

ABSTRACT

MUHAMAD FAHRI. 2025. ***IN SILICO* ANALYSIS OF *Andrographis paniculata* (BURM. F.) WALL. EX NEES) AS A POTENTIAL ANTIMALARIAL AGENT FOR SUPPLEMENTARY BIOLOGY TEACHING SUPPLEMENT.** Department of Biology Education, Faculty of Teacher and Education, Siliwangi University, Tasikmalaya

Andrographis paniculata, a member of the Acanthaceae family, commonly known as “Sambiloto” or “King of Bitters,” has long been used in traditional Oriental and Ayurvedic medicine. The public believes that the decoction of *A. paniculata* leaves serves as an herbal remedy for malaria. This study aims to analyze the antimalarial potential of *A. paniculata* through an in silico molecular docking approach. The research was conducted from March to June. Compounds from *A. paniculata* were extracted using the maceration method with ethyl acetate as the solvent. The selection of leaves was based on the dominance of active compounds, such as terpenoids, alkaloids, and phenolic compounds in that part. The extraction results were tested using Gas Chromatography - Mass Spectrometry (GC-MS). A total of 59 compounds were identified. These compounds were screened based on literature, thereby reducing them to 8 secondary metabolite compounds that have potential as antimalarial agents, including squalene, beta-sitosterol, stigmasterol, dasycarpidan-1-methanol, (E)-Labda-8(17),12-diene-15,16-dial, isosteviol methyl ester, retinoic acid, and dl- α -tocopherol. The eight compounds were analyzed against the *Plasmodium falciparum* aminopeptidase M1 (PfA-M1) receptor (PDB ID: 4ZW6), with compound 9q as the control ligand. The results showed that all test compounds had affinity for PfA-M1 with the best binding affinity value shown by stigmasterol (-9.6 kcal/mol), exceeding the PfA-M1 control ligand (-9.1 kcal/mol). All test compounds met Lipinski's criteria, showed good pharmacokinetic properties, and exhibited relatively safe toxicity profiles (stigmasterol class 4; others class 4 and 5), thus meeting the requirements as oral drugs. The research results will be compiled in the form of a booklet as a supplement teaching material for Bioinformatics courses.

Keywords: Antimalaria; *A. Paniculata*; Secondary Metabolites Compound; PfA-M1 Receptor