



An *in-silico* investigation into the bacterial exotoxins affecting cell death for designing a new generation of anti-cancer drugs

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Abstract:

Statistical information about the incidence of cancer malignancies, reminded a high degree of importance in providing innovative approaches for diagnosis, prevention and treatment of these type of disease. In this regard, targeting cancerous cells with bacterial and non-bacterial toxins which are termed immunotoxin, leading to the opening of a new window in the field of cancer target therapy. Accordingly, designing, development and evaluation a new generation of immunotoxins were considered in this study based on *in-silico* survey. In this regard, a profile of bacteria exotoxins with the ability to induce cell death (CDTs) via cell cycle disruption was collected. Subsequently, these toxins were evaluated based on analyzed the affecting molecular mechanisms of them in cell death and effective dosage. Moreover, NCBI, BLAST, PatchDock, MEGA6, Pymol, Swissmodel, Interproscan, Sulfinator, NetPhos and NetNGlyc programs and databank were used for assessment the structure, function as well as homologues sequences of selected toxins. The results of the structural evaluation of the sequences led to reveal physicochemical properties of them as well as endonuclease-conserved domains in some toxins derived of genus of the bacteria including *Escherichia*, *Haemophilus*, *Aggregatibacter* and *Shigella*. On the other hand, the analysis of Cycle inhibiting factor (CIF) did not reveal any conserved domains in *Yersinia* and *Escherichia* as well as in homologues strains of the bacteria. Moreover, some CDTs showed high potential for induction death in cancerous cells with suitable domains in length, immunogenicity and binding affinity to targets that are considering for immunotoxins designing in our group.

Keywords:

Cancer, toxin, domain, immunotoxin, *In-silico* investigation

