



Designing and evaluation a new generation of the effective immunotoxins for sarcoma based on *in-silico* Investigation

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Immunotoxins therapy is among the promising prospects for the treatment of cancer diseases based on detection the cancerous cells surface specific antigens (SCSAs) as well as on the using of toxins that are derived from bacterial and non-bacterial microorganisms. Bearing in mind, a thorough understanding of the structural and functional characteristics of these toxins and specific antigens of the cancer cells as well as corresponding ligands will be provided a new generation of immunotoxins that has been considered for sarcomas in this study. In this regard, SCSAs of the sarcoma and corresponding ligands were gathered. Selected sequences were retrieved from corresponding databases. Virtual measurement of the expression of the selective antigens was determined by ProteinAtlas. Host range of the selective toxins and relationship of them were performed by Blast and MEGA6 programs, respectively. CD Search and Motif Scan were then applied with the aim of detection of the structural and functional properties of the protein sequences. Furthermore, structural modeling was carried out via Modeller program. Cluspro and PatchDock programs were applied for binding affinity assessment. Subsequently, assembling the selected domains; 3D structure as well as immunogenic properties of designed constructs were performed and then considered for codon optimization and virtual expression. Generally, the results of this study lead to introduce some strains of the bacteria with efficient toxins, capable domains within the Diphtheria, high efficiency of the IL2 for targeting a wide range of malignancies as well as a new immunotoxin construct with suitable in structure and function properties, named as P-DT-(GGGS)3-H- IL2.

