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In the Name of God

This is to certify that Mohammad Fatehi abdol abadi

Presented the poster entitled " AN INVESTIGATION ON THE STABILITY OF THE CATALYTIC DOMAIN OF DIPHTHERIA TOXIN IN SEPARATED SITUATION " at the 17th International & Iranian Congress of Microbiology , Tehran, Iran, 23-25 August 2016

Dr. Abbas Ali Imami Fooladi
Imami Fooladi
Executive Secretary

Dr. Pejvak Khaki
Khaki
Scientific Secretary

**P124 - 933: AN INVESTIGATION ON THE STABILITY OF THE CATALYTIC DOMAIN OF
DIPHTHERIA TOXIN IN SEPARATED SITUATION**

Mohammad Fatehi abdol abadi¹, Aliakbar Haddad-Mashadrizeh², Jafar Saeidi³

1. Department of Biology, Science and Research branch, Islamic Azad University, Khorasan Razavi, Neyshabur, Iran
2. Cell and Molecular Biotechnology Research Group, Institute of Biotechnology, Ferdowsi University of Mashhad, Mashhad, Iran and Department of Biology, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran
3. Department of Biology, Science and Research branch, Islamic Azad University, Khorasan Razavi, Neyshabur, Iran

Background and Aim: Diphtheria toxin, as a critical therapeutic factor in immunotoxins development, is consisting of two parts A and B. The A fragment is containing the active site of this toxin, which are considered in this study for the evaluation the stability of it in separated situation.

Methods: At the first step, 3D structure of the toxin with the ID: 1XTD was retrieved from PDB. Discovery Studio3.0 Client was used for removing the water molecules, ligands and catalytic domain from the intact toxin. Simulation of catalytic domain compared to intact diphtheria toxin, were performed using GROMACS5.07, gromos96 43a1 force field. It was performed in 310°K for NVT, NPT, MD; and 2ns of time for MD step. RMSD and RMSF plots were drawn by excel. Moreover, the alignment structures of the catalytic domain and intact toxin were shown by Pymol software.

Results: The result of RMSF plot indicate that the about 11% of the amino acids of the catalytic domain is more than of them in the native structure. On the other hand, this plot showed that the differences in the RMSF values for about 15 amino acids is greater than 0.1. More analysis demonstrate that the RMSF values of five amino acid from six of them, which are situated in the active site of the catalytic domain, are less than of them in the intact toxin.

Conclusion: In general, the results of this investigation indicate that the stability of the catalytic domain as well as active site, in separated form, is more than of them in intact toxin.

Keywords: DiphtheriaToxin, Therapeutic factor, Catalytic domain, Active site, GROMACS-5.0.7