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Structural And Functional Optimization Of SS1P
Based On In-Silico Simulation

Sara Malekzadeh

Chairman, NCCP
Dr. M. Taghi Mirahmadi

Scientific Chair(Basic)
Dr. M. R. Abbaszadegan

Scientific Chair(Clinical)
Dr. A. Allahyari

Nastaran Center for Cancer Prevention

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Structural And Functional Optimization Of SS1P Based On In-Silico Simulation

1. **Sara Malekzadeh** (Department Of Biology, Payam Noor University Of Mashhad, Mashhad, Iran)
2. **Aliakbar Haddad-Mashadrizeh** (Cell And Molecular Biotechnology Research Group, Institute Of Biotechnology, And Department Of Biology, Faculty Of Science, Ferdowsi University Of Mashhad, Mashhad, Iran)
3. **Majid Rajabiyan Noghondar** (Department Of Biology, Payam Noor University, Tehran, Iran)

Abstract

Immunotoxin (IT) therapy is promising approach for targeted cancer therapy with the minimal side effects. These types of drugs are chimeric proteins with two main parts including death and ligand domains. Accordingly, structural and functional characterization of these types of drugs, based on in-silico simulation, could be providing suitable context for optimization as well as innovation in common immunotoxins. Bearing in mind, structural optimization of SS1P immunotoxin was considered in this study. In this regard, the protein sequence of the SS1P was retrieved from corresponding database such as Google patent. Structural characterization of the immunotoxin was performed via Intrproscan5 and Blast programs. On the other hand, the protein sequence of the mesothelin as specific target of this drug was retrieved from NCBI databank. MODELLER9.15 were used for structural modeling of the sequences. PROTEINATLAS database were used for assessment the expression of the antigen. Furthermore, HADDOCK were used for evaluation the binding affinity. Finally, all statistical analysis were expressed with SPSS 21.0 (SPSS Inc., Chicago, IL, USA). The results of the sequence characterization of the SS1P lead to obvious two main parts in the sequence context including dsfv and PE which are linked to each other with G2S1. Moreover, the structure stability of the protein were confirmed after simulation under 300°K, 100ps of the time for NVT and NPT steps and 20000ps (20ns) for MD step. On the other hand, molecular docking of the mesothelin to the modeled IT as well as optimized IT were confirmed after simulation. Taken together, the results of the present study provide in-silico approaches for optimization as well as innovation in the common sequence context of its for novelty in drugs design.

Corresponding Author: Aliakbar Haddad-Mashadrizeh (Cell and Molecular Biotechnology Research Group, Institute of Biotechnology, and Department of Biology, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran)