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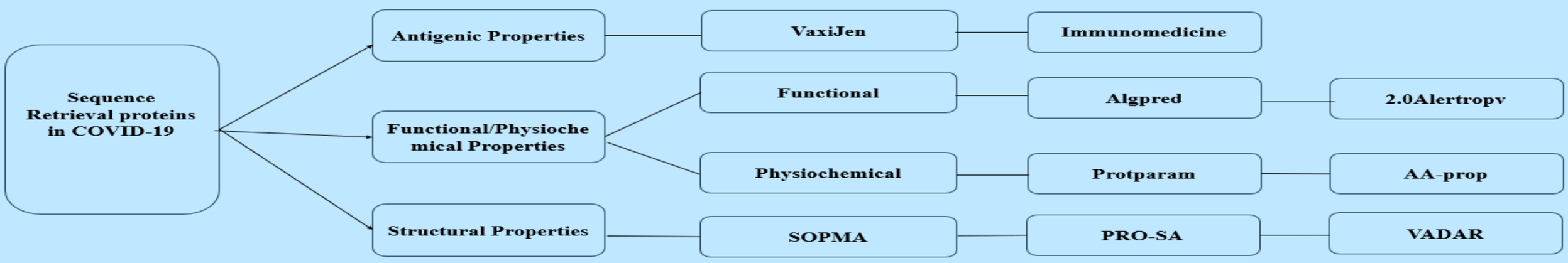
Insilico Analysis of *Catharanthus roseus* Phytochemicals for their Antiviral potential against COVID-19

INTRODUCTION

- **COVID-19, short for "Coronavirus Disease 2019," is an infectious respiratory illness caused by the novel coronavirus SARS-CoV-2. *COVID-19* symptoms vary but can include fever, cough, shortness of breath, fatigue, loss of taste or smell, and sore throat.**
- **The medicinal properties of *Catharanthus roseus* and its inherent alkaloids, such as vincristine and vinblastine have been used in the treatment of certain cancers**
- **Remdesivir is an antiviral medication that has been used in the treatment of COVID-19. Some of the drawbacks and considerations associated with Remdesivir include; nausea, vomiting, and changes in liver enzymes, which may require monitoring during treatment.**
- **The present research introduces an *insilico* approach to identify a novel potential ligand to target the disease causing S-glycoprotein of COVID-19 thereby giving a futuristic perspective to develop a novel sustainable medication against COVID-19.**

Symptoms of COVID-19

MATERIALS AND METHODS



RESULTS

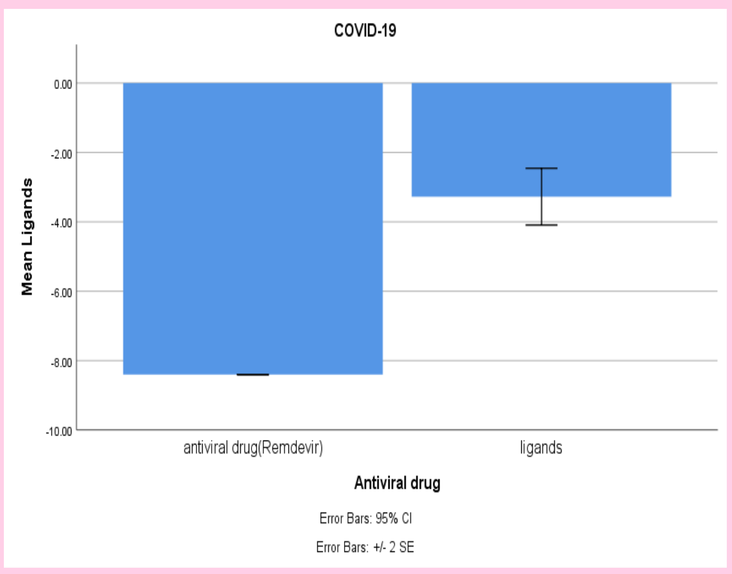


Fig. 1. Bar chart representing the mean binding affinity of Remdevir and Ligand

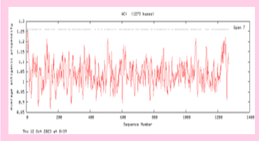
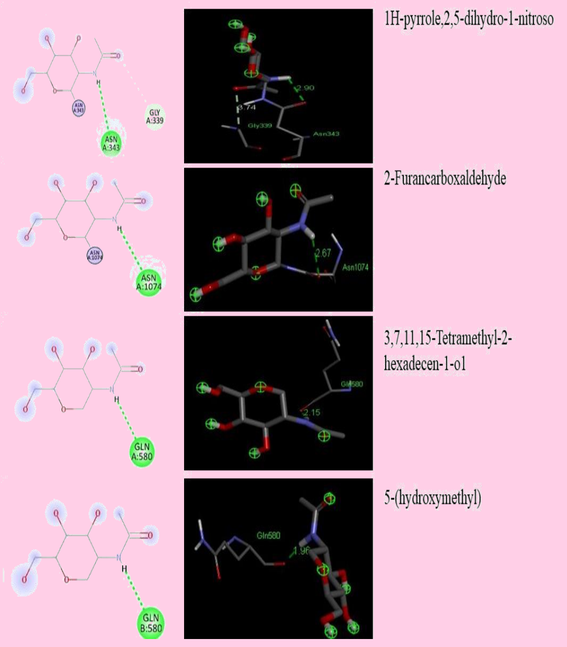
.	Antigenic properties				
Protein sequence	VaxiJen		Immunomedicine		
	Antigenic score Threshold = 0.4	Antigenic nature	Average antigenic propensity	Antigenic determinants	Antigenic plot sequence
s-glycoprotein	0.4592	Probable antigen	1.0411	63	

Table . Antigenic Properties of the selected epitopes of COVID-19



2D and 3D representations of docking results of COVID-19

DISCUSSION AND CONCLUSION

- **Four compounds were identified through GC-MS analysis and were subjected as a ligand for docking docking studies. The identified ligands are 2-Furancarboxaldehyde, 5-(hydroxymethyl), 1H-pyrrole, 2,5-dihydro-1-nitroso, and 3,7,11,15-Tetramethyl-2-hexadecen-1-ol.**
- **The secondary protein structures with access to the number of alpha helices, beta turns, and coils of the antigenic chains of S-glycoprotein were obtained from tabulated SOPMA findings.**
- **The comparison between the antidrug against COVID-19 as control group and ligands of *Catharanthus roseus* as study group indicates a statistical significance between the two groups ($p=0.018$, $p < 0.05$)**
- **From structural and epitope modelling, the epitope with PDB ID 6VYB was found to be the best suited receptor for targeting antiviral drug against COVID-19.**
- **The current study merely demonstrates an immunoinformatic method for assessing a potential drug as an alternative to Remdesivir and their interactions with the phytochemicals found in *C.roseus*, which will spur further *insilico* research to develop an effective COVID-19 antiviral drug.**

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