Molecular Insights Into M.L.C.E Larvicide: Garcinia mangostana Pericarp and Citrus aurantifolia Leaves Combined Extracts as a Novel Natural Larvicide for Aedes aegypti Larvae

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Aedes aegypti is a mosquito species that transmit diseases, including dengue fever, Zika virus and chikungunya. The control of A. aegypti populations is essential to prevent the spread of these diseases. However, the current mosquito control involving synthetic chemicals may lead to negative impact to the environment, plus the larvae might have increased resistance towards the chemicals. Previously, M.L.C.E Larvicide is developed towards A. aegypti larvae, by combining Garcinia mangostana pericarp extract and Citrus aurantifolia leaves extract. The exposure to M.L.C.E Larvicide caused significant behavioural changes of larvae, thus leading to larval inactivation and death. This study aims to explore its underlying mechanism of action through molecular docking and binding affinity studies with key target proteins in the larvae, such as Sterol Carrier Protein-2 (SCP2), Glutathione S-transferases (GST), and trypsin. The bioactive compounds from both plant extracts exhibited strong binding affinities, with Copaene from G. mangostana pericarp extract showing a binding affinity of -9.6 kcal/mol to SCP-2 and Beta-eudesmol from C. aurantifolia leaves extract showing -8.1 kcal/mol to acetylcholinesterase. These results could explain the morphological alterations of treated larvae in previous experiments. In short, M.L.C.E Larvicide demonstrates the potential as a promising, environmentally friendly and natural alternative to synthetic chemical larvicides for A. aegypti control, offering a sustainable solution to combat vector-borne diseases. At the same time, it can also contribute to Sustainable Development Goal, particularly No. 3 Good Health and Well-Being and World Health Organization Road map for Neglected Tropical Diseases 2021-2030.

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