OMICS Group Conferences
Accelerating Scientific Discovery

World Congress on
Biotechnology

BIOTECHNOLOGY-2011
doi:10.4172/jpb.1000240

Structural analysis of ES-31 serine protease from *Mycobacterium tuberculosis* by using bioinformatic tools

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Mycobacterium tuberculosis is an intracellular pathogen, occuring in macrophages of host & persists there for a long time. In general, external proteases in bacteria are associated with bacterial pathogenic virulence, however little information is available on *M. tuberculosis* secreted proteins. A diagnostically important secreted antigen, Excretory Secretory-31(TB ES-31) with serine protease activity was isolated from different *M. tuberculosis* strains culture filtrate. It is reported that catalytic triad is similar both in serine protease and some lipase enzymes. To confirm whether the active site of ES-31 serine protease and ES-31 of lipase is same or not; its inhibition of serine protease activity by lipase inhibitor and inhibition of lipase activity by serine metallo-protease inhibitors has to confirm. Some lipases use the same catalytic triad as that of serine protease and also hydrolyze ester bond by same mechanism. Previous studies had shown that ES-31 is highly sensitive to commercial anti obesity drug Orlistat for both serine protease and lipase activity and thus orlistat can be used to inhibit the action of ES-31. Orlistat binds to the active site of pancreatic lipase,which leads to some conformational changes and abolish its activity.The exact mechanism can be studied using bioinformatics tools.

After purifying the enzyme the sequences and molecular weight can be determend using mass spectrometry,and then the sequences we will built a homology model of ES-31.. In order to validate the sequence-structure alignment, to remove bad contacts derived from homology modelling and to achieve a good starting structure, the model was subjected to exhaustive molecular dynamics simulation with software. Furthur the model quality can be assessed by the geometric quality of backbone conformation, the residues interaction, the residue contact and the energy profile of the structures using various bioinformatic tools. To evaluate the predictive ability of the *M. tuberculosis* ES-31 homology model and its suitability for use in the structure based drug designing a docking study was conducted. As stated ES-31 can be inhibited by Orlistat, in the present studies docking studies can be very useful to gain insights into the most probable binding conformation of ES-31 with Orlistat. In conclusion these results may help in the understanding of the mechanism of action of *M. tuberculosis* ES-31 antigen. Further it will provide information about more improved selective ES-31 antigen blockers for the treatment of tuberculosis disease.