Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Fast and easy conversion of *ortho* amidoaryldiselenides into the corresponding Ebselen-like derivatives driven by theoretical investigations.

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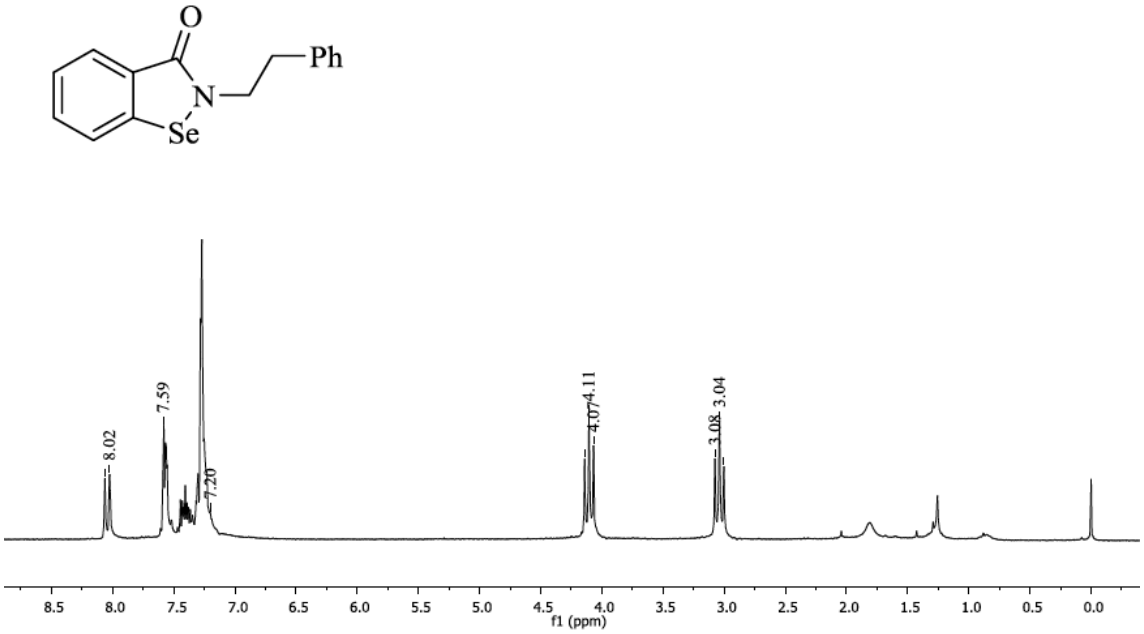
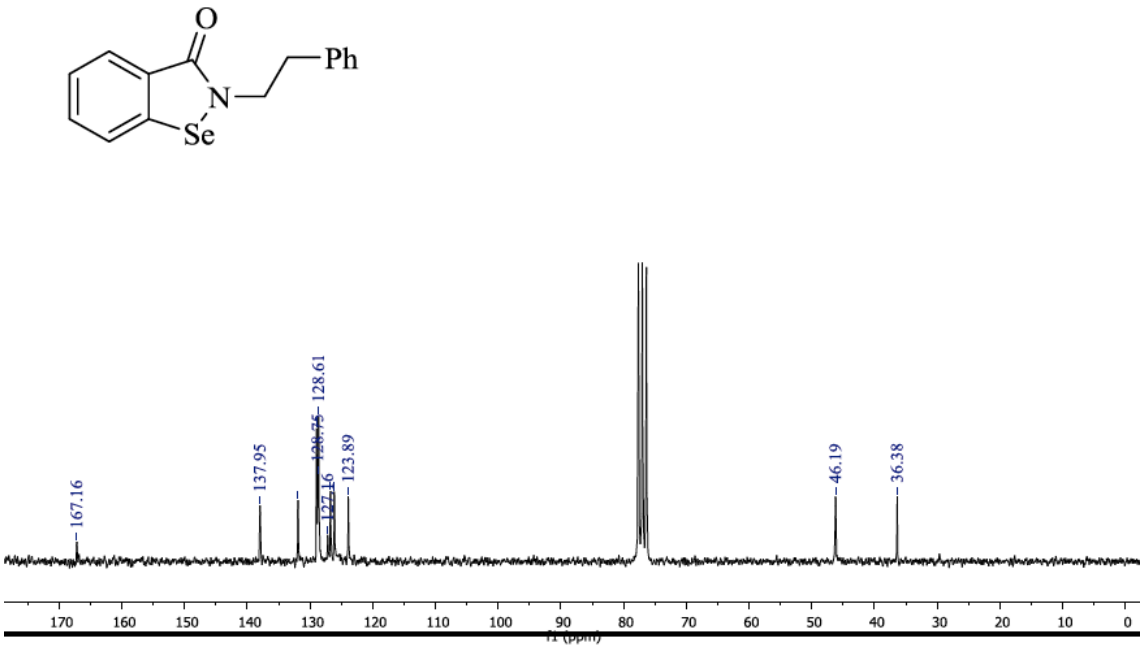
Supporting Information

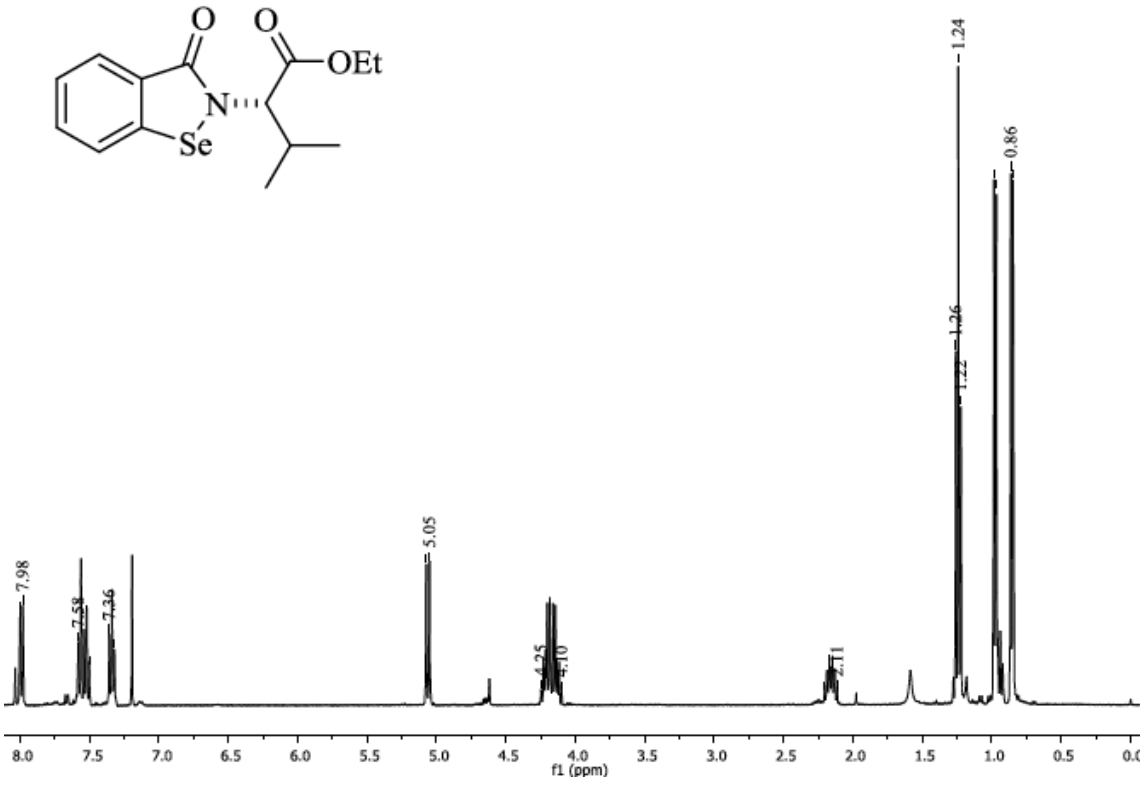
^{1}H ^{13}C and mass spectra of the new compounds

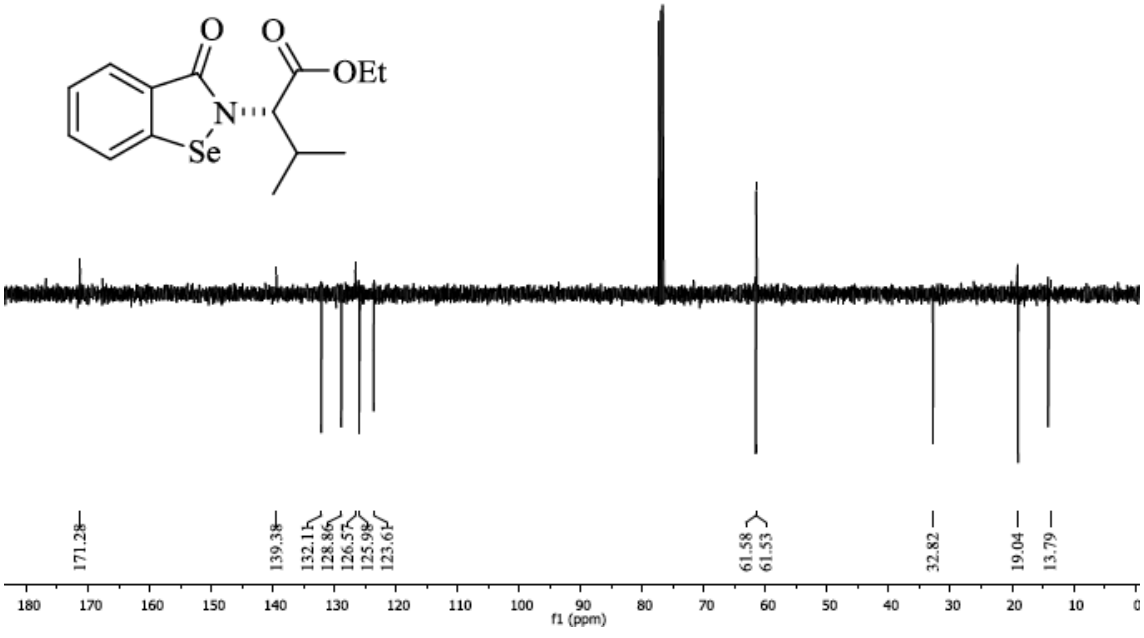
2-(1-phenylpropan-2-yl)benzo[d][1,2]selenazol-3(2H)-one (**9b**)



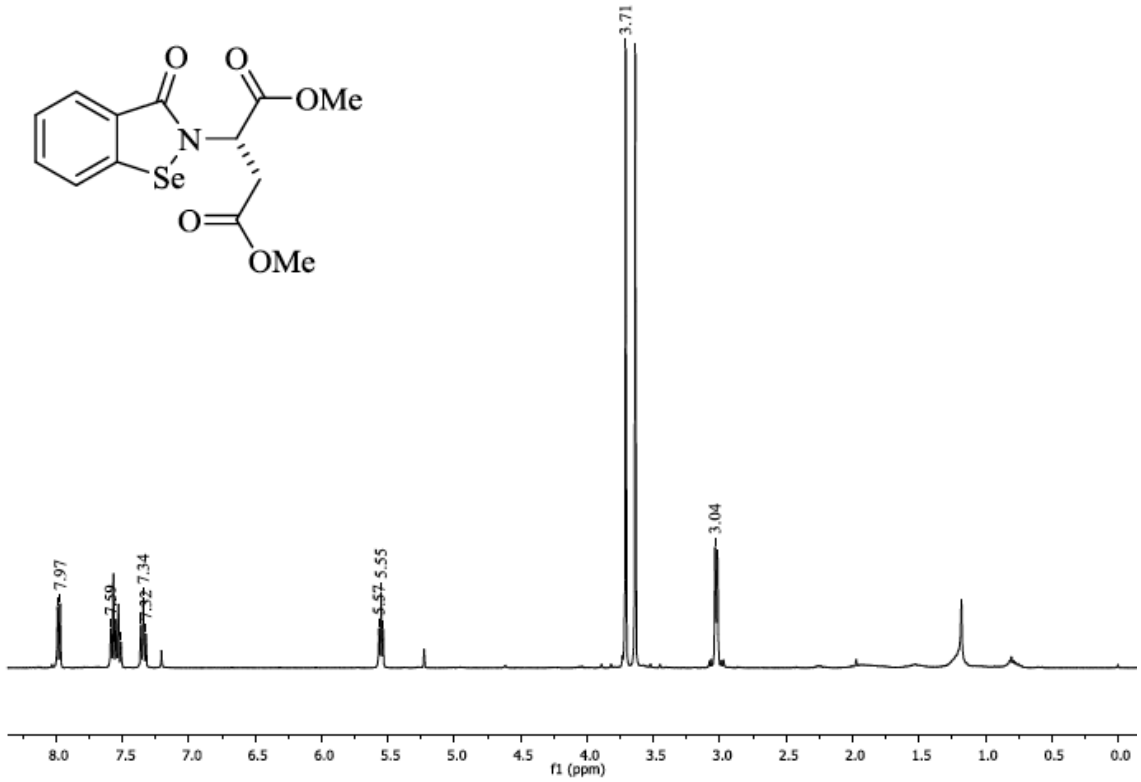


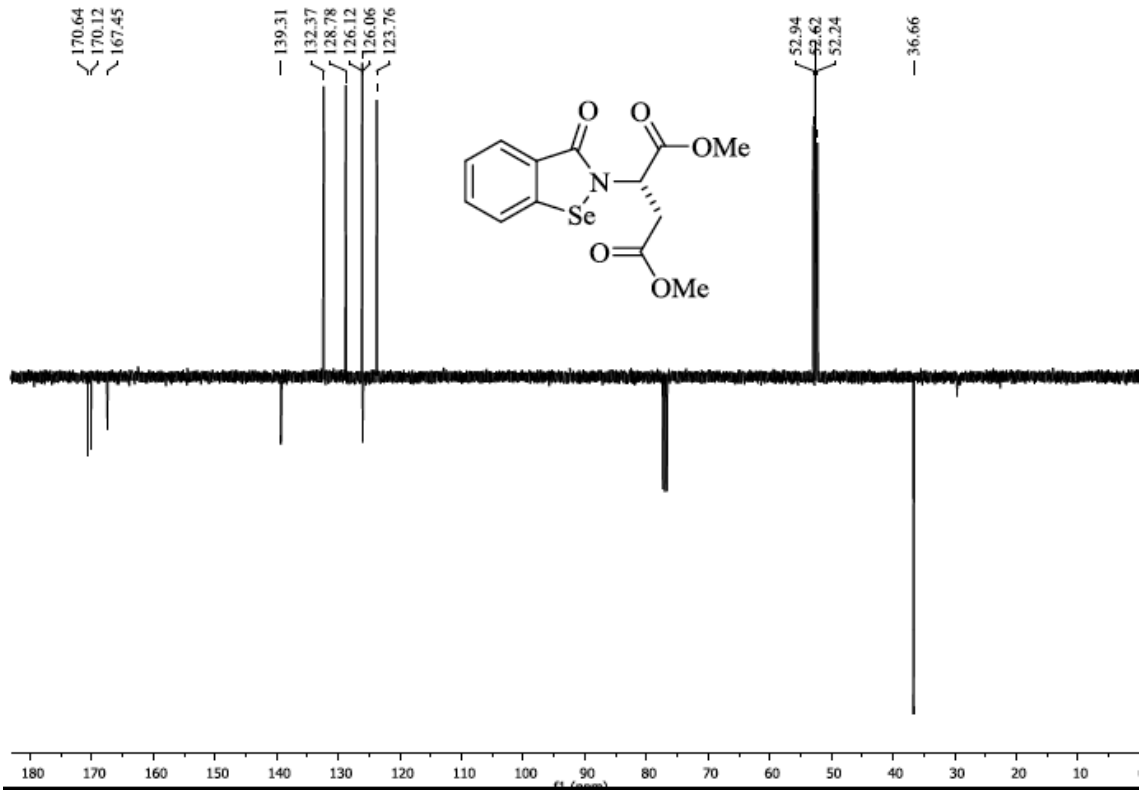
(S)-ethyl 3-methyl-2-(3-oxobenzo[d][1,2]selenazol-2(3H)-yl)butanoate (**9e**)



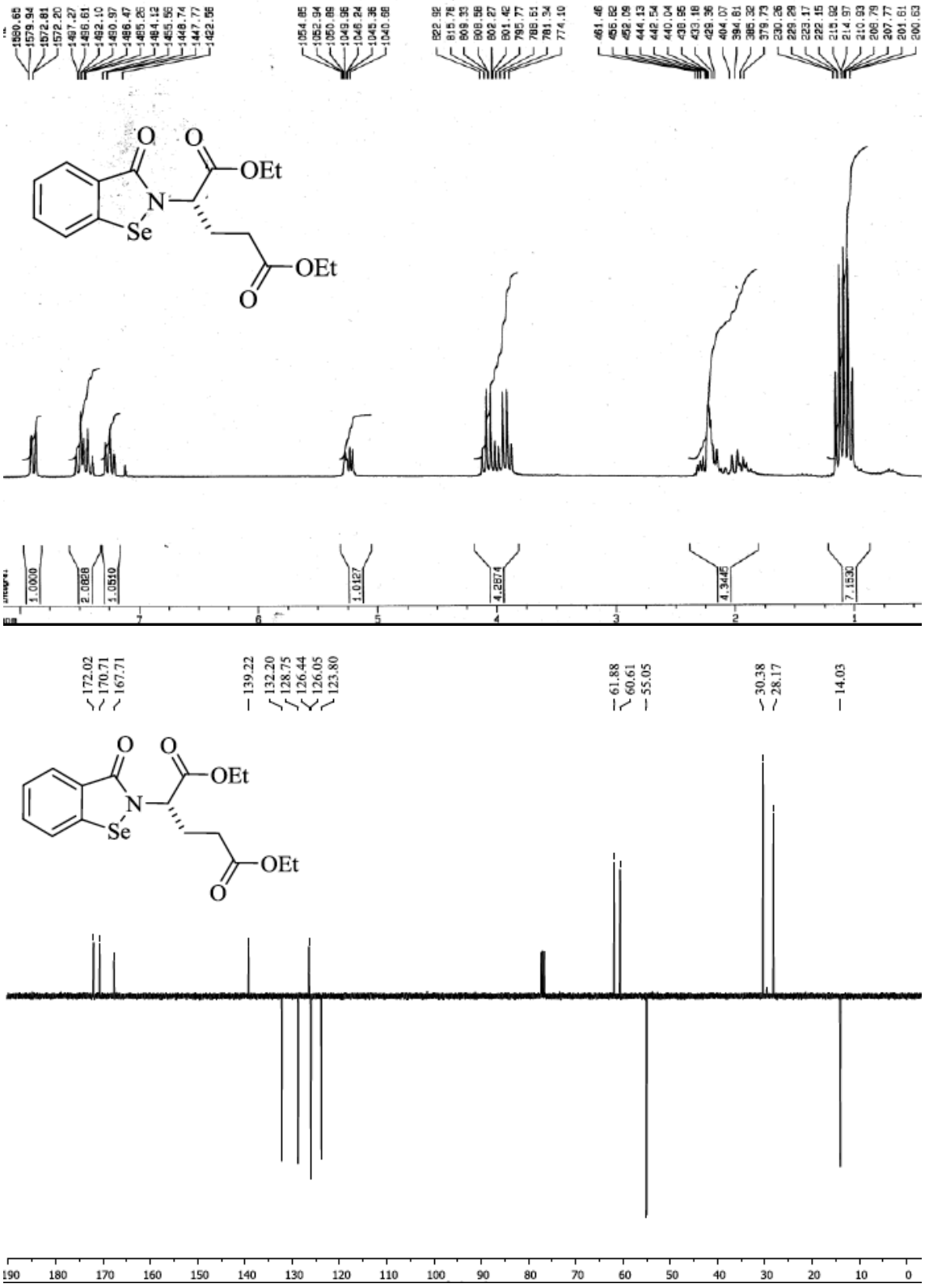


(S)-dimethyl 2-(3-oxobenzo[d][1,2]selenazol-2(3H)-yl)succinate (**9g**)

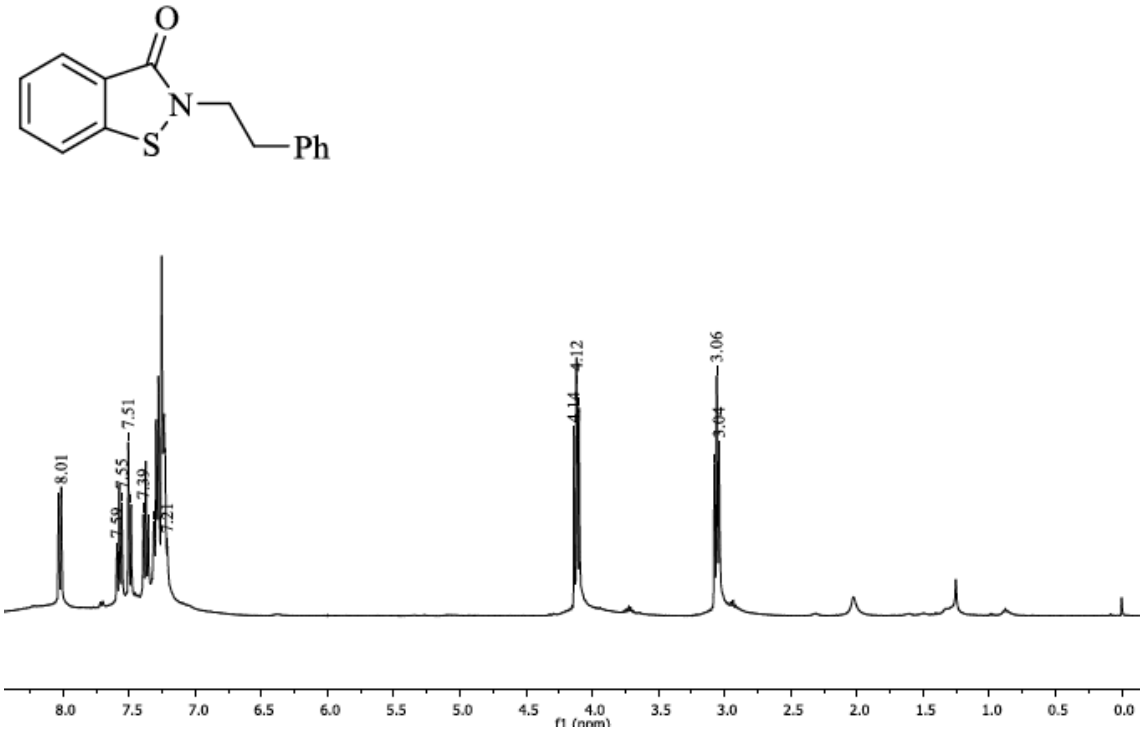


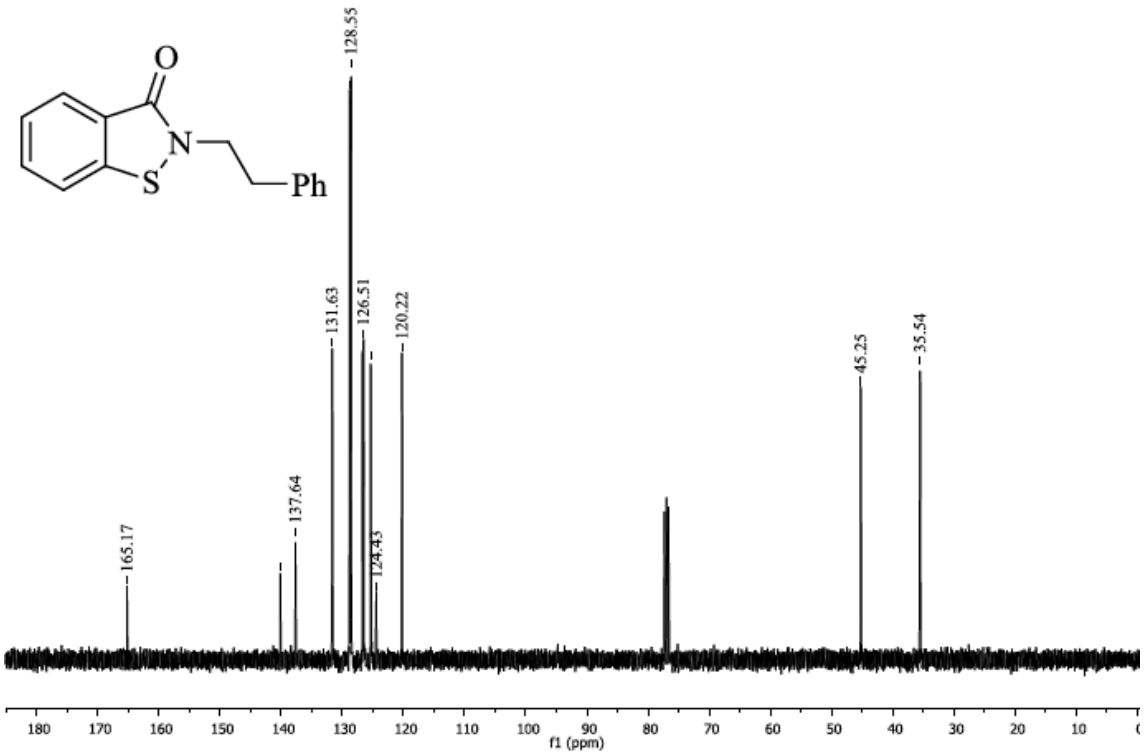


(S)-diethyl 2-(3-oxobenzo[d][1,2]selenazol-2(3H)-yl)pentanedioate (**9h**)



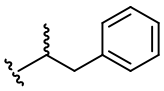
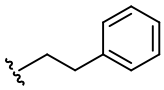
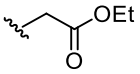
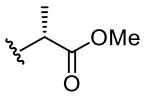
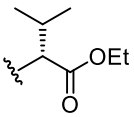
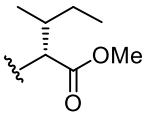
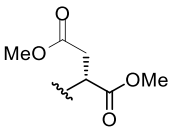
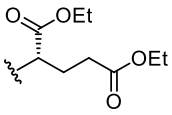
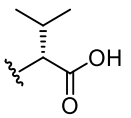
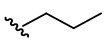
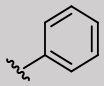
2-(1-phenylpropan-2-yl)benzo[d]isothiazol-3(2H)-one (**9l**)





Glutathione-peroxidase-like activity assay

The experiments to measure the catalytic activity of the ebselen and its derivatives as mimetics of the GPx enzyme were carried out according to the Tomoda method [9–11]. In a quartz cuvette, the selenium catalyst (final concentration = 0,01mM), thiophenol (final concentration = 5 mM) and MeOH at 25(± 3) ºC were mixed.

Entry	R	Ch	Product	Vel rel to 9k
1		Se	**9a**	0.97
2		Se	**9b**	0.83
3		Se	**9c**	0.82
4		Se	**9d**	1.11
5		Se	**9e**	1.10
6		Se	**9f**	1.07
7		Se	**9g**	0.96
8		Se	**9h**	0.87
9		Se	**9i**	1.08
10		Se	**9j**	0.82
11		Se	**9k**	1.0

The spectrophotometer was programmed to promote the reading of UV light absorbance at a wavelength of 305 nm every 10 seconds due the formation of the PhSSPh. After around 120 seconds of the beginning of the experiment, the catalytic GPx model reaction (H_2O_2 + 2PhSH -> $2H_2O$ + PhSSPh) was initiated by the addition of H_2O_2 (final concentration: 10mM). The reaction was monitored for more 150 seconds. Each analysis was done in triplicate.

***Comparison of the catalytic activity (GPx-like) of 8k and* 9k**

The experimental procedure used was analogous to the previous one with the same concentration of thiophenol (final concentration = 5 mM) and H_2O_2 (final concentration: 10mM). However, the volume of methanol used was 0.66 ml and the experiment was started after 100 seconds. Furthermore, the reaction was monitored for more 200 seconds. The selenium catalysts used were ebselen and ebselen diselenide, where the concentrations were varied according to the tests below.

Selenium catalyst	**Test 1 (final concentration [mM])**	**Test 2 (final concentration [mM])**	**Test 3 (final concentration [mM])**	**Test 4 (final concentration [mM])**
9k	0.020	0.010	0.100	0.050
8k	0.010	0.005	0.050	0.025

Calculation of T50

The stoichiometric ratio between PhSSPh and PhSH is 1:2, respectively. The rate of PhSSPh formation is known from the linear portion of peroxidase-like activity spectrophotometric quantification. Thus, from the total concentration of PhSH and the rate of PhSSPh formation, the calculation was performed by a extrapolation the time required to consume 50% of PhSH, that is, the T50.

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