#### **MAJOR PROJECT REPORT**

# ASSESSMENT OF SMALL MOLECULE BINDING POCKETS OF Clostridium perfringens

Submitted by NEELAKSHI SAINI 09/BINF/2010 M.Tech BioInformatics, 4<sup>th</sup> semester

SUBMITTED IN PARTIAL FULFILLMENT OF THE AWARD OF DEGREE OF

#### MASTER OF TECHNOLOGY IN BIOINFORMATICS



## DEPARTMENT OF BIOTECHNOLOGY DELHI TECHNOLOGICAL UNIVERSITY (FORMERLY DELHI COLLEGE OF ENGINEERING)

### Certificate

This is to certify that the project entitled – "ASSESSMENT OF SMALL MOLECULE BINDING POCKETS OF *Clostridium perfringens*" has been carried out by *Ms. Neelakshi Saini* at the Department of Biotechnology, Delhi Technological University, (formerly Delhi College of Engineering), Delhi in partial fulfilment for the degree of Master of Technology in Bioinformatics from Delhi Technological University, (formerly Delhi College of Engineering), Delhi.

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#### Declaration

I *Neelakshi Saini*, M.Tech Bioinformatics student hereby declare that the project entitled *"ASSESSMENT OF SMALL MOLECULE BINDING POCKETS OF Clostridium perfringens"* submitted for the partial fulfilment of the degree Master of Technology in Bioinformatics is a record work done by me, during the period Jan, 2012 - June, 2012 and has not formed the basis for the award of any Degree or other similar titles under any University in India or Abroad.

Neelakshi Saini

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#### ABSTRACT

Here we report a study that focuses on methodology for assessing the Drugability of all small-molecule binding pockets in a pathogen *Clostridium perfringens*. The approach incorporates accurate pocket identification, sequence conservation with host as well as similar organism and structure resolution. The method was applied to 15 structures from pathogen *Clostridium perfringens* as a result around 71 appropriate pockets were identified, which were then scored and ranked. About 6 new targets were identified, which further need to be analysed for their Drugability potential.

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