Assessment the lethal dosage of bacterial toxins for designing a series of novel immunotoxins

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Abstract:

Cancer which is the result of unusual growth of abnormal cell and the extension of them to other parts of the body, considered as the major challenges of health in human societies. These kinds of diseases could be diagnosed, prevented as well as treated via various methods, especially with molecular approaches. In this regard, development the novel anti-cancer drugs such as immunotoxins, with the capability to targeted transmission of the bacterial and nonbacterial toxins to the cancer cells are a new approach. Bearing in mind, an investigation on the potent toxins, their structure and functions as well as on lethal doses could be providing suitable approaches for immunotoxins designing, which are considered in this study. In this regard, a profile of pore forming as well as disruptive protein synthesis of the bacterial toxins was collected, and effective dosage of them was determined. The selective sequences were retrieved from NCBI, EMBL and Uniprot databanks and then were analyzed with CDSearch and Motifscan for detection structural and functional features of them. 3D structures of selected sequences were retrieved from PDB and Pubchem and or modeled via Modeller program. Cluspro and PatchDock were used to evaluate the binding affinity of toxins to the ratio of lethal dosage. In general, the results of this study led to reveal various toxins with a variety of mechanism, including Alpha, aerolysin, Beta, leukotoxin, LF, Microcin, Hemolysin, pvl, vvc, vacA, shiga, Verotoxin, Diftheria toxin, Exotoxin A, CPE, distending toxin, Hdcdt with different effective dose ranging from 2ng/ml up to 25µg/ml belonging to Beta toxin of *Clostridium perfringens* and Exotoxin of *Streptococcus pyogenes*, respectively. Moreover, led to introduce a series of effective domains with the capability of designing of the novel immunotoxins.

Keywords

Cancer, immunotoxin, toxin, effective dosage, *In-silico* biology