

## **Supplementary Material**

# **Deciphering the Potential of Pre and Pro-Vitamin D of Mushrooms against Mpro and PLpro Proteases of COVID-19: An In Silico Approach**

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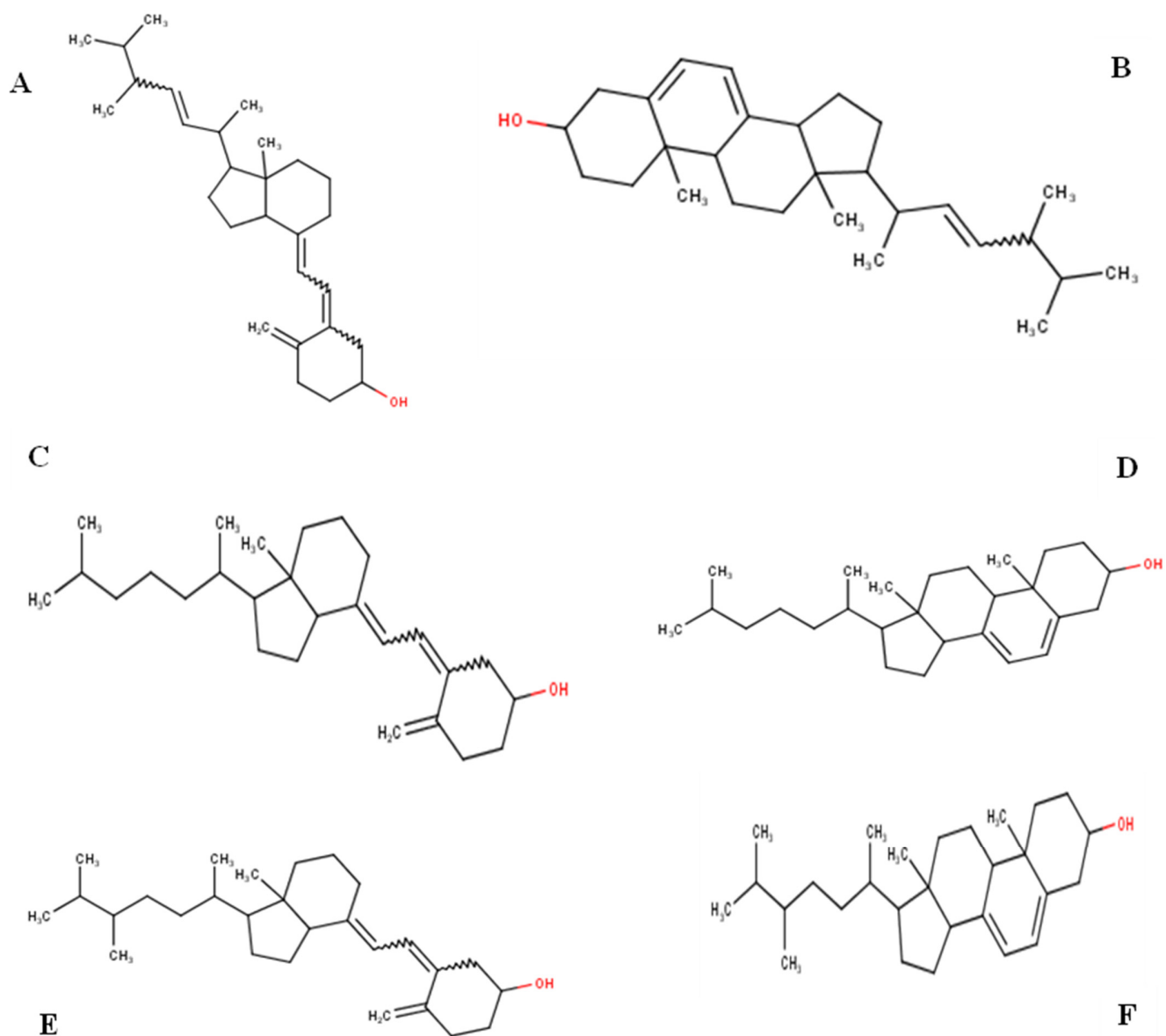
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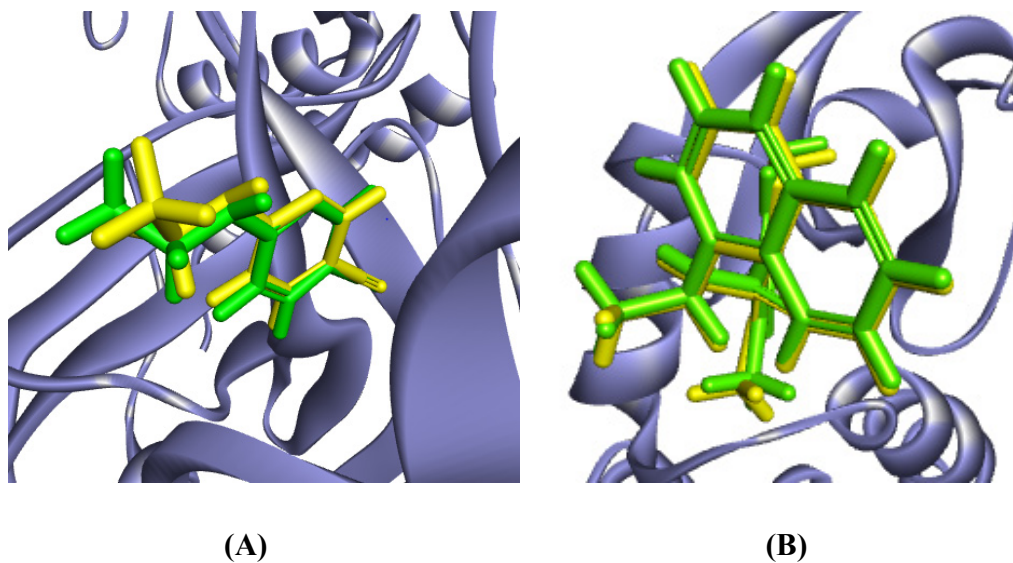
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**Supplementary Figure S1:** 2D structures of pre-and pro-vitamin Ds molecules (**A**) Ergocalciferol (pre-vitamin-D<sub>2</sub>) (**B**) Ergosterol (pro-vitamin-D<sub>2</sub>) (**C**) Cholecalciferol (pre-vitamin-D<sub>3</sub>) (**D**) 7-Dehydrocholesterol (pro-vitamin-D<sub>3</sub>) (**E**) 22,23-dihydroergocalciferol (pre-vitamin-D<sub>4</sub>) (**F**) 22,23-Dihydroergosterol (pro-vitamin-D<sub>4</sub>)



**Supplementary Figure S2:** Result of re-docking experiments green colored pose represents original conformation and yellow color represents docked conformation of co-crystallized ligand (A) 6-(ethylamino)pyridine-3-carbonitrile (RZS) of Mpro and (B) 5-amino-2-methyl-N-[(1R)-1-naphthalen-1-ylethyl]benzamide (TTT) for PLpro.