T Jebasingh, J Proteomics Bioinform 2015, 8:8
http://dx.doi.org/10.4172/0974-276X.S1.077

OMICS International
conferenceseries.com

5th International Conference on
Proteomics & Bioinformatics
September 01-03, 2015 Valencia, Spain

In silico design of drug and vaccine for leptospirosis

T Jebasingh
Madurai Kamaraj University, India

Leptospirosis is a worldwide zoonotic disease caused by the gram-negative spirochete *Leptospira*. During its course of infection, it causes multi-organ complications. In the current study, the membrane protein (LipL32) and collagenase of *Leptospira* were analyzed *in silico* to design a vaccine and a drug for leptospirosis. The available vaccines against leptospirosis are of limited use because of their low efficacy, inability to induce long term protection and cross protection against the different serovars of pathogenic *Leptospira*. Four sequential and conformational B-cell epitopes from the crystal structure of LipL32of *Leptospira interrogans* serovar Copenhageni str. Fiocruz L1-130 were mapped by using *in silico* tools like IEDB Elipro, ABCpred and BCPRED and VaxiJen servers. The structure of Cardamom Mosaic Virus (CdMV) was predicted and used as a platform to display the predicted epitopes of LipL32 at C, N and both the termini. Based on the type of amino acids, length, surface accessibility and docking energy with CdMVCP model, the epitope 1 displayed at the N-terminus of CdMV CP was predicted to be a promising vaccine candidate when compared to other epitopes displayed at the C-terminus or at both the termini. Collagenase, an extracellular protease plays a pivotal role in pathogenesis of *Leptospira* during invasion by degrading the host collagen fibers in the extracellular matrix. The model of *Leptopsira* collagenase was built by threading method with the crystal structure of collagenase and further refined by SPDB viewer and 3Drefine. Three ligand binding sites of collagenase at N-terminus, catalytic site and C-terminus were predicted by Metapocket server. Among sixty seven inhibitors for collagenase fetched from the ChEBI and Zinc databases, Protohypericin which binds at the catalytic site was predicted to be the best inhibitor for *Leptospira*l collagenase. Hence protohypericin can be used as a potential candidate drug to combat the disease progression in leptospirosis.

Biography

T Jebasingh has completed his PhD from Madurai Kamaraj University, India and Post-doctoral studies from Weizmann Institute of Sciences, Israel. He is currently working as assistant professor at School of Biological Sciences, Madurai Kamaraj University. His research is focused to develop vaccine for leptospirosis and to unravel the role of proteases in invasion of *Leptospira*. He has published nearly 10 papers in reputed journals.

jebasinghs@gmail.com

Notes: