

Biochemical Efficacy, Molecular Docking and Inhibitory Effect of 2,3-Dimethylmaleic Anhydride on Acetylcholinesterases

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Abstract : Evolution has caused many insects to develop resistance to several synthetic insecticides. This problem along with the persisting concern regarding the health and environmental safety issues of the existing synthetic insecticides has urged the scientific fraternity to look for a new plant-based natural insecticide with inherent eco-friendly nature. *Colocasia esculenta* var. *esculenta* (L.) Schott (Araceae family) is widely grown throughout the South- East Asian Countries for its edible corms and leaves. Various physico-chemical and spectroscopic techniques (IR, ¹H NMR, ¹³C NMR and Mass) were used for the isolation and characterization of isolated bioactive molecule named 2, 3-dimethylmaleic anhydride (3, 4-dimethyl-2, 5-furandione). This compound was found to be highly toxic, even at low concentration, against several storage grain pests when used as biofumigant. Experimental studies on the mode of action of 2, 3-dimethylmaleic anhydride revealed that the biofumigant act as inhibitor of acetylcholinesterase enzyme in cockroach and stored grain insects. The knockdown activity of bioactive compound is concurrent with in vivo inhibition of AChE; at KD99 dosage of bioactive molecule showed more than 90% inhibition of AChE activity in test insects. The molecule proved to affect the antioxidant enzyme system; superoxide dismutase (SOD), and catalase (CAT) and also found to decrease reduced glutathione (GSH) level in the treated insects. The above results indicate involvement of inhibition of AChE activity and oxidative imbalance as the potential mode of action of 2, 3-dimethylmaleic anhydride. In addition, the study reveals computational docking programs elaborate the possible interaction of 2, 3-dimethylmaleic anhydride with enzyme acetylcholinesterase (AChE) of *Periplaneta americana*. Finally, the results represent that toxicity of 2, 3-dimethylmaleic anhydride might be associated with inhibition of AChE activity and oxidative imbalance.

Keywords : 2,3-dimethylmaleic anhydride, *Colocasia esculenta* var. *esculenta* (L.) Schott, Biofumigant, acetylcholinesterase, antioxidant enzyme, molecular docking

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