

**NOVEL APPROACH TO TARGET PERIODONTITIS
AND ATHEROSCLEROSIS BY INHIBITION OF
ARGININE GINGIPAINS**

A Major Project Dissertation is submitted

in partial fulfilment of the requirement for the degree of

Master of Technology

In

Bioinformatics

Submitted by

Komal Chouhan

(2K13/BIO/08)

Delhi Technological University, Delhi, India

Under the supervision of

Dr. Asmita Das



Department of Biotechnology
Delhi Technological University
(Formerly Delhi College of Engineering)
Shahbad Daultapur, Main Bawana Road, Delhi-110042, INDIA



CERTIFICATE

This is to certify that the M. Tech. Project entitled “**Novel approach to target Periodontitis and Atherosclerosis by inhibition of Arginine gingipains**”, submitted by **Komal Chouhan (2K13/BIO/08)** in partial fulfilment of the requirement for the award of the degree of Master of Technology, Delhi Technological University (Formerly Delhi College of Engineering, University of Delhi), is an authentic record of the candidate’s own work carried out by her under my guidance.

The information and data enclosed in this dissertation is original and has not been submitted elsewhere for honouring of any other degree.

Date:

Dr. Asmita Das

(Project Mentor)

Department of Bio-Technology

Delhi Technological University

(Formerly Delhi College of Engineering, University of Delhi)

Prof. D.Kumar

Head of Department

Department of Bio-Technology

DECLARATION

I, **KOMAL CHOUHAN**, hereby declare that the work entitled “**Novel approach to target Periodontitis and Atherosclerosis by inhibition of Arginine gingipains**” has been carried out by me under the guidance of Dr. Asmita Das, in Delhi Technological University, Delhi.

This Major Project is part of partial fulfilment for the degree of M.Tech in Bioinformatics. This is the original work and has not been submitted for any other degree in any other university.

Komal Chouhan

Roll no. : 2K13/BIO/08

ACKNOWLEDGEMENT

I would like to acknowledge my deep sense of gratitude to **Professor D.Kumar (Head of Department), Department of Biotechnology, Delhi Technological University, Delhi-110042** for giving me an opportunity to study and work in this prestigious institute.

I am extremely thankful to my mentor, **Dr. Asmita Das, Assistant Professor, Department of Biotechnology, Delhi Technological University, Delhi-110042** for her exemplary guidance, monitoring and constant encouragement. I would also like to thank her for sparing the efforts in compiling the work presented here.

Komal Chouhan

2K13/BIO/08

CONTENTS

S.No.	TOPIC	PAGE No.
	<i>LIST OF FIGURES</i>	<i>i</i>
	<i>LIST OF TABLES</i>	<i>ii</i>
	<i>LIST OF ABBREVIATIONS</i>	<i>iii</i>
1	ABSTRACT	1
2	INTRODUCTION	2-4
	2.1 Periodontal diseases	2
	2.2 Atherosclerosis	3
	2.3 Relation between periodontal disease and atherosclerosis	3
	2.4 Vaccine development	4
	2.5 Emerging concepts regarding vaccine development	4
3	REVIEW OF LITERATURE	5-9
	3.1 Periodontitis and Atherosclerosis	5
	3.2 Inflammatory disease	6
	3.3 Gingipains produced by P.gingivalis	6
	3.4 TG2 is an important mediator in P.gingivalis infection	7
	3.5 Developing strategies for vaccines	7
	3.6 Immunization against porphyromonas gingivalis	8
	3.7 Designing vaccine against periodontitis: Polymicrobial infection	9
4	MATERIALS AND METHODS	10-14
	4.1 Microorganisms involved	10
	4.2 Retrieval of nucleotide sequences from NCBI	10
	4.3 Phylogenetic analysis	10
	4.4 Retrieval of protein sequences NCBI	10
	4.5 Similarity searches using BLAST	10
	4.6 Conserved domains NCBI	10
	4.7 Structure prediction using PHYRE2	11
	4.8 Binding sites predicted PredictProtein	11
	4.9 Visualisation by PYMOL	11
	4.10 B cell epitope prediction by: ABCpred Prediction Server, Discotope, Bepipred Linear Epitope Prediction	11
	4.11 Antigenecity, Flexibility, Surface Accesability Prediction	12
	4.12 T cell epitope prediction by: Multipred, NetMHC, CTLpred, PrediVac	13
	4.13 Prediction of TAP regions by: TAPpred	13
	4.14 Proteosomal sites prediction using PAProc	14
	4.15 Vaccine stretch prediction according to geographical area by: PrediVac- Population coverage prediction	14
5	RESULTS	15-33
	5.1 Retrieval of Accession number and GI number	15
	5.2 Retrieval of nucleotide seq. from NCBI & performing BLAST	15
	5.3 Phylogenetic Analysis	16

	5.4	Transglutaminase2 (TG2)	16
	5.5	Prediction of 3D structure of TG2 using PHYRE2 tool	17
	5.6	Prediction of protein binding regions or binding sites of TG2 using PredictProtein tool	19
	5.7	B-cell epitope prediction using different tools	20
	5.8	Antigenecity, Flexibility and Surface Accesibility prediction	23
	5.9	T-cell epitope prediction using different tools	25
	5.10	Predicting vaccine stretches according to geographical area – PrediVac population coverage prediction	29
	5.11	Prediction of TAP binding regions by TAPPred	30
	5.12	Prediction of proteosomal cleavage sites by PAMPro	31
	5.13	Visualisation of predicted epitopes	32
6	CONCLUSION		34
7	DISCUSSION AND FUTURE PERSPECTIVE		34-36
8	ANNEXURE		37-44
9	REFERENCES		45-49