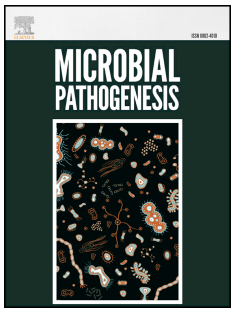
Accepted Manuscript



An *in silico* study: Novel targets for potential drug and vaccine design against drug resistant *H. pylori*

Pasala Chiranjeevi, Chilamakuri Chandra Sekhar Reddy, Katari Sudheer Kumar, Nalamolu Ravina Madhulitha, Aparna R. Bitla, Amineni Umamaheswari

PII: S0882-4010(17)30890-2

DOI: 10.1016/j.micpath.2018.05.037

Reference: YMPAT 2976

To appear in: *Microbial Pathogenesis*

Received Date: 21 July 2017

Revised Date: 19 May 2018

Accepted Date: 22 May 2018

Please cite this article as: Chiranjeevi P, Reddy CCS, Kumar KS, Madhulitha NR, Bitla AR, Umamaheswari A, An *in silico* study: Novel targets for potential drug and vaccine design against drug resistant *H. pylori*, *Microbial Pathogenesis* (2018), doi: 10.1016/j.micpath.2018.05.037.

An *in silico* study: Novel targets for potential drug and vaccine design against drug resistant *H. pylori*

Pasala Chiranjeevi[1], Chilamakuri Chandra Sekhar Reddy [2], Katari Sudheer Kumar[1], Nalamolu Ravina Madhulitha[1], Aparna R. Bitla[3] and Amineni Umamaheswari*[1]

[1]Bioinformatics Centre, Department of Bioinformatics, SVIMS University, Tirupati-517507, India

[2]Cancer Research UK Cambridge Institute, University of Cambridge, Cambridge, CB2 0RE, UK

[3]Department of Biochemistry, SVIMS University, Tirupati-517507, (A.P), India

[1]*Corresponding author: Tel: 0877-2287727; E-mail: svims.btisnet@nic.in

Abstract

Gastric cancer risk and adverse ramifications by augmented multi-drug resistance (MDR) of *Helicobacter pylori* are alarming serious health concern. Combating through available drugs is a difficult task due to lack of appropriate common targets against genetically diverse strains. To improve efficacy, the effective targets should be identified and critically assessed. In the present study, we aim to predict the potential novel targets against *H. pylori* strains by employing computer aided approach. The genomic dataset of 53 *H. pylori* strains was comparatively processed and eventually predicted 826 'conserved gene products'. Further, we performed subtractive genomic approach in search of promising crucial targets through the combination of *in silico* analyses. Codon adaptation index (CAI) value calculation and literature surveys were also done in order to find highly expressed gene products with novelty. Consequently, four enzymes and three membrane proteins were prioritized as new therapeutic and vaccine targets respectively which found to have more interactors in network with high-confidence score, druggability, antigenicity and molecular weight <110 kDa. Therefore, our results underpin the importance of new targets may counteract with false–positive / negatives and facilitate appropriate potential targets for a new insight of reliable therapeutic development.

Keywords *H. pylori*, common proteins, metabolic pathways, network analysis, druggability, therapeutic targets.

Abbreviations

CAI: Codon adaptation index; CELLO: subCELlular LOcalization predictor; COGdb: Cluster of orthologous groups database; CP: chokepoint proteins; DEG: Database of Essential Genes;