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*Abstract*

# Molecular Docking Studies of Antimalarial Compounds from the Acetonic Extract of *Cecropia obtusifolia* †

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**Abstract:** Malaria is a disease that affects many people in the world. In Mexico, malaria is still a disease with active zones, especially in the states of Chiapas and southern Chihuahua where several communities are affected year after year. According to previous studies, a moderate antimalarial effect has been attributed to some *Cecropia* species in several countries, such as Brazil, Panama, and Colombia. To date in Mexico, no studies have evaluated the possible antimalarial activity of *Cecropia Obtisifolia* Bertol. The objective of the present study was to identify the main metabolites present in the acetonic extract of *C. Obtusifolia* and to evaluate their possible antimalarial activity in silico analysis. An acetonic extraction of *C. Obtusifolia* leaves was performed using Thin-Layer Chromatography (TLC) and high performance liquid chromatography HPLC, and the main compounds were identified. The identified compounds were evaluated with specific molecular docking studies using four different malarial targets with the PDB codes 1CET, 1PZ4, 2BL9, and 4ZL4; the evaluation was performed using AutodockVina and visualized using LigPlot and PyMOL. From the acetone extract, the compounds were found to be ursolic acid, α-amyrin, chrysin, and isoorientin using TLC and HPLC. The docking studies showed that the ligands docked well with the targets, resulting in the following strongest binding energies between the ligands and the targets (kcal/mol): isoorientin–1CET (−9.1), chrysin–1PZ4 (9.6 kcal/mol), isoorientin–2BL9 (−8.8), and chrysin–4ZL4 (−9.6). These binding affinities were stronger than the control ligands. An analysis of the results suggests that isoorientin and chrysin could act as anti-malarial agents.

**Keywords:** malaria; *Cecropia obtusifolia*; molecular docking; ethnopharmacology; anopheles; Plasmodium; acetona extract



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