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Research Article

Pongaglabrone as a Potential Lead Molecule Targeting the Matrix Protein of Nipah virus: A Molecular Docking Study

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ABSTRACT

Nipah virus is a zoonotic pathogen was firstly identified in Malaysia country in 1998 and spread all over world including West Bengal, India in 2001. The severity is causing fatal infections and mortality in humans, it is very important to discover novel inhibitor with natural sources. The current Insilco study gives antiviral flavonoid against nipah virus. The Structure of nipah virus has surface glycoproteins (G and F) for host attachment and fusion and matrix (M) protein located beneath the viral lipid envelope that plays a crucial role in virus assembly, budding, and structural organization. The study focuses on matrix protein inhibition using flavonoids. The selected flavonoid-derived phytochemical Lanceolatin, Pongaglabrone, Pongaglabol, Flavone, and Isopongaglabol were evaluated for their inhibitory potential against the target protein represented by 7SKT protein structure using molecular docking analysis. Among the tested compounds, Pongaglabrone demonstrated the highest binding affinity with a docking score of −8.07 kcal/mol, followed by Pongaglabol with −7.14 kcal/mol. Isopongaglabol and Lanceolatin exhibited moderate binding energies, whereas Flavone showed the lowest binding affinity. The inhibition occurs in the more repeated binding regions PHE283, ARG286 and ILE243.These findings indicate that flavonoid-based phytochemicals, particularly Pongaglabrone, may serve as promising lead compounds for the development of antiviral agents targeting Nipah virus proteins. Further in vitro and in vivo studies are required to validate their therapeutic potential.

1. Introduction

Nipah virus is a zoonotic pathogen was firstly identified in Malaysia country in 1998 and spread all over world including India in 2001.Since then till 2026 several outbreaks were spread in different states like Kerala and west Bengal, the outbreaks also include eastern states like Bangladesh, Nepal, and Bhutan(Rathish & Nguyen, 2026).There were 754 human NiV cases and 435 deaths reported globally. The severity is causing fatal infections and mortality in humans. Nipah virus (NiV) is classified under the Paramyxoviridae family and belongs to the Henipavirus genus(L. Wang et al., 2024). Natural reservoirs of NiV include fruit bats, with transmission also occurring in pigs and humans, which lead to consider this NiV a level 4 pathogen with a high risk compatibility. Virus encoding structural proteins (N, P, M, F, G, L) and accessory proteins (C, V, W) that facilitate viral replication.

Beyond structural roles, NiV The matrix (M) protein has been reported to suppress host antiviral defence mechanisms by disrupting the nuclear transport of immune signaling molecules, thereby dampening type I interferon production and contributing to immune evasion (Ciancanelli & Basler, 2006). This dual role coordinating viral assembly while suppressing innate immunity makes M protein a central determinant of viral replication efficiency and pathogenicity. Experimental studies indicate that M protein deletion or functional inhibition reduces viral budding and impairs NiV propagation, highlighting its potential as a therapeutic target (Y. E. Wang et al., 2010). The respiratory system serves as a major entry point and replication site for the virus. Respiratory pathogenesis involves direct viral cytopathic effects, immune-mediated injury, and endothelial dysfunction (Talukdar et al., 2023).

Antiviral drugs like acyclovir and ribavirin were used to treat Nipah infections during previous outbreaks in Singapore and Malaysia. However, they were not fully effective in curing

Nipah-infected individuals (Chan et al., 2025) (Sharma et al., 2019). Other compounds currently under evaluation include remdesivir, favipiravir, griffithsin, chloroquine, and acyclovir (Lo et al., 2019). For highly lethal pathogens like Nipah, conducting human challenge trials poses safety and ethical concerns that make the approach highly unlikely (Hope & McMillan, 2004). The goal of this work is to identify superior natural components as possible treatments for the Nipah virus using computational approaches. In order to identify compounds with higher binding affinity and stronger inhibitory capacity than existing drugs, this study will undertake in silico molecular docking of Swiss similar analogues generated by Swiss similarity against M protein.

Materials and Methods

2.1. Materials used for the Insilico studies

The softwares used to accomplish the Insilico work are autodocktools-1.5.7 for molecular docking, Discovery studio 2025 client used for optimising protein and ligand also used for visualising 2D and 3D structures. UCSF-Chimera 2025 used for detecting the active site prediction and surface structure visualization. The Swiss dock web server for homology structure similar molecules optimizing. The database used is IMPPAT for studying and retrieving phytochemicals. All software was run on personal computer. The Open Babel software was used to convert file formats into a form readable by Auto Dock.

2.1.1. Immunogenicity and protein modelling

The target protein is the matrix protein. The matrix protein is primarily responsible for morphogenesis and budding of new virions from the viral particle. The protein structure weight is 87.92 kDa. There were 2 chains present in its structure A and B with a sequence length of 398 amino acids. The protein crystal structure is derived from experimental data obtained through X-Ray Diffraction with a resolution of 2.05 Å, which made the protein a reliable molecule for these studies. The protein is retrieved from RCSB protein database by a PDB id 7SKT. The specific catalytic activity was concealed in the protein. This makes it more interesting, only the small molecules can be used as ligands. The protein file is saved in PDB format from RCSB PDB and optimized with removing additional chains and heta atoms using Discovery Studio 2025. Using Auto Dock Tools 1.5.7 (Trott & Olson, 2010) kollaman charges and Gasteiger charges were assigned to the protein to ensure proper electrostatics for molecular docking. Hydrogen atoms and nonpolar hydrogens were assigned. The protein prepared is now saved in PDBQT format for further grid and dock files formation.

2.1.2. Selection and preparation of phytochemical

According to prior research, a selection of 30 flavonoids was identified through a Swiss similarity search. Among these 30 flavonoids, only 5 were chosen for further analysis based on their binding scores and ADMET properties. These 5 flavonoids were obtained from the IMPPAT database in SDF format and subsequently converted to PDB format using Open Babel. The flavonoids that exhibited noteworthy results were sourced from three medicinal plants: Pongamia pinnata, Tephrosia apollinea, and Arachis hypogaea which were retrieved from IMPPAT database(Vivek-Ananth et al., 2023).

2.1.3. Docking procedure

The molecular docking simulations were conducted by first establishing a precisely defined search space to facilitate optimal ligand navigation toward the binding pocket. A grid box consisting of 628,725 total points with dimensions of 95 × 75 x 82 and a grid spacing of 0.625 Å was utilized for all five phytochemicals. The grid centred was strategically positioned at coordinates X = -4.35, Y = -18.28, and Z = -16.85. Following the generation of the Grid Parameter Files (GPF), docking was executed via the Lamarckian Genetic Algorithm (LGA) with a population size of 150, a maximum of 27,000 generations, and an energy evaluation limit of 2.5 million. All other parameters were maintained at software defaults within the Docking Parameter Files (DPF). The resulting Docking Log Files (DLG) were subsequently analysed to determine the binding orientations and thermodynamic stability of the resulting complexes.

2.1.4. ADMET prediction

ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) plays a crucial role in evaluating the pharmacodynamics properties of a proposed molecule for its

Table-1. Molecular docking analysis of selected flavonoids

Flavonoid	Hydrogen bond interactions	Other bonds	Medicinal plant	Inhibition constant	Binding energy (kcal/mol)
Pongaglabrone	Asn60, Leu298	Asn182, Leu181, His277, Ile186, Cys299, Ile278,	*Pongamia pinnata*	1.23 uM	-8.07
Pongaglabol	Tyr250, Val243, Arg287	Lys258, Cys255, Phe242, Ser285, Arg245, Tyr254,	*Pongamia pinnata*	5.88 uM	-7.14
Isopongaglabol	Thr51, Gly53	Ile320, Leu268, Glu319, Ser267, Cys318, Leu350, Lys351, Pro52, Ile49	*Pongamia pinnata*	11.97 uM	-6.62
Lanceolatin A	Thr51	Leu268, Ser267, Ile320, Lys48, Ser317, Cys318, Leu350, Lys351, Phe266	*Tephrosia apollinea*	14.11 uM	-6.72
Flavone	Ser301	Phe300, Ile305, Leu194, Asp304, Met188, Arg191, Ile189, Leu237, Met236	*Arachis hypogaea*	80.44 uM	-5.59

potential use as a drug. These properties were predicted using swissadme (Daina et al., 2017) and protox browsers (Banerjee et al., 2024). These were free web browsers available. The best hits were observed using these browsers by uploading SMILES in the search bar.

3. Results and Discussion

In comparison to the common medication Lanceolatin A, the molecular docking investigation of five possible phytochemicals against M protein provided important information about their binding affinities, interaction patterns, and inhibitory potential. The findings show that a number of substances have better binding properties, indicating their potential as more potent matrix protein inhibitors for the treatment of Nipah virus.

3.1. Medicinal Plant Source:

The flavonoids analysed in this study are derived from different medicinal plants, highlighting their natural origin and pharmacological relevance. Pongaglabrone, pongaglabol, and isopongaglabol are derived from Pongamia pinnata, while lanceolatin A is obtained from Tephrosia apollinea, and flavone is associated with Arachis hypogaea. These plants are known for their traditional medicinal uses, supporting the potential therapeutic relevance of the studied compounds.

3.2. Binding Energy:

The Binding energy offers valuable information regarding the stability of ligand–protein complexes. Among the flavonoids analysed, the binding energies varied between −5.59 and −8.07 kcal/mol. The binding energy that indicated the greatest favourability belonged to pongaglabrone (−8.07 kcal/mol), suggesting the creation of a highly stable complex with the target protein. Pongaglabol also displayed a relatively strong binding affinity (−7.14 kcal/mol), followed by lanceolatin A (−6.72 kcal/mol) and isopongaglabol (−6.62 kcal/mol), which exhibited moderate interaction strengths. Flavone had the least favourable binding energy (−5.59 kcal/mol), implying a weaker interaction and reduced stability of the complex.

3.3. Inhibition Constant (Ki):

The inhibition constant (Ki) indicates the affinity of a ligand for its target protein, with lower values representing stronger inhibition. The Ki values measured varied between 1.23 µM and 80.44 µM. Pongaglabrone exhibited the lowest Ki value (1.23 µM), indicating it has the most significant inhibitory potential among the compounds evaluated. Pongaglabol revealed moderate inhibition (5.88 µM), while isopongaglabol and lanceolatin A displayed comparatively weaker inhibition with Ki values of 11.97 µM and 14.11 µM, respectively. Flavone had the highest Ki value (80.44 µM), reflecting the least inhibitory activity.

3.4. Hydrogen Bond:

Hydrogen bonding plays a critical role in stabilizing ligand–protein interactions and enhancing binding specificity. The analysed compounds formed hydrogen bonds with key amino acid residues within the active site. Residues such as ASN60, LEU298, TYR250, VAL243, ARG287, THR51, GLY53, and SER301 were prominently involved in hydrogen bonding. The presence of multiple hydrogen bond interactions contributes significantly to the stability and proper orientation of the ligands within the binding pocket.

3.5. Other Intermolecular Interactions:

In addition to hydrogen bonds, hydrophobic interactions and van der Waals forces were observed between the ligands and various amino acid residues, including LEU, ILE, PHE, CYS, LYS, and SER (Fig-1). These interactions complement hydrogen bonding by enhancing the overall binding affinity and stabilizing the ligand within the protein's active site. Compounds with a greater number of such interactions tend to exhibit improved binding stability. The Table.2 presents a detailed assessment of the physicochemical characteristics, drug-likeness, and toxicity of selected compounds, including pongaglabrone, pongaglabol, isopongaglabol, lanceolatin A, and flavone, which are vital factors in the initial phases of drug discovery (Table 1). The molecular weights of the selected compounds range from 222.24 to 336.38 g/mol, remaining within acceptable limits for drug-like properties. The quantity of hydrogen bond acceptors (HBA: 2–5) and donors (HBD: 0–1) stays within the acceptable range set by Lipinski's rule of five, signifying a well-balanced ability for intermolecular interactions without hindering membrane permeability. Topological polar surface area (TPSA) values lie between 30.21 and 63.58 Å², which are indicative of good intestinal absorption and potential oral bioavailability, as compounds with TPSA below 140 Å² are generally considered permeable. The high

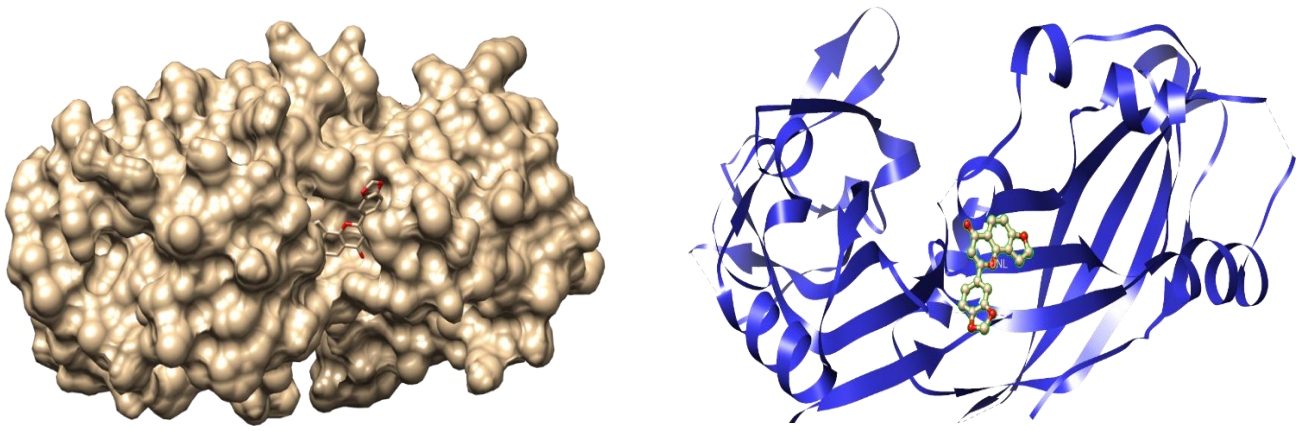

Fig-1. Binding interactions of Pongaglobrone with binidng pocket of M protein Nipah virus.
A) Sureface representation; B) Three-dimentional view

Table-2. Physicochemical properties, drug-likeness, and lipophilicity profiles of selected compounds (pongaglabrone, pongaglabol, isopongaglabol, lanceolatin A, and flavone), including molecular weight (MW), hydrogen bond acceptors (HBA), hydrogen bond donors (HBD), topological polar surface area (TPSA), gastrointestinal (GI) absorption, Lipinski's rule of five violations, bioavailability score, and consensus log P (octanol/water partition coefficient and toxicity)

compound	Physicochemical properties					drug likeliness			Toxicity	
	MW	HBA	HBD	TPSA	Consensus Log Po/w	GI Absorption	Lipinski Violations	Bioavailability score	Predicted LD50	Predicted toxicity class
Pongaglabrone	306.27	5	0	61.81	3.23	High	0	0.55	4000mg/kg	5
Pongaglabol	278.26	4	1	63.58	3.17	High	0	0.55	4000mg/kg	5
Isopongaglabol	292.29	4	0	52.58	3.39	High	0	0.55	4000mg/kg	5
Lanceolatin A	336.38	4	1	59.67	3.63	high	0	0.55	2570mg/kg	5
Flavone	222.24	2	0	30.21	3.18	High	0	0.55	2500mg/kg	5

gastrointestinal (GI) absorption predicted for all compounds further supports their suitability for oral administration.

Importantly, none of the compounds show any violations of Lipinski's rule, reinforcing their classification as drug-like molecules with favourable pharmacokinetic profiles (Table-2). The bioavailability score of 0.55 for all compounds suggests a moderate probability of achieving adequate systemic exposure upon oral dosing. Lipophilicity, expressed as consensus log P (Po/w), ranges from 3.17 to 3.63, indicating an optimal balance between aqueous solubility and membrane permeability. Compounds with log P values in this range are typically associated with efficient passive diffusion across biological membranes while maintaining sufficient solubility. Among the compounds, lanceolatin A exhibits the highest lipophilicity (log P = 3.63), which may enhance membrane permeability but could slightly reduce aqueous solubility. In contrast, pongaglabol shows relatively lower lipophilicity (log P = 3.17), potentially favouring better solubility. Flavone, with the lowest MW and TPSA, may demonstrate rapid absorption and distribution.

The toxicity which was predicted from protox web browser shows the oral toxicity prediction of the compound. The LD50 is 4000mg/kg for the first three flavonoids and 2570mg/kg and 2500mg/kg for lanceolatin A and flavone compounds. The selected molecules were classified under toxicity class 5, indicating low acute toxicity, though harmful effects may occur if consumed in high doses. Collectively, these findings indicate that all studied compounds possess favourable physicochemical and pharmacokinetic attributes, supporting their potential as promising candidates for further optimization and drug development studies.

This study highlights the effectiveness of in-silico molecular docking in identifying potential inhibitors of the matrix protein of Nipah virus infection. Among the screened ligands, Pongaglabrone exhibited the strongest binding affinity, followed by pongaglabol, indicating their promise as antiviral candidates. These findings are consistent with several recent computational studies on Nipah virus, where phytochemicals and small molecules have demonstrated binding energies typically ranging between −6.0 to −8.5 kcal/mol against key viral proteins. The binding affinities observed in this study fall within or exceed this range, suggesting comparable or improved inhibitory potential. Similar studies have reported that compounds with lower binding energies and favourable inhibition constants tend to form more stable ligand–protein complexes, supporting effective disruption of viral assembly and replication.

Compared to earlier reported ligands, Pongaglabrone stronger binding profile indicates a potentially higher specificity and stability within the active site. However, computational approaches alone cannot fully replicate biological complexity. Consistent with previous research, further validation through in vitro enzymatic assays, blood–brain barrier permeability studies, and in vivo evaluations remains essential to confirm pharmacological activity and safety. Overall, this study aligns with and extends existing research by identifying phytochemicals with competitive binding characteristics, reinforcing their potential as lead compounds for developing effective therapies against Nipah virus infection.

4. Conclusion

This study successfully employed in-silico modelling and molecular docking to identify a novel matric protein inhibitor with superior binding affinity. Among the five investigated ligands, Pongaglabrone exhibited the strongest binding energy (-8.00 kcal/mol) and the lowest inhibition constant (1.23uM), indicating greater potency. Similarly, pongaglabol demonstrated remarkable binding characteristics (-7.14 kcal/mol, Ki = (-5.88uM), reinforcing its potential as a promising matrix protein inhibitor. These findings align with recent advancements in Nipah virus inhibiting drug design. While results are promising, further *in vitro* enzymatic assays, blood-brain barrier permeability. The ADMET predictions were also done using swissadme and protox browsers, every parameter is favourable. The identified phytochemical represents a strong candidate for preclinical development, potentially leading to more effective treatments for Nipah virus

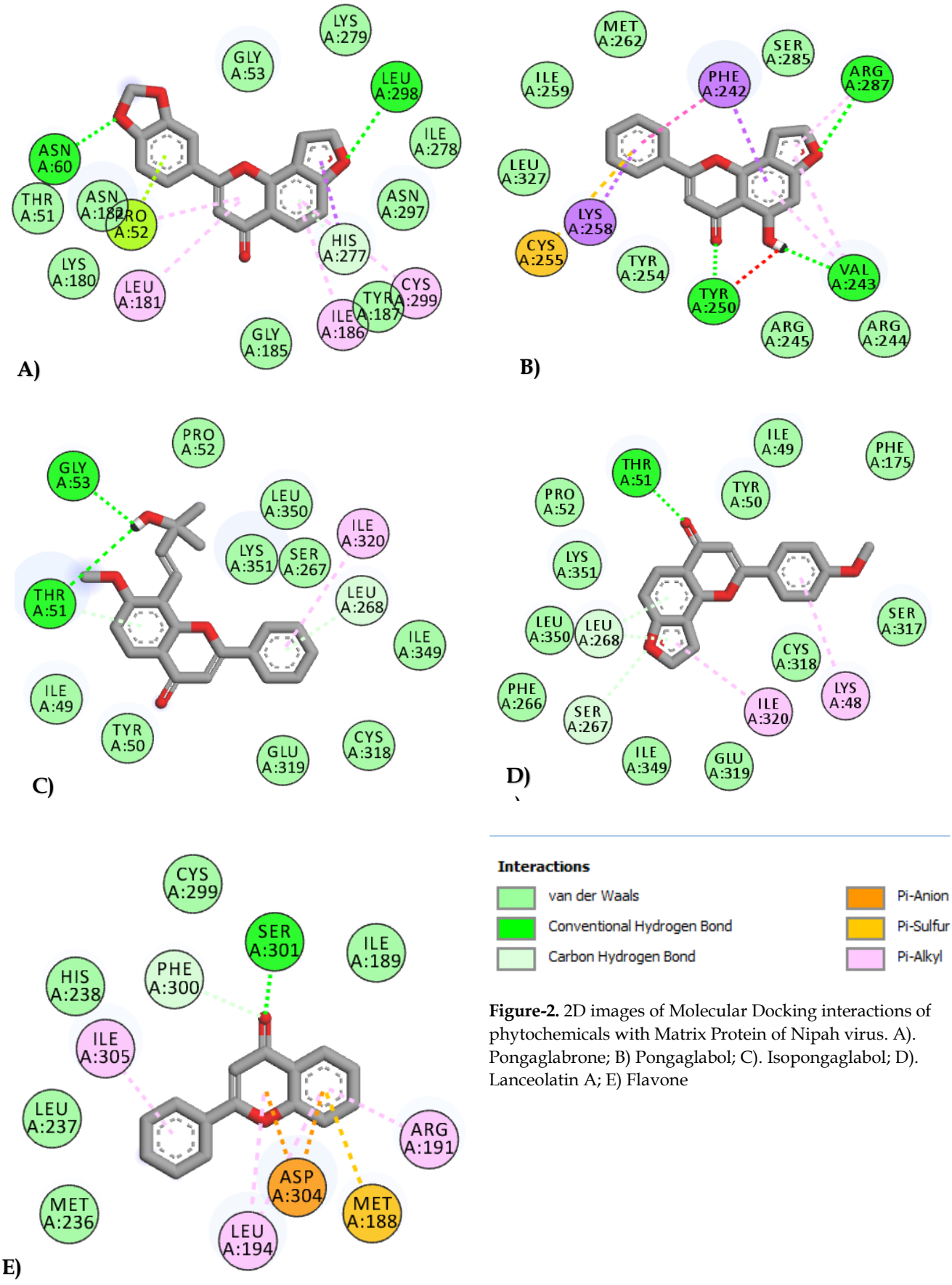

Figure-2. 2D images of Molecular Docking interactions of phytochemicals with Matrix Protein of Nipah virus. A). Pongaglabrone; B) Pongaglabol; C). Isopongaglabol; D). Lanceolatin A; E) Flavone

infection with improved target engagement and fewer side effects than current therapies. This study underscores the power of structure-based drug discovery in accelerating the identification of next-generation matrix protein inhibitors, offering hope for better management of Nipah virus debilitating symptoms.

Declarations

Ethics approval and consent to participate: Not applicable

Competing interests:

The authors declare that they have no competing interests

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