"The contributed chapters in the book written by the faculties of science stream in the light of the recent thinking and developments in the field of science and education.- Science& Technology is now dominates almost every field of our activities.In summary, The faculties (Science stream) of GEMS Arts & Science college have made an excellent attempt to bring about this book Homo Scientia", covering almost all the important areas from biological sciences to artificial intelligence. Every article has its own merits in both academic and research fronts..I record my grateful appreciation and thanks to the contributors of this book for their untiring efforts."

Dr. Balagopalan Unni

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HOMO SCIENTIA

Dr. Balagopalan Unni,
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Smitha Pramod V

GEMS

HOMO SCIENTIA

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Brief Biography

Dr. B.G.Unni, (Balagopalan Unni) Ph.D
(Allahabad central University)
FRES (London), FIANSc , FISAgBc, FICCE

Former Chief Scientist and Area Coordinator (Biotechnology & Biological Sciences) DADD and Fulbright Fellow retired from CSIR service in 2015 after 38 years of research career at CSIR North East Institute of Science & Technology Jorhat Assam. Appointed at Assam down town University as Director-Research in March 2015 and continued up to June 2019 and then re-designated as Adviser Research in August 2019). Back in Kerala, Dr.Unni is appointed as Director Academic & Research at GEMS College of Arts & Science affiliated to University of Calicut from August 2019. Both the positions are on honorary basis to strengthen the institutions in research areas. He did his BSc Biology (1972-74, Ewing Christian College, Alld University), MSc in Biochemistry(1974-76)(Second Rank) and Ph.D in Biochemistry from Allahabad University(1976-80) and PDF in Molecular Biology from Texas A&M University, USA(1988-91). Dr. Unni is specialized in Biochemistry, Molecular Biology, and Biotechnology and well established in his area of research and completed more than 40 years of research in both basic and applied fields of research. Dr.Unni got more than 130 research papers, 190 abstracts, 35 papers in proceedings, 7 patents,1 technology.18 chapters in books, edited 3 books and 29 students

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received PhD degrees under his guidance and supervision. Dr. Unni had completed more than 20 projects sponsored by Commonwealth Science Council, London, Ministry of Non conventional Energy Sources, Department of Non conventional Energy Sources Govt of India, North Eastern Council Govt of India, Department of Science &Technology, Department of Biotechnology, Central Silk Board,GB Pant Institute of Himalayan Environment and Development, CSIR and DRDO, Ministry of Defense, Govt of India during his scientific tenure at CSIR NEIST. Dr Unni received- Fulbright Travel Award/ Fellowship (USA) Dr. B.M. Das Memorial Science award, Hebrew University Award , H.R. Cama Memorial Travel Award,COSTED Travel Award,. DAAD- fellowship-Germany, Well Mark International Scholarship (USA) & Technology award in life sciences by CSIR,Govt of India . Best Fulbright Alumni Chapter Leader-South Asia Selected by the United States Education Foundation In India (USIEF), New Delhi .Nominated to represent India at the International Fulbright Scholars meet at Marrakech, Morocco- Nominated by United States Education Foundation In India, New Delhi . Dr. Unni is in the editorial board of more than eight indexed journal in the country .Dr.Unni was nominated to various state and central committees such as High power committee for development of sericulture activities Muga, Eri,Tassar and Mulberry in Assam nominated by Governor of Assam, .Expert in the area of non mulberry sericulture, Ministry of Textiles, Advisory Board, Post graduate Biotechnology programme, Academic Council, Assam Agricultural University, Research Council, Central Silk Board, Ministry of Textiles , DBT's Nominee for Biosafety Committee ,Vice President SBC (India) Indian Institute of Science Bangalore, Vice President Indian Academy of Neuro-sciences, Member Fulbright Academy of Science & Technology, USA, Board of studies- Botany Nagaland University and Biotechnology Saugar University Madhya Pradesh., Fellow, Indian Academy of Neurosciences & Indian Society of Agricultural Biochemists, Fellow Royal Entomological Society, London UK and Scientific

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Advisor International Foundation of Science, Sweden, Member, Board of Studies Raiganj University (2017----), Member Research Review committee Tea Board of India (2016-2019), Member Advisory Committee Cancer Research Advisory Board, North East Cancer Hospital & Research Institute (2017--) President, Tea Improvement Consortium, Ltd, Tocklai Assam (2018-2020) .

Dr.Unni visited USA, Germany, Israel, Jordan, France, Morocco ,UK, Thailand ,Jordan, Singapore , China and UAE under various exchange program.

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Preface

I am very happy to learn that, the GEMS Arts & Science College is bringing out a series of books written by the faculty in this academic year. The college is occupying a very important position among the colleges in Kerala, the same way the college is having unique standing in both academic and research fronts too. This is because of the excellent management, faculties and the best performances of the students.. I have full confident that in the course of time, and with the sincere commitment and dedication of the faculties , students and with management , the college will attain high level perfection and excellence and became a model college in the state of Kerala

This book entitled " Homo Scientia" had comprehensive research topics in various aspects in the topics of cyber security, biotechnology, microbiology and geology.A brief description about the cybersecurity, the protection of computer set up such as hardware, software data from several threats have been described in the chapter The best practices for deploying and managing IPS network security tools have been explored. The integration of intrusion prevention system (IPS) solutions, adherence to security policies, regular updates, monitoring and the implementation of incident response procedures are considered to be the essential components of a comprehensive network security framework. The risk management in cyber security, various cyber-attack kinds, malware, and some strategies to tackle these attacks are also explained by the authors. A comprehensive overview of the evolution of computer graphics, exploring the advancements in hardware, software, algorithms, and techniques that have propelled the field from its early pixel-based beginnings to the current state of realism etc also described. Optical character recognition has been extensively investigated in the past few years, and has been proven that high recognition rates can be achieved in specific

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application scenarios using some standard and well-studied methods such as neural network, support vector machine (SVM), etc. The possibility of learning an appropriate set of features for designing optical character recognition (OCR) has been investigated

Biotechnology is an interdisciplinary science using modern technologies to construct biological processes in research, agriculture, formulation of pharmaceutical products and other related fields. The better understanding of advances in plant genetic resources, genome modifications, omics technologies to generate new solutions for food security under changing environmental scenarios etc have been discussed in this chapter. The increasing demand for food had a great impact on the agriculture sector to address the various challenges associated with crop productivity. The tremendous advancement in plant research helps in understanding plant biology for sustainable food security, functional ecosystems, crop improvement and human health. One of the sustainable farming techniques is the use of fertilizer at nano level. Nanomaterials that enhance plant nutrition could be considered as an alternative to the conventional chemical fertilizers. one chapter covered the importance of nano fertilizer to enhance metabolic processes in plants and reviewed the concerns in developing nanotechnological methods in the future. Metabolomics has now emerged as a powerful tool for the comprehensive analysis of metabolites within biological systems. One of the chapters provides a review on metabolomics, encompassing its methodologies, applications, potential impact on personalized medicine ,and discusses further the need for advancements in analytical technologies. The antifungal activity of mangroves, particularly Rhizophora species are one of the main sources for fungicidal compounds due to the presence of high concentration of phenols. The antifungal activity of Rhizophora species has been elucidated, and could be further utilized as biocontrol agents for fungal disease in agricultural crops. One of the chapters discussed the species identification and its impact on economical and ecological level in the species like Nutmeg, one of the important medicinal plants that had a greater attention ,however, it was very difficult to differentiate the sexual identity

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in the seedling stages. But the protein content screening among the studied plantlets had differentiated the sexes in the species as explained by the author.

AI (Artificial Intelligence) or machine intelligence enables farmers to enhance the quality and ensure a quick go-to market strategy for crops, and adoption of these algorithms to improve food industries. Artificial intelligence (AI) has also the potential to revolutionize education, from personalized learning to assessment and grading. Additionally, AI-powered tools can provide greater accessibility to students with disabilities, while also enabling more engaging and interactive content. AI continues to develop and become more prevalent in education, towards responsible and equitable implementation. However the negative and positive part of the AI may also be looked into.

The chapters related to microbiological aspects have also been incorporated in this book . Carbapenem-resistant A. baumannii (CRAb), bacteria that cause multi-infections in humans and resistant to multiple drugs too. The study attempted to isolate and characterize the bacterial species from the clinical specimens using biochemical techniques. The enzyme, carbapenemase produced by the bacteria was isolated and determined by different assays. Another study identified the antibacterial, antioxidant and anticancer activities of Ganoderma lucidum by various chromatographic techniques. Anticancer activity was also assessed on HeLa cell lines using MTT assay and DPPH assay. In one of the chapters,the author discussed L-asparaginase, one of the widely exploited enzymes for the treatment of acute lymphoblastic leukemia (ALL). Also attempted to isolate and characterize the enzyme from soil samples collected from different locations at Kerala. The study indicated that soils can provide a rich source for L-asparaginase which has got ample application in pharmaceutical industries.

The studies on various geological aspects with respect to different geographical areas in Kerala soil has been included in the book. The vertical geochemical variation and elemental mobility of the lateritic terrain in the Makkaraparamba of Malappuram District, Kerala has been very well investigated. Under extremely oxidizing and leaching conditions, laterite

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soil transformed into a variety of rocks and further developed into stable secondary product in the existing humid tropical and subtropical environments. The hydrogeological conditions in Kumbala- Kaliyar river basin, Kasaragod district, Kerala was assessed by means of Vertical Electrical Sounding (VES). The digital spatial data output of the present study would be much helpful for planning and management of surface and sub-surface water resources of Kasaragod River basin in which the Kasaragod township is centrally located

The contributed chapters in the book written by the faculties of science stream in the light of the recent thinking and developments in the field of science and education.Science& Technology is now dominates almost every field of our activities. In summary , The faculties (Science stream) of GEMS Arts & Science college have made a n excellent attempt to bring about this book Homo Scientia".covering almost all the important areas from biological sciences to artificial intelligence. Every article has its own merits in both academic and research fronts..I record my grateful appreciation and thanks to the contributors of this book for their untiring efforts.

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STRUCTURAL CHARACTERIZATION OF PHOSPHOTRANSACETYLASE ENZYME IN PORPHYROMONAS GINGIVALIS: IN –SILICO APPROACH

Silva Shihab
Assistant Professor
PG Department of General Biotechnology

ABSTRACT

Porphyromonas gingivalis is an oral anaerobic, black-pigmented, immotile Gram-negative microbe.Itbelongs to large number of species of bacteria that resides in the buccal cavity that plays a major role in the periodontal disease pathology, which is an inflammatory infection that damages the tissues that support the tooth, sometimes leading to dental deterioration. *Porphyromonas gingivalis* is a common dental biofilm bacterium, However, in periodontal injuries, it can be exceedingly damaging and grow in vast numbers of cells. This is a kind of bacterium that ferments amino acids such as glutamate and aspartate to obtain its metabolic energy. Phosphotransacetylase is one the major enzymes which is produced by this bacterium and it plays a significant part in the production of ATP. A better understanding on structural characteristics of this enzyme from *Porphyromonas gingivalis* aids to more information on ATP production mechanism in these bacteria. The crystal structures of phosphotransacetylase from *Porphyromonas gingivalis* is identified earlier but the structural details and validation of this enzyme is not determined. In this study we have performed with the structural characterization and validation of phosphotransacetylase from *Porphyromonas gingivalis* through in-silico screening by employing bioinformatics methods

like homology modeling, 3D structure prediction and other modeling approaches. The results of the 3D structure prediction and modeling approaches of the enzyme phosphotransacetylase from *Porphyromonas gingivali* could be useful for various therapeutic studies in this field of research.

INTRODUCTION

Porphyromonas gingivalis is an oral anaerobic, black-pigmented, immotile Gram-negative microbe. It belongs to large number of species of bacteria that resides in the buccal cavity that plays a major role in the periodontal disease pathology, which is an inflammatory infection that damages the tissues that support the tooth, sometimes leading to dental deterioration. The periodontal pathogen *Porphyromonas gingivalis* has the ability to invade primary gingival epithelial cell cultures. It may infiltrate periodontal tissues on a limited level, eluding host defence mechanisms. This utilizes a series of virulence factors that enable the immunological and inflammatory responses to be unregulated. One of the key virulence features of this oral pathogen is the presence of adhesive filamentous extensions known as fimbriae. Fimbriae are made with the subunits of polymerized fimbrillin (FimA) that plays a critical role in *Porphyromonas gingivalis*' capacity to colonise and infiltrate periodontal tissue as well as cause alveolar bone deterioration. Both in animal and human models, it has been found in a variety of diseased organs and tissues Following the oral delivery, P. gingivalis translocates to distant tissues such as the liver or joint and it is also detected in the brains of individuals suffering Alzheimer's disease. This has sparked a renewed interest in figuring out how *P. gingivalis* plays a role in chronic inflammatory illnesses

Before its recategorization as a new genus *Porphyromonas*, it was known as *Bacteroides gingivalis*. The term *Porphyromonas* is a combination of the Greek adjective porphyrios, which means purple, and the Greek noun monas, which means unit.Since the colonies on blood agar plates appear black after 6 to 10 days due to the buildup of heme, the term *Porphyromonas* means porphyrin cell.. The pathogenic capability of the *Porphyromonas*

gingivalisis also due to the generation of biofilms and the functions of bacterial dipeptidyl peptidase IV. Furthermore, the development of biofilms can uplift the virulence of *Porphyromonas gingivalis* through an increase in the DPPIV activity. The major pathways for ATP and energy synthesis in *Porphyromonas gingivalis* are still unknown. *Porphyromonas gingivalis* cannot ferment carbohydrates like glucose; however it can use modest amounts of glucose monomers for polymer production. Therefore, *Porphyromonas gingivalis* depends on amino acid catabolism to create metabolic energy. In many bacteria, Acetate kinase and phosphotransacetylase form a critical route for producing ATP from excess acetyl coenzyme A. Phosphotransacetylase catalyzes the reversible conversion of the acetyl group from the acetyl phosphate to coenzyme A resulting in the formation of inorganic phosphate and acetyl-CoA. Pta converts acetyl-CoA to acetyl phosphate which is then transformed to acetate by Ack, resulting in the synthesis of ATP via substrate-level phosphorylation.

Understanding the 3-D structure of proteins, as well as their interactions with certain other chemicals like ligands, would help with their fractional function. In addition, the recognition of their 3D structures relies on logical modification and protein engineering. The 3D protein structures may be utilized to create drugs and vaccines, as well as anticipate conformational epitopes. The need to classify tertiary protein structures relative to the negligible amount of structural annotation is highlighted by a massive number of identified protein sequences. Because of their high failure rate, empirically determining protein structures is a big challenge. Additional approaches should be developed since determining 3D protein structures experimentally is costly and time-consuming.

Purification and crystallization are additional challenges for outer membrane proteins, in addition to the conventional experimental determination of 3D protein structures. Today's biologists are very interested in bioinformatics instruments. One of the major applications of these instruments is the 3D structure prediction of proteins. To predict the protein structure, there are numerous methodologies and algorithms, and one of those is homology modeling. Homology modelling is an in-

silico method for predicting 3D protein structures that employs well-known homologous protein molecules as a template. In this study, we have performed the 3D structure determination and validation of the protein Phosphotransacetylase produced by *Porphyromonas gingivalis* ATCC 33277.

METHODOLOGY

Retrieval and alignment of sequences

The protein sequence of *Porphyromonas gingivalis* ATCC 33277 phosphotransacetylase was obtained in FASTA format from the NCBI structure database at https://www.ncbi.nlm.nih.gov/Structure/index.shtml and used as a query for BLAST against a non-redundant protein database at http://blast.ncbi.nlm.nih.gov/Blast.cgi. Putative conserved domains of the query were also checked. The protein sequence was used as an input to PSI-BLAST against the protein data bank at http://blast.ncbi.nlm.nih.gov/Blast.cgiin order to find homologous structures.

Topology and signal peptide prediction

The integral transmembrane topology protein prediction provides valuable information about the protein's functionality. TopCons predicts membrane protein and signal peptide consensus topology at http://topcons.cbr.su.se/.TMHMM predicts transmembrane helices structure at http://www.cbs.dtu.dk/services/TMHMM/.PRED-TMBB predicts the geometry of loops by locating gram-negative bacteria's transmembrane strands in the structure at http://biophysics.biol.uoa.gr/PRED-TMBB/.

Analysis of primary sequence and subcellular localization

Protparam at http://expasy.org/tools/protparam.html is a free web tool used to compute molecular weight, theoretical pI, amino acid composition, instability index, aliphatic index, GRAVY and Vaxijen score. Similarly, to predict subcellular localization CELLO at http://cello.life.nctu.edu.tw/is used. Also, PSLpred at http://crdd.osdd.net/raghava/pslpred/for predicting cytoplasmic, periplasmic, inner membrane, outer membrane or extracellular localization is used.

Secondary structure prediction

To improve the accuracy of protein secondary structure prediction, the self-optimized prediction technique http://npsa-pbil.ibcp.fr/cgibin/npsaautomat.pl?page=npsasopma.html is used. This server's parameters were set as 4 conformational states (helix, sheet, turn, and coil), 8 similarity threshold, and 17 window width.

Homology Modeling

PS2v2 at http://ps2.life.nctu.edu.tw/is an automated homology modeling server that predict 3D structures, selects a template and aligns target-template. SWISS-MODEL, a fully automated protein structure homology-modeling server at https://swissmodel.expasy.org/and Swiss PDB-Viewer are both available on the ExPASy web portal

Other modeling methods

The I-TASSER server predicts structures and functions of protein at http://zhanglab.ccmb.med.umich.edu/I-TASSER/. Multiple-threading alignments and ab initio models are used to create 3D models. LOMETS at I-TASSER Server generates tertiary structure

Ligand binding site prediction

COFACTOR predicts the biological function in the I-TASSER server based on structure and protein interactions. This server also predicts amino acids involved in the ligand binding site.

Model Evaluation

The structural assessment in Swiss model was used to create ramachandran plots for the protein and its template https:// swissmodel.expasy.org/assess.

Orientation of the Protein in membrane

The OPM server at https://opm.phar.umich.edu/ppm_ server_ybrc was used to locate the rotation of transmembrane and peripheral proteins in membranes that use the tertiary structure (PDB coordinate file) as an input. Many membrane-associated proteins from the PDB have previously been calculated and are available in the OPM database.

Identification of functionally and

structurally important residues

InterProSurf (http://curie.utmb.edu/pattest9.html) is used to predict functional locations on the protein surface. The 3D structure of protein was used as the server's input file.

Cleft analyses

Clefts and grooves in the protein surface were predicted using Profunc at http://www.ebi.ac.uk/thornton-srv/databases/profunc/. This server can also forecast the depth of clefts and the amino acids found in the clefts

Surface accessible pockets and cavities

CastP server (http://sts.bioe.uic.edu/castp/)gives information on the accessible and inaccessible pockets for proteins and other compounds, as well as their sizes. Depth (http://mspc.bii.a-star.edu.sg/tankp/help.html) calculates and predicts depth, cavity sizes, ligand binding sites, and PKA. The closest distance between a residue/atom and the bulk solvent is also measured by depth

RESULTS AND DISCUSSION

Sequence alignment and template search

The phosphotransacetylase protein sequence was saved in FASTA format contains 340 amino acids. Protein sequences used as a BLAST query yielded a list of sequences with the highest similarity. A BLAST search of the phosphotransacetylase protein sequence yielded many hits. PSI-BLAST findings against the Protein Data Bank revealed numerous homologous structures. The first hit was chosen as a homology modelling template with the highest score. Protein with PDB code 6IOW_A was the top hit for phosphotransacetylase sequence (100 % identity). Within this sequence, putative conserved domains were discovered.

Topology and signal peptide prediction

Based on expected inner, transmembrane, and exterior sections of the protein, a 2D topological model of phosphotransacetylase was created (Fig. 1). A transmembrane antiparallel β-strand makes up this protein. In its original state, the protein appears to have a β-barrel shape, according to the model. The strands that make up the β-barrel are connected by a loop on the outside or twists on the inside. TOPCONS use the

TMHMM, SPOCTOPUS, and Signal P algorithms to predict the absence of transmembrane helices across the protein sequence, as well as the absence of a signal peptide at the protein's N terminus. The entire protein is made up of two domains: a cork domain at the N terminus and a transmembrane barrel at the C terminal.

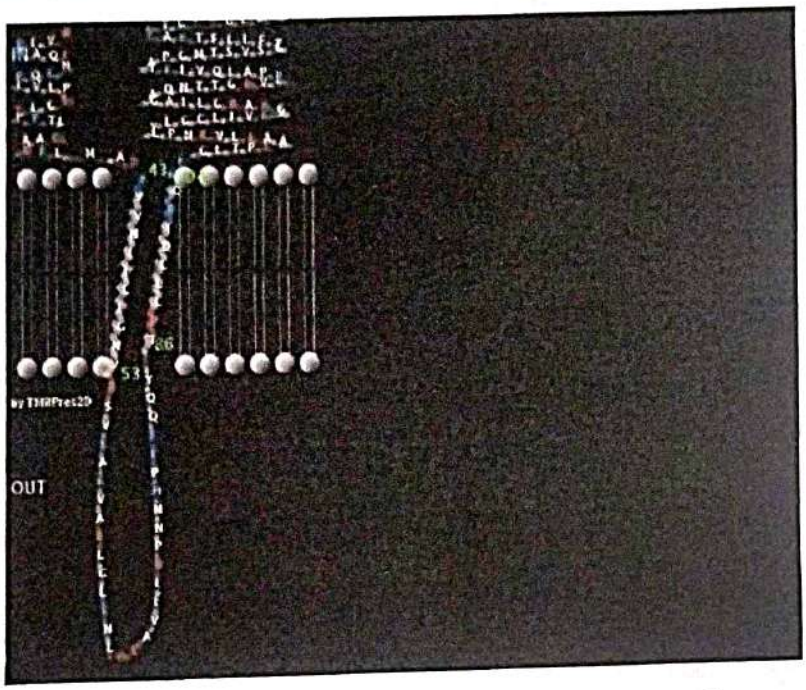


Fig 1. A 2D topology model of phosphotransacetylase

Primary sequence analysis and subcellular localization

Physical and chemical properties were calculated using protein sequences. Phosphotransacetylase contains 340 residues. There are 43 (Asp + Glu) negatively and 37 (Arg + Lys) positively charged residues respectively. Table 1 summarises the molecular weight, theoretical pI, instability index, aliphatic index, grand average of hydropathicity indicates protein solubility, and Vaxijen score. The aliphatic index of a protein is volume occupied by the aliphatic side chains. It could be considered to increase thermostability of globular proteins. The instability index is used to calculate the protein's stability. The GRAVY value is calculated by dividing the sum of the

hydropathy values of all amino acids in a peptide or protein by the number of residues in the sequence. The protein sequence subcellular localization predicted by CELLO was cytoplasmic with the highest reliability of 4.543. With 90.2 % precision, PSLpred predicted the protein sequence as cytoplasmic protein.

Table 1: Protparam and Vaxijen primary sequence analysis

Protein name	Vaxijen score	Number of amino acids	Mole cular weight	Theore tical pI	Insta bility index	Alipha tic index	Grand average of hydro pathicity (GRAVY)
Phosp hotran sacetylase	**0.4508**	**340**	36107.82	**5.34**	**25.08**	**108.53**	**0.039**

Secondary Structure Prediction

The secondary structure of a protein is made up of coils, helixes, and strands. The tertiary structures might be validated using the secondary structure. It was shown as alpha helix (45.59%), extended strand (13.53%), beta turn (5.00%) and random coil (35.88%). The structure is represented in colors as alpha-helix, beta strand, beta turn and coils are shown in Fig. 2.

Fig. 2 Secondary structure of Phosphotransacetylase

Homology Modeling

Swiss model and Ps2v2 (template-based prediction server)

identified 2 models as 6IOW_A and 2AF4_C respectively through homology modeling. Their models were selected for further scrutiny.

Other modeling methods

Each server and software used for homology modelling imposed new models on its own. I-TASSER created five models that were ranked according to their C-scores. The best model with the highest C-score was chosen for validation analyses from the available models. The LOMETS server a meta threading approach also predicted ten models. The models were also taken to be examined further.

Ligand binding site prediction

COFACTOR tool predicts the involvement of conserved residues between the crock domain and the large extracellular loop of barrel in the binding site is found to have highest C-score of 0.46 2AF4_C is shown in Fig. 3. C-score is the predicted binding site's confidence score.

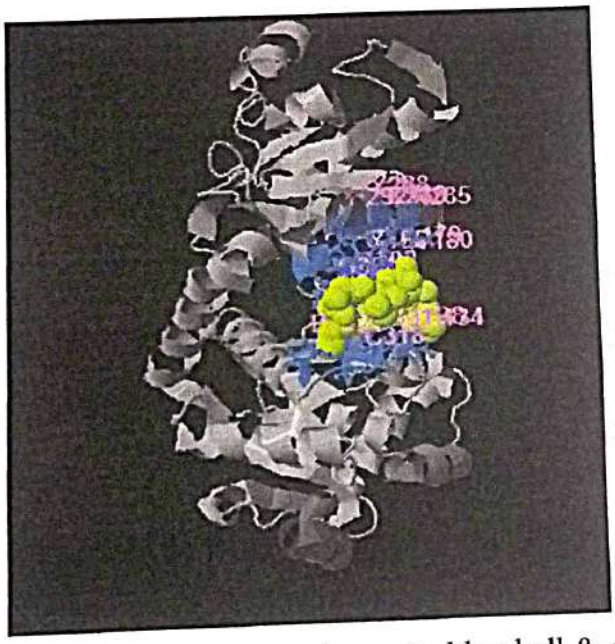


Fig 3. Binding residues are shown in blue ball & stick and the predicted binding ligand is shown in green yellow sphere.

Model evaluation

Swiss models assess the quality of 3D models using

structural evaluation. In the Ramachandran plot of models, the % residues were found in the favoured and outlier areas. It depicts the torsion angles of the protein backbone in two dimensions. In the Ramachandran map, the phi and psi angles cluster into distinct regions, each corresponds to a different secondary structure. The chosen model had maximum percent of preferred favoured residue (approximately 98.22 %) as well as with zero outlier residue is shown in Fig. 4.

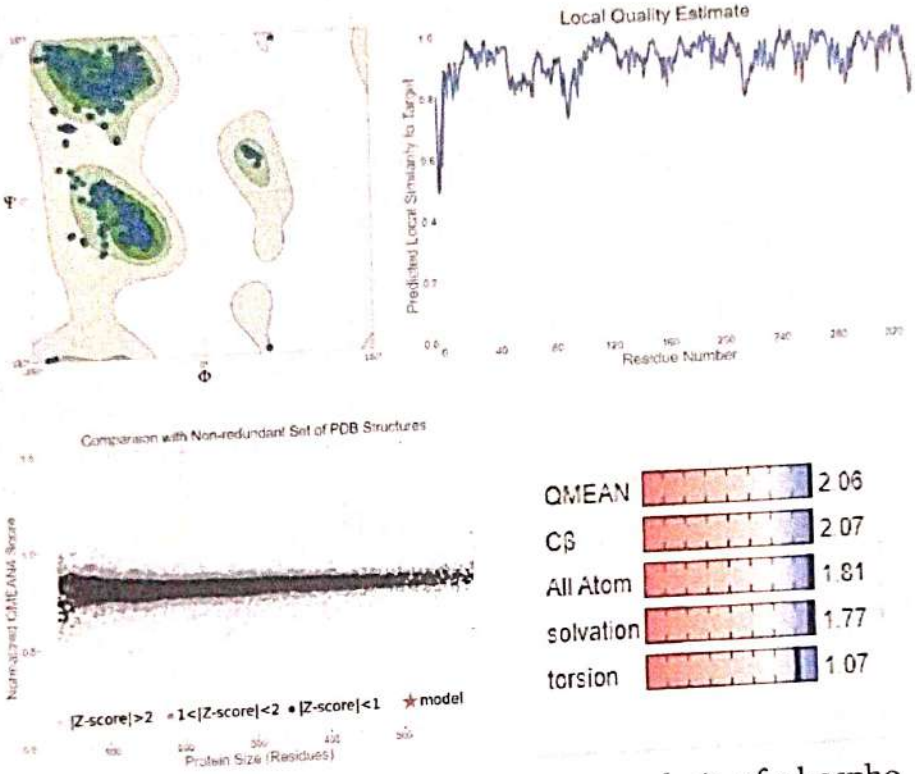


Fig. 4. Ramachandran plot and Z-Score analysis of phospho transacetylase

Orientation of the Protein in membrane

Both PDB specific structures of transmembrane protein complexes and peripheral proteins, as well as membrane-bound peptides, are currently included in the OPM database, along with their calculated membrane boundaries. The precision of calculated hydrophobic thicknesses and tilt angles are 1.5 ± 3.1 Å and 89.± 8.° respectively. The global minimum of transfer energy

is -1.7 kcal/mol. The determined tilt angles in homologous proteins vary depending on the protein's size, oligomeric state, and sequence identity percentage. The cytoplasmic protein showing hydrophobic boundaries of the lipid bilayer is shown in Fig.5.

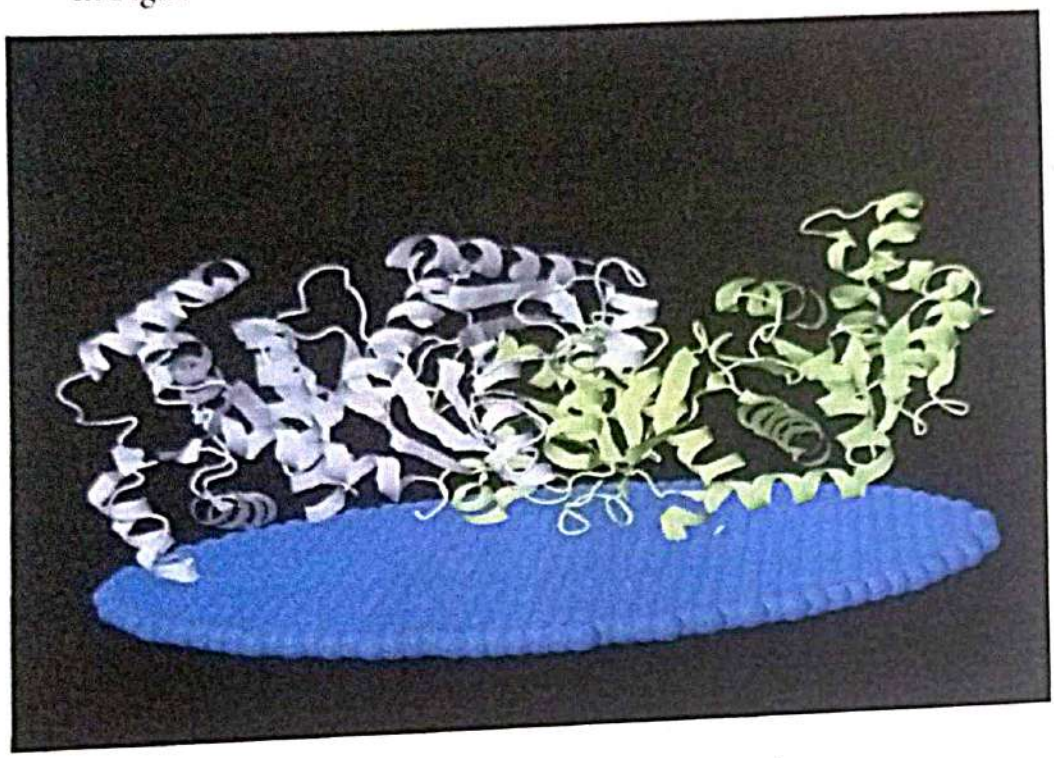


Fig. 5. Orientation of protein in cell membrane

Identification of functionally and structurally important residues

A globular cytoplasmic protein was predicted. Interprosurf's findings show that functional regions on the surface of protein structures. According to these findings, the outer membrane loop and the cork domain are the most functional areas in the protein structure. The top functional residues are indicated in red and others is highlighted in green sticks in Fig.6.

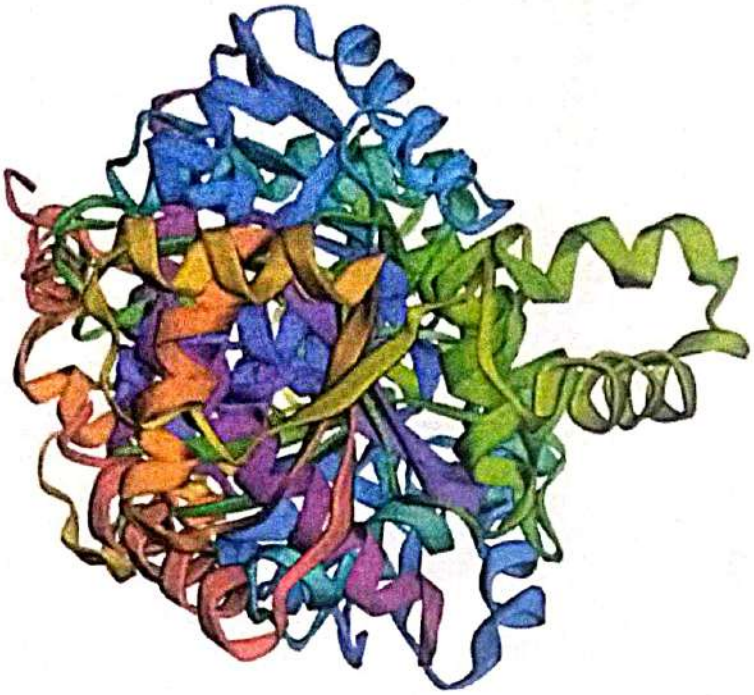


Fig. 6. Top functional residues of predicted protein are highlighted in red sticks and others are highlighted in green sticks

Cleft analyses

A total of 10 gap regions were found.Profunc proposed a region with an average depth of 21.88 Å, accessible vertices of 67.74 Å, and buried vertices of 12.03 Å, with the greatest and deepest cleft of this protein having RI ratio 1.14.

Surface accessible pockets and cavities

The CastP server calculates the top ten structural regions of a protein, area and volume of each pocket and cavity, both on a solvent-exposed surface and on a molecular surface, using analytical methods. Biologically relevant functional residues are discovered and shown in PDB structures. Fig.7 shows the atoms of annotated residues that lie in the pocket are highlighted.

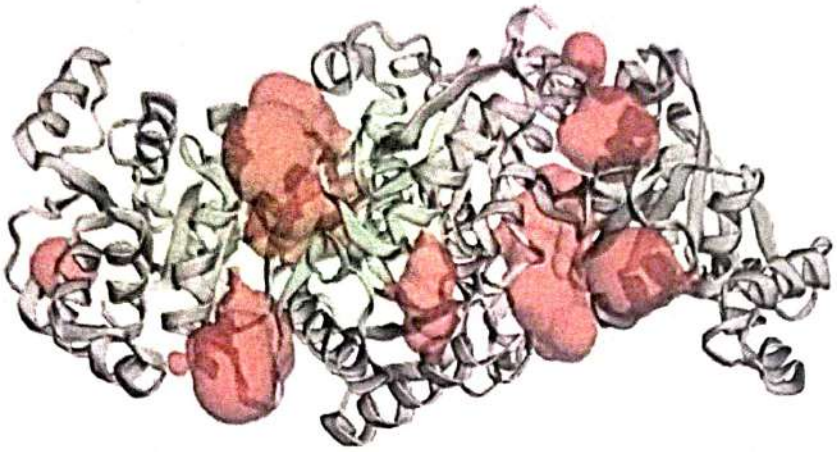
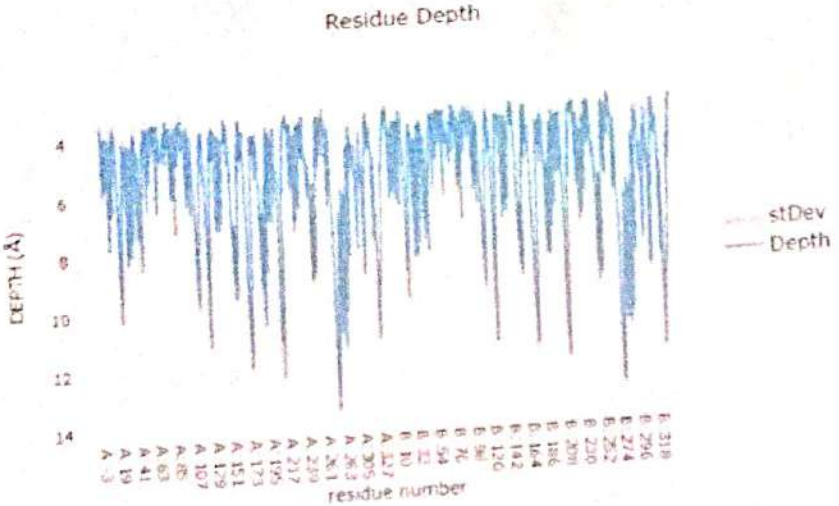
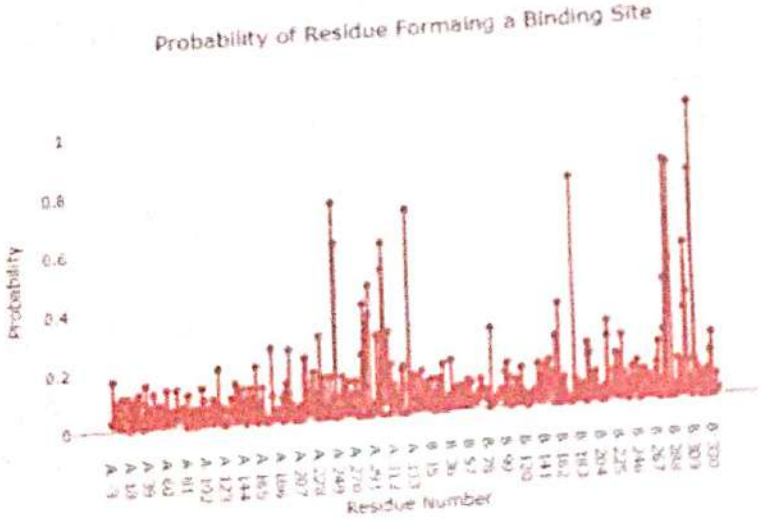


Fig. 7. CastP results showing surface accessible pockets and residues are colored based on area and volume size. The important one illustrate in red respectively

Protein binding sites are residues/atoms on the surface of proteins that directly interact and are close to ligand binding sites. A binding cavity is a protein substructure having complementary geometrical and chemical properties to the bound ligand. High-resolution crystal structures, residue depth, and solvent-accessible area values were determined for all residues using a set of ligands. The pair of residue depth accessible area value pairs determine the chance of specific amino acids being included in the binding cavity. The programme calculates the likelihood of a binding cavity for each protein residue. The depth values mean and standard deviation are depicted in the graph. The probability of a residue forming a binding site, as well as the depth plot and residues of binding cavity, depth, and accessible surface area, are shown in Fig. 8.





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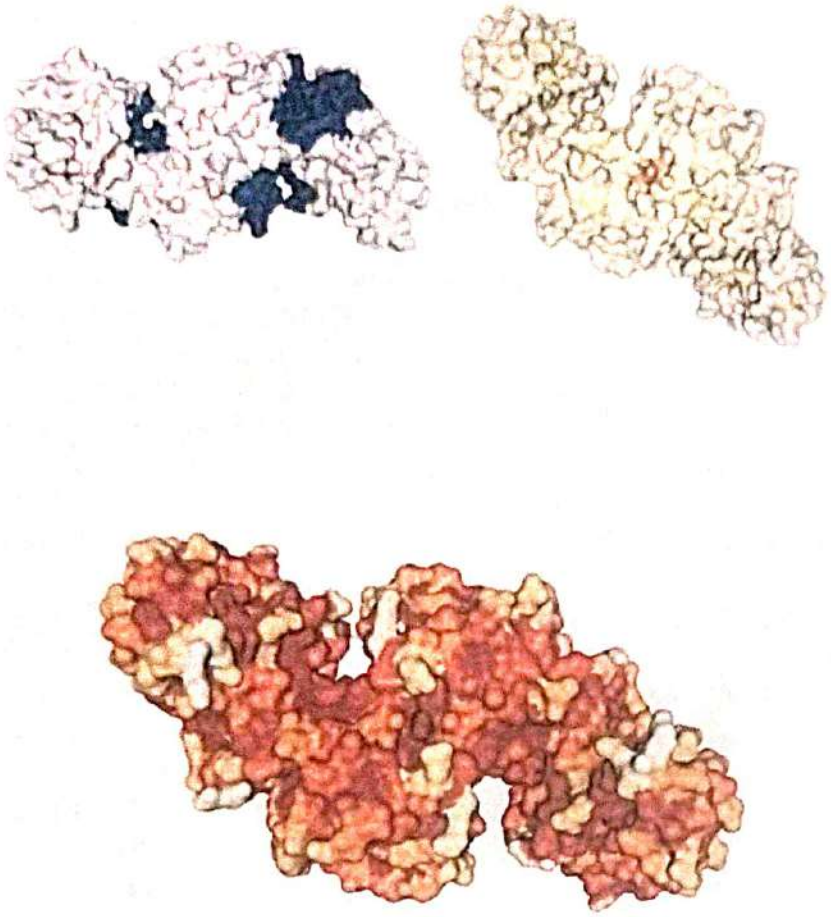

Fig. 8. Probability of residue forming a binding site and residue depth plot is shown. Top: probability of residue forming a binding site and residue depth plot. Below: Residues of the predicted binding cavity, depth and accessible surface area is shown

DISCUSION

Porphyromonas gingivalis, which causes periodontal inflammatory disorders, is one of the anaerobic bacteria found in the oral cavity. The present study aimed at studying the characteristics of this bacterium using an in-silico analysis. By using protein sequences as an input for BLAST, a

collection of sequences was constructed as the highest similar sequence.. BLAST research revealed multiple hits in the protein sequence of phosphotransacetylase. For homology modelling the protein with PDB code 6IOW-A was the top hit for the phosphotransacetylase chain (100 percent identity). A 2D topological model of phosphotransacetylase was created based on the expected structure inside the transmembrane and outer sections of the protein. The model suggests that the protein is organized in the native form of β-barrels. Protein sequences were used to compute a variety of physical and chemical properties. There are 340 residues in phosphotransacetylase. There are 43 negatively charged residues (Asp + Glu) and 37 positively charged residues (Arg + Lys). While analyzing the primary structure Molecular weight, aliphatic index, theoretical pI, instability index, and large hydropathicity average were included in the computed parameters. The protein sequence subcellular localization predicted by the CELLO was cytoplasmic with the highest reliability of 4.543. The protein sequence was predicted by PSLpred with 90.2 percent precision as a cytoplasmic protein. While prediction of secondary structures attribution of secondary structure components in the protein is alpha helix (45.59%), extended strand (13.53%), beta turn (5.00%) and random coil (35.88%). For 3D structure prediction, the Swiss model and Ps2v2 has recruited 2 models known as 6IOW-A and 2AF4-C respectively for homology modeling. Their models have been chosen for further scrutiny. And other modeling methods were also employed which included I-TASSER which has built five models and it was ranked based on their C-scores. The best model with the highest C-score was chosen for validation analyses from the available models. The LOMETS meta server predicted ten models for the protein. The models were also taken to be examined at further thoroughly.

Ligand binding sites were calculated using COFACTOR software which indicated the presence of retained residues in the binding site with the highest C-score of 0.46 of 2af4C between the crock domain and the broad extracellular barrel loop. The 3D models were estimated qualitatively by structural assessment in Swiss model. Orientation of the 3D structure of protein in membrane was determined and the accuracy of

computed hydrophobic thicknesses and tilt angles are 1.5 3.1 and 89. 8 °, respectively, and the global minimum of transfer energy is -1.7 kcal/mol. The findings of the search for functionally and structurally relevant residues revealed that the outer membrane loop and the cork domain are the most functionally important sites in the protein structure.

In cleft analysis the total number of gap regions analyzed was 10 and an area with an average depth of 21.88 Å, accessible vertices of 67.74 Å and buried vertices of 12.03 Å was suggested by Profunc, with the highest and deepest cleft in this protein being RI ratio 1.14. CastP server has predicted the top ten areas in protein structure. On both a solvent accessible surface (SA, Richard's surface) and a molecular surface, this server has estimated the area and volume of each pocket and cavity (MS, Connolly surface).

CONCLUSION

The bioinformatics methods are being investigated as a viable strategy for closing the gap between the amount of protein sequences and the 3D protein structure. Many important processes are conducted during the screening of innovative drug candidates to rule out substances that have negative effects or interact with other medications. In-silico approaches have been extremely useful in identifying targets and predicting the efficacy of new medications. Our approach of using 3D structure prediction and the outcomes of many predictions should pave the door for additional structural, functional, and therapeutic study in the sector.