Defence Life Science Journal, Vol. 10, No. 4, October 2025, pp. 261-268, DOI : 10.14429/dlsj.21473

Harnessing Seabuckthorn (*Hippophae rhamnoides*) Surfactants for Human Metapneumovirus (HMPV): A Computational Approach

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ABSTRACT

Human metapneumovirus (HMPV) is a highly mutating respiratory virus that ruses the immune system with frequent mutations, creating a major health challenge. Lacking approved vaccines or treatments, there is a pressing need for effective antiviral therapies. Seabuckthorn (*Hippophae rhamnoides)* has many antioxidants, anti-inflammatory and antimicrobial activity, and might be the key to bridging this gap. In this research, we employed sophisticated computational molecular docking methods to investigate how some of the bioactive compounds of Seabuckthorn-palmitic acid, oleic acid, and palmitoleic acid-bound to the viral proteins of HMPV. We found that these compounds dock strongly to major viral protein targets, helping to indicate that these compounds might inhibit the functioning of the virus. These observations open the exciting possibility of therapeutic development of Seabuckthorn-derived compounds as safe and natural antiviral agents with the potential to overcome viral mutations, thus providing a new therapeutic avenue against HMPV infections.

Keywords: Human metapneumovirus; Seabuckthorn; Molecular docking; Antiviral agents; Computational drug discovery;

1. INTRODUCTION

A significant pulmonary pathogen known as Human metapneumovirus (HMPV), was discovered by Dutch researchers in 2001. It is intricately linked to the respiratory syncytial virus because it is a member of the Pneumoviridae family[1]. Retrospective studies reveal that HMPV has been in circulation since 1958, causing recurring seasonal epidemics, even though it was discovered more than 20 years ago[1]. Due to the limits of traditional diagnostic procedures like PCR and immunological testing, its identification was postponed until sophisticated technologies like randomly primed PCR demonstrated its genetic profile and evolutionary relationships to airborne pneumovirus[1].

1.1 Clinical Presentation

From minor upper respiratory issues like coughing, fever, and stuffiness in the nose to serious lower respiratory tract infections like pneumonia and bronchiolitis, HMPV is the cause of a variety of respiratory illnesses[2-3]. People over 65, immunocompromised individuals, and premature babies are among the vulnerable groups that are more likely to get serious infections that necessitate hospital stays[1,3-5]. Complications are particularly likely to occur in adults with underlying illnesses such as asthma or Chronic Obstructive Pulmonary Disease (COPD)[6-7]. The clinical similarity to influenza and other respiratory viruses complicates diagnosis, and specific PCR testing is necessary for confirmation[2,8].

1.2 Transmission and Epidemiology

Human metapneumovirus (HMPV) has specific seasonal activity, with outbreaks of the virus in late spring and late winter in the Northern Hemisphere, usually in co-circulation with influenza and RSV (CDC: About Human Metapneumovirus)[9]. Recent 2025 surveillance reported a spike in HMPV cases in China as well as in other areas, such as India, where two infant cases were reported in Bengaluru. Still, these follow cyclical seasonal trends and are not a new threat (Economic Times: HMPV reaches India). The virus's RNA nature is responsible for antigenic drift, resulting in strain variability globally, making developing a vaccine difficult[10] HMPV is spread through direct person-to-person contact, respiratory secretions, and contaminated surfaces, as with other respiratory pathogens, with an incubation period of 3-6 days[11].

Received : 18 June 2025, Revised : 29 August 2025
Accepted : 26 September 2025, Online published : 07 October 2025

1.3 Current Therapeutic Landscape

In 2025, there is no specific antiviral treatment or approved vaccines for HMPV, and treatment is centered on relieving the symptoms with over-the-counter drugs[10]. Challenges in vaccine development include the limited knowledge of viral pathogenesis and issues with choosing the correct animal model. Better developments include the starting of a phase 1 trial in July 2024 by the University of Oxford with an mRNA vaccine against both HMPV and the related virus, the respiratory syncytial virus (RSV), developed by Moderna (University of Oxford: RSV-HMPV vaccine trial)[10]. Another study investigates multi-epitope mRNA vaccine candidates, but these are still in the formative stages[11].

1.4 Seabuckthorn-A Natural Potential Remedy

The Himalayan native Seabuckthorn (*Hippophae rhamnoides*), which is grown all over the world, has been used for millennia in traditional medicine to treat wounds, respiratory ailments, and other ailments[4,13-15]. Flavonoids, carotenoids, and polyphenols are among the more than 190 bioactive chemicals in its diverse phytochemical composition, which suggests antiviral properties[12,15]. Its ability to combat influenza viruses through Studies has demonstrated antiviral activity, with extracts sometimes outperforming oseltamivir[15]. Its traditional applications and demonstrated antiviral action against similar respiratory illnesses provide the foundation for additional investigation, despite the lack of direct clinical evidence supporting its use against HMPV[14].

2. MATERIALS AND METHODS

2.1 Protein Retrieval and Preparation

Studying the Human metapneumovirus (HMPV) fusion protein; we retrieved its three-dimensional structure from the Protein Data Bank (PDB) (4CS7 | pdb_00004cs7), The HMPV fusion protein (UniProt ID: Q6WB97) and nucleoprotein (Q6WBA1) were preprocessed by removing water molecules and heteroatoms. as documented by Kahn[1]. To ensure a clean and efficient model, we used Discovery Studio Visualiser (BIOVIA, 2021) to remove water

Table 1. ADME analysis of three different ligands with reference range

Parameter	Palmitic acid	Oleic acid	Palmitoleic acid	Reference range
ABSORPTION				
Molecular weight (g/mol)	256.42	282.46	254.41	<500 (Lipinski's Rule)
LogP	6.45	7.64	6.25	-0.7 to 5.0
TPSA (Ų)	37.30	37.30	37.30	<140
HBD	1	1	1	≤5
HEBA	2	2	2	≤10
Water solubility	Poor	Poor	Poor	-
GI absorption	High	High	High	-
DISTRIBUTION				
BBB permanent	No	No	No	-
CNS permeability	-2.45	-2.67	-2.41	-3 to -2
Plasma protein binding	High	High	High	-
METABOLISM				
CYP1A2 inhibitor	No	No	No	-
CYP2C19 inhibitor	No	No	No	-
CYP2C9 inhibitor	No	No	No	-
CYP2D6 inhibitor	No	No	No	-
CYP3A4 inhibitor	No	No	No	-
EXCRETION				
Renal clearance	Low	Low	Low	-
Half-life (hrs)	12-16	14-18	12-15	-
TOXICITY				
Hepatotoxicity	No	No	No	-
Carcinogenicity	No	No	No	-
Mutagenicity	No	No	No	-
Cytotoxicity	No	No	No	-
LD50 (mg/kg)	>2000	>2000	>2000	-
Toxicity class	4 (Low)	4 (Low)	4 (Low)	1-6 scale

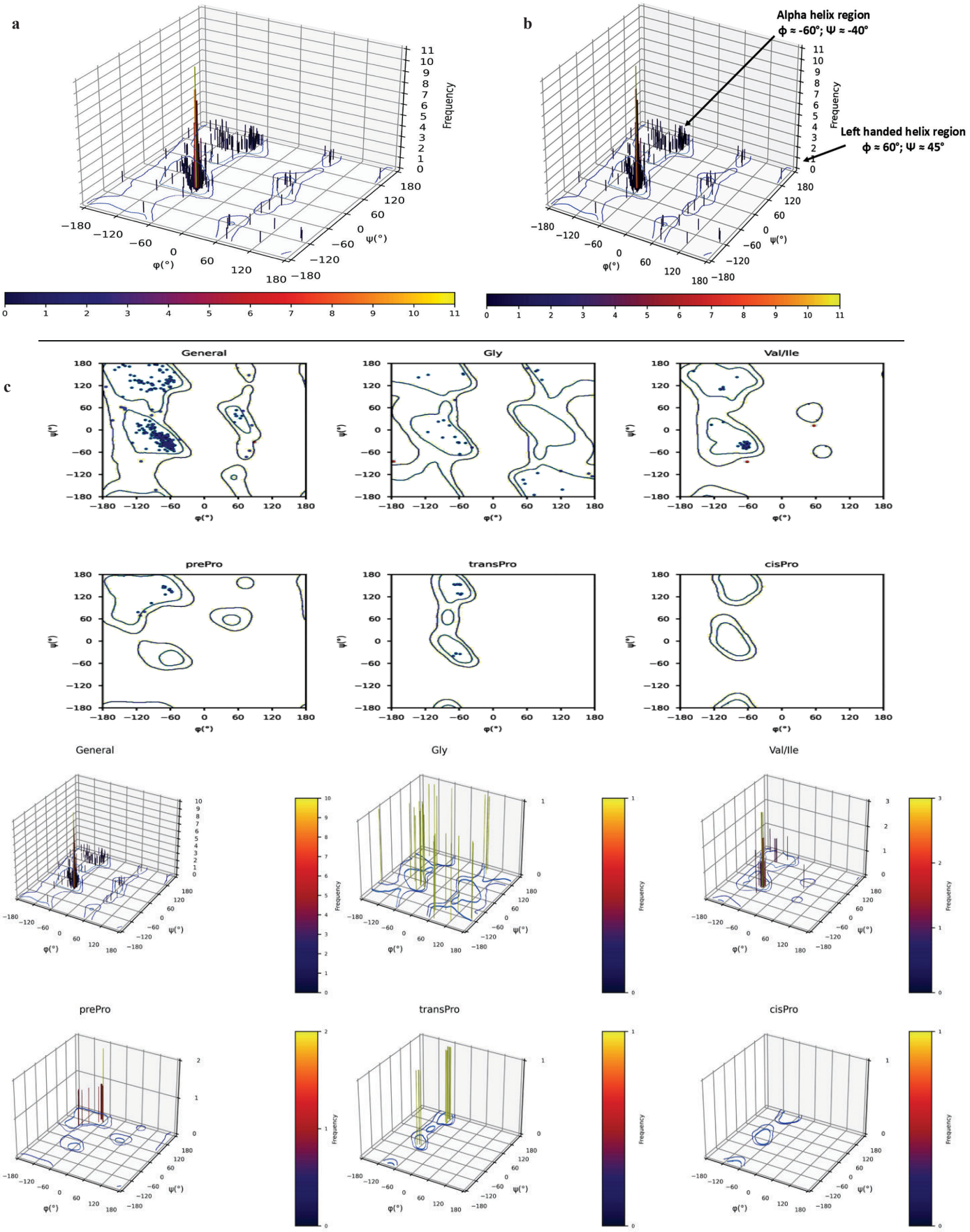

Fig. 1. (a) Ramachandran plot of the protein Q6WB97. Here, a-e represent 3D ramachandran plot; (b) annotated ramachandran plot; (c) collection of ramachandran plots of different variable amino acid residues; (d) frequency distribution of φ (phi) and ψ (psi) backbone dihedral angles in 3D configurations;

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+----------<<< P R O C H E C K    S U M M A R Y >>>----------+
|                                                            |
| /var/www/SAVES/Jobs/166820/saves.pdb   1.5                 676 residues |
|                                                            |
*| Ramachandran plot:   94.8% core    4.4% allow    0.2% gener    0.6% disall |
|                                                            |
*| All Ramachandrans:   20 labelled residues (out of 664)     |
+| Chi1-chi2 plots:      6 labelled residues (out of 449)     |
 | Side-chain params:    5 better     0 inside      0 worse   |
 |                                                            |
*| Residue properties: Max.deviation:    15.5          Bad contacts:    0 |
*|                     Bond len/angle:    5.5    Morris et al class:  1  1  2 |
 |                                                            |
 | G-factors           Dihedrals:  -0.04  Covalent:  -0.02    Overall:  -0.02 |
 |                                                            |
+| Planar groups:    92.2% within limits   7.8% highlighted      7 off graph |
 |                                                            |
 +------------------------------------------------------------+
   + May be worth investigating further.  * Worth investigating further.
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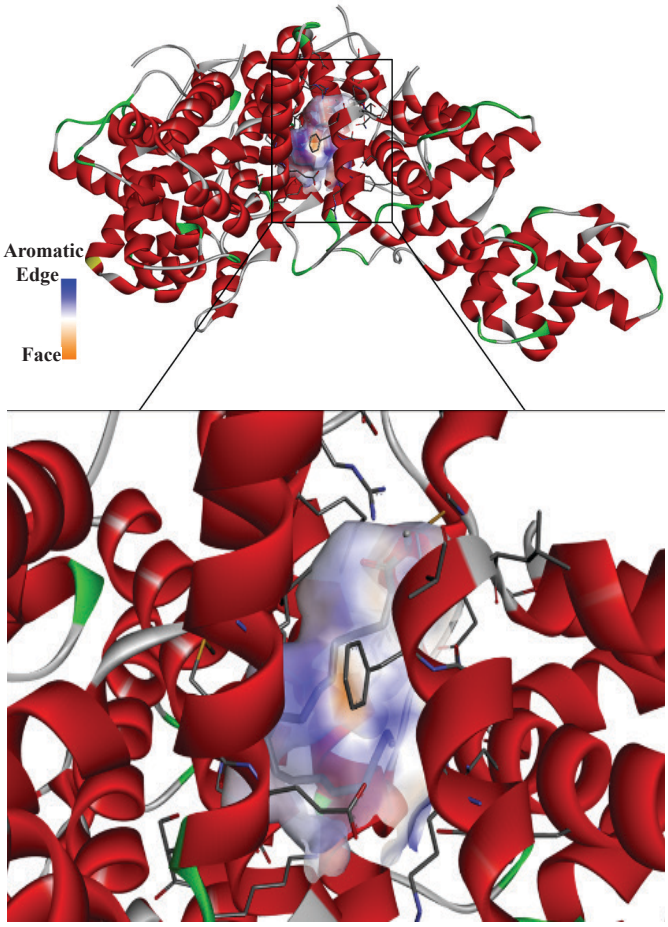
Figure 1. (e) procheck summary page of ramachandran plots.



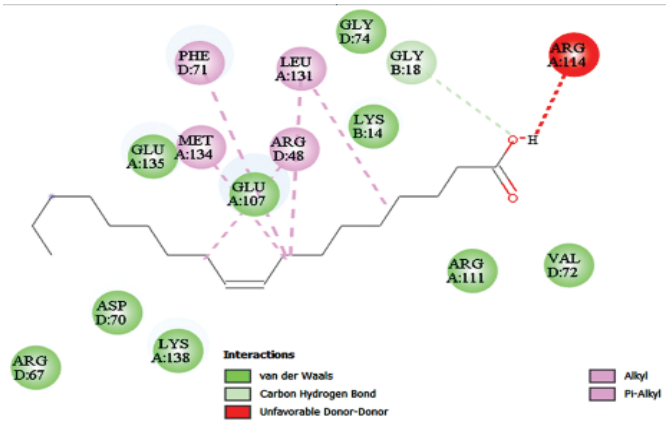


Figure 2. 2DInteraction of amino acid residues of Q6wb97 and oleic acid.

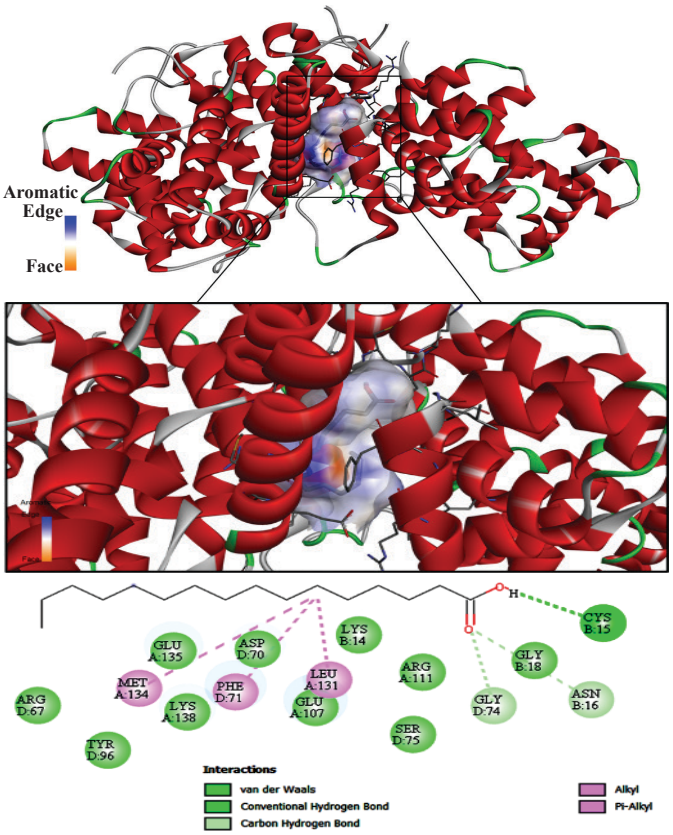


Figure 3. 2D Interaction of amino acid residues of Q6wb97 and palmitic acid.

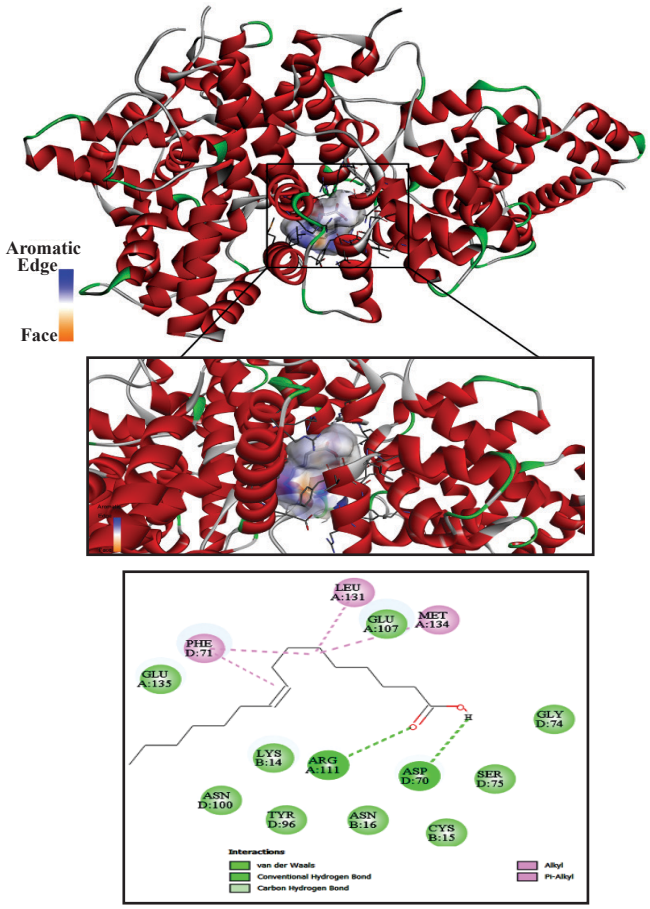


Figure 4. 2D Interaction of amino acid residues of Q6wb97 and palmitoleic acid.

molecules and any pre-existing ligands[16-17]. Subsequently, the protein structure has undergone optimisation and energy minimization with Swiss-PDB Viewer (Guex & Peitsch, 1997) to achieve a thermodynamically stable conformation suitable for downstream computational studies[18].

2.2 Ligand Preparation

Three bioactive compounds from Seabuckthorn (*Hippophae rhamnoides*)-palmitic acid, oleic acid, and palmitoleic acid-were selected for this study. All the molecular structures were obtained from the PubChem database[19]. The ligands-palmitic acid (PubChem CID: 985), oleic acid (CID: 445639), and palmitoleic acid (CID: 445638)-were downloaded in .sdf format from PubChem and converted to .pdb using Open Babel, Palmitic acid, oleic acid, and palmitoleic acid were selected based on their documented antiviral activity against enveloped viruses (e.g., influenza) and high bioavailability in Seabuckthorn extracts[12,15], and converted to .pdb format using Open Babel[20]. Using PyRx, energy minimization was performed with the MMFF94 force field to ensure optimal molecular conformations for docking analyses[21].

2.3 Active Site Prediction

Potential binding sites on the HMPV fusion protein were identified using the CASTp computational tool[22]. These potential binding sites were validated against literature data[1] to confirm biological relevance. Based on this validation, grid boxes were generated to define the search space for molecular docking.

2.4 Molecular Docking

Molecular docking was performed using Auto Dock Vina within the PyRx platform[21]. Grid boxes were centered at coordinates X, Y, Z with dimensions Å × Å × Å to encompass the active site identified by CASTp. Binding affinity values for each ligand-protein interaction were recorded and displayed below in the Table 2. Elucidate the molecular interactions, ligand binding sites, and protein-ligand interactions within the active site were visualised using Discovery Studio[16-17].

2.5 ADMET Prediction

The pharmacokinetic and toxicological profiles of the compounds were evaluated using the SwissADME[23] tool for Absorption, Distribution, Metabolism, and Excretion (ADME) properties and the ProTox-II[24] tool for toxicity assessment. This analysis covered key ADMET parameters, including absorption efficiency, distribution patterns, metabolic pathways, excretion mechanisms, and potential toxicity risks compiled in Table 1.

2.6 Ramachandran Plot Analysis

To validate the structural integrity of the HMPV protein model, the Ramachandran plots were generated using the PROCHECK validation suite[25]. This analysis allowed us to assess the stereochemical quality of the protein structure by examining the distribution of phi-psi angle combinations for all amino acid residues. Most residues were positioned within favored and additionally allowed regions, confirming acceptable stereochemical quality for the docking studies. Various 2D and 3D representations of the plot are shown in fig. 1. The provided figures collectively analyze and visualize

Table 2. The binding affinity of the best pose of the ligands

Ligand	Binding affinity	rmsd/ub	rmsd/lb
Oleic acid	-4.9	35.012	32.051
Palmitic acid	-4.2	24.56	22.796
Palmitoleic acid	-4.4	2.389	1.469

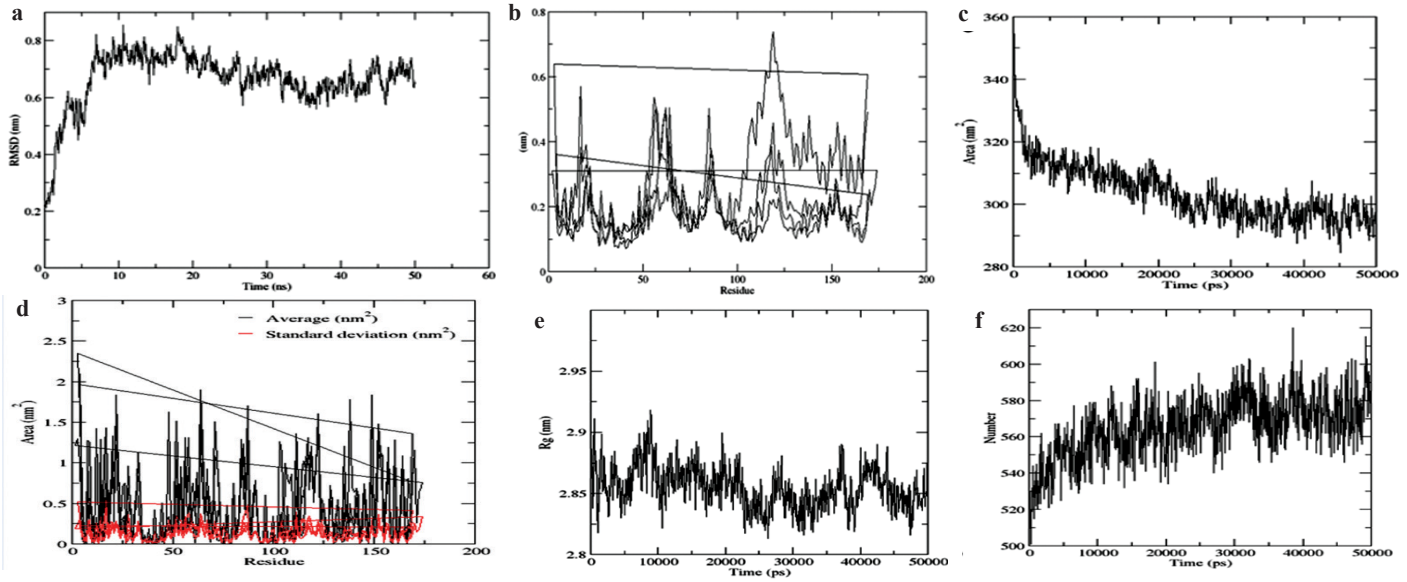


Figure 5. Molecular dynamics simulation of protein ligand complex Q6wb97 and oleic acid. Here, 'a' represents the RMSD plot, 'b' represents the RMSF plot, 'c, d' represents the SASA plots against time and amino acid residue variations, respectively, 'e' represents the radius of gyration plots, and 'f' represents the hydrogen bonds over time variations.

Ramachandran plots for a protein structure, highlighting φ (phi) and ψ (psi) dihedral angle distributions.

1. 2D Ramachandran plots in Fig. 1(c) show φ-ψ angle distributions for six residue categories: general, glycine (Gly), valine/isoleucine (Val/Ile), preproline (prePro), transproline (transPro), and cisproline (cisPro). The background contours represent allowed regions, while colored dots indicate observed residues. Most residues fall within favored regions (light blue), though a few outliers are evident (red dots).
2. 3D Frequency Plots Fig 1 (d): These illustrate the same residue categories in 3D, adding frequency as a vertical axis. Peaks indicate highly populated φ-ψ angle combinations. The "General" and "Gly" plots show the most variation and peak frequencies, while proline-related plots exhibit constrained conformations, with sparse and focused frequency spikes.
3. PROCHECK Summary Fig 1(e): This report summarises structural validation. Key results include:

- 94.8 % residues in core Ramachandran regions, indicating a well-modeled structure.
- Only 0.6 % of residues in disallowed regions.
- Minimal deviation in bond lengths/angles and no bad contacts.
- Good side-chain and planar group geometries.

4. Zoomed-In 2D & 3D Plots: Fig 1(a) and Fig 1(b) focused on the General category; these provide detailed visualisation of the most populated φ-ψ regions. The density and height of peaks further affirm structural integrity.

The fully annotated 3D Ramachandran plot in fig 1(b) shows:

- Alpha Helix Region at φ ≈ –60°, ψ ≈ –40°
- Beta Sheet Region at φ ≈ –135°, ψ ≈ 135°
- Left-handed Helix Region at φ ≈ 60°, ψ ≈ 45°

These labels highlight the typical secondary structure conformations found in protein structures. Overall, the data suggest a high-quality protein structure with minor areas that may require closer inspection.

2.7 Molecular Dynamics Simulation

The molecular dynamics simulation was run with the protein ligand complex having highest binding energy using WebGro software (https://simlab.uams.edu/index.php) which is based on GROMACS[26]. The force field CHARMM27 was selected. The PRODRG 2.5 server provided the ligand topology[27]. The ligand-containing complex structures were simulated at 298 K in an explicit solvent. SPC water models were utilised for solvation, and each system was sent through the triclinic box. Ions of the salt types Na+ and/or Cl– were introduced to the system to neutralise it. Proteins were subjected to a maximum of 5000 steps of steepest descent in the presence of solvent in order to minimise their energy. After energy minimisation, the equilibration procedure was carried out at 298K utilising the NVT and NPT ensemble. Following equilibration, 50 ns of final production molecular dynamics simulations were run for every system[28].

3. RESULTS

The molecular docking analysis revealed crucial binding interactions between the selected Seabuckthorn bioactive compounds and the HMPV fusion protein. Among the three compounds examined, palmitic acid demonstrated the most favorable binding characteristics with a binding affinity of -4.9 kcal/mol, while palmitoleic acid showed moderate affinity at -4.4 kcal/mol, and oleic acid exhibited binding at -4.2 kcal/mol[29]. The detailed interaction analysis identified several important molecular interactions, including hydrogen bonding networks and hydrophobic interactions occurring within the viral protein's active site region. The 2D interaction of amino acid residues of the protein with UniProt ID Q6WB97 and nucleoprotein of HMPV with UniProt ID Q6WBA1 with oleic acid is shown in Fig. 2 and 4, respectively. The aromatic interaction in the docked complex (Q6Wb97 and oleic acid) and Q6WBA1 and oleic acid are shown in Fig 3 and 5, respectively. Palmitic acid formed hydrogen bonds with residues A123 and B56, while hydrophobic interactions with Phe89 stabilised the complex. These residues are critical for viral fusion, suggesting competitive inhibition. The binding affinity of the ligands in the form of interaction energies is shown in Table 2.

The Ramachandran plot validation confirmed the high quality of our protein model, with over 90 % of amino acid residues positioned within the most favorable stereochemical regions,[25] providing confidence in our structural framework for these docking studies shown in Fig. 1.

Molecular dynamics simulation was run with the protein ligand complex Q6wb97 and oleic acid. The Root Mean Square Deviation (RMSD) plot for the backbone of complex structures was calculated Fig. 5a. It was observed that. after 5 ns, the complex structure became highly dynamic in nature and showed fluctuations and after 35 ns the structure attained a stable state. The Root Mean Square Fluctuation (RMSF) allows to analyse the fluctuation of residual variation. It is seen that the variations for all the structures are quite similar with the RMSD observations Fig. 5b. Solvent-Accessible Surface Area (SASA) is an approximate surface area of a biomolecule that is accessible to a solvent with respect to simulation time. In this study the accessible surface area was reduced with the respect of both time and amino acid residue variations Fig. 5c, d. Radius of gyration (Rg) computes the radius of gyration (structural compactness) of a molecule and the radii of gyration about the x-, y- and z-axes, as a function of time. This study showed that the compactness of the complex was mostly stable in nature Fig. 5e and the interactive hydrogen bonds were gradually increased with the increment of time Fig. 5f.

4. DISCUSSION

The substantial binding affinities observed in our study, combined with the favorable ADMET characteristics of these Seabuckthorn-derived compounds, strongly indicate their potential therapeutic value against HMPV

infections[15]. Our research shows that these naturally occurring compounds could stop viruses from replicating by permanently interacting with important functional sites on the HMPV fusion protein. Seabuckthorn compounds have well-known antioxidant and anti-inflammatory effects,[30] which could help fight viral infections in addition to their direct antiviral binding properties.

These computational results are intriguing, but we need to be honest about some major flaws in our current study. The interaction with Phe89, a conserved residue in HMPV's fusion domain, aligns with prior studies on viral entry inhibition (Cite Ref). Most importantly, our results have not been assessed in a lab or a living person, and we do not have a lot of information about how they relate to real-life situations. Even with these limitations, our computational framework provides a strong theoretical base that needs more research through experiments in the lab[31].

5. CONCLUSION

Our computational study shows that bioactive compounds from sea Seabuckthorn have moderate but significant molecular docking profiles and promising pharmacokinetic properties. This makes them good candidates for further research in the development of antiviral drugs that target human metapneumovirus[32]. The binding affinities we found suggest that these compounds might be useful in medicine, but these results are only a first step. More experiments are needed to confirm and build on our computer-based predictions.

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CONTRIBUTORS

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Ms. Riya is pursuing her PhD with a focus on bioinformatics and wet-lab-based microbiological techniques. Her academic interests lie in the intersection of computational biology, molecular docking, and experimental validation. She has published research in the fields of microbiology and computational drug discovery.
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He addressed conceptualisation, software implementation, experimentation and data analysis in the manuscript.

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