



**PROTEIN STRUCTURE PREDICTION AND PROTEIN STRUCTURE COMPARISON
BY ALIGNMENT OF SARS-COV-2 SPIKE GLYCOPROTEIN AND ANGIOTENSIN-
CONVERTING ENZYME 2 (ACE2) FROM DIFFERENT ORGANISM'S HOST**

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ABSTRACT

Coronavirus disease (covid-19) is an infectious Disease caused by severe acute respiratory syndrome (SARS-cov-2) previously known as "ncov-19" has been associated with The recent epidemic of acute respiratory distress syndrome. the first cases were seen in Wuhan, China in December 2019 before spreading Globally recent studies have suggested that Angiotensin-converting enzyme 2 (ACE2) is more likely to be the cell receptor through which the SARS-COV-2 virus invades the host cell using the spike glycoprotein. in the present work we make the protein Structure alignment and calculates the RMSD score in between the SARS-COV-2 spike glycoprotein and ACE2 receptor from Different organism's host. To make the protein Structure alignment and the calculation of RMSD score we use the Pymol Structure visualization tool.

KEYWORDS: SARS-COV-2, Structure Prediction, Structure Alignment.

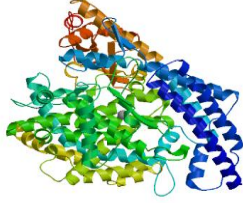

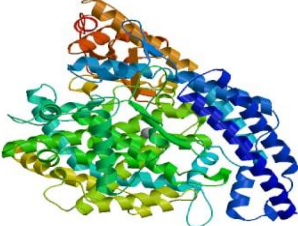
INTRODUCTION

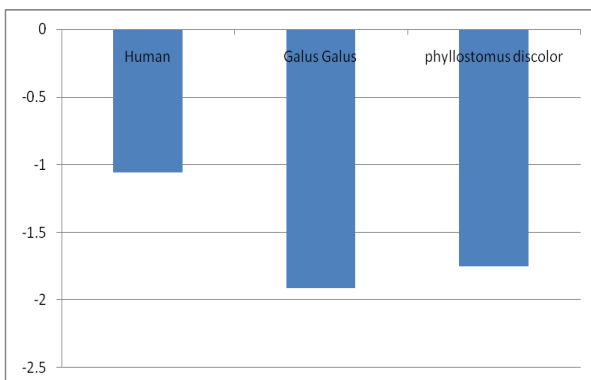
The Spread of Covid-19 is caused by the SARS-COV-2 has been associated with the recent epidemic of acute respiratory distress syndrome. the present Study revealed that Angiotensin-converting enzyme 2 (ACE2) is more likely to be the cell receptor through which the SARS-COV-2 virus invades the host cell using the spike glycoprotein. In the present work, we provide an 3 dimensional protein Structure by calculating it's Q-mean score and also gives us the structure alignment by calculating it's RMSD Score between SARS-COV-2 spike glycoprotein from different coronavirus isolates with host ACE2 protein. Finally, we Studied the variations of ACE2 Protein from targeted organism's host (human, galus galus & Phyllostomus discolor) against the SARS-COV-2 Spike glycoprotein by Calculating the RMSD Score.

Programs: Different protocols, methods and programs are available through which the target sequences are obtained in specific fasta file format (developed by W. Pearson) using the biological database NCBI. Further we predict the 3 dimensional protein structure from the obtained protein sequences using the Swiss model server. After prediction of 3 dimensional Protein Structure we make the protein Structure alignment and calculates the RMSD Score between targeted protein structures using the 'Pymol' Protein Structure Visualization tool.

Structure Prediction: Protein Structure Prediction is a research field which aims to create 3 dimensional models from the amino acid sequence. Protein Structure Prediction from amino acid sequence is one of the high focus problems in Bioinformatics today because the biological function of the protein is determined by it's 3 dimensional structure thus, the 3 dimensional structure prediction is a fundamental area of Bioinformatics. for the 3 dimensional structure Prediction we took the SARS-COV-2 spike glycoprotein and ACE2 protein from Different organism's host. usually, Q-mean shows the Quality score of the predicted structure as nearer to zero shows good Quality of the structure shown in (graph:1).

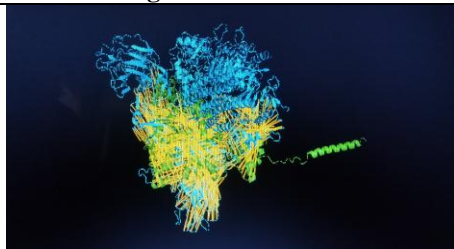
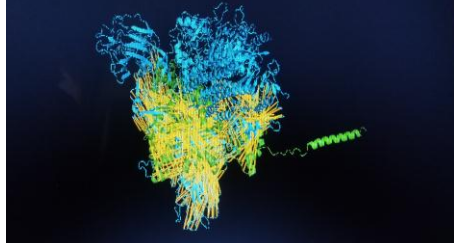
Table 1: Shows organisms name with it's Q-mean score.

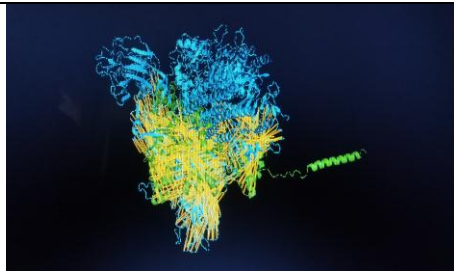
Sr.no	Organism Name	NCBI Accession	Protein Structure	Q-mean Score
1	Human	BAB40370.1		-1.06
2	Galus Galus	QEQ50331.1		-1.91
3	Phyllostomus discolor	XP_028378317.1		-1.75

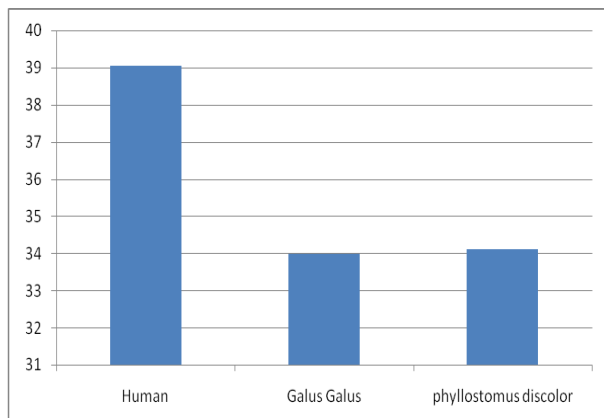
**Graph 1: Shows the Q-mean score.**

Structure Alignment: Structural Alignment is a fundamental approach for Homology Detection, functional annotation of novel protein structures. Protein structural alignment provides the evolutionary relationship between two or more protein structures. for the structural alignment we took the SARS-COV-2 spike glycoprotein and ACE2 protein from Different organism's host. And their alignment scores are given in the forms of RMSD score, RMSD shows the alignment score of the said structures ranging from 33.988 to 39.052, usually, lowest RMSD values shows better the model is in the comparison to the target Structure shown in (Graph:2).

Table 2: Shows alignment between SARS-COV-2 glycoprotein and host ACE2 Protein.

Sr_no	Organism name	Alignment Structure	RMSD score
1	Human		39.052
2	Galus Galus		33.988

3	Phyllostomus discolor		34.118
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Graph 2: shows RMSD score between SARS-COV-2 glycoprotein and host ACE2 Protein.

RESULT AND CONCLUSION

In these study we implement Different Bioinformatics methods, programs and tools to predict the 3 dimensional Protein Structure from the sequence and also do the protein structure alignment and calculate the RMSD score between targeted Structures i.e SARS-COV-2 spike glycoprotein and ACE2 from Different host organisms. Q-mean shows the Quality score of the predicted structure as nearer to zero shows good Quality of the structure shown in (graph:1). RMSD shows the degree of the structural similarity between two or more structures usually, lowest RMSD values shows better the model is in the comparison to the target Structure shown in (Graph:2).

it will lead practitioners to study the coevolution and relationship in between the virus (SARS-COV-2) & host (human, galus galus & Phyllostomus discolor), also to study the conserved Domains between SARS-COV-2 spike glycoprotein and targeted host ACE2 receptor based on protein structure alignment and root mean square deviation (RMSD) score.

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