

Supplementary material

Antioxidant activity, *In Silico* Study on NADPH Oxidase, and ADMET Prediction of the Chemical Constituents of *Allium sativum* L. (Garlic) Essential Oil

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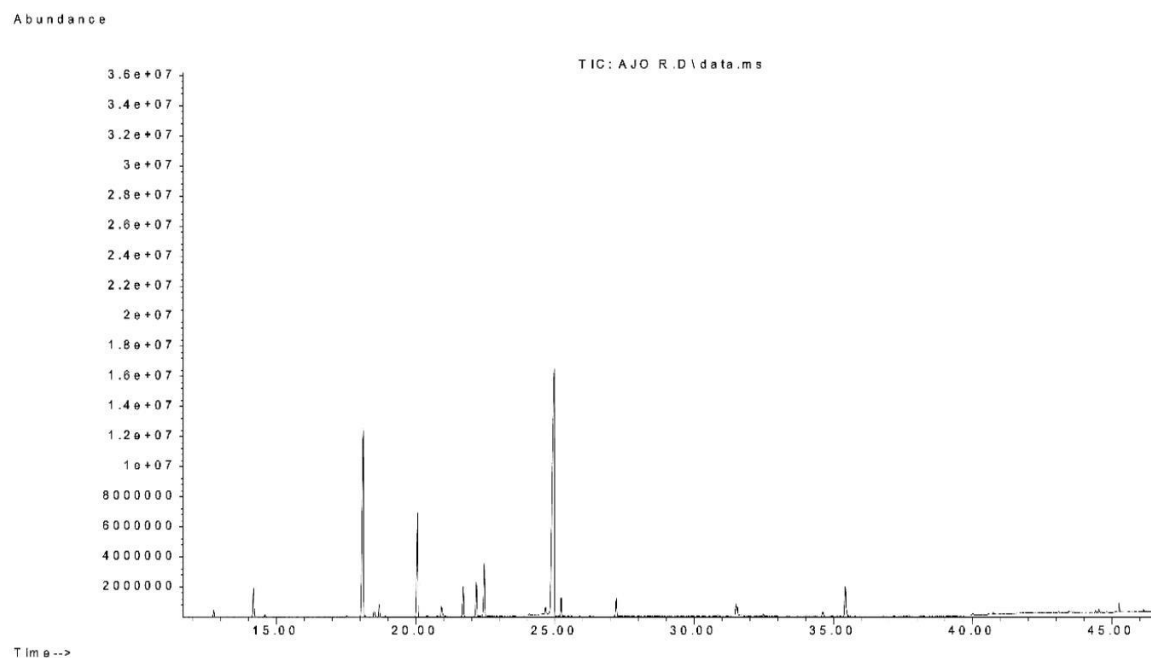


Figure S1. GC chromatogram of the essential oil from garlic

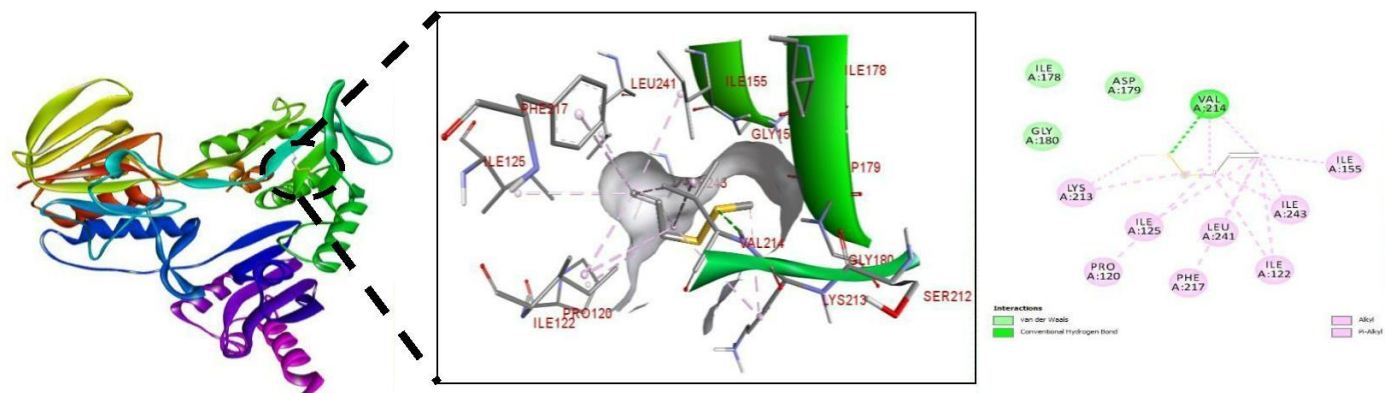


Figure S2. Molecular interaction studies of Allyl methyl disulfide with NADPH-oxidase (PDB ID: 2CDU), surface view (Left panel), and 2D (Right panel) interactions.

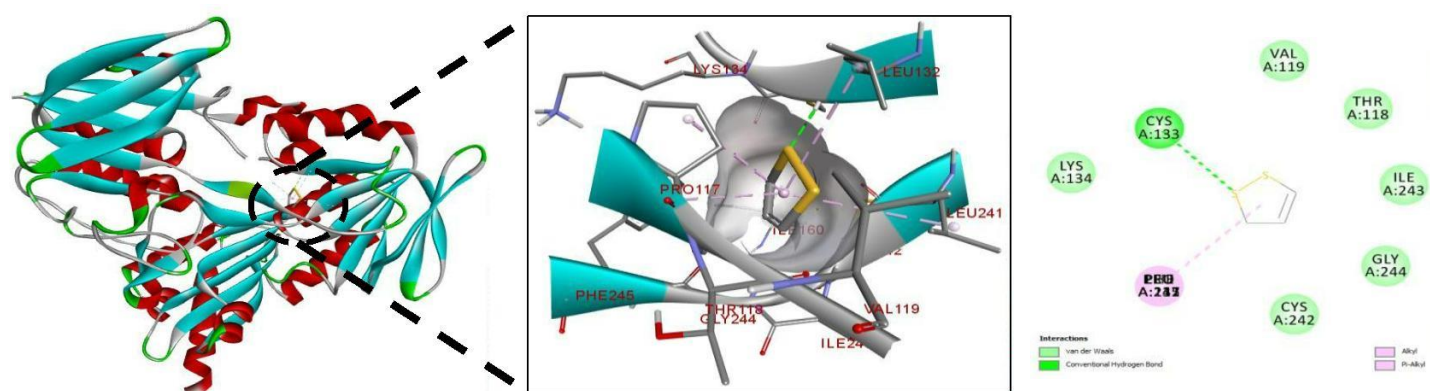


Figure S3. Molecular interaction studies of 3H-1,2-dithiole with NADPH-oxidase (PDB ID: 2CDU), surface view (Left panel), and 2D (Right panel) interactions.

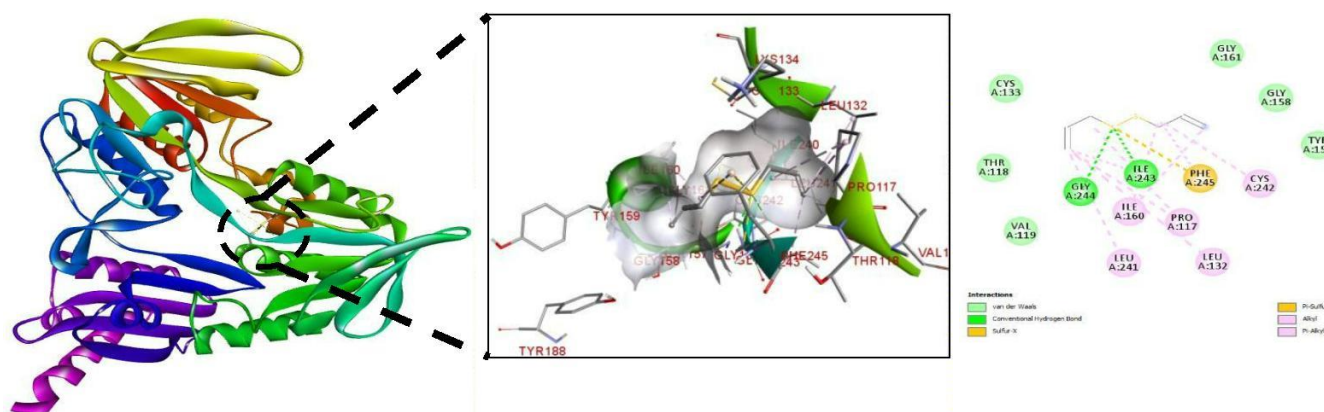


Figure S4. Molecular interaction studies of Diallyl disulfide with NADPH-oxidase (PDB ID: 2CDU), surface view (Left panel), and 2D (Right panel) interactions.

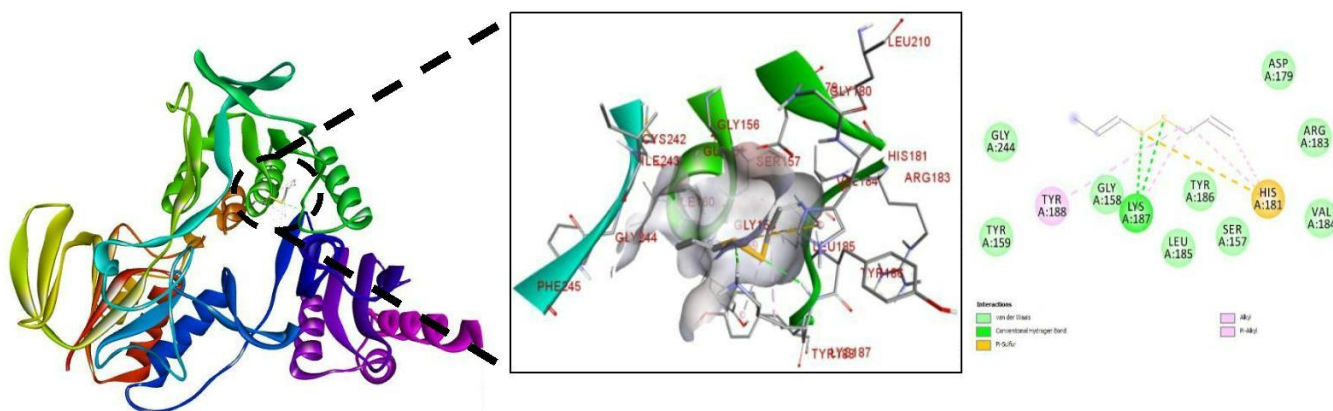


Figure S5. Molecular interaction studies of 1-propenyl 2-propenyl- (E) -disulfide with NADPH-oxidase (PDB ID: 2CDU), surface view (Left panel), and 2D (Right panel) interactions.

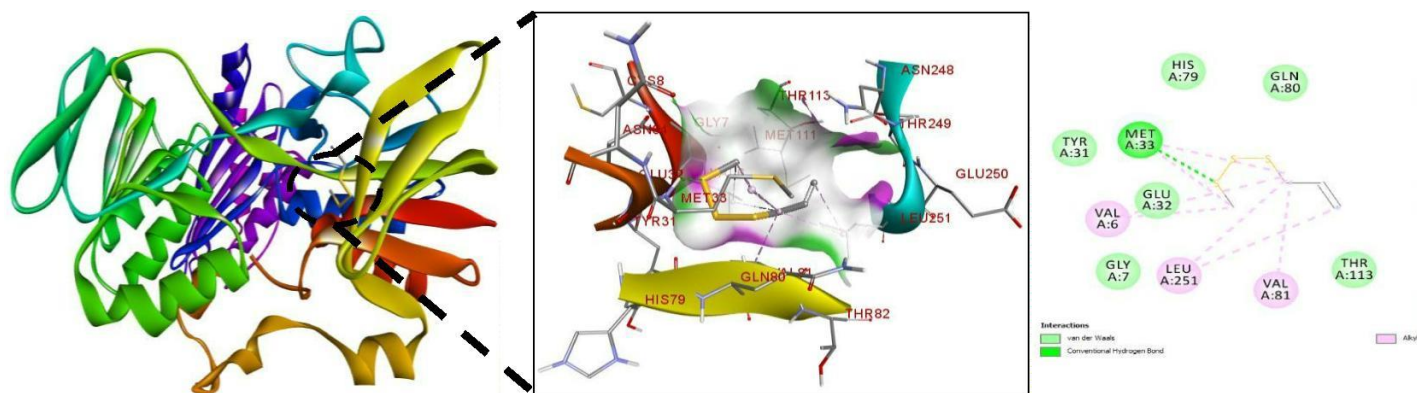


Figure S6. Molecular interaction studies of Allyl methyl trisulfide with NADPH-oxidase (PDB ID: 2CDU), surface view (Left panel), and 2D (Right panel) interactions.

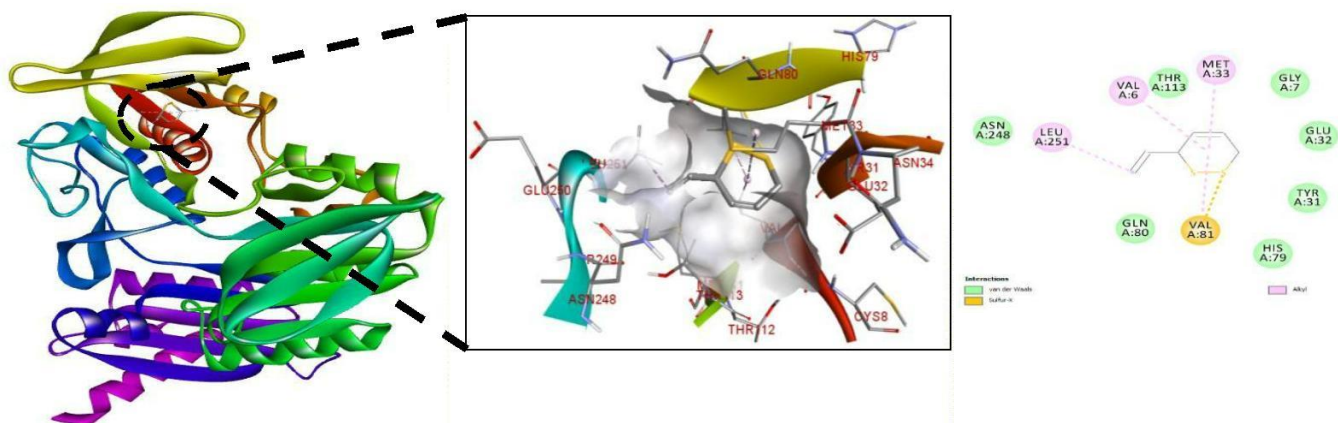


Figure S7. Molecular interaction studies of 3-Vinyl-1,2-dithiacyclohex-4-ene with NADPH-oxidase (PDB ID: 2CDU), surface view (Left panel), and 2D (Right panel) interactions.

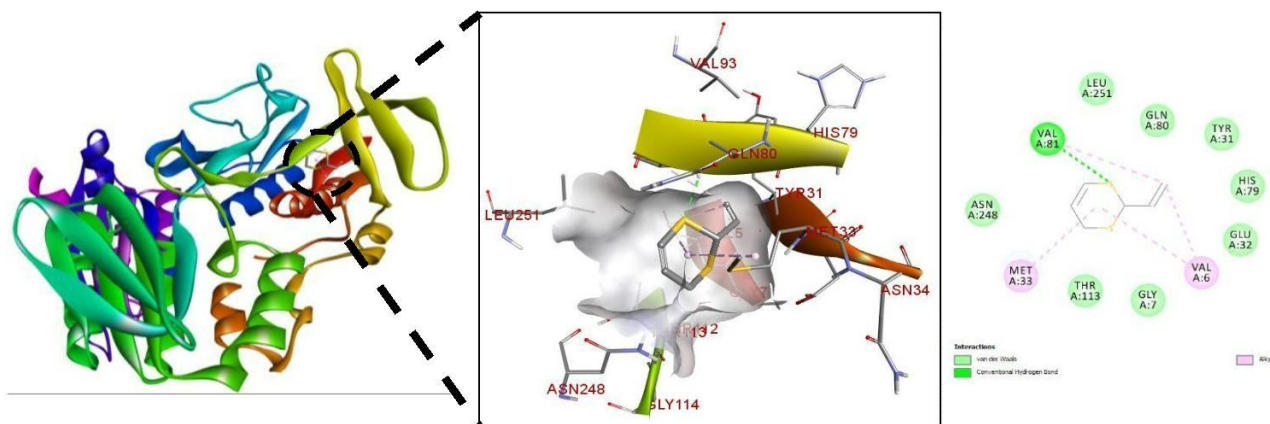


Figure S8. Molecular interaction studies of 2-Vinyl-4H-1,3-dithiine with NADPH-oxidase (PDB ID: 2CDU), surface view (Left panel), and 2D (Right panel) interactions.

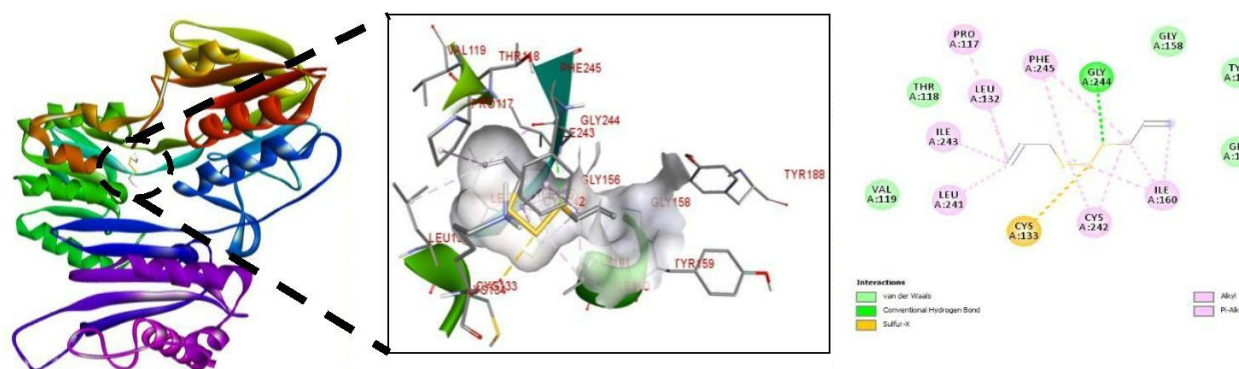


Figure S9. Molecular interaction studies of Diallyl trisulfide with NADPH-oxidase (PDB ID: 2CDU), surface view (Left panel), and 2D (Right panel) interactions.

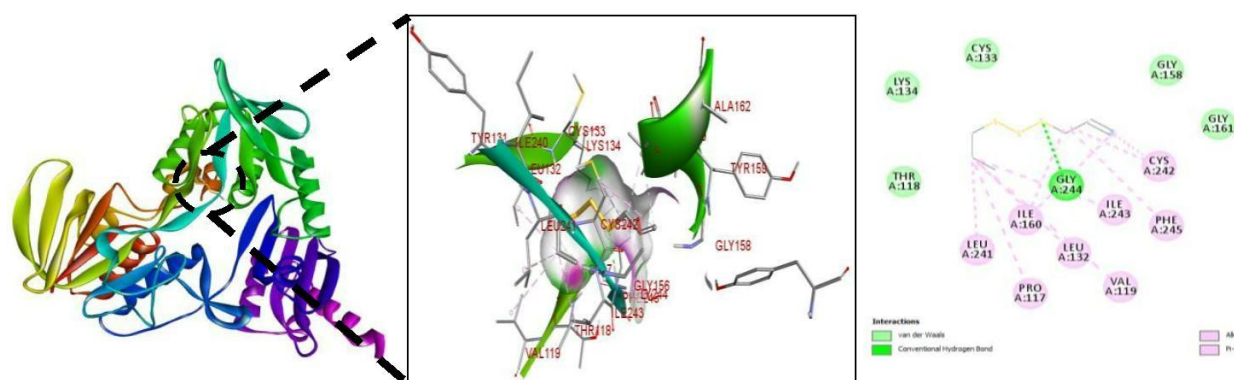


Figure S10. Molecular interaction studies of 1-Allyl-3-propyltrisulfan with NADPH-oxidase (PDB ID: 2CDU), surface view (Left panel), and 2D (Right panel) interactions.

