Digital Defense: Using Molecular Docking to Combat the Mountain Pine Beetle Epidemic in North American Forests

Paliwal, Aayush (School: Pine Creek High School)

The ongoing outbreak of the Mountain Pine Beetle (Dendroctonus ponderosae) has caused the destruction of 125 million acres of pine forests across North America, increasing wildfire risk and releasing megatons of carbon dioxide as dead trees decay. Under normal conditions, these beetles help maintain forest health by targeting older trees. However, current overpopulation has led to widespread infestation of pine trees of all ages. This project aims to identify a natural, non-lethal inhibitor of the beetle's Cytochrome P450 enzyme, which is important for breaking down the host tree's defenses. A group of nine phytochemicals were selected based on structural similarity to P450's substrate and their medical and therapeutic properties. Molecular docking was performed to evaluate binding affinity (kcal/mol) using Autodock Vina. The results showed that apigenin had the strongest binding affinity, with a score of -8.3 kcal/mol, suggesting it may act as a competitive inhibitor of Cytochrome P450. This could limit the beetle's ability to process chemicals produced by pine trees, reducing damage to the forest. These findings show a promising, natural approach to reducing the impact of Mountain Pine Beetle infestations without disrupting the ecosystem. With further testing, this strategy could help protect forests, sustain the Pine Beetle population at an ideal number, lower wildfire risk, and reduce carbon emissions on a larger scale.

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