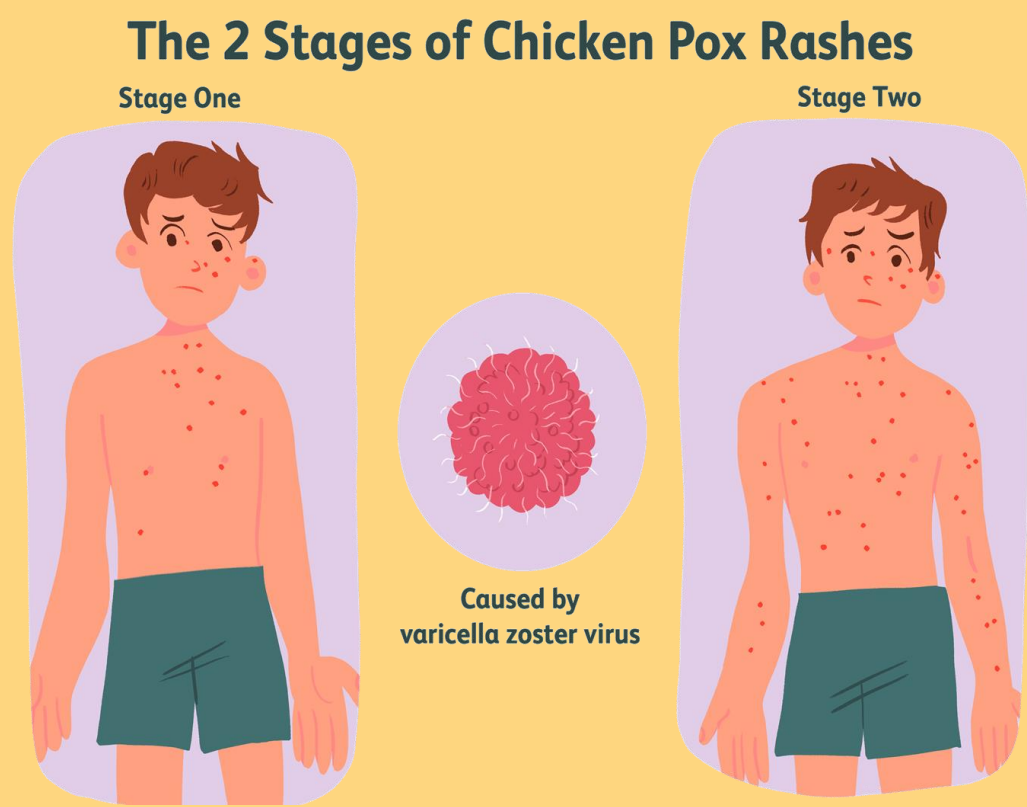


A Comparative *Insilico* Study in *Catharanthus roseus* Phytochemicals against Chickenpox

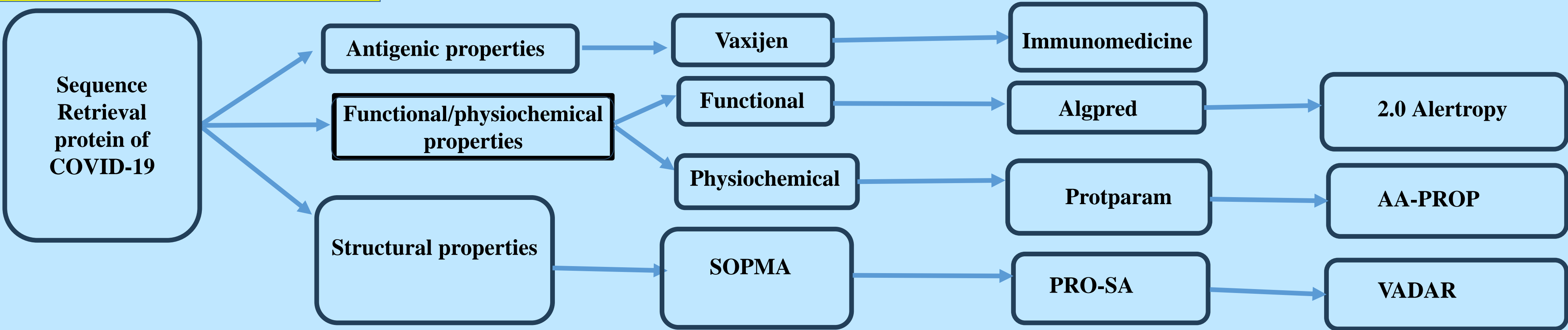
INTRODUCTION

- Chickenpox, also known as varicella, is a highly contagious viral infection primarily caused by the Varicella-Zoster virus. It is most common in children under the age of 10 but can affect individuals of all ages.
- Symptoms may include fever, headache, and a general feeling of malaise before the rash appears and virus spread through by direct contact of rashes.
- Commercially acyclovir drug has been used for chickenpox viral infection, it is specifically designed to target herpesviruses and may not be effective against other viral infections.
- The medicinal properties of *Catharanthus roseus* and its inherent alkaloids, such as vincristine and vinblastine have been used in the treatment of certain cancers.
- The present research focuses on developing a novel protein ligand complex through *insilico* docking studies by using *Catharanthus roseus* through leaf extraction



Stages of chickenpox and its characteristics

MATERIALS AND METHODS



RESULTS

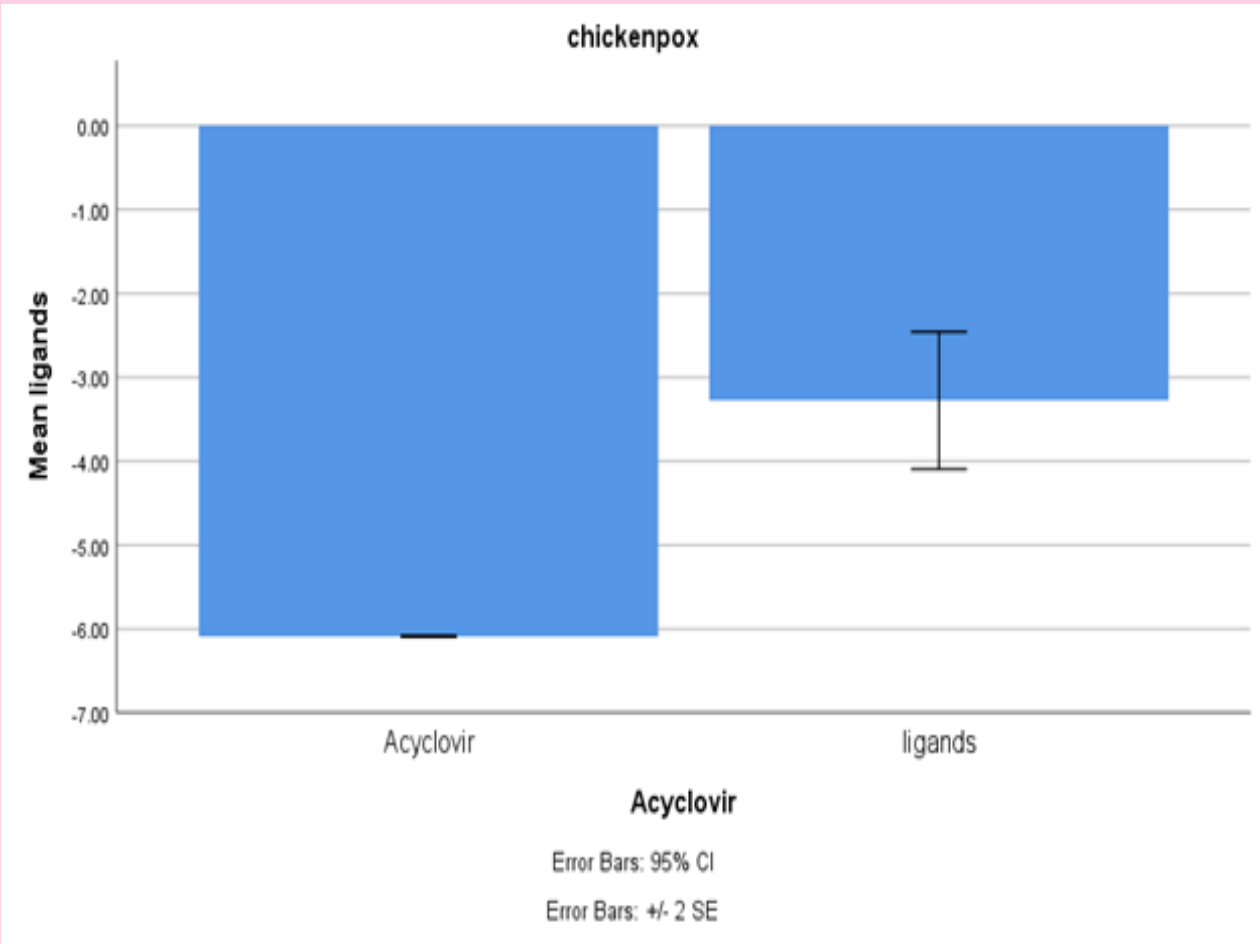


Fig. 1. Bar chart representing the mean binding affinity of Acyclovir and Ligand

Protein sequence	Antigenic properties				
	VaxiJen		Immunomedicine		
	Antigenic score Threshold = 0.4	Antigenic nature	Average antigenic propensity	Antigenic determinants	Antigenic plot sequence
ORF61	0.4772	Probable antigen	1.0189	16	

Table 1. Antigenic Properties of the selected epitopes of chickenpox

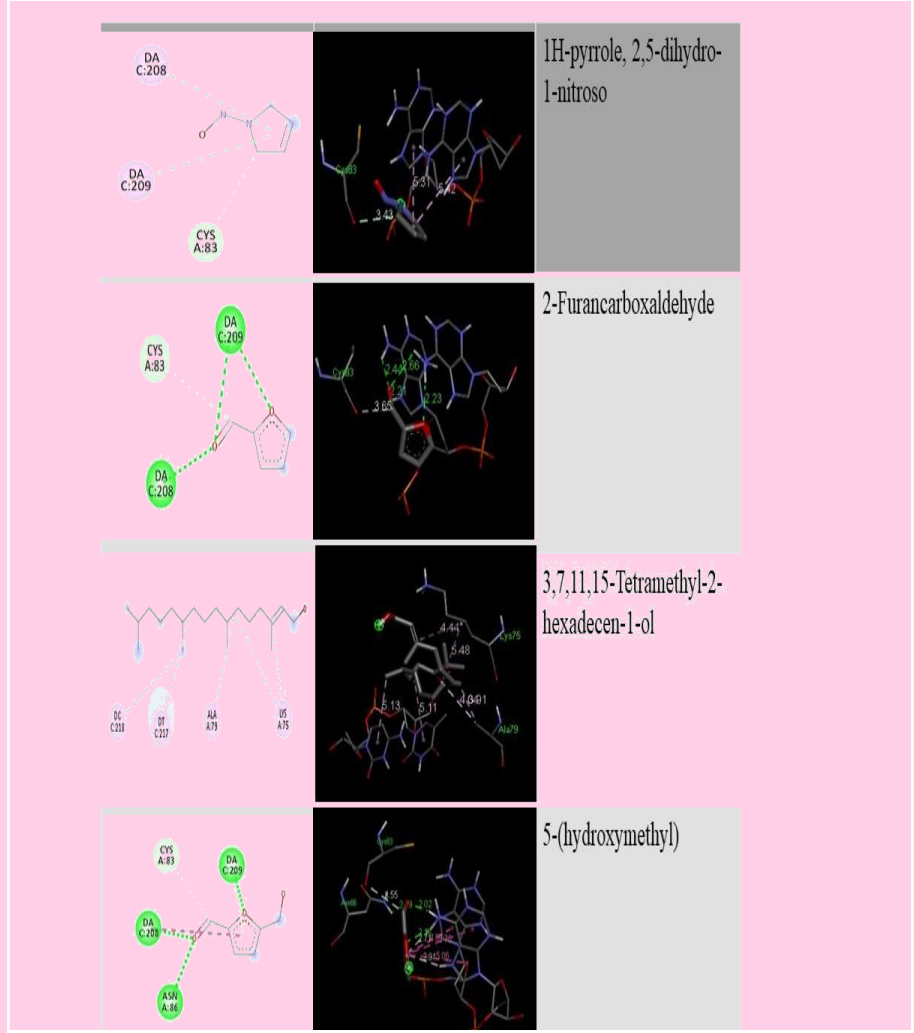


Table 2. 2D and 3D representations of docking results of Chickenpox

DISCUSSION AND CONCLUSION

- The epitope with PDB ID 1IF1 was shown to be the most suitable receptor for targeting an antiviral medication against chickenpox based on structural and epitope modelling with the highest binding affinity of -5.1kcal/mol.
- The comparison between the antidrug against Chickenpox as control group and ligands of *Catharanthus roseus* as study group indicates a statistical significance between the two groups (p=0.018, p < 0.05)
- After being discovered by GC-MS analysis, four compounds were used as ligands in docking experiments. 2-Furancarboxaldehyde, 5-(hydroxymethyl), 1H-pyrrole, 2,5-dihydro-1-nitroso, and 3,7,11,15-Tetramethyl-2-hexadecan-1-ol are the ligands that have been found.
- The current study merely demonstrates an immunoinformatic method for assessing a potential drug as an alternative to Acyclovir and their interactions with the phytochemicals found in *C.roseus*, which will spur further *insilico* research to develop an effective Chickenpox antiviral drug.
- The secondary protein structures with access to the number of alpha helices, beta turns, and coils of the antigenic chains of ORF61 were obtained from tabulated SOPMA.

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