In Silico Evaluation of the Repellent Efficacy of Selected Citrus Terpenoids Against *Aedes Albopictus* OBP 1 Protein Using Molecular Docking Techniques

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Mosquito-borne diseases pose a major global health threat, affecting billions each year. Rising resistance to synthetic pesticides and the lack of antiviral treatments, especially for illnesses like dengue, emphasize the need for alternative prevention methods. Natural plant compounds, particularly citrus-derived terpenoids, have shown promise as eco-friendly mosquito repellents. This study used an *in silico* approach to assess the binding efficiency of selected citrus-based phytochemicals against Odorant Binding Protein 1 (OBP1) of *Aedes albopictus*, with the synthetic repellent DEET as a reference. Key compounds analyzed included limonene, α-pinene, β-pinene, linalool, citronellol, myrcene, citral, and neral—chosen for their known repellent activity and abundance in citrus extracts. The OBP1 active site was identified using CASTp, and molecular docking was performed using AutoDock 4.2.6 with standard parameters (Kollman charges and merged non-polar hydrogens). Docking was tested at exhaustiveness levels 8, 30, 50, and 100 to validate results. Additional virtual screening was conducted with Vina, and interactions were visualized using Discovery Studio and ChimeraX. Limonene showed the highest binding affinity at –6.8 kcal/mol, surpassing DEET (–5.0 kcal/mol). Other compounds like α-pinene and β-pinene also exhibited stronger affinities than DEET. The docking interactions included hydrogen bonds, alkyl, and π-alkyl interactions, suggesting favorable structural compatibility with OBP1. While no significant statistical differences were observed across exhaustiveness levels, minor variations in binding affinity were noted. Overall, the findings highlight the potential of citrus-derived terpenoids, particularly limonene, as effective natural alternatives to synthetic mosquito repellents. The study demonstrates the value of computational docking in screening plant-based bioactive compounds for mosquito control strategies.

Keywords: Odorant binding protein 1 (OBP1), *In silico analysis, Aedes albopictus, c*itrus-derived terpenoids, molecular docking

Acknowledgement: *This abstract was supported by the Science and Technology Human Resource Development Project, Ministry of Higher Education, Sri Lanka, funded by the Asian Development Bank (Grant No. R2RJ4).*