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Abstract

Bioinformatics approaches for molecular characterization and structural elucidation of a hypothetical protein of *Aedes albopictus* †

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Abstract: The most critical issues in computational biology are characterizing and predicting uncharacterized proteins' secondary and tertiary structures from their uploaded amino acid sequences in databases. *Aedes albopictus*, sometimes referred to as the Asian tiger mosquito or forest mosquito and the carrier of dengue-like diseases, has many proteins, many of which are still poorly understood. The current work aimed to elucidate the physicochemical properties and structures of the as-yet-uncharacterized *Aedes albopictus* protein AEW48448.1. ExPASy Protparam, CD Search, SOPMA, PSIPRED, and other advanced computerized tools were used following the standard flowchart for characterizing a hypothetical protein to ascertain the roles and structures of AEW48448.1. After identifying the protein's secondary and tertiary structures, the structures were evaluated for quality using tools like PROCHECK and the ProSA-web. Later, the active site was also discovered using CASTp v3.0. The protein is more stable because it has a higher aliphatic index value and more negatively charged residues than positively charged. Multiple bioinformatics tools' modeling of the proteins' 2D and 3D structures confirmed that they had domains, indicating that they were functional proteins with the host's antiviral, cytokine, and interferon production pathways. Additionally, the protein was revealed to have active regions where ligands may bind. The work aimed to elucidate the characteristics and structures of an uncharacterized *Aedes albopictus* protein that may serve as a therapeutic target for creating antiviral candidates and vaccines.

Keywords: *Aedes albopictus*; functional annotation; protein-protein interactions; molecular characterization

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