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Computational Kinetic Modeling of the Selenol Catalytic Activity as the Glutathione Peroxidase Nanomimic

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ABSTRACT

Density functional theory and solvent-assisted proton exchange methods have been applied for computational modeling of the catalytic cycle of selenol zwitterion anion from the kinetic and thermodynamic viewpoints. Selenol zwitterion anion has been represented as an effective glutathione peroxidase nanomimic. It reduces peroxides through a three-step pathway. In the first step, seleninic acid is produced through deprotonating of the selenol zwitterion anion in the presence of the hydrogen peroxide. Seleninic acid reacts with a thiol to form selenylsulfide in the second step. In the last step, selenylsulfide is reduced by the second thiol and regenerates selenolate anion through disulfide formation. Selenol zwitterion anion in comparison to more widely studied compounds such as ebselen has a good activity to react with hydrogen peroxide and producing seleninic acid. The energy barrier of this reaction is 11.7 kcal.mol^{-1} which is smaller than the reported enzyme mimics. Moreover, the reactions of seleninic acid and selenylsulfide with