Supplementary Data

Bio-active components of *Cymbopogon martinii* essential oil as therapeutics targeting bacterial Penicillin-Binding-Proteins (PBPs): Aroma profile, in silico-docking, pharmacokinetics, and wet-lab validation

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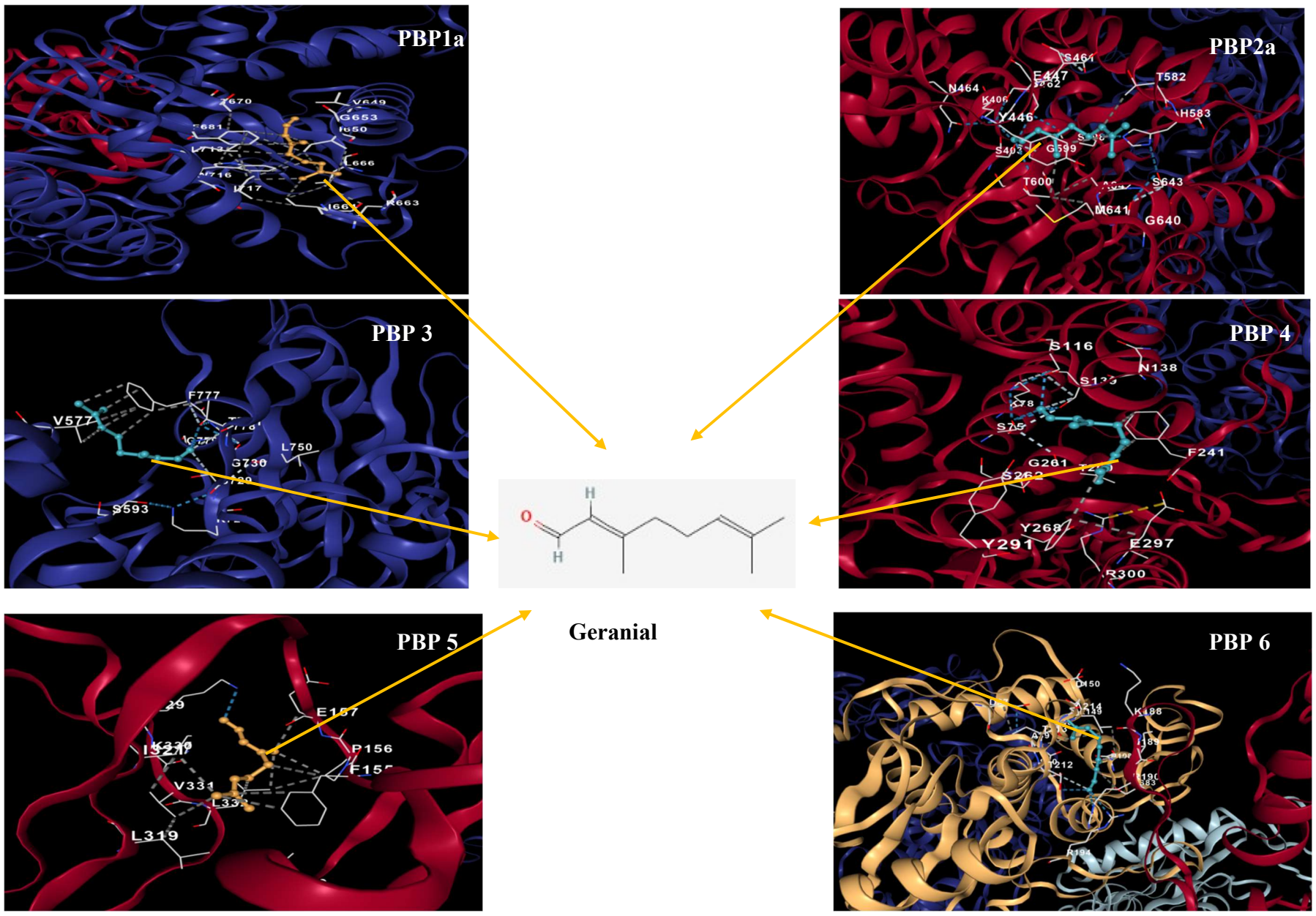


Figure S1. *Molecular Docking of Geranial with six bacterial PBPs.*

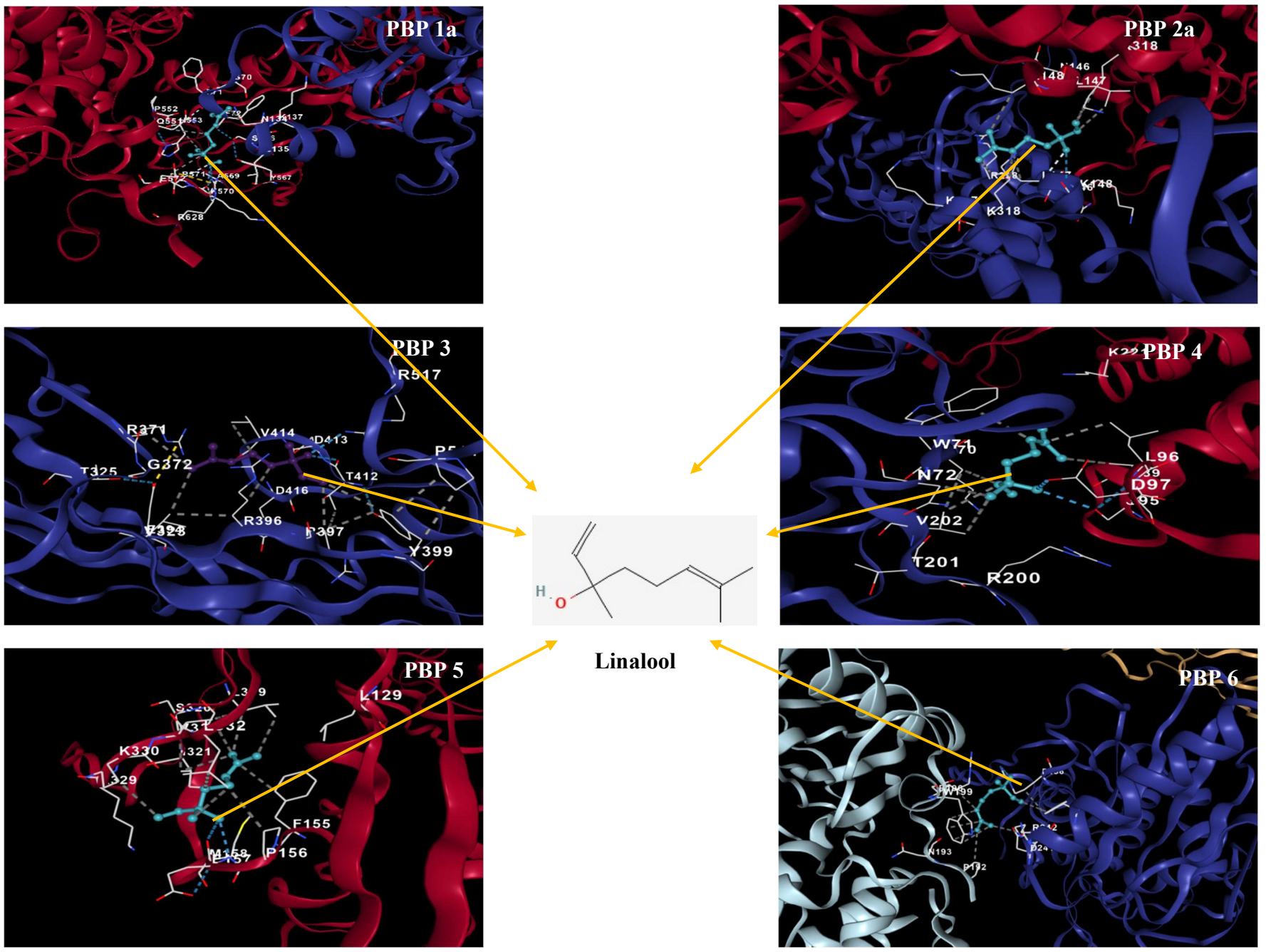


Figure S2. *Molecular Docking of Linalool with six bacterial PBP's.*

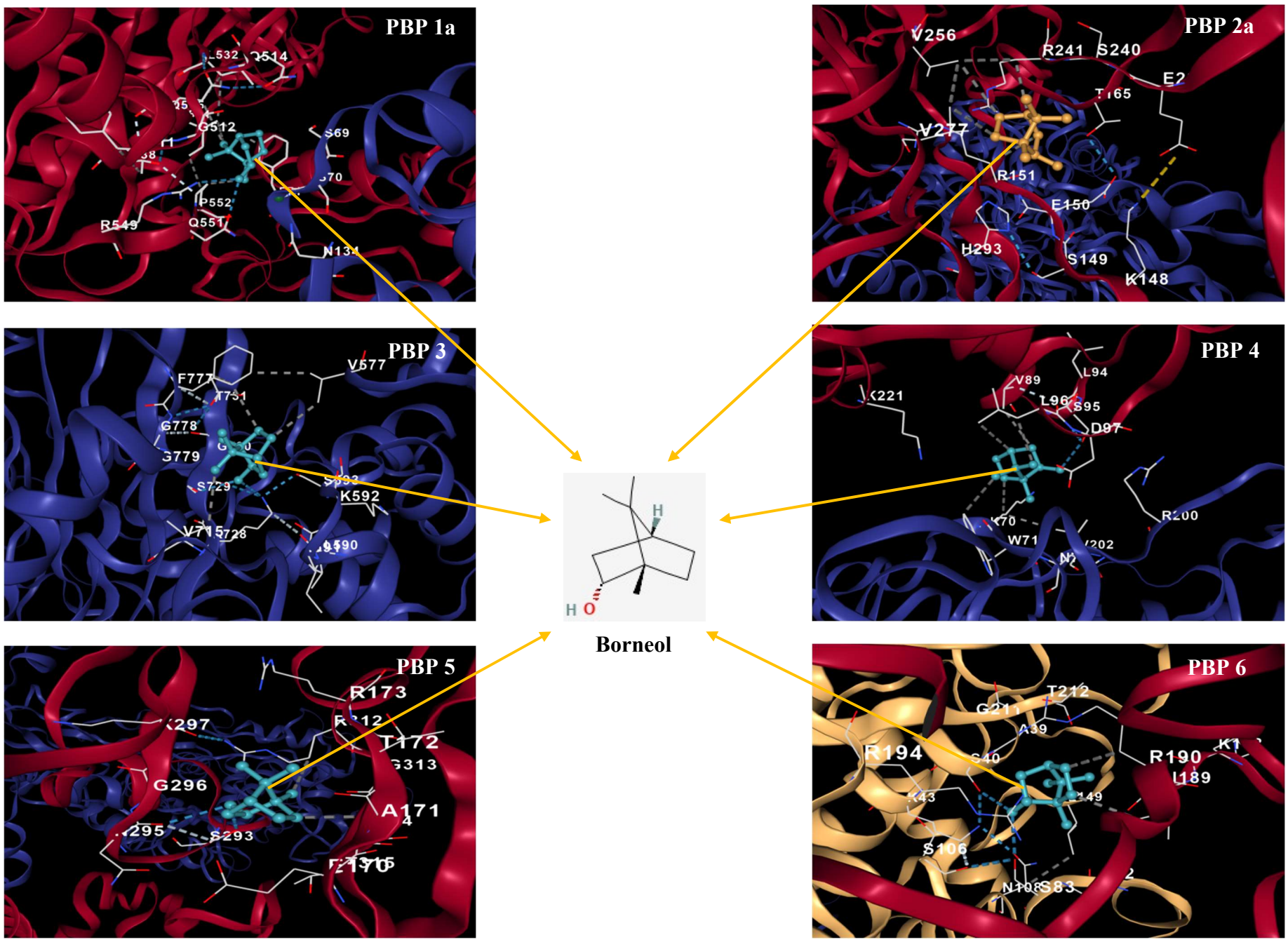


Figure S3. *Molecular docking of Borneol with six Penicillin Binding Proteins.*

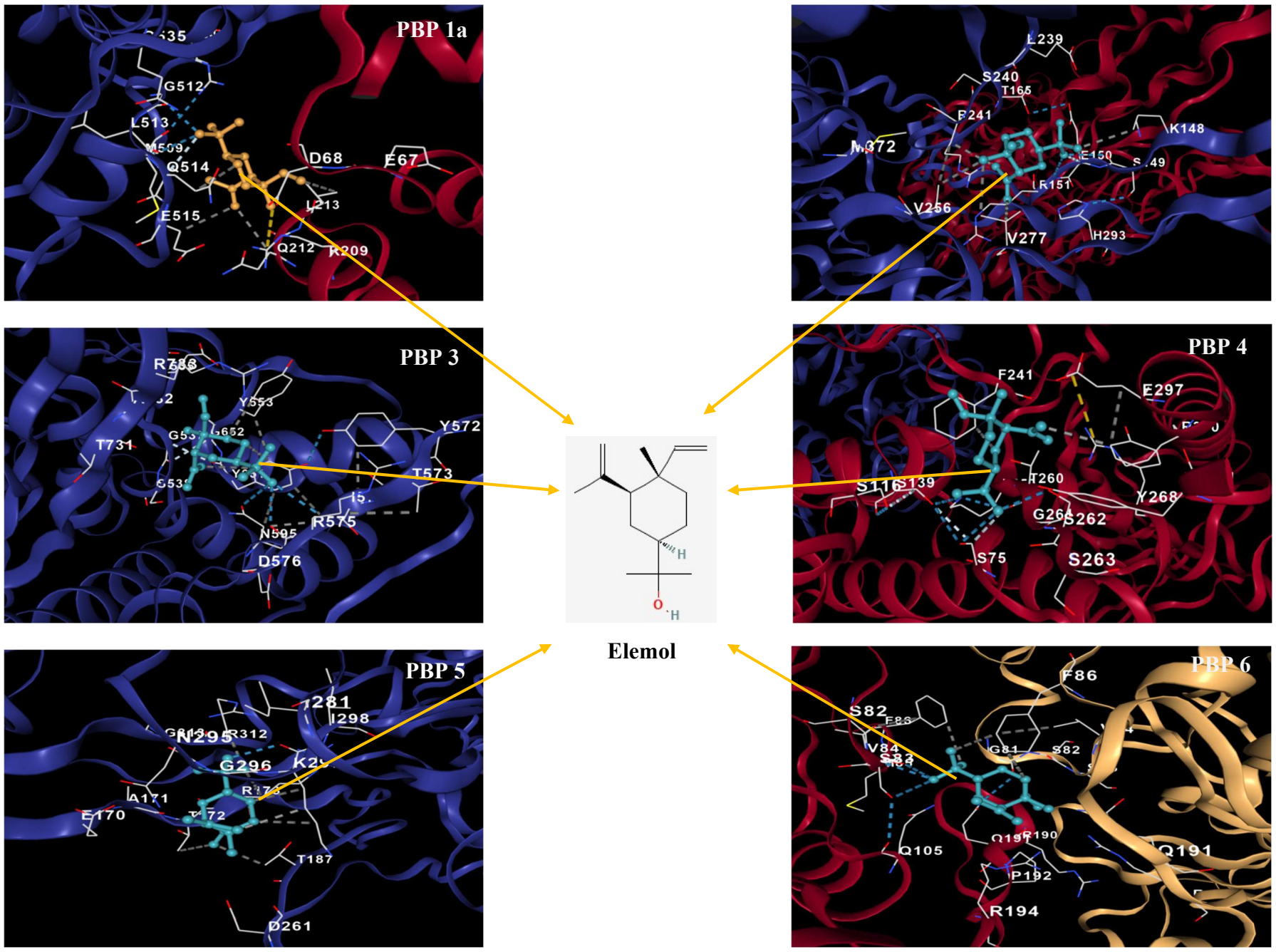


Figure S4. *Molecular docking of Elemol with six Penicillin Binding Proteins.*

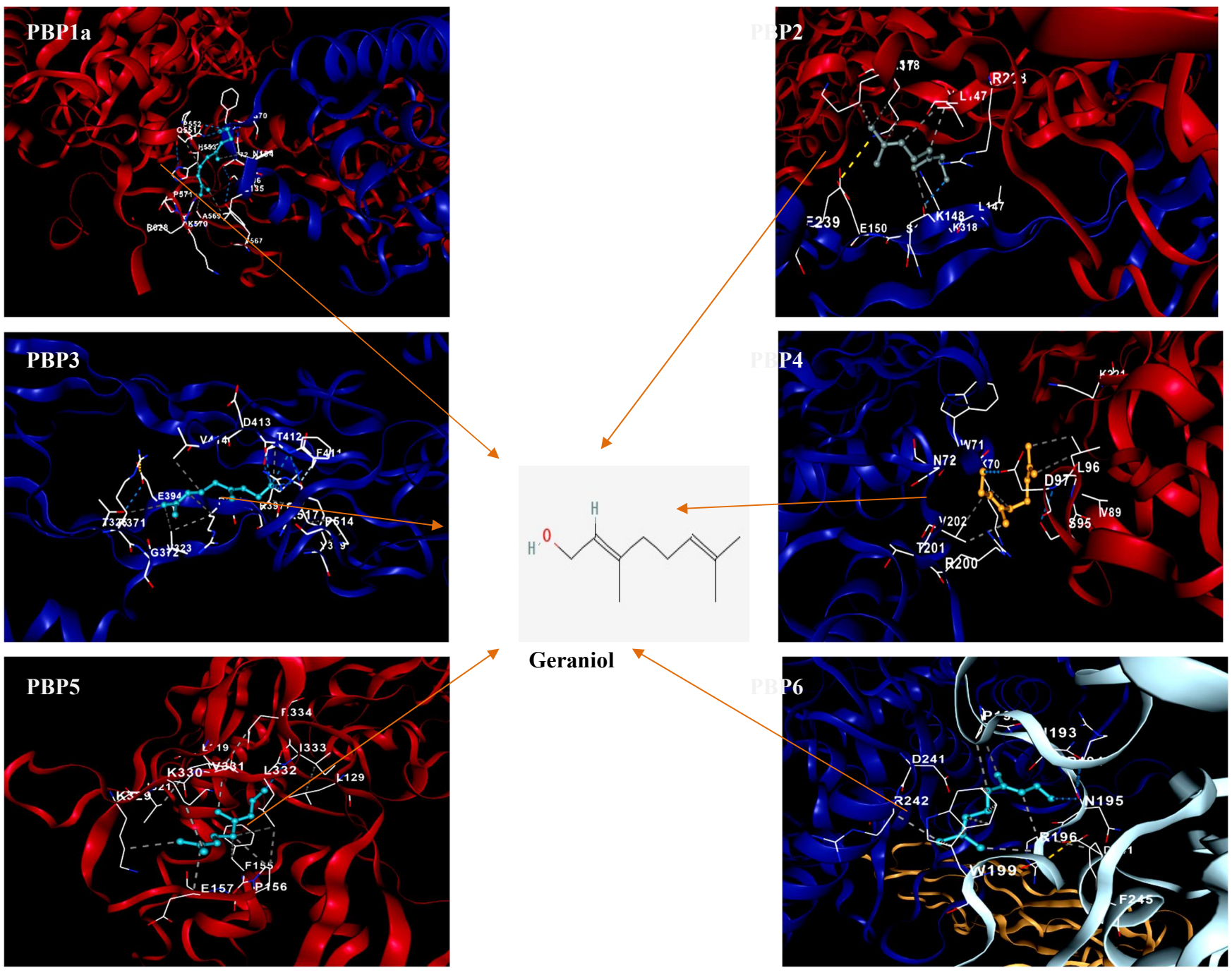


Figure S5. *Molecular Docking of Geraniol with six bacterial cell wall proteins.*

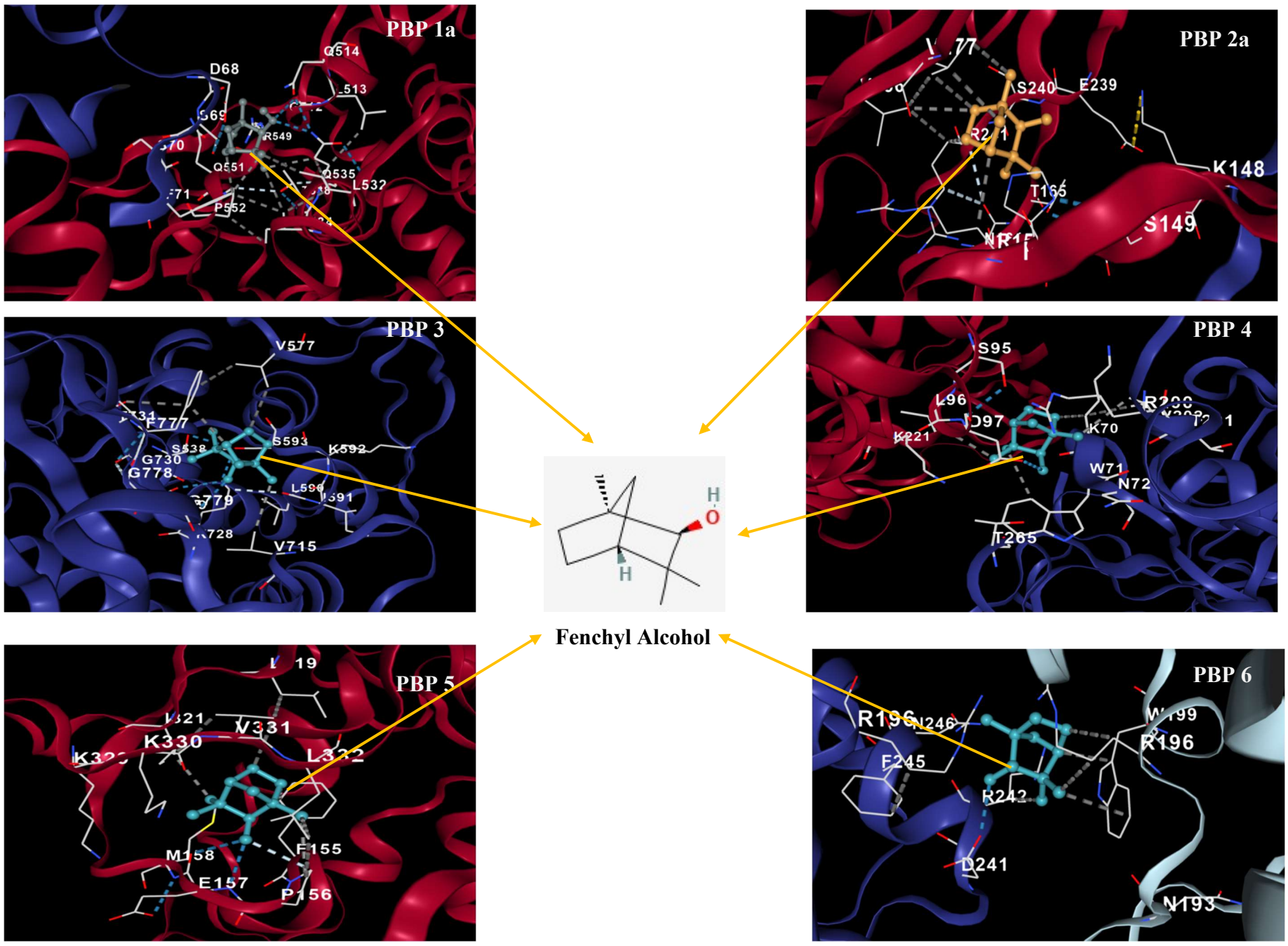
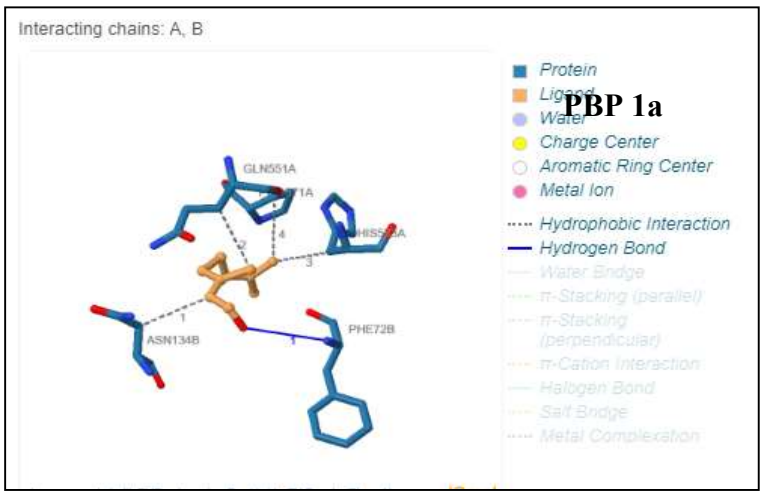
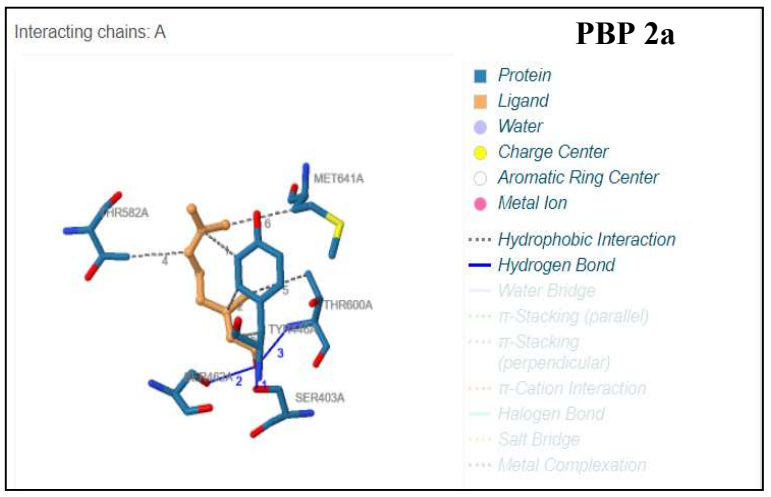
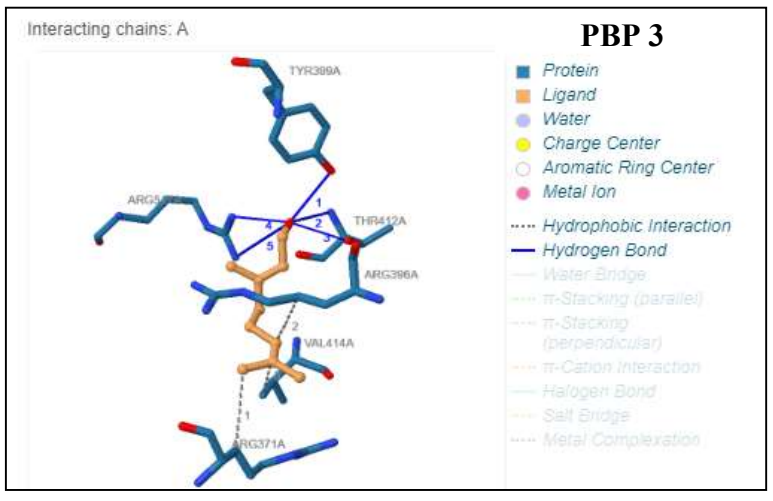


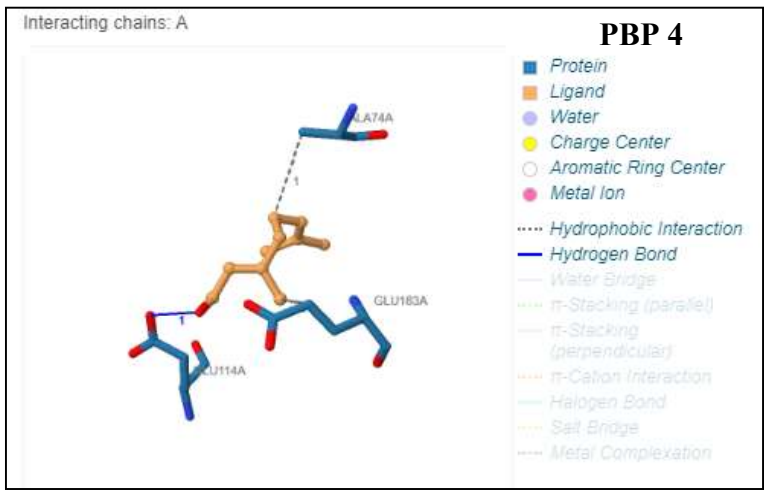
Figure S6. *Molecular docking of Fenchyl alcohol with six Penicillin binding Proteins.*

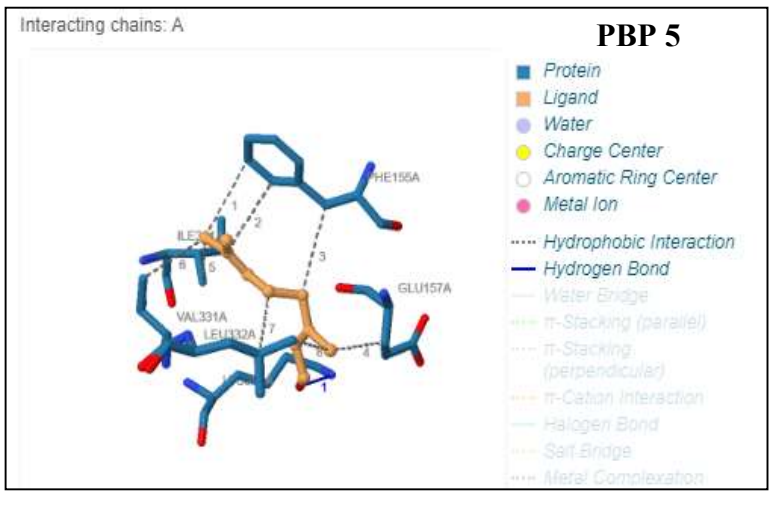
Figure S7. *Molecular docking of 6-methyl-hept-5-en-2-one with six Penicillin binding Proteins.*











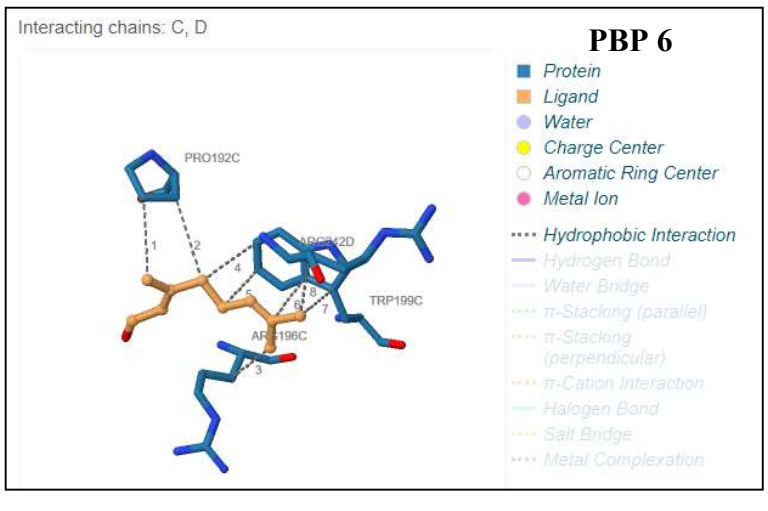
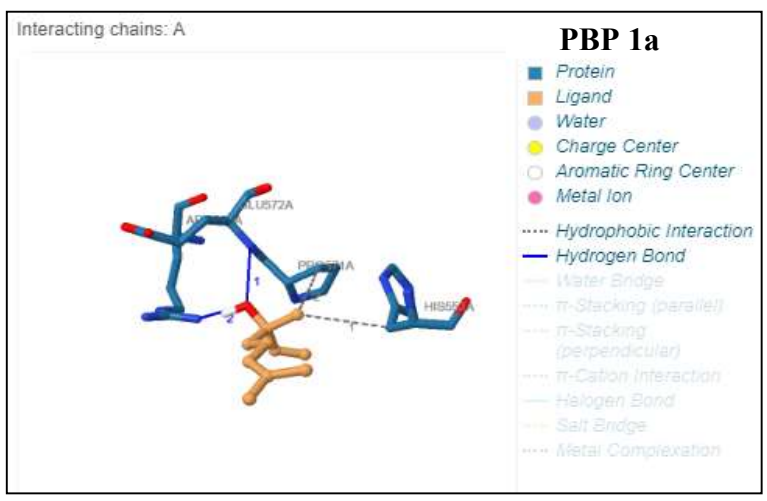
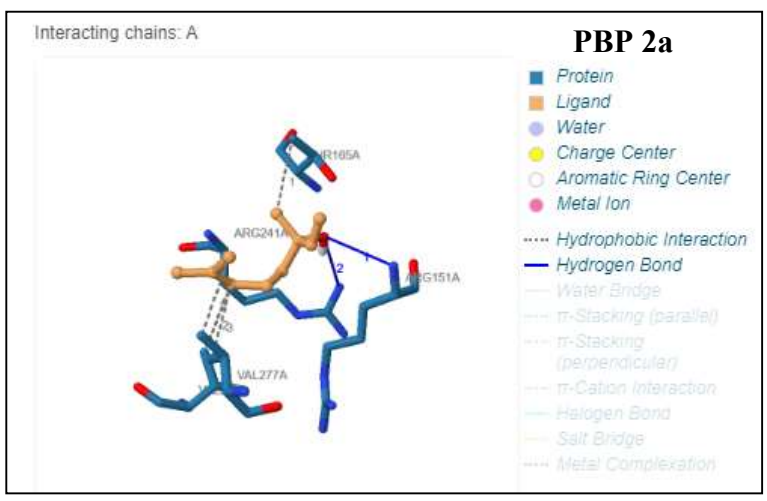
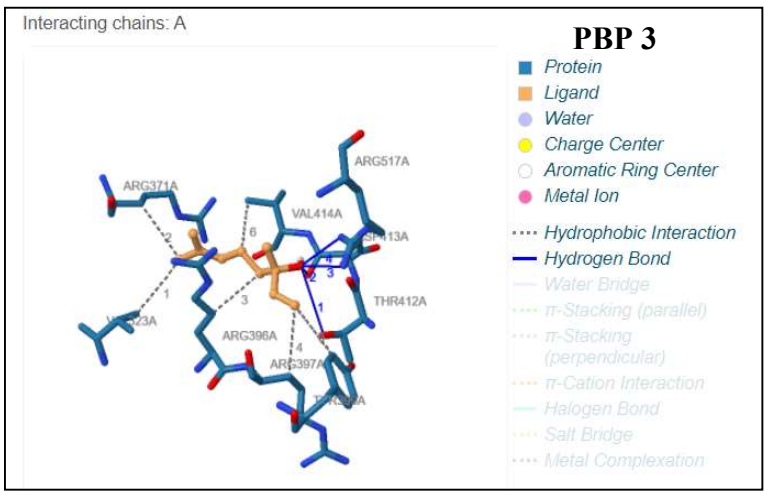
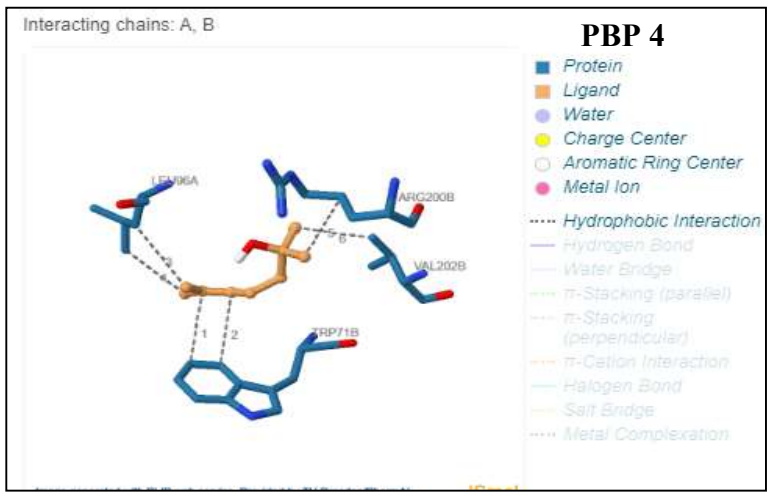


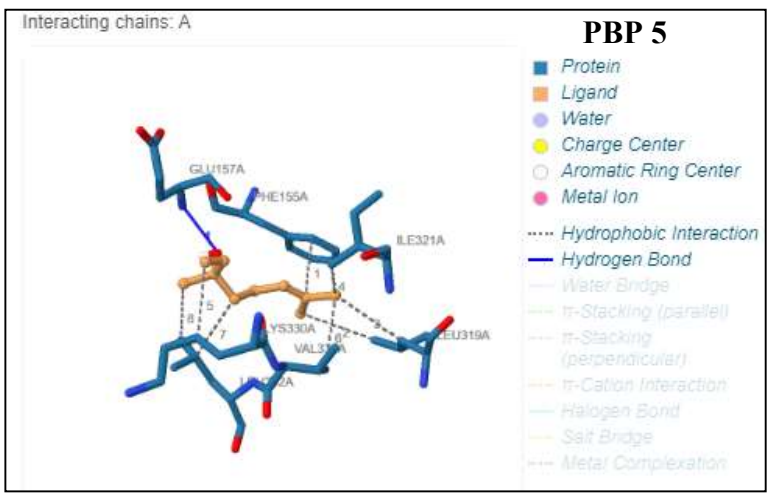
Figure S8. *3-D interactions of geranial with protein receptors.*











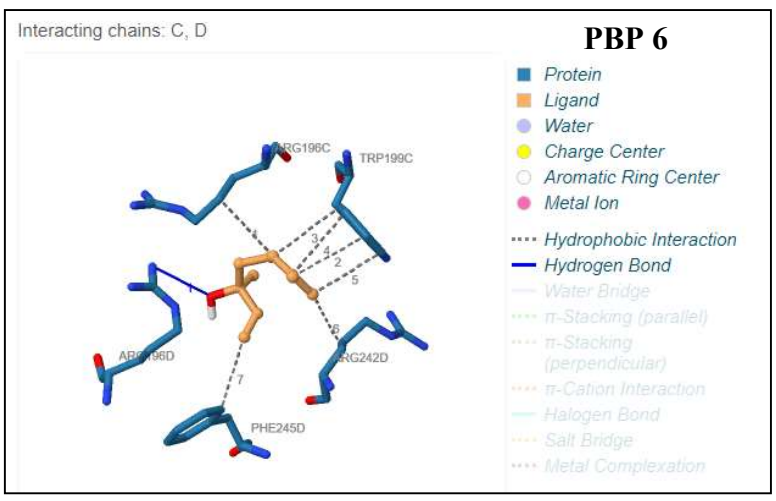
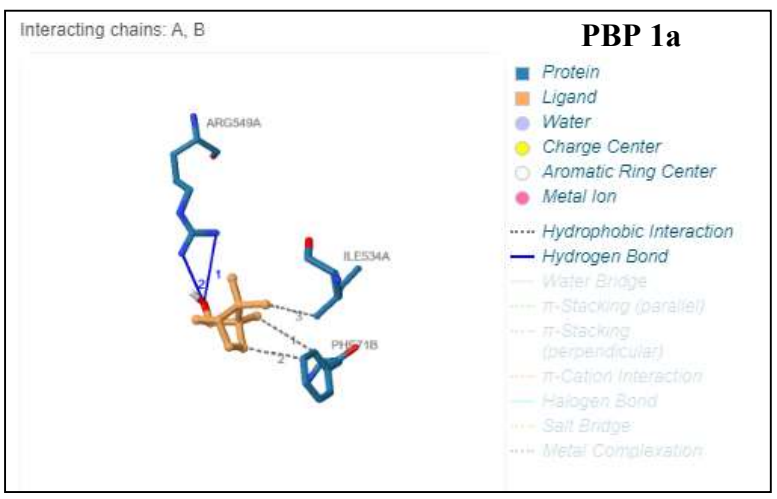
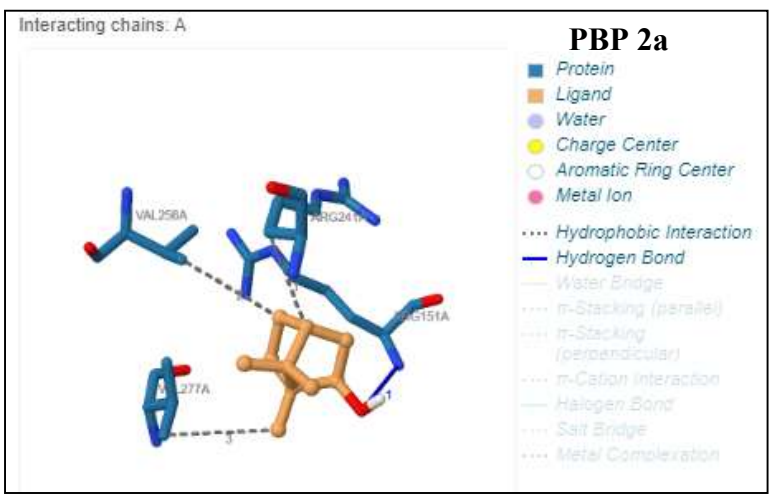
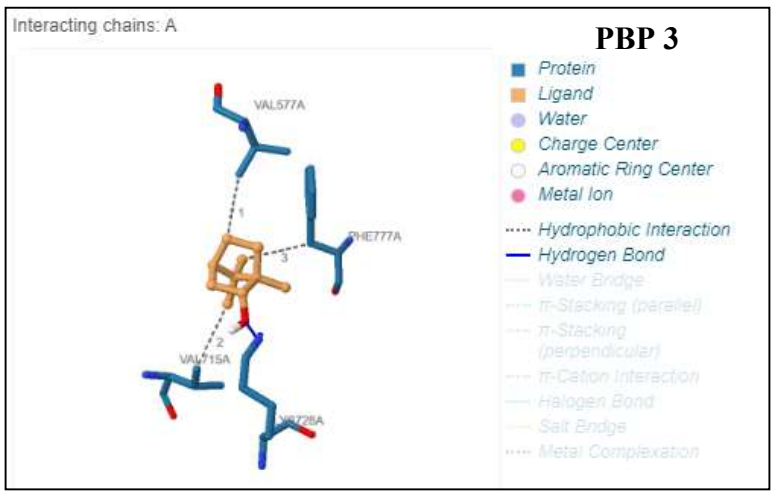
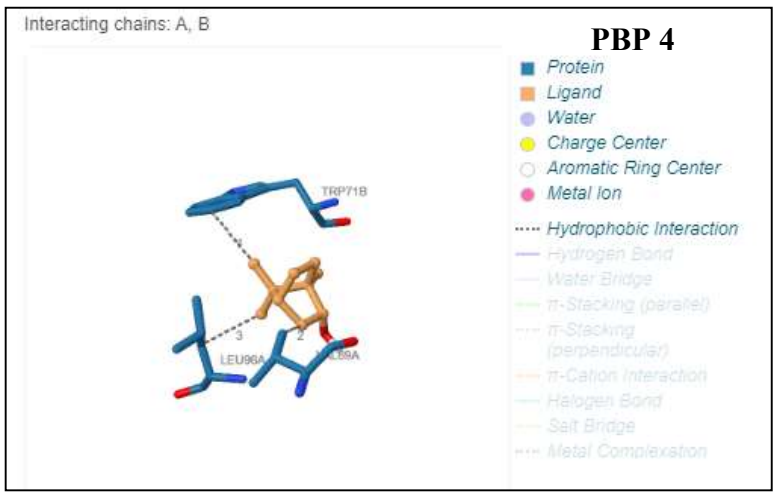


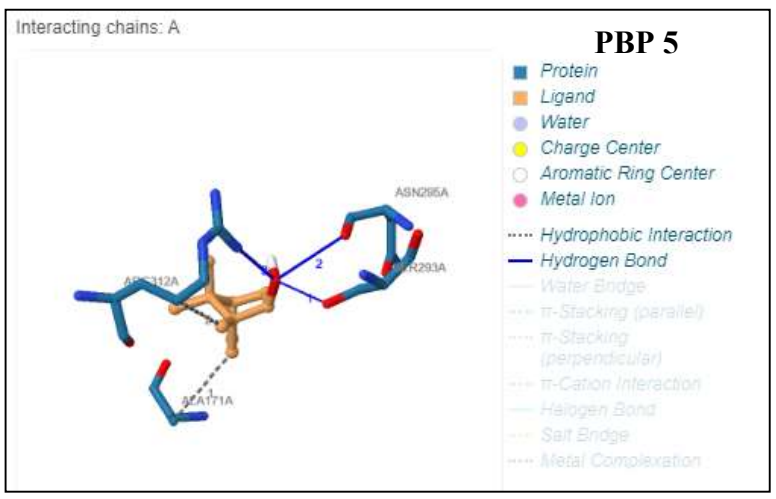
Figure S9. *3-D interaction of Linalool with protein receptors.*











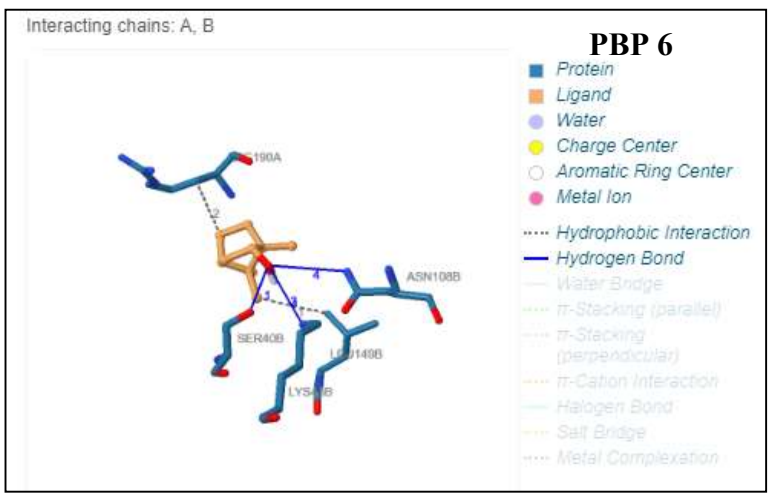
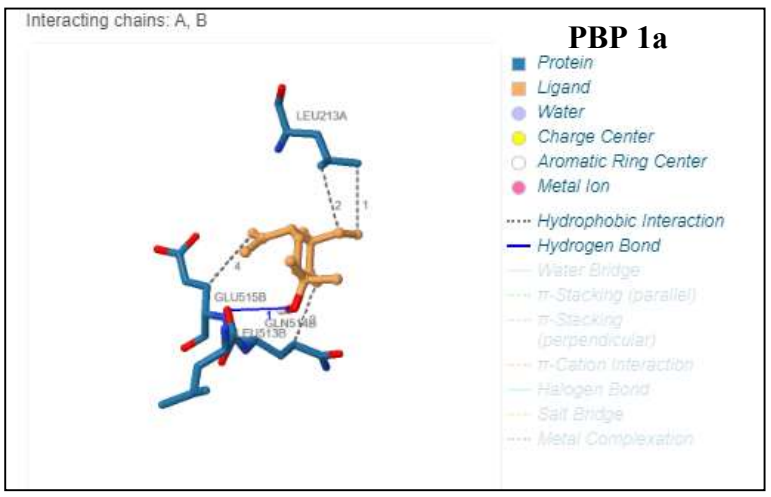
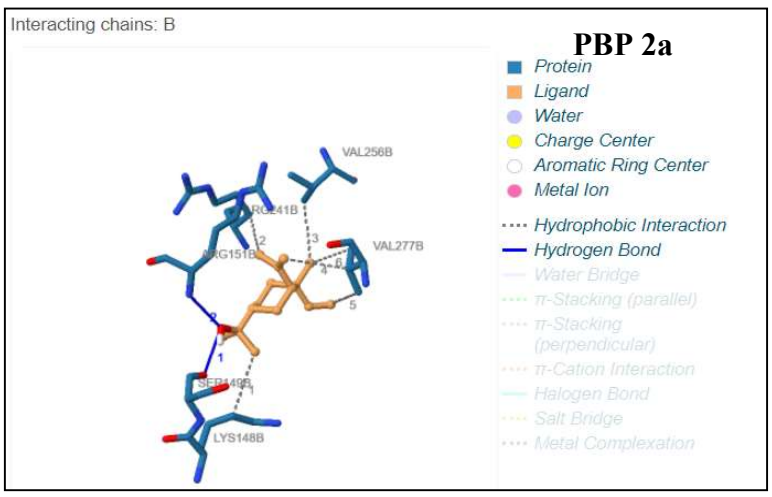
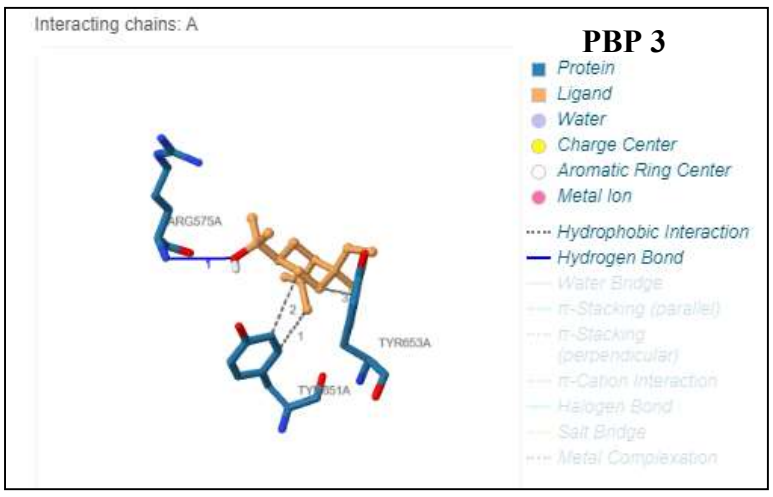
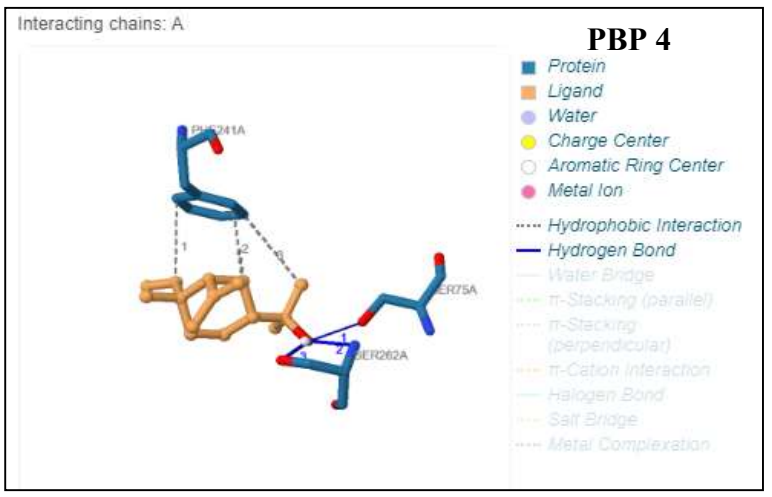


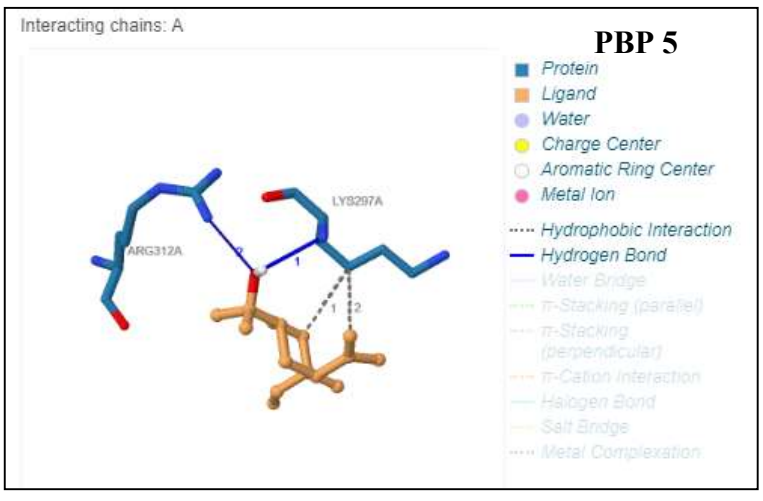
Figure S10. *3-D interactions of Borneol with protein receptors.*











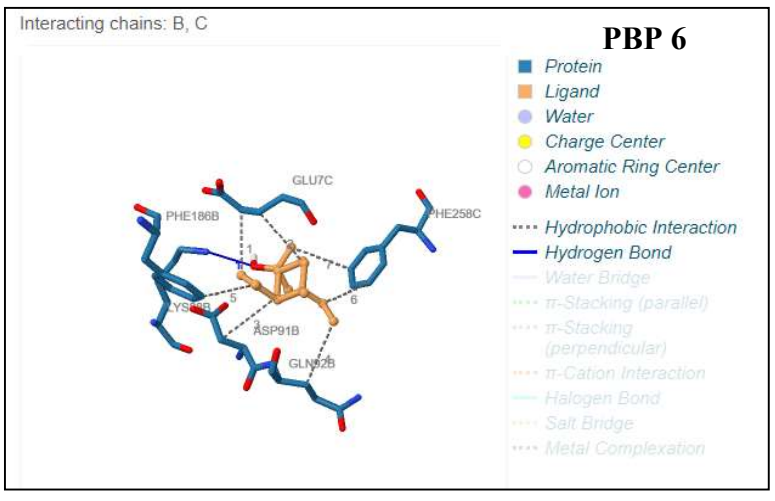
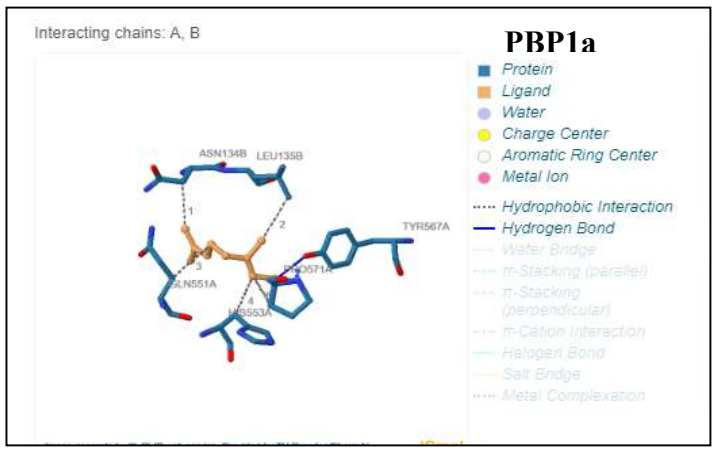
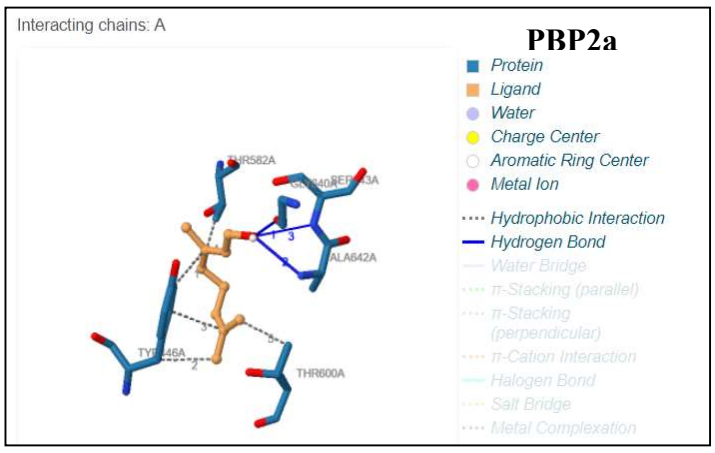
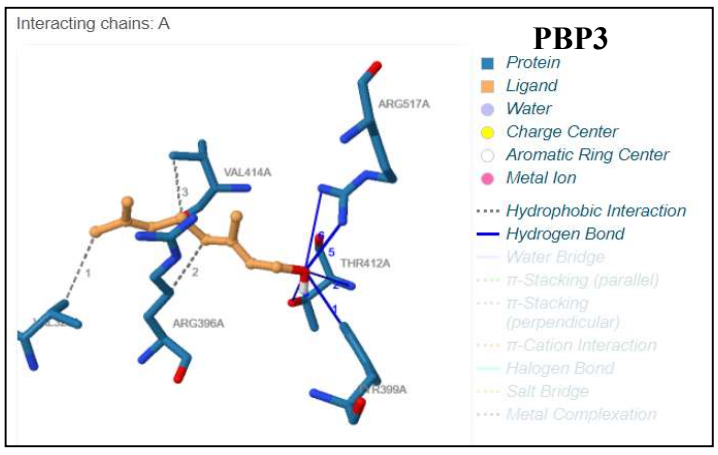
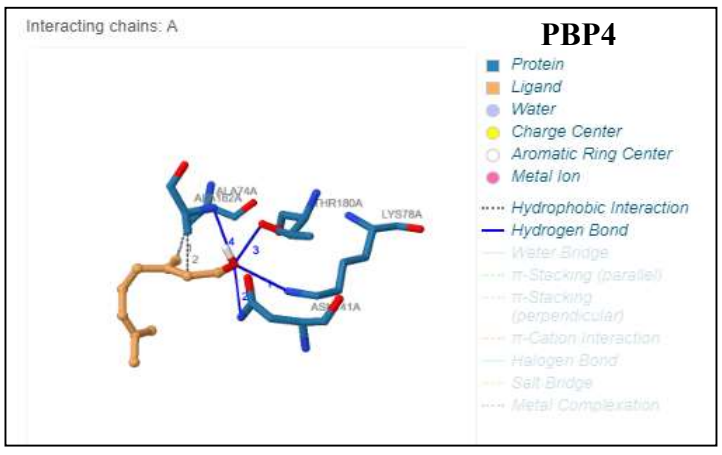


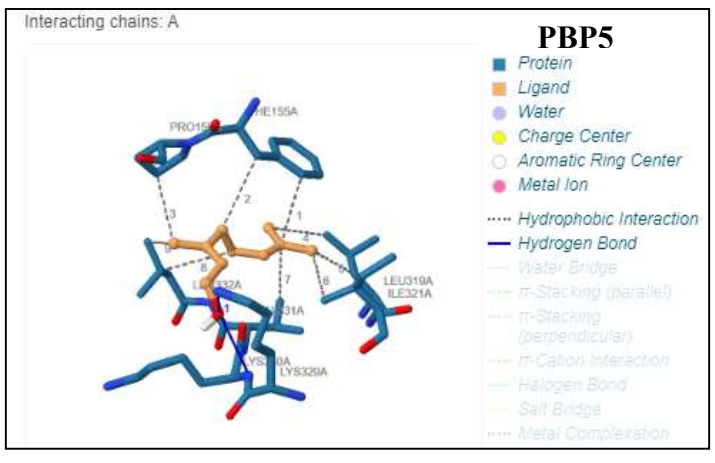
Figure S11. *3-D interactions of Elemol with protein receptors.*











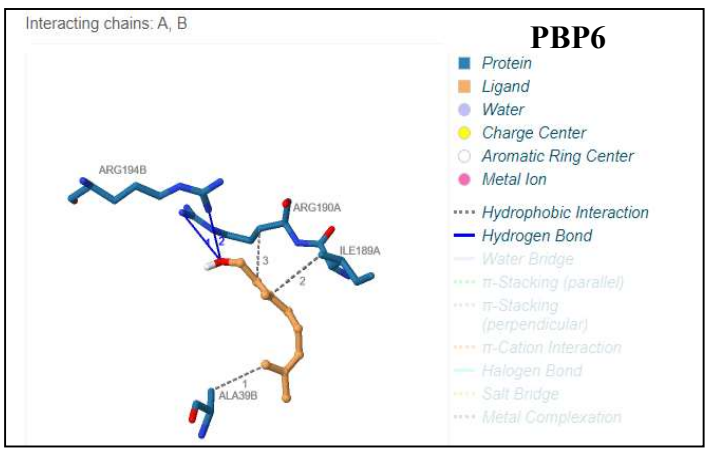
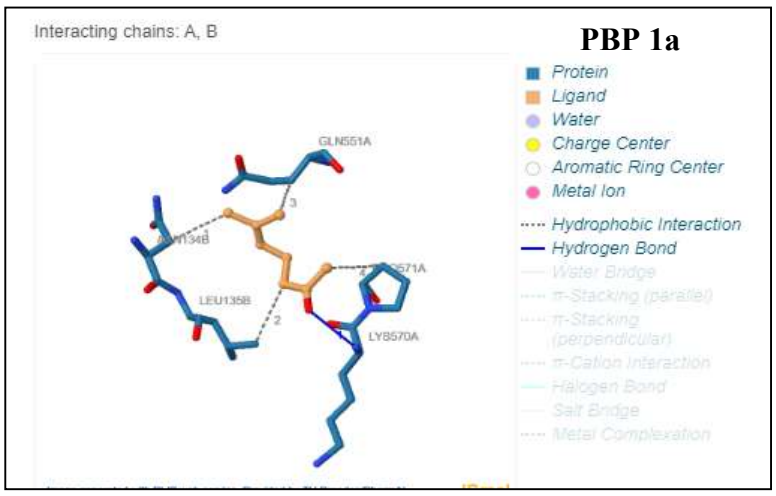
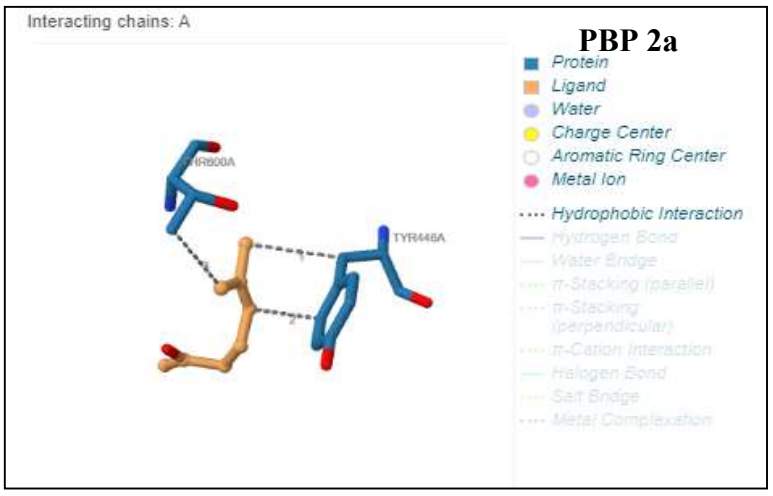
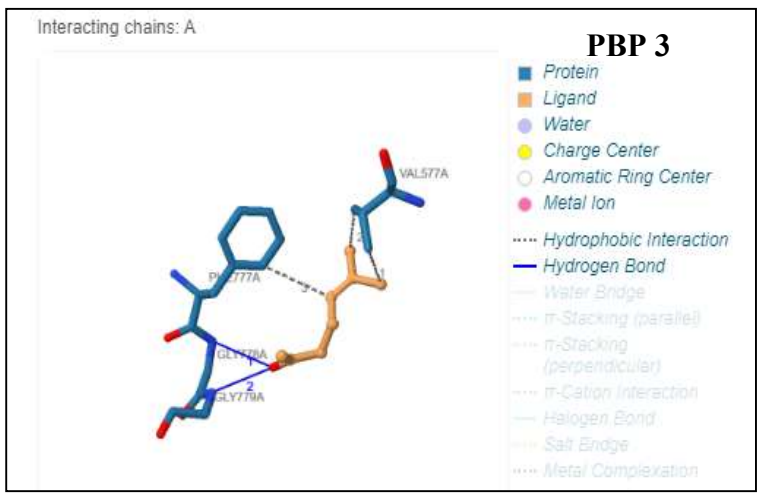
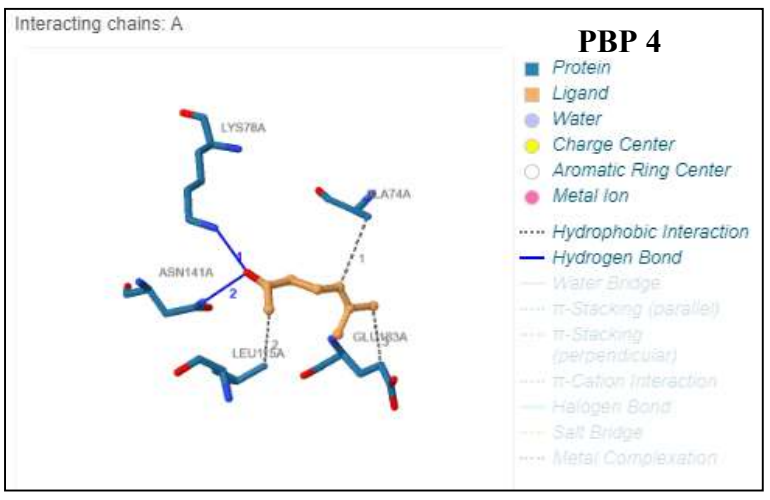


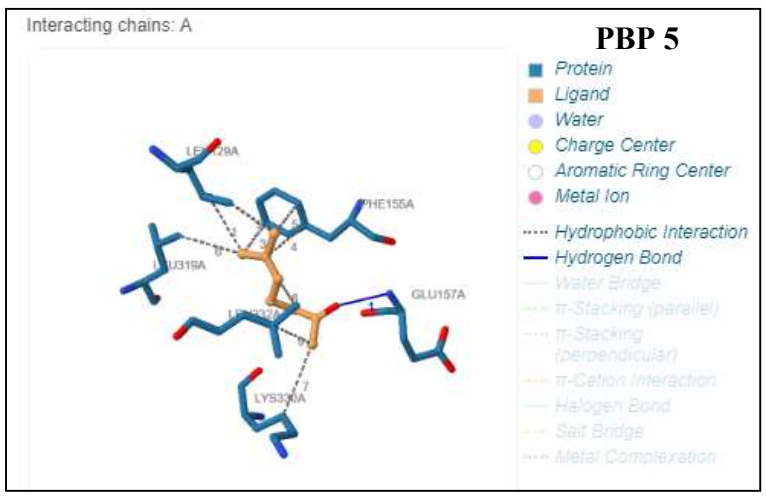
Figure S12. 3D interactions of Geraniol with protein receptors.











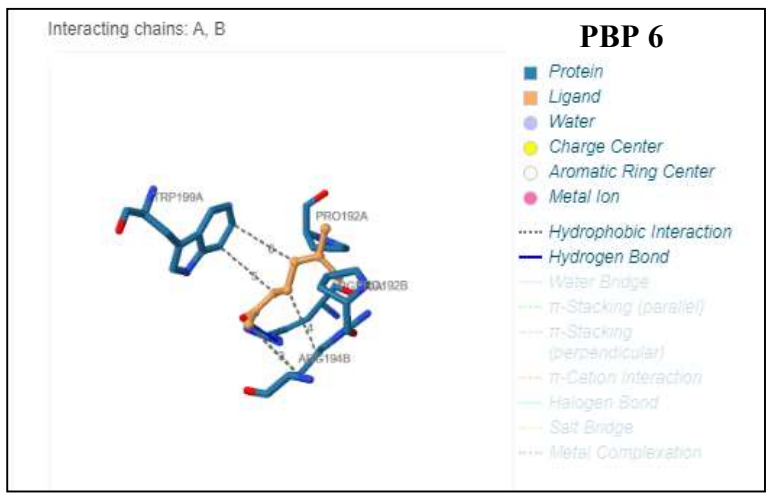
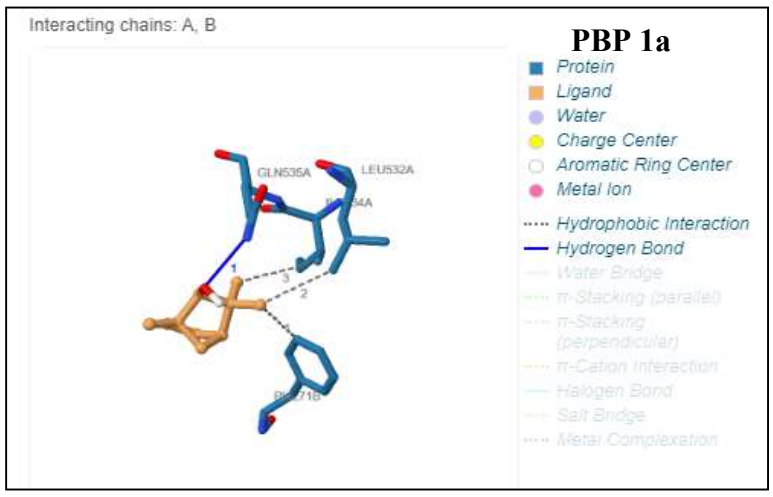
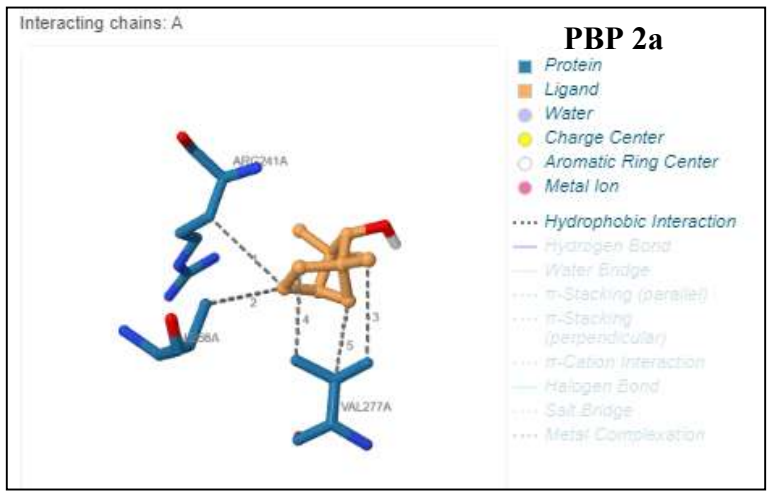
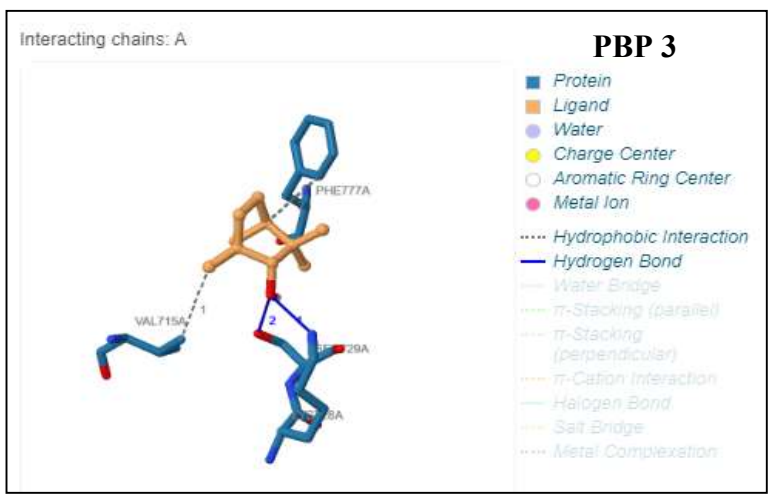
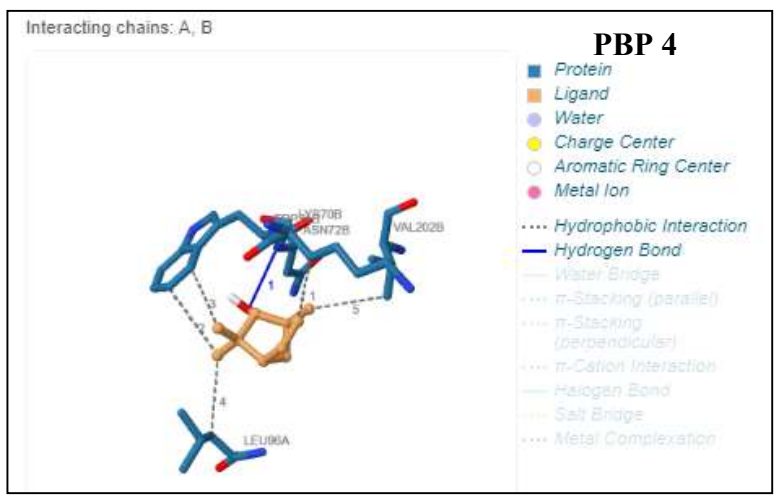


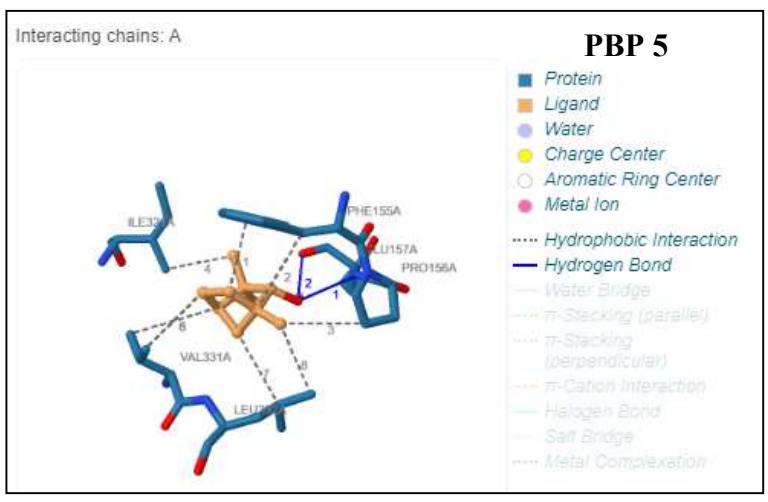
Figure S13. *3-D interactions of 6-methyl-hept-5-en-2-one with protein receptors.*











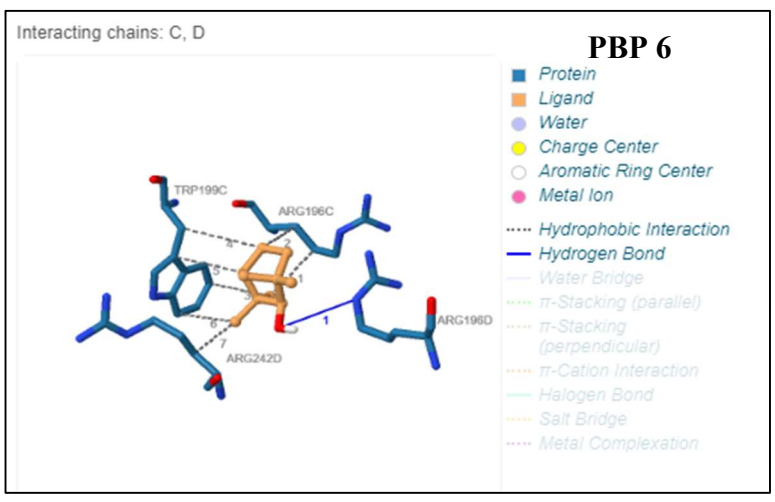


Figure S14. *3-D interactions of Fenchyl alcohol with protein receptors.*

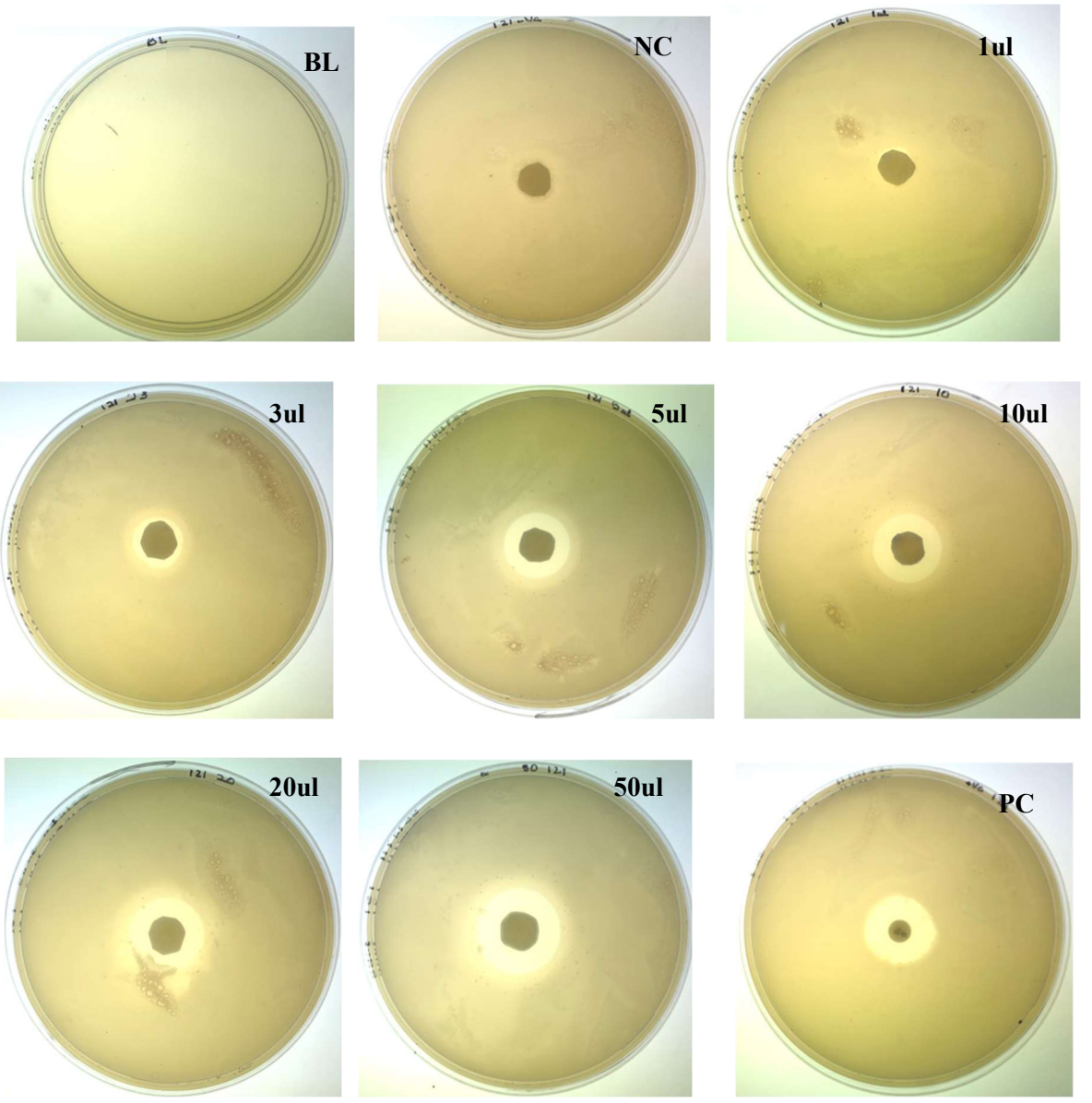


Figure S15. *Anti-microbial activity of PRO against MTCC 121.BL: Blank (Only Media) NC: Negative Control (empty disc) PC: Positive Control (Streptomycin 10 mg/disc)*

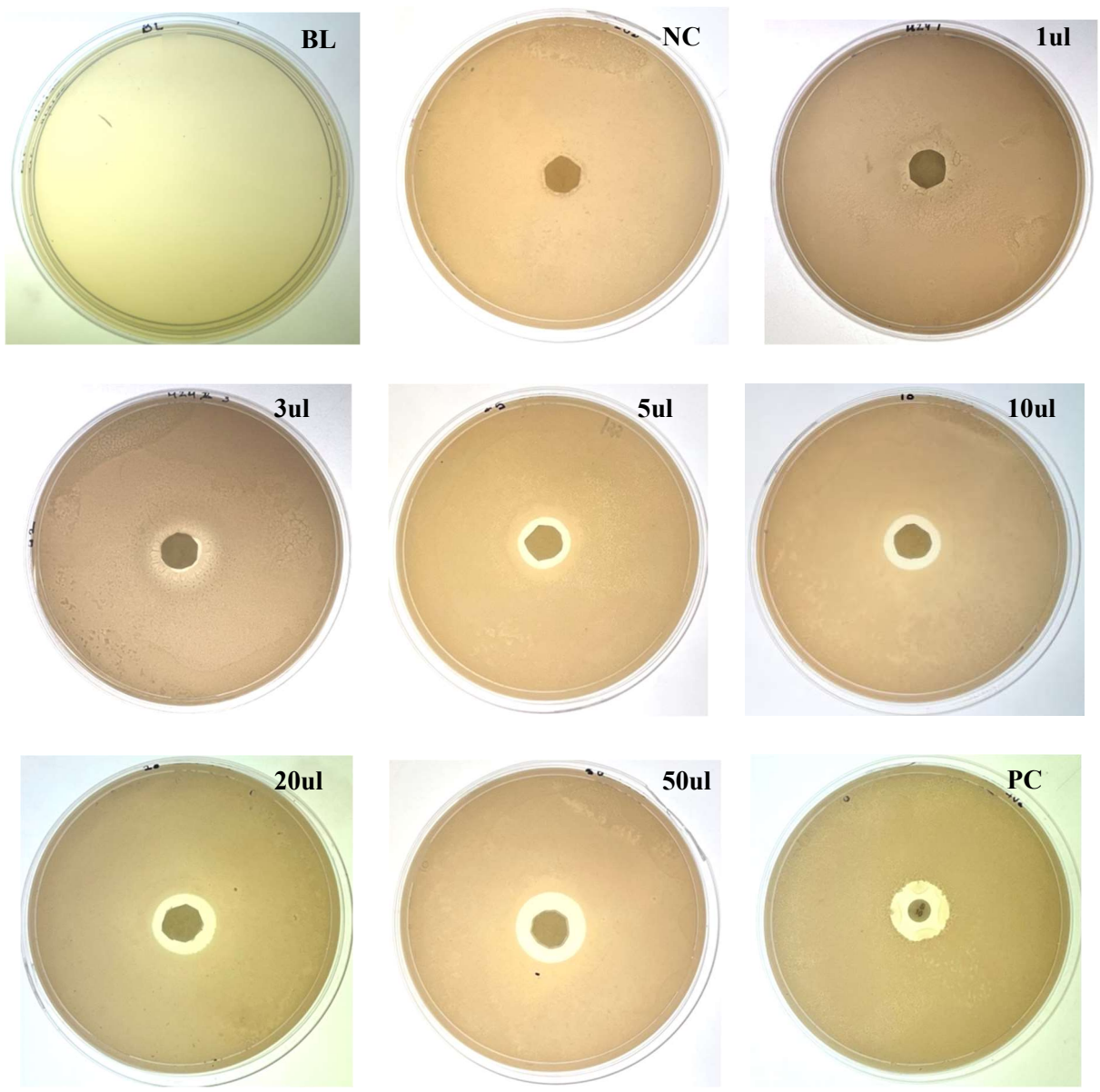


Figure S16. *Anti-microbial Activity of PRO against MTCC424 BL: Blank (Only Media), NC: Negative Control, PC: Positive Control (Streptomycin 10 mg/disc).*

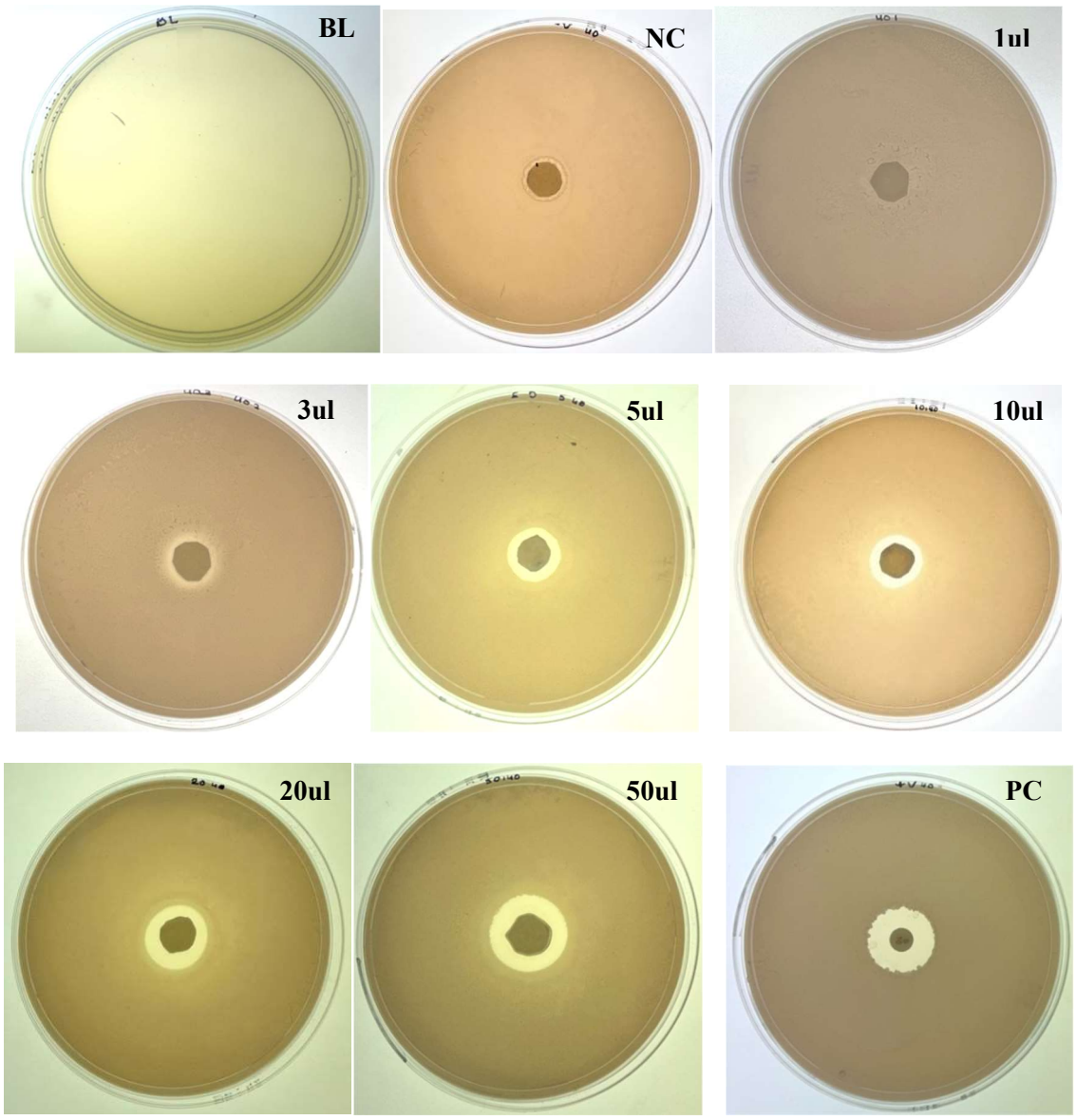


Figure S17. *Showing Anti-microbial Activity of PRO against MTCC40. NC: Negative control (empty disc), PC: Positive Control (Streptomycin 10mg/disc, BL: Blank (only media).*

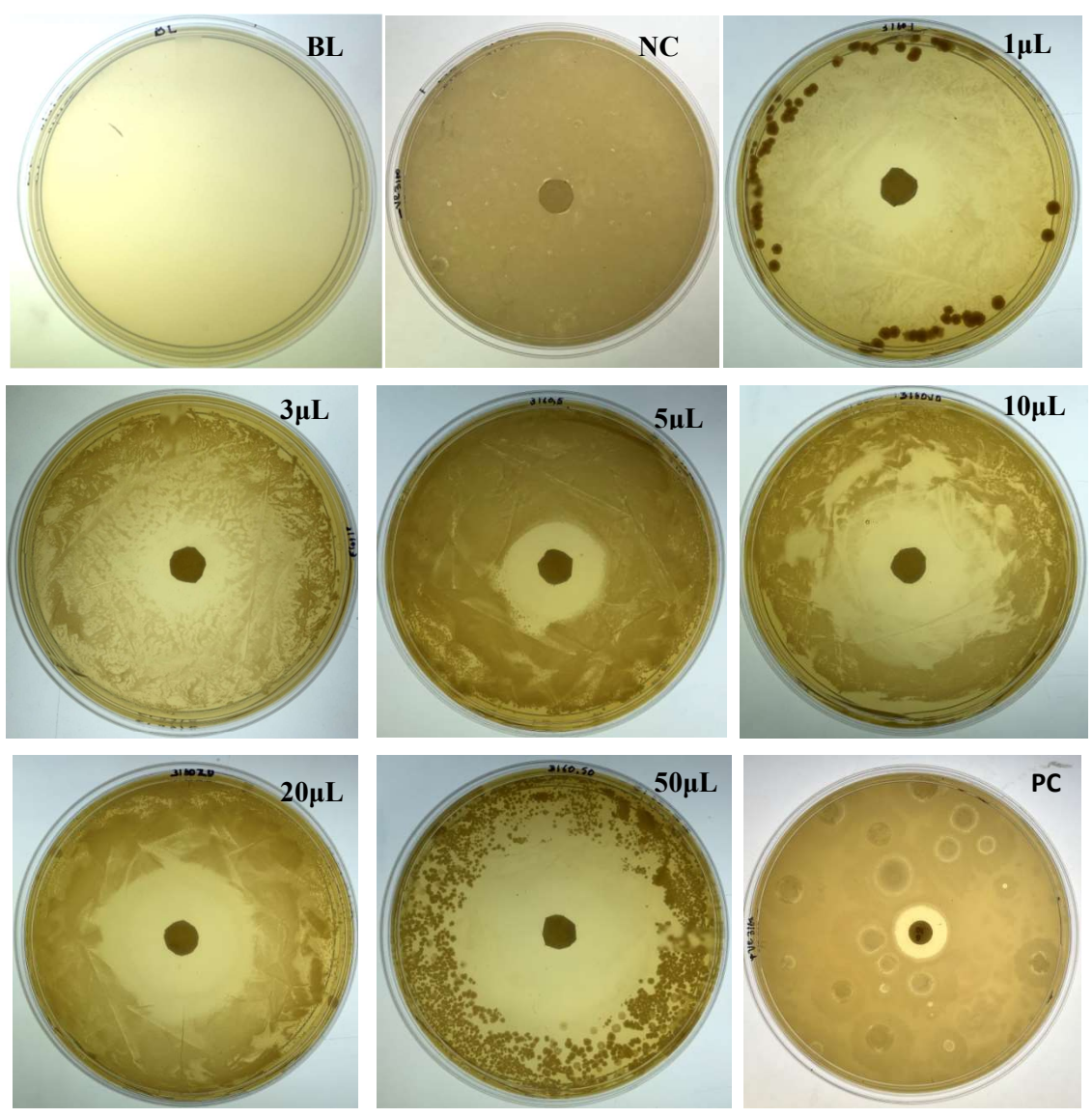


Figure S18. *Anti-microbial Activity of PRO against MTCC3160. BL: Blank (Only Media) NC: -ve Control, PC: +ve Control.*