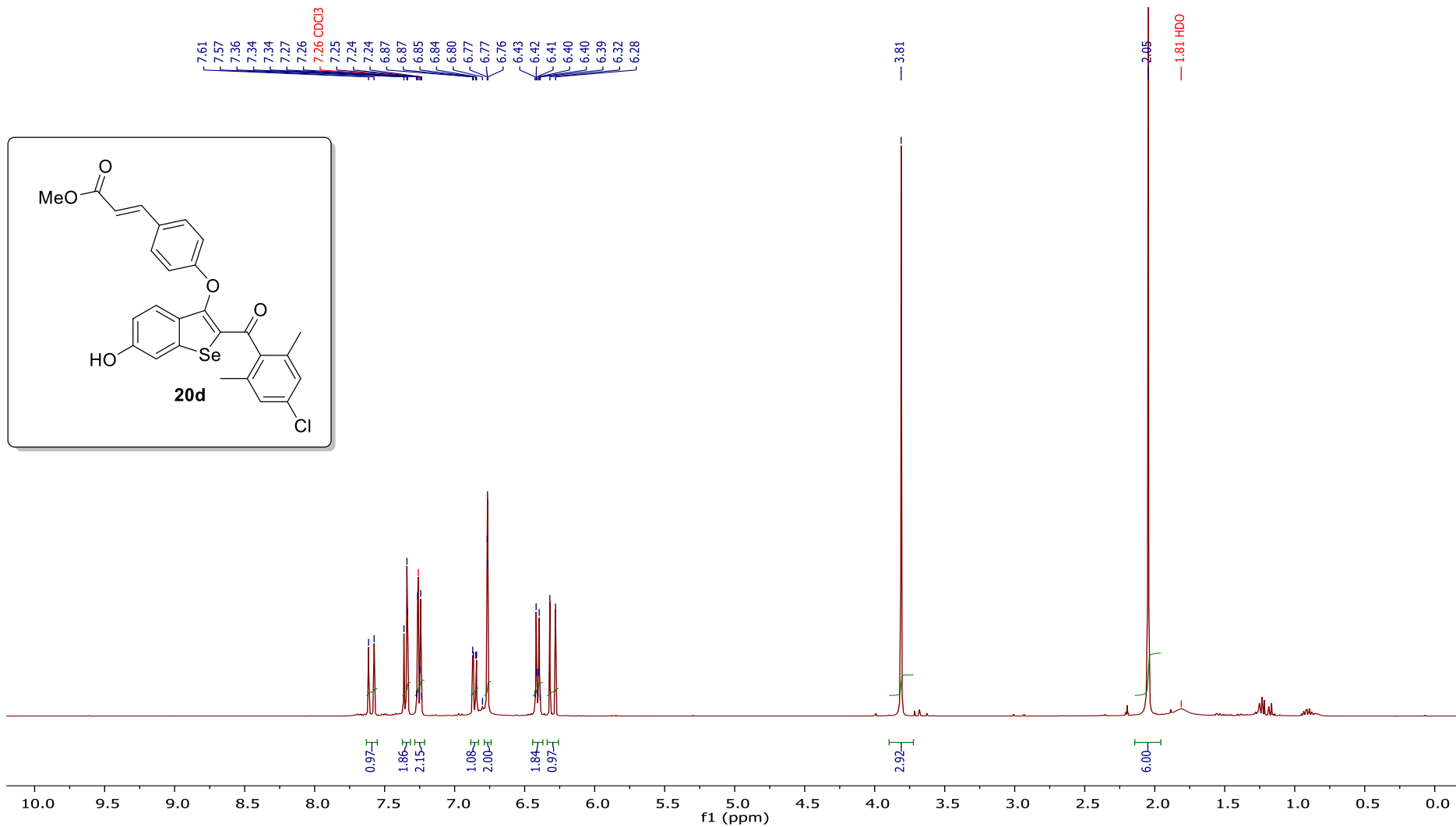
-106.98
-107.00
-107.01
-107.02
-107.04
-107.05
-107.06



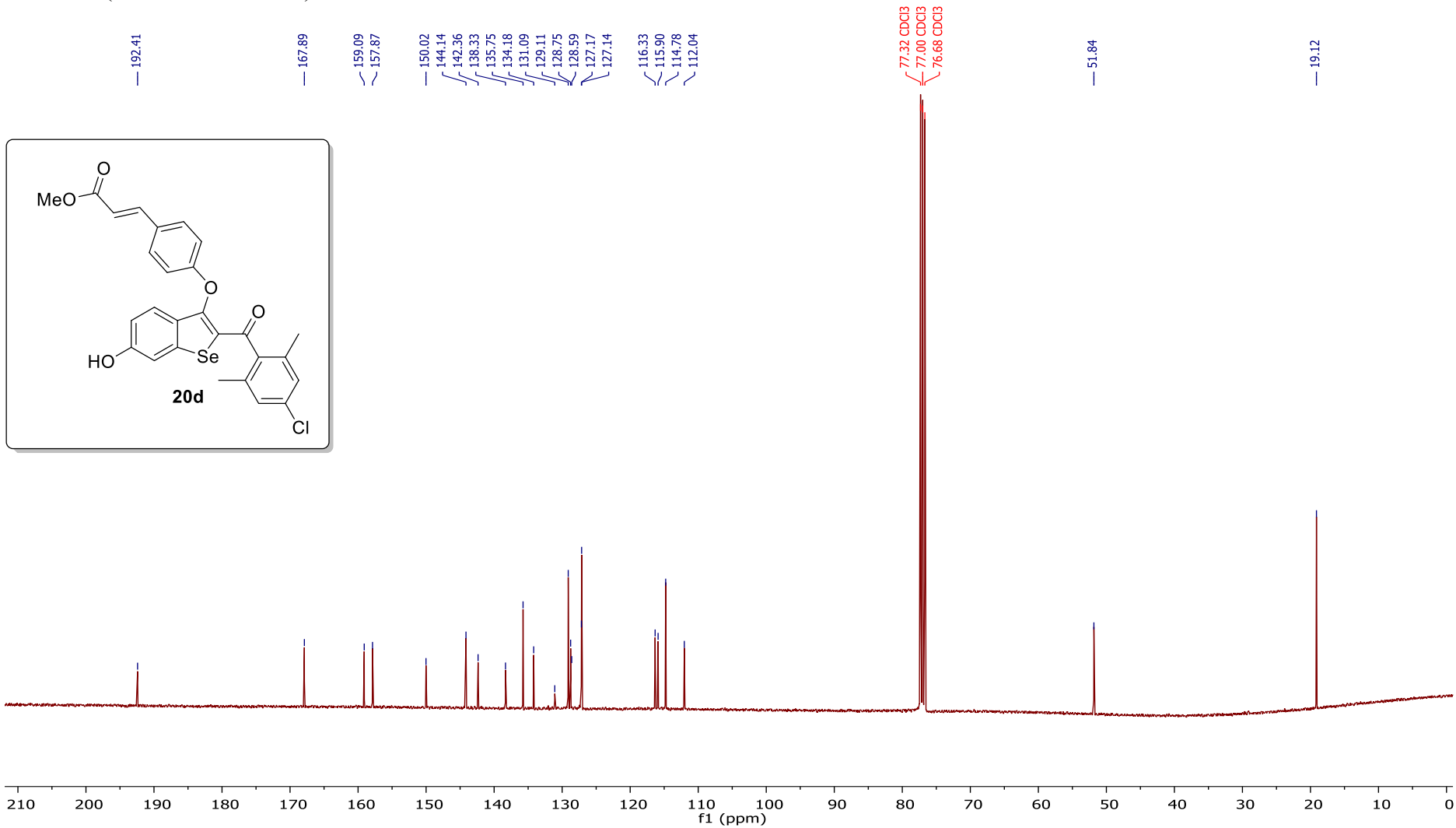
^{77}Se NMR (76.37 MHz, DMSO- d_6):



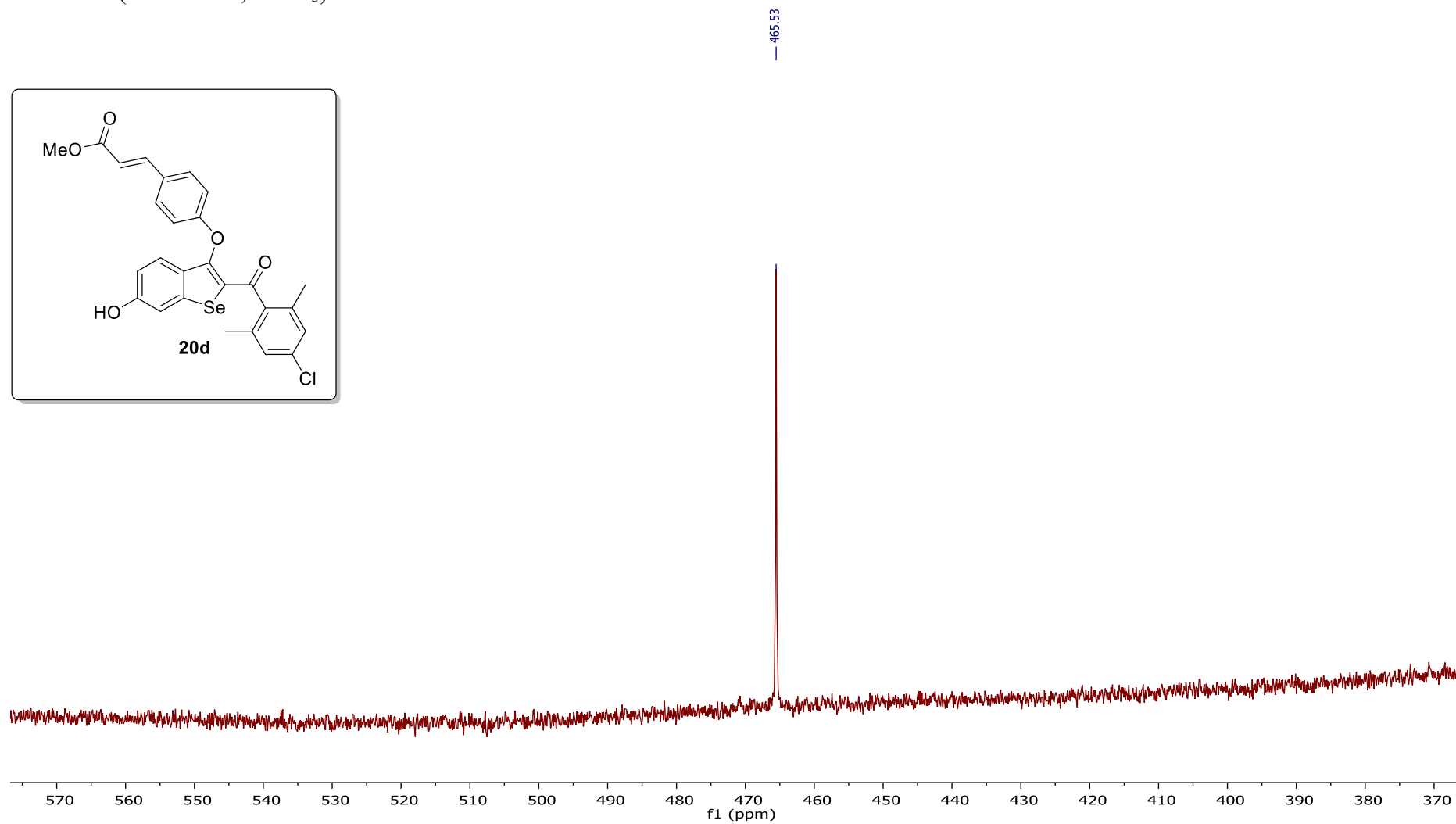
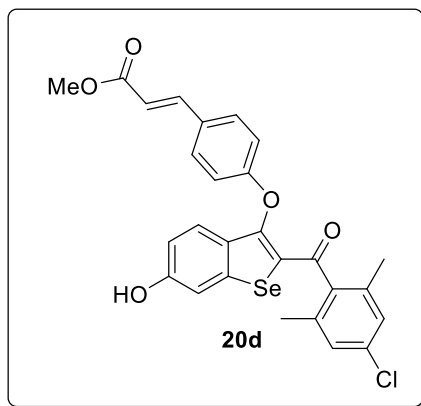
^1H NMR (400 MHz, CDCl_3):



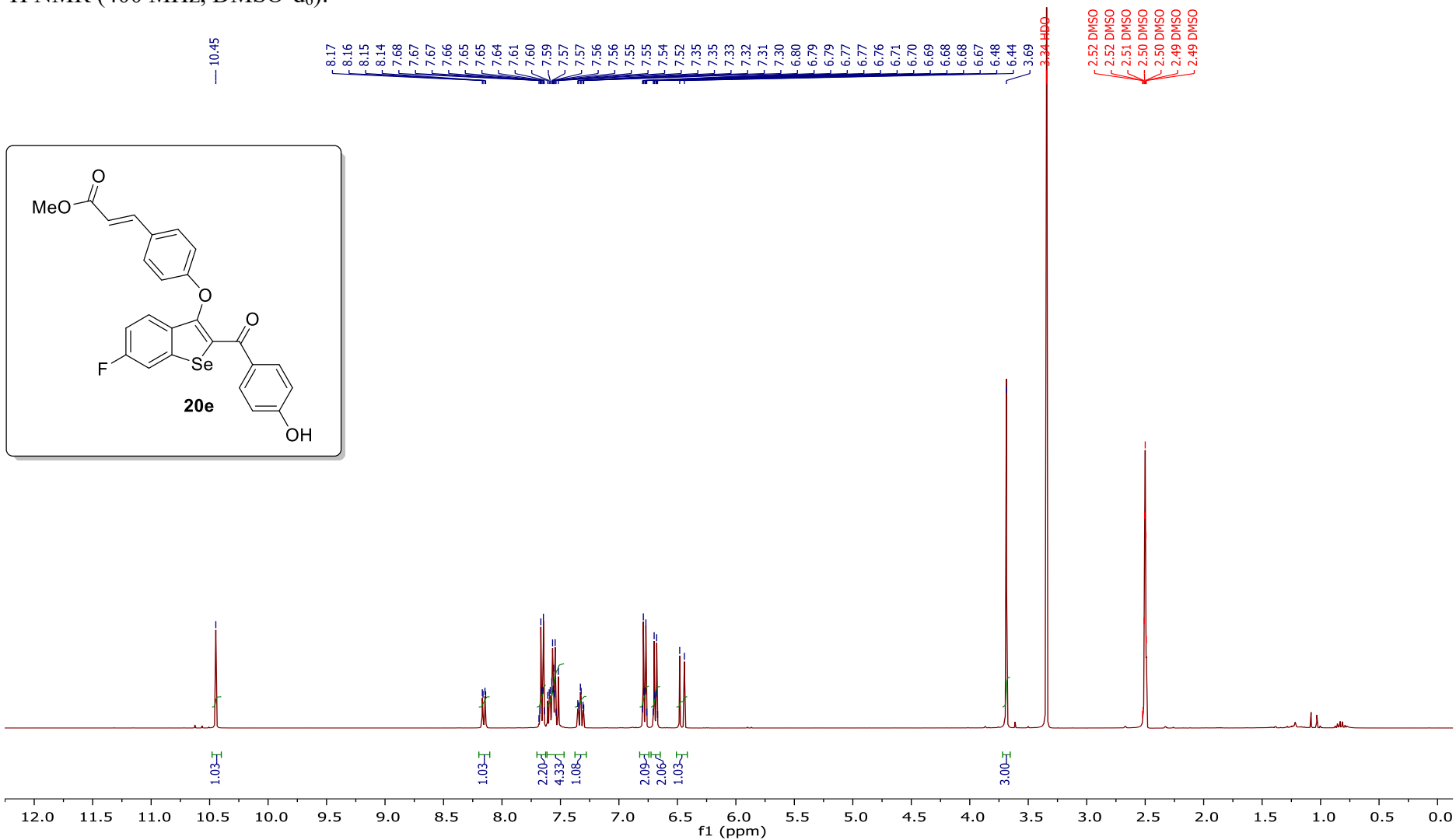
^{13}C NMR (100.6 MHz, CDCl_3):



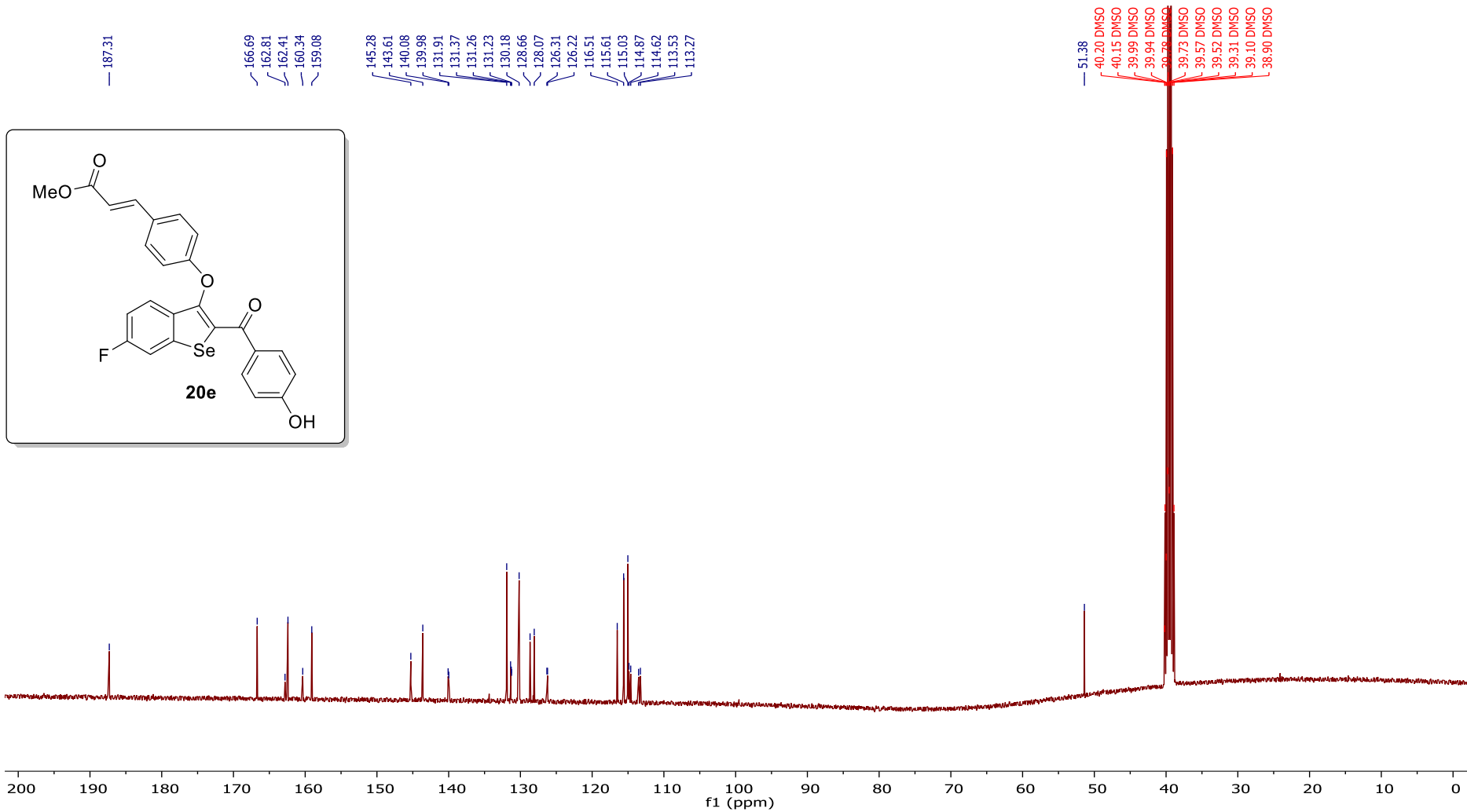
^{77}Se NMR (76.37 MHz, CDCl_3):



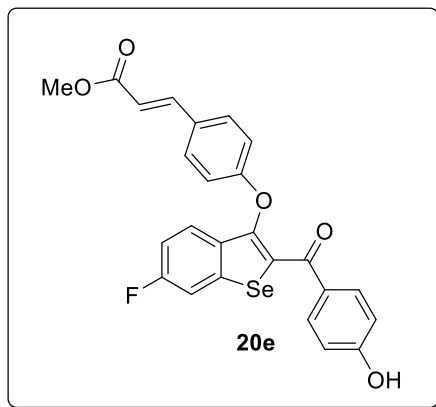
^1H NMR (400 MHz, DMSO- d_6):



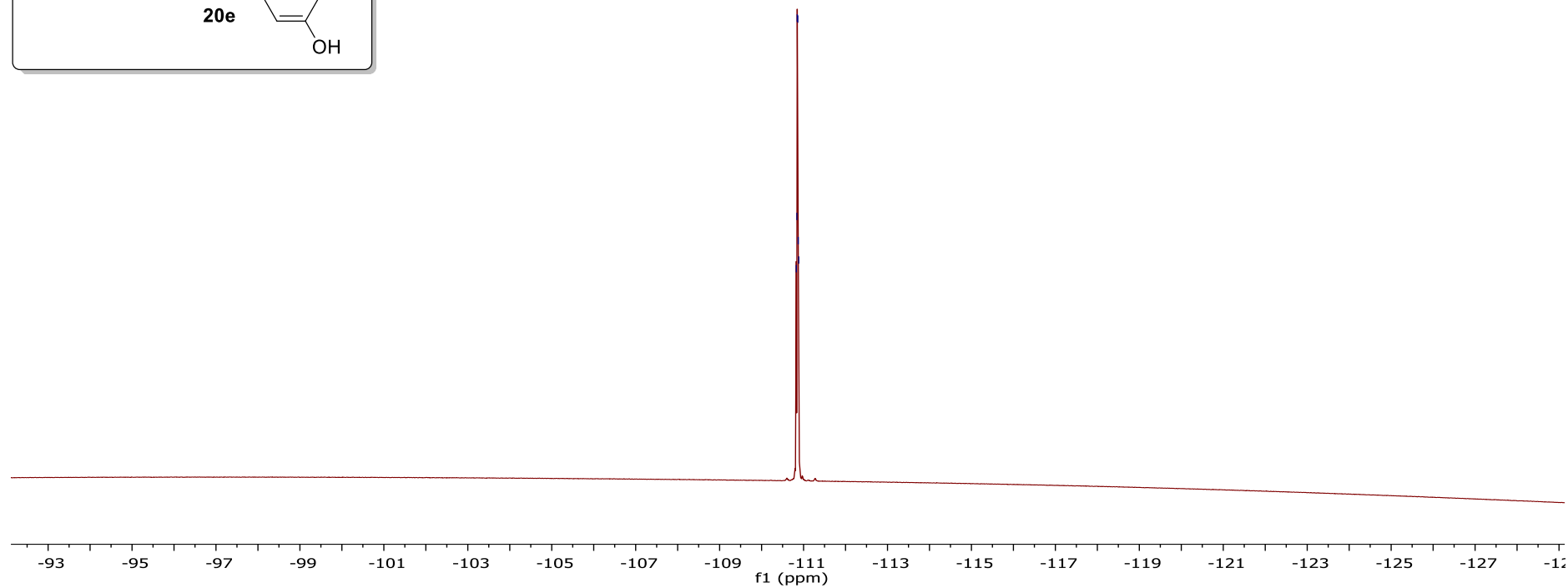
^{13}C NMR (100.6 MHz, DMSO- d_6):



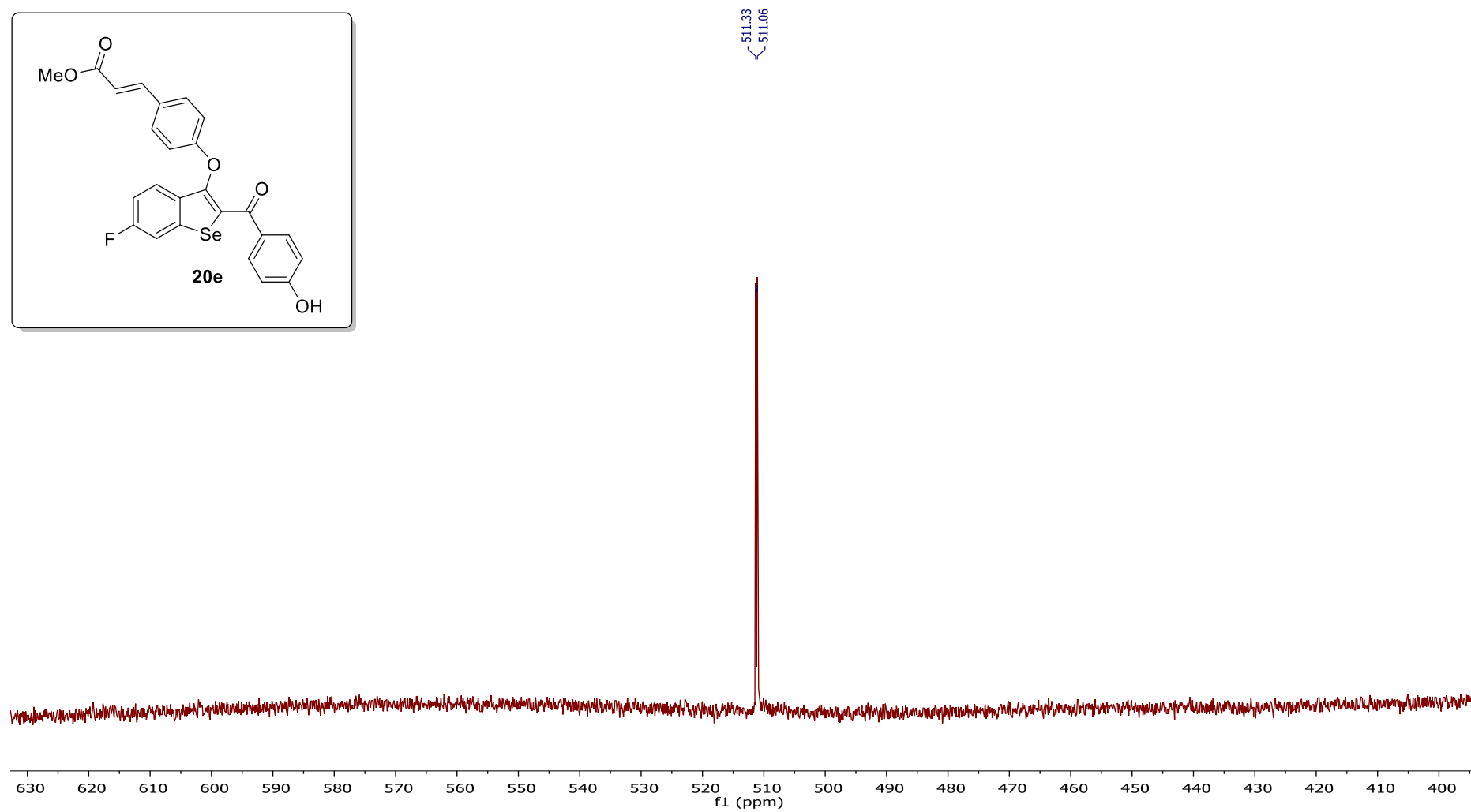
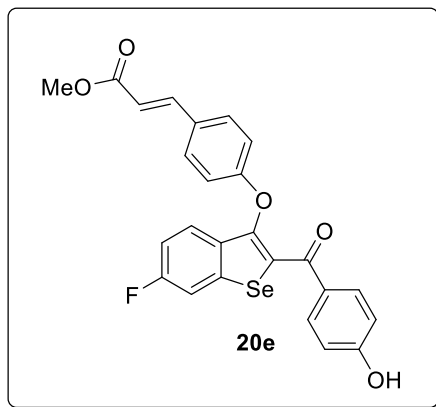
^{19}F NMR (376.21 MHz, DMSO-d_6):



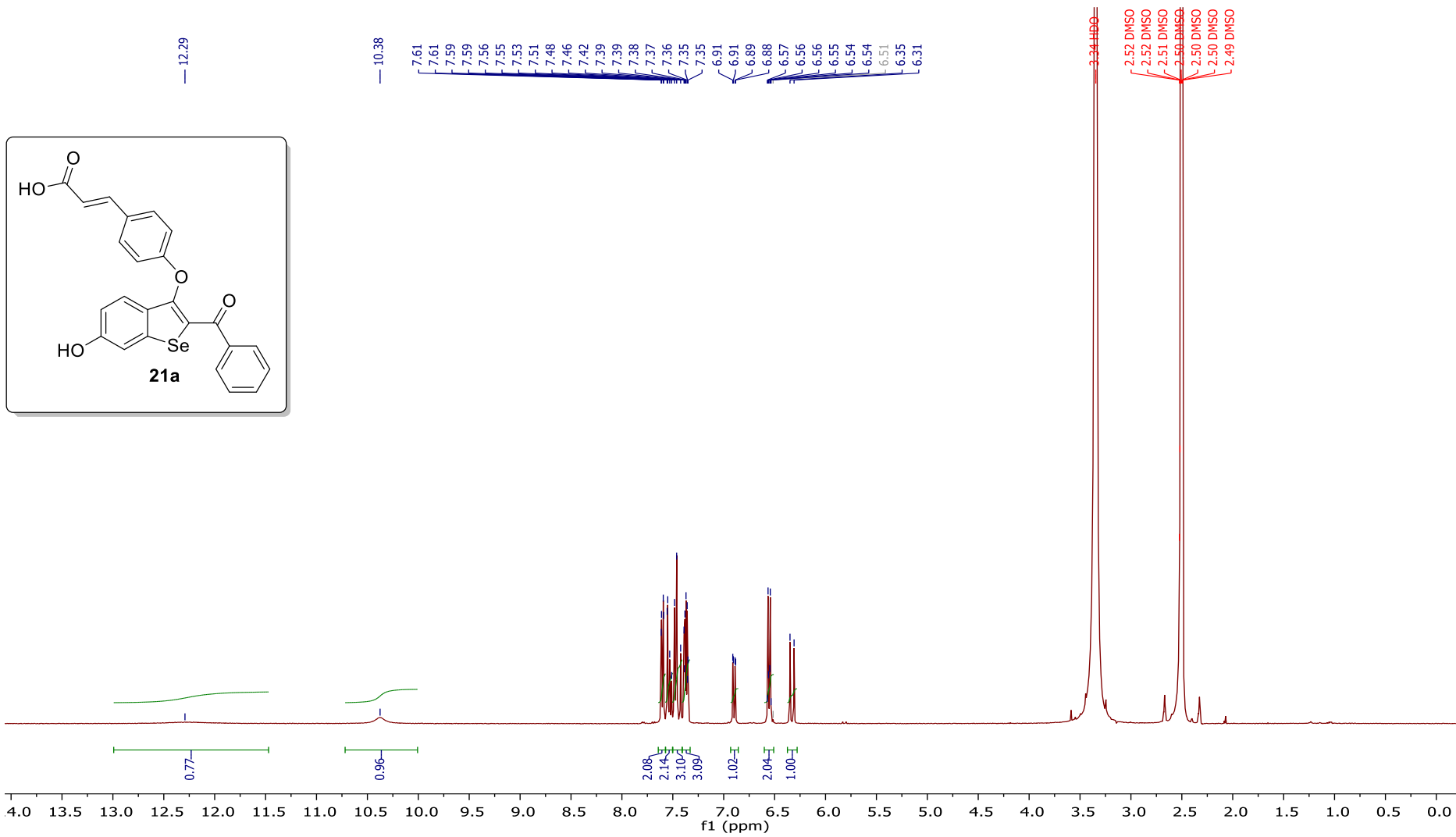
-110.83
-110.84
-110.85
-110.86
-110.87
-110.89



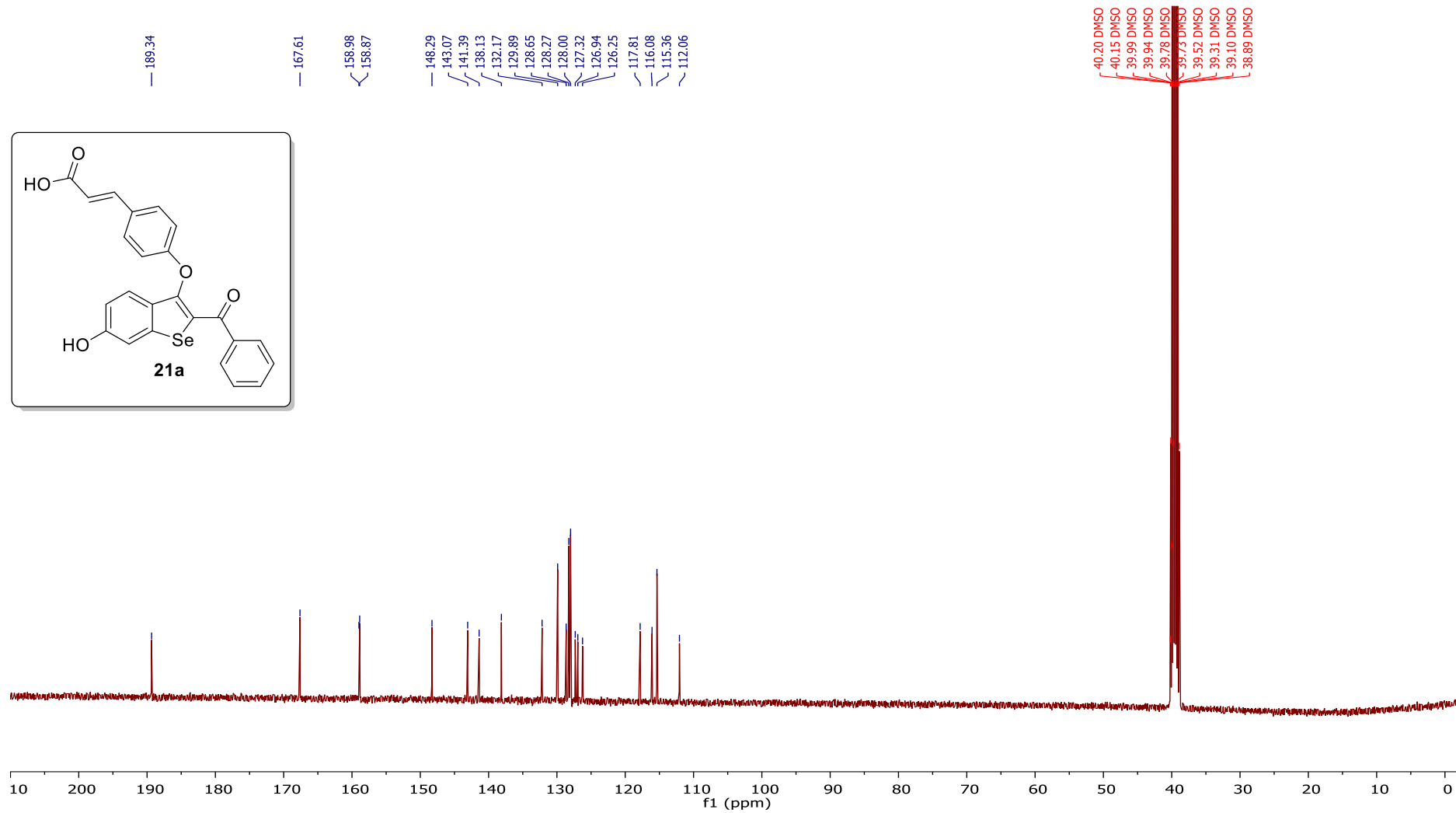
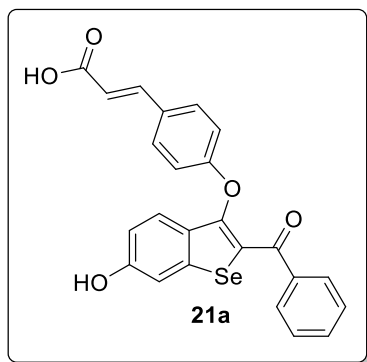
^{77}Se NMR (76.37 MHz, DMSO- d_6):



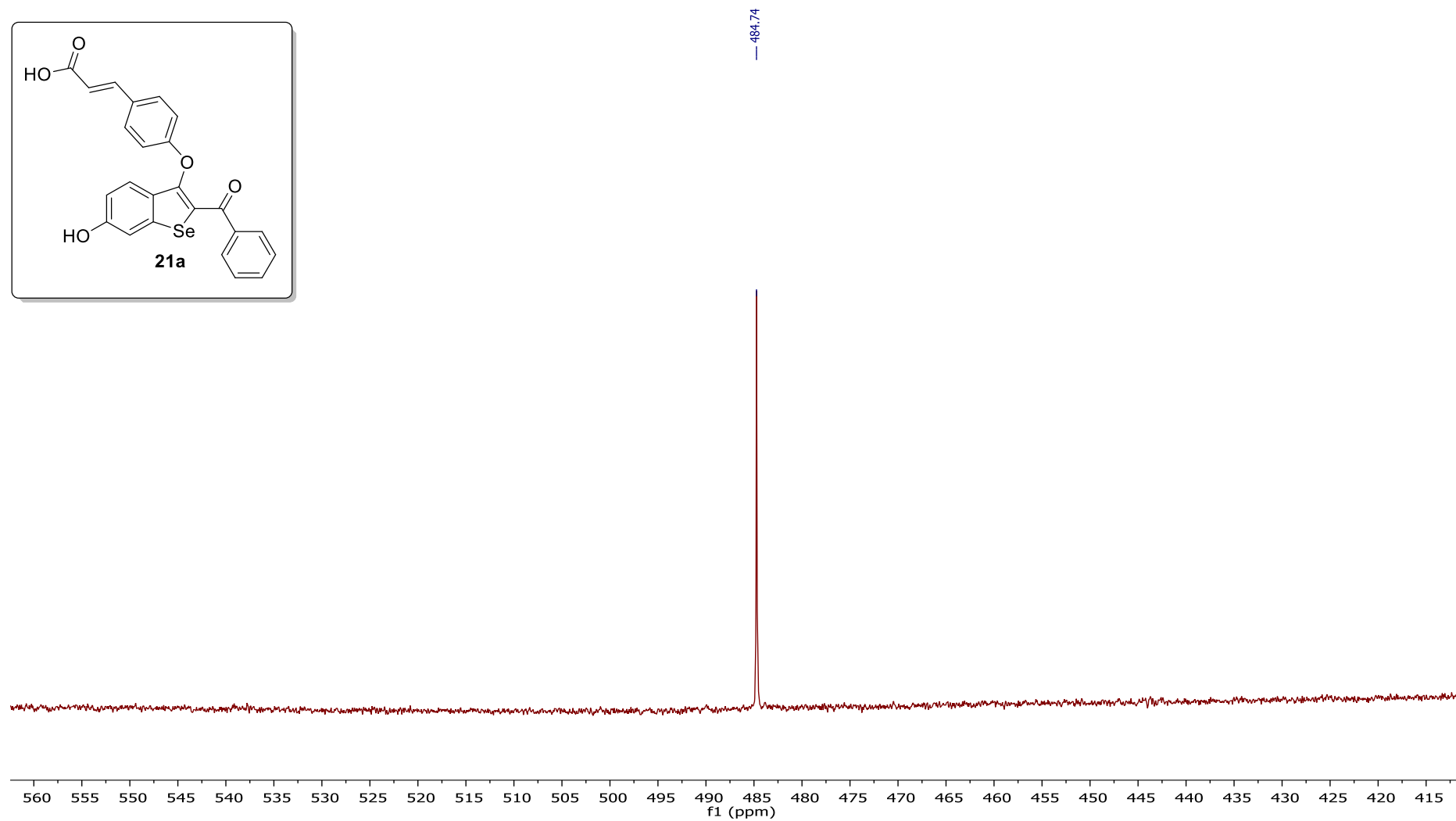
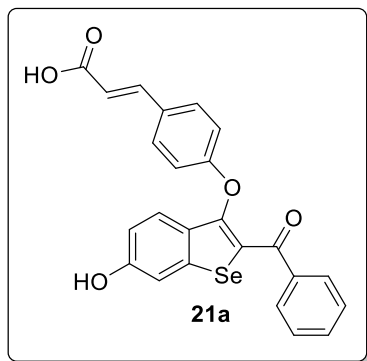
^1H NMR (400 MHz, DMSO- d_6):



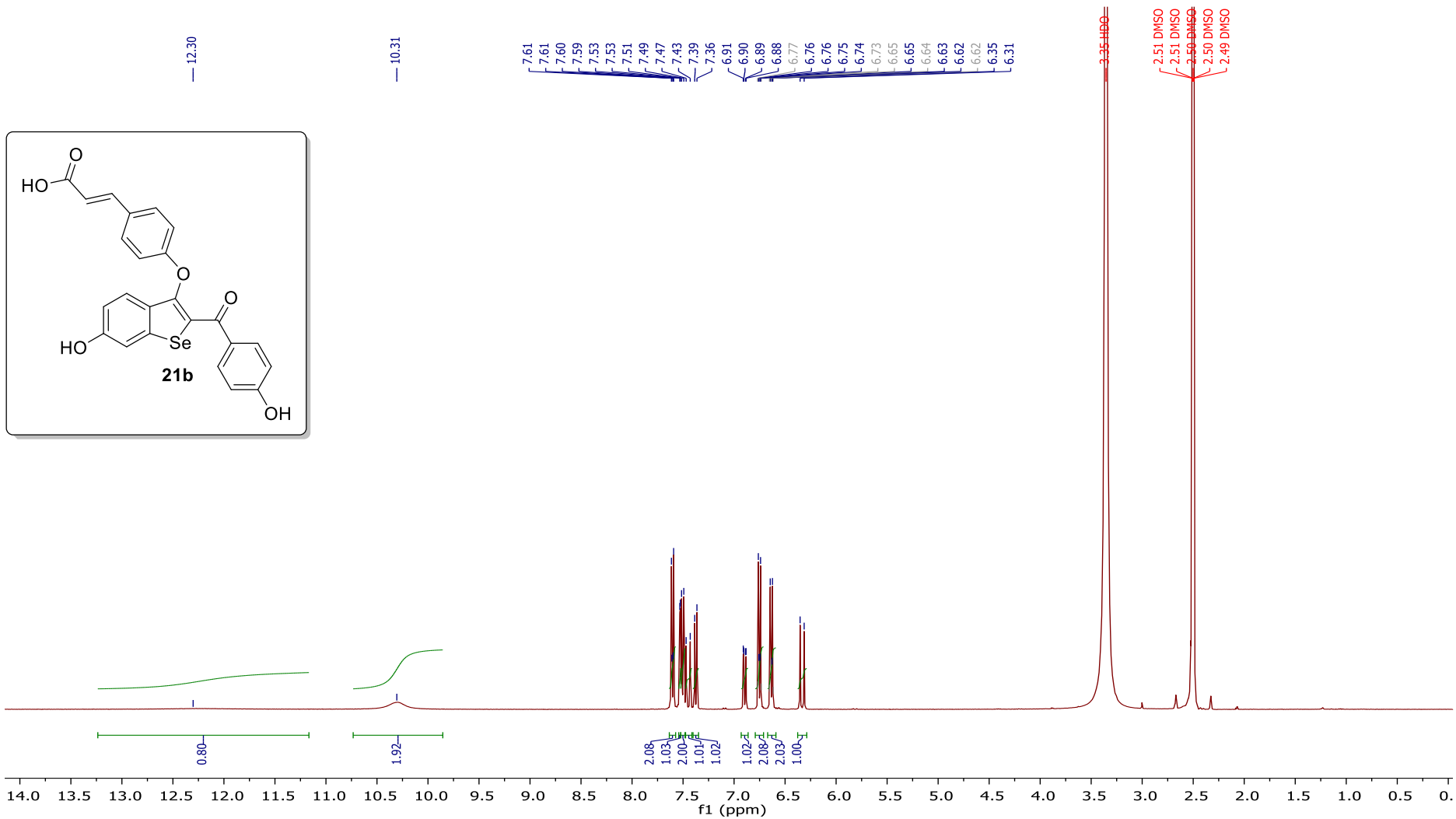
^{13}C NMR (100.6 MHz, DMSO- d_6):



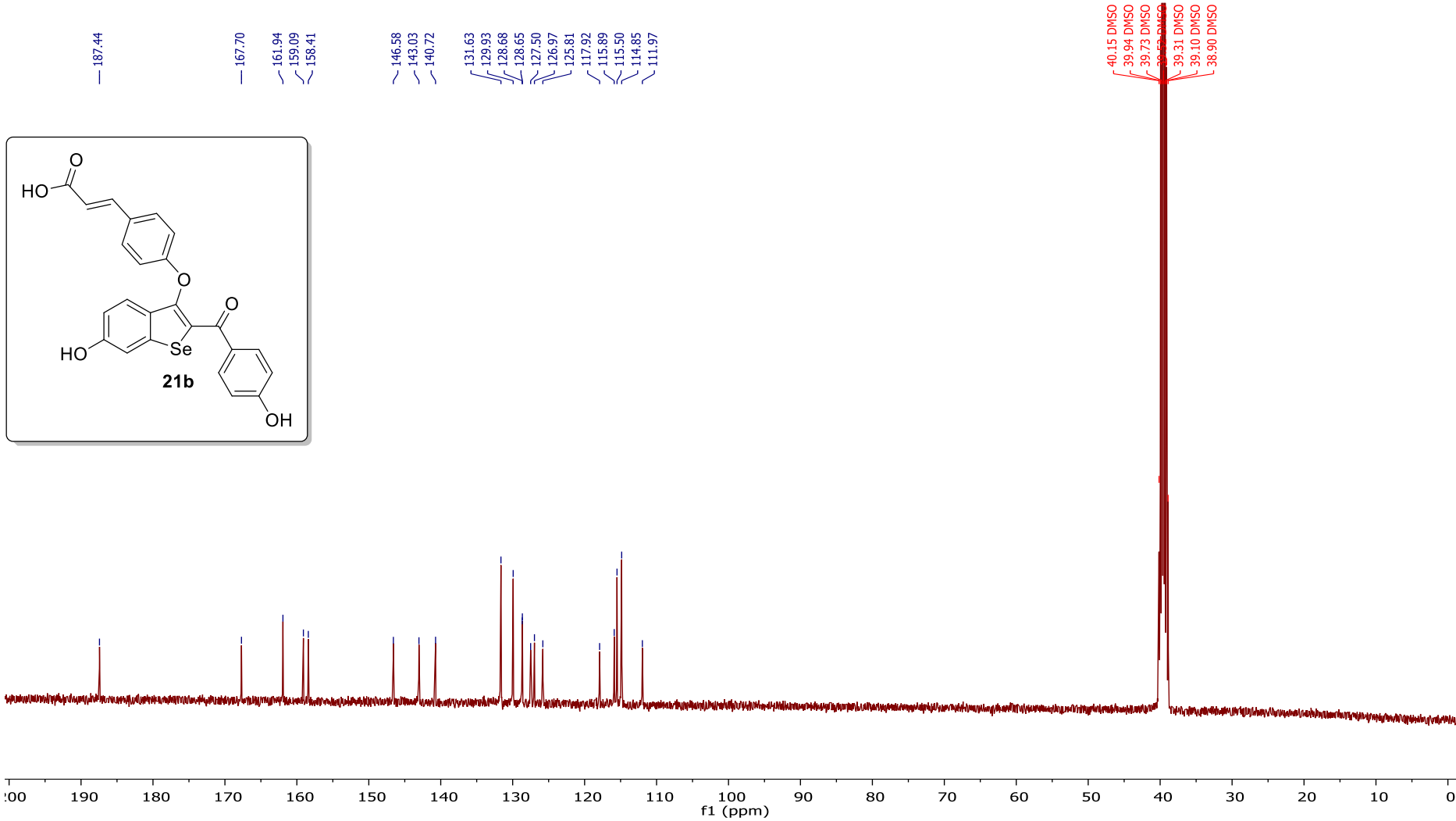
^{77}Se NMR (76.37 MHz, DMSO- d_6):



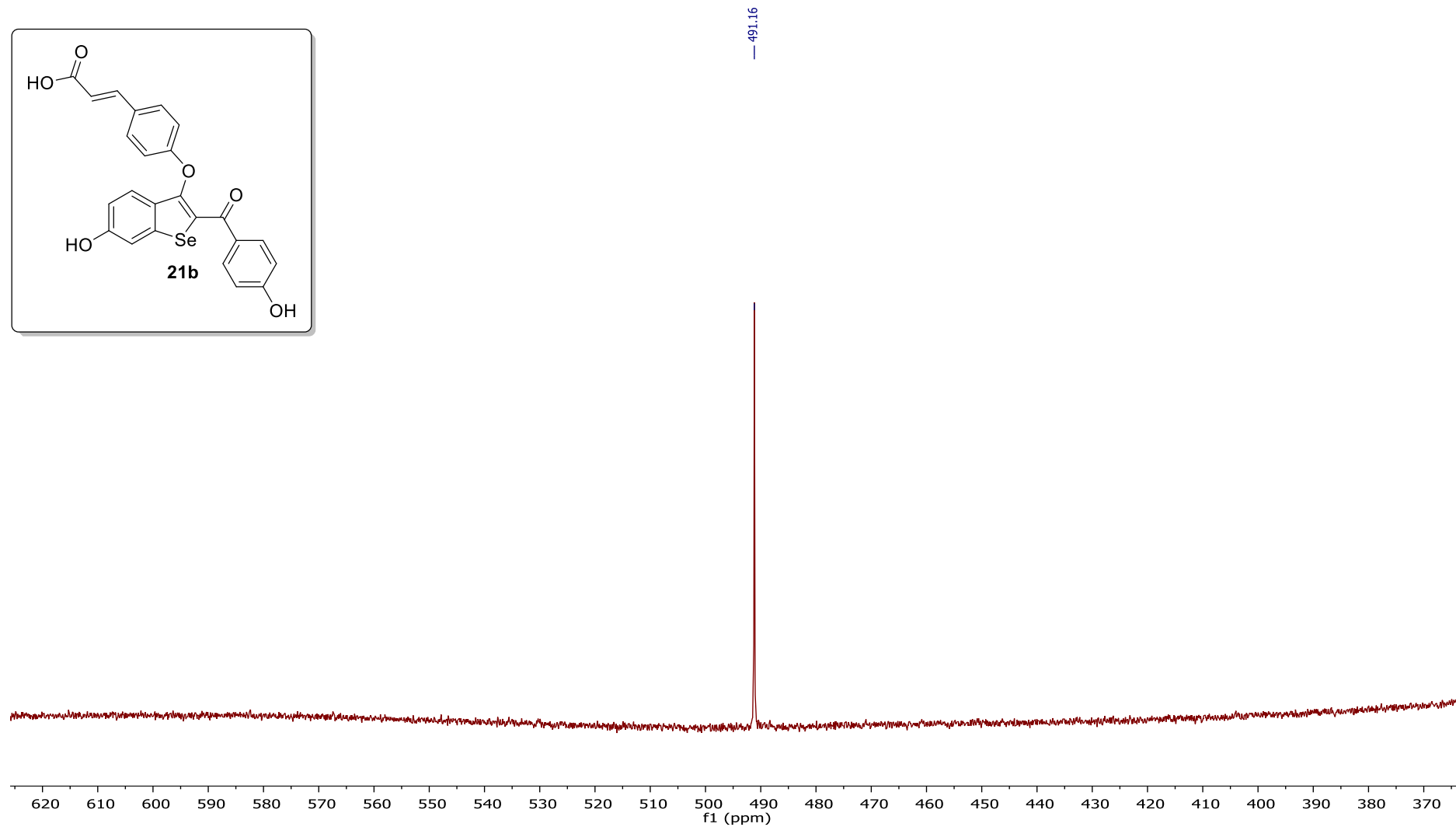
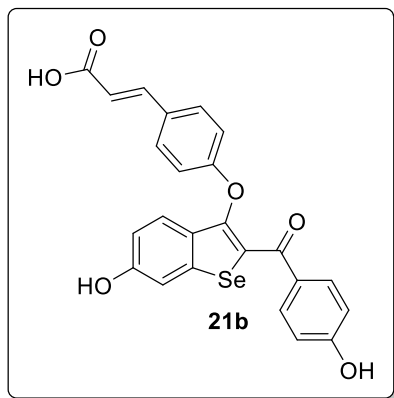
^1H NMR (400 MHz, DMSO- d_6):



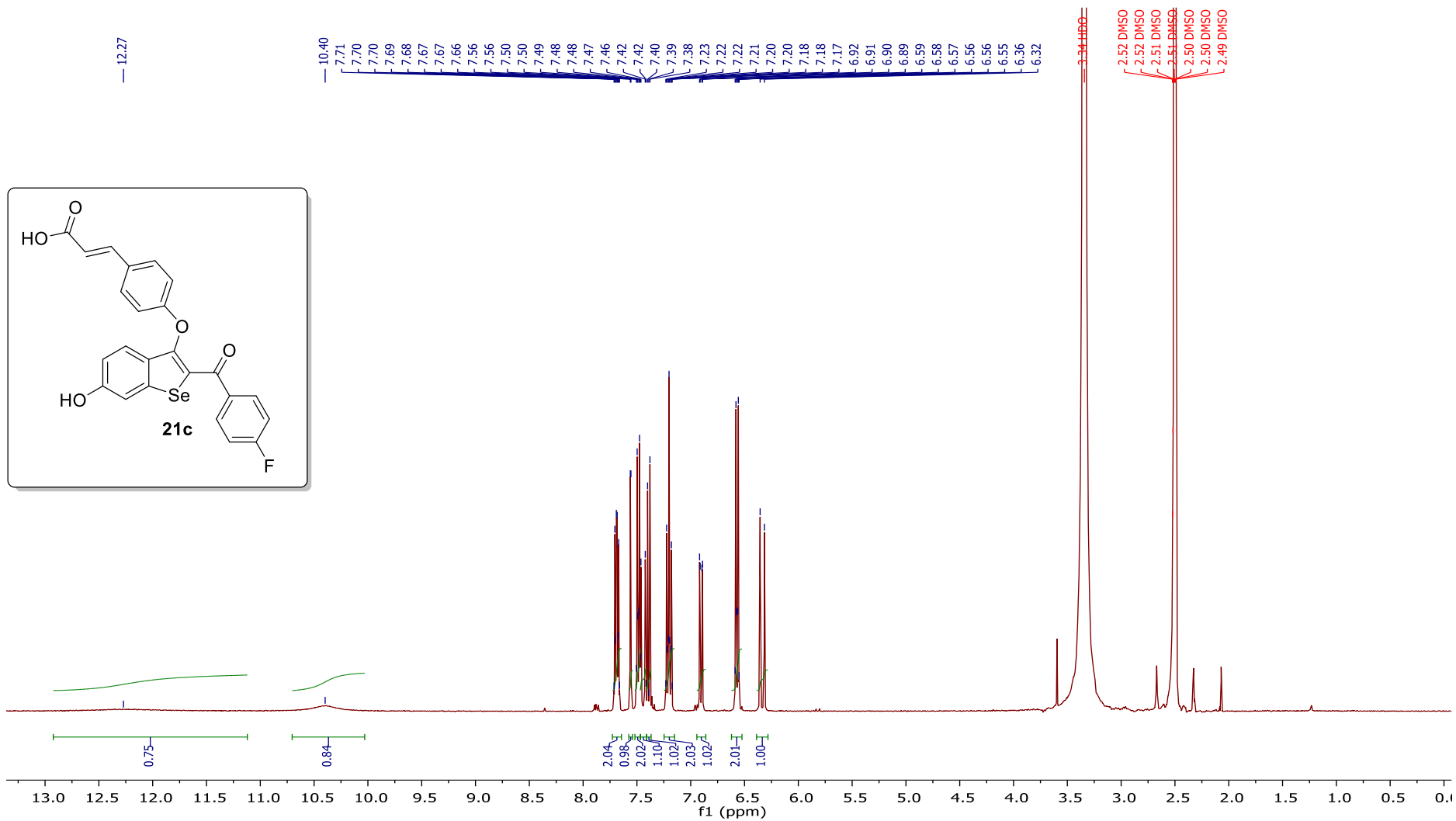
^{13}C NMR (100.6 MHz, DMSO- d_6):



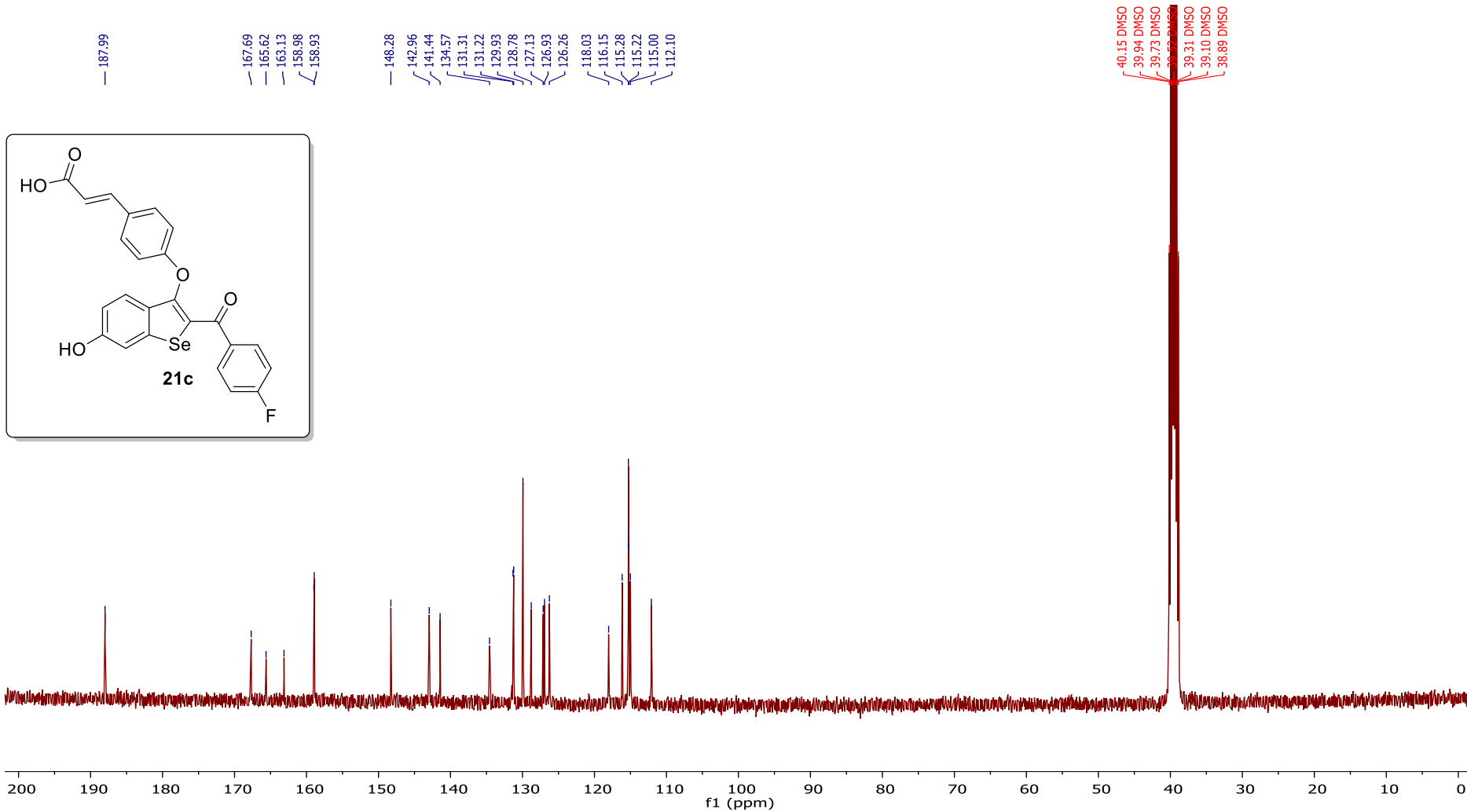
^{77}Se NMR (76.37 MHz, DMSO- d_6):



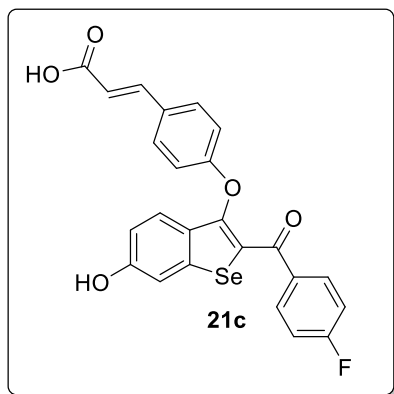
^1H NMR (400 MHz, DMSO- d_6):



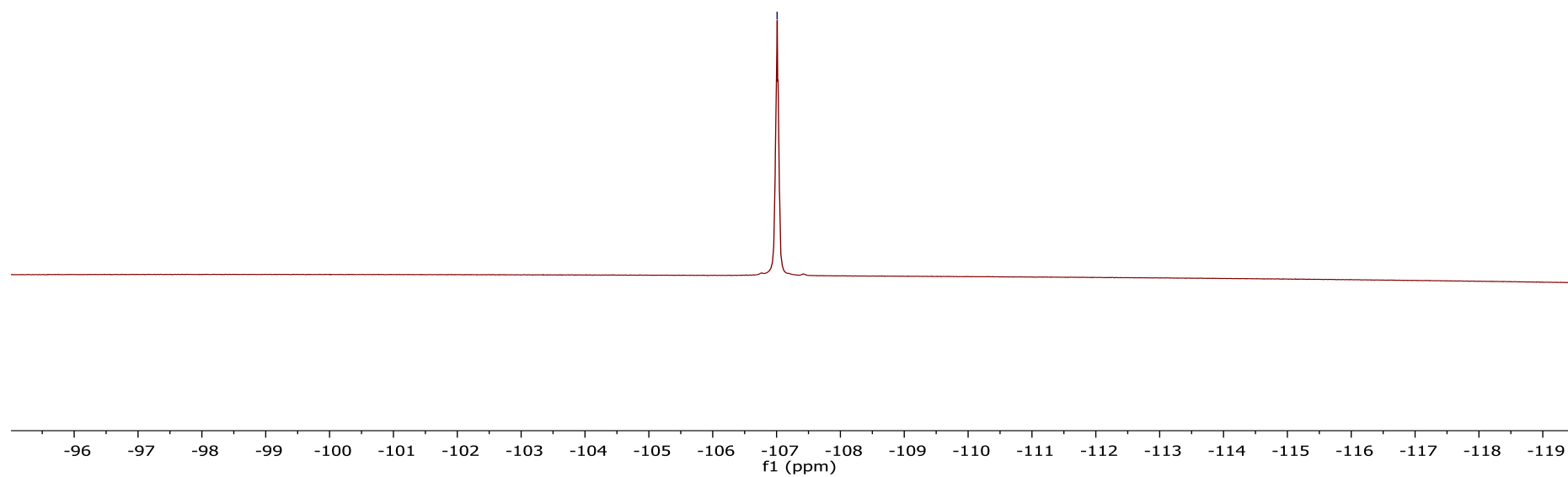
¹³C NMR (100.6 MHz, DMSO-d₆):



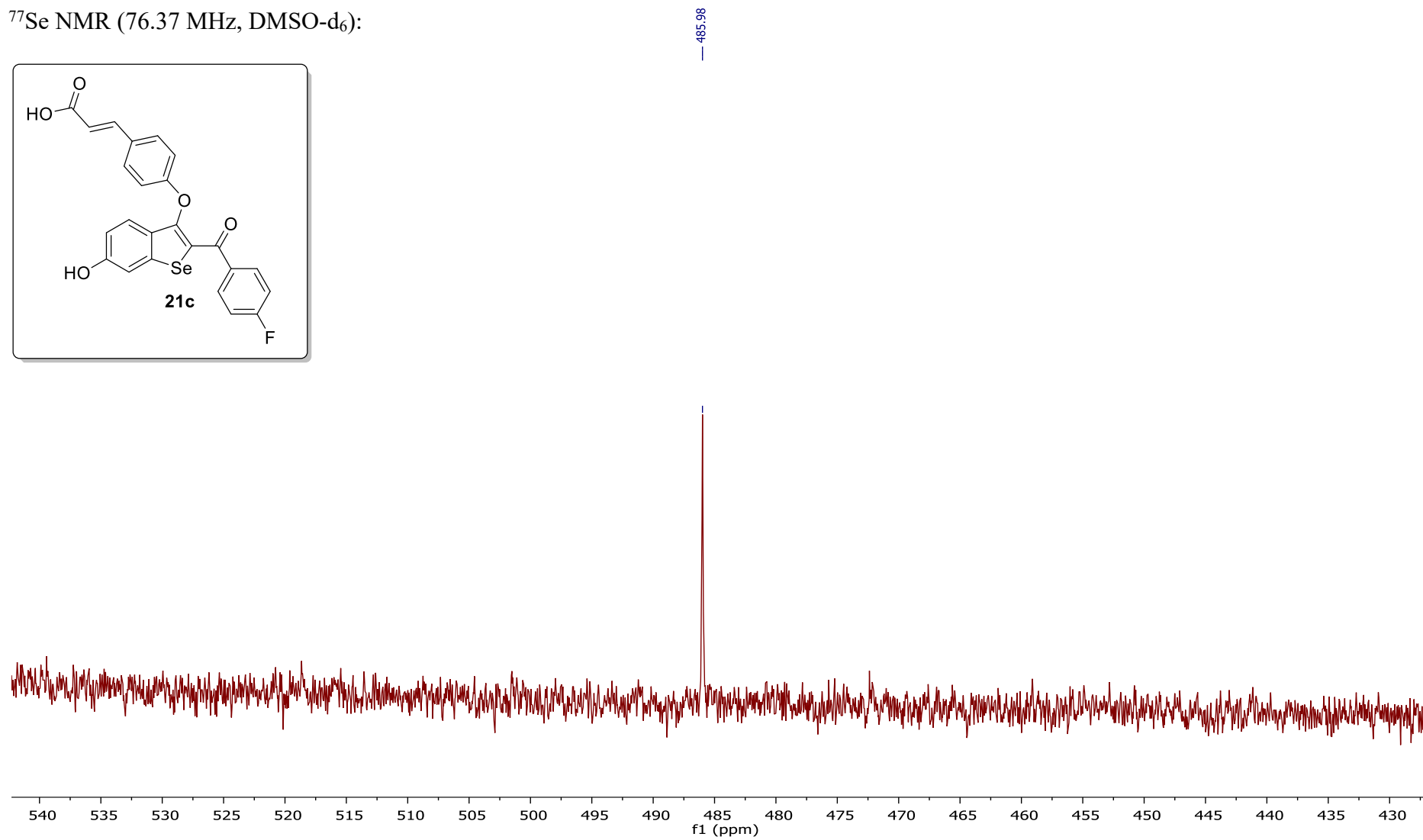
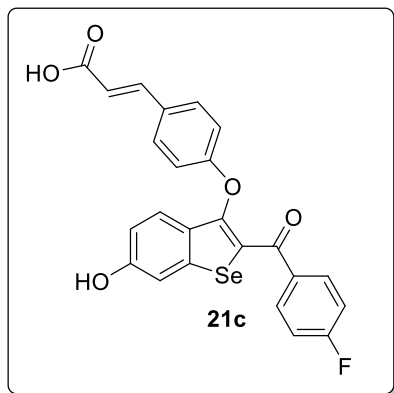
^{19}F NMR (376.21 MHz, DMSO-d_6):



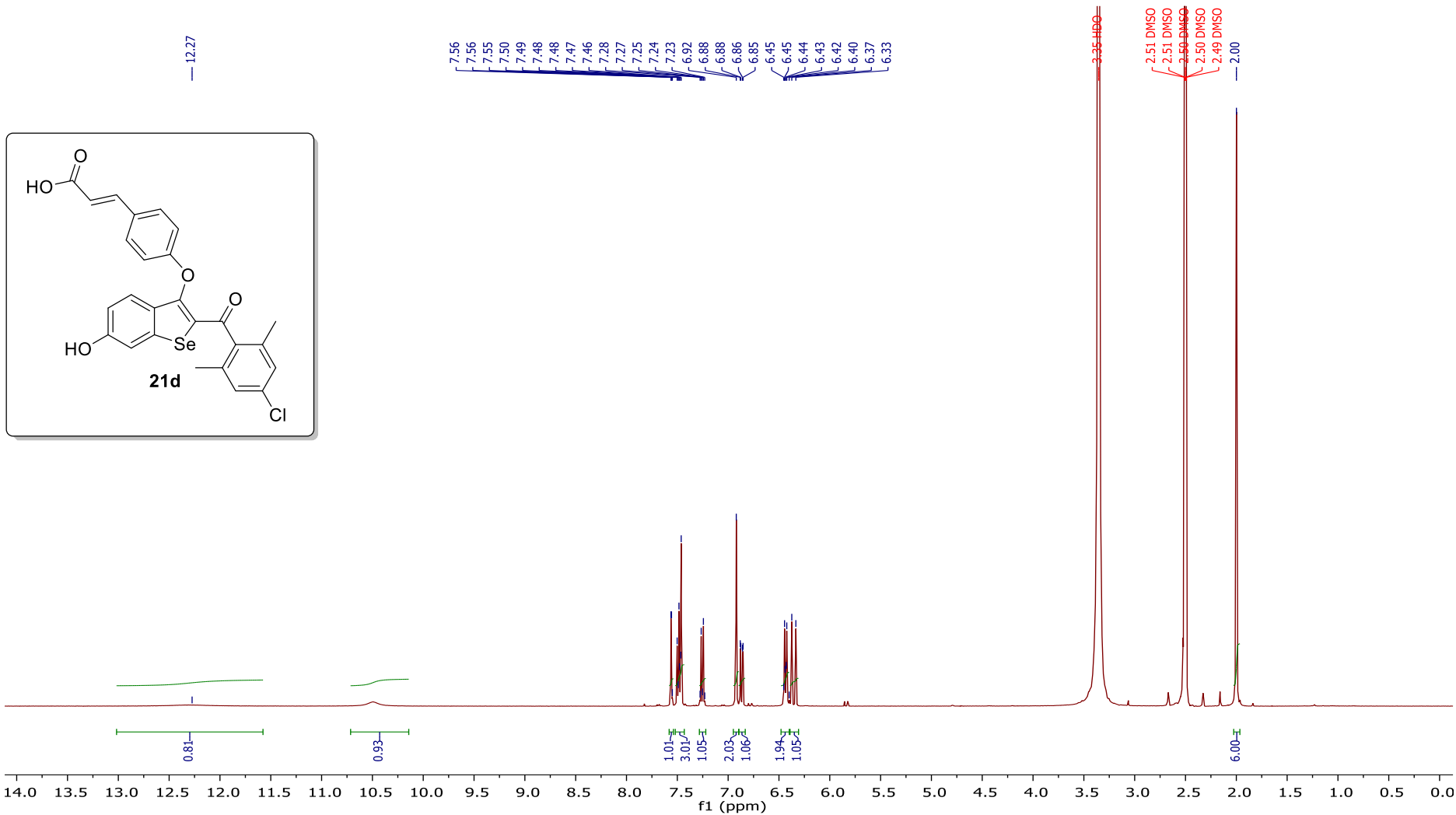
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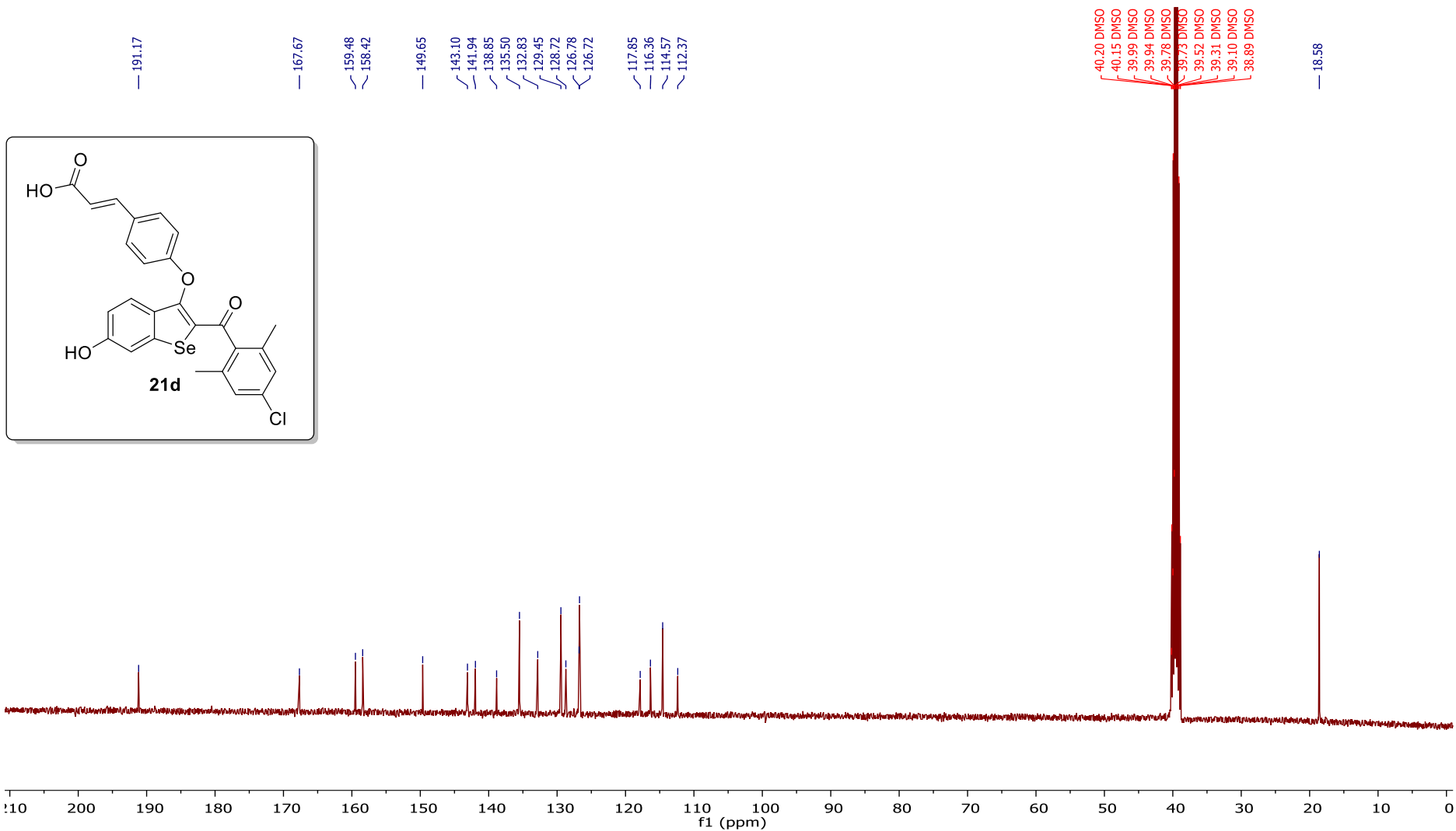
^{77}Se NMR (76.37 MHz, DMSO- d_6):



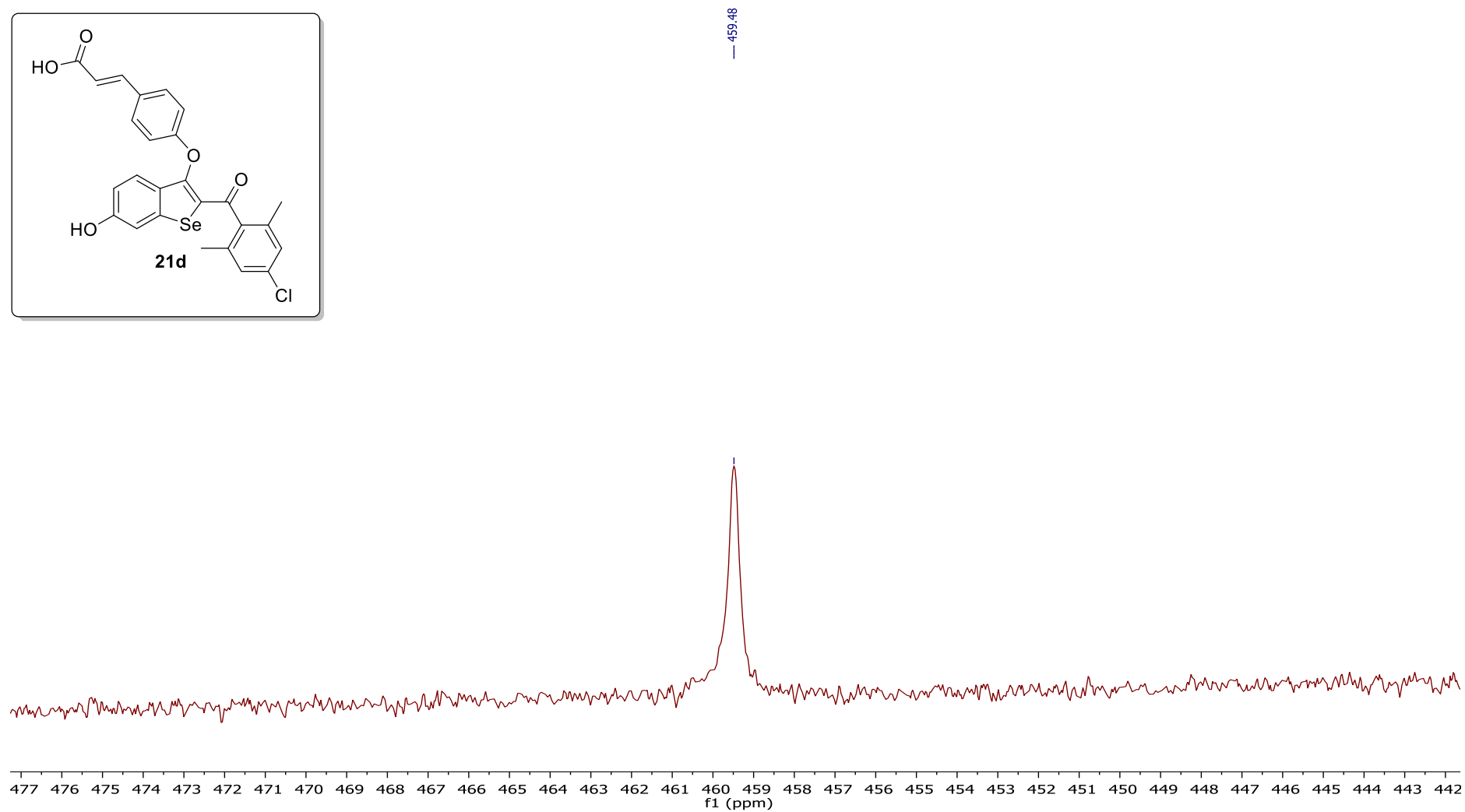
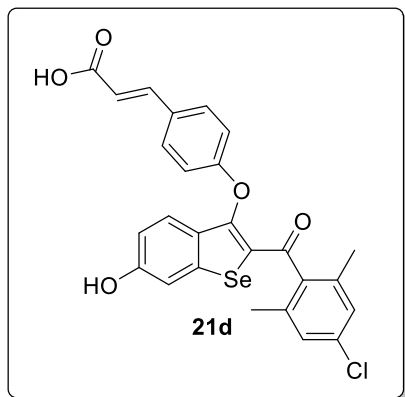
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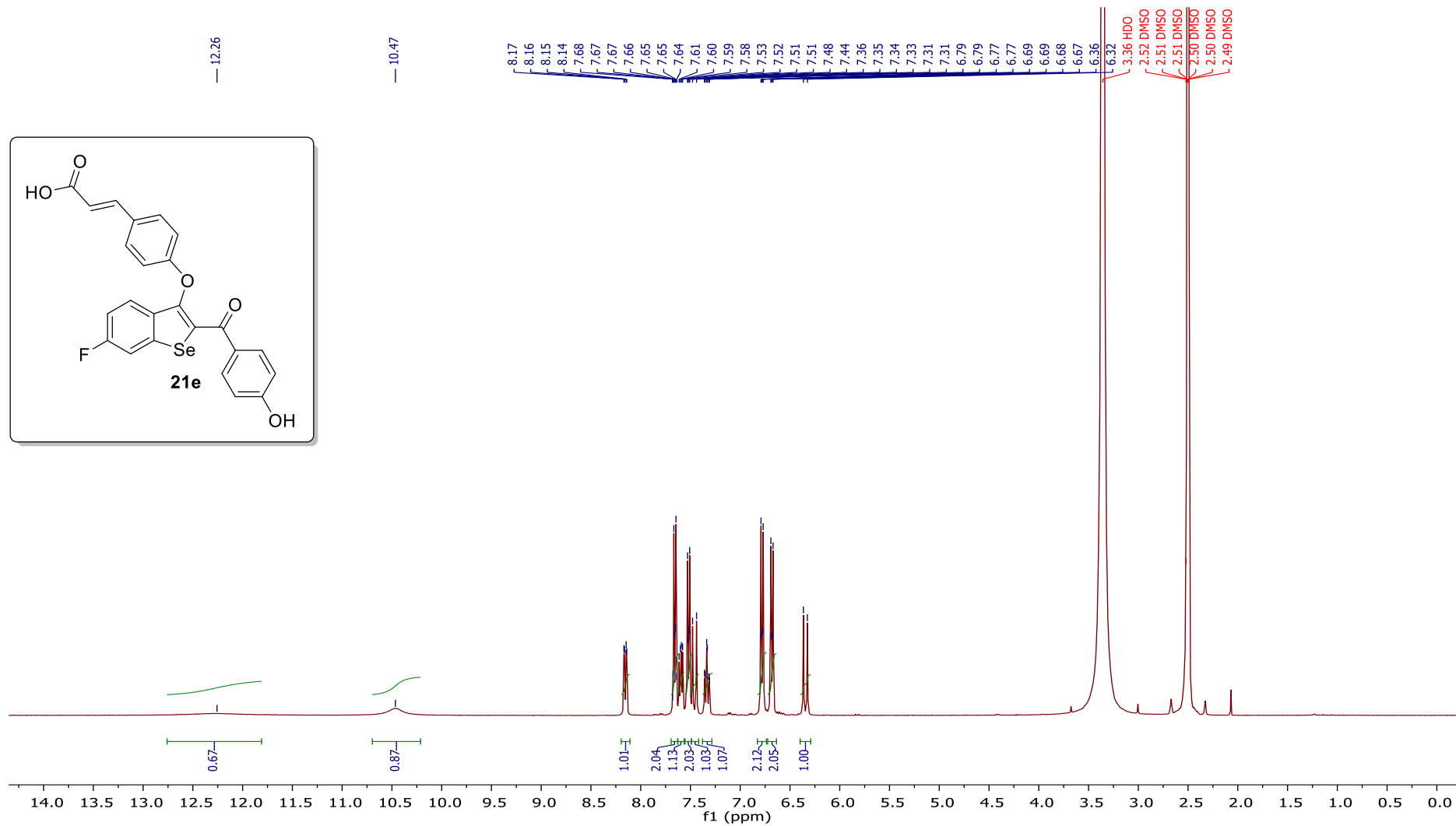
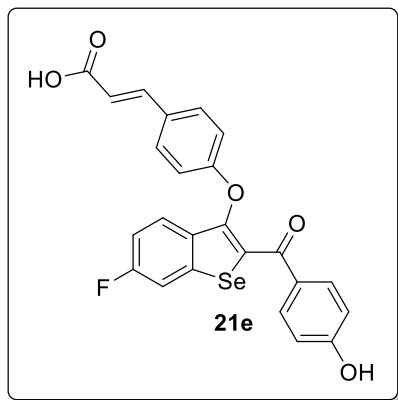
^{13}C NMR (100.6 MHz, DMSO- d_6):



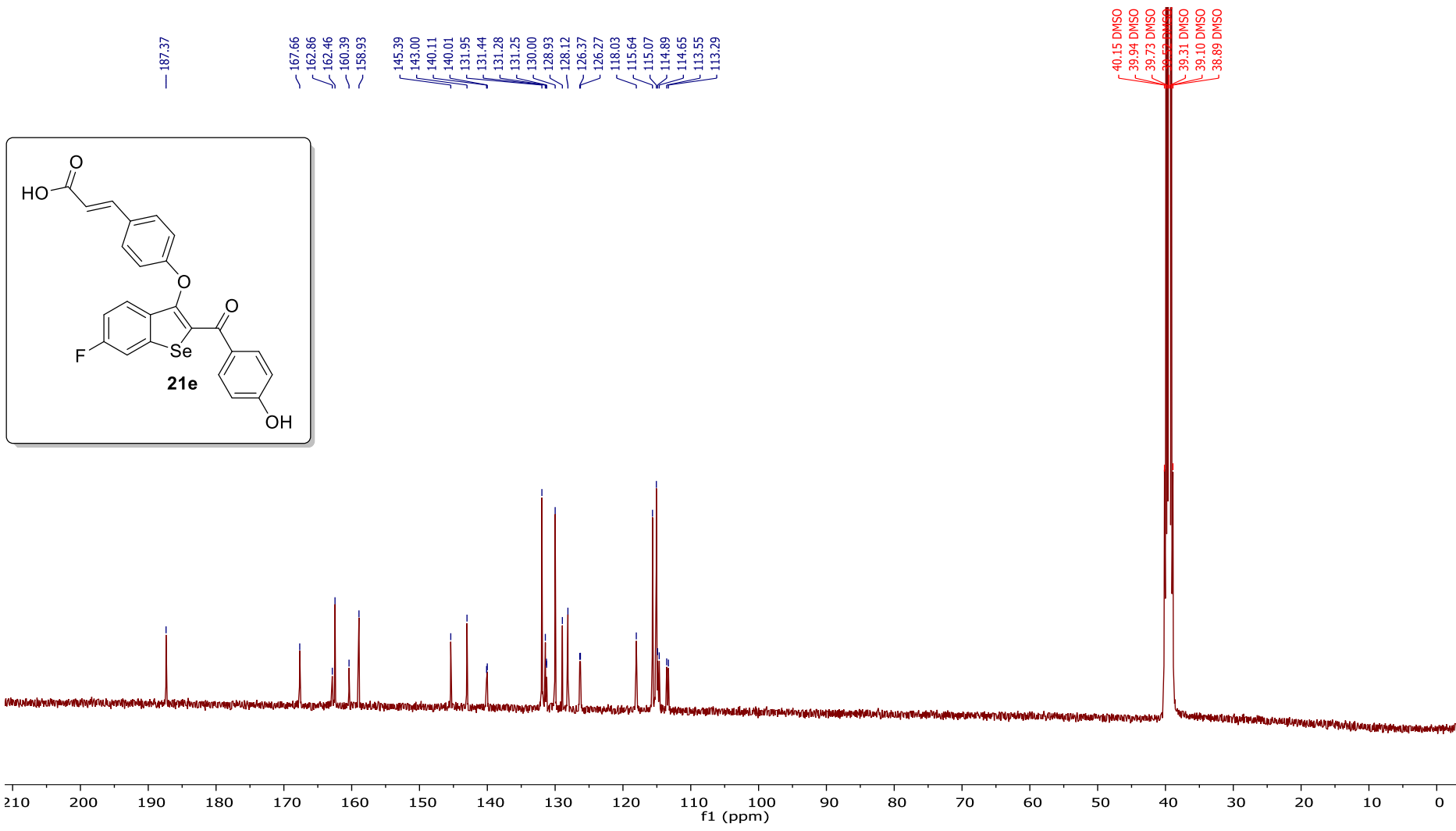
^{77}Se NMR (76.37 MHz, DMSO- d_6):



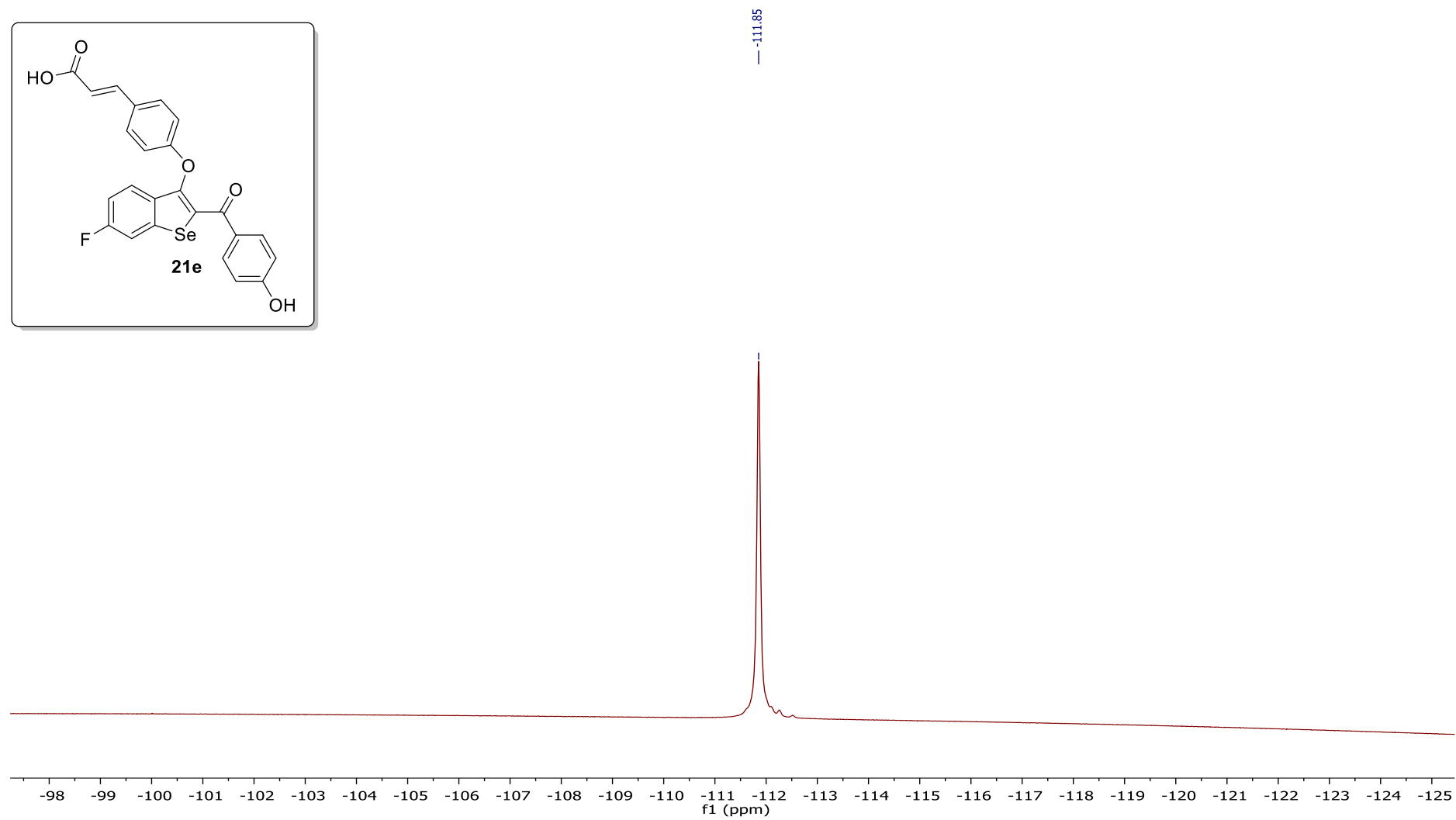
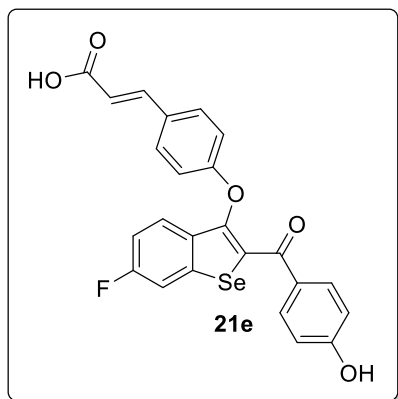
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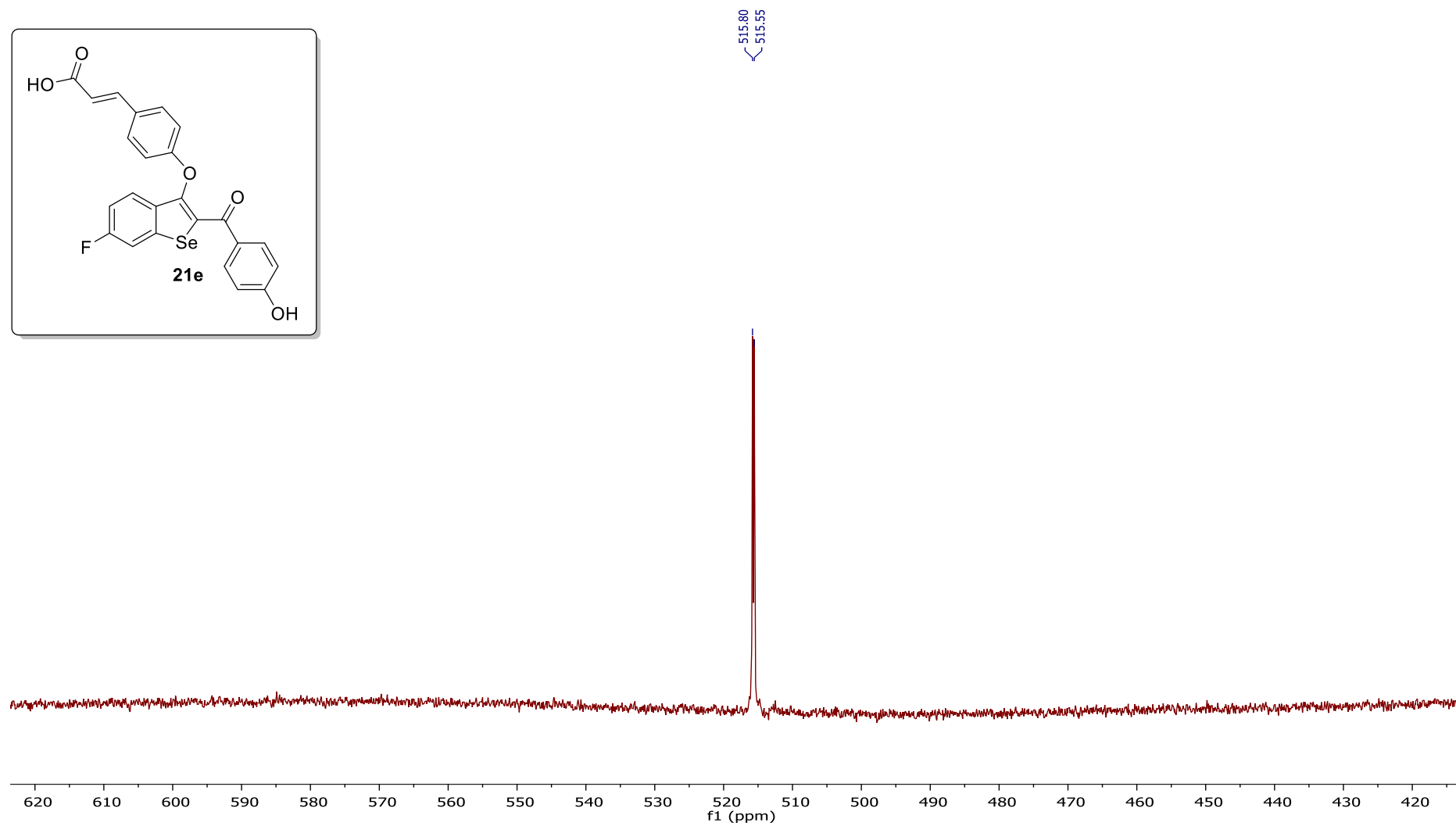
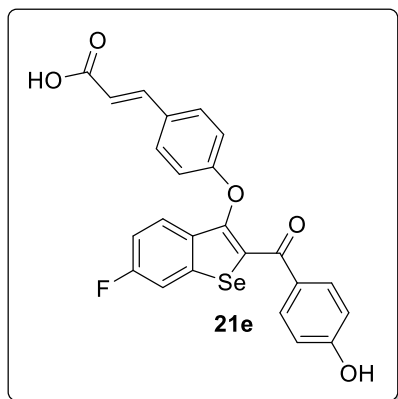
^{13}C NMR (100.6 MHz, DMSO- d_6):



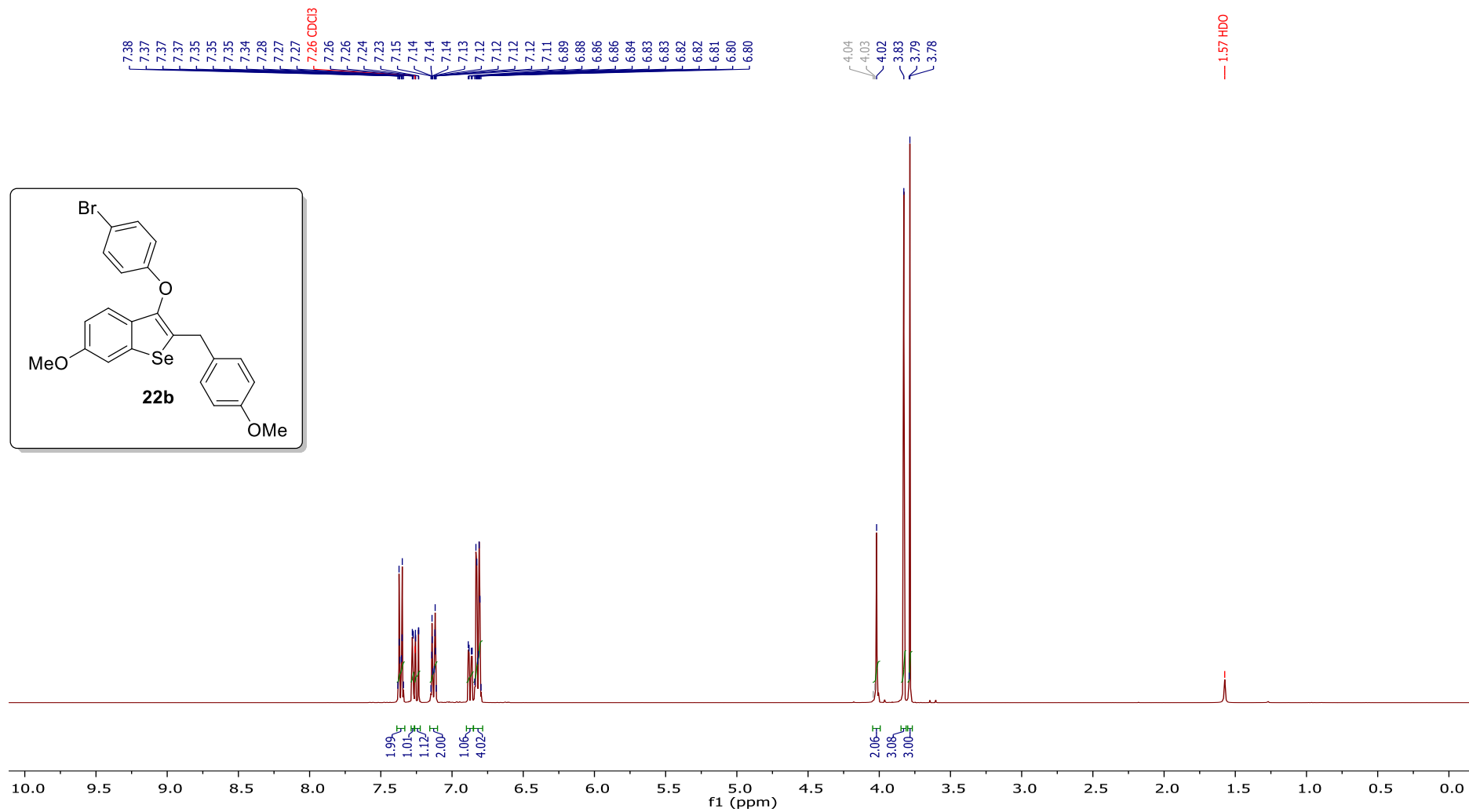
^{19}F NMR (376.21 MHz, DMSO-d_6):



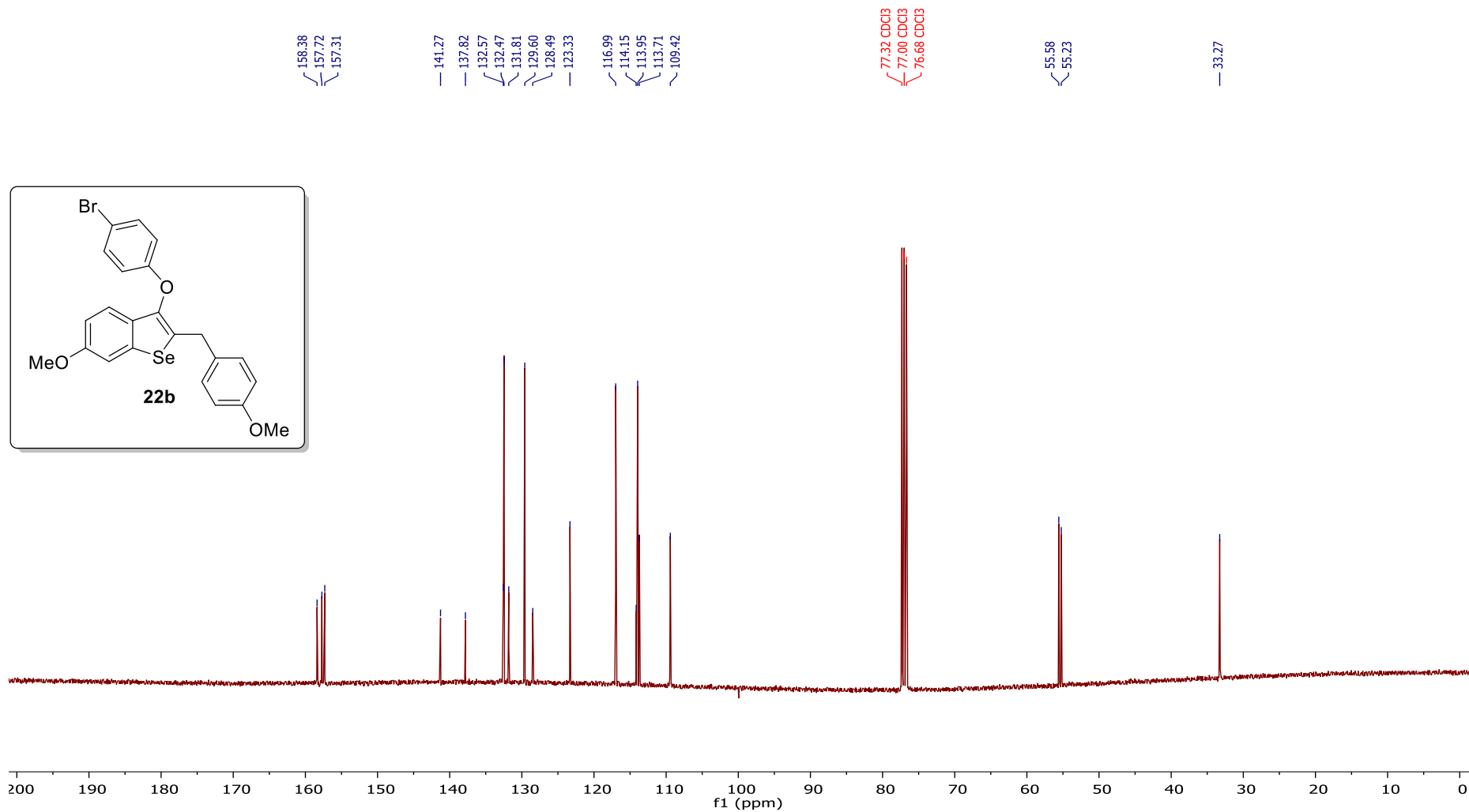
^{77}Se NMR (76.37 MHz, DMSO- d_6):



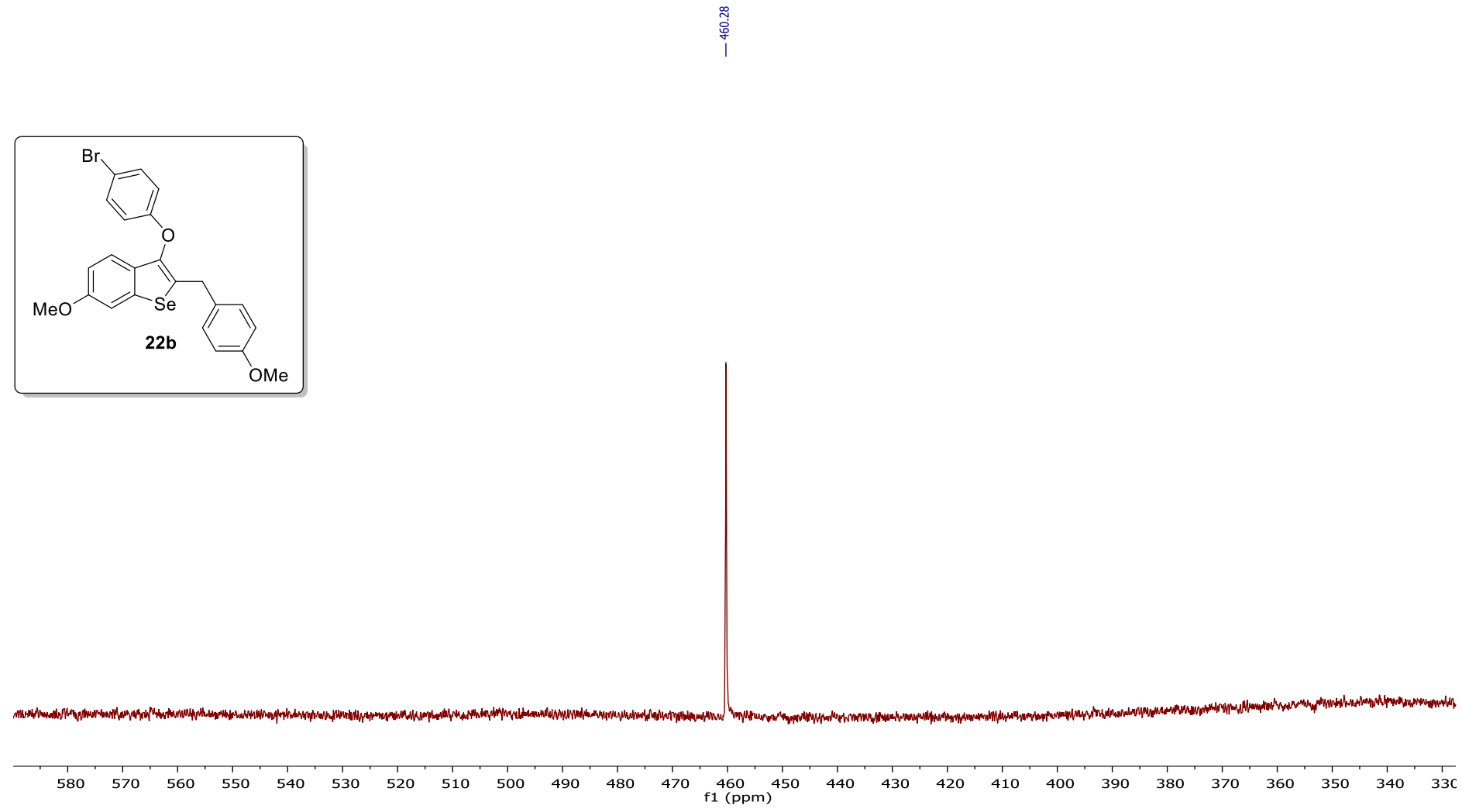
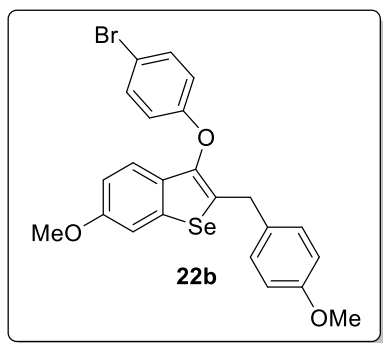
$^1\text{H NMR}$ (400 MHz, CDCl_3):



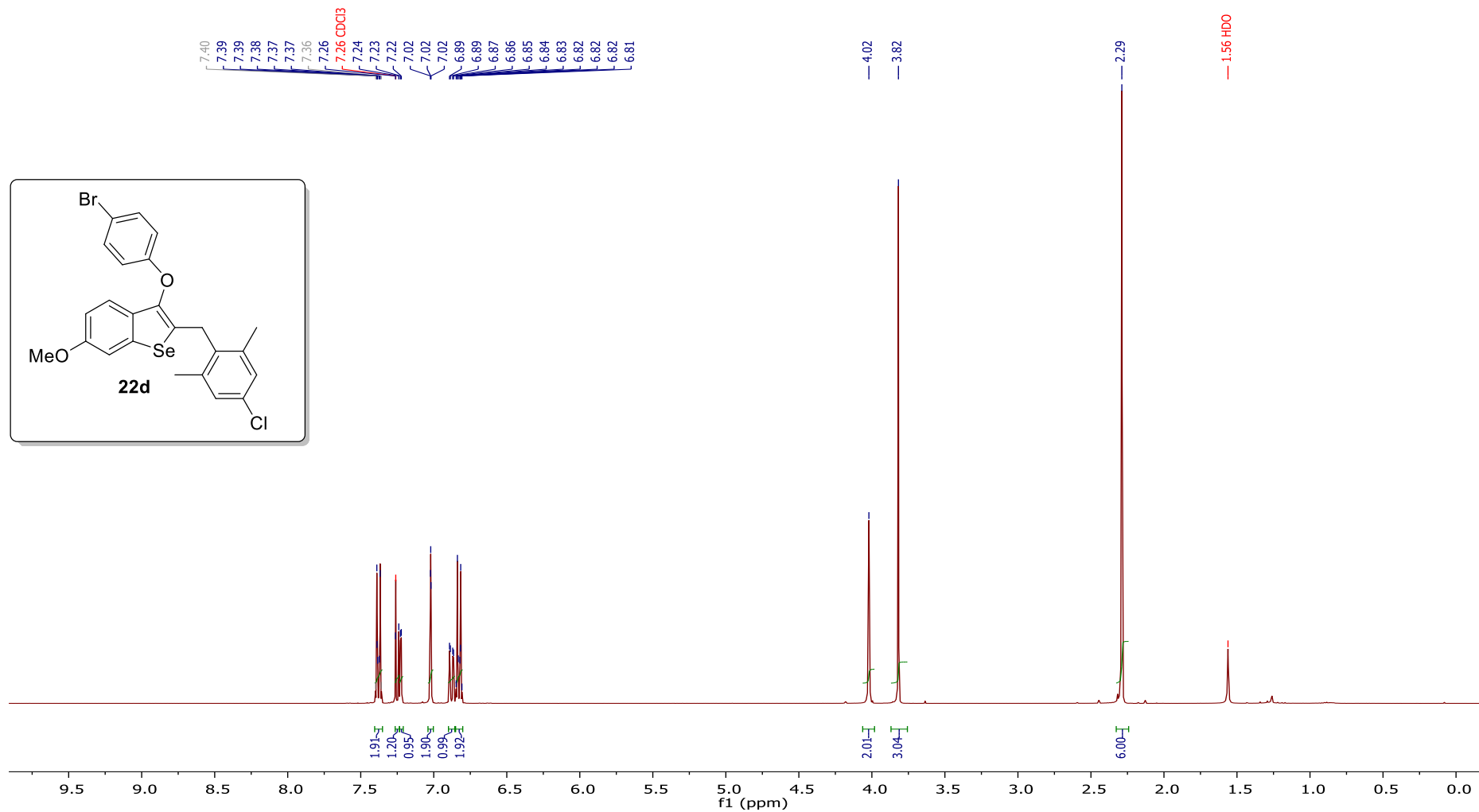
^{13}C NMR (100.6 MHz, CDCl_3):



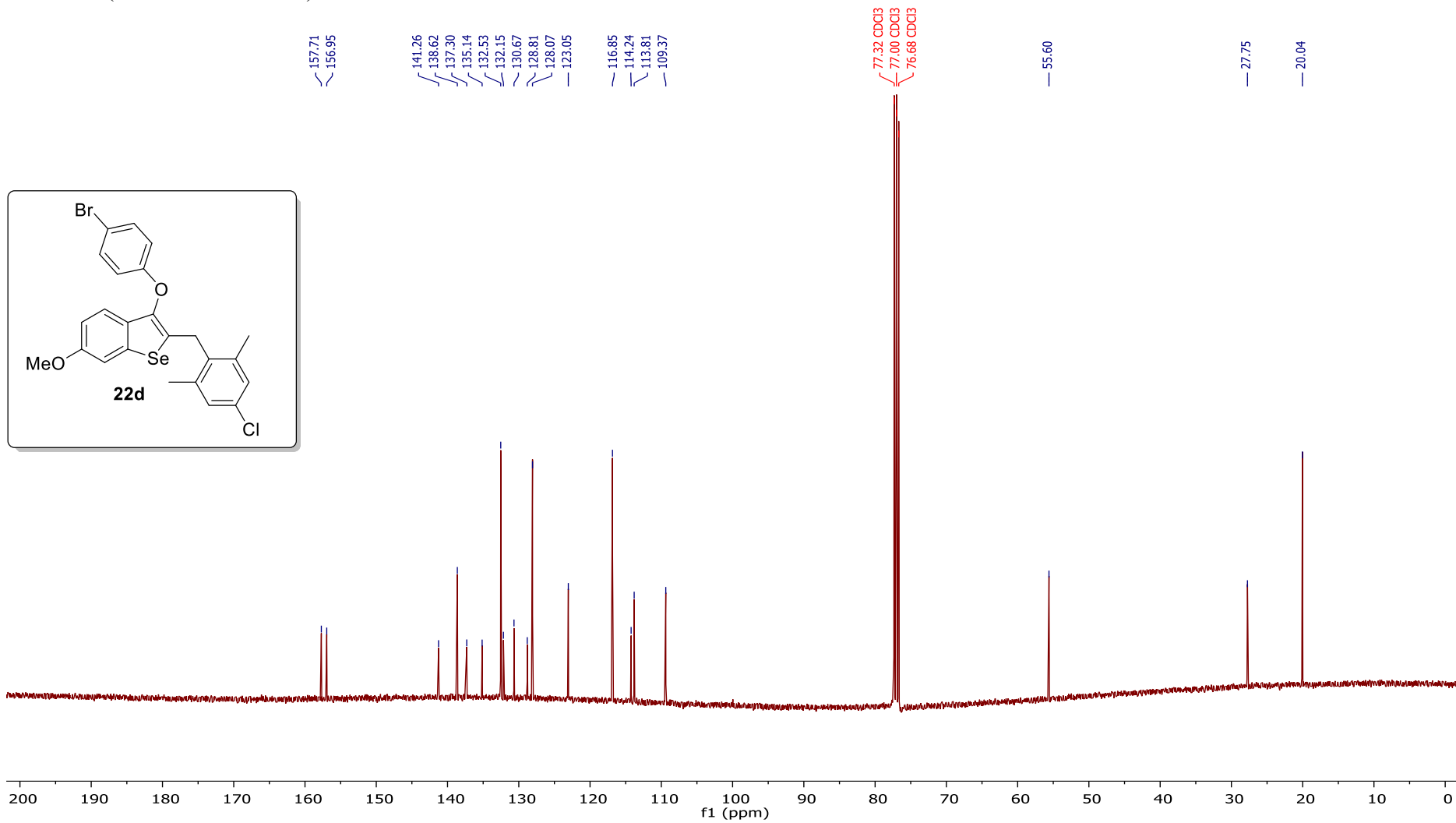
^{77}Se NMR (76.37 MHz, CDCl_3):



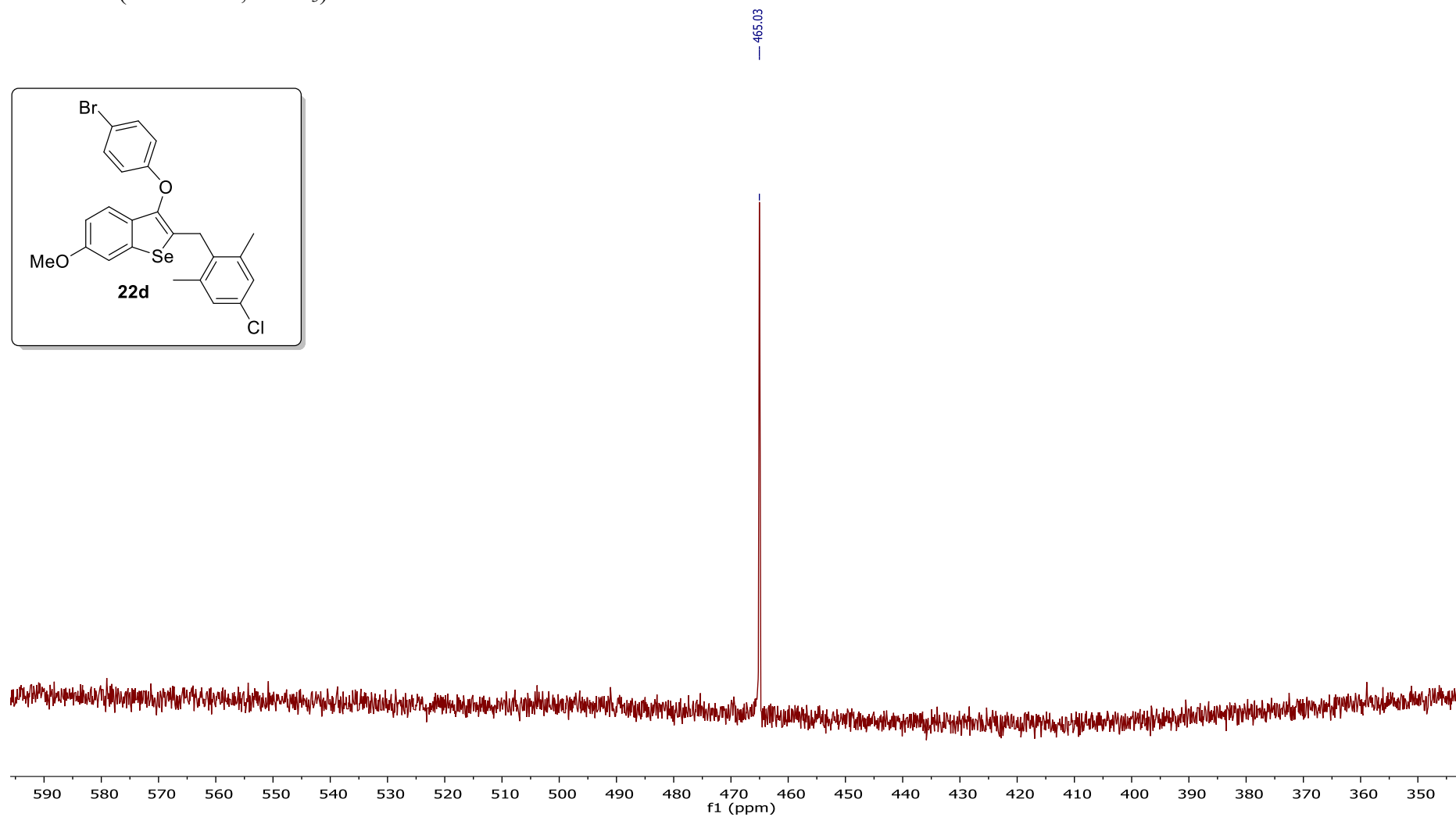
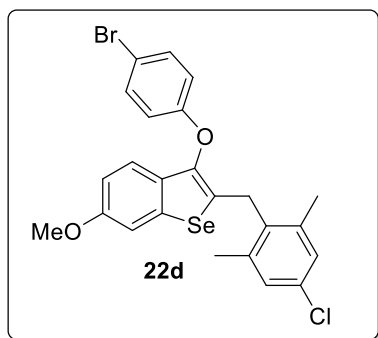
^1H NMR (400 MHz, CDCl_3):



^{13}C NMR (100.6 MHz, CDCl_3):



^{77}Se NMR (76.37 MHz, CDCl_3):

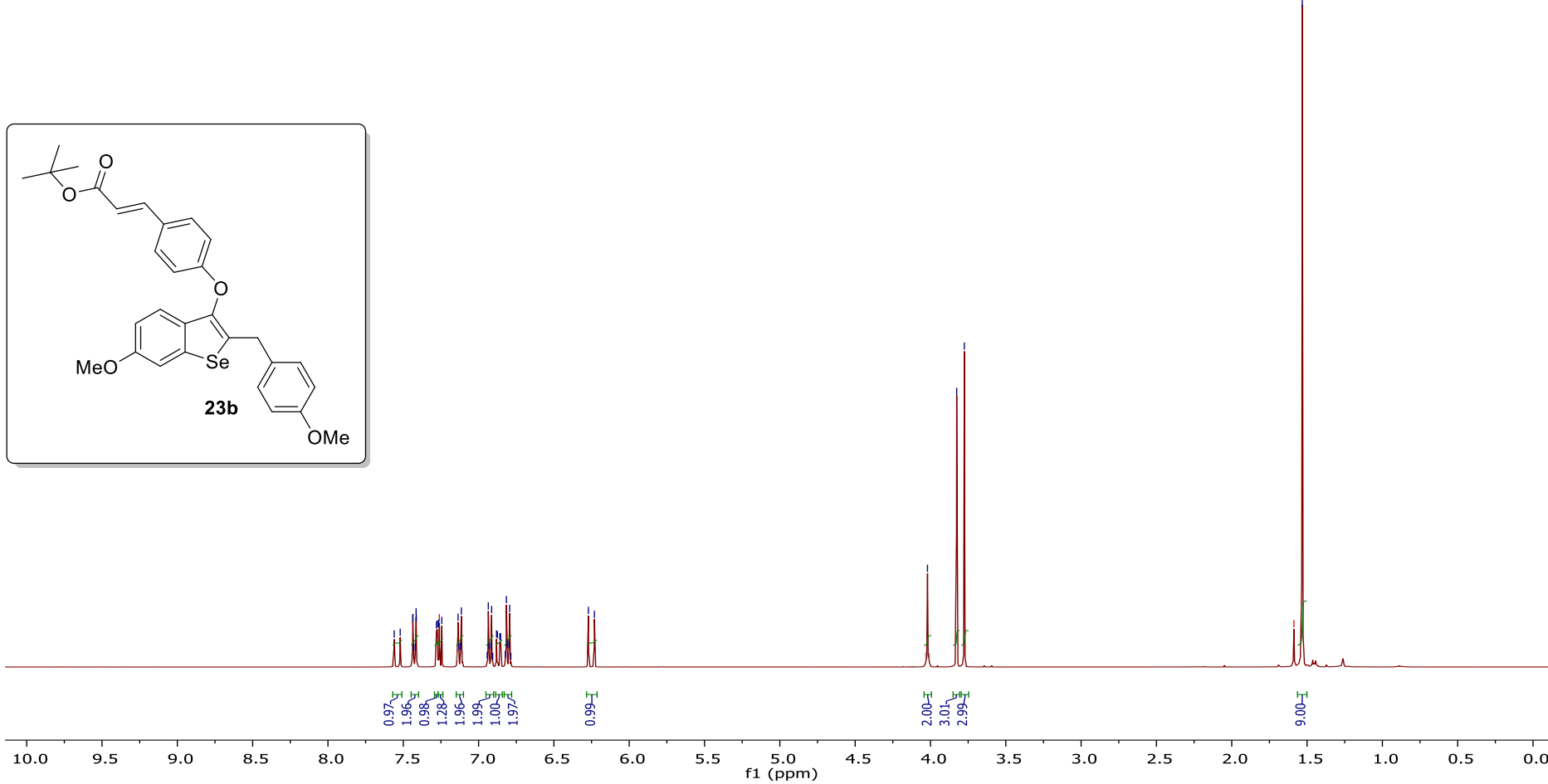
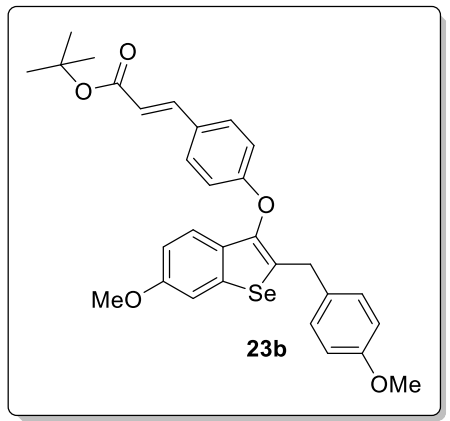


^1H NMR (400 MHz, CDCl_3):

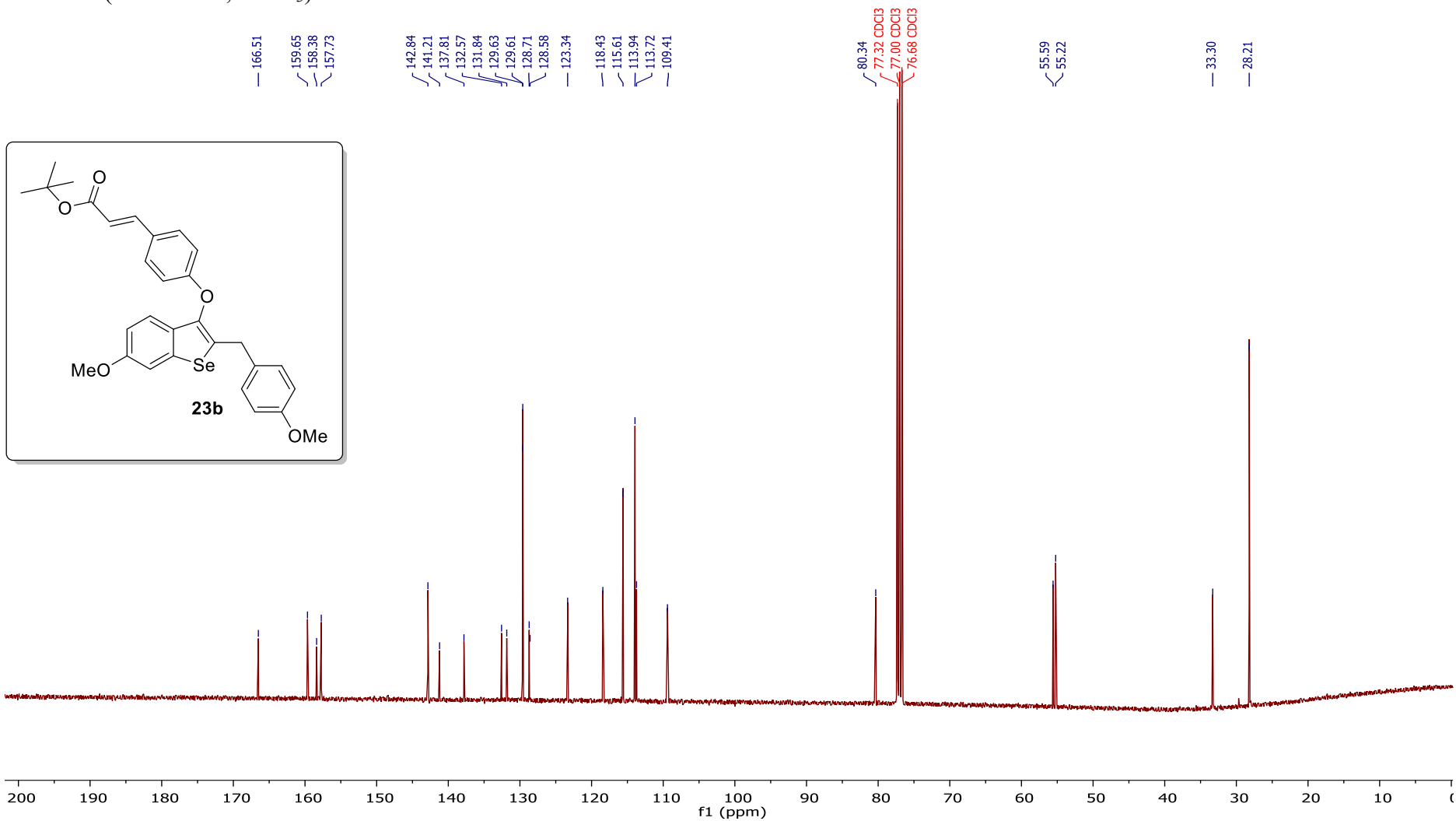
7.56
7.52
7.44
7.44
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7.42
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7.41
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7.28
7.27
7.27
7.26 CDCl_3
7.24
7.14
7.13
7.12
7.11
6.94
6.94
6.93
6.92
6.91
6.88
6.88
6.86
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4.02
4.01
3.83
3.78

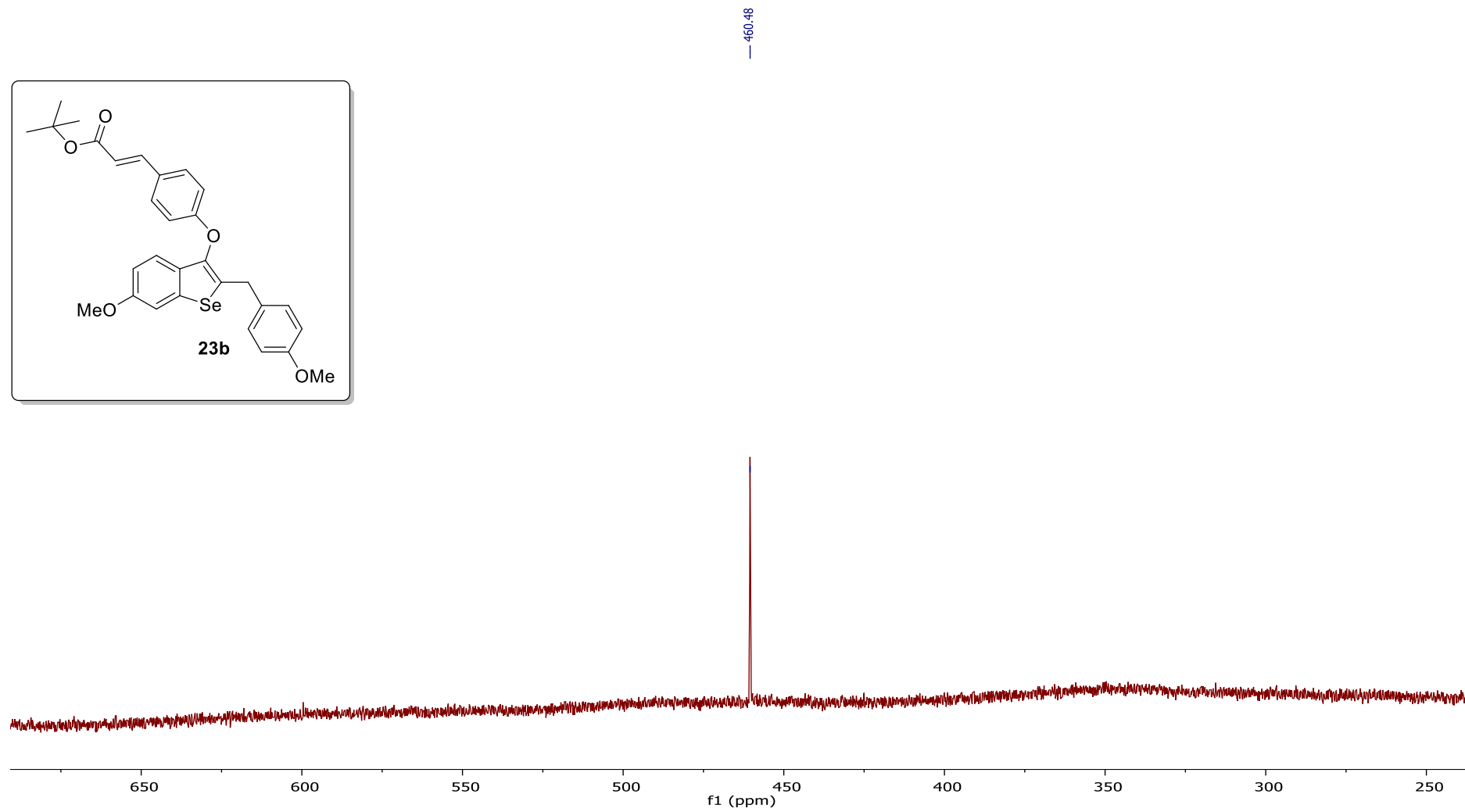
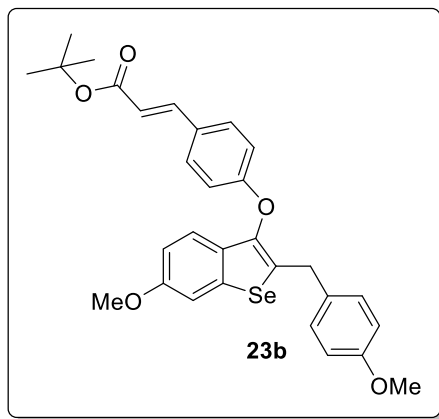
1.59 H₂O
1.53



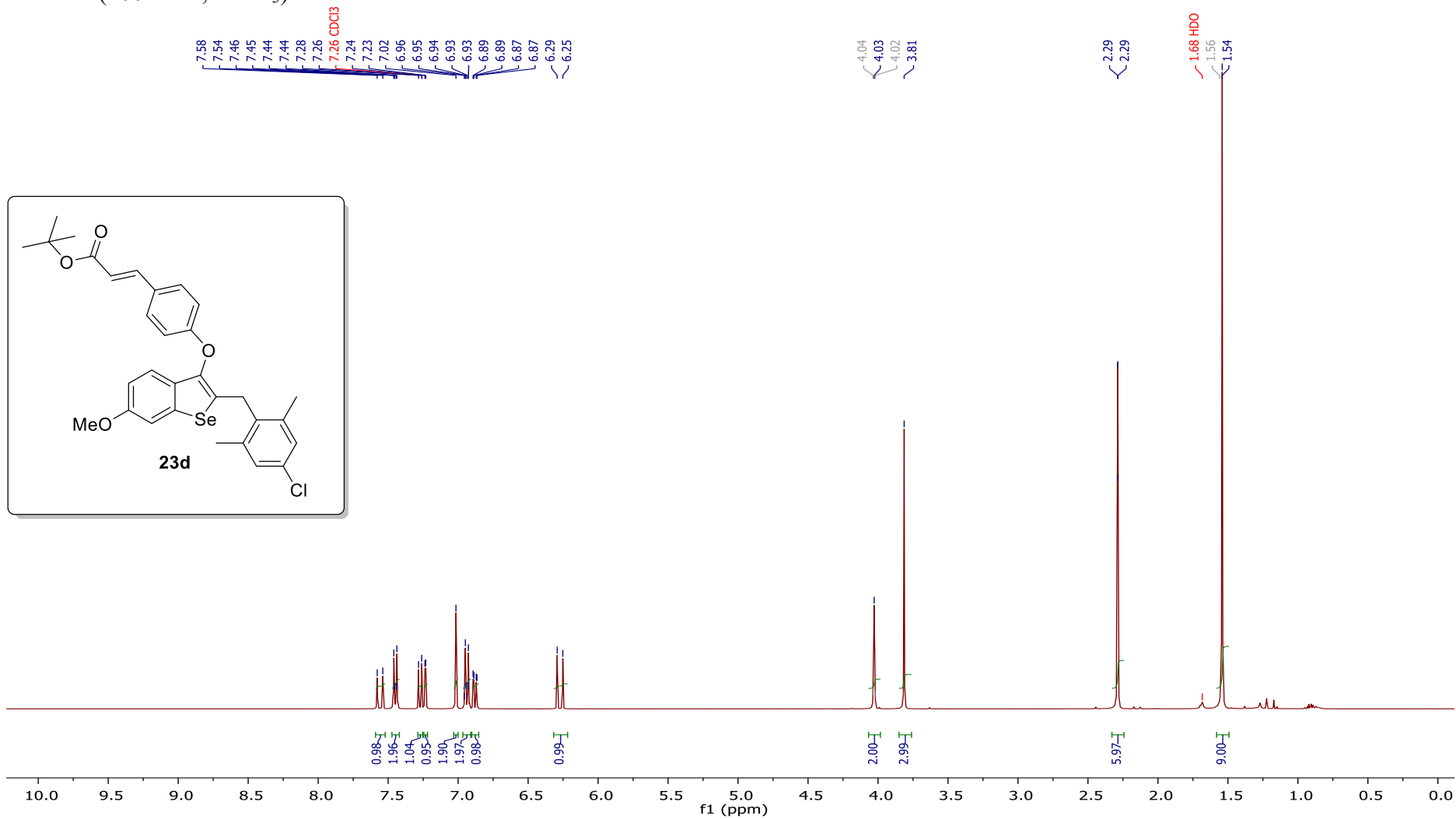
^{13}C NMR (100.6 MHz, CDCl_3):



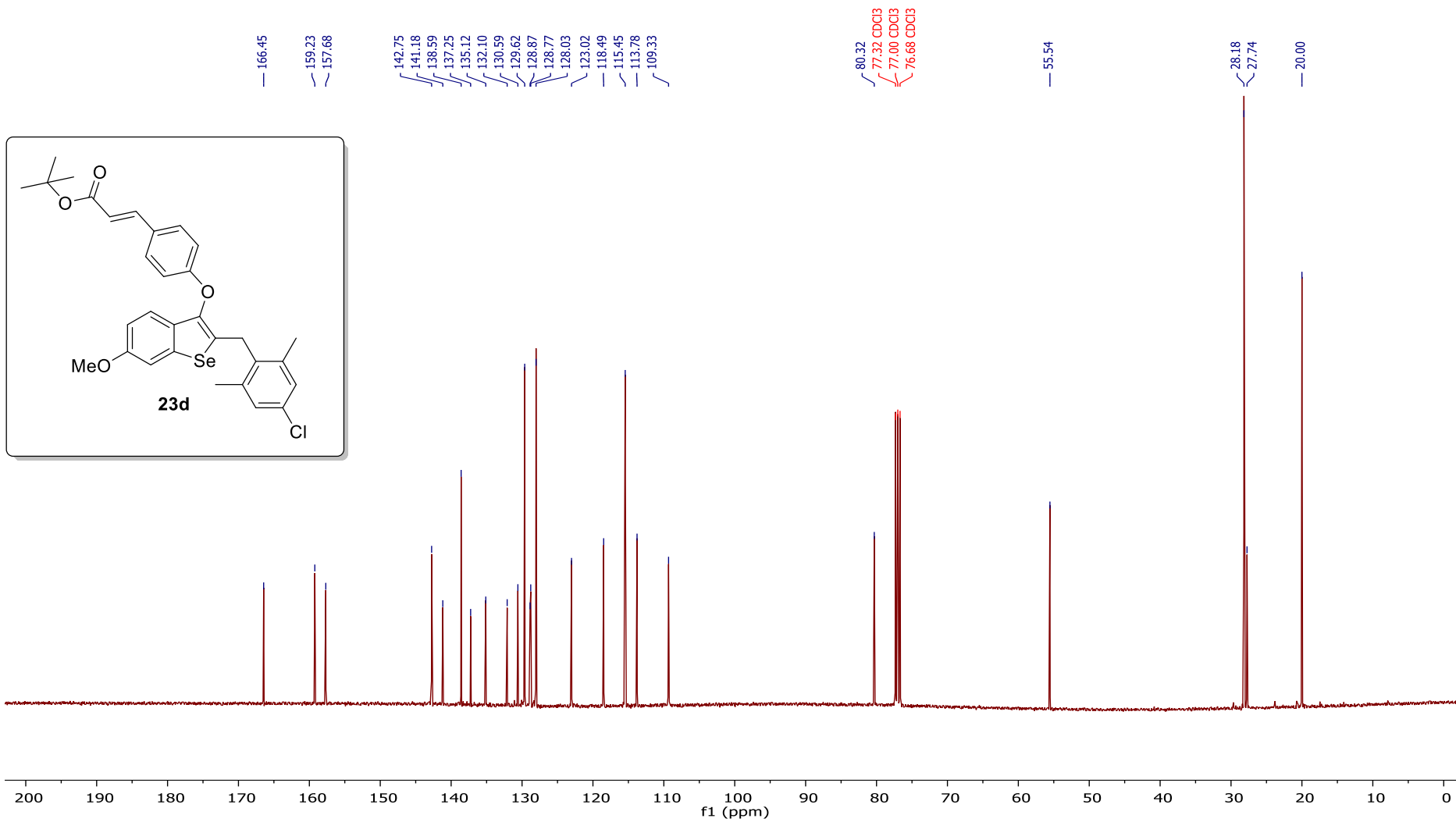
^{77}Se NMR (76.37 MHz, CDCl_3):



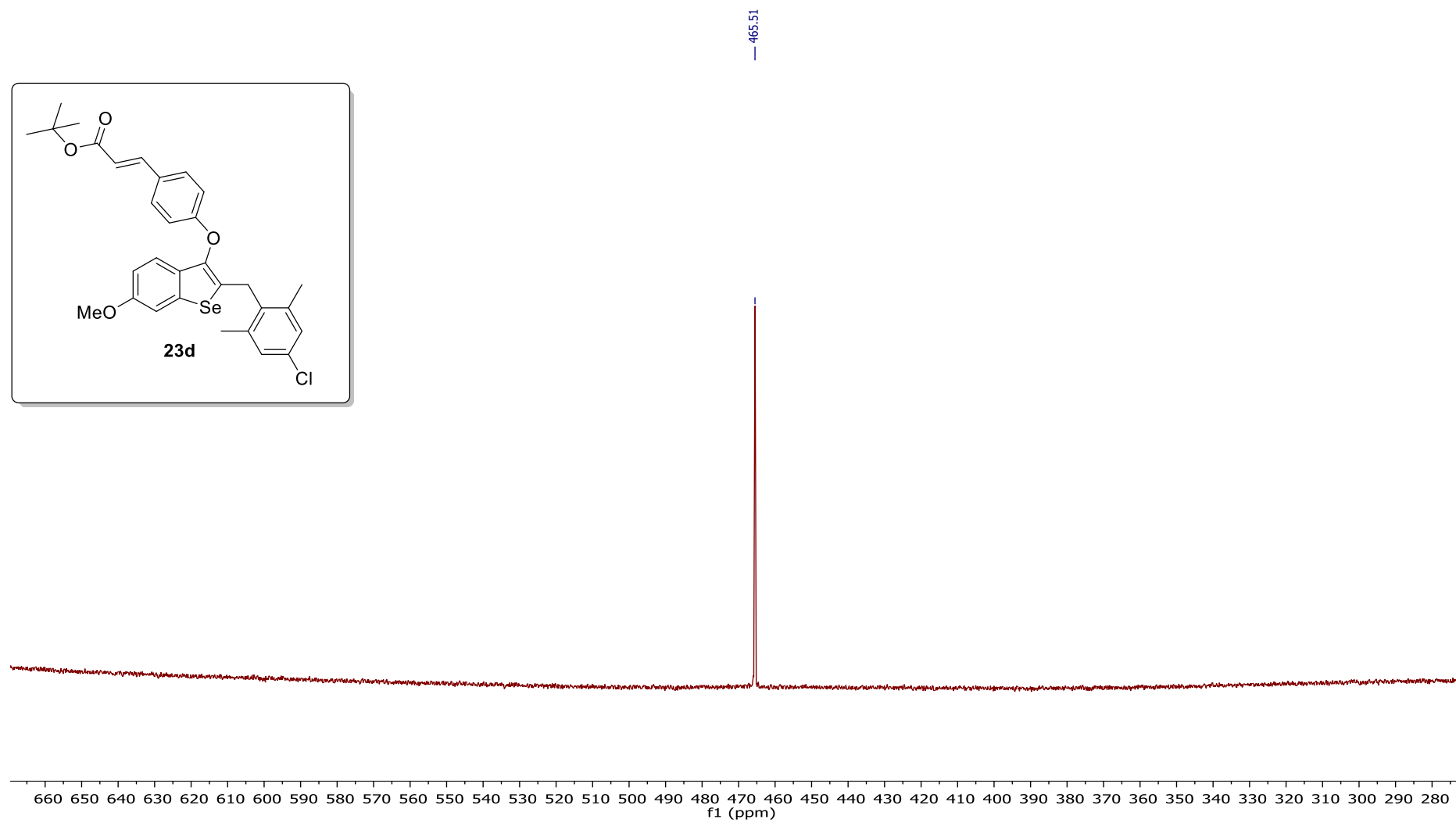
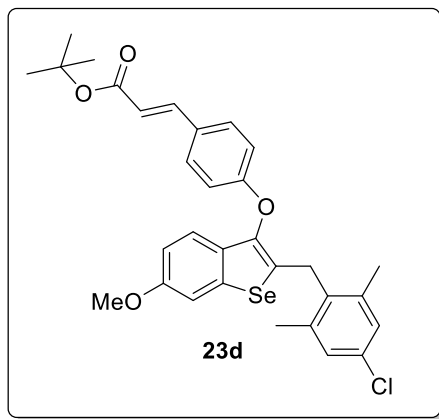
¹H NMR (400 MHz, CDCl₃):



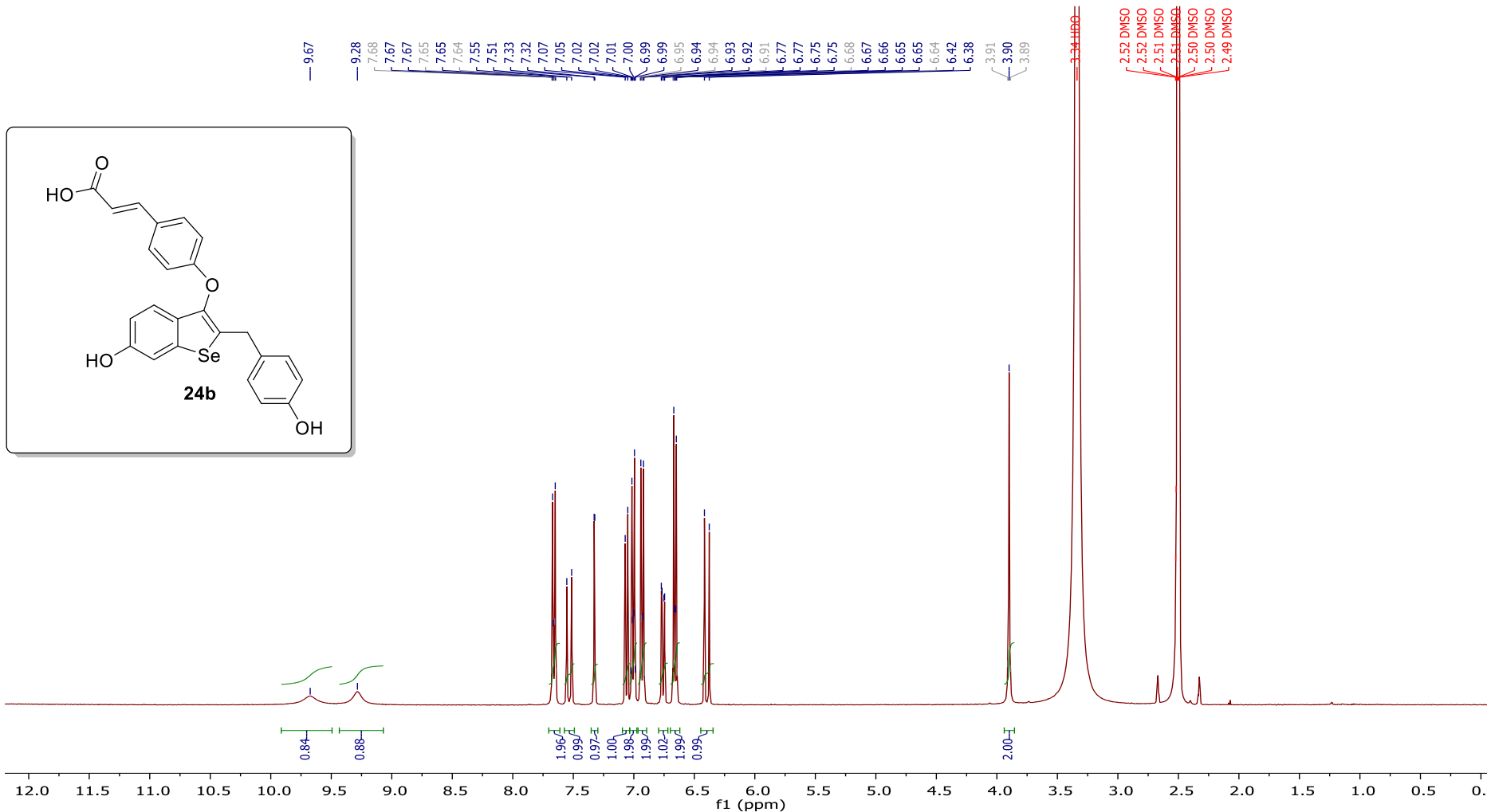
^{13}C NMR (100.6 MHz, CDCl_3):



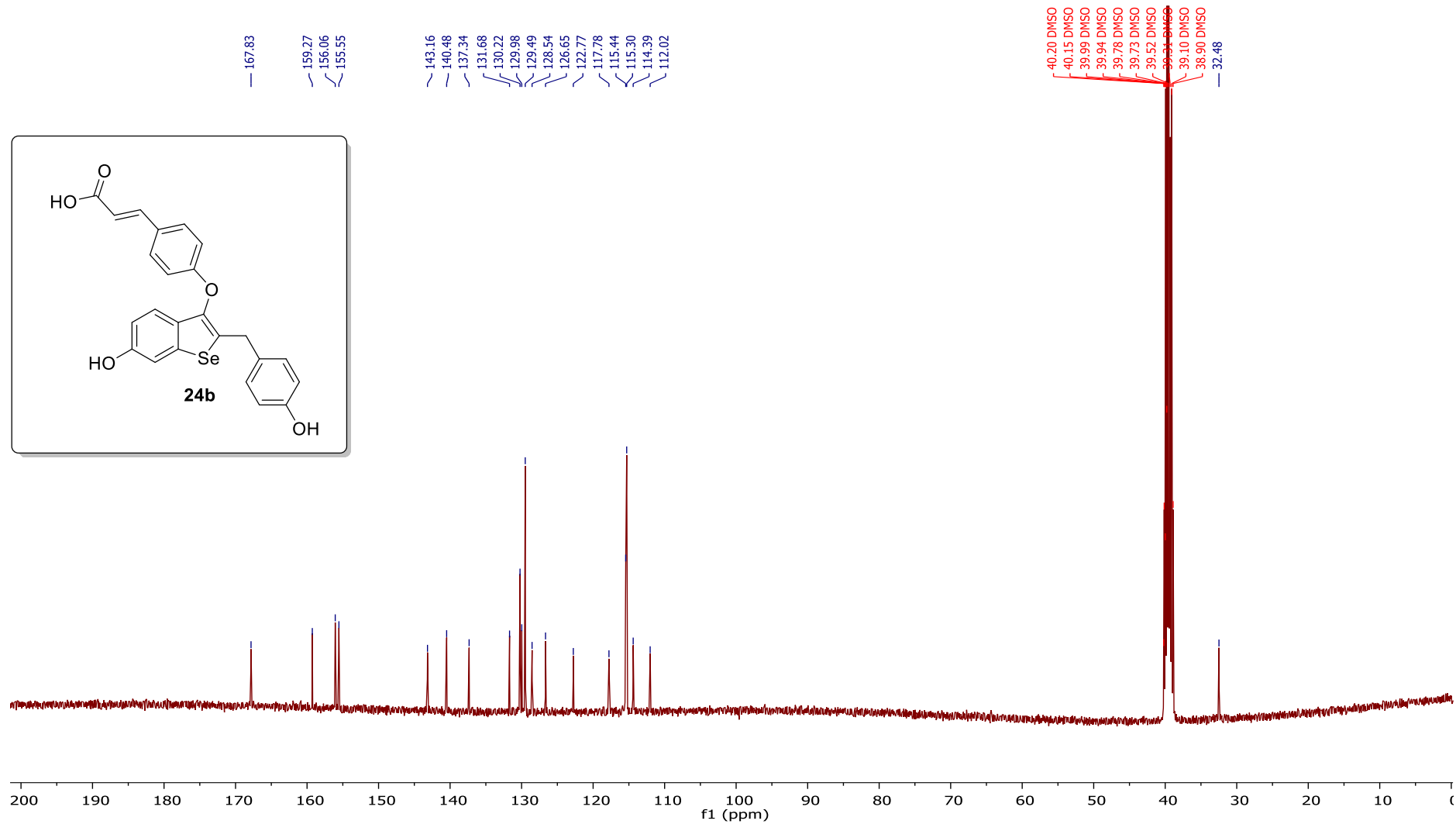
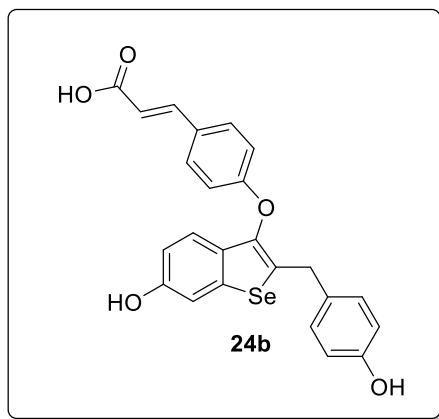
^{77}Se NMR (76.37 MHz, CDCl_3):



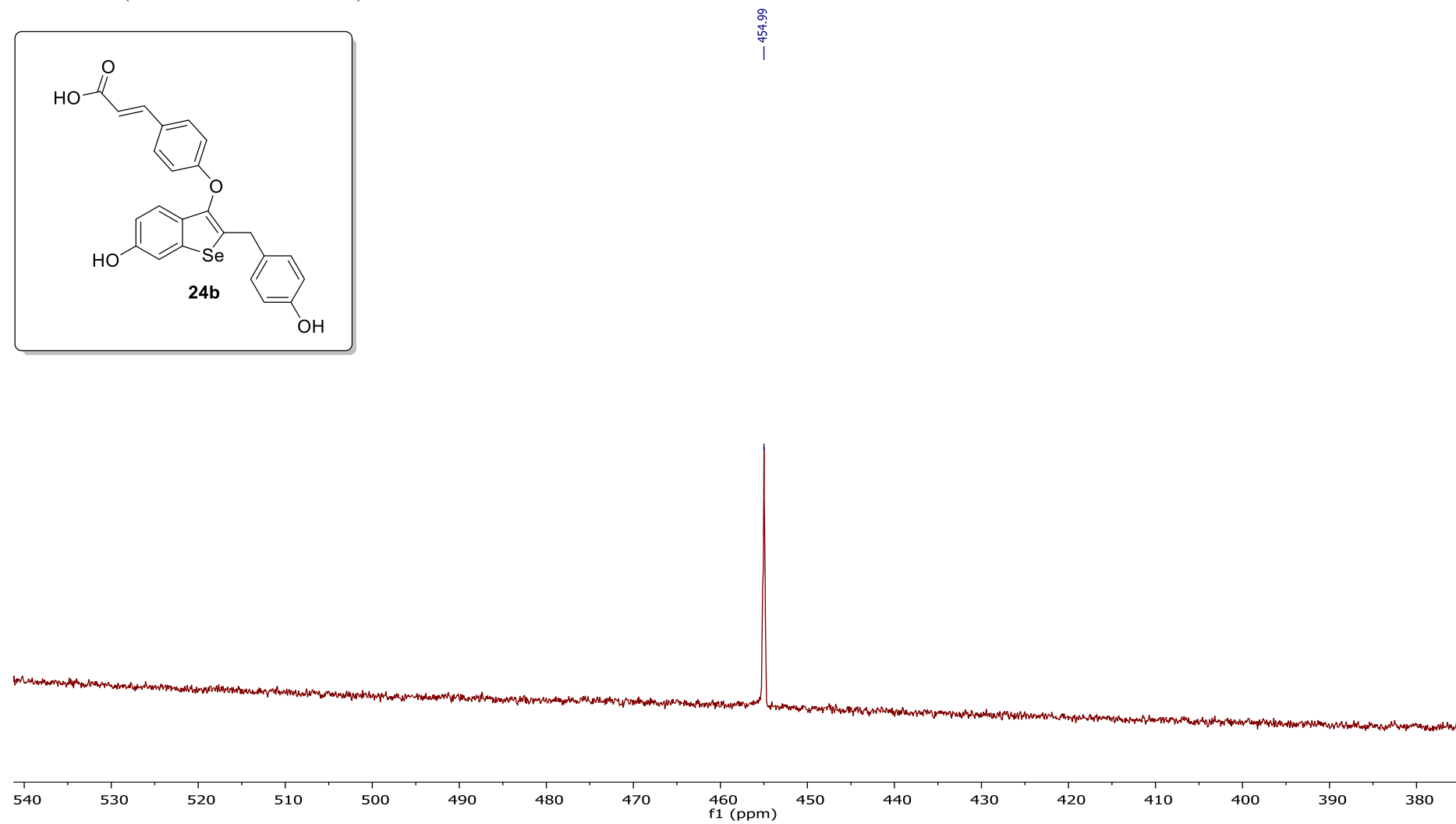
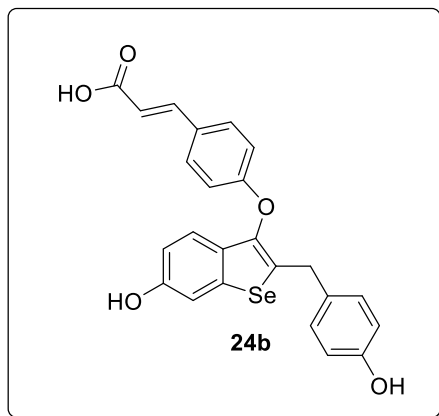
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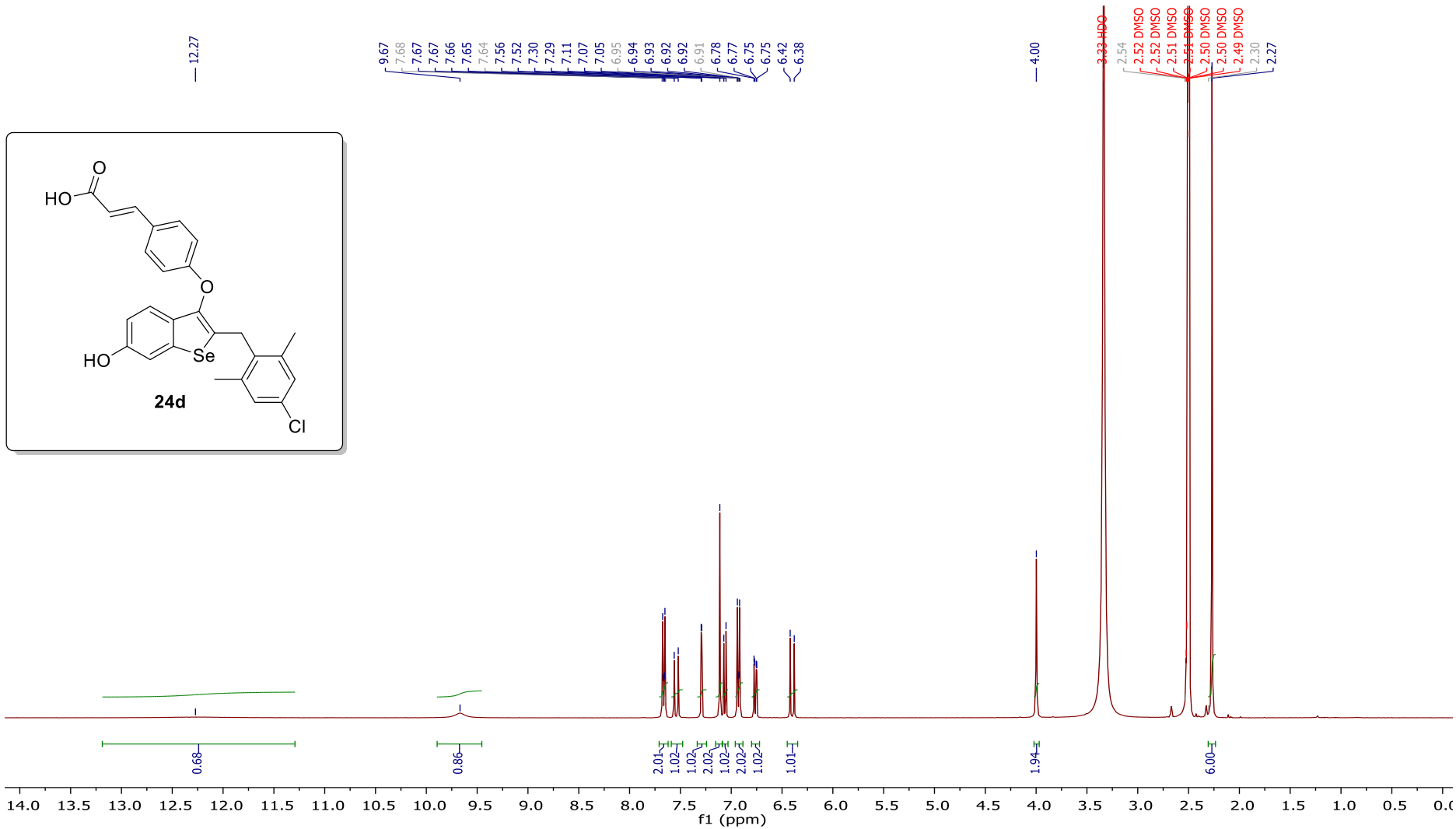
^{13}C NMR (100.6 MHz, DMSO- d_6):



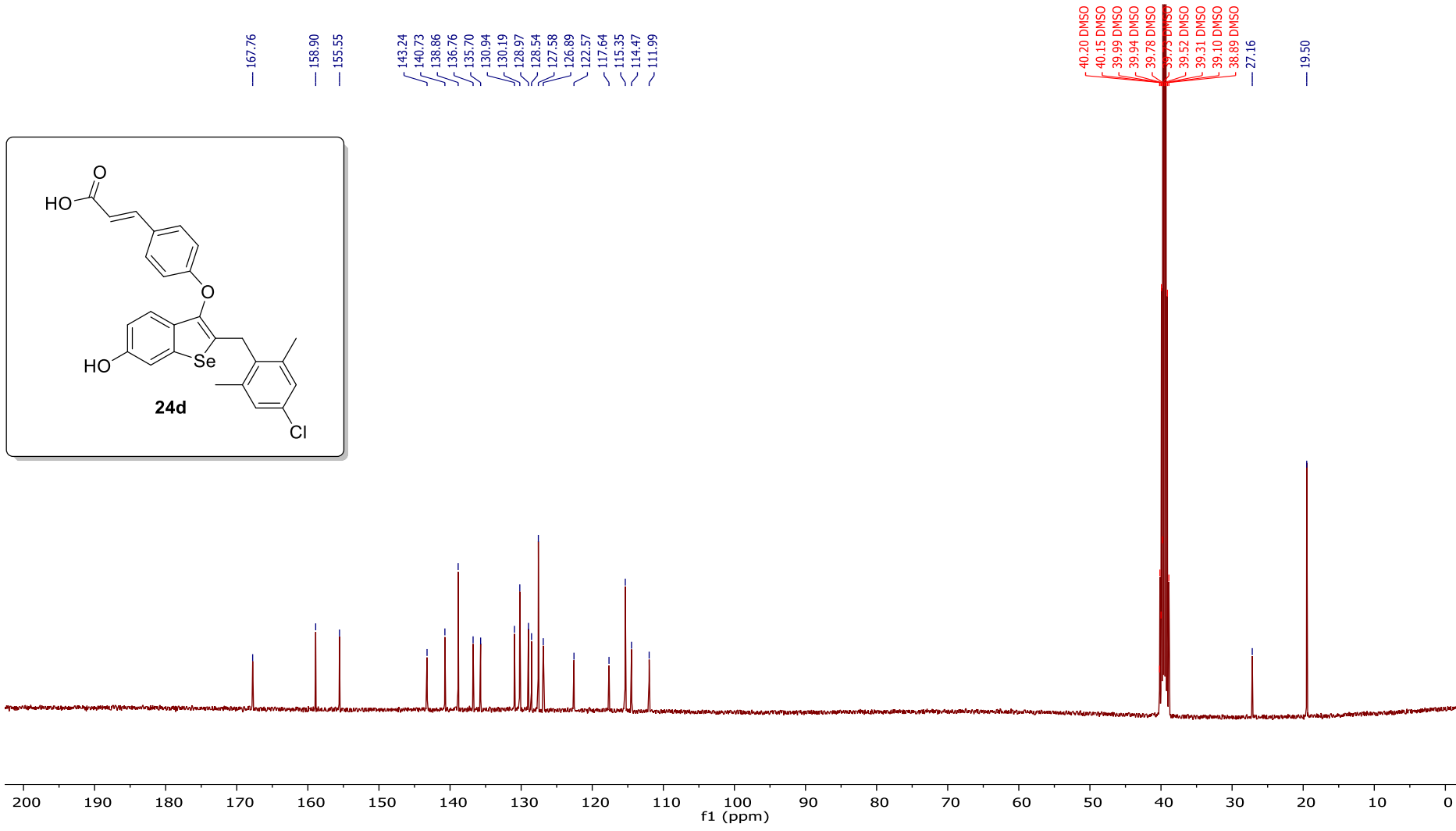
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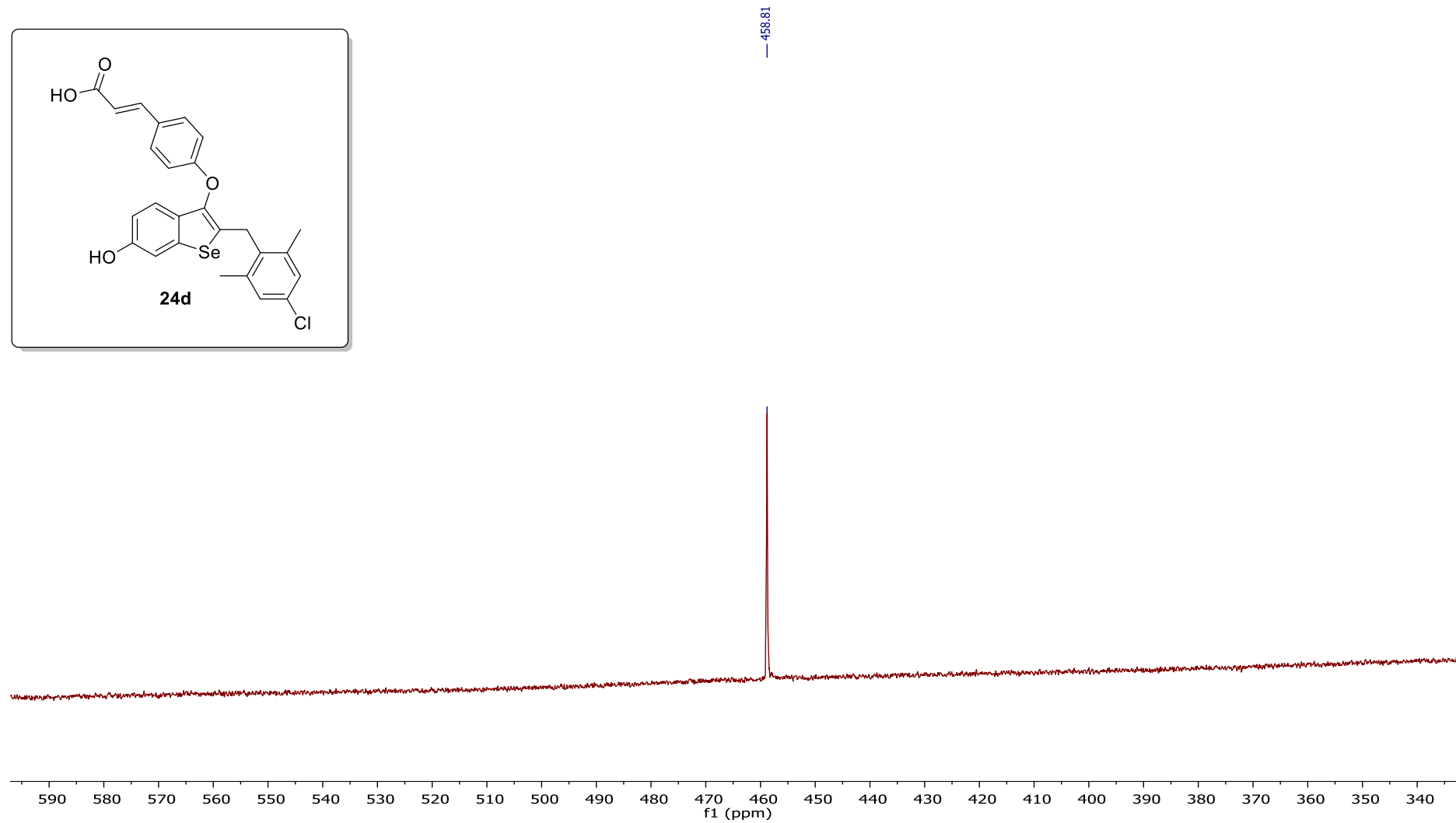
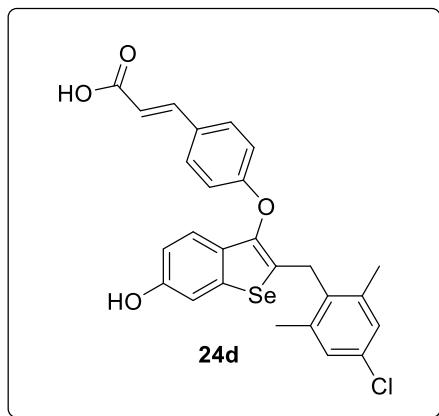
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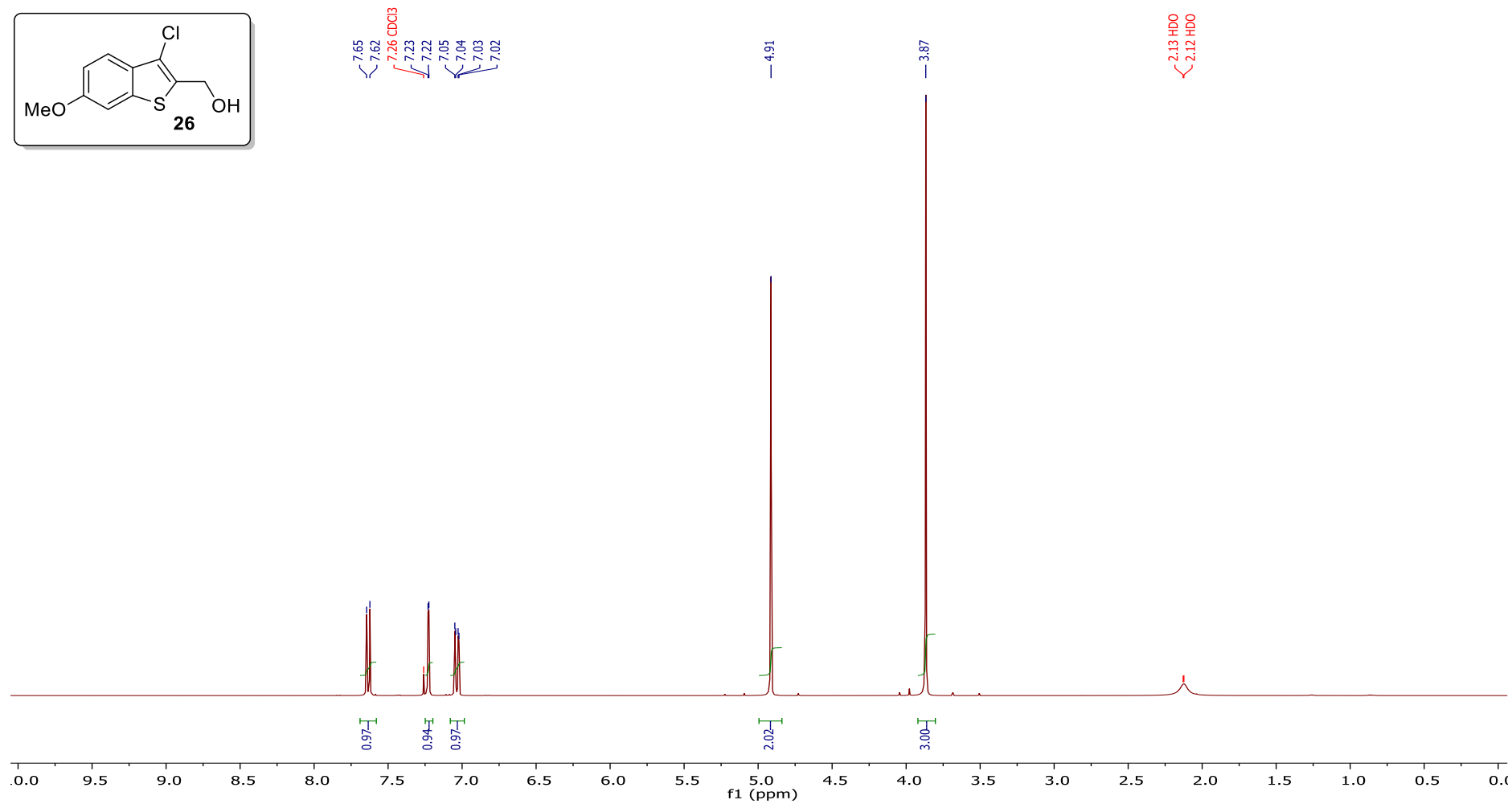
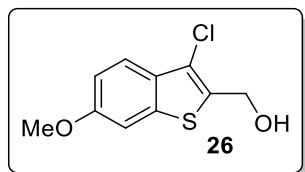
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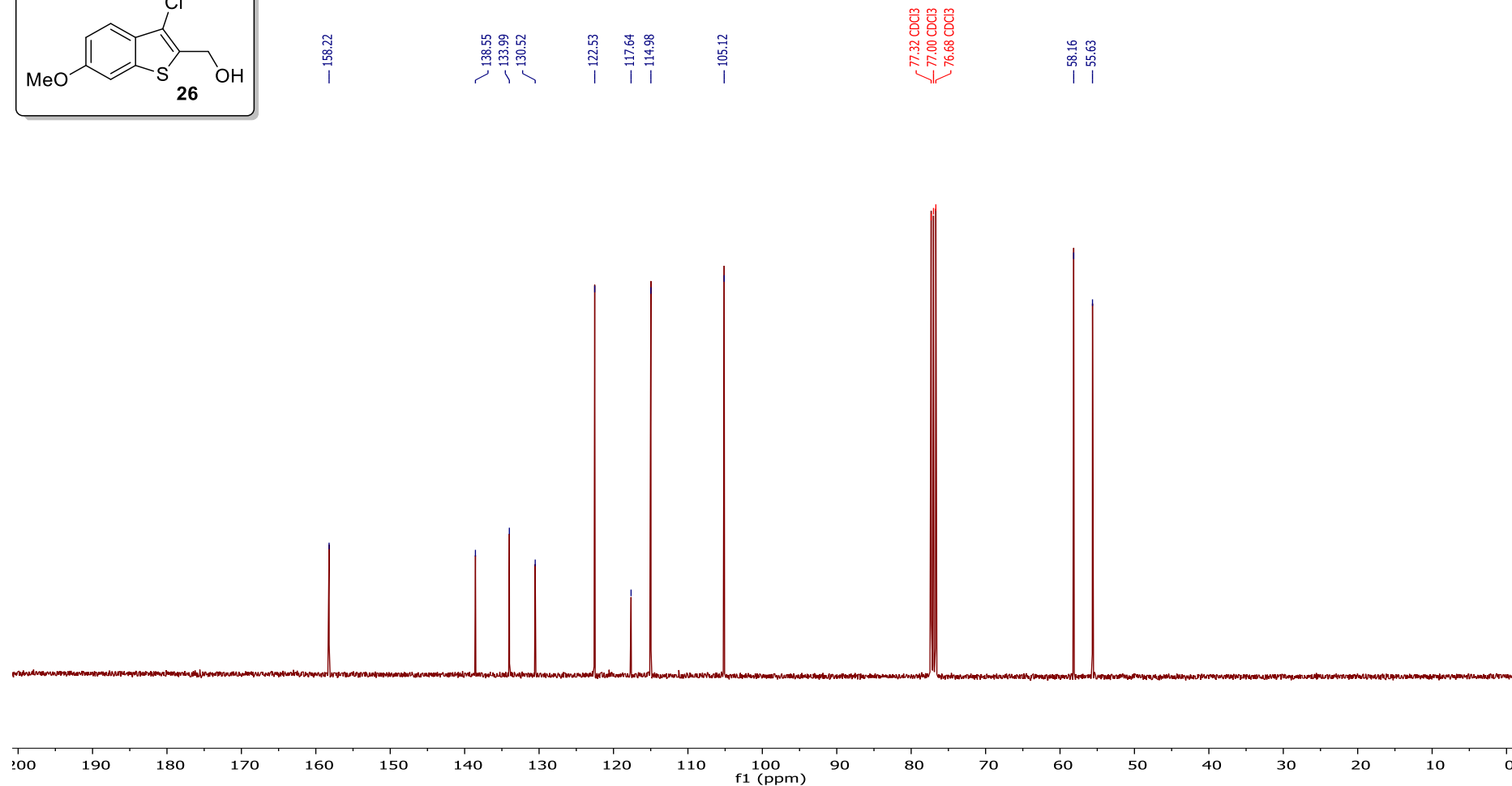
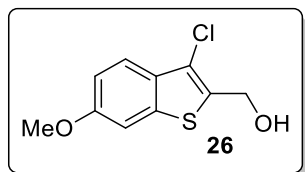
^{77}Se NMR (76.37 MHz, DMSO- d_6):



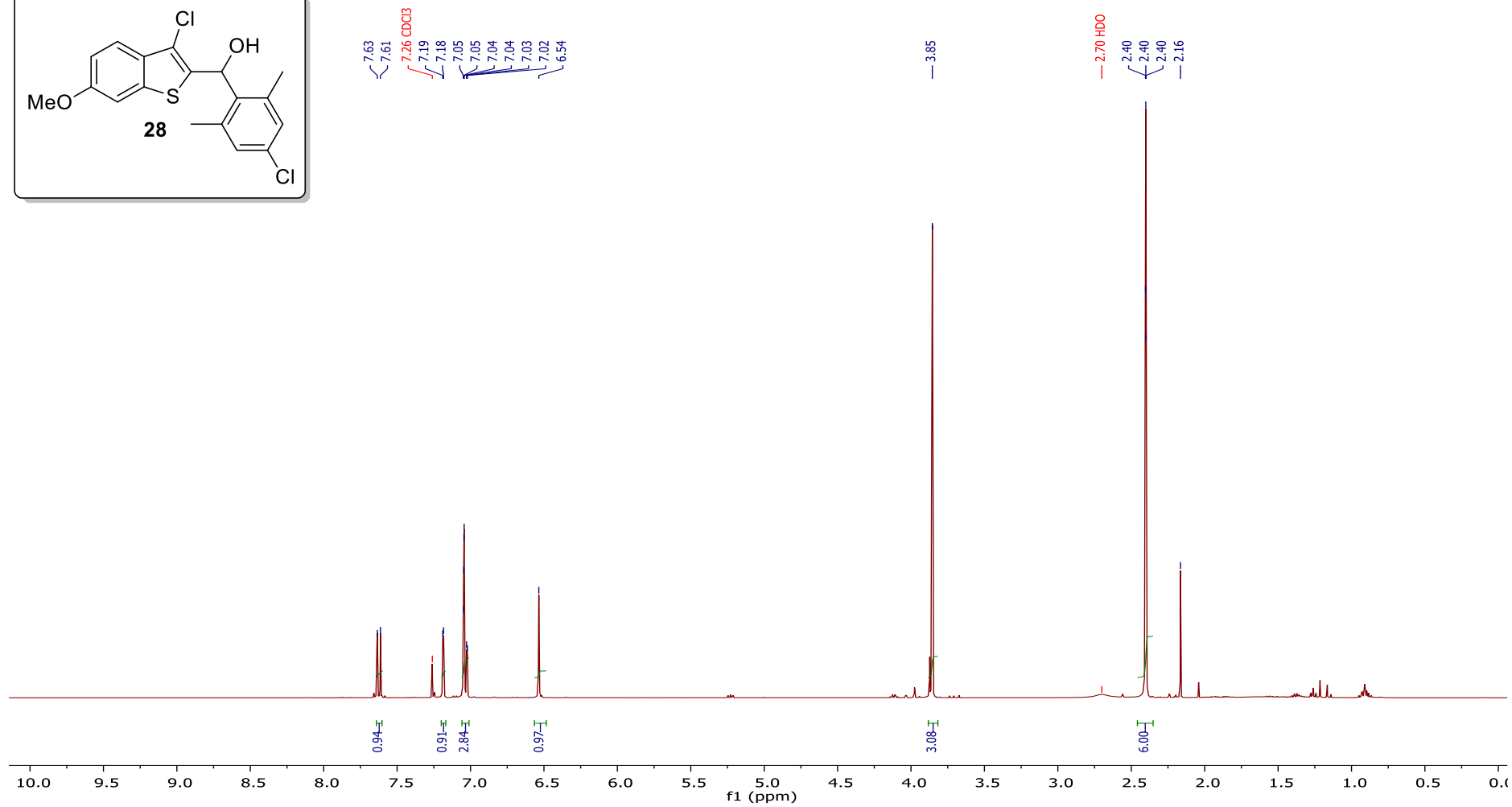
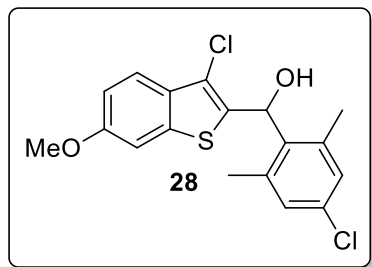
^1H NMR (400 MHz, CDCl_3):



^{13}C NMR (100.6 MHz, CDCl_3):



^1H NMR (400 MHz, CDCl_3):



^{13}C NMR (100.6 MHz, CDCl_3):

