STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 76 (2020)

Supporting information for article:

Supramolecular insight into the substitution of sulfur by selenium, based on the crystal structures, quantum-chemical calculations and biosystem recognition

Ivana S. Đorđević, Marko Popadić, Mirjana Sarvan, Marija Petković-Benazzouz and Goran V. Janjić

Supporting information

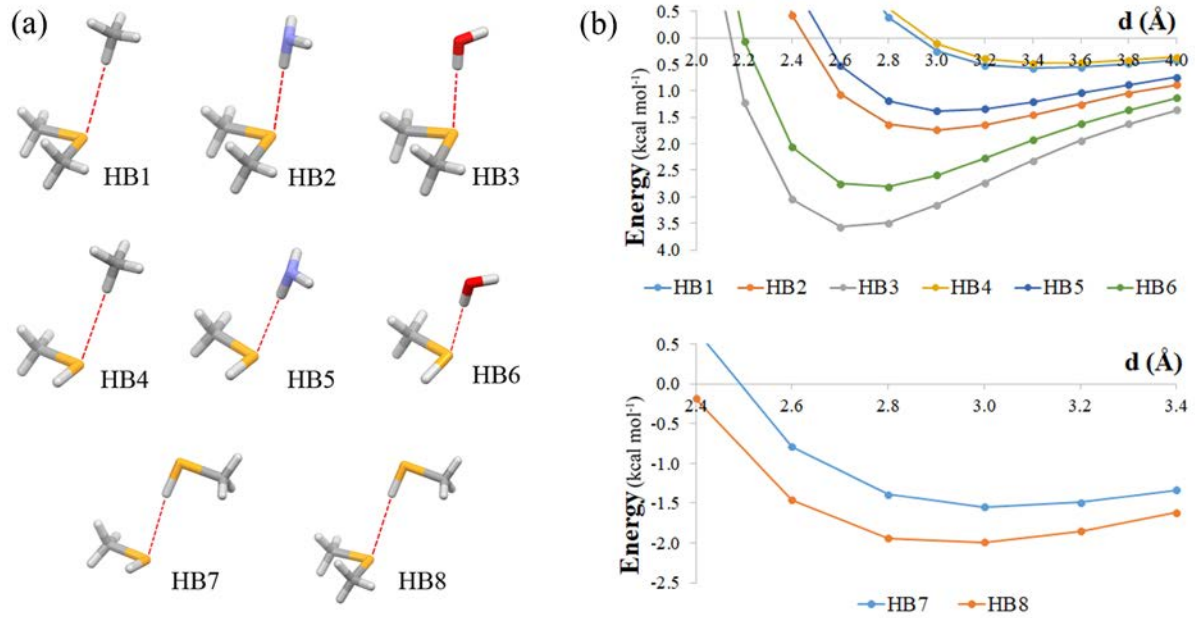

Figure S1 (a) Model systems used for evaluations of the strength of Se hydrogen bonds and (b) energies graphics: $CH_4\cdots CH_3SeCH_3$ (HB1), $NH_3\cdots CH_3SeCH_3$ (HB2), $H_2O\cdots CH_3SeCH_3$ (HB3), $CH_4\cdots CH_3SeH$ (HB4), $NH_3\cdots CH_3SeH$ (HB5), $H_2O\cdots CH_3SeH$ (HB6), $CH_3SeH\cdots CH_3SeH$ (HB7), $CH_3SeH\cdots CH_3SeCH_3$ (HB8).

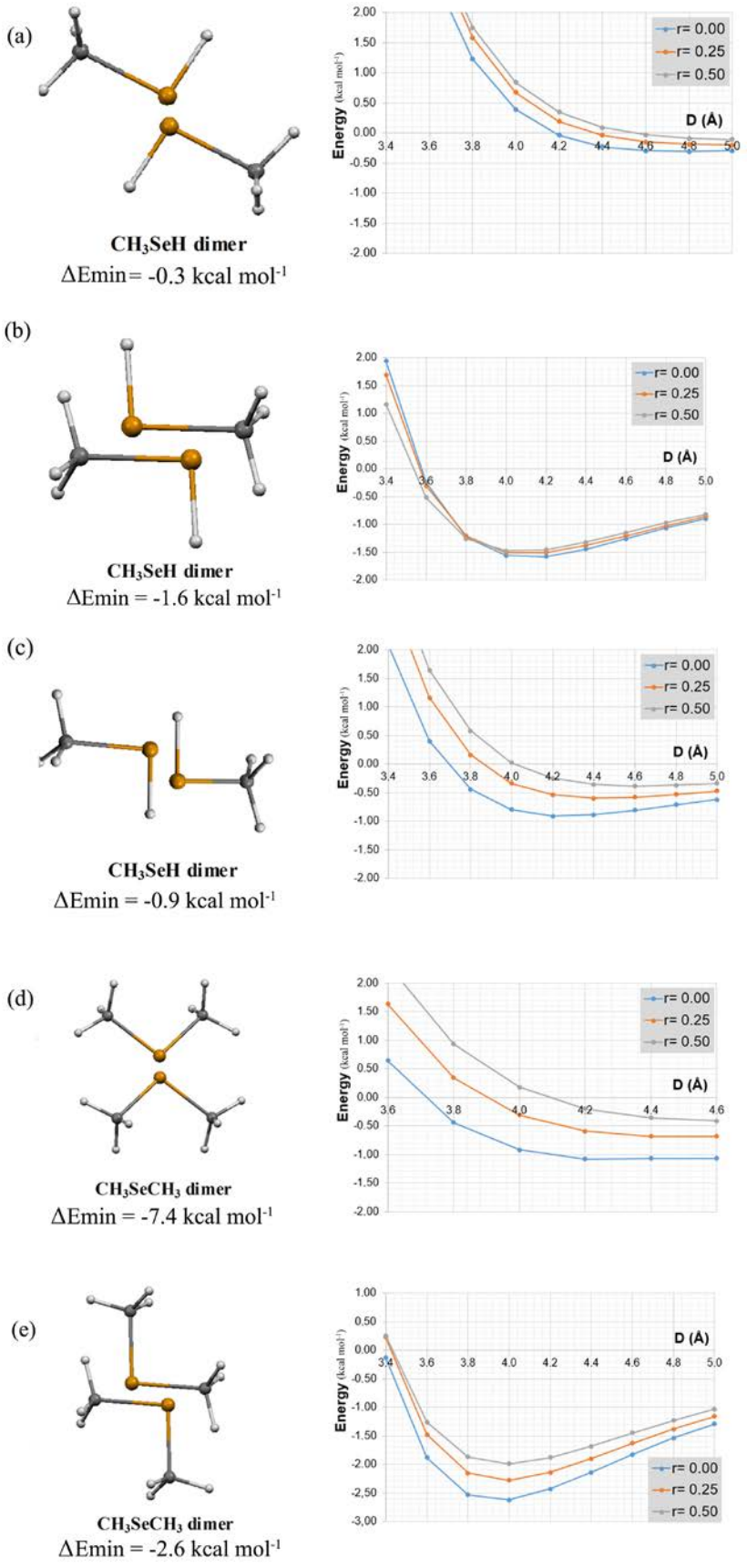

Figure S2 Model systems used for evaluations of the strength of parallel interactions and energies graphics: a) P1, b) P2, c) P3, d) P4 and e) P5 systems.

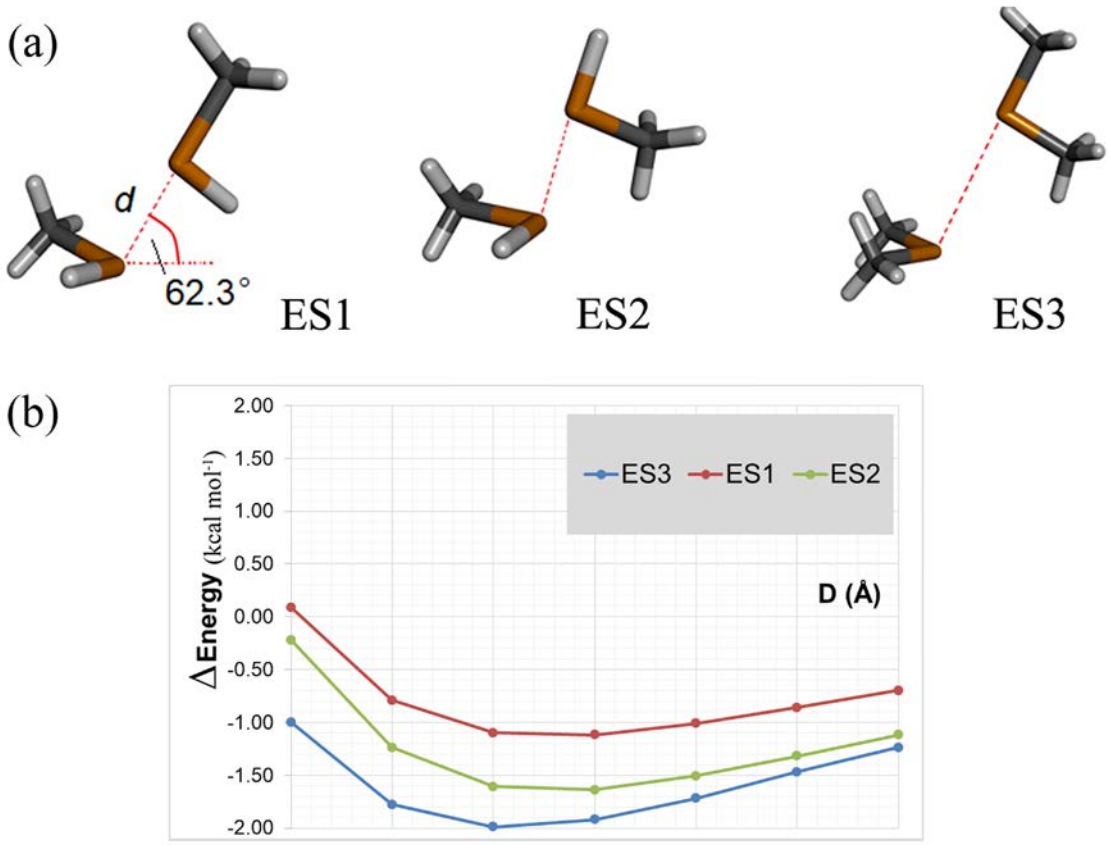

Figure S3 Model systems used for evaluations of the strength of σ/π interactions and energies graphics: ES1, ES2 and ES3.

S1. Docking study on INOs (inducible nitric oxide synthase)

Crystal structure of human INOs (inducible nitric oxide synthase) is obtained from Protein data bank (PDB ID: 4NOS). Validation of docking procedure by AutoDock Vina program was confirmed by redocking. Inhibitor ITU (iodotubercidin) was primarily extracted along with molecule H4B. This cleaned structure was then redocked again with inhibitor ITU. Docking results showed that iodotubercidin binds on the same site (position 1 on **Figure S4)**, in the narrow cleft within the larger active-site cavity containing heme complex.

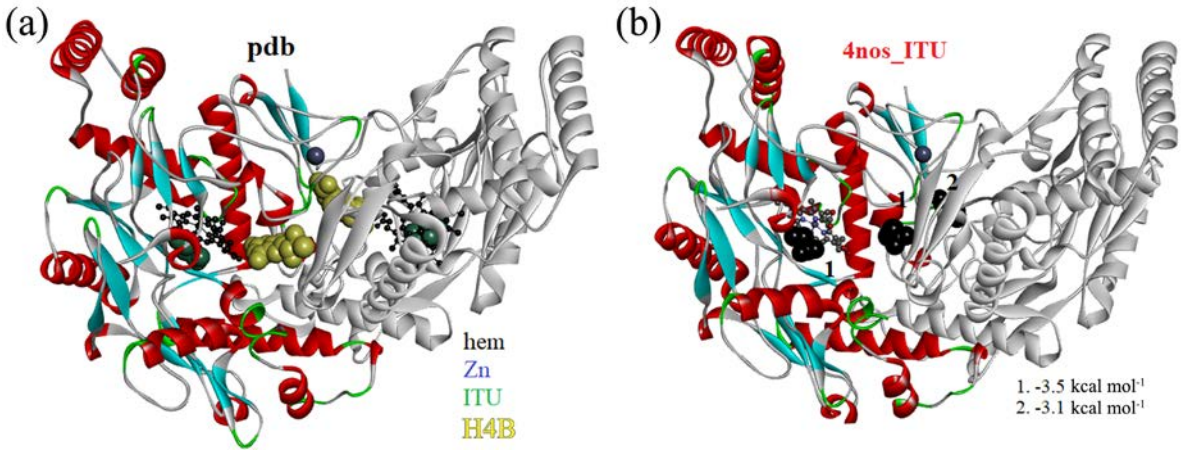

Figure S4 3D structure of 4NOS enzyme (a) obtained form PDB with: Zn atom, ITU, H4B and hem. Binding sites and binding energies of inhibitor ITU at active site of 4NOS enzyme (b).

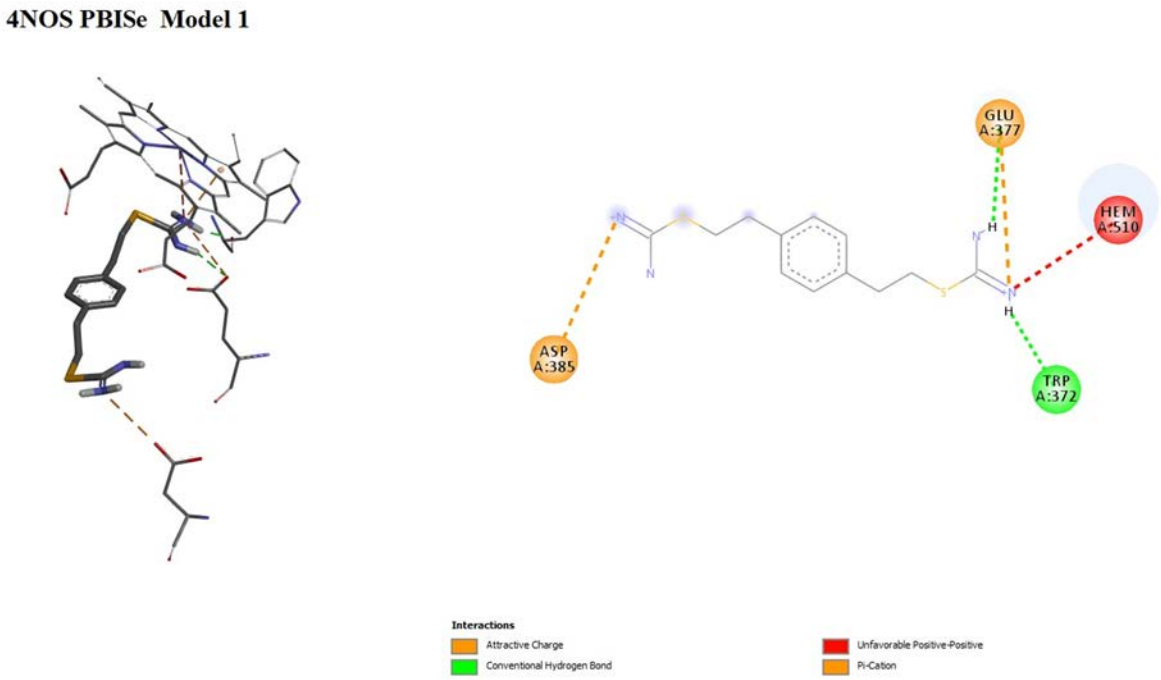

Figure S5 Binding site of PBISe at 4NOS and the distributions of amino-acid residues for position 1.

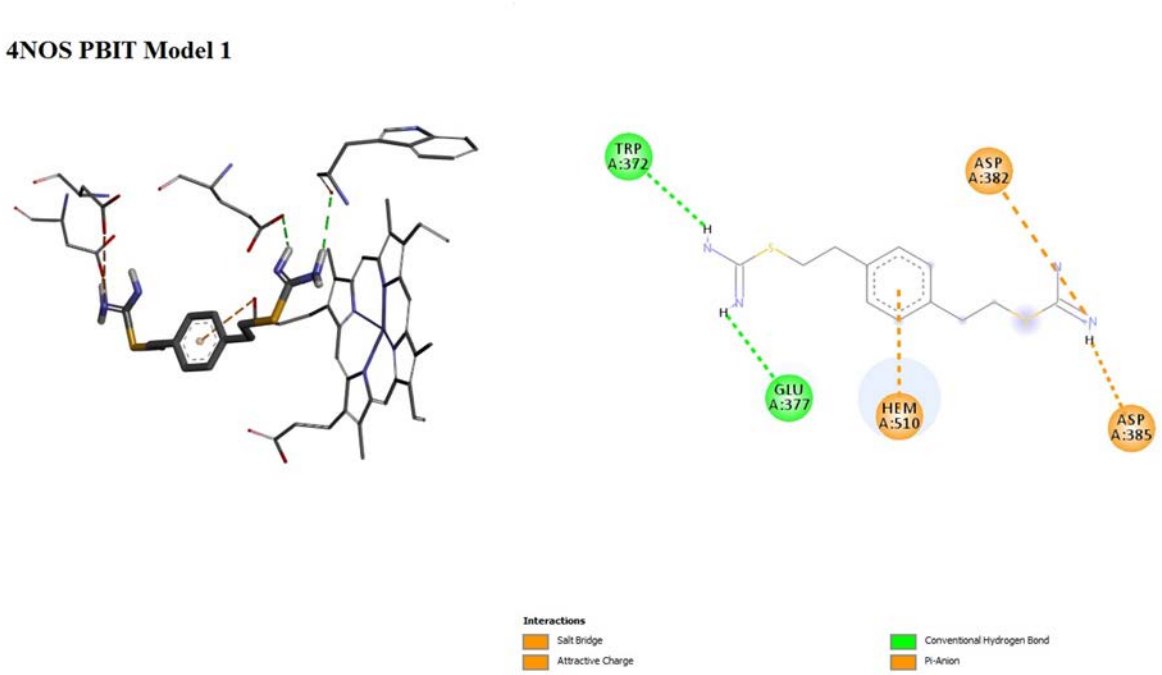

Figure S6 Binding site of PBIT at 4NOS and the distributions of amino-acid residues for position 1.

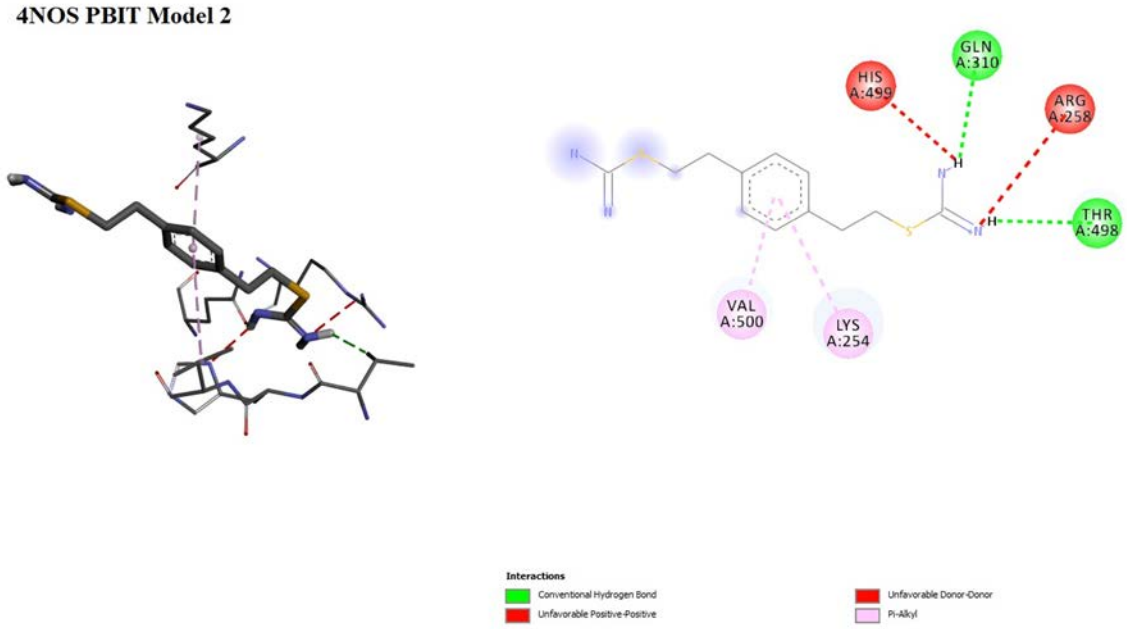

Figure S7 Binding site of PBIT at 4NOS and the distributions of amino-acid residues for position 2.

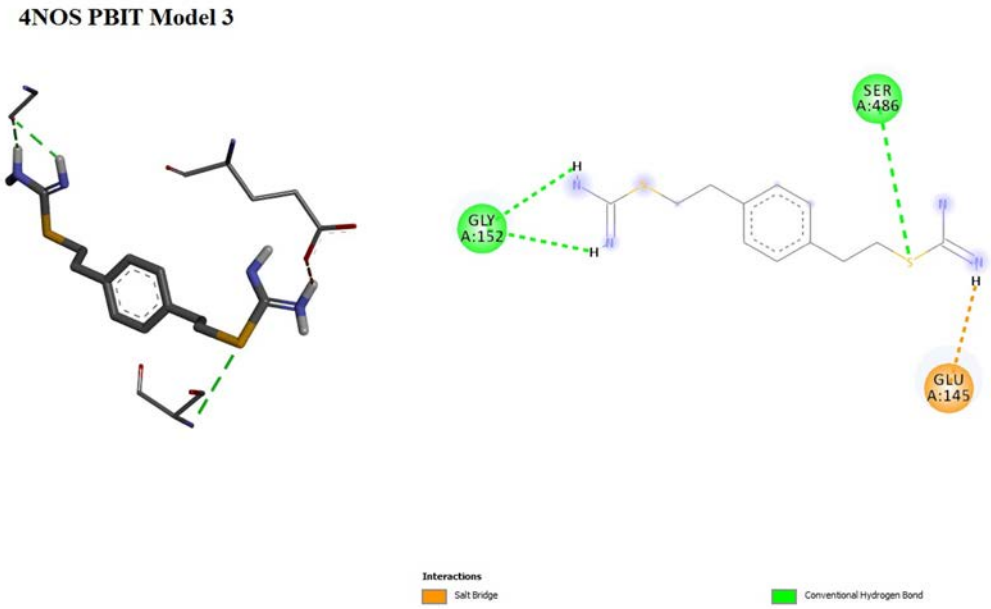

Figure S8 Binding site of PBIT at 4NOS and the distributions of amino-acid residues for position 3.

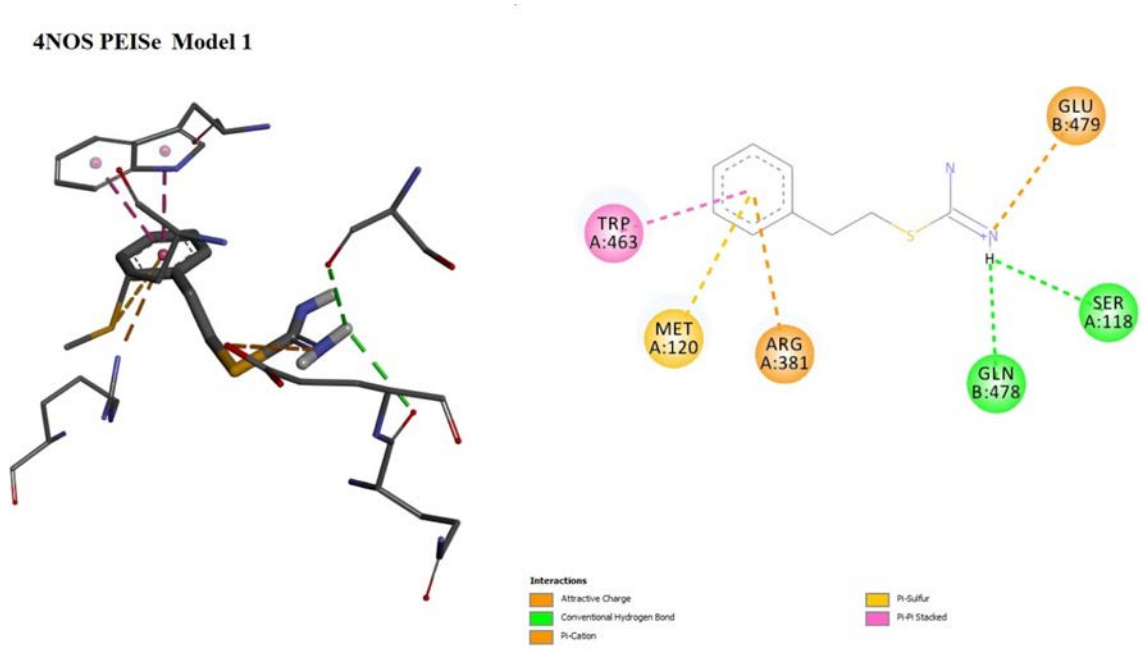

Figure S9 Binding site of PEISe at 4NOS and the distributions of amino-acid residues for position 1.

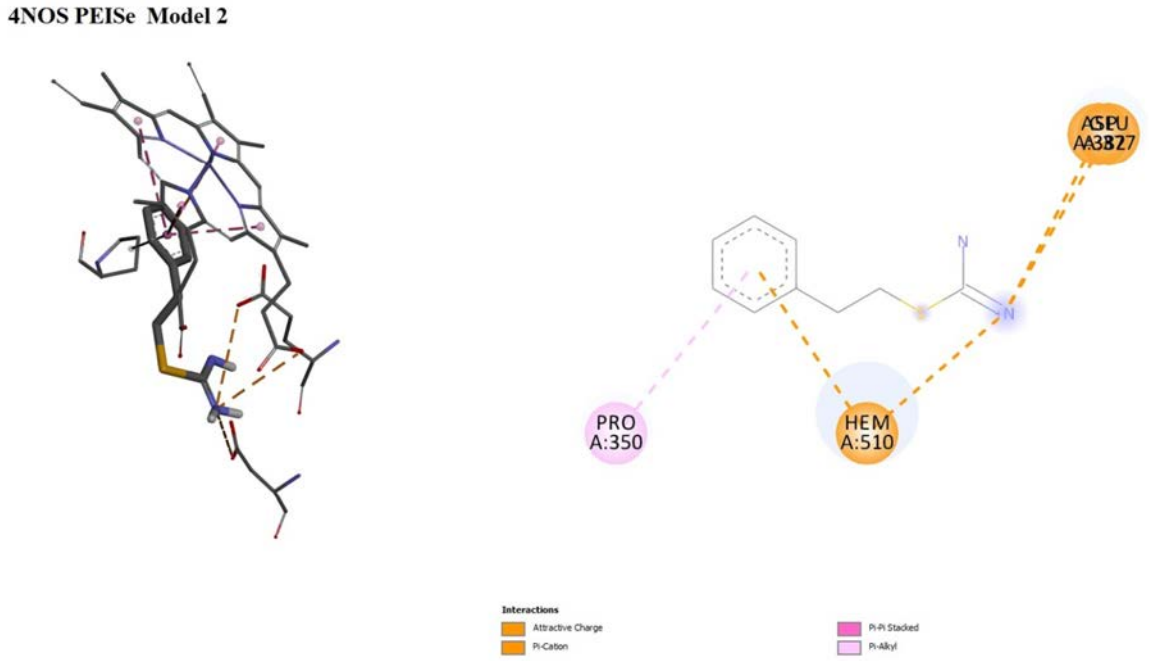

Figure S10 Binding site of PEISe at 4NOS and the distributions of amino-acid residues for position 2.

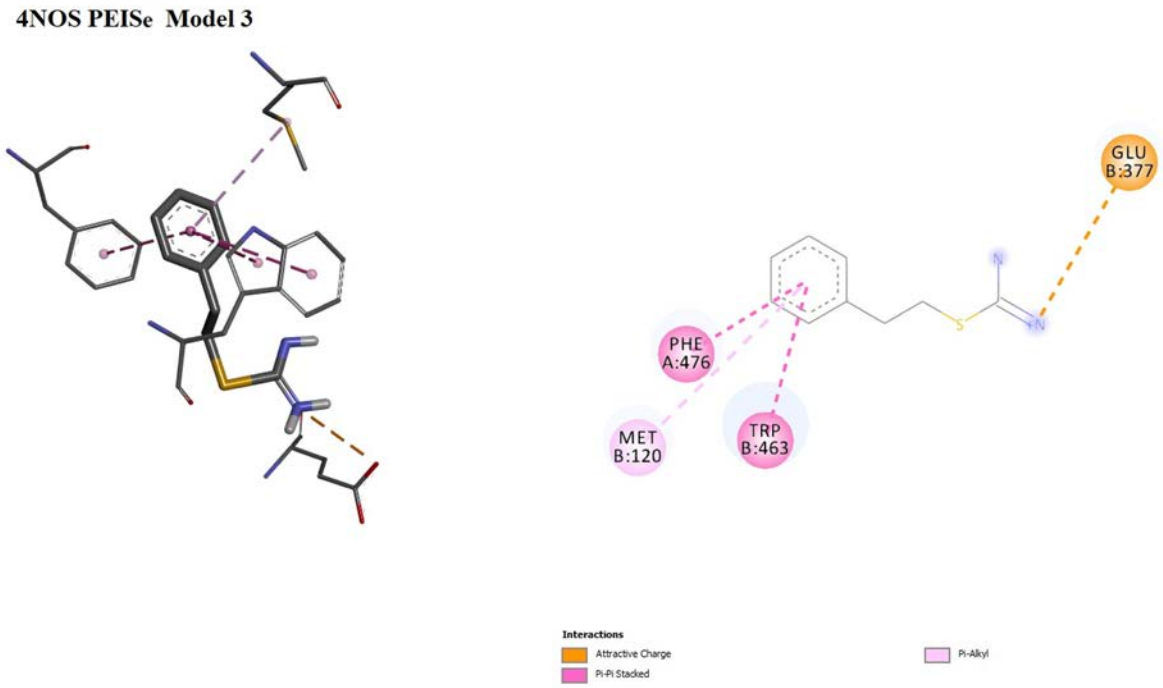

Figure S11 Binding site of PEISe at 4NOS and the distributions of amino-acid residues for position 3.

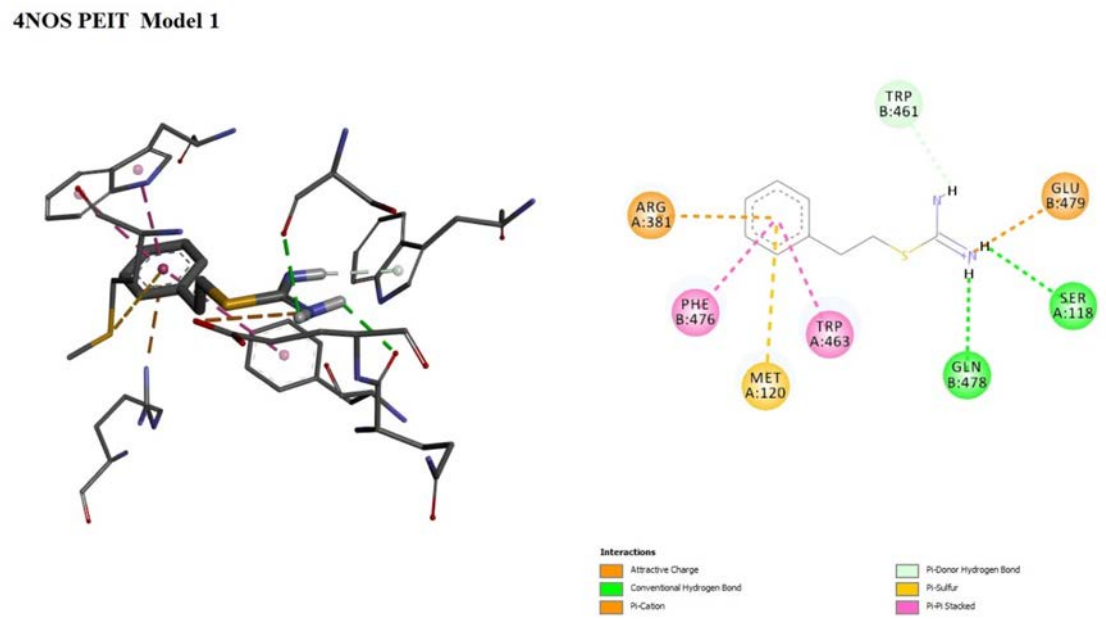

Figure S12 Binding site of PEIT at 4NOS and the distributions of amino-acid residues for position 1.

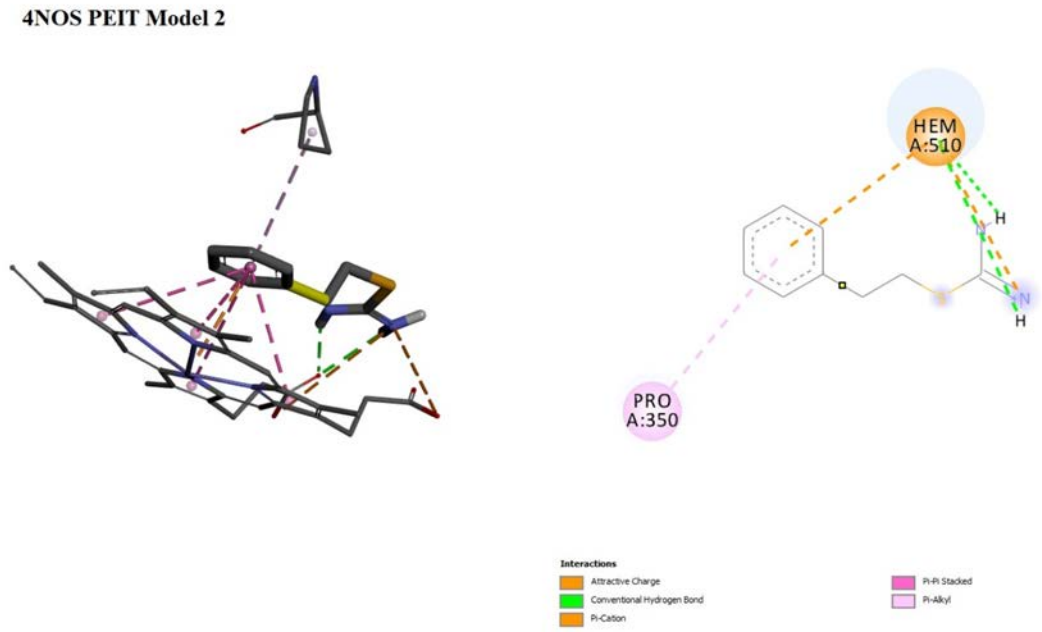

Figure S13 Binding site of PEIT at 4NOS and the distributions of amino-acid residues for position 2.

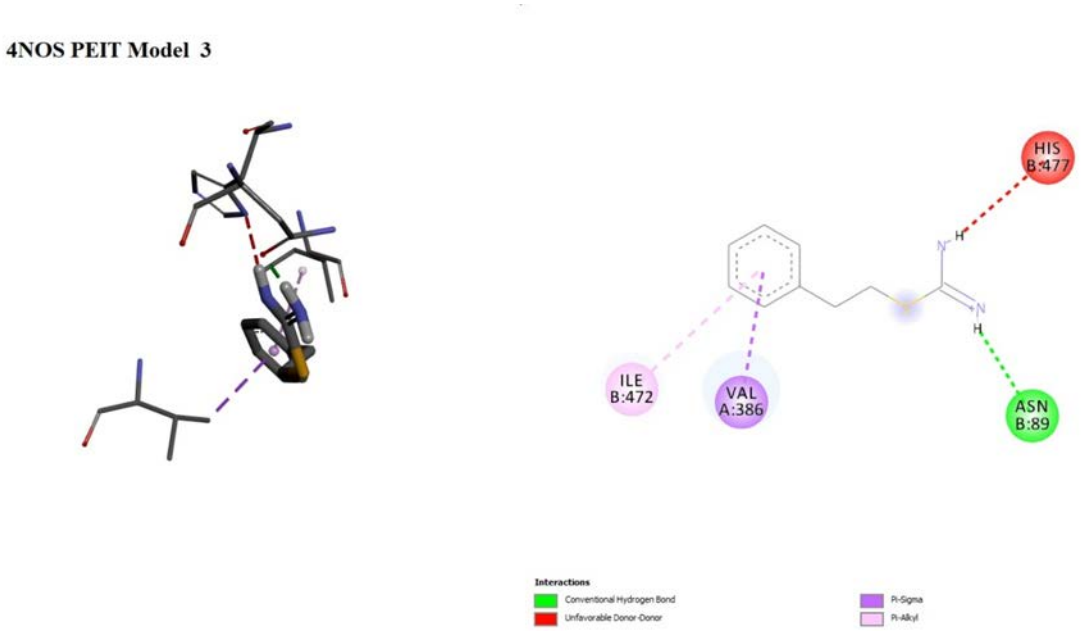

Figure S14 Binding site of PEIT at 4NOS and the distributions of amino-acid residues for position 3.

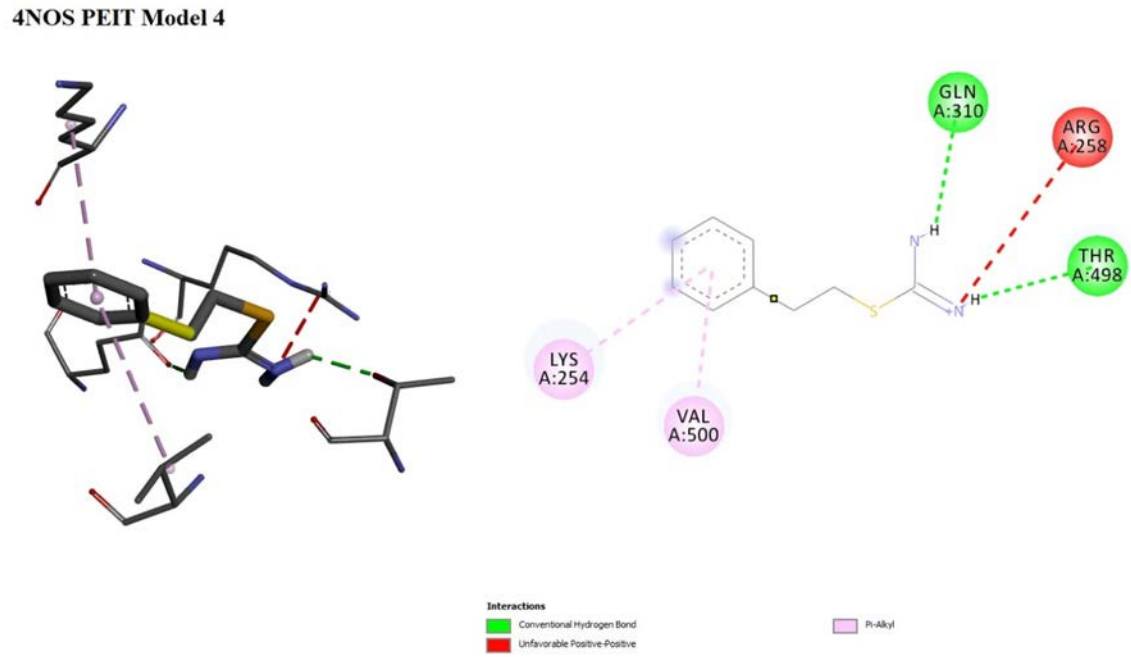

Figure S15 Binding site of PEIT at 4NOS and the distributions of amino-acid residues for position 4.

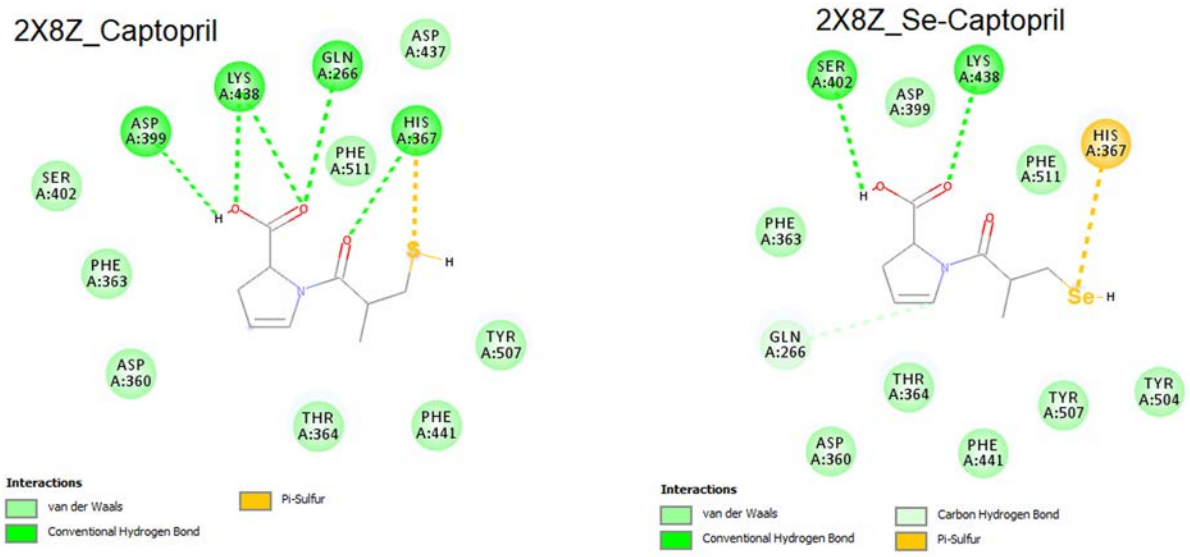

Figure S16 The distributions of amino-acid residues for the most stabile orientation for binding Captopril and Se-Captopril to ACE enzyme (pdb code: 2X8Z).

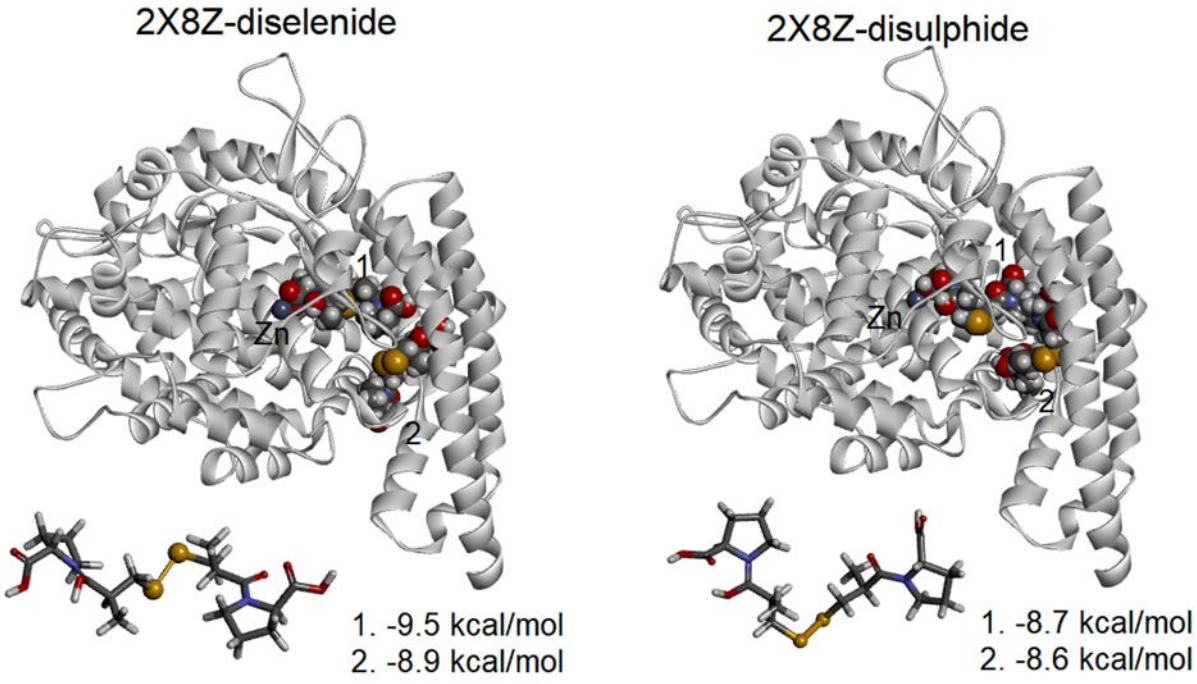

Figure S17 Binding sites and binding energy of disulphide and diselenide derivatives of Captopril and Se-Captopril at Angiotensin I-converting enzyme (ACE) (pdb code 2X8Z, Bhuyan & Mugesh, 2011).

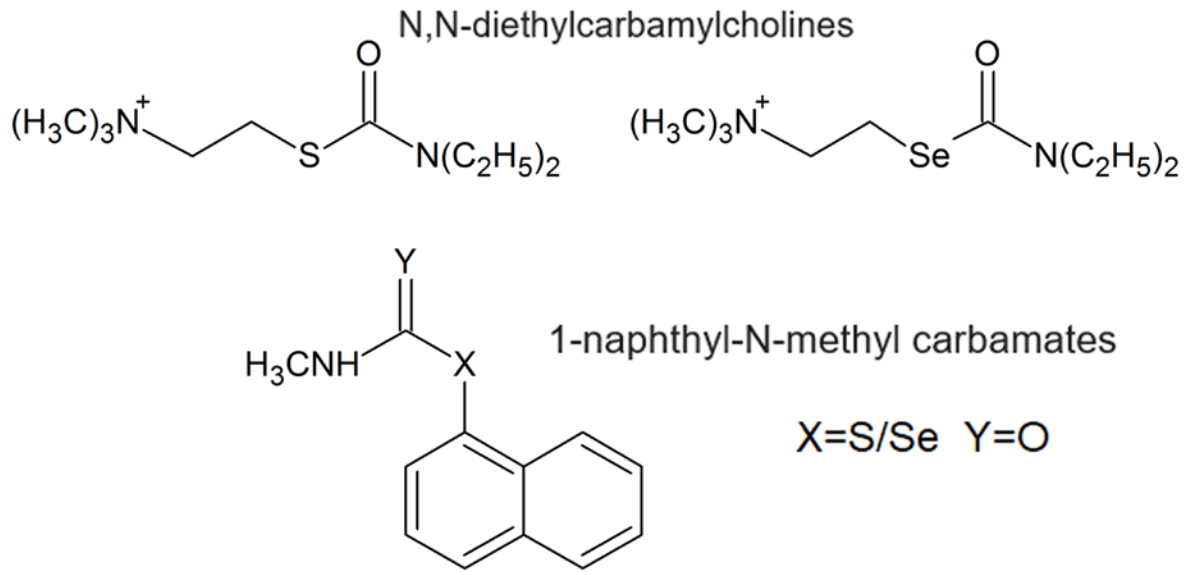

Figure S18 Sulfur and selenium derivatives of N,N-diethylcarbamylcholine and carbaryl, used for studying the inhibiting activity towards electric eel acetylcholinesterase.

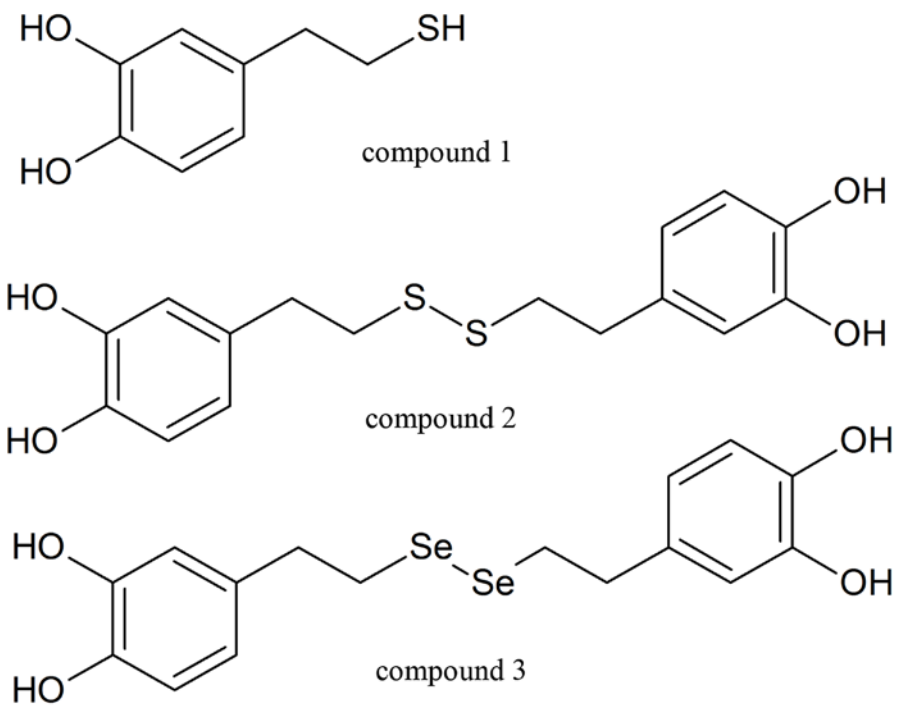

Figure S19 Sulfur and selenium derivatives of phenols from hydroxytyrosol used for studying the inhibition activity towards lipid peroxidation.