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Vitex negundo L. Essential Oil: Odorant Binding Protein Efficiency Using Molecular Docking Approach and Studies of the Mosquito Repellent

Bamidele Joseph Okoli [1,*], Zakari Ladan [2], Fanyana Mtunzi [3] and Yayock Chigari Hosea [4]

[1] Department of Chemical Sciences, Faculty of Science and Technology, Bingham University, New Karu 961105, Nasarawa State, Nigeria
[2] Department of Chemistry, Faculty of Science, Kaduna State University, Tafawa Balewa Way, Kaduna 800283, Kaduna State, Nigeria; zakari.ladan@kasu.edu.ng
[3] Institute of Chemical and Biotechnology, Vaal University of Technology, Southern Gauteng Science and Technology Park, Private Bag X021, Vanderbijlpark 1911, South Africa; fanyana@vut.ac.za
[4] Department of Biological Sciences, Faculty of Science, Kaduna State University, Tafawa Balewa Way, Kaduna 800283, Kaduna State, Nigeria; yayock.hosea@kasu.edu.ng
* Correspondence: okolibj@binghamuni.edu.ng; Tel.: +234-27767619418

Simple Summary: Malaria fever kills millions of people annually in the tropical and subtropical countries of Africa and Asia. Because there is no effective vaccine, malaria prevention is exclusively dependent on avoiding human-vector interaction. The interaction of *Vitex negundo* essential oil constituents with *Anopheles gambiae* Odorant Binding Proteins (OBP), as well as its compositional variation, repellent efficacy, and toxicity profile, are investigated in this work. The oils were subjected to GC-MS analysis, a mosquito behavioral test, OBP-ligand interactions, *Anopheles* species authentication, and toxicity profile. Docking protocol validation was achieved by redocking the co-crystallized ligands and root mean square deviation (RMSD) calculation. The oil yields and compositions are climate–soil dependent with ≈71.39% monoterpenes and ≈16.32% sesquiterpene. Optimal repellency is achieved at 15 min at ED_{50} 0.08–0.48% *v*/*v* while the RMSD was estimated to be within 0.24–1.35 Å. Strong affinities, −6.4 to −5.4 kcal/mol, were demonstrated by α-pinene, citronellal, linalool, and myrcene for OBP1, OBP7, OBP4, and OBP. respectively. The hydrophobic interactions involve Leu17, Cys35, ALA52, Leu73, Leu76, Ala88, Met91, Lys93, Trp114, Phe123, and Leu124 receptors on α-helixes 1–7 within the binding cavities, and may block the olfactory receptors resulting in disorientation. α-pinene, linalool, and myrcene are safe and suitable for use in the development of green and innovative repellents because their ligand efficiency metrics, ADME/tox, and repellency screening are all within the threshold values.

Abstract: (1) Background: Malaria fever affects millions of people yearly in Africa and Asia's tropical and subtropical areas. Because there is no effective vaccine, malaria prevention is solely dependent on avoiding human-vector interaction. (2) Aim: This study examines the interaction between the constituents of *Vitex negundo* essential oil and *Anopheles gambiae* Odorant Binding Proteins (OBP) as well as the compositional variation, repellent efficacy, and toxicity profile. (3) Methods: The oils were subjected to GC-MS and mosquito behavioral analysis. OBP–ligand interactions, *Anopheles* species authentication, and the toxicity profile were determined by molecular docking, PCR assay and in silico ADME/tox tool. Docking protocol validation was achieved by redocking the co-crystallized ligands into the protein binding pocket and root mean square deviation (RMSD) calculation. (4) Results: The oil yields and compositions are climate–soil dependent with ≈71.39% monoterpenes and ≈16.32% sesquiterpene. Optimal repellency is achieved at 15 min at ED_{50} 0.08–0.48% *v*/*v* while the RMSD was estimated to be within 0.24–1.35 Å. Strong affinities were demonstrated by α-pinene (−6.4 kcal/mol), citronellal (−5.5 kcal/mol), linalool (−5.4 kcal/mol), and myrcene (−5.8 kcal/mol) for OBP1, OBP7, OBP4, and OBP; respectively. The hydrophobic interactions involve Leu17 (α-helix 1), Cys35 (α-helix 2), ALA52 (α-helix 3), Leu73, Leu76(α-helix 4), Ala88, Met91, Lys93, Trp114 (α-helix 5), Phe123 (α-helix 6), and Leu124 (α-helix 7) receptors within

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