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Targeting Human Bocavirus: *In-Silico* Identification of Promising Antiviral Peptides

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Abstract
Human bocavirus (HBoV) is a significant pathogen associated with respiratory and gastrointestinal diseases in children. Developing antiviral medications for HBoV is essential for effectively managing infections and minimizing complications in this vulnerable population. Antiviral peptides offer a promising strategy for precise and efficient treatment against HBoV. This study utilized in-silico methods to identify potential antiviral peptides for HBoV, focusing primarily on the VP1 protein, which plays a crucial role in viral infection by facilitating viral entry, replication, and pathogenesis. The protein sequence of VP1 was retrieved from the UniProt database, and its secondary and three-dimensional structures were predicted using PSIPRED and AlphaFold2, respectively. The predicted protein structure was refined using the GalaxyRefine server and assessed for structural integrity and quality using the PROCHECK and ProSA servers. Promising antiviral peptides were identified from the CAMPR4 database, and their three-dimensional structures were obtained from the PDB database. These antiviral peptides were subjected to docking studies with the VP1 protein of HBoV. The docking studies showed that the MBD-4 (11-40) / P9 [H21R, K23R, K28R] P9R peptide had the highest binding energies, making it the most effective antiviral peptide, followed by VP1-1RPB (Rp 71955), VP1-2FBS (LL-37), VP1-1BDS (Antihypertensive protein BDS-1), VP1-2MM6 (Alstotide S1), and VP1-2DD6 (Dermaseptin-4). This study establishes a foundation for future *in vitro* and *in vivo* research, aiming to develop potent antiviral treatments for HBoV.
Key words:

Keywords
Antiviral peptides, Human bocavirus, anti-microbial peptides, three-dimensional structure, in-silico studies.

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INTRODUCTION
Human Bocavirus is classified as a member of the Bocaparvovirus genus in the Parvoviridae family. It has been associated to acute respiratory infections, mainly in children between the ages of 6 and 24 months. HBoV was first identified in nasopharyngeal aspirates (NPA) from children with respiratory tract infections (RTI) in 2005 using PCR screening and subsequent sequencing techniques (Allander et al., 2005). There are four distinct species of the virus that have been identified: HBoV1, HBoV2, HBoV3, and HBoV4. HBoV1 is commonly linked to respiratory infections, (Kapoor et al., 2009; Arthur et al., 2009; Kapoor et al., 2010). HBoV1 has been detected in children with RTI that occur both in non-hospital settings and in various hospital studies, with a prevalence ranging from 2.2% to 18.4% (Christensen et al., 2010; Wu et al., 2014; Calvo et al., 2016;

Principi et al., 2015; Uršič et al., 2012). The presence of the virus has been identified in multiple countries, such as Australia, Canada, Croatia, France, Hong Kong, Pakistan, Saudi Arabia, and Tunisia (Ljubin-Sternak et al., 2021). Research has shown that HBoV can exist simultaneously with other viruses such as human rhinovirus, human adenovirus, and respiratory syncytial virus. The virus has been identified in respiratory and fecal samples, indicating its capacity to cause infections in various bodily systems (Arden et al., 2006; Weibrich et al., 2006).

HBoV is a linear single-stranded DNA virus with a genome of approximately 5 kb in length (Deng et al. 2014). The capsids of HBoV consist of major capsid protein VP2 and minor capsid protein VP1, with VP2 thought to constitute 95% of the whole capsid structure (Kim & Kim, 2016).

The VP1 protein of HBoV is crucial for viral infection as it contributes to the infectivity and replication of the virus. VP1, a capsid protein, is primarily responsible for the infectivity of HBoV. It contains essential motifs and regions necessary for viral entry, replication, and pathogenesis. The nuclear localization signal (NLS) within the VP1 protein guides the viral genome to the nucleus, facilitating viral replication and gene expression (Tu et al. 2015). Studies have identified phospholipase A2 motifs within the VP1-unique (VP1u) region of HBoV genomes, which are essential for viral infectivity. These motifs, along with other structural elements like the calcium-binding loop and catalytic residues, are critical for the replication and spread of the virus (Kapoor et al., 2010). Additionally, the VP1 protein is involved in the expression of viral capsid proteins (VP1, VP2, and VP3), highlighting its role in the assembly of infectious virions (Zou et al., 2016). The VP1 unique region (VP1u) of HBoV has been associated with virus infectivity and induction of inflammation in host cells. This region contains motifs and activities like secreted phospholipase A2 (sPLA2), contributing to the pathogenesis of lower respiratory tract illnesses (Chiu et al., 2014). Furthermore, the VP1 protein is essential for preventing premature termination of transcription of the cap mRNA from the native genome, demonstrating its importance in viral gene expression and replication (Yan et al., 2019).

Antiviral peptides exhibit significant promise in the treatment of human bocavirus owing to their specificity, efficacy, and potential for inducing fewer adverse effects in comparison to traditional antiviral medications (Xia et al., 2018). Antiviral therapy is essential because HBoV infections can be severe, and there are no specific treatment or vaccine that specifically combat this virus. Antiviral peptides have the capacity to specifically target viral proteins or essential viral replication processes, resulting in potent inhibitory effects against viral infections (Xia et al., 2018). Antiviral medication is essential for the treatment of human bocavirus (HBoV) infections, especially in children, due to the potential for severe respiratory illnesses such as acute wheezing, bronchiolitis, and pneumonia (Allander et al., 2007; AL-Iede et al., 2023). The efficacy and broad-spectrum utility of antiviral peptides in combating various viruses, including coronaviruses, influenza viruses, and herpes simplex viruses, is exemplified by their utilization. This encompasses their potential efficacy against HBoV (Xia et al. (2018).

The importance of developing antiviral peptides for human bocavirus medication lies in their capacity to deliver precise therapy, suppress viral replication, and bolster the host immune response against the virus (Xia et al., 2018). Antiviral peptides have the ability to interrupt the process of viral entry, hinder the replication of viruses, and regulate the immune responses of the host in order to effectively combat viral infections (Xia et al., 2018).

Therefore, this study aims to predict antiviral peptides against Human Bocavirus (HBoV) using in-silico approaches. These findings will be valuable for subsequent in-vitro and in-vivo studies to develop a novel therapeutic approach for HBoV. For this purpose, the VP1 protein of HBoV was selected to identify potential antiviral peptides.

The development of antiviral peptides targeting the VP1 protein of Human Bocavirus (HBoV) is considered novel due to several key factors. The VP1 protein of HBoV plays a crucial role in viral infectivity, replication, and pathogenesis (Shao et al., 2021). Targeting VP1 with antiviral peptides presents a unique opportunity to disrupt essential viral functions, potentially inhibiting viral entry, replication, and spread.

MATERIALS AND METHODS

Collection of Sequences

The VP1 protein sequence of HBoV1 was retrieved from the Uni Prot database: (https://www.uniprot.org/uniprotkb?query=%28+human+bocavirus+%29).

The sequence was analysed using Prot Param to determine its phytochemical characteristics. Additionally, sequences of antimicrobial peptides (AMPs) were collected from the CAMPR4 database (Collection of Anti-Microbial Peptides, http://www.camp.bicnirrh.res.in/seqDb.php?page=0). Criteria for selecting AMPs included sequence

length (1-100 mer), experimental validation, experimentally elucidated structure, antiviral activity, natural and synthetic origins, and viral taxonomy.

Screening of Antiviral Peptides

The obtained peptide sequences were further investigated for their AMP probability using the Antimicrobial Peptide Scanner vr.2 (https://www.dveltri.com/ascan/v2/), with a threshold cutoff value of >0.5.

Study of Physiochemical Properties of AMPs

The potential antiviral peptide (AMPs) sequences were analysed using the ProtParam tool (https://web.expasy.org/protparam/) to determine their key physicochemical properties, including molecular weight, theoretical pI, instability index, net charge, and grand average of hydropathicity (GRAVY). Peptides with a theoretical pI greater than 40 were selected for further study. Further, the peptides were evaluated for hydrophobicity and hydrophilicity using the PEPTIDE 2.0 server (https://www.peptide2.com/N_peptide_hydrophobicity_hydrophilicity.php).

Additionally, the solubility of the peptides was assessed using the Protein-Sol server (https://protein-sol.manchester.ac.uk/). Peptides which were shown hydrophobicity and hydrophilicity more than 30% were considered for further docking studies. This comprehensive evaluation ensures the selection of peptides with optimal properties for antiviral activity and stability.

Study of Physiochemical Properties of VP1

The retrieved VP1 protein of HBoV was subjected to ProtParam to determine its physiochemical properties, as mentioned above. Structure Prediction and Validation of VP1 of HBoV. The secondary structure of VP1 of HBoV was initially predicted using PSIPRED (http://bioinf.cs.ucl.ac.uk /psipred/) and SOPMA (https://npsa-pbil.ibcp.fr/cgibin/npsa_automat.pl?page=/NPSA/npsa_sopma.html). The three-dimensional structure of VP1 was then predicted using AlphaFold 2 (Jumper et al., 2021) and refined using the GalaxyRefine module (https://galaxy.seoklab.org/cgibin/submit.cgi?type=REFINE). The predicted and refined 3D structure of VP1 was evaluated using the PROCHECK (http://bioinf.cs.ucl.ac.uk/psipred/&uuid=56b7f320-1e5b-11ef-80c1-00163e100d53) and ProSA (https://prosa.services.came.sbg.ac.at/prosa.php) servers. Molecular Docking of VP1 and AMPs Molecular docking is an essential step to understand the interaction between the ligand and receptor. In this study, VP1 was considered the receptor and the potential AMPs as ligands. Protein-protein docking was conducted using the ClusPro server (https://cluspro.org/login.php) (Kozakov, D. et al., 2017). Initially, the selected potential AMPs' three-dimensional structures were collected from the PDB structure database, further refined using the Galaxy Refine server, and used as ligands in this study. Based on the binding energies between VP1 and the antiviral peptides, the most potential candidate was chosen.

RESULTS AND DISCUSSION

The development of effective antiviral treatments for Human Bocavirus is imperative for various reasons. HBoV is a notable pathogen that causes respiratory and gastrointestinal illnesses in children, resulting in severe symptoms, hospitalizations, and long-term health problems (Alam et al., 2015). Young children and individuals with pre-existing conditions are at a higher risk of experiencing severe complications, such as bronchiolitis, pneumonia, and asthma exacerbations, as a result of HBoV (Calvo et al., 2015). At present, there are no specific antiviral treatments or vaccines accessible for HBoV, underscoring the necessity for the development of focused antiviral therapies (Chow & Esper, 2009). Administering efficient antiviral treatments can decrease the occurrence of illness and death related to these infections in children (Mietzsch et al., 2017). In this context, this study aims to predict potential antiviral peptides against HBoV using in-silico approaches. To meet this objective, the VP1 protein was selected as the target due to its significant role in virus entry, replication and pathogenicity. The VP1 sequence of HBoV (Q3YPH4) was retrieved from the UniProt database, containing 671 amino acid residues with a molecular weight of 75,085.21 Da. The ProtParam server predicted the physicochemical characteristics of the protein, including a theoretical pI of 8.30, an instability index (II) of 34.54, an aliphatic index of 60.64, and a grand average of hydropathicity (GRAVY) of -0.658. The instability index value suggests that the protein is stable.

The instability index (II) is a crucial metric used to assess the stability of proteins. An instability index value below 40 indicates protein stability, while a value exceeding 40 suggests protein instability (Dauda et al., 2017; Shukla et al., 2018). This threshold of 40 serves as a critical point in determining whether a protein is likely to be stable or unstable.

Table 1. Section of antimicrobial peptides from CAMP$_{R4}$ database.

Title	UniProt_id	Camp_ID	PDBID	Source_Organism	Seqence	Length	Prediction_Class	Prediction_ Probability
Dermaseptin-4	P80280	CAMPSQ 467	2DCX,2DD6	Phyllomedusa sauvagii	ALWMTLLKKVLKAAAKALNAVLVGANA	27	AMP	1
Mytilin-B	P81613	CAMPSQ 564	2EEM	Mytilus edulis	SCASRCKGHCRARRCGYYVSVLYRGRCYCKCL RC	34	AMP	1
Human Defensin-5	Q01523	CAMPSQ 730	1ZMP,3I5W,4E82,4E8 3,4E86	Homo sapiens	ATCYCRTGRCATRESLSGVCEISGRLYRLCCR	32	AMP	1
Rp 71955	P37046	CAMPSQ 754	1RPB	Actinomycete Sp9440	CLGIGSCNDFAGCGYAVVCFW	21	AMP	1
Palicourein	P84645	CAMPSQ 762	1R1F	Palicourea condensata	GDPTFCGETCRVIPVCTYSAALGCTCDDRSDG LCKRN	37	AMP	1
Vhl-1	P84522	CAMPSQ 763	1ZA8	Viola hederacea	CGESCAMISFCFTEVIGCSCKNKVCYLNSIS	31	AMP	1
Kalata-B8	P85175	CAMPSQ 956	2B38	Oldenlandia affinis	GSVLNCGETCLLGTCYTTGCTCNKYRVCTKD	31	AMP	1
Reptilian Defensin	P0CAP0	CAMPSQ 1028	2B5B	Caretta caretta	EKKCPGRCTLKCGKHERPTLPYNCGKYICCVP VKVK	36	AMP	1
Melittin	P01501	CAMPSQ 1142	1BH1,2MLT	Apis mellifera	GIGAVLKVLTTGLPALISWIKRKRQQ	26	AMP	1
Antihypertensiv e protein BDS-1	P11494	CAMPSQ 1178	1BDS,2BDS	Anemonia sulcata	AAPCFCSGKPGRGDLWILRGTCPGGYGYTSN CYKWPNICCYPH	43	AMP	1
Vhl-1	P84522	CAMPSQ 3000	1ZA8	Viola hederacea	SISCGESCAMISFCFTEVIGCSCKNKVCYLN	31	AMP	1
Retrocyclin-2		CAMPSQ 3108	2LZI	Synthetic construct	GICRCICGRRICRCICGR	18	AMP	1
Antiviral lectin scytovirin	P86041	CAMPSQ 3781	2QT4	Scytonema varium	GSGPTYCWNEANNPGGPNRCSNNKQCDGA RTCSSSGFCQGTS	95	AMP	1

Title	UniProt_id	Camp_ID	PDBID	Source_Organism	Seqence	Length	Prediction_Class	Prediction_ Probability
LL-37	P49913	CAMPSQ 11864	2FBS,2FBU,2FCG,2K6O,2LMF	Homo sapiens	RKPDPGPKGPTYCWDEAKNPGGPNRCSNSK QCDGARTCSSSGFCQGTAGHAAA LLGDFFRKSKEKIGKEFKRIVQRIKDFLRNLVPR TES	37	AMP	0.999
Human Defensin-5/HD5 [E21R]	Q01523,	CAMPSQ 19763	4RBX	Synthetic construct	ATCYCRTGRCATRESLSGVCRISGRLYRLCCR	32	AMP	1
Rev (34-50)	P05866	CAMPSQ 21860	1ULL	Synthetic construct	TRQARRNRRRRWRERQR	17	AMP	0.635
Antifungal protein PAFB	D0EXD3	CAMPSQ 23410	2NC2	Penicillium chrysogenum	KFGGECSLKHNTCTYLKGGKNHVVNCGSAA NKKCKSDRHHCEYDEHHKRVDCQTPV	56	AMP	0.999
MBD-4 (11-40) / P9 [H21R, K23R, K28R], P9R	P82019	CAMPSQ 23847	6M56	Synthetic construct	NGAICWGPCPTAFRQIGNCGRFRVRCCRIR	30	AMP	1
Alstotide S1	A0A1P7TZ77	CAMPSQ 24145	2MM6	Alstonia scholaris	CRPYGYRCDGVINQCCDPYHCTPPLIGICL	30	AMP	1

To achieve the objective of this study, antiviral peptides were collected from the CAMPR4 (Collection of Anti-Microbial Peptides) database, adhering to criteria such as sequence length (1-100 amino acids), experimental validation, elucidated structure, antiviral activity, natural or synthetic nature, and viral taxonomy. Based on these criteria, 24 AMP sequences were obtained (Table 1). The physicochemical properties of these peptides were analysed using the ProtParam server (Table 2).

Table.2 Physiochemical properties of antimicrobial peptides collected from CAMP$_{R4}$ database.

Title	Molecular weight	Theoretical pI	Net charge	Instability index		GRAVY
Dermaseptin-4	2779.47	10.48	4	10.38	stable	1.004
Mytilin-B	3981.76	9.58	9	44.3	unstable	-0.344
Human Defensin-5	3588.19	8.96	4	13.79	stable	-0.113
Rp 71955	2185.53	3.8	-1	33.82	stable	1.157
Palicourein	3928.43	4.78	-1	60.26	unstable	-0.189
Vhl-1	3340.94	6.1	0	45.6	unstable	0.69
Kalata-B8	3307.81	7.76	1	27.53	stable	-0.023
Reptilian Defensin	4080.98	9.39	7	31.6	stable	-0.608
Melittin	2847.49	12.02	5	44.73	unstable	0.273
Antihypertensive protein BDS-1	4714.42	8.64	3	29.18	stable	-0.309
Vhl-1	3340.94	5.85	0	56.12	unstable	0.69
Retrocyclin-2	2041.58	9.3	5	36.55	stable	0.517
Antiviral lectin scytovirin	9722.48	8.59	4	30.61	stable	-1.1
LL-37	4493.32	10.61	6	23.34	stable	-0.724
Human Defensin-5/HD5 [E21R]	3615.26	9.49	6	7.77	stable	-0.144
Rev (34-50)	2437.77	12.6	9	207.8	unstable	-3.459
Antifungal protein PAFB	6300.08	8.83	4	41.35	unstable	-1.121
MBD-4 (11-40) / P9 [H21R, K23R, K28R], P9R	3412.05	10.46	6	12.8	stable	-0.15
Alstotide S1	3373.96	6.7	0	37.59	stable	0.063

Table 3. Hydrophobicity and solubility of antimicrobial peptides.

Title	Hydrophobic	Acidic	Basic	Neutral	solubility
Dermaseptin-4	70.37%	0%	14.81%	14.81%	76.70%
Rp 71955	42.86%	4.76%	0%	52.38%	69.20%
LL-37	37.84%	13.51%	29.73%	18.92%	77.50%
MBD-4 (11-40) / P9 [H21R, K23R, K28R], P9R	36.67%	0%	20%	43.33%	62.70%
Alstotide S1	33.33%	6.67%	10%	50%	37.70%
Antihypertensive protein BDS-1	32.56%	2.33%	11.63%	53.49%	70.70%
Reptilian Defensin	27.78%	5.56%	27.78%	38.89%	0.863
Retrocyclin-2	22.22%	0%	27.78%	50%	--
Antiviral lectin scytovirin	22.11%	6.32%	11.58%	60%	0.795
Human Defensin-5	21.88%	6.25%	18.75%	53.13%	72.10%
Human Defensin-5/HD5 [E21R]	21.88%	3.13%	21.88%	53.13%	72.10%
Kalata-B8	16.13%	6.45%	9.68%	67.74%	71.50%

Using an AMP prediction probability cutoff value of >0.5 and considering 19 peptides ranging from 17 to 95 amino acids were selected. These were further screened based on the instability index, with a cutoff value of 40. Peptides with an instability index less than 40 were considered stable, resulting in the selection of 12 peptides. Their hydrophobicity and solubility were then analysed using the PEPTIDE 2.0 and SolPro servers.

In the Peptide Hydrophobicity/Hydrophilicity Analysis, peptides showing hydrophobicity above 30% were selected for further docking studies with VP1 of HBoV. The final 6 selected AMPs were Dermaseptin-4, Rp 71955, LL-37, MBD-4 (11-40) / P9 [H21R, K23R, K28R], P9R, Alstotide S1, and Antihypertensive protein BDS-1. The three-dimensional structures of these peptides were retrieved from the PDB database and used for docking studies (Fig.1).

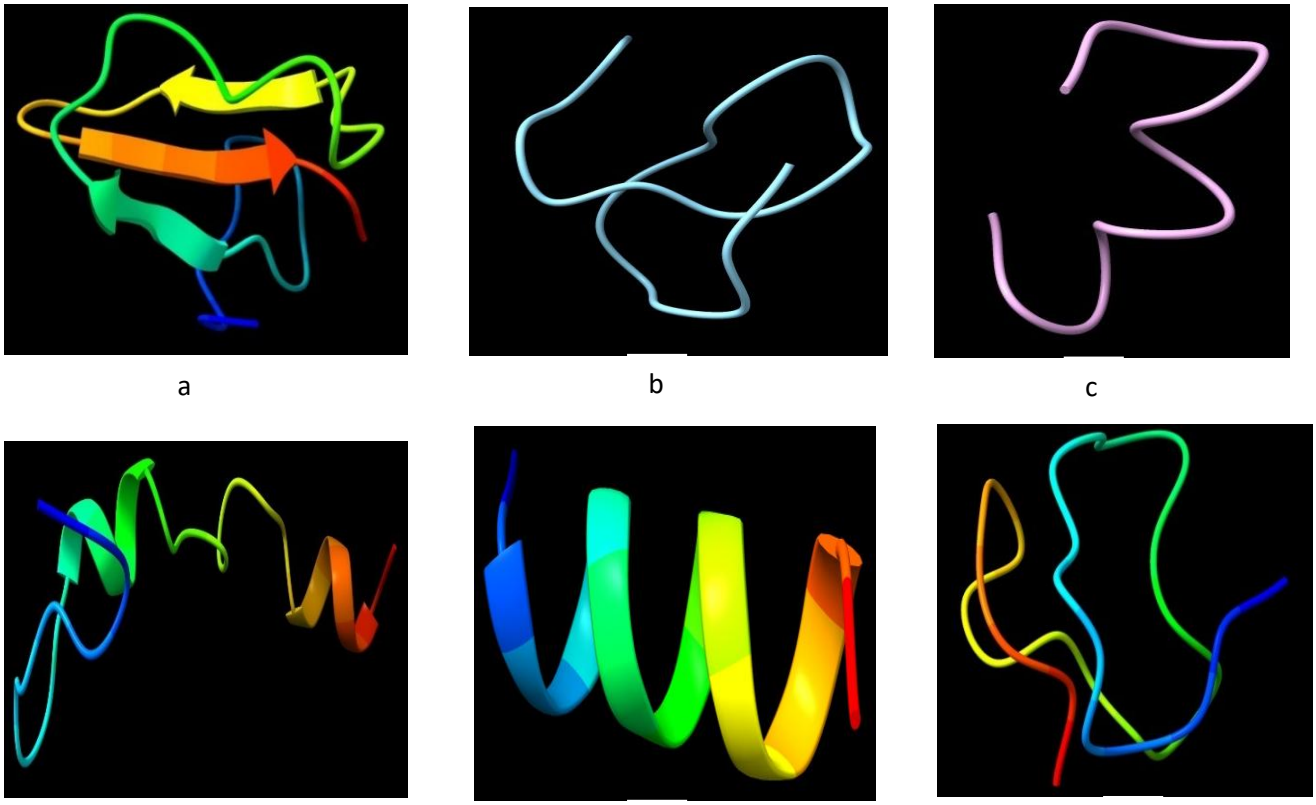

Fig.1 Antiviral peptides (AMPs) a) BDS, b)1RPB, c) 2DDB, d) 6M56, e) 2FBS, f) 2MM6

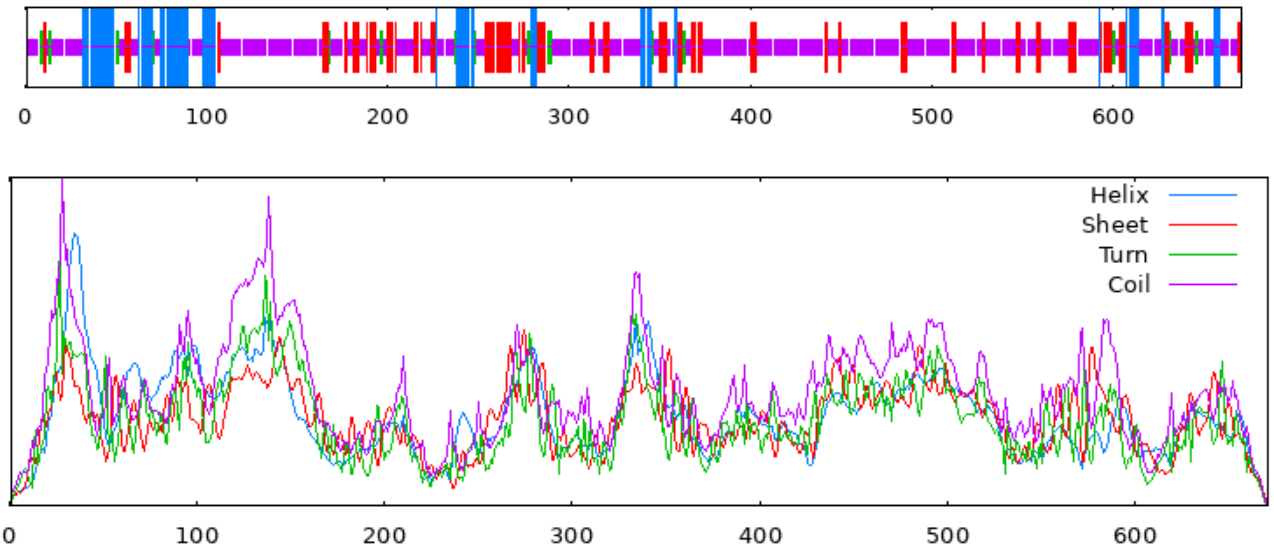

Fig.2 Secondary structure prediction of VP1 of HBoV by SOPMA.

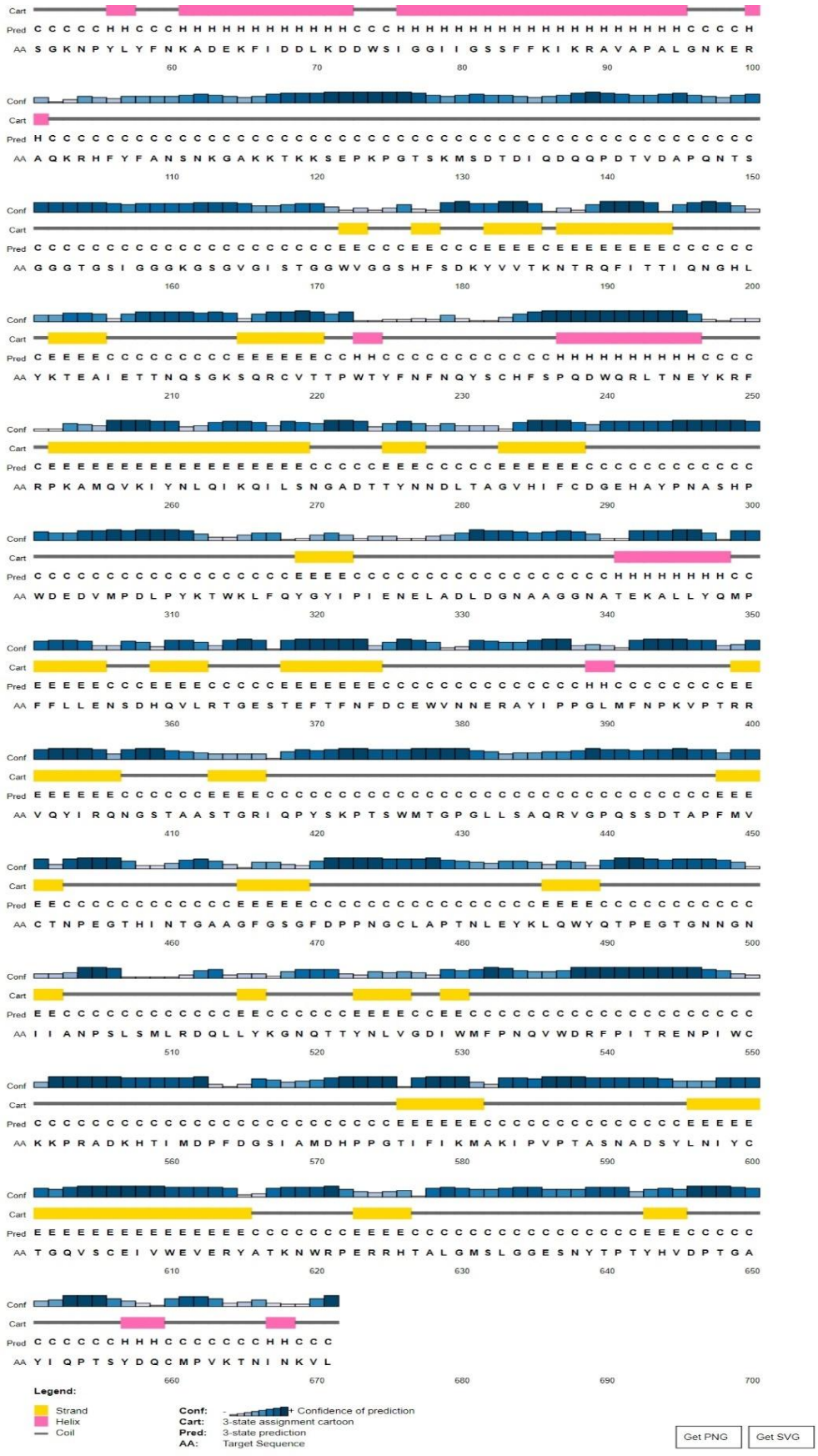

Fig.3 Secondary structure prediction of VP1 of HBoV by PSIPRED.

The secondary structure of the VP1 sequence was predicted using PSIPRED and SOPMA (fig.2&3), revealing that the sequence consists of alpha helices (12.97%), extended strands (18.93%), beta turns (3.73%), and random coils (64.38%). The 3D structure was predicted using AlphaFold 2 (fig.4). Developed by DeepMind, AlphaFold 2 has significantly transformed the field of structural biology by predicting the three-dimensional configurations of proteins with exceptional precision (Yang et al., 2023; Hegedüs et al., 2022). This AI system can accurately predict the atomic-level structure of proteins based on their amino acid sequences (Akdel et al., 2022). AlphaFold 2 has greatly expanded the range of protein sequences that can be structurally analysed due to its highly accurate predictions (Beuming et al., 2022). The model has demonstrated superior performance in predicting previously unknown protein structures, surpassing conventional methods such as standard docking approaches (Wilson et al., 2021; Lin et al., 2022).

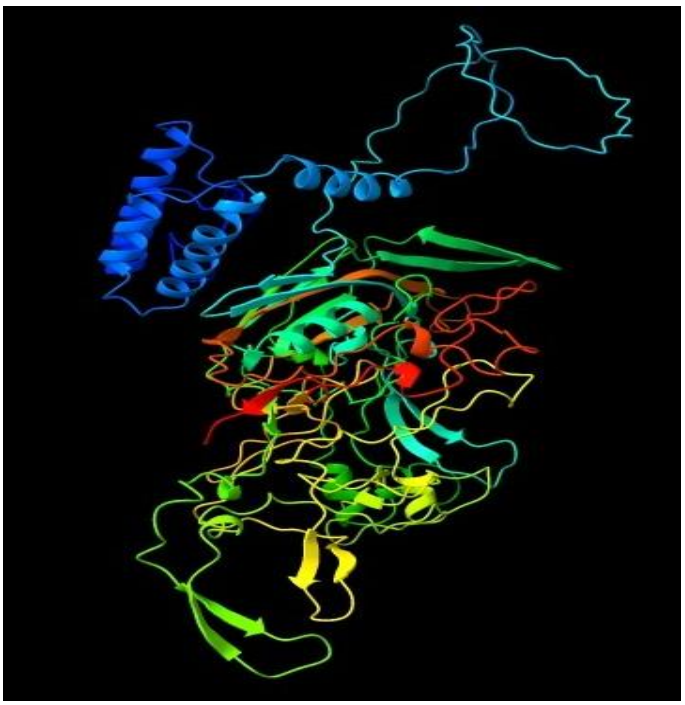

Fig.4 Prediction of 3D structure of VP1 protein of HBoV1 predicted by Alphafold2

The 3D structure that was designed underwent evaluation using PROCHECK and ProSA servers. These two servers are indispensable tools for assessing protein structures. PROCHECK is a software application created to evaluate the stereochemical accuracy of protein structures (Laskowski et al., 1993). This study conducts a thorough analysis of the stereochemistry of protein structures, providing valuable insights into possible inaccuracies or abnormalities in the arrangement of amino acids. PROCHECK is a commonly utilized tool for verifying the geometry and overall excellence of protein models, guaranteeing their adherence to established structural standards.

ProSA is an important tool for identifying errors in three-dimensional protein structures. Prosa, an abbreviation for Protein Structure Analysis, is a highly utilized software that assists in the improvement and verification of experimental protein structures. It is essential in the processes of structure prediction, modelling, and refinement, as it assists researchers in identifying and correcting structural inaccuracies or anomalies.

In the Ramachandran plot from PROCHECK analysis (fig.5a), the residues were distributed as follows: most favored regions (452 residues, 80.9%), additional allowed regions (66 residues, 11.8%), generously allowed regions (19 residues, 3.4%), and disallowed regions (22 residues, 3.9%). After further refinement of 3D structure using the GalaxyRefine server, the distribution improved to most favoured regions (522 residues, 93.4%), additional allowed regions (32 residues, 5.7%), generously allowed regions (2 residues, 0.4%), and disallowed regions (3 residues, 0.5%).

ERRAT analysis showed an overall quality factor of 89.9, and Verify3D analysis indicated that 80.48% of the residues had an averaged 3D-1D score of ≥0.1, suggesting the structure is "pass." The ProSA server provided a Z-score of -8.21, indicating that the

structure is close to those determined by X-ray crystallography (fig.5b). All these evaluation parameters suggest that the 3D structure of the VP1 protein of HBoV is of high quality and accuracy, comparable to experimentally determined structures.

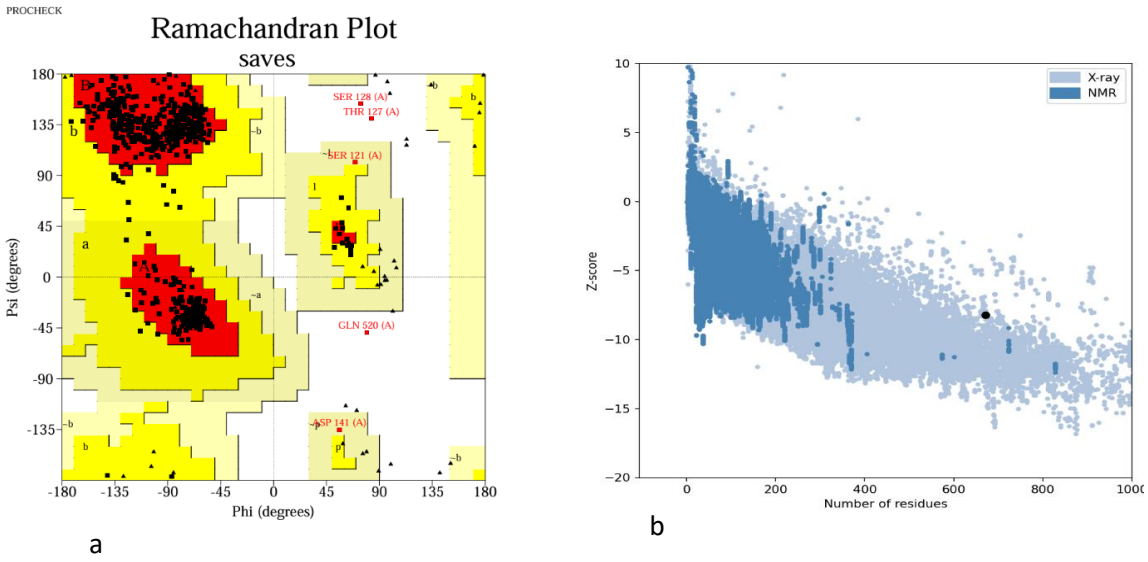

Fig.5 Evaluation of 3D structure of VP1 of HBoV. a) Ramachandran plot of VP1 structure of HBoV. b) Plot is generated by ProSA server to VP1 protein structure representing the Z score (-8.21)

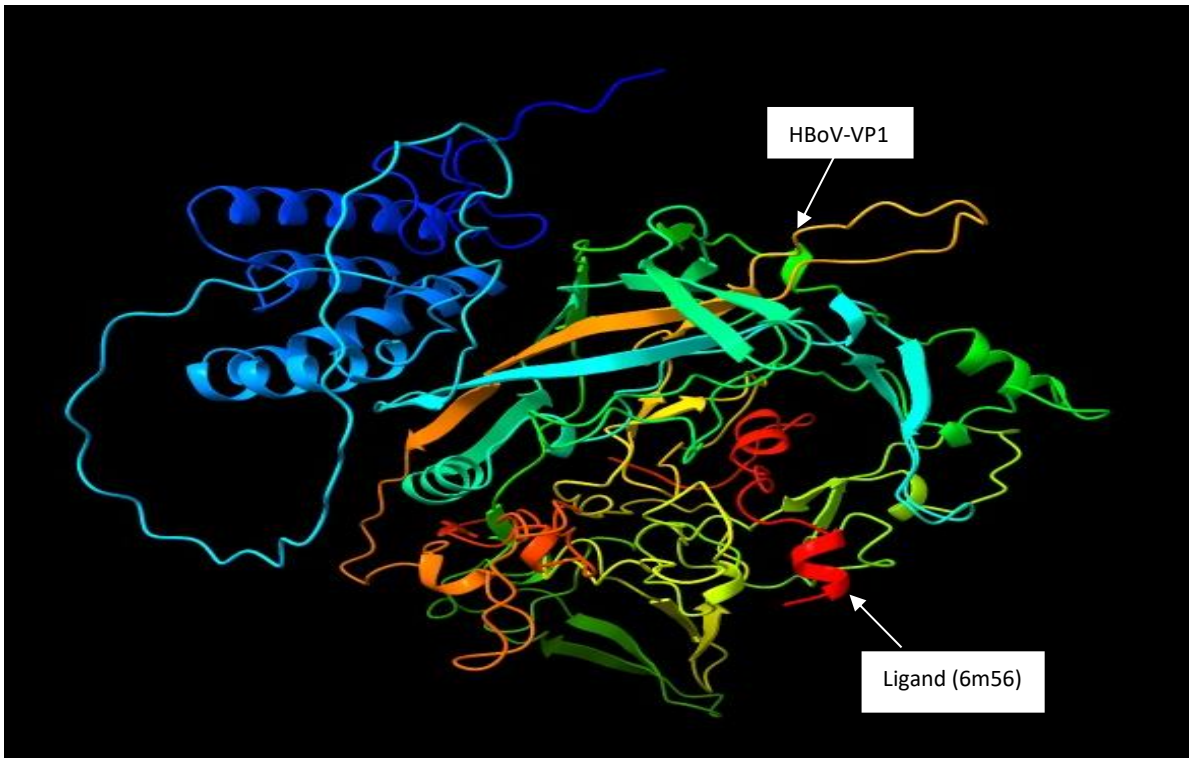

Fig.6 Molecular docking between HBoV-VP1 and 6M56 by ClusPro.

Protein-protein docking studies were conducted between the predicted VP1 3D structure and the validated AMPs with the following PDB structures (fig.6): Dermaseptin-4 (2DD6), Rp 71955 (1RPB), LL-37 (2FBS), MBD-4 (11-40) / P9 [H21R, K23R, K28R] P9R (6M56), Alstotide S1 (2MM6), and

Antihypertensive protein BDS-1 (1BDS). The VP1 protein structure acted as the receptor, while the AMP structures served as ligands. After successful docking, the binding energies for the complexes between VP1 and the AMPs were identified as follows: VP1-2DD6 (-790.2), VP1-1RPB (-1219.3), VP1-2FBS (-1019.5), VP1-6M56 (-1345.3), VP1-2MM6 (-955.7), and VP1-1BDS (-977.9).

The strength of interactions between a ligand and a receptor can be assessed by the binding energy values. In the context of ligand-receptor interactions, more negative binding energy values indicate stronger interactions between the ligand and receptor (Hermans & Wang, 1997). The free energy of binding decreases as the binding energy becomes more negative, signifying a more stable interaction between the ligand and the receptor (Hermans & Wang, 1997). These results suggest that the VP1-6M56 (MBD-4 (11-40) / P9 [H21R, K23R, K28R] P9R) complex had the lowest energy for interaction, indicating the strongest binding, followed by VP1-1RPB (Rp 71955),VP1-2FBS (LL-37), VP1-1BDS (Antihypertensive protein BDS-1), VP1-2MM6 (Alstotide S1), and VP1-2DD6 (Dermaseptin-4). This ranking highlights the potential effectiveness of these peptides, with VP1-6M56 being the most promising candidate for further investigation and development as an antiviral agent against Human Bocavirus (HBoV).

CONCLUSION

This study focuses on identifying potential antiviral peptides for human bocavirus (HBoV). Based on the role of VP1 in viral entry, replication, and pathogenesis, VP1 is considered the most promising target for antiviral strategies. Therefore, in-silico methods were used to predict potential antiviral peptides against the VP1 3D structure. Docking studies between thoroughly screened and selected antiviral peptides and HBoV's VP1 protein revealed that the most promising antiviral peptide was MBD-4 (11-40) / P9 [H21R, K23R, K28R] P9R. This research provides a foundation for further studies in both in vitro and in vivo settings to develop effective antiviral therapies against HBoV.

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Conflict of Interests

The authors declare no conflict of interest.

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