Interaction Between TNF and SVMPs of PI Class: Molecular Modeling and Docking at a Glance

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Abstract

TNF (Tumor Necrosis Factor) produced mainly by monocytes, is a proinflammatory cytokine that plays an important role in modulating inflammatory responses and host defense mechanisms. At increased levels such cytosine is closely related to degenerative diseases such as rheumatoid arthritis. Metalloproteases are enzymes characterized by their zinc catalytic structure at their active site, snake venom metalloproteases (SVMPs) are responsible for inducing haemorrhage and disturbances in the prey blood coagulation cascade. However, certain SVMPs do not have hemorrhagic activity (PI class SVMPs), thus having effects such as inhibition of platelet aggregation, apoptosis induction and pro anti-inflammatory activities. Previous studies carried out in silico and in vitro with the enzyme BmooMP-alpha-I isolated from snake venom Bothrops moojeni a metalloprotease class PI have demonstrated its ability to directly inhibit TNF in immunopathologies like colitis.The aim of this study is to perform in silico studies to elucidate the interaction between tumor necrosis factor and metalloproteases class PI present in snake venom. For this will be carried out protein-protein interaction dockings of TNF and SVMPs, structural alignments and molecular modeling will be performed. As result, it is expected to be obtained Ligand Root Mean Square Deviation LRMS = 5.0 or Interactive Root Mean Square Deviation IRMS = 2.0 . At the end of this project we hope to contribute to the understanding of the interaction between TNF and SVMPS class PI and their therapeutic applications.

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