AFLATOXINS INHIBITORY MECHANISM OF *ASPERGILLUS PARASITICUS* USING BIOINFORMATICS

BY

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ABSTRACT

Natural inhibition of toxins, pesticides and carcinogenic components is currently global scope to protect the environment. There are many challenges for fighting many problems confronting human, animals, plants and even microorganisms. At the interface between agriculture and nutrition, the aflatoxin contamination of food and feed touches on agriculture, health and economy. For more than three decades aflatoxin problems have been researched in Africa. The diversity of aflatoxin structures induces various toxic effects in human, animal, poultry, fish and plants. The main fungi that produce aflatoxins are *Aspergillus parasiticus* and *Aspergillus flavus*, which are numerous in warm and humid regions of the world. Aflatoxins are the most carcinogenic naturally occurring compounds which make worth complications on health, including hepatocellular carcinoma, acute intoxication, immune system disorder and growth retardation in children. Therefore, aflatoxin contamination is a global threat to human and animal health. Finding solution for aflatoxin inhibition is one of the key safety indexes for health and agriculture. The aim of this study was to find an essential enzyme in aflatoxin biosynthesis pathway in *Aspergillus* species and using some bioinformatics tools to inhibit this enzyme by using natural components. The *in silico* docking technique is one of the most applicable tools used in enzyme inhibition. In this investigation, about 700 natural compounds were examined, analogized and docked to examine their ability for inhibiting the most effective three domains (Acyl Carrier protein (ACP), product template (PT) and thioesterase

(TE)) in polyketide synthesis enzyme which is representing the backbone of aflatoxin pathway biosynthesis. About forty natural components showed the best results with the three domains which attached to the active sites for the three domains, and gave the best results including the lowest binding energy and the best chemical interactions. From the docking results, the top ten natural components from each domain were analyzed and examined for their toxicity. Finally, the three natural compounds gave the best docking results; bromodeoxytopsentin which gave binding energy reached to -9 and two covalent hydrogen bond interactions with ACP domain, kraussianone 6 which gave binding energy reached to -11.2 and two covalent hydrogen bond interactions with PT domain and pinocembrin which gave binding energy reached to -7.3 and one covalent hydrogen bond interactions with TE domain.

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