

## Supplementary Materials

# Click Chemistry of Selenium Dihalides: Novel Bicyclic Organoselenium Compounds Based on Selenenylation/Bis-Functionalization Reactions and Evaluation of Glutathione Peroxidase-like Activity

Maxim V. Musalov \* and Vladimir A. Potapov

A. E. Favorsky Irkutsk Institute of Chemistry, Siberian Division of The Russian Academy of Sciences,  
1 Favorsky Str., 664033 Irkutsk, Russia

\* Correspondence: musalov\_maxim@irioch.irk.ru

## Table of Contents

Experimental (General Information)	2
Examples of $^1\text{H}$ and $^{13}\text{C}$ -NMR Spectra	3-11
Examples of $^1\text{H}$ and $^{13}\text{C}$ -NMR Spectra	11-22
Examples of $^{77}\text{Se}$ -NMR and $^1\text{H}$ - $^{77}\text{Se}$ -HMBC NMR Spectra	22-25
Examples of Mass Spectra	26-29

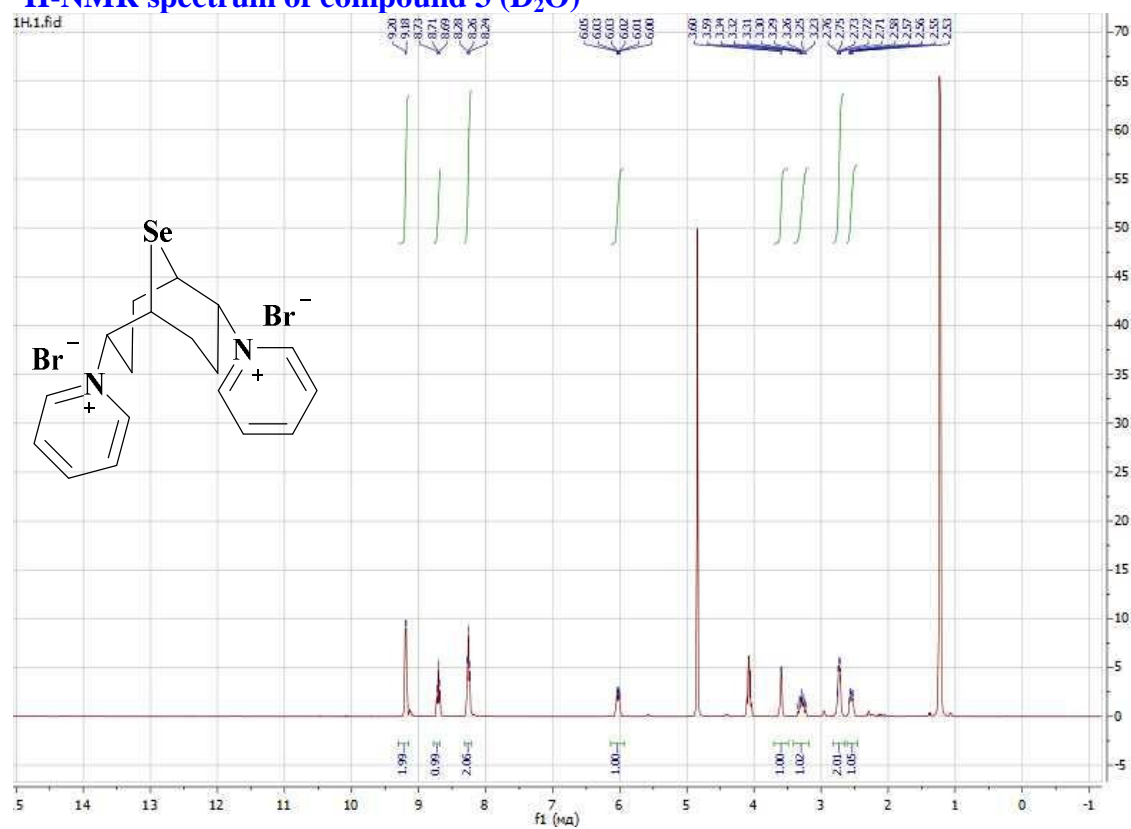
## Experimental (General Information)

The  $^1\text{H}$  (400.1 MHz),  $^{13}\text{C}$  (100.6 MHz), and  $^{77}\text{Se}$  (76.3 MHz) NMR spectra were recorded on a Bruker DPX-400 spectrometer (Bruker BioSpin GmbH, Rheinstetten, Germany) and referred to the residual solvent peaks of  $\text{CDCl}_3$  ( $\delta = 7.27$  and  $77.16$  ppm in  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR, respectively), DMSO ( $\delta = 2.50$  and  $39.50$  ppm for  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR, respectively) or  $\text{D}_2\text{O}$  ( $\delta = 4.79$  ppm for  $^1\text{H}$ -NMR) and dimethyl selenide ( $^{77}\text{Se}$ -NMR).

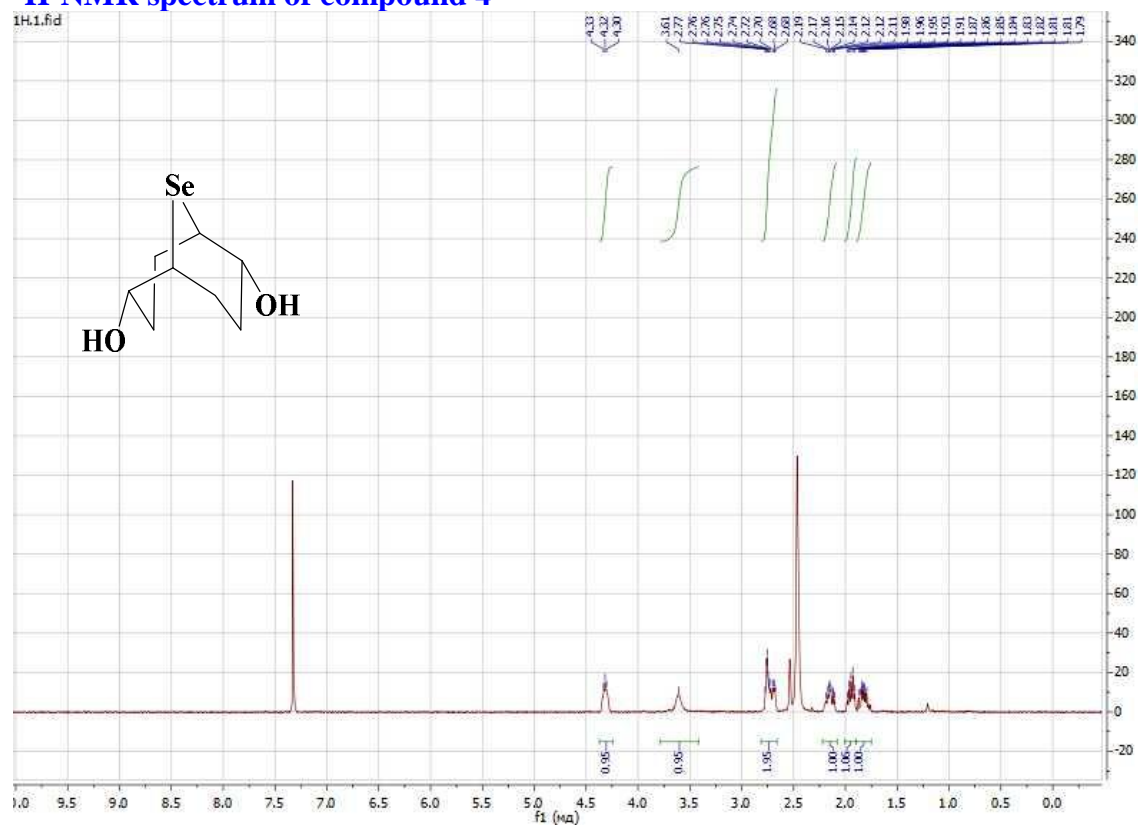
The mass spectra were recorded on a Shimadzu GCMS-QP5050A (Shimadzu Corporation, Kyoto, Japan) with electron impact (EI) ionization (70 eV).

## Examples of $^1\text{H}$ -NMR Spectra

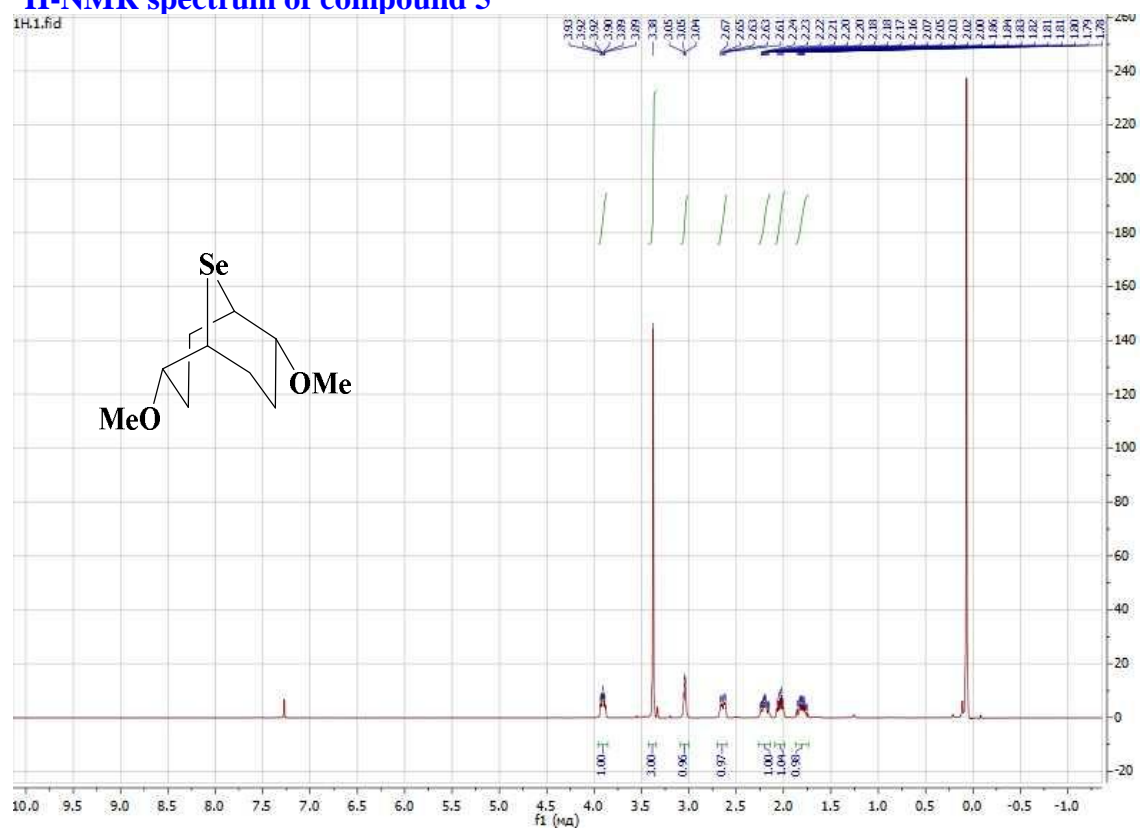
### $^1\text{H}$ -NMR spectrum of compound 3 ( $\text{D}_2\text{O}$ )



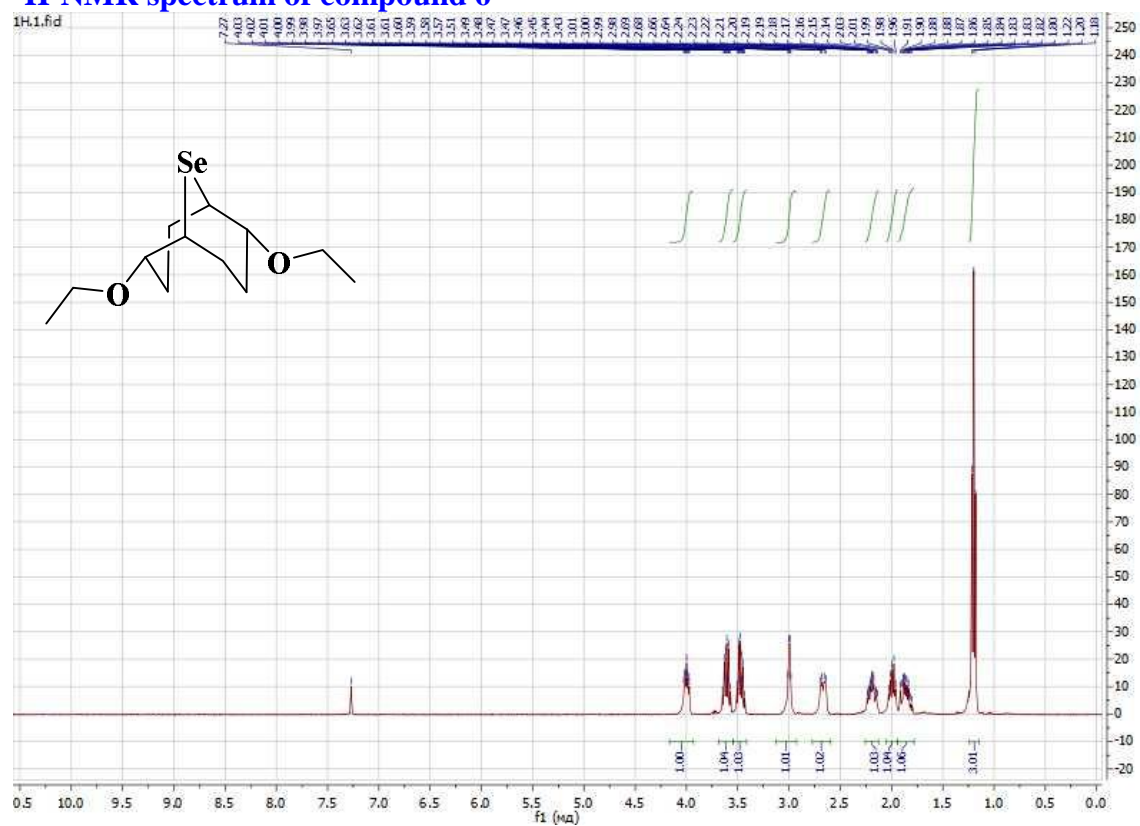
### $^1\text{H}$ -NMR spectrum of compound 4



### <sup>1</sup>H-NMR spectrum of compound 5

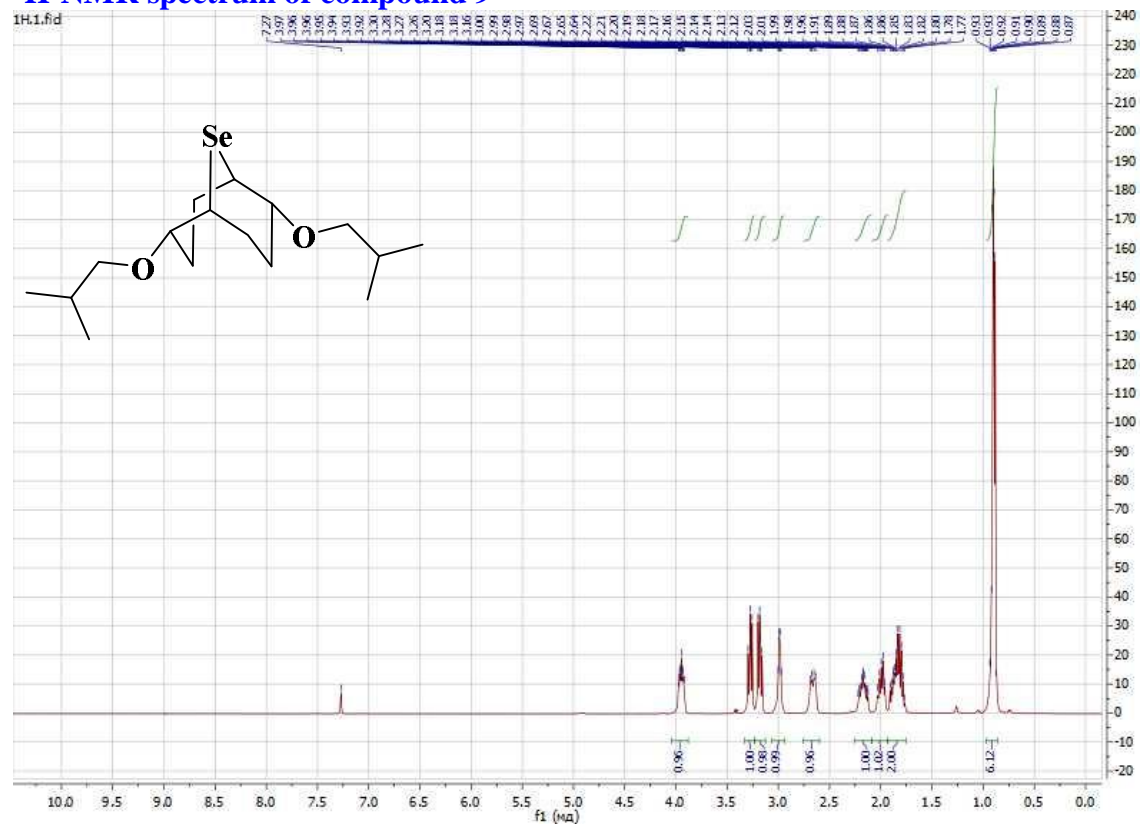


### <sup>1</sup>H-NMR spectrum of compound 6

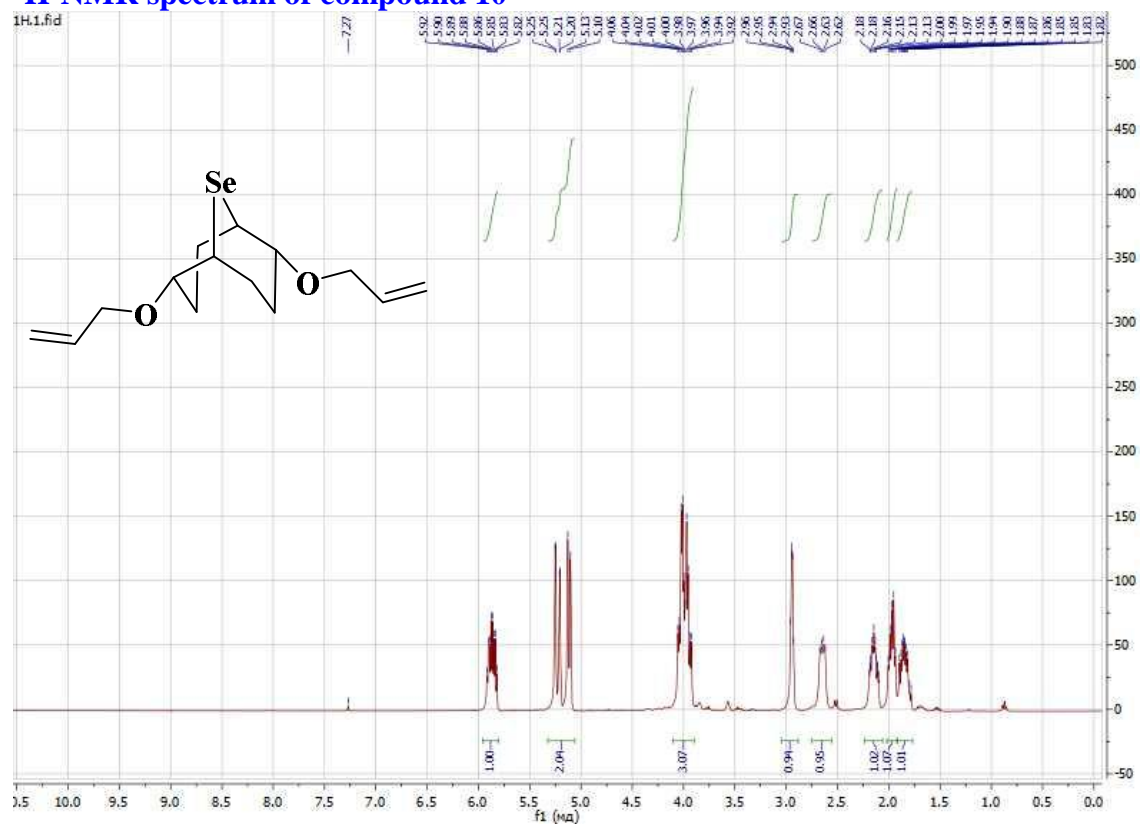




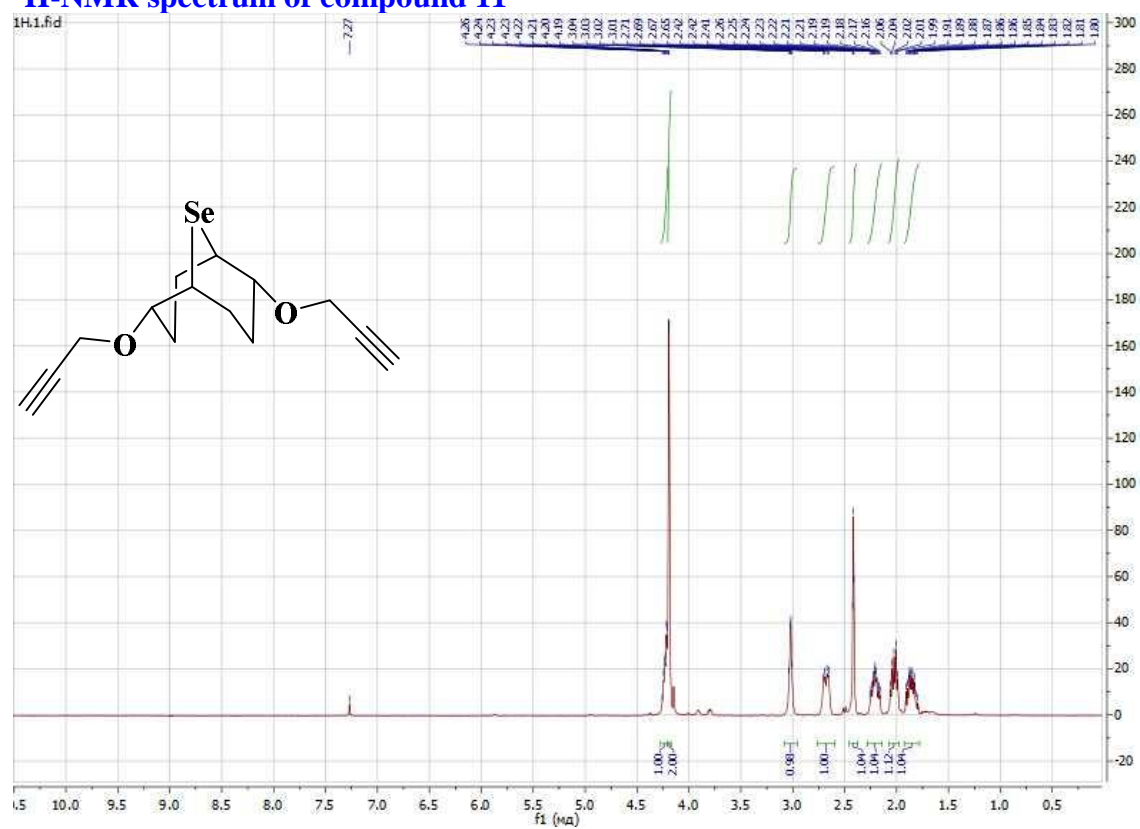
# <sup>1</sup>H-NMR spectrum of compound 9



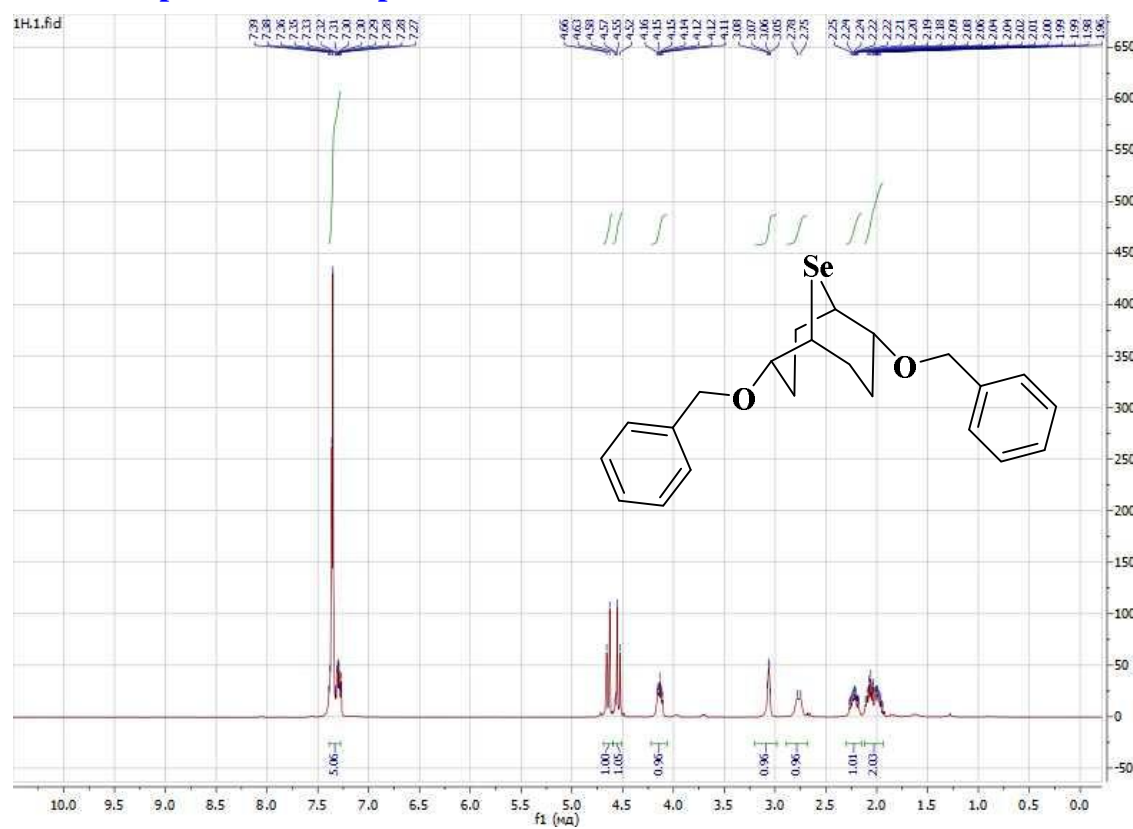
# <sup>1</sup>H-NMR spectrum of compound 10



# <sup>1</sup>H-NMR spectrum of compound 11

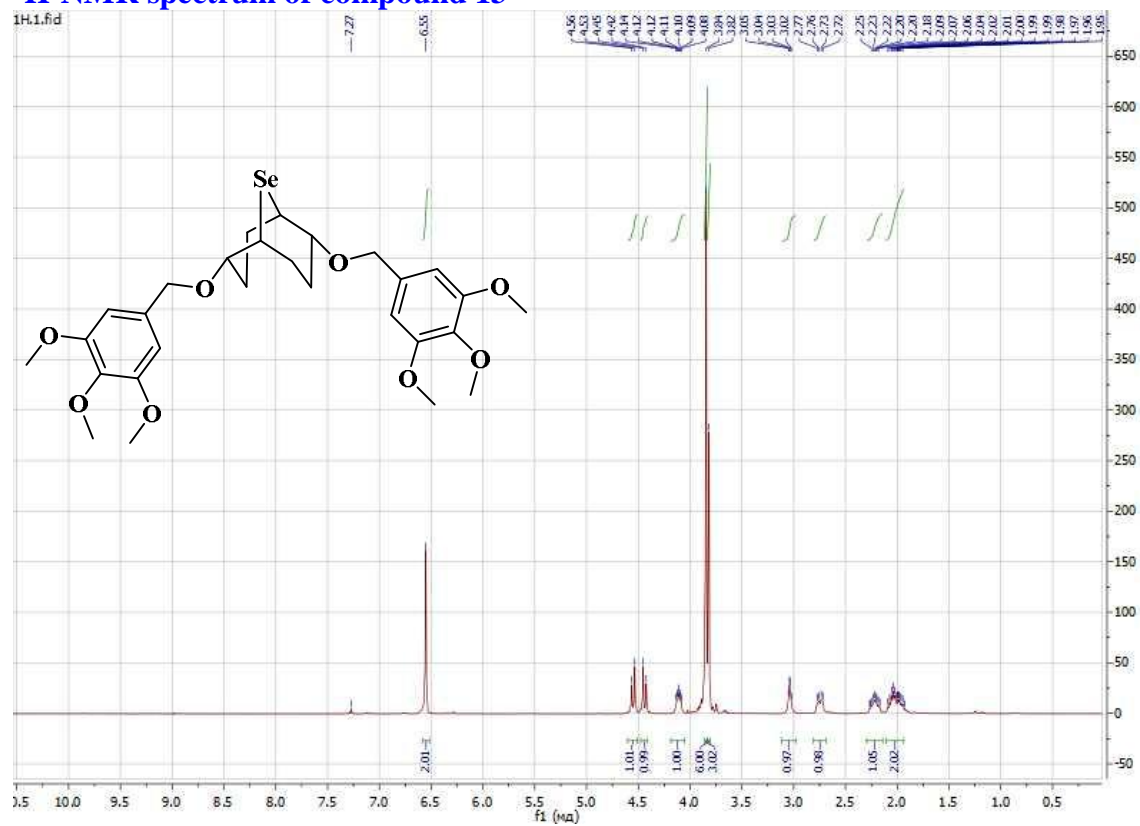


# <sup>1</sup>H-NMR spectrum of compound 12

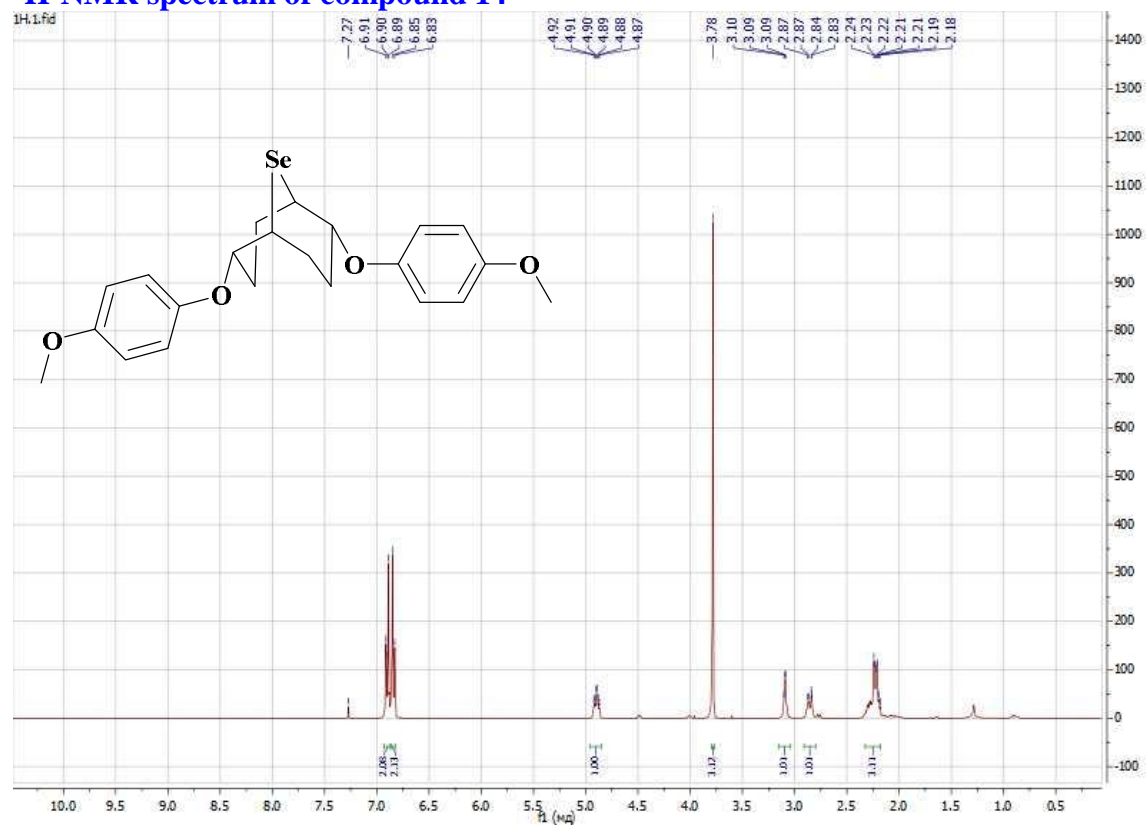




# <sup>1</sup>H-NMR spectrum of compound 13

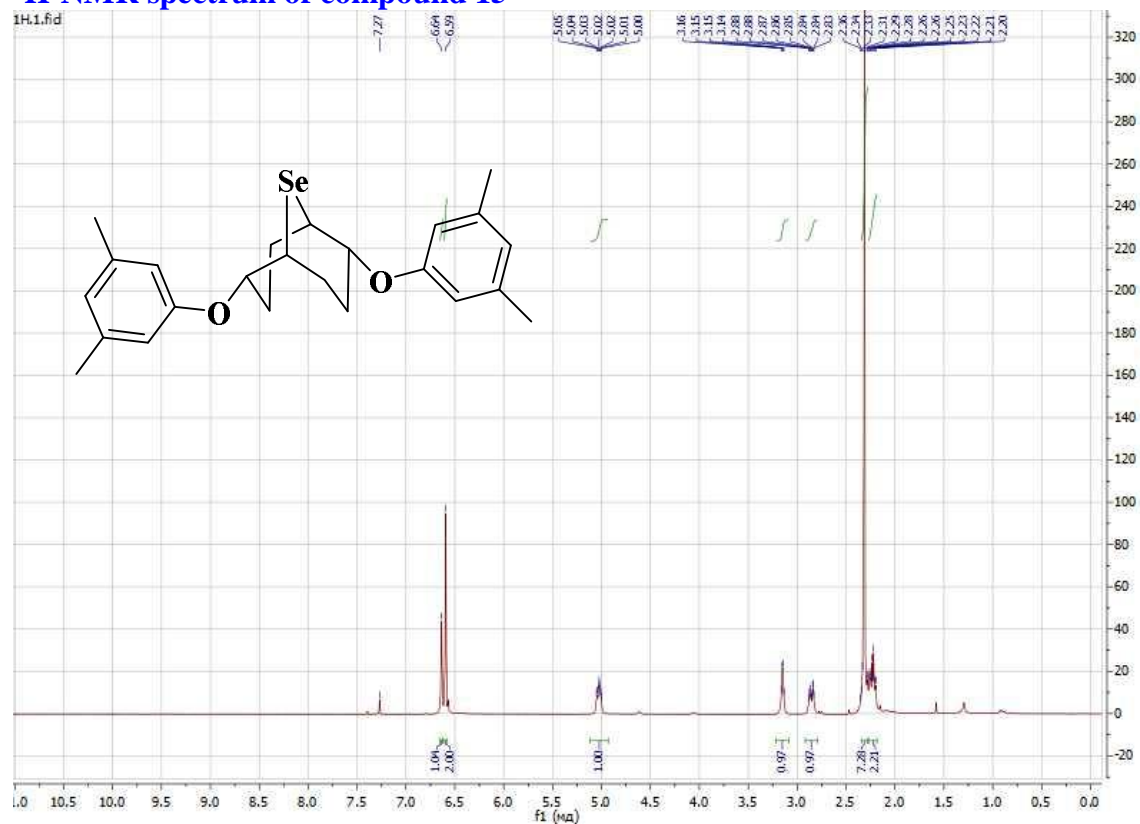


# <sup>1</sup>H-NMR spectrum of compound 14

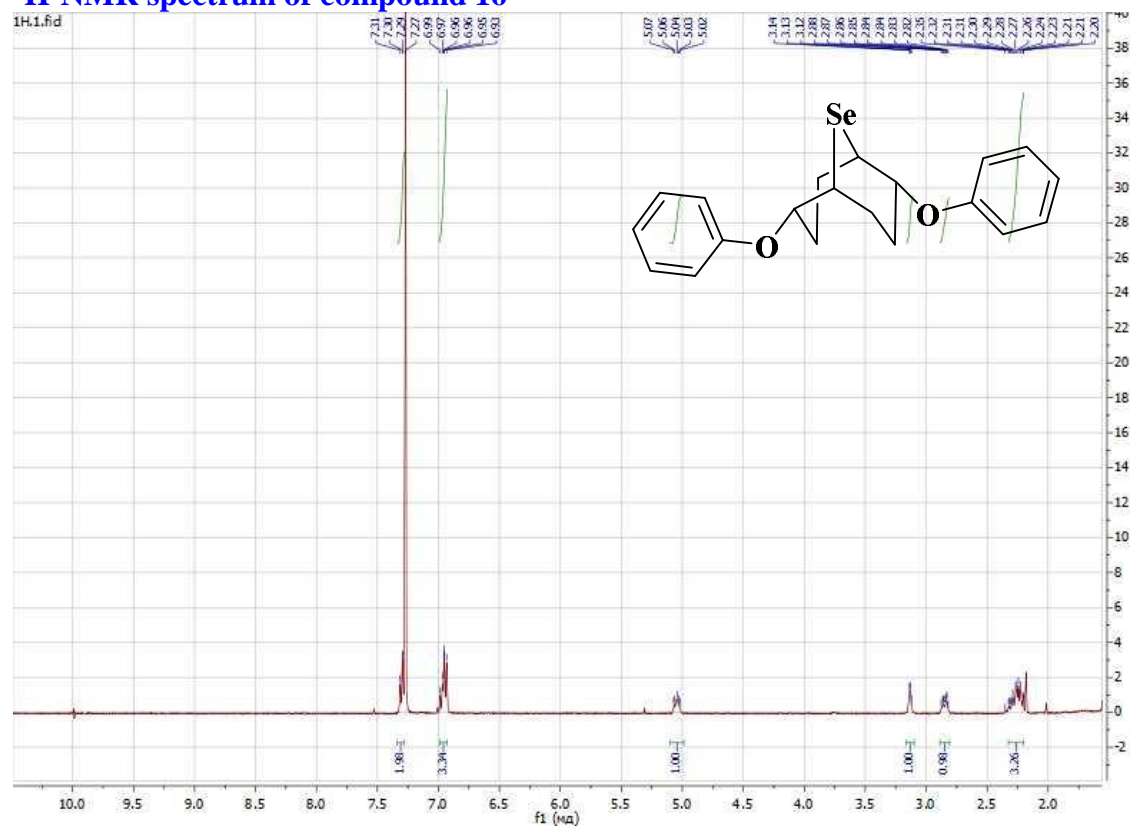




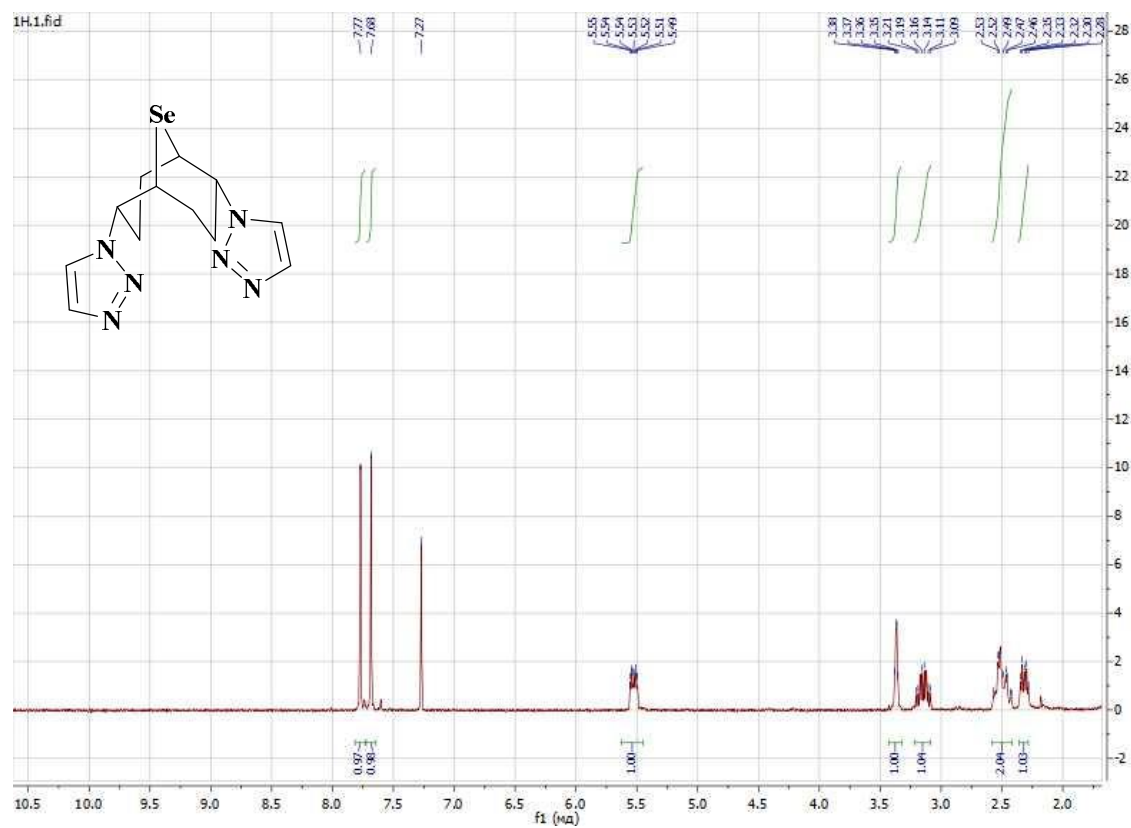
# <sup>1</sup>H-NMR spectrum of compound 15



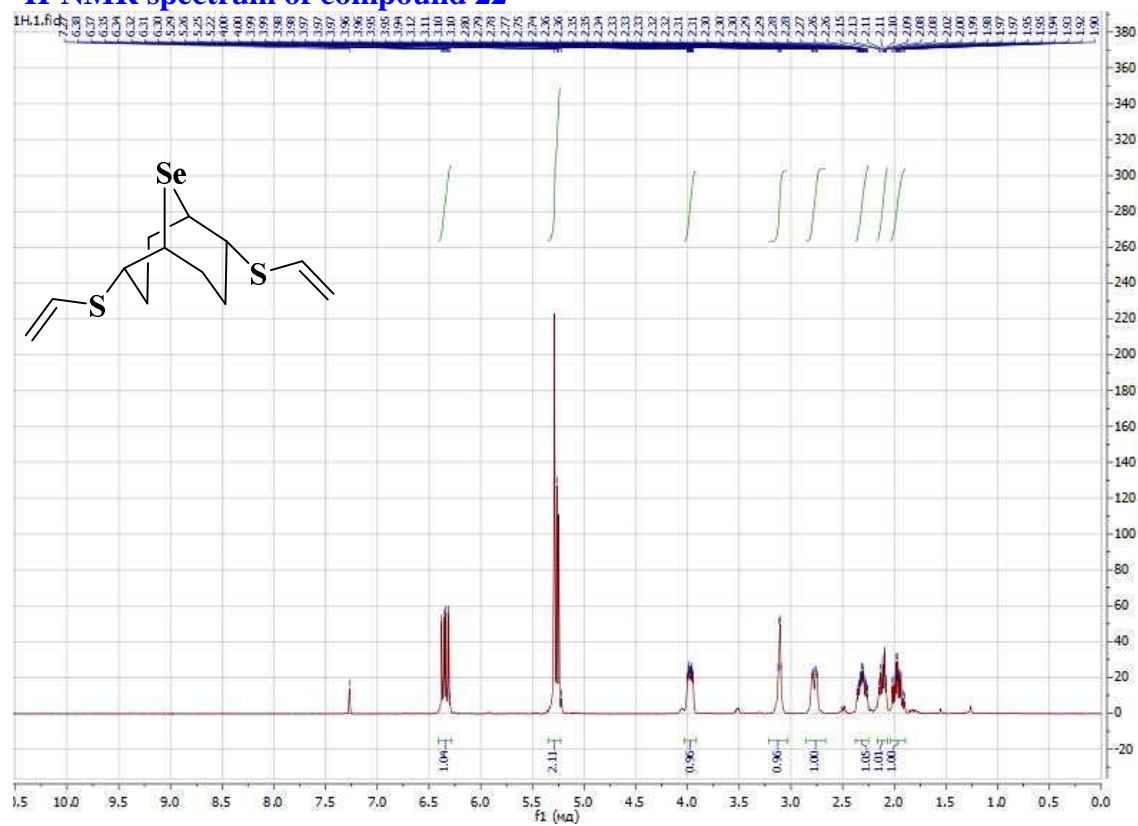
# <sup>1</sup>H-NMR spectrum of compound 16



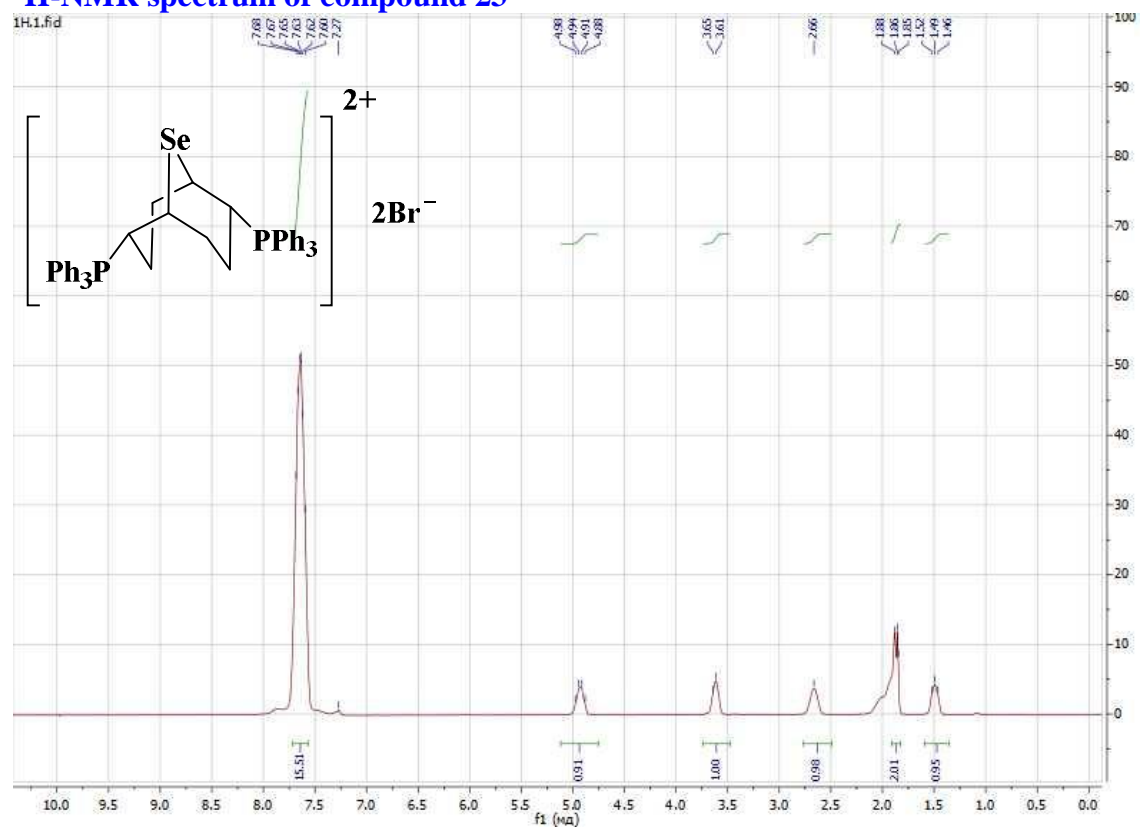
# <sup>1</sup>H-NMR spectrum of compound 18



# <sup>1</sup>H-NMR spectrum of compound 22



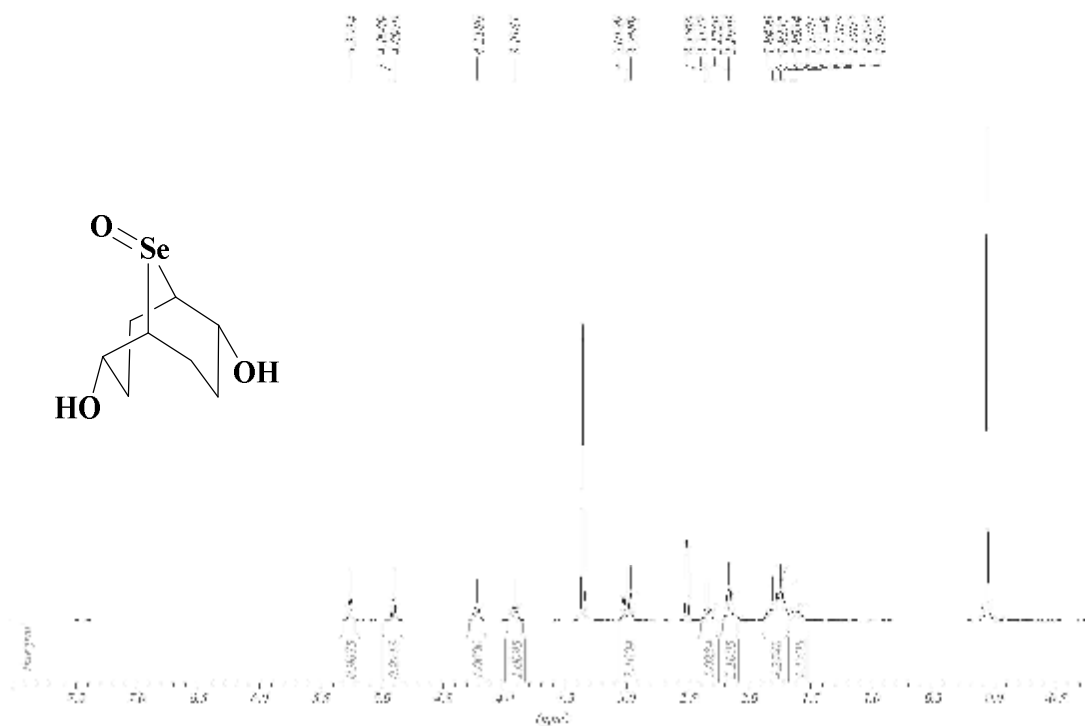
# <sup>1</sup>H-NMR spectrum of compound 23



# <sup>1</sup>H-NMR spectrum of compound 24

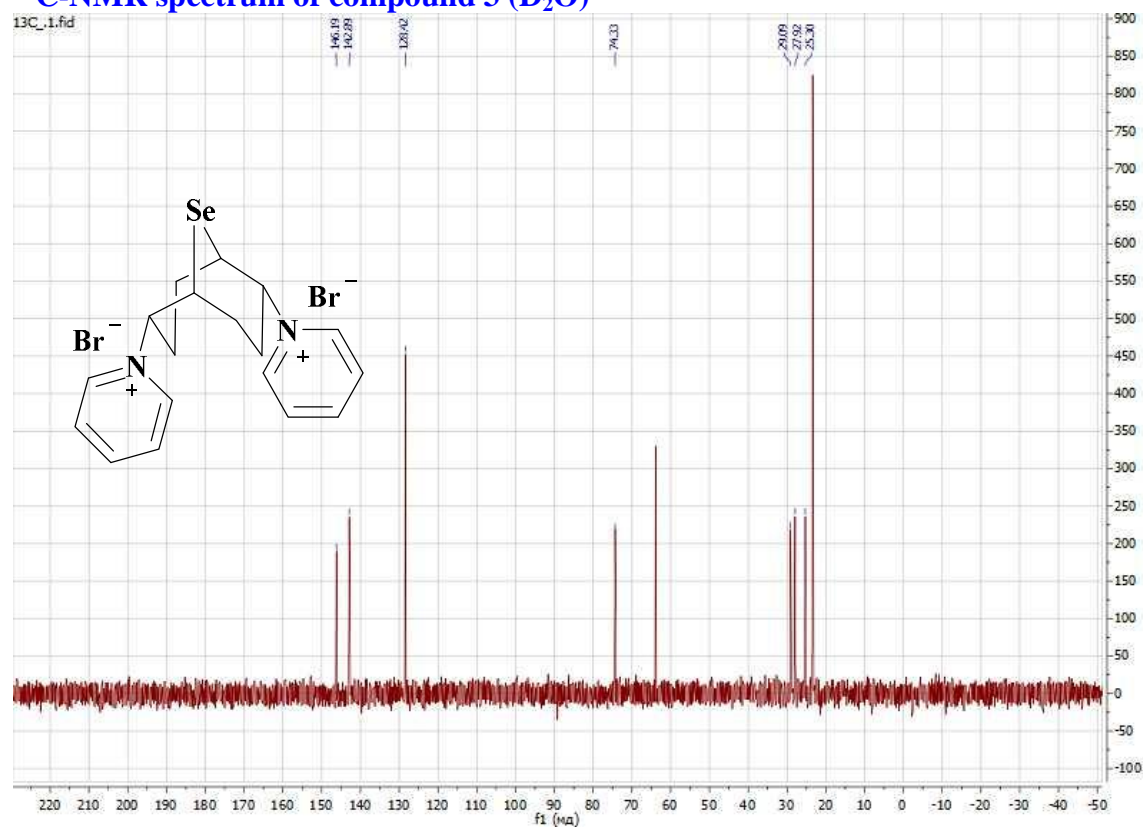


### <sup>1</sup>H-NMR spectrum of compound 25

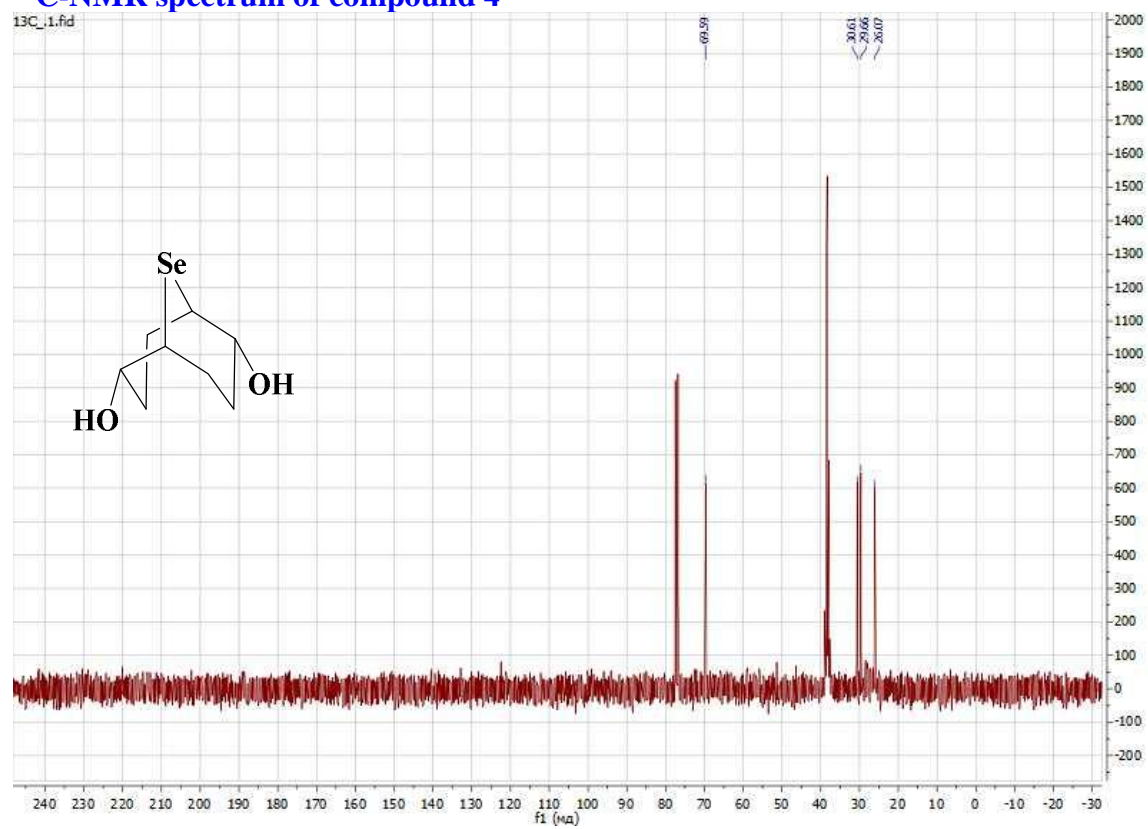


## Examples of <sup>13</sup>C-NMR Spectra

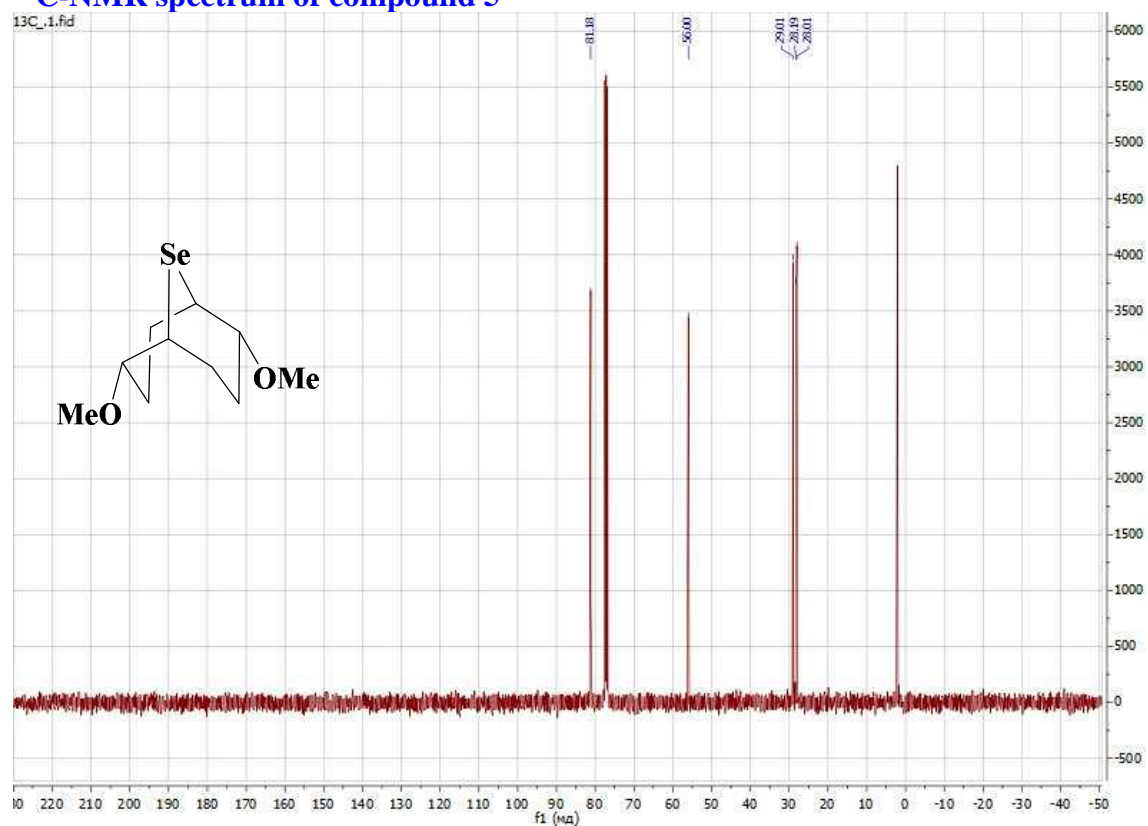
### <sup>13</sup>C-NMR spectrum of compound 3 (D<sub>2</sub>O)



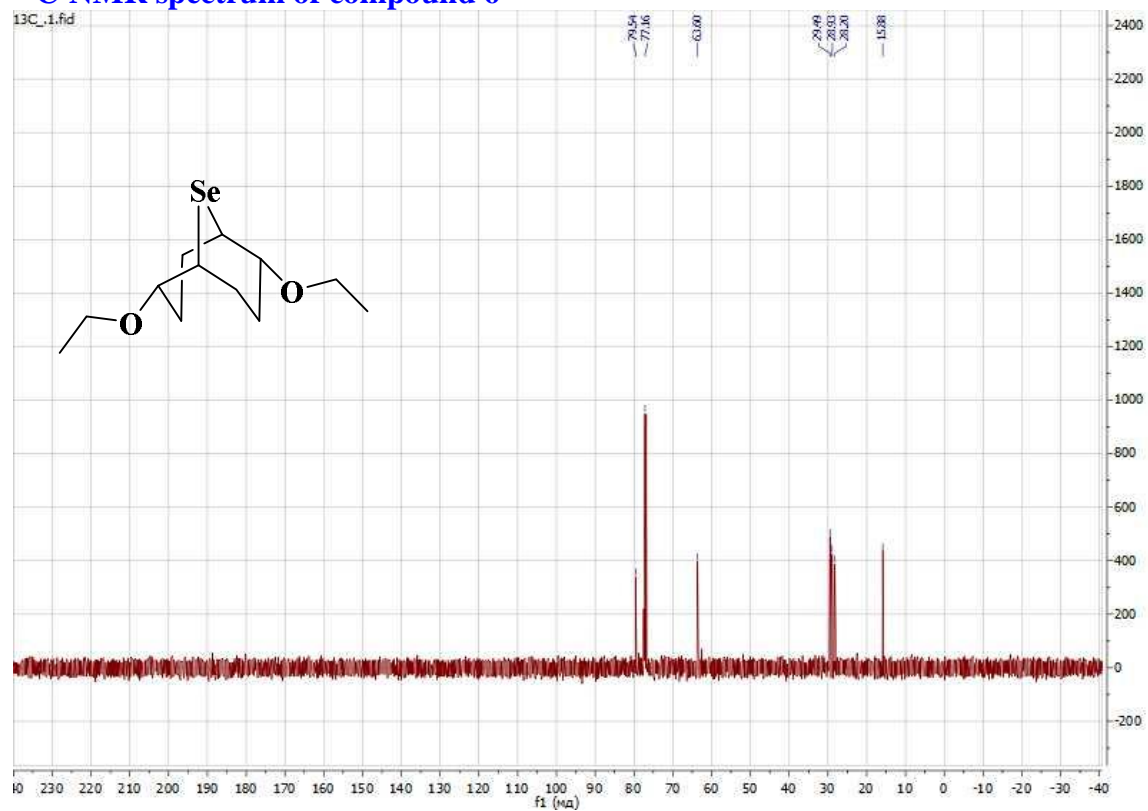
### $^{13}\text{C}$ -NMR spectrum of compound 4



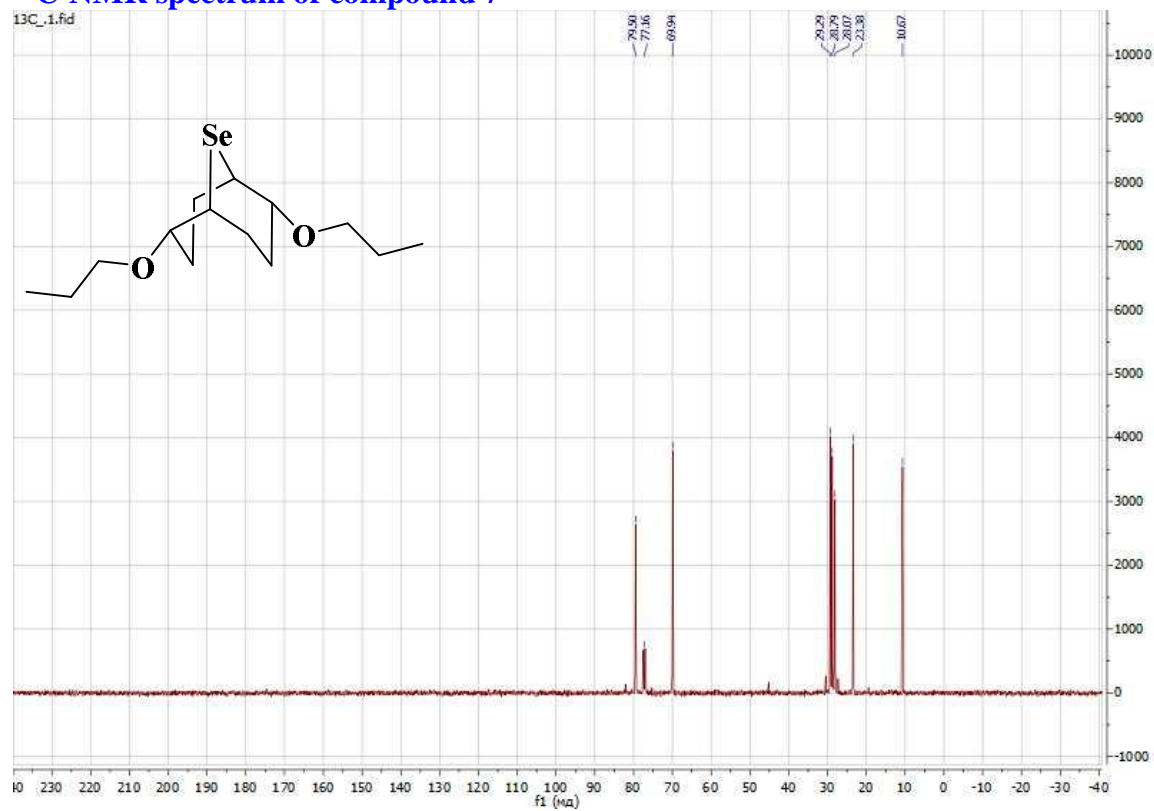
### $^{13}\text{C}$ -NMR spectrum of compound 5



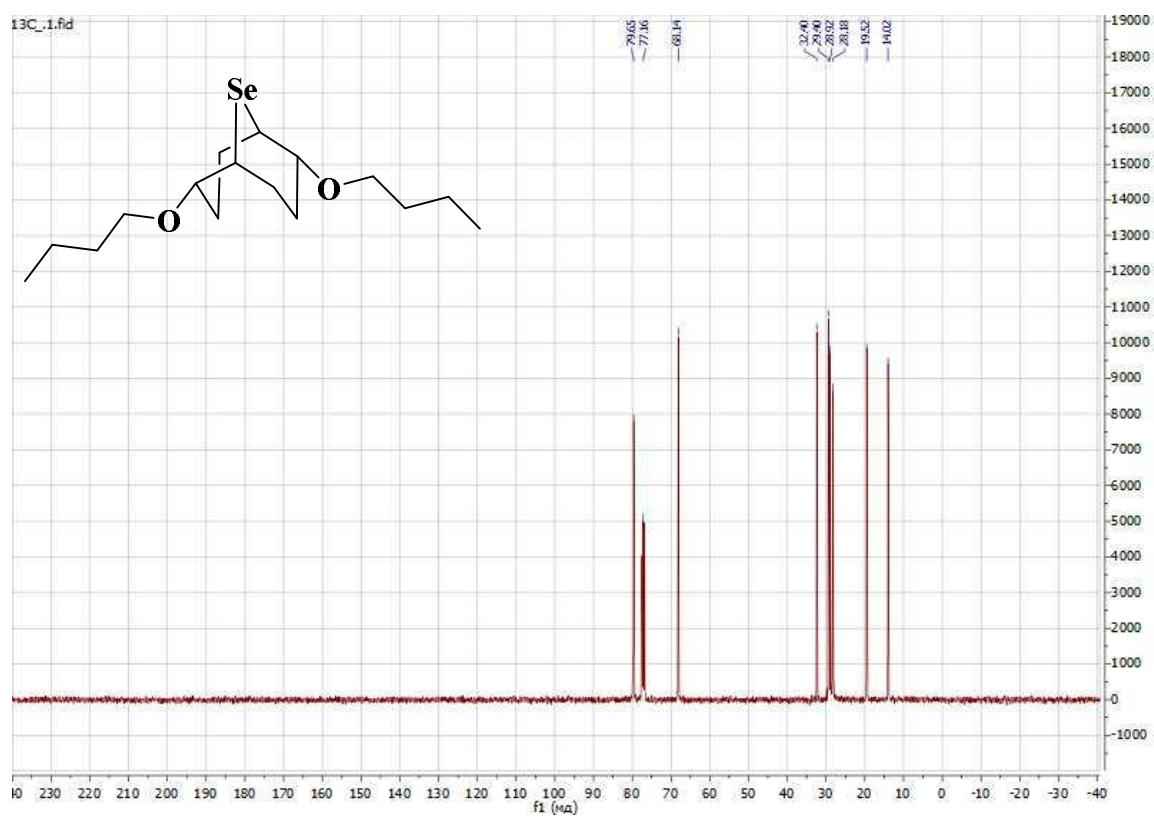
**$^{13}\text{C}$ -NMR spectrum of compound 6**



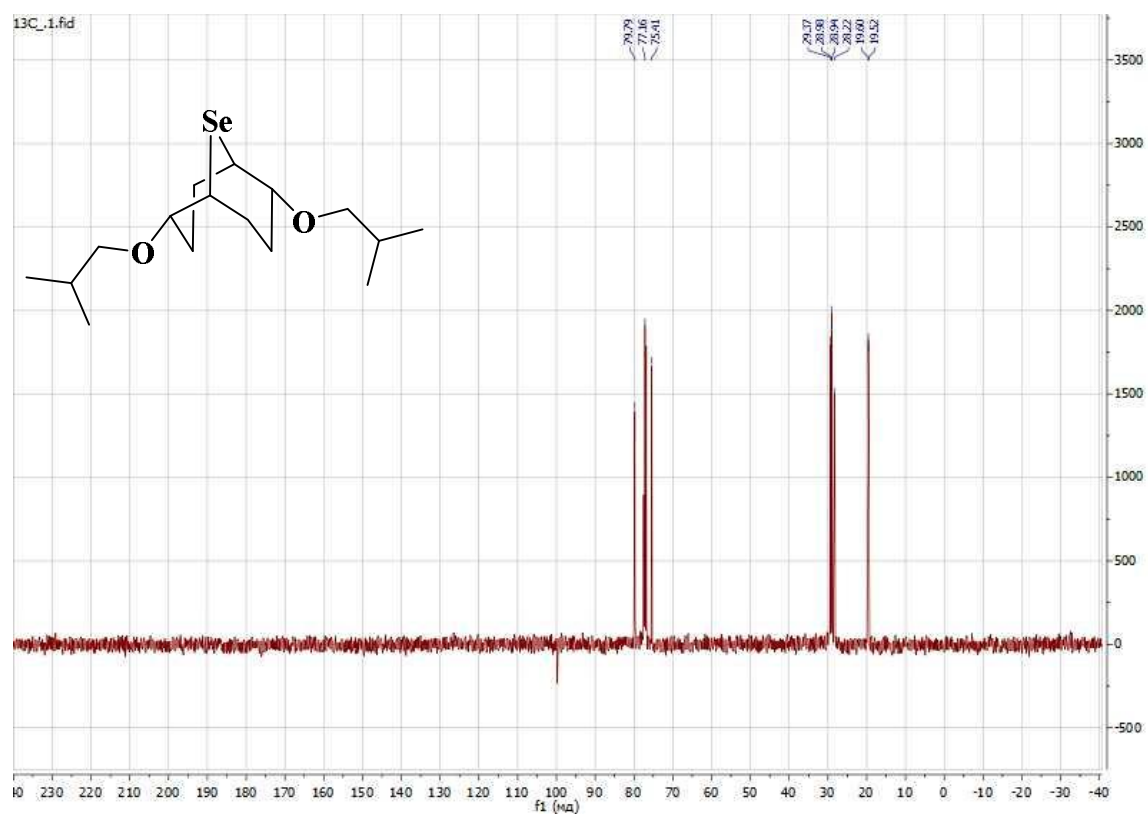
**$^{13}\text{C}$ -NMR spectrum of compound 7**



### $^{13}\text{C}$ -NMR spectrum of compound 8

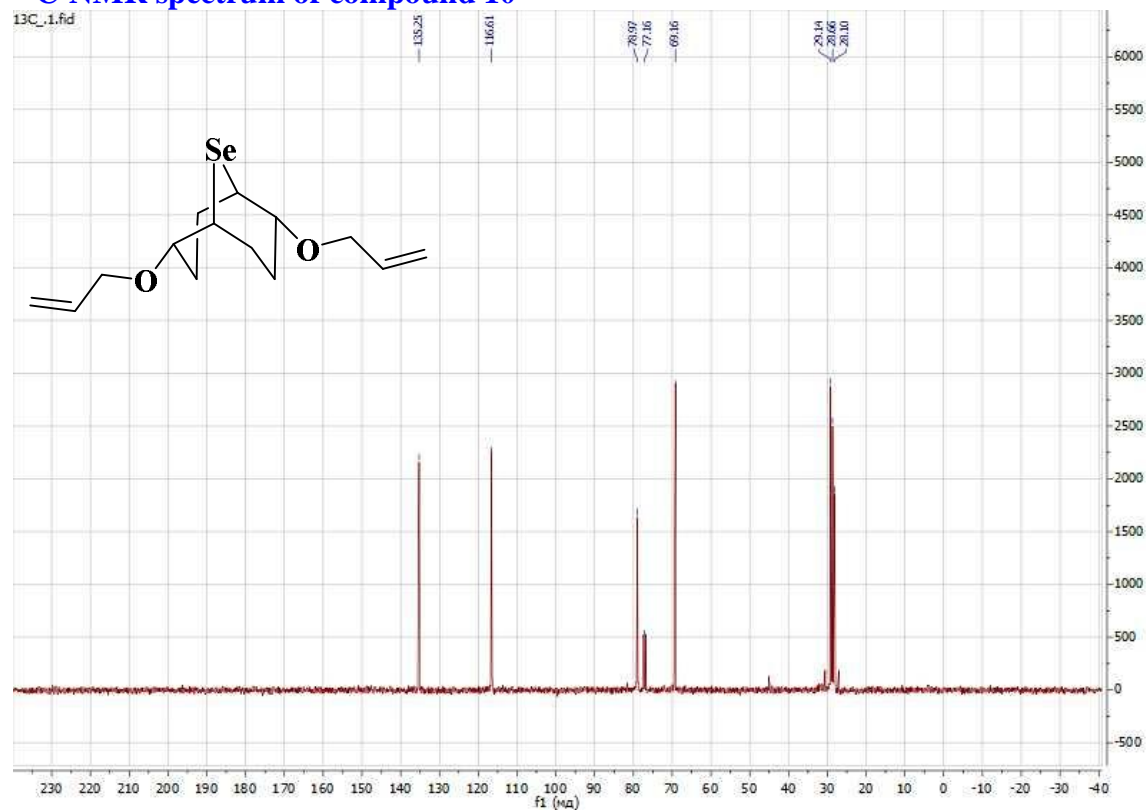


### $^{13}\text{C}$ -NMR spectrum of compound 9

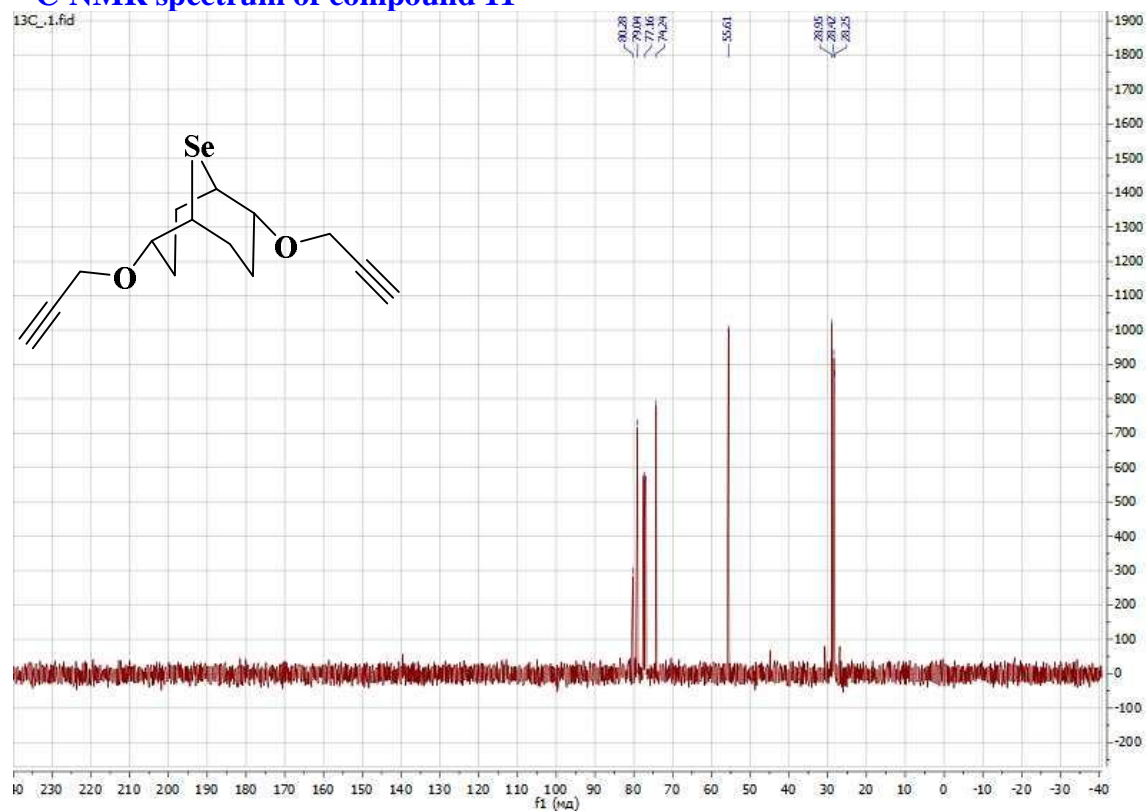




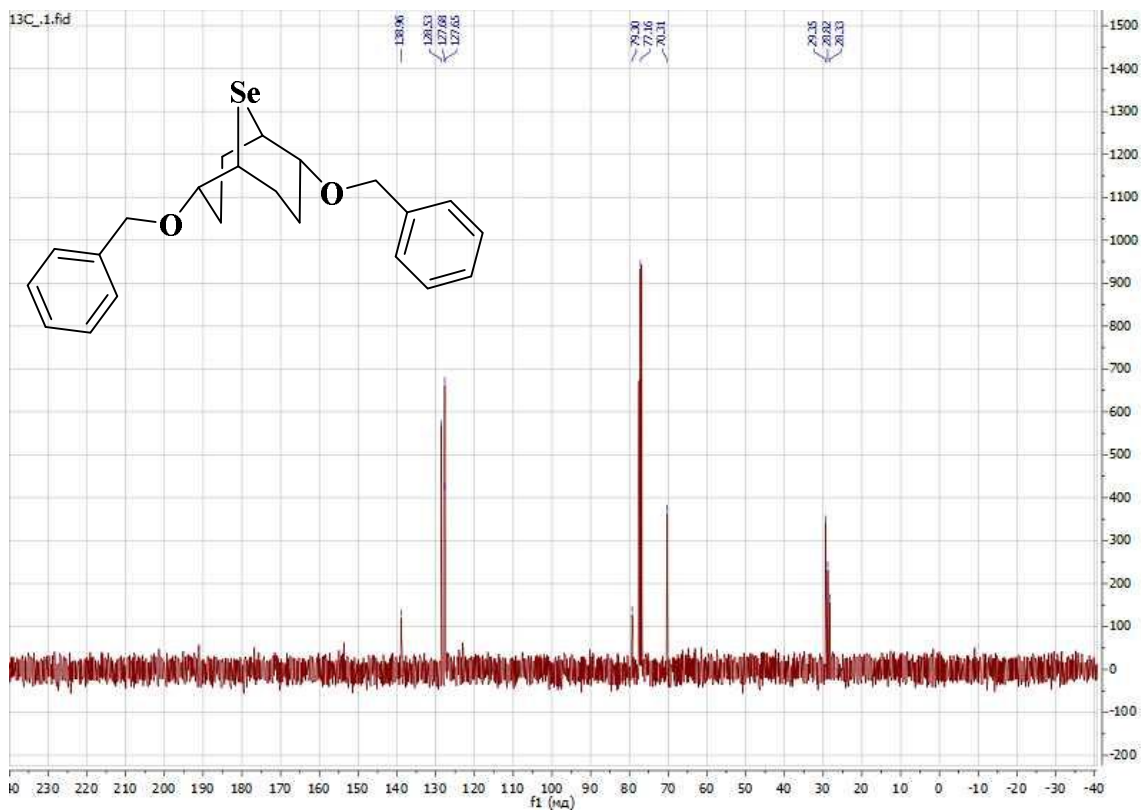
### $^{13}\text{C}$ -NMR spectrum of compound 10



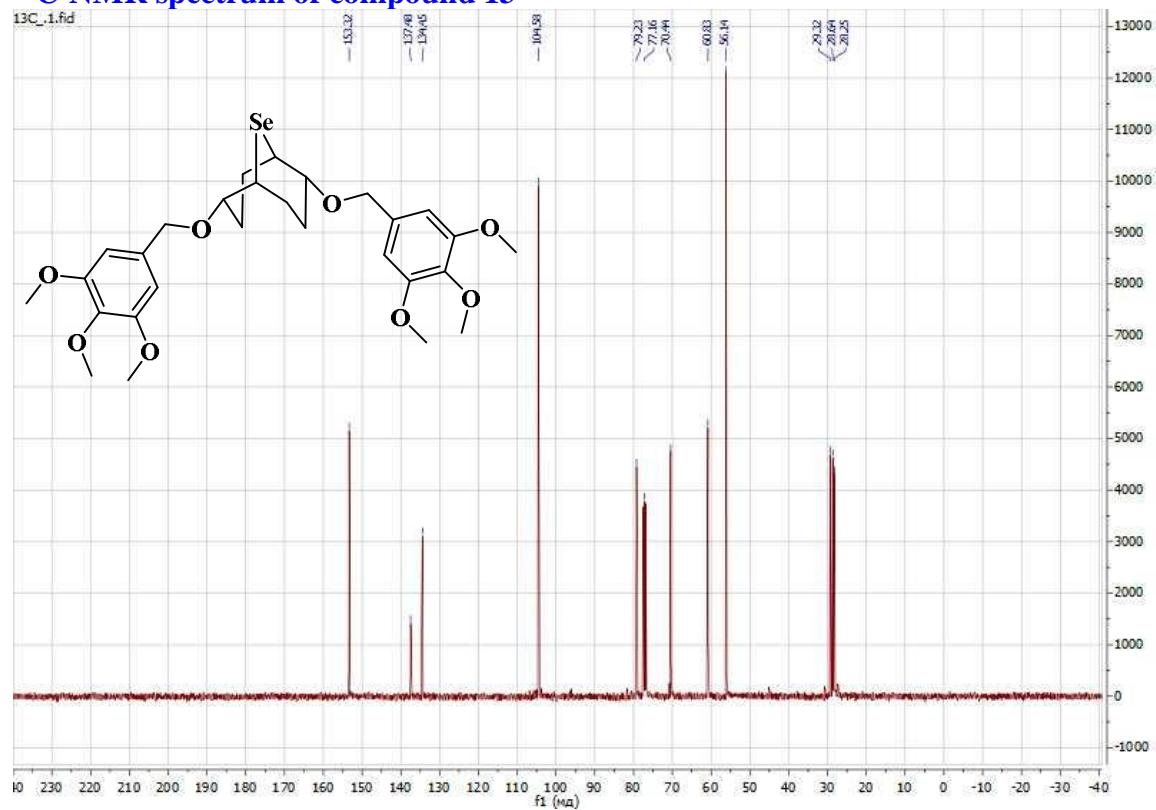
### $^{13}\text{C}$ -NMR spectrum of compound 11



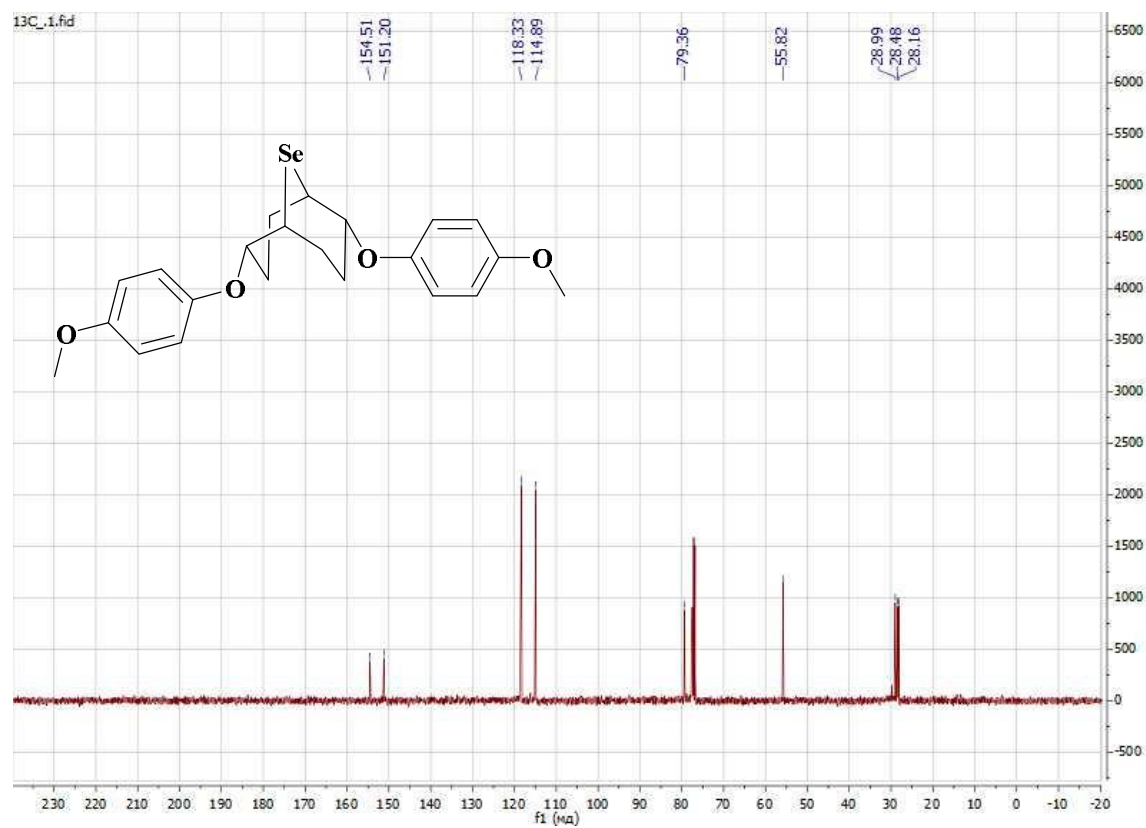
### $^{13}\text{C}$ -NMR spectrum of compound 12



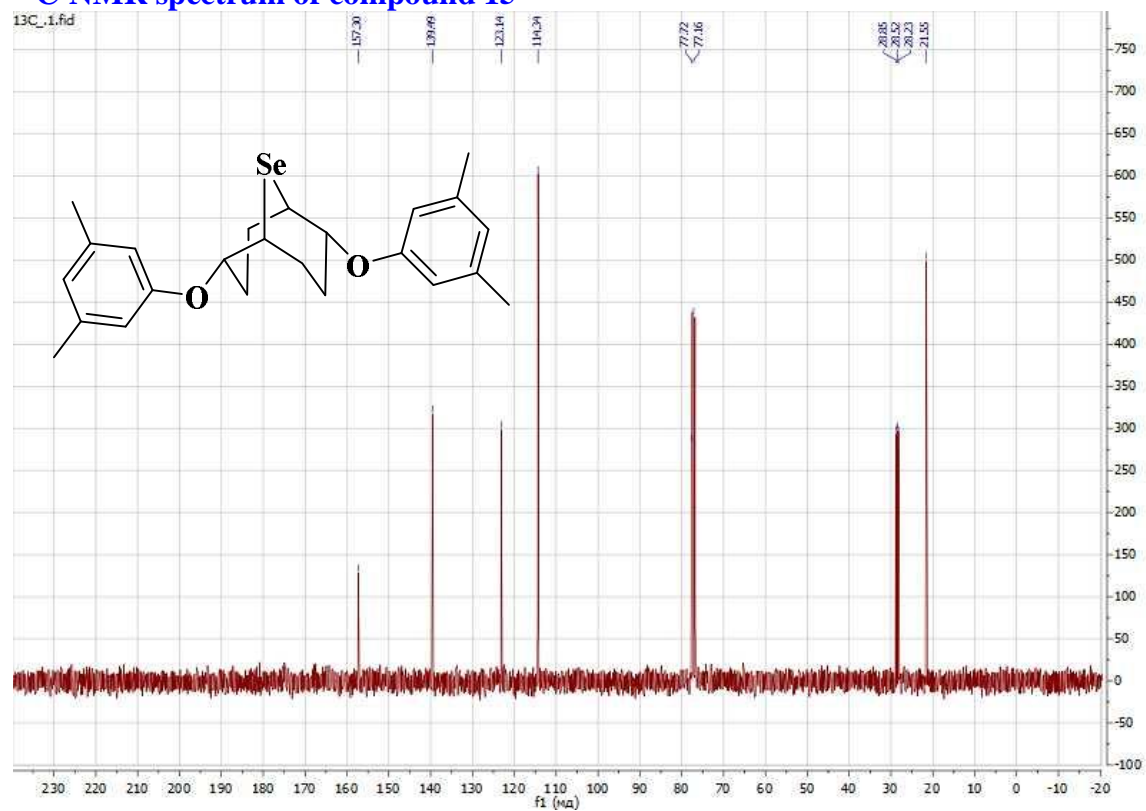
### $^{13}\text{C}$ -NMR spectrum of compound 13



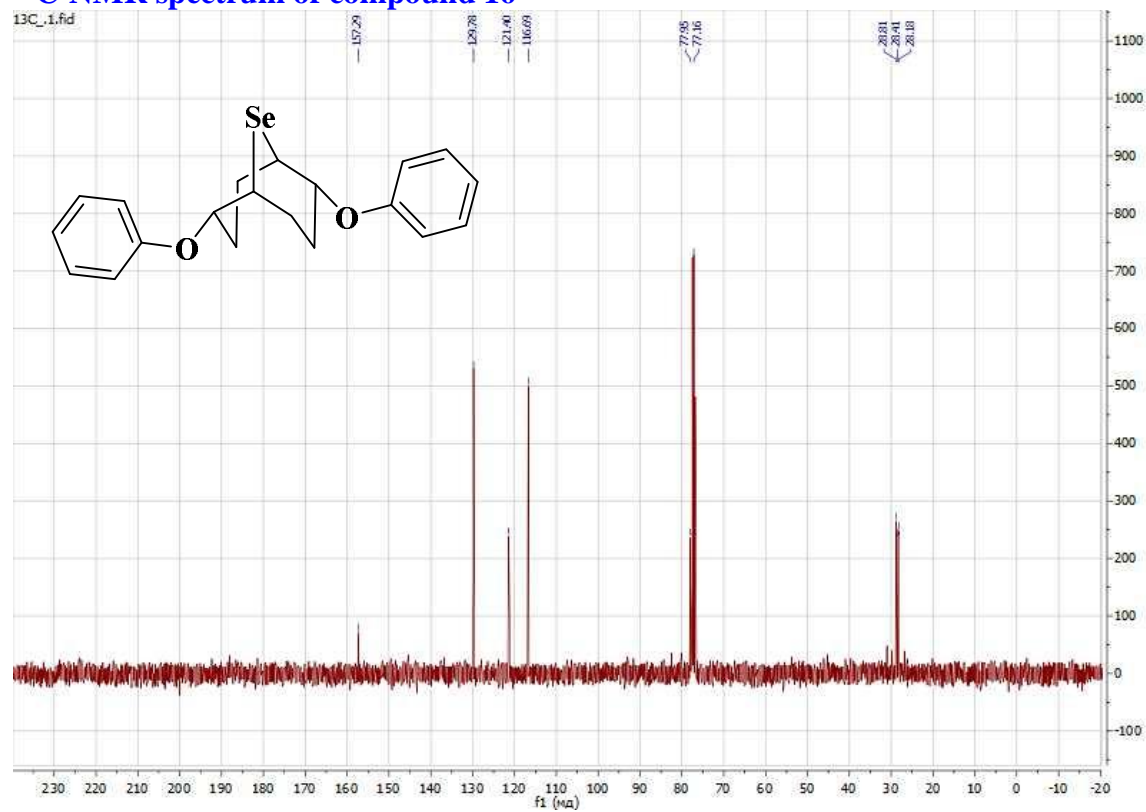
### <sup>13</sup>C-NMR spectrum of compound 14



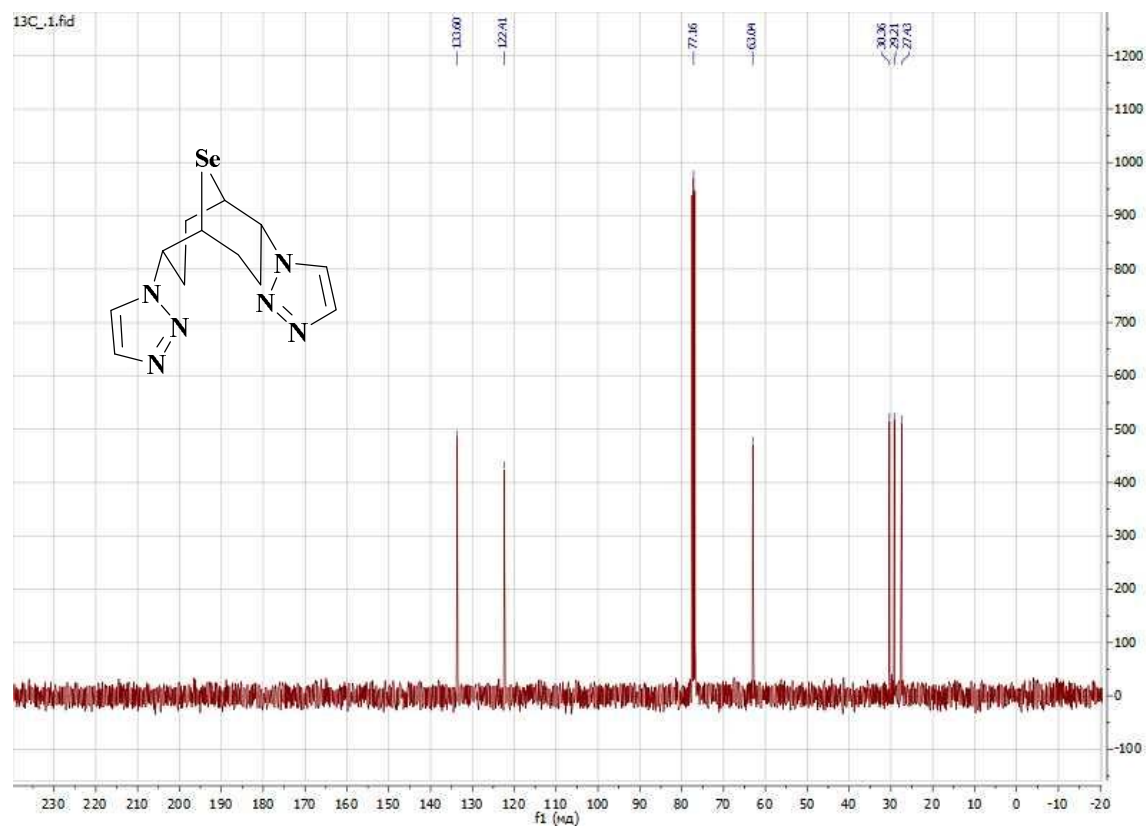
### <sup>13</sup>C-NMR spectrum of compound 15



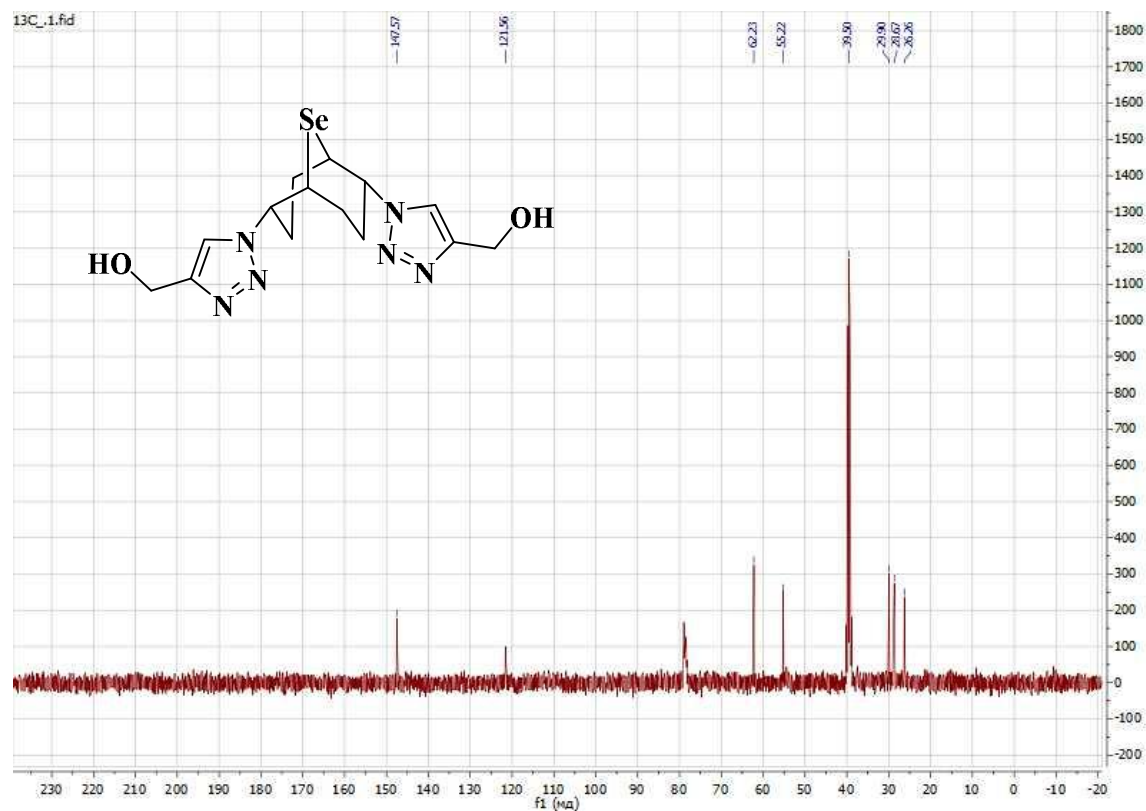
**$^{13}\text{C}$ -NMR spectrum of compound 16**



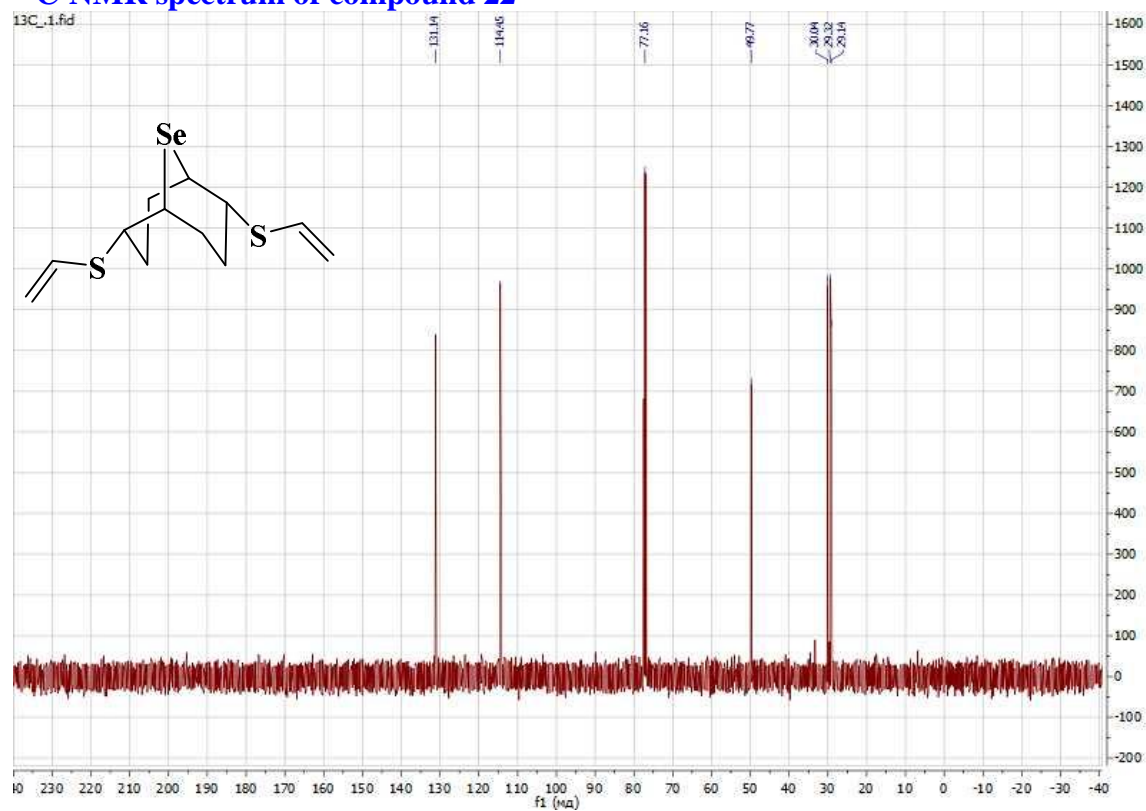
**$^{13}\text{C}$ -NMR spectrum of compound 18**



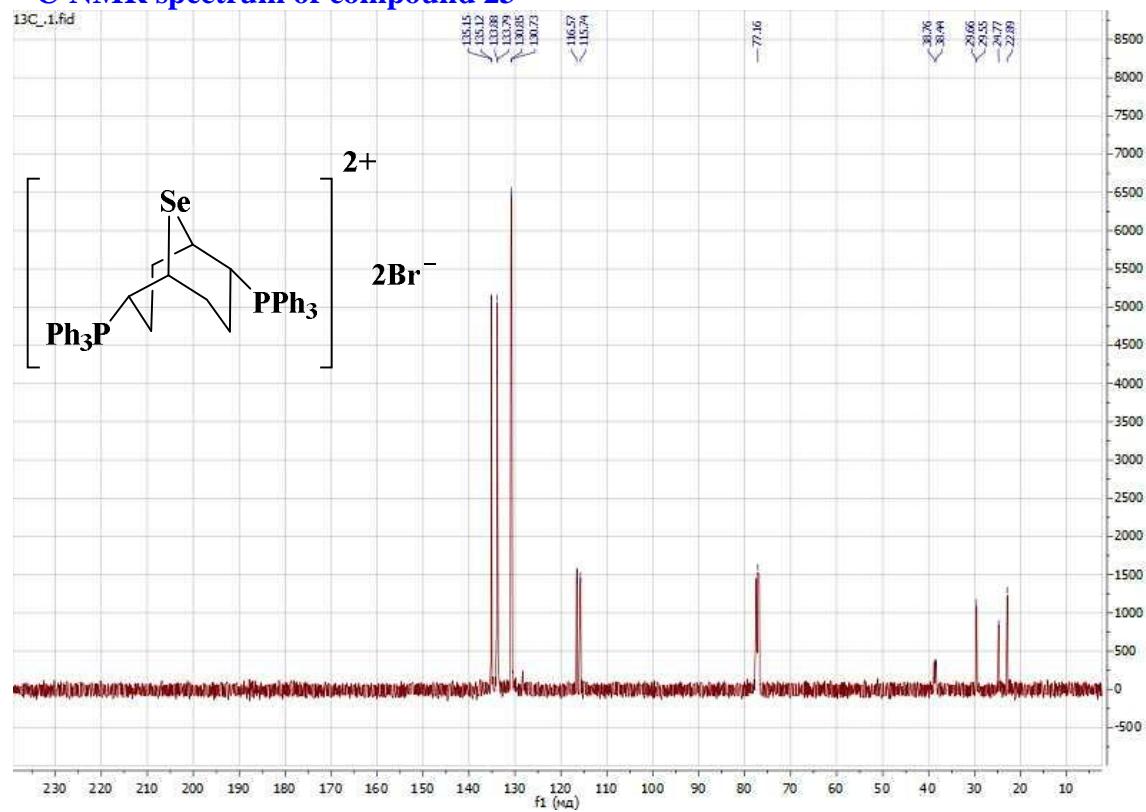
**$^{13}\text{C}$ -NMR spectrum of compound 19 (DMSO- $d_6$ /CDCl $_3$ )**



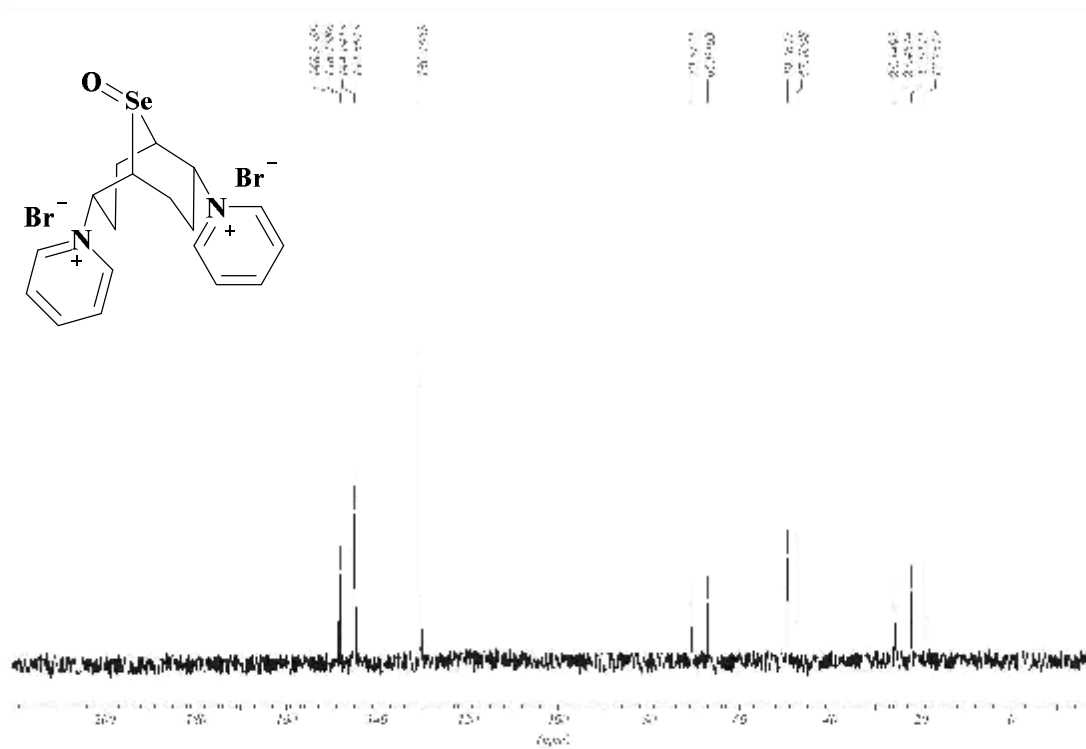
**$^{13}\text{C}$ -NMR spectrum of compound 22**



### $^{13}\text{C}$ -NMR spectrum of compound 23

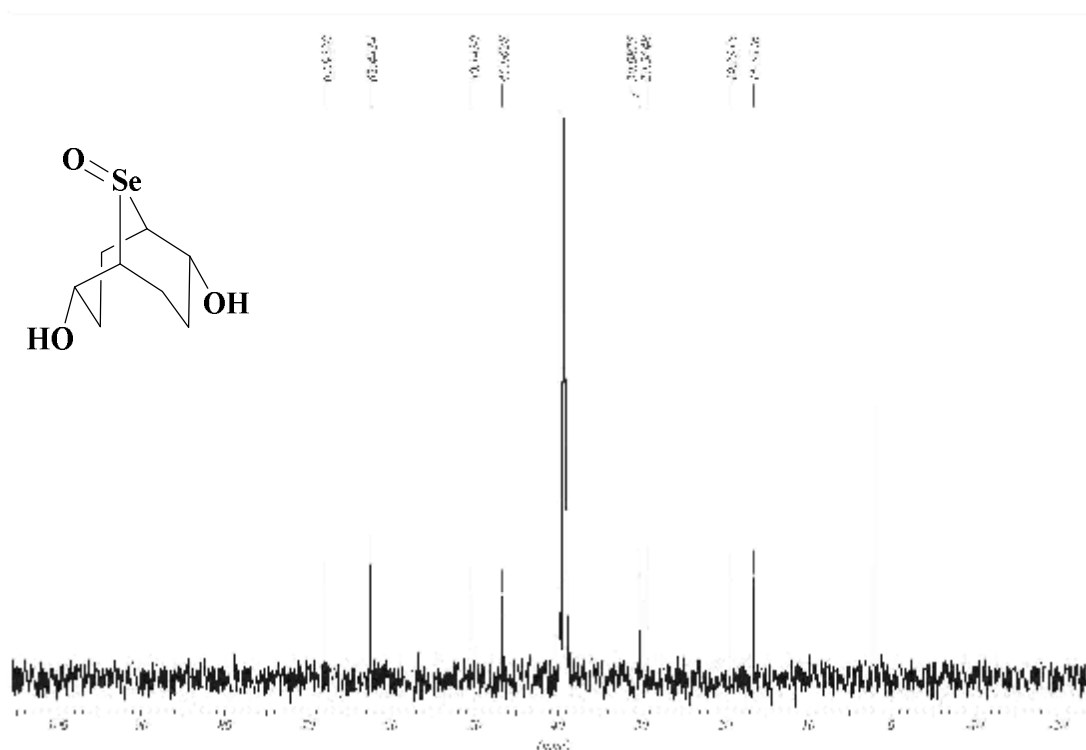


### $^{13}\text{C}$ -NMR spectrum of compound 24



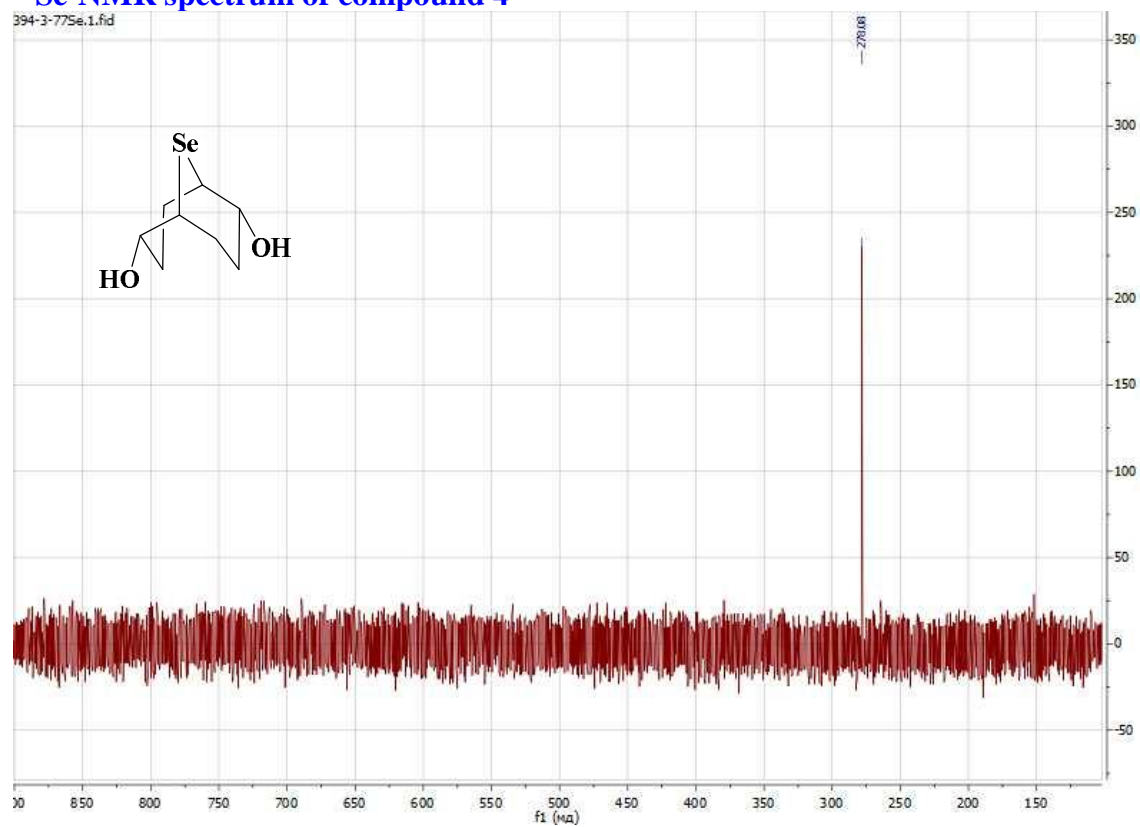


## $^{13}\text{C}$ -NMR spectrum of compound 25

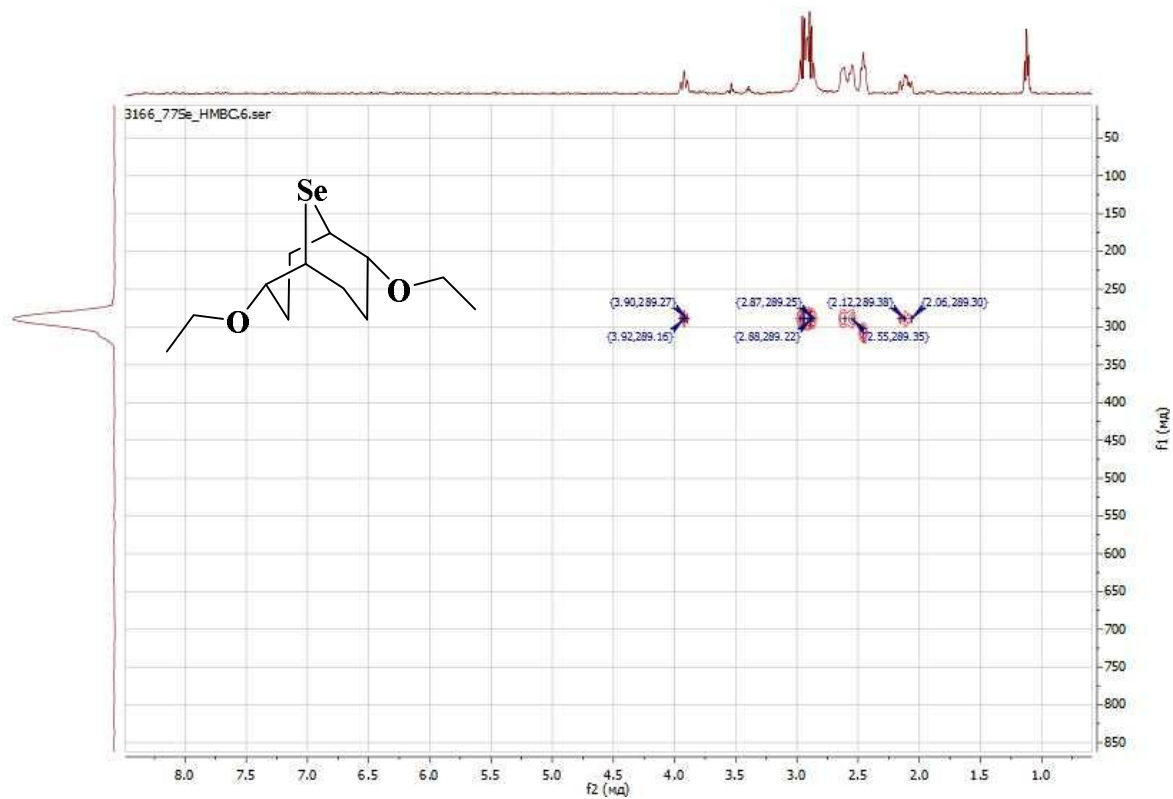
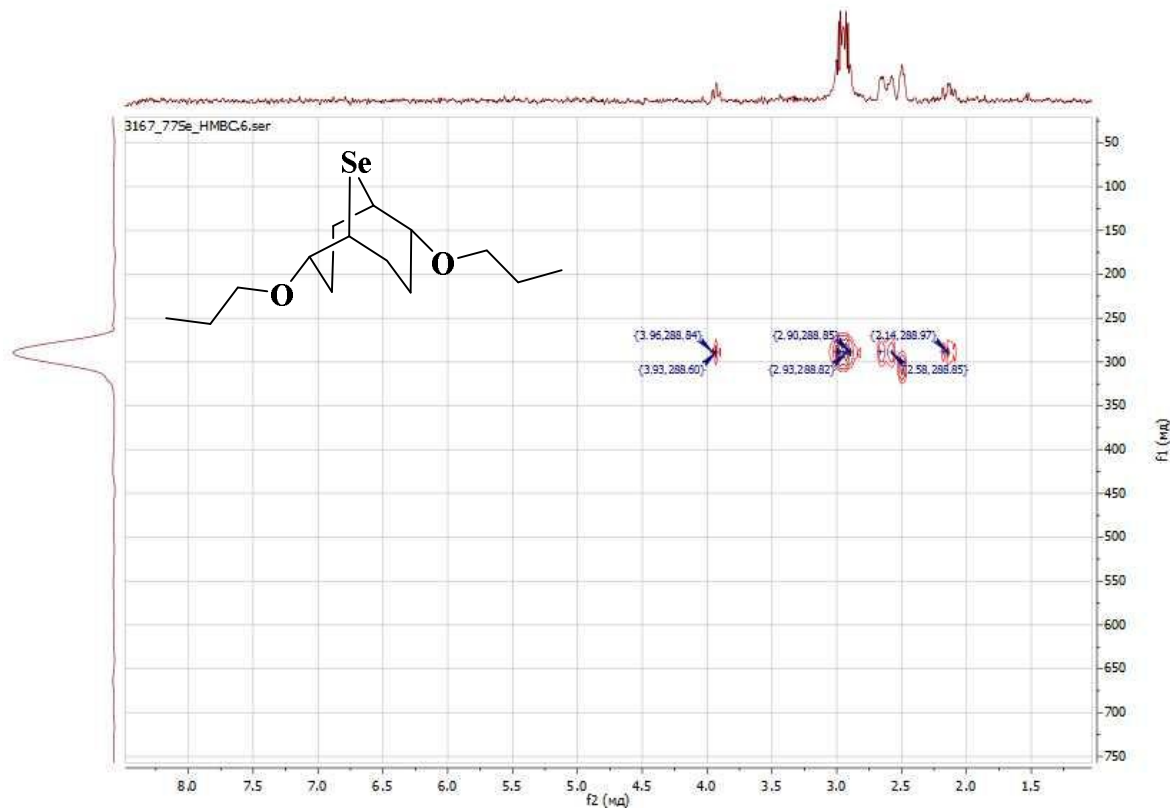


## Examples of $^{77}\text{Se}$ -NMR and $^1\text{H}$ - $^{77}\text{Se}$ -HMBC NMR Spectra

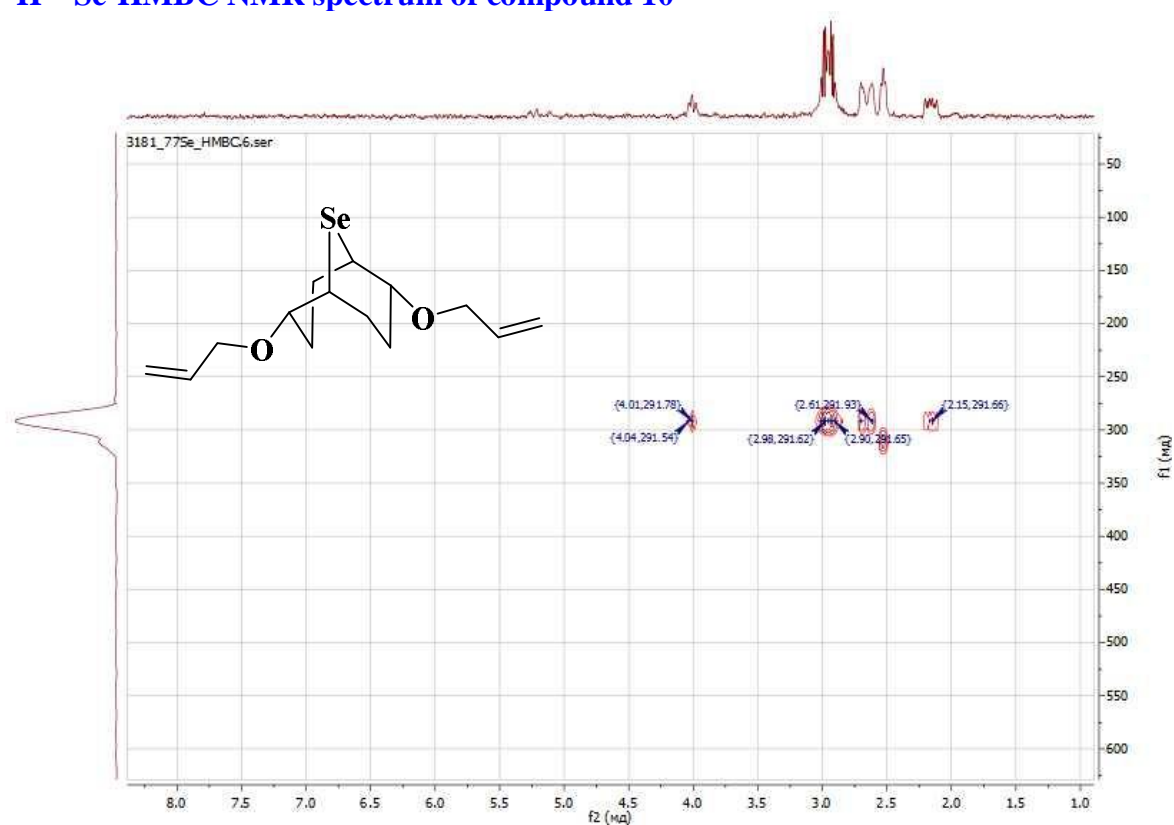
### $^{77}\text{Se}$ -NMR spectrum of compound 4



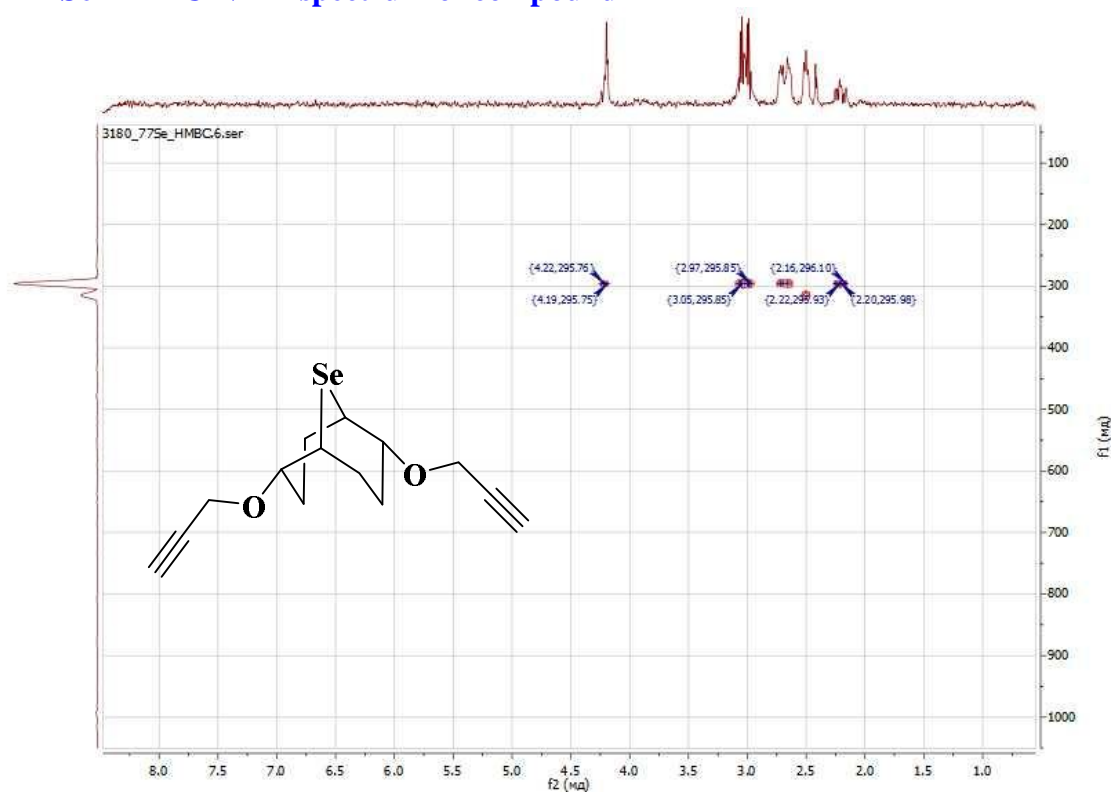


<sup>1</sup>H-<sup>77</sup>Se-HMBC NMR spectrum of compound 6 $^1\text{H}$ - $^{77}\text{Se}$ -HMBC NMR spectrum of compound 7

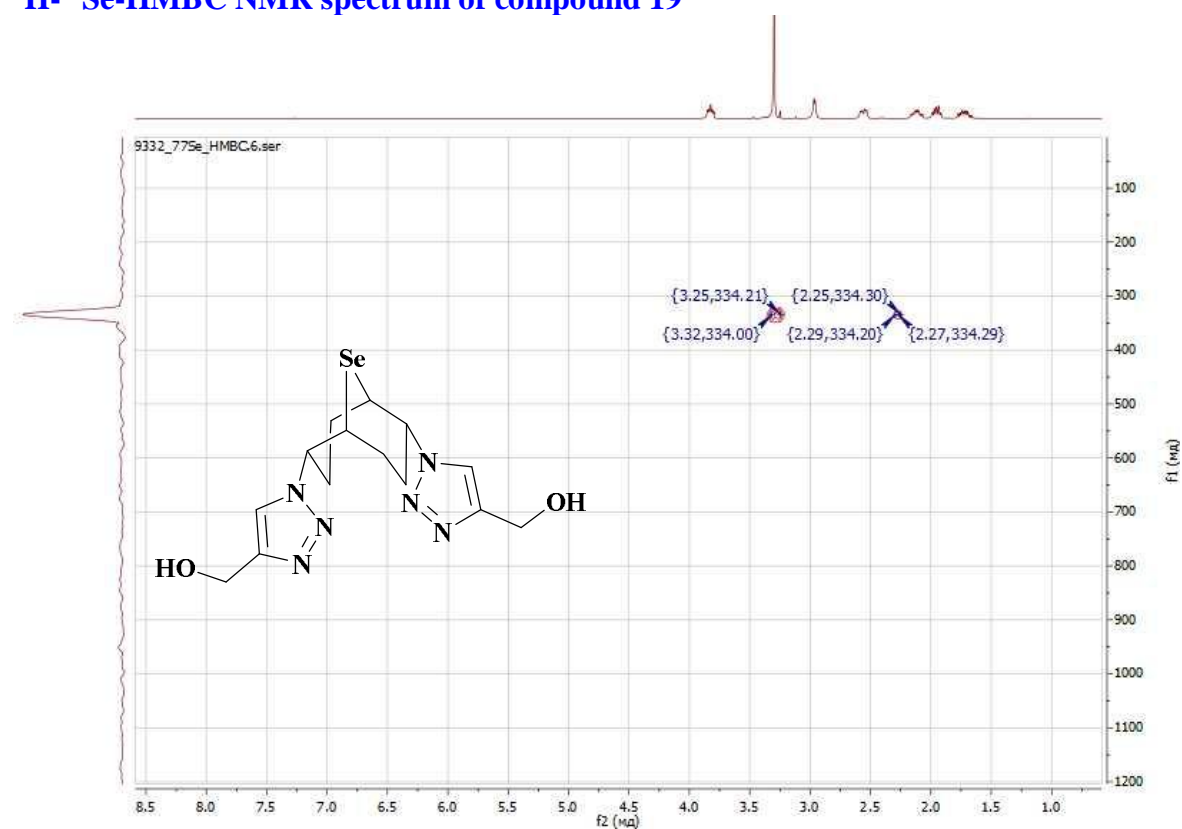
**$^1\text{H}$ - $^{77}\text{Se}$ -HMBC NMR spectrum of compound 10**



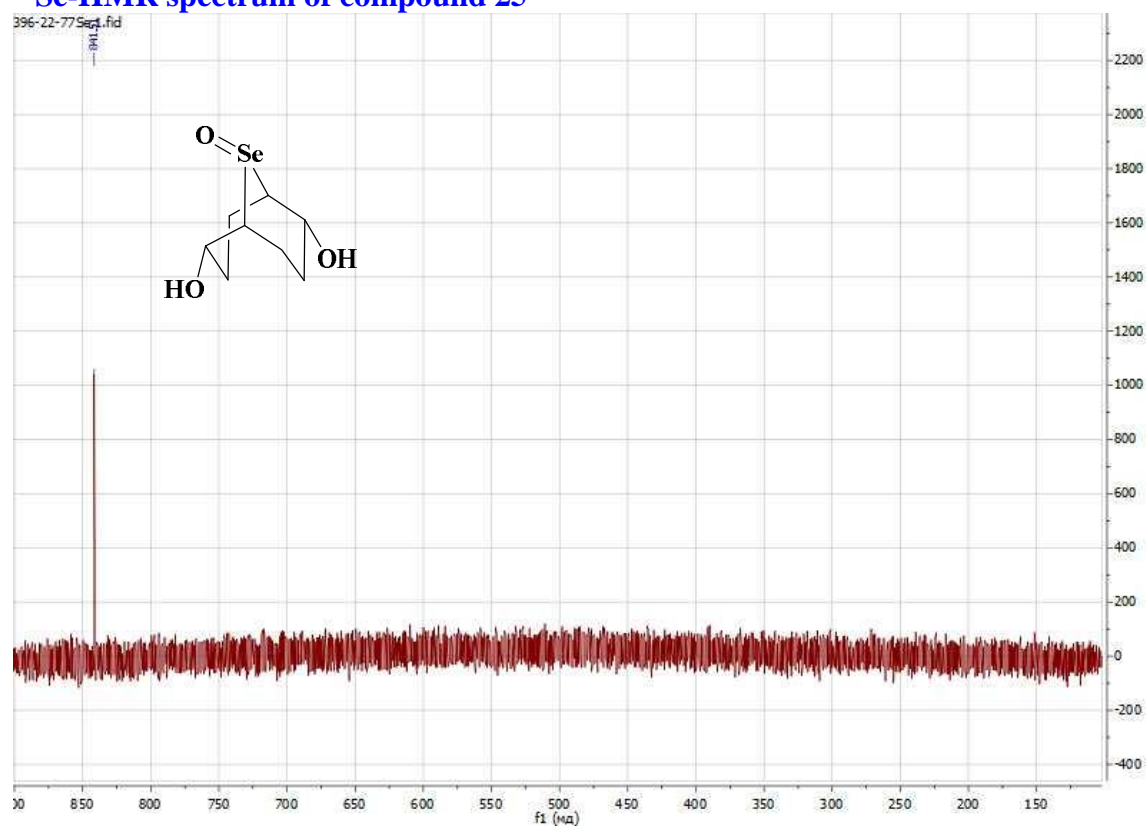
**$^1\text{H}$ - $^{77}\text{Se}$ -HMBC NMR spectrum of compound 11**



**$^1\text{H}$ - $^{77}\text{Se}$ -HMBC NMR spectrum of compound 19**

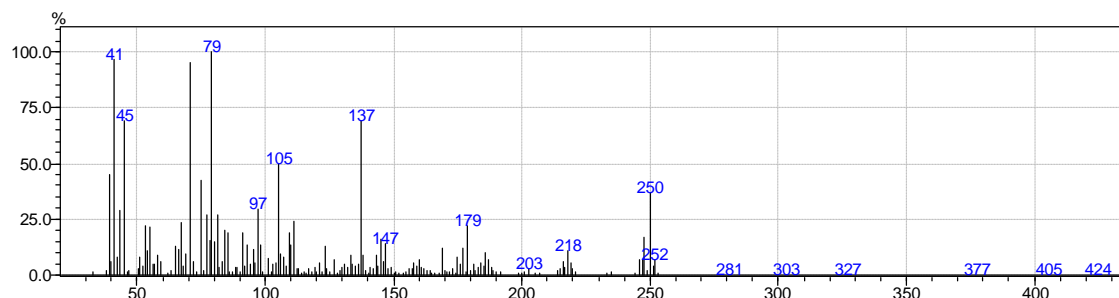


**$^{77}\text{Se}$ -HMR spectrum of compound 25**

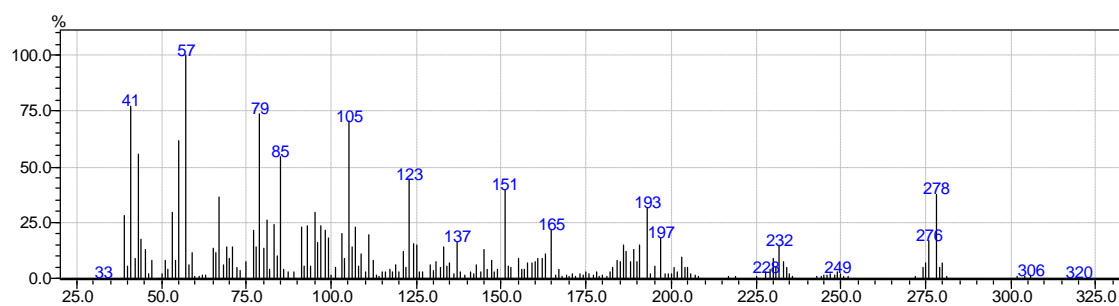


## Examples of Mass Spectra

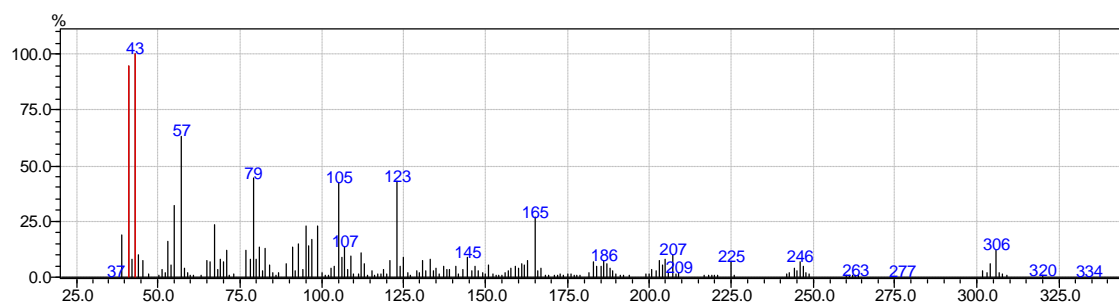
Mass spectrum of bis(methoxy) derivative 5 ( $M^+ = 250$ )



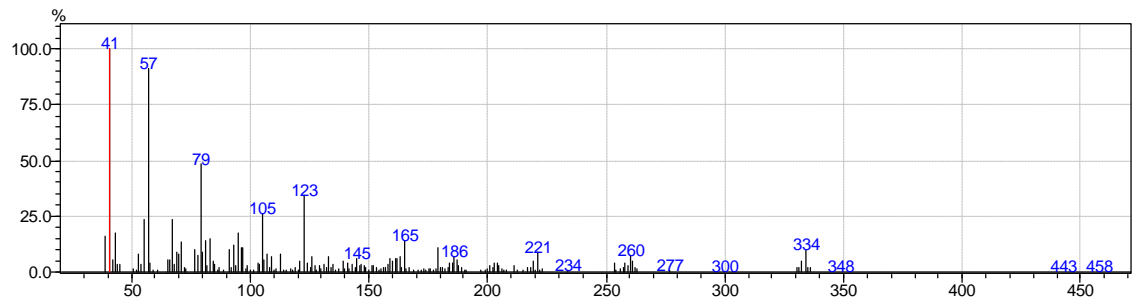
Mass spectrum of bis(ethoxy) derivative 6 ( $M^+ = 278$ )



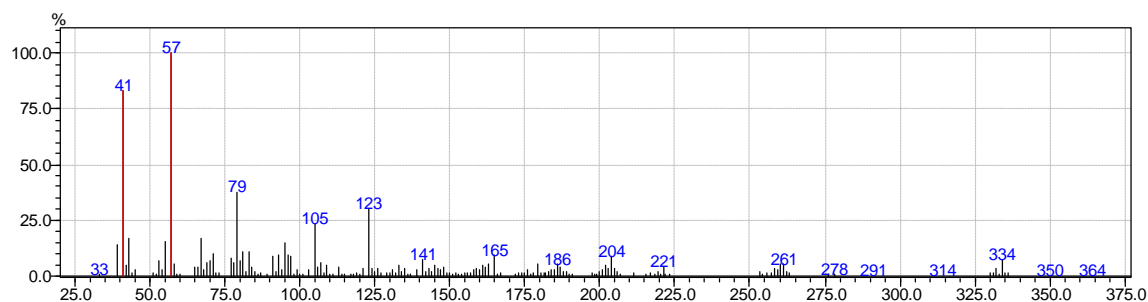
Mass spectrum of bis(propoxy) derivative 7 ( $M^+ = 306$ )



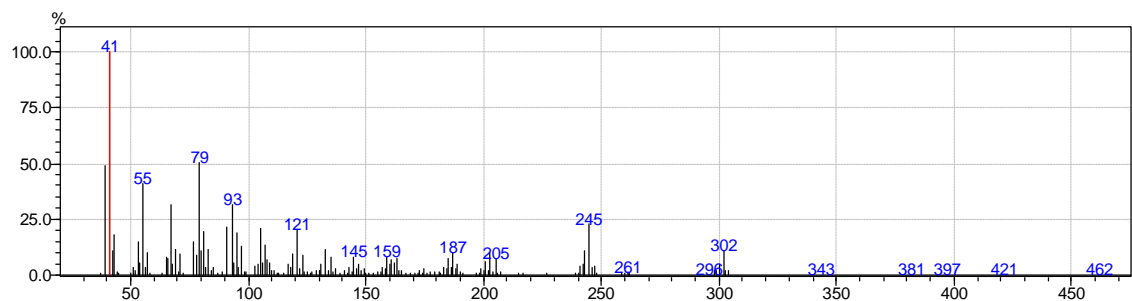
**Mass spectrum of bis(butoxy) derivative 8 ( $M^+ = 334$ )**



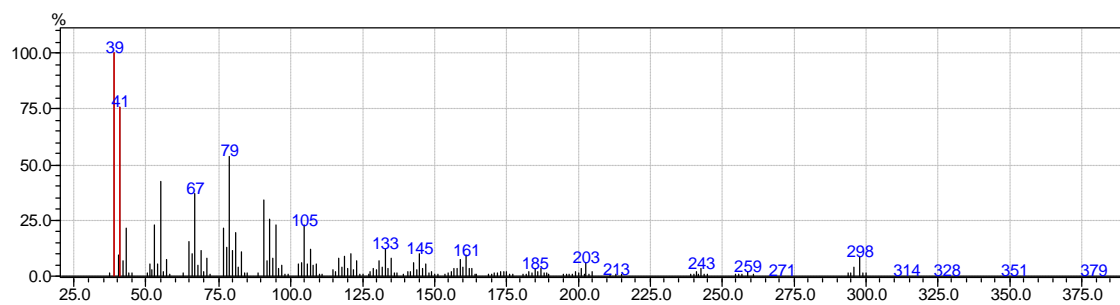
**Mass spectrum of bis(isobutoxy) derivative 9 ( $M^+ = 334$ )**



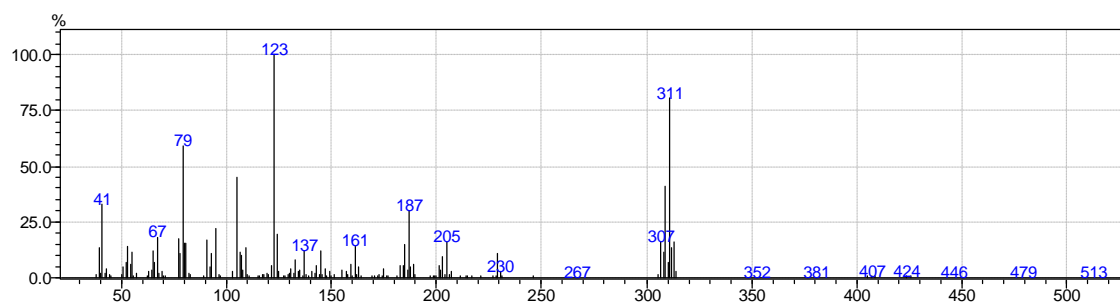
**Mass spectrum of bis(allyloxy) derivative 10 ( $M^+ = 302$ )**



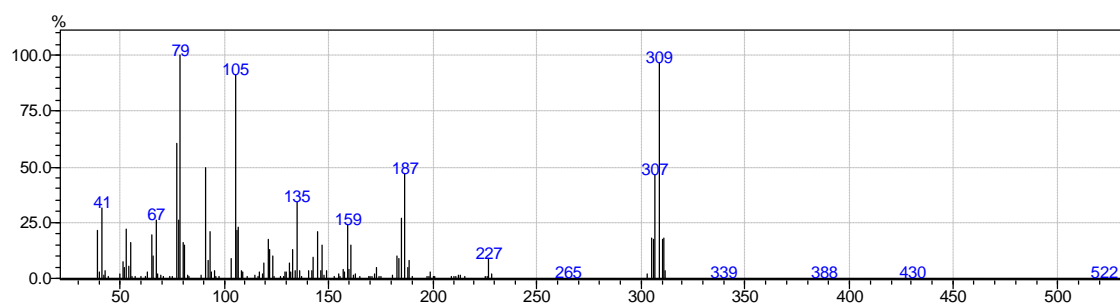
**Mass spectrum of bis(propargyloxy) derivative 11 ( $M^+ = 298$ )**



**Mass spectrum of bis(4-methoxyphenoxy) derivative 14 ( $311 = [M^+ - \text{MeOC}_6\text{H}_4\text{O}]$ )**



**Mass spectrum of bis(3,5-dimethylphenoxy) derivative 15 ( $309 = [M^+ - \text{Me}_2\text{C}_6\text{H}_3\text{O}]$ )**



**Mass spectrum of bis(phenyloxy) derivative 16 ( $281 = [M^+ - C_6H_5O]$ )**

