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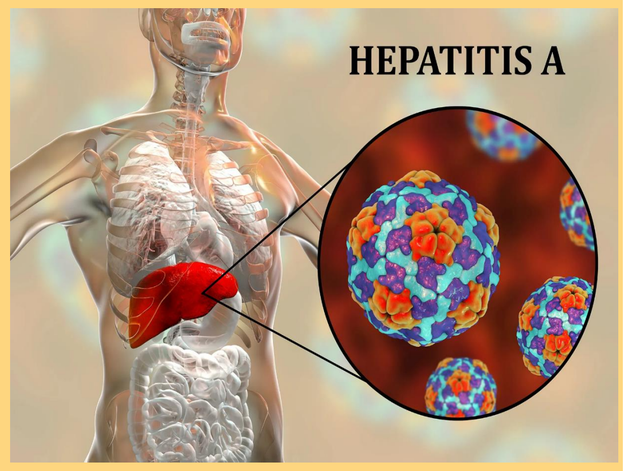
Assessing the Potential of Anti Hepatitis-A activity of *Catharanthus roseus* Phytochemicals using Immunoinformatics

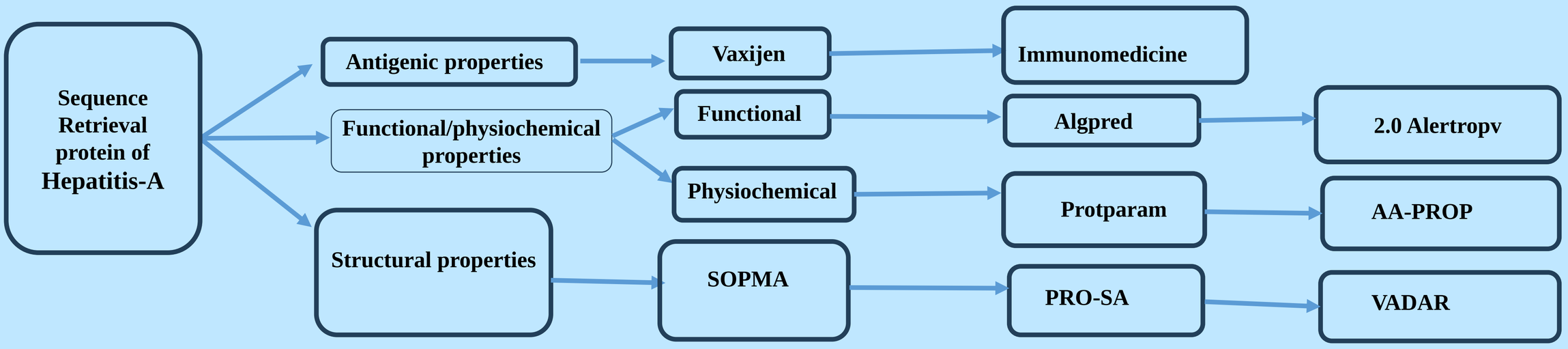
INTRODUCTION

- Hepatitis A is a highly contagious liver infection caused by the hepatitis A virus (HAV). It is typically transmitted through the ingestion of contaminated food or water or through close contact with an infected person.
- Existing commercially available antiviral drug for Hepatitis-A include Havrix that contains inactivated hepatitis A virus. The main drawback of using the Havrix vaccine is that it provides protection specifically against hepatitis
- A virus infection but not against other forms of hepatitis, such as hepatitis B or C.
- The medicinal properties of *Catharanthus roseus* and its inherent alkaloids, such as vincristine and vinblastine have been used in the treatment of certain cancers
- *Catharanthus roseus* also plays a major role in traditional medicine in various culture for treating a range of ailment.
- 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.



Characteristics of Hepatitis-A Virus

MATERIALS AND METHODS



RESULTS

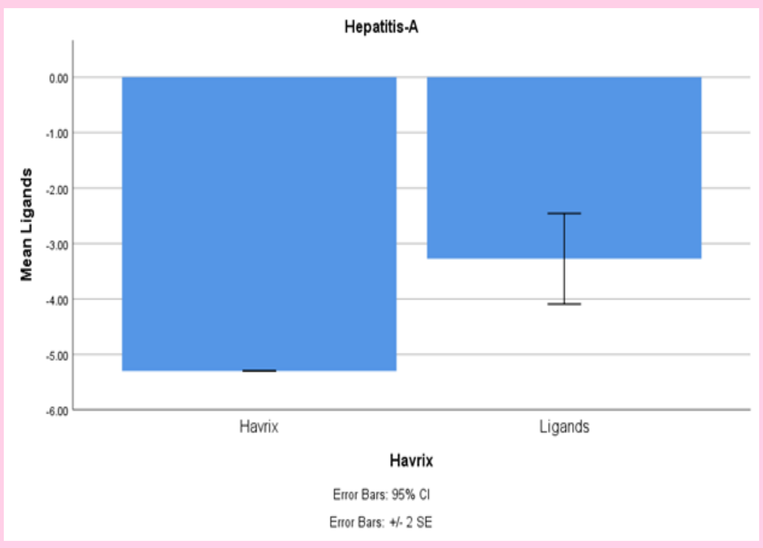


Fig. 1. Bar chart representing the mean binding affinity of Havrix and Ligand

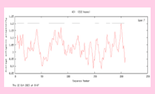
Protein sequence	Antigenic properties				
	VaxiJen		Immunomedicine		
	Antigenic score Threshold = 0.4	Antigenic nature	Average antigenic propensity	Antigenic determinants	Antigenic plot sequence
3C protease	0.4981	Probable antigen	1.0296	7	

Table 1. Antigenic Properties of the selected epitopes of Hepatitis-A virus

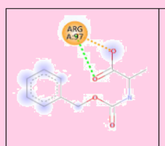
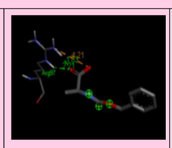
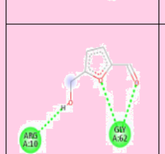
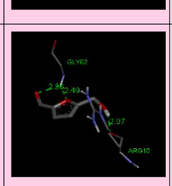
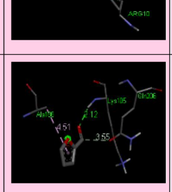
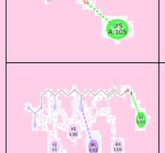
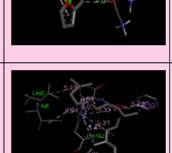
		1H-pyrrole, 2,5-dihydro-1-nitroso,
		2-Furancarboxaldehyde
		3,7,11,15-Tetramethyl-2-hexadecen-1-ol
		5-(hydroxymethyl)

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

DISCUSSION AND CONCLUSION

- Four compounds were identified through GC-MS analysis and were subjected as a ligand for docking studies, the highest binding affinity of -5.1 kcal/mol was observed.
- The secondary protein structures with access to the number of alpha helices, beta turns, and coils of the antigenic chains of HAV 3C protease were obtained from tabulated SOPMA findings.
- The comparison between the antidrug against Hepatitis-A as control group and ligands of *Catharanthus roseus* as study group indicates a statistical significance between the two groups ($p=0.018$, $p < 0.05$)
- Table 2. shows the 2D and 3D representations of docking findings of phytochemical substances docked to HAV 3C protease of Hepatitis.
- According to structural and epitope modelling, the epitope with PDB ID 2CXV is the most suitable receptor for antiviral medication targeting in the treatment of hepatitis-A.
- The current study merely demonstrates an immunoinformatic method for assessing a potential drug as an alternative to Havrix and their interactions with the phytochemicals found in *C.roseus*, which will spur further *insilico* research to develop an effective Hepatitis-A antiviral drug.

BIBLIOGRAPHY

- Ciocca, Emily T., Kristen A. Staggers, Jennifer Carey, Antone R. Opekun, F. Blaine Hollinger, Wendy A. Keitel, Robert L. Atmar, Hana M. El Sahly, and Jennifer A. Whitaker. 2024. “Delays in Hepatitis A Vaccination in People with HIV in Houston, Texas between 2010 and 2018.” Vaccine: X 16 (January): 100422.
- Syeda, Anjum Mobeen, and K. Riazunnisa. 2020. “Data on GC-MS Analysis, in Vitro Anti-Oxidant and Anti-Microbial Activity of the Catharanthus Roseus and Moringa Oleifera Leaf Extracts.” *Data in Brief* 29 (April): 105258.
- Maynard, J. E. 1990. “Hepatitis B: Global Importance and Need for Control.” *Vaccine* 8 Suppl (March): S18–20; discussion S21–23.
- Rosner, B. n.d. “Fundamentals of BioCistatistics (The 7th Edition).” *Boston, MA: Brooks/Cole*.
- Derived from Catharanthus Roseus in the Active Site of Trypanosoma Cruzi by Molecular Docking.” *Research, Society and Development* 11 (5): e23711528114–e23711528114.