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RESEARCH ARTICLE
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MOLECULAR DOCKING FOR THE IDENTIFICATION OF NIPAH VIRUS "G" SITE INHIBITORS FROM VARIOUS MEDICINAL PLANTS

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Abstract

Objective: Recently to see the rapid spread of the Nipah virus in the world. NiV is first discover in Malaysia. Bats are the main reservoir as a viral source particularly,fruits and date palm sap are contaminated by their saliva. It is spread in India last year also. This disease does not have any particular treatment and vaccines to treat against the virus to cure the infected person. In 2023, the mortality rate of this virus in Bangladesh is 85%. Now a days the common antiviral drugs like Ribavirin,Monoclonal antibody and Favipiravir are used. Some significant consequences are produced. In this study, we focus alternative remedy to against the Nipha virus.

Materials and methods:. The plant phytoconstituents of *Aloe barbadensis*, *Curcuma longa* is predicted to be against Niv using a molecular docking study using the Schrodinger Maestro 12.7 version. Also performing ADME screening is the Qikprop tool. The field is quickly evolving, the novel possible active principle to inhibit the Nipah virus.

Results: Out of 99 phytoconstituents 6-Deoxy-L-Mannopyranose has a higher docking score -6.65Kcal/mol and Vanillic acid -6.305kcal/mol than the standard Ribavirin-5.519Kcal/mol.

Conclusion: Hence it can be utilized as a lead compound to control Nipah virus. Therefore, it is concluded to be fit for human consumption without adverse effects.

Keywords: *Aloe barbadensis, Curcuma longa*, phytoconstituents, Nipah virus, Molecular docking and ADME analysis.

INTRODUCTION:

The Nipah virus is a recent one that has spread over the world. It is an RNA virus with the Genus: Henipavirus and was recently described as Cedar virus. It belongs to the Family: Paramyxoviridae. It first emerged in Malaysia in 1998 and has since caused several outbreaks in South and Southeast Asia. NiV is highly pathogenic as well as person-to-person transmission(1). The virus was named after Kampung Sungai Nipah village in Malaysia. NiV is a zoonotic disease. The genome of the Nipah virus consists of a non-segmented negative-sense single-stranded RNA. It encodes the six structural proteins as Nucleocapsid (N), Phosphoprotein (P), Matrix protein (M), Fusion protein (F), Glycoprotein (G), and RNA polymerase (L) (2). Still no available particular treatment for NiV, so we

focused on the natural source for the treatment of NiV, in this study. Indian traditional medicines use the plants *Aloe barbadensis and Curcuma longa* which have various therapeutic benefits. *Aloe barbadensis* is one of the medicinal plants. It is also called a Miracle plant. There are over 250 types of Aloe vera only some of these plants are used in medicines. It is a succulent plant that belongs to the Family: Xanthorhoeaceae. It originated in India, East and South Africa, West Indies. The phytoconstituents of Aloe vera are Amino acids, Anthraquinones, Enzymes, Minerals, Salicylic acid, Saponin, Steroids, Sugars, and Vitamins (3). The reported pharmacological effects of *Aloe barbadensis* included Antiviral activity, Immunomodulatory action, Anti-asthmatic activity, Antipyretic activity, Antitussive, Laxative effect, Wound healing, Anti-inflammatory activity, Antibacterial activity, Antidiabetic activity, Anti hyperlipidemic activity, Anticancer activity (4). *Curcuma longa* is one of the most common medicinal plants. It can be used in many utilizations for food, pharmaceutical industry, and animal. It is widely used in India, China and Southeast Asia. It is used as a spice, food preservative and colouring material. Curcuma is traditionally involved in Ayurvedic. It belongs to the Family: of Zingiberaceae. The phytoconstituents of curcuma are Curcumin, Sodium curcuminate, Methyl curcumin, Curcumin glucuronide, Curcumin sulphate, Dihydrocurcumin, Demethoxycurcumin, Bis- demethoxycurcumin, Ar-tumerone, Hexahydrocurcumin, Hexahydrocurcuminol, Dihydroferulic acid (5). The reported pharmacological effects of *Curcuma longa* are Anti-inflammatory, Antioxidant, Anticancer, Anti-mutagenic, Antifungal, and Antiviral activity (6). Molecular docking entails arranging molecules properly to interact with receptors (7). Some software was created in the last ten years, with well-known examples including Auto Dock, Auto Dock vina, Dock Thor, GOLD, FleXX, and virtual docking software. Computer-aided drug discovery (CADD) is used by fashionability in pharmaceutical research and administration. We consider that they streamline the procedure and make it easier to accelerate medication development and discovery (8). This study could also examine the possible natural medicinal ligands and receptor complexes using molecular docking (9).

MATERIALS AND METHODS:

In this study, we use the Schrodinger Maestro Software 12.7 version. New York LLC, USA, Academic version.

Protein preparation:

The protein structure of the 2VSM (NiV Envelope glycoprotein) was retrieved from the RCSB Protein Data Bank (PDB) at https://www.rcsb.org/. The X-ray diffraction technique, which has a resolution value of 1.80 Å, was used to determine the atomic and molecular structure of the crystal. The 416 amino acids (AA) long and anticipated molecular weight (MW) of the NiV envelope glycoprotein, with the PDB ID 2VSM, is 46.84 kDa. The protein's A chain was generated by removing the extra chains, co-crystallized ligands, and solvent molecules for further study. The protein structure was prepared using protein preparation wizard with the default setting, the protein's bond ordering has been imposed, hydrogens and missing side chains have been added, and the water molecule has been removed. For this protein preparation, we used the OPLS3e force field (10).

Ligand preparation:

The Ligprep tools were created to construct high-quality ligand preparations from the phytoconstituents of *Aloe barbadensis, Curcuma longa*, and all the ligands two-dimensional (2D) or three-dimensional (3D) SDF (Structures Data Files) structures were obtained at the workspace. Optimized Potential for Liquid Stimulations (OPLCs)-2005 force field carried out the geometric minimization (11).

Docking analysis:

With flexible docking on Maestro between Ligands and the target protein active site, a molecular docking investigation of 58 phytocompounds from the *Aloe barbadensis, Curcuma longa* medicinal

plant was conducted against the Nipah virus. For docking, an additional accuracy mode is provided. While Ligands were flexible, the protein was fixed during molecular docking (12).

ADME Analysis:

The Qikprop tool in the Maestro suite is used to predict the "drug-likeness" features of phytocompounds from selected phytocompounds. Filtered unsuitable phytocompounds based on the "rule of three" (Jongenson's rule) and Lipinski's rule of five (13).

RESULTS:

From this study, accordingly to collected 58 phytochemicals from the plant, they were arranged and formatted by afore mentioned methods. The phytoconstituents are listed in table 1 and 2.

Table 1: Total phytoconstituents of *Aloe barbadensis*:

Phytoconstituents	PubChem ID	Molecular formula
Salicylic acid	338	$C_7H_6O_3$
Glycine	750	$C_2H_5NO_2$
Phosphoenolpyruvate	1005	$C_3H_5O_6P$
Pyridoxine	1054	$C_8H_{11}NO_3$
Uric acid	1175	$C_5H_4N_4O_3$
Emodin	3220	$C_{15}H_{10}O_5$
Hydroxyproline	5810	$C_5H_9NO_3$
Alanine	5950	$C_3H_7NO_2$
Aspartic acid	5960	$C_4H_7NO_4$
L-Lysine	5962	$C_6H_{14}N_2O_2$
Tyrosine	6057	$C_9H_{11}NO_3$
Methionine	6137	$C_5H_{11}NO_2S$
Phenylalanine	6140	$C_9H_{11}NO_2$
Histidine	6274	$C_6H_9N_3O_2$
Valine	6287	$C_5H_{11}NO_2$
Threonine	6288	$C_4H_9NO_3$
Aloe-emodin	10207	$C_{15}H_{10}O_5$
Anthranol	10731	$C_{14}H_{10}O$
6-Deoxy-L-Mannose	25310	$C_6H_{12}O_5$
Glutamic acid	33032	$C_5H_9NO_4$
Mannose	82308	$C_6H_{12}O_6$
Glutathione	124886	$C_{10}H_{17}N_3O_6S$
Proline	145742	$C_5H_9NO_2$
Arachidonic acid	444899	$C_{20}H_{32}O_2$
Gamma lineolic acid	5280933	$C_{18}H_{30}O_2$
Alkaline phosphatase	18985873	$C_{21}H_{36}N_8O_6$
Ascorbic acid	54670067	$C_6H_8O_6$

Table 2: Total phytoconstituents of *Curcuma longa*:

Phytoconstituents	PubChem ID	Molecular formula
Glycine	750	$C_2H_5NO_2$
Eugenol	3314	$C_{10}H_{12}O_2$
Hydroxychloroquine	3652	$C_{18}H_{26}ClNO_3$
L-serine	5951	$C_3H_7NO_3$
Tyrosine	6057	$C_9H_{11}NO_3$
L-Methionine	6137	$C_5H_{11}NO_2S$
L-Phenylalanine	6140	$C_9H_{11}NO_2$
L-Valine	6287	$C_5H_{11}NO_2$
Alpha Pinene	6654	$C_{10}H_{16}$
Vanillic acid	8468	$C_8H_8O_3$
Azulene	9231	$C_{10}H_8$
Terpinoline	11463	$C_{10}H_{16}$
Beta Pinene	14896	$C_{10}H_{16}$
6-Deoxy - L-Mannopyranose	25310	$C_6H_{12}O_5$
Catechin	73160	$C_{15}H_{14}O_6$
2-(hydroxymethyl)anthraquinone	87014	$C_{15}H_{10}O_3$
Cinnamic acid	444539	$C_9H_8O_2$
Ferulic acid	445858	$C_{10}H_{10}O_4$
p-coumaric acid	637542	$C_9H_8O_3$
Caffeic acid	689043	$C_9H_8O_4$
Curcumin	969516	$C_{21}H_{20}O_6$
Quercetin	5280343	$C_{15}H_{10}O_7$
Luteolin	5280445	$C_{15}H_{10}O_6$
Kaempferol	5280863	$C_{15}H_{10}O_6$
Bixin	5281226	$C_{25}H_{30}O_4$
T3Bisdemethoxycurcumin	5315472	$C_{19}H_{16}O_4$
T2Demethoxycurcumin	5469424	$C_{20}H_{18}O_5$
Cinnamate	5957728	$C_9H_7O_2$
N7Dihydroxydimethoxyflavone	13889021	$C_{17}H_{14}O_6$
Ascorbic acid	54670067	$C_6H_8O_6$
T4-Cyclocurcumin	69879809	$C_{21}H_{20}O_6$

Results of ADME analysis of *Aloe barbadensis & Curcuma longa* phytoconstituents:

Qikprop software was used to do ADME testing on the chosen 27 phytoconstituents of *Aloe barbadensis* and 31 phytoconstituents of *Curcuma longa*. The ADME features of phytochemicals are based on their molecular parameters, including their molecular weight, CNS, logHERG, QPlog BB, (#metab) numerous potential metabolic processes, and (% human) predicted (human oral absorption). The "drug-likeness" of a few substances is terrible. They were therefore eliminated, preventing the harsh chemicals from passing through the cellular membrane. Only 20 phytoconstituents of *Aloe barbadensis* and 17 phytoconstituents of *Curcuma longa* were found to pass the limit in the ADME investigation. These are listed in table 3 and 4.

Table 3: Results of ADME analysis of *Aloe barbadensis*:

S.no	PubChem	BI(CNS)	BJ(Mol. wt)	BR(Donor HB)	BS(Accept HB)	CA(QPlogpo\w0	CB(QPlogS)	CD(QPlogHERG)	CE(QPPlogCaCo)	CF(QPlogBB)	CH(QPlogKp)	CL(QPlogKhsa)	CM(Human oral absorption)	CN(Percent human oral absorption)	CQ(PSA)	CS(Rule of five)	CT(Rule of three)
		-2 inactive 2 active	130.0-725.0	0.0-6.0	2.0-20.0	(-2.0)-6.5	(-6.5)-0.5	Concern below (-5)	<25 poor >500 great	(-3.0)-1.2	(-8.0)-(-1.0)	(-1.5)-1.5	1-low 2-medium 3-high	>80%high <25%poor	7.0-200.0	Max 4	Max 3
01	338	-1	138.123	1	2.5	-0.2227	0.114	-1.97	932.309	-0.319	-3.322	-0.861	3	78.767	44.844	0	0
02	750	-2	75.067	4	3.4	-1.315	-0.59	-4.704	375.134	-1.043	-4.187	-1.072	2	65.318	58.228	0	0
03	1054	-1	169.18	3	2.75	0.111	-1.474	-3.829	798.292	-0.541	-3.549	-0.683	3	66.581	49.408	1	0
04	1175	-2	168.112	0.25	2.25	-0.742	-0.349	-2.299	90.683	-1.016	-5.481	-0.762	2	57.639	89.818	0	0
05	3220	-1	270.241	1	4.25	0.131	-0.969	-3.204	340.865	-0.812	-3.699	-0.699	2	73.042	67.747	0	0
06	5810	-1	131.131	3	3.4	-0.807	-0.848	-3.85	362.843	-0.872	-4.215	-0.882	2	55.079	62.102	1	0
07	5950	-1	89.094	3	1.75	-0.53	-0.772	-4.659	536.964	-0.864	-3.884	-0.947	2	72.706	53.266	0	0
08	5960	-2	133.104	2	2.5	-0.815	-0.637	-3.732	130.539	-1.328	-4.982	-0.856	2	60.038	80.285	0	0

09	6057	-2	181.191	6	2.75	-0.829	-0.7	-3.744	265.67	-1.04	-4.382	-1.015	2	52.524	68.354	1	0
10	6137	-1	149.207	6	1.25	-0.283	-0.949	-4.505	649.86	-0.673	-3.723	-1.079	3	75.631	51.062	0	0
11	6140	-1	165.191	5	2	-0.207	-0.86	-3.661	777.163	-0.527	-3.572	-0.898	3	77.467	49.477	0	0
12	6274	-2	155.156	5	2	-0.522	-1.213	-4.348	260.538	-1.125	-4.494	-0.903	2	67.127	71.493	0	0
13	6287	-1	117.147	3	0.25	0.004	-0.135	-3.124	879.375	-0.406	-3.467	-0.898	2	66.706	46.447	1	0
14	6288	-1	119.12	3.25	1.5	-0.902	0.532	-1.922	357.962	-0.561	-4.226	-1.006	2	54.417	62.496	1	0
15	10731	1	194.232	1	0.75	1.902	-1.323	-3.416	5033.613	0.277	-1.122	-0.33	3	100	14.387	0	0
16	25310	-1	164.158	4.5	5.5	-1.322	-1.501	-4.628	430.589	-0.901	-4.166	-0.938	2	53.392	58.649	1	0
17	33032	-2	147.13	3	3.5	-0.885	-1.435	-4.496	94.76	-1.685	-5.252	-0.831	2	57.14	85.308	0	0
18	82308	-2	180.157	5	7	-1.789	-1.694	-4.348	204.901	-1.172	-4.793	-0.894	2	44.882	76.355	1	0
19	145742	-1	115.132	4	3.9	-0.886	-0.519	-3.363	961.017	-0.402	-3.393	-0.927	3	75.145	45.754	0	0
20	54670067	-2	176.126	2	4.5	-0.957	-1.39	-4.662	148.645	-1.528	-4.872	-0.906	2	47.263	78.784	1	0

Table 4: Results of ADME analysis of *Curcuma longa* selected phytoconstituents:

PubChem	BI (CNS)	BJ (Mol. wt 0	BR (Donor HB)	BS (AcceptHB)	CA (QPlogpo\w)	CB (QPlogS)	CD (QPlogHERG)	CE (QPlogCaCo)	CF (QPlogBB)	CH (QPlogKP)	CL (QPlohKhsa)	CM (Human oral absorption)	CN (Percent human oral absorption)	CQ (PSA)	CS (Rule of five)	CT (Rule of three)
	-2(inactive) 2(active)	130.0-725.0	0.0-6.0	2.0-20.0	(-2.0)-6.5	(-6.5)-0.5	Concern below (-5)	<25 poor >500great	(-3.0)-1.2	(-8.0)-(-1.5)	(-1.5)-1.5	1-low 2-medium 3-high	>80% high <25% poor	7.0-200.0	Max 4	Max 3
6057	-2	181.191	6	2.75	-0.829	-0.7	-3.744	265.67	-1.04	-4.382	-1.0155	2	52.524	68.354	1	0
6140	-1	165.191	5	2	-0.207	-0.86	-3.661	777.163	-0.527	-3.572	-0.898	3	77.467	49.477	0	0
8468	-1	168.149	1	2.5	0.271	-0.969	-2.946	639.279	-0.562	-3.641	-0.638	3	78.749	51.088	0	0
25310	-1	164.158	4.5	5.5	-1.322	-1.501	-4.628	430.589	-0.901	-4.166	-0.938	2	53.392	58.649	1	0
444539	0	148.161	1	1.5	0.514	-0.735	-2.395	1251.938	-0.202	-3.169	-0.592	3	85.396	36.851	0	0
445858	-1	194.187	2	2.25	0.184	-0.948	-2.714	460.12	-0.648	-3.918	-0.619	3	75.686	55.727	0	0

637542	-1	164.16	2	2.25	-0.125	-0.536	-2.518	427.97	-0.645	-3.979	-0.725	2	73.312	55.728	0	0
689043	-2	180.16	3	3	-0.667	-0.385	-2.596	184.9	-1.01	-4.592	-0.83	2	63.614	72.375	0	0
969516	-1	368.385	2	5.5	1.278	-3.574	-4.265	529.858	-0.851	-3.799	-0.201	3	70.227	59.071	1	0
5280343	-2	302.24	1	3.75	0.409	-2.498	-4.796	58.829	-2.074	-5.125	-0.459	3	61.013	91.897	0	0
5280445	-2	286.24	1	4	0.017	-1.409	-3.587	90.833	-1.473	-4.855	-0.614	3	62.092	80.53	0	0
5280863	-2	286.24	1	4	0.41	-2.107	-4.334	136.169	-1.502	-4.513	-0.52	3	67.543	75.25	0	0
5315472	-1	308.333	2	5.5	0.71	-2.914	-4.138	458.45	-0.89	-3.921	-0.403	3	78.733	59.071	0	0
5469424	-1	338.359	2	5.5	0.993	-3.241	-4.199	492.88	-0.871	-3.86	-0.303	3	80.952	59.07	0	0
13889021	-1	314.294	2.5	6	0.154	-2.044	-3.271	601.816	-0.561	-3.74	-0.546	3	64.634	45.833	1	0
54670067	-2	176.126	2	4.5	-0.957	-1.39	-4.662	148.645	-1.528	-4.872	-0.906	2	47.263	78.784	1	0
69879809	-1	368.385	2.5	6.25	1.073	-3.412	-4.037	772.322	-0.587	-3.577	-0.263	3	71.958	45.512	1	0

Molecular docking results of *Aloe barbadensis* and *Curcuma longa* phytoconstituents:

The selected phytocompounds of the docking score, glide energy, glide$_{evdw}$, interaction residues, pi-pi stacking, and pi-cation of the ligand, which are shown in table 5 and 6. *Aloe barbadensis* docking results of 6-Deoxy-L-mannopyranose were -6.65 kcal/mol docking score, -28.962 kcal/mol for glide energy and -17.137 kcal/mol for glide$_{evdw}$ energy, and the total 5 H-bonds involved such as VAL 484, SER 486, ARG 495, LEU 526 and THR 538 are the following interaction residues they are shown in **Figure 1.** The docking score values for the following salicylic acid molecule are -6.329 kcal/mol, -

29.127 glide energy kcal/mol and -17.137 kcal/mol for $glide_{evdw}$ and four H-bonds are VAL 484, ARG 495, LEU 526, SER 486 the interaction aminoacid residues shown in **Figure 2.** Glycine received a docking score of -5.8 kcal/mol, a glide energy of -29.127 kcal/mol, and a $glide_{evdw}$ of -13.934kcal/mol. The interaction residues are LYS 465,THR 462,SER 457,ASN 509,TYR 454, total five H- bonds are occurred depicted in **Figure 3.** For *Curcuma longa* docking results of Vanillic acid was -6.305 kcal/mol docking score, -31.333 kcal/mol for glide energy and -13.143kcal/mol for $glide_{evdw}$ and the interaction residue is SER 468. The pi-cation involved in ARG 495 shown in **Figure 4.** The docking score value of L-Phenylalanine -5.184kcal/mol, -25.061kcal/mol of glide energy, -14.135 kcal/mol of $glide_{evdw}$ and the three H-bonds interaction residues are ARG 495, LEU 526, SER 486. The pi-cation was ARG 495 and ARG 548 they are shown in **Figure 5**. The docking score of Tyrosine -4.373 kcal/mol, -30.555 kcal/mol of glide energy, -9.781/mol of $glide_{evdw}$ and the interaction residues are LEU 526. The pi-cation was ARG 495. They are shown in **Figure 6**. The Ribavirin was interacted with Nipha virus also depicted in **Figure 7**.

Table 5: The Docking results of *Aloe barbadensis* selected phytoconstituents:

S.no	Phytoconstituents name	Docking score Kcal/mol	Glide energy Kcal/mol	Glideevdw	Interaction Residues	Pi cation
1	6-Deoxy-L-mannopyranose	-6.65	-28.962	-17.137	VAL 484, SER 486, ARG 495, LEU 526, THR 538	-
2	Salicylic acid	-6.329	-29.127	-14.939	VAL 484, ARG 495, LEU 526,,SER 486	-
3	Glycine	-5.8	-26.499	-13.934	LYS 465, THR462, SER 457, ASN 509, TYR 454	-
4	Phenylalanine	-5.185	-25.061	-14.135	LEU 526, ARG 495, SER 486	ARG 548, ARG 495
5	Proline	-4.999	-23.324	-19.411	ARG 495, SER 486	-
6	Alanine	-4.99	-24.426	-14.53	VAL 484, SER 486, LEU 526, ARG 495	-
7	Pyridoxine	-4.928	-28.17	-17.937	VAL 484, SER 486, ARG 495	ARG 495
8	Valine	-4.811	-21.962	-15.077	ARG 495, SER 486, VAL 484	-
9	Threonine	-4.091	-22.655	-18.863	ARG 495, SER 486	-
10	Tyrosine	-3.966	-25.538	-15.626	LEU 526,VAL 484	ARG 495
Std.drug	**Ribavirin**	**-5.519**	**-30.576**	**-20.001**	**GLN 559, GLY 506**	**-**

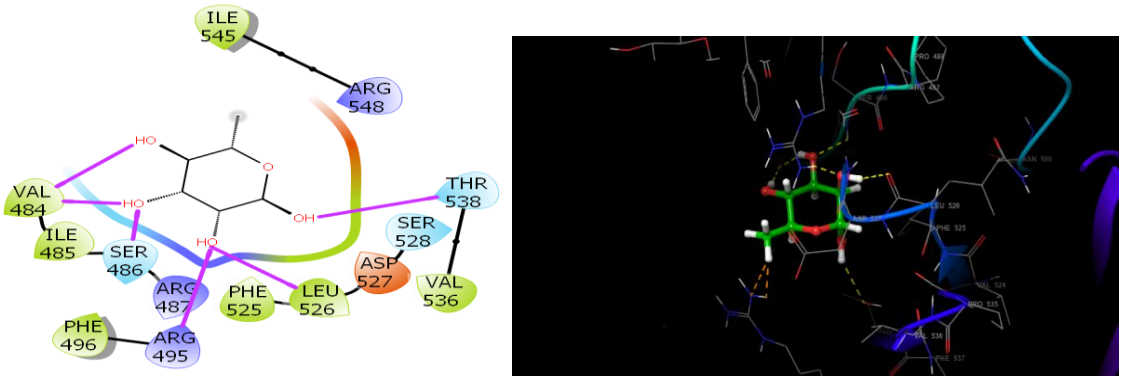

Figure 1: 2D and 3D Structure of docking interaction of 6-Deoxy-L-Mannopyranose with Nipah virus

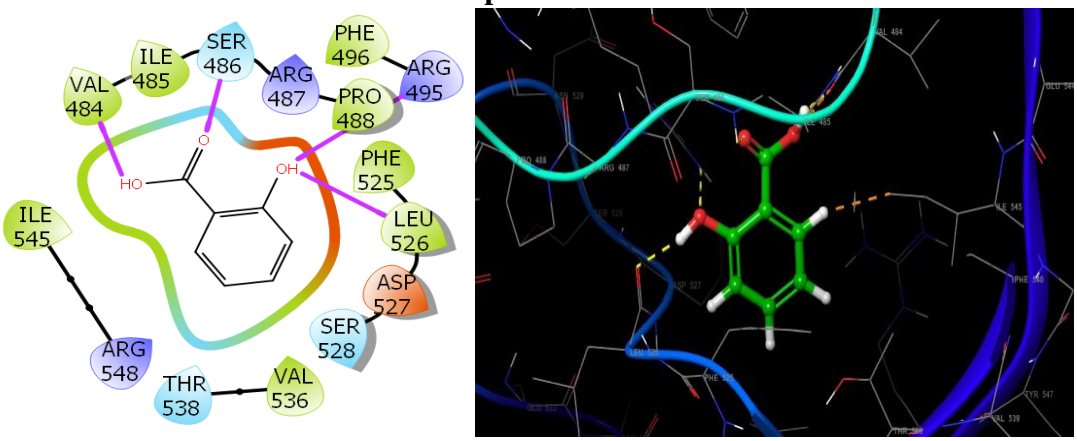

Figure 2: 2D and 3D Structure of docking interaction of Salicylic acid with Nipah virus

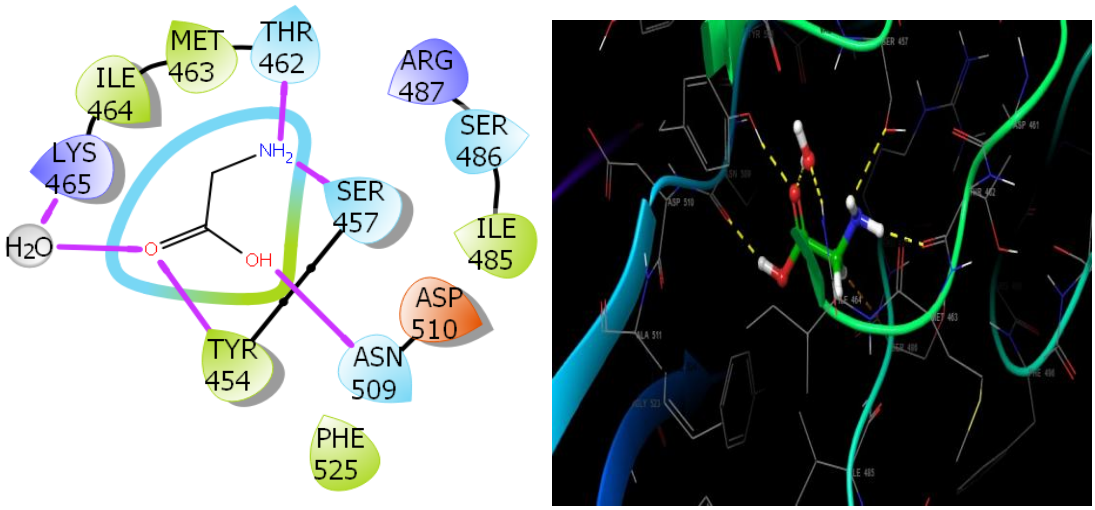

Figure 3: 2D and 3D Structure of docking interaction of Glycine with Nipah virus

Table 6: The Docking results of *Curcuma longa* selected phytoconstituents

S.NO	Phytoconstituents name	Docking score Kcal/mol	Glide energy Kcal/mol	Glidee vdw	Interaction Residues	Pi cation
1	Vanillic acid	-6.305	-31.333	-13.143	SER 468	ARG 495
2	L-Phenylalanine	-5.184	-25.061	-14.135	ARG 495, LEU 526, SER 486	ARG 495, ARG 548
3	Tyrosine	-4.373	-30.555	-9.781	LEU 526	ARG 495
Std.drug	**Ribavirin**	**-5.519**	**-30.576**	**-20.001**	**GLN 559, GLY 506**	-

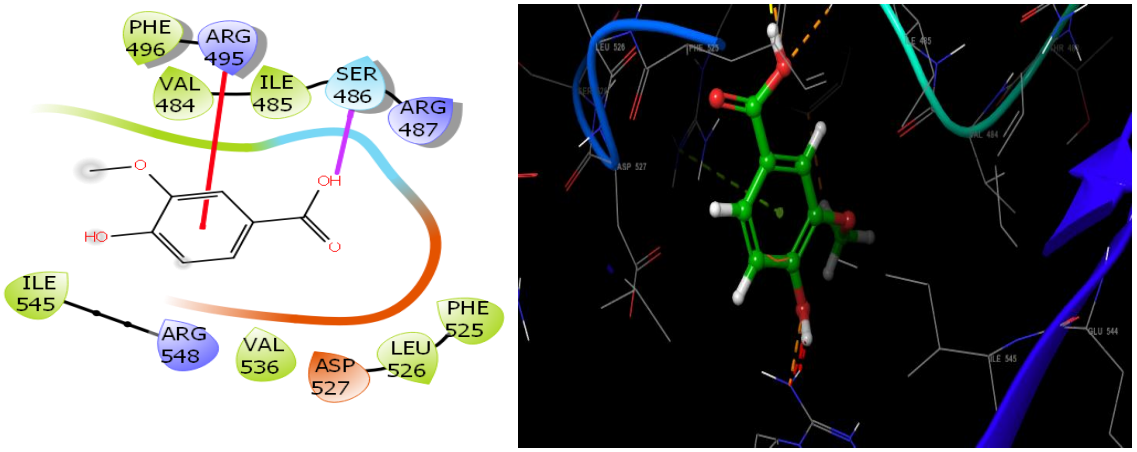

Figure 4: 2D and 3D Structure of docking interaction Vanillic acid with Nipah virus

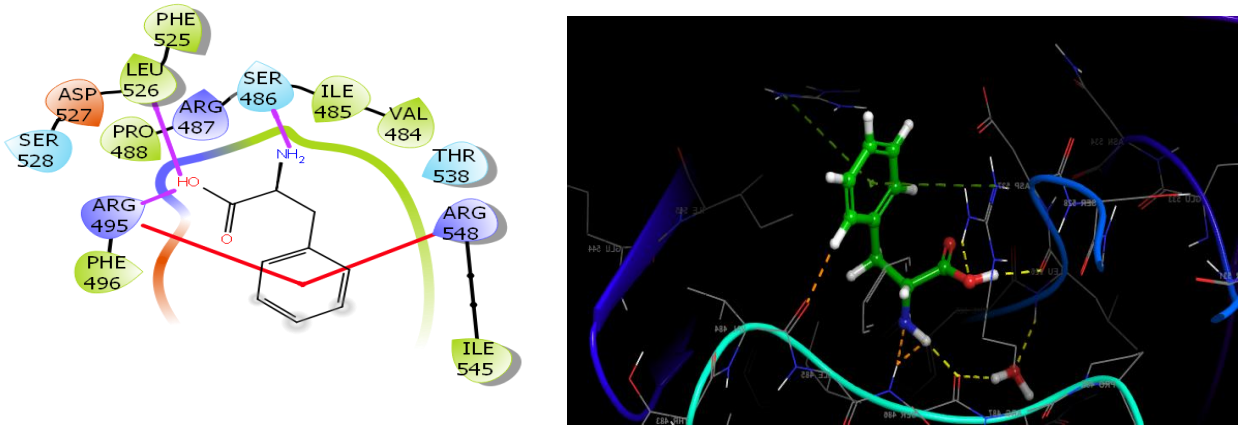

Figure 5: 2D and 3D Structure of docking interaction L-Phenylalanine with Nipah virus

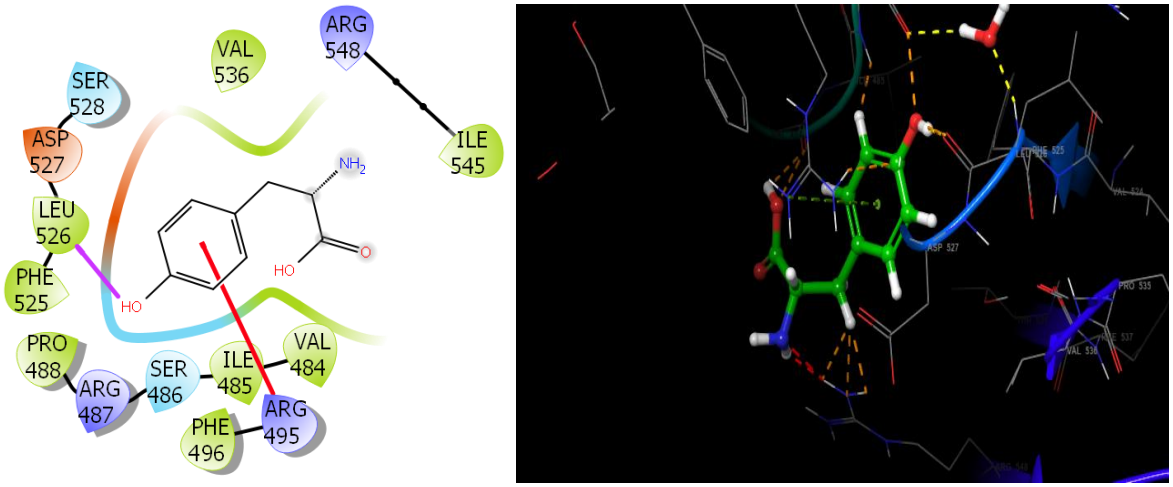

Figure 6: 2D and 3D Structure of docking interaction Tyrosine with Nipah virus

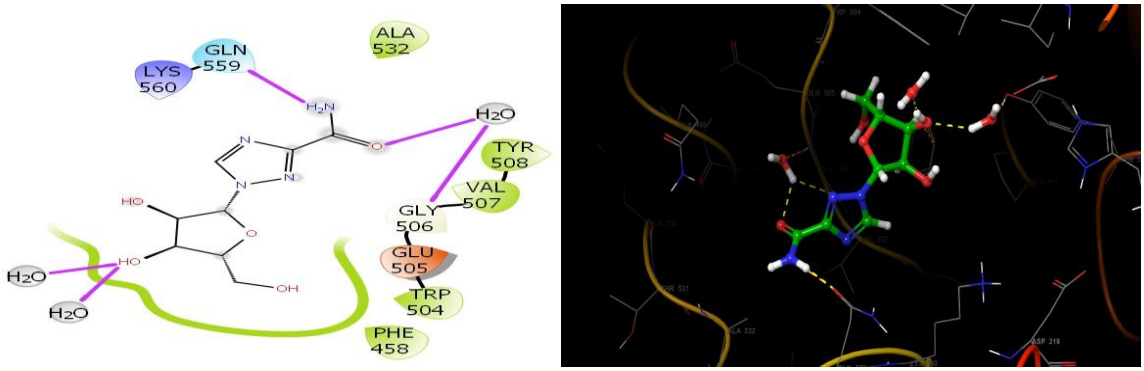

Figure 7: 2D and 3D Structure of docking interaction Ribavirin with Nipah virus

DISCUSSION:

The genome of the virus consists of a non-segmented negative-sense single-stranded RNA. The G protein mediates virus attachment and binds to the host cellular Ephrin-B2 and B3 receptors. The Ephrin-B2 is expressed in neurons, endothelial cells and smooth muscle surrounding arteries, placental tissue, spleen, and sinusoidal lining of lymph nodes. These tissues have been reported to be targets of Henipavirus infection. Ephrin-B3 is expressed in lymphoid cells, which may account for the NiV- infection-induced acute lymphoid necrosis. The NiV G was truncated into five fragments. They are NiV G1, consisting of amino acids 71-181, it is the stalk region. The other four truncated regions were within the globular head domain, constituted by amino acids 152-311(G2), 278-429(G3), 396-602(G4), and 498-602(G5), respectively (14). 6-Deoxy-L-Mannopyranose and Vanillic acid has less binding energy than the other phytoconstituents. Also, compared to the standard reference Ribavirin, which had a docking score of -5.519kcal/mol. 6-Deoxy-L-Mannopyranose of CNS value was within the limit value. So, it does not cause any toxicity in the CNS. The $\log_{HERG}$ attained less than -5. The molecular weight of 6-Deoxy-L-Mannopyranose and Vanillic acid were 164.1 and 168.149 respectively, all remaining parameters reached the recommended value. Our top-hit phytoconstituents(6- Deoxy- L- Mannopyranose and Vanillic acid) interact with G-site particularly G-4 and G-5 (484,486,495,526,536) and G-4 (486) aminoacid residues. Glycoprotein mainly involved in RNA replication. So in our study we promise active phytoconstituents inhibit the RNA replication of Nipah virus.

CONCLUSION:

Nipah virus spread last before two months in India. It does not have any proper vaccines and treatments against the virus to cure the infected person. The initial stage of this virus infects the lungs which travels in the brain, spleen and kidneys. So, we treat this disease by alternative methods of traditional plants like *Aloe barbadensis* and *Curcuma longa* against the viral activity. From the result,

we conclude that 6-Deoxy-L-Mannopyranose and Vanillic acid could excellent pharmacological drug candidate for effective attachment inhibitors. Consequently, it was thought that consuming it would be safe for people.

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CONFLICT OF INTEREST:
The author confirms no conflict of interest for this manuscript.

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