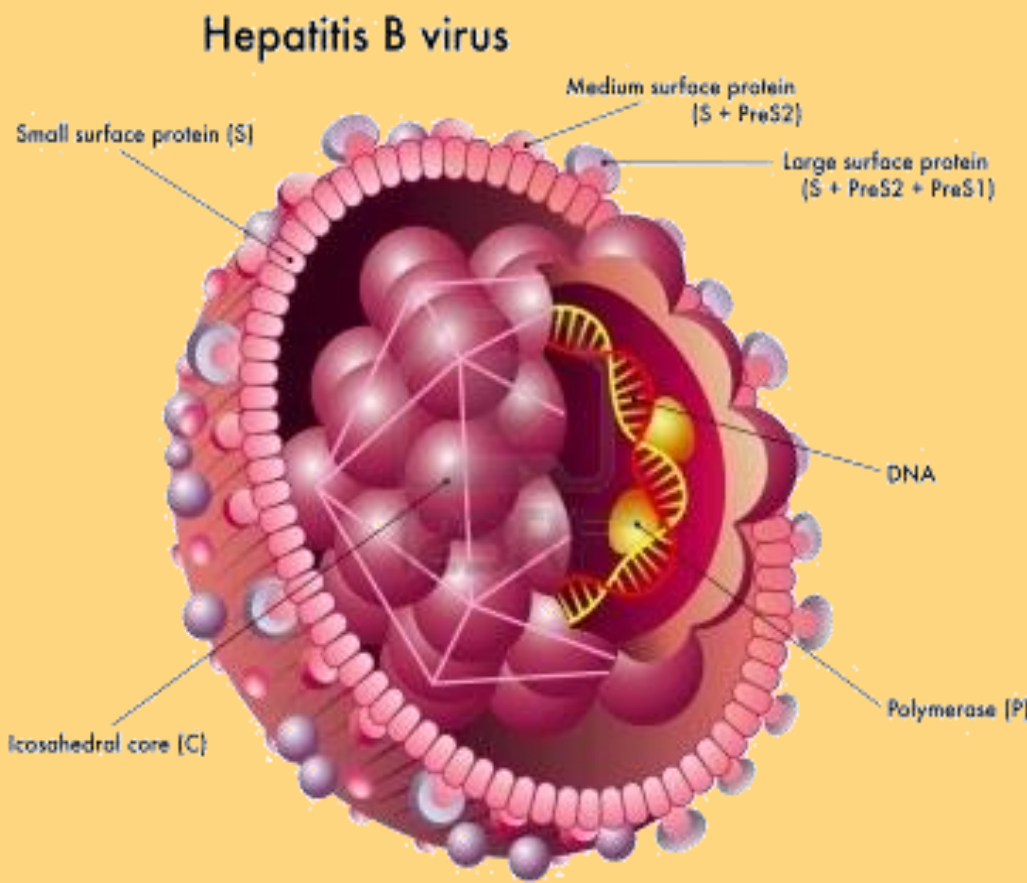


Phytochemical profiling of *Catharanthus roseus* for Potential Anti Hepatitis-B activity, an *Insilico* Approach

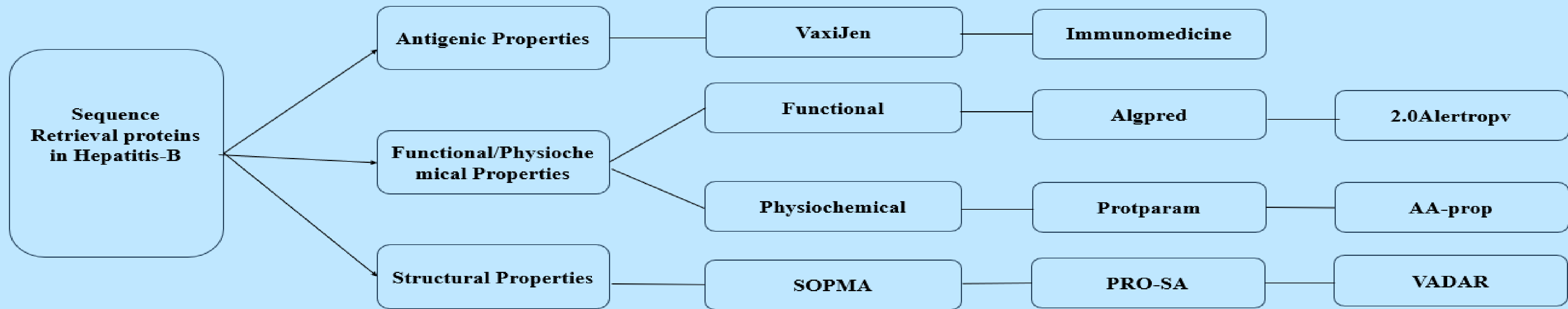
INTRODUCTION

- Hepatitis B can lead to acute and habitual liver complaints being a major cause of liver- related complications, including cirrhosis and liver cancer.
- Common modes of HBV include unprotected sexual intercourse, sharing needles or syringes, mother-to-child transmission during childbirth, and exposure to infected blood or open sores.
- Tenofovir is an antiviral medication that is commonly used in the treatment of chronic hepatitis B infection. Available in two forms: tenofovir disoproxil fumarate (TDF) and tenofovir alafenamide (TAF)
- 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 aim of this present research introduces an *insilico* approach to identify a novel potential ligand to target the disease causing protein thereby giving a futuristic perspective to develop a novel sustainable medication against effective diseases.



Hepatitis B Virus characteristics

MATERIALS AND METHODS



RESULTS

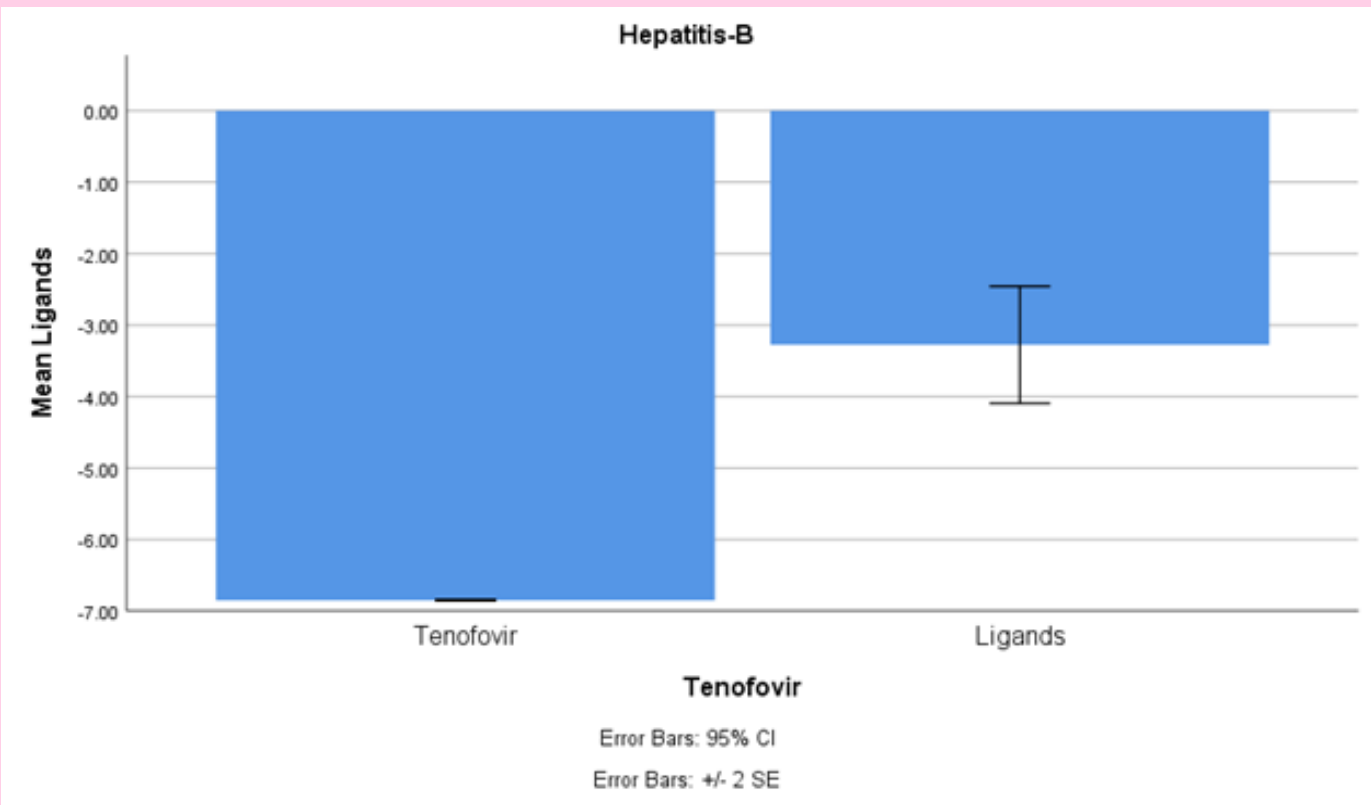
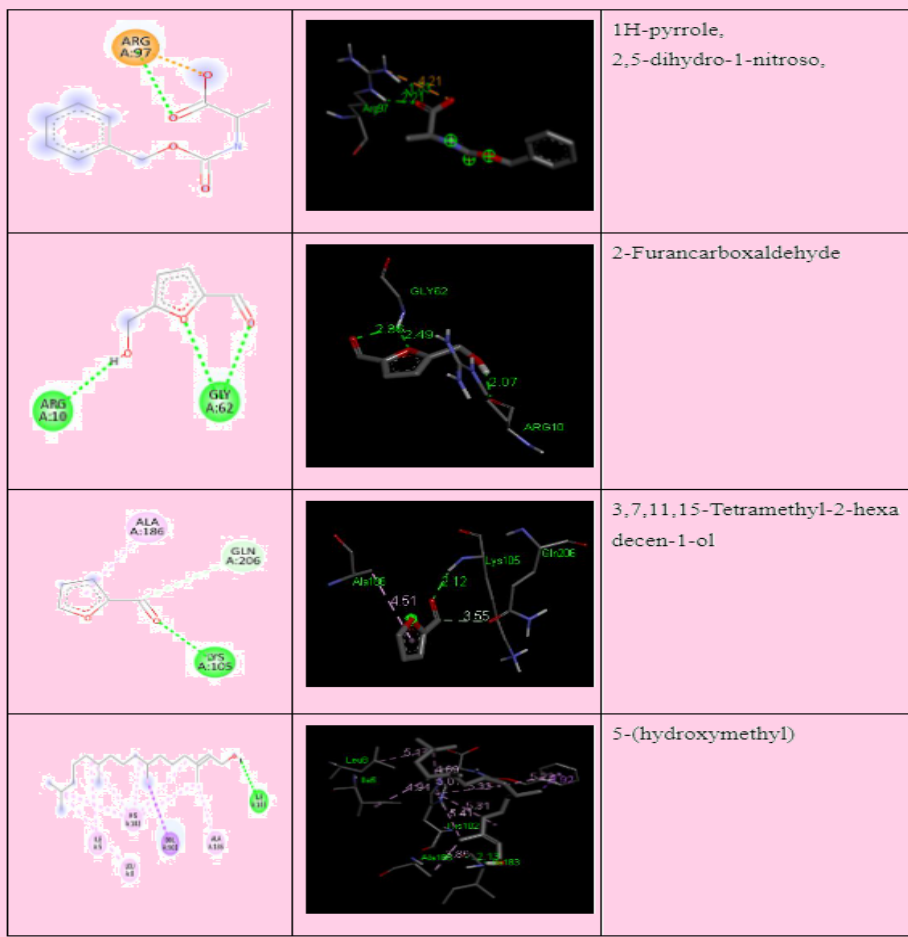


Fig. 1. Bar chart representing the mean binding affinity of Tenofovir and Ligand

Protein sequence	Antigenic properties				
	VaxiJen		Immunomedicine		
	Antigenic score Threshold = 0.4	Antigenic nature	Average antigenic propensity	Antigenic determinants	Antigenic plot sequence
DNA protease	0.5872	Probable antigen	1.0488	35	

Table . Antigenic Properties of the selected epitopes of Hepatitis-B virus



2D and 3D representations of docking results of HBV

DISCUSSION AND CONCLUSION

- GC-MS analysis was used to identify four compounds, which were then used as ligands in docking tests. 2-Furancarboxaldehyde, 5-(hydroxymethyl), 1H-pyrrole, 2,5-dihydro-1-nitroso, and 3,7,11,15-Tetramethyl-2-hexadecen-1-ol are the ligands that have been found.
- The secondary protein structures with access to the number of alpha helices, beta turns, and coils of the antigenic chains of DNA protease were obtained from tabulated SOPMA findings.
- The comparison between the antidrug against Hepatitis-B 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)
- The epitope with PDB ID 2HN7 was discovered to be the most suitable receptor for targeting antiviral medication against Hepatitis-B.
- The current study merely demonstrates an immunoinformatic method for assessing a potential drug as an alternative to Tenofovir and their interactions with the phytochemicals found in *C.roseus*, which will spur further *insilico* research to develop an effective Hepatitis-B antiviral drug.

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