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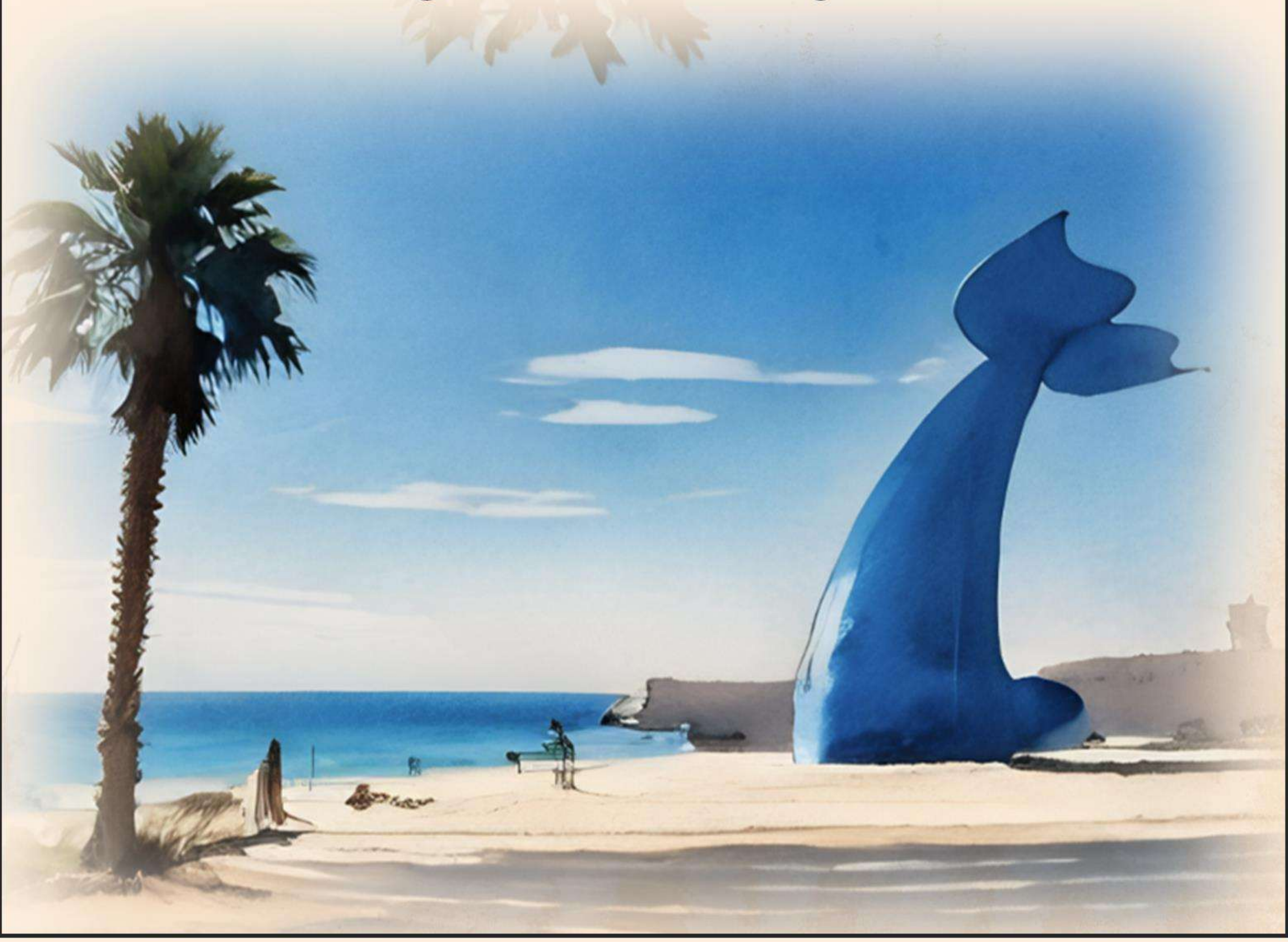

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Poster 42

Computational Insights into the Impact of Non-Synonymous Mutations in the ABC Transporter Gene of *Apis mellifera*

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Non-synonymous mutations lead to amino acid substitutions that can affect a protein's structure and function, thereby influencing biological processes such as detoxification. ATP-binding cassette (ABC) transporters (an important superfamily of detoxification genes) play a critical role in the efflux of toxic compounds in honey bees (*Apis mellifera*), essential for their survival in environments exposed to natural and synthetic xenobiotics. In this study, non-synonymous mutations in 21 ABC transporter genes were identified. Then, computational tools were employed to investigate the structural and functional consequences of a non-synonymous mutation in the protein encoded by the ABC transporter gene LOC411997. Protein structures were generated from a FASTA file using AlphaFold3, converted from mmCIF to PDB format, and visualised in PyMOL, where mutations were introduced. Functional site predictions were performed using Proteins Plus, and molecular dynamics simulations were conducted in YASARA to assess stability and conformational changes. Our findings suggest that a mutation that replaces threonine with isoleucine alters the protein dynamics by modifying its energy landscape and stability. The total potential energy of the wild-type protein was calculated as -3,640,842 kcal/mol. In contrast, this value increased to -3,443,695 kcal/mol for the mutant protein. This difference suggests that the mutation may affect conformation, flexibility, and biological function of the protein encoded by the ABC transporter gene LOC411997. Understanding these conformational changes at the molecular level will contribute to strategies for improving honey bee's resilience and conservation.