

**IN-SILICO INVESTIGATION OF  
INHIBITOR PHYTOCHEMICALS OF  
*GLYCYRRHIZA GLABRA* TARGETING  
FUSION GLYCOPROTEIN OF NIPAH  
VIRUS**

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## IN-SILICO INVESTIGATION OF INHIBITORY PHYTOCHEMICALS OF *GLYCYRRHIZA GLABRA* TARGETING FUSION GLYCOPROTEIN OF NIPAH VIRUS

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### Abstract

Nipah virus, a pathogenic zoonotic virus belongs to genus Henipavirus and family Paramyxoviridae responsible for encephalitis and significant threat to global health due to its high death rate, limited therapeutic option, and possible to transmission by multiple mode. First outbreak identify in Malaysia and Singapore in year 1998 in around pig farm. Currently no FDA approved drugs available in market but several research and clinical trials is underdevelopment to discover medication on urgent basis for preventive action in future outbreak. It is type of zoonotic virus so it transmitted by mostly animals and most common animals are pigs, fruit bats, some time dogs and also transmitted by contaminated date, palm, and horse meat.

Nipah virus structurally contain six protein, Fusion glycoprotein is one of them which is associate in viral entry into host cell by fusion with host cell membrane. Targeting fusion protein and understanding structure activity relationship with various potential phytochemicals is a promising strategy for antiviral drug development.

In this studies, use of medicinal plant '*Glycyrrhiza glabra*' which is usually known in india as a mullaithi and licorice for their medicinal value and their traditional uses in fever, sexual debility, cough, respiratory disorders, hyperdipsia, paralysis, stomach ulcers, rheumatism, skin disease and hemorrhagic disease because of various bioactive phytochemicals and selected 25 of them. Aim to investigate potential therapeutic drugs by molecular docking and ADMET studies. For In-silico investigation of fusion glycoprotein structure has downloaded from Protein Data Bank with ID 5EVM, a library of 25 phytochemicals from *Glycyrrhiza glabra* which identified by IMPPAT and downloaded by Pubchem and tool which use in study that is Biovia discovery studio, PyRx and SwissADME.

The result shows that all phytochemicals are good binding affinity whereas top six phytochemicals on the basis of their binding affinity such as Hispaglabridin B,

Glabrene, Shinpterocarpin, 3-Hydroxyglabrol, Glychionide A and Licoflavone B and their binding affinity is -9.8, -9.6, -9.5, -9.4, and -9.4 respectively make them a potential therapeutic drug for inhibition of Nipah virus.

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**List of Abbreviation**

NiV	Nipah virus
WTO	World Health Organization
BC	Before Christ
vRNA	Virus ribonucleoprotein
IMPPAT	Indian Medicinal Plants, Phytochemistry And Therapeutics
PDB	Protein Data Bank
ADME	Adsorption Distribution Metabolism and Excretion

# CHAPTER 1

## INTRODUCTION

### 1.1 Background

Nipah virus is a highly pathogenic which classified within the genus Henipavirus of the family Paramyxoviridae. The virus was initially isolated in 1998 during an outbreak of severe encephalitis near pig farming area in Malaysia and Singapore. Epidemiological investigations confirmed that transmission virus from infected pigs to humans, with a reported case death rate of around 40% [1]. The index cases were linked to occupational exposure in swine farms, with subsequent molecular characterization confirming NiV as a novel paramyxovirus. Fruit bats of the genus Pteropus were later recognize as the natural depository host [1].

Nipah virus exhibits multiple routes of zoonotic transmission to humans. Primary spillover events occur through direct contact with infected reservoir hosts, specifically fruit bats a member of genus Pteropus, or intermediate domestic animal hosts such as domestic pigs and goat [2]. Secondary transmission in humans population happen via intimate touch with infected individuals and primarily via respiratory droplets or bodily fluids. Infection of virus and mode of transmission has documented during eruption in Bangladesh and India [2].

NiV infection in human and exhibit several symptoms including fever, headaches, sore throat, vomiting, muscle pain these are early symptom of respiratory disease and acute encephalities, some time patient often go to coma and death in acute encephalities. The symptom of acute encephalities are most of neurological like vertigo, somnolence, and altered mental status [3]. These symptoms demonstrate the systemic involvement and neuroinvasive potential of the virus. Case fatality rates vary by outbreak, with documented mortality reaching 75% in certain epidemics. The high pathogenicity of NiV is associated to its neurotropic and systemic tropism, leading to multiorgan failure in fatal cases [3].

At current time unavailability of licensed vaccines or targeted antiviral therapy available for Nipah virus infection in clinical practice. Experimental approaches have yielded some promising results, particularly the monoclonal antibody m102.4, which has demonstrated neutralizing capacity against viral glycoproteins in animal studies. The antiviral compound ribavirin has shown modest therapeutic benefits in certain cases, though its efficacy remains inconsistent. These potential treatments require further rigorous evaluation through systematic clinical trials to determine their safety, optimal dosing, and therapeutic effectiveness in human populations [4].

The WHO made the Nipah virus a Priority Pathogen in its Research and Development Blueprint because of its high potential for epidemics and the development of medicinal for counter measures on the urgent basis. This categorization highlights the virus's potential to spread globally and create high-mortality epidemics, making immediate investments in the development of vaccines and antiviral medications necessary [5].

Nipah virus, a negative-sense single strand RNA virus contains the size of genome ~18,250 nucleotides belonging to the Paramyxoviridae family. It encodes total nine proteins, P gene contain four protein information (phosphoprotein (P), W, V, C protein) and other five such as nucleoprotein, matrix-protein, fusion-glycoprotein, attachment glycoproteins and a large polymerase protein [6].

By coordinated actions of two envelope glycoproteins, the Nipah virus infects host cells. By binding to cell receptors, the G glycoprotein causes the F glycoprotein to carry out membrane fusion [7].

Henipaviruses contain two surface spike glycoprotein. Spike glycoprotein bind with host cell surface receptor. After binding, F glycoprotein activated and preform virus-host cell membrane fusion and help virus to enter cell. Henipavirus F glycoprotein, a trimeric class I transmembrane glycoprotein produced as a precursor of F0 and undergo for post-translational split by host cell cathepsin-L in endosomal compartment and gives fusion promoting subunit F1 and F2 which are bind with disulfide bond. F glycoprotein change a metastable pre-fusion state to a high thermodynamically stable postfusion phase for farther activation. This state favour for viral envelop, interaction with host cell membrane and help membrane fusion for viral entry [7]. The structural examination of NiV virus membrane fusion

glycoprotein bind with human cell surface receptor Ephrin- B3 and help in viral entry. By focusing fusion glycoprotein structure, identify potential antiviral therapeutic phytochemicals on the basis of protein-ligand interaction [8].

In Indian history, the use of medicinal plants has been an integral part in maintaining human health and preserving cultural customs.

Medicinal plants contain therapeutic potential for drug discovery and also proven in history [9]. In past years, use of synthetic compounds as a source of API discovery declined in trend whereas natural compounds such as phytochemicals are most studied by the scientific community [9]. Now a large number of experiments are going on to isolate phytochemicals as potential drugs for specific targets by in-silico [9]. According to WHO, eight out of ten world population faith in medicinal plants for their primary health, medicinal plants have low cost, are environmentally friendly as compared to synthetic compounds [10][11]. Ancient Indian knowledge-books like Rig-Veda, Atharva-Veda, Charak Samhita and Sushruta Samhita also contain plants as primary sources of food as well as use in healthcare [11]. Use of medicinal plant *Glycyrrhiza glabra* from thousands of years in different countries including China, ancient Egypt, Greece and Rome [12]. Habitat of *Glycyrrhiza glabra* in Russia, UK, USA, Italy, France, Germany, Spain, China, Northern India (Punjab and Sub-Himalayan tracts) and Southern Europe [12]. *Glycyrrhiza glabra* belongs to the fabaceae (Pea) family and tracheophyta phylum.

Medicinal value of plant '*Glycyrrhiza glabra*' based on bioactive chemical substances, these substances are triterpenoid, saponin, flavonoids, tannins, alkaloids and phenolic substances [13]. Name of *Glycyrrhiza glabra* derived from ancient Greek term glykos means sweet and rhiza means root. In North India these plants are known as mullaithi and in Mediterranean and certain parts of Asia known as licorice or sweetwood [13] [14]. Some medicinal claims by traditional healers that this plant is effective in pathological conditions such as water pill, cholagogue, coughs, cold, and inflammation [13].

## 1.2 Objective of Study

1. In-silico screening of *Glycyrrhiza glabra* phytochemicals and fusion glycoprotein of Nipah virus.
2. visualization of *Glycyrrhiza glabra* phytochemicals and fusion glycoprotein of Nipah virus.
3. ADME studies of *Glycyrrhiza glabra* phytochemicals.

## **CHAPTER - 2**

### **Literature Review**

#### **2.1 Structure Nipah Virus and Mechanism of Host Cell Entry**

Nipah virus genetic sequence is a non-segmented, negative strand RNA virus which is transcribed and replicated by help of viral polymerase and generate capped and polyadenylated monocistronic corresponding to each of the viral genes at time of transcription [6] [16]. Genome of NiV i.e RNA , contains consecutive arranging from 3'-5;' direction. The RNA structure having six genes nucleocapsid, phosphoprotein, matrix-protein, fusion-glycoprotein, attachment-glycoprotein and long polymerases. Three genes i.e N, P and L makes (vRNA) by attaching together. G and F glycoprotein work as attachment and fusion respectively and host cell entry [6] [17].

Mechanism of NiV infection into its host cell by with two glycoprotein that is G-glycoprotein and Fusion glycoprotein protein. The G-glycoprotein help virus in attachment to host cell surface receptor whereas fusion glycoprotein make fusion between virus and cell membrane and help virus to enter into cell [16].

The G-glycoprotein protein of NiV trigger the fusion glycoprotein by binding to host ephrin B2/3 receptor and induce structure change in G-glycoprotein. The refolding of fusion glycoprotein demonstrates that monomeric ephrinB2 binds to fusion protein, causing an allosteric alteration in NiV G glycoprotein that aids in complete activation. This virus enters host cells by a receptor [7] [16] [17].

Recent studies shows that viral regulation of host cell machinery inhibit nucleolar Treacle protein that increase Henipavirus (Hendra and Nipha virus) production by targeting DNA-Damage Response (DDR) pathway [17].

#### **2.2 Transmission, Epidemiology, Pathology and Treatment of Nipah Virus**

Bats contains different types of high risk pathogen like Nipah, Rabies and Marburg viruses and serve as a reservoir hosts and transmit infection by directly or indirectly.

Other transmission of Nipah virus from bats to animal like pigs, human infected by pigs and palm juice. Fruit bats acts as main natural transmitting agent of Nipah virus and other transmission ways like viral contaminated date palm sap, Pteropus species, infected fruits are consumed by pigs and pet animals, NiV infected exported pork meat and close contact with Nipah virus infected human also spread to other human [17].

The first recognized case of human infection by Nipah virus in the Malaysian village of Sungai Nipah in 1998 and isolated from nose and oropharynx of pigs. Another outbreak identified in outside Malay peninsula in human by consuming horse meat and fruit contaminated with body fluid of bats [18]. Indian first NiV case reported in Siliguri, West Bengal in year 2001 at time of the eruption in Bangladesh and after that another outbreak reported from Nadia district West Bengal in 2007 [17]. Most recent outbreak documented in Kozhikode district, Kerala, and source of transmission identified as fruit bats [15] [17].

At time of autopsies on Malaysian patient, lesions found in their brain with disseminated microinfarction this caused vasculitis-induced thrombosis and directly affect neurons [19]. Vasculitic lesions also found in respiratory tract, heart and kidneys and these all patients were positive for Nipah virus. NiV affects mostly on medium size and small blood vessels and display endothelial multinucleated syncytia and fibrinoid necrosis [19].

In Malaysia, Ribavirin one of effective compounds used to treat other paramyxovirus patients [20]. But ineffective against animal model. However unavailability of effective antiviral drugs NCDC suggests Ribavirin use of oral and parental for all confirmed cases [20].

Broad-spectrum antiviral drug, Favipiravir a ribonucleotide well known ability to target viral RNA polymerase enzyme, it blocks the replication and transcription pathway of RNA virus [21]. A guanosine analogue Acyclovir, used to diagnose encephalitis in Singapore in year 1999 eruption [21]. Remdesivir used against Nipah virus [21]. Balapiravir, a nucleoside analogue shows an effective treatment against NiV [21]. Some of vaccine is going on in development like subunit vaccines, targeting certain section of G and F glycoprotein [21].

### 2.3 Fusion Glycoprotein as Potential Molecular Target for NiV Drug Discovery

At time of NiV enter human cells, two most important protein work together that protein is G glycoprotein and F glycoprotein. Fusion glycoprotein one of potential target for drug design which inhibit NiV. Type I transmembrane protein i.e fusion protein contain 546 amino acid. F0 precursor is split into two disulfide bond components i.e F1 and F2. F1 contains multiple function and responsible for fixing the F protein in lipid membrane and around twenty hydrophobic amino acid include fusion peptide at N-terminal area of F1 subunit. Fusion peptide is crucial for biological activity of F glycoprotein and F glycoprotein protein is responsible for initiation of host membrane fusion and cellular entry [22]. Fusion glycoprotein structurally identify as a potential antiviral therapeutic target for drug development and discovery by bioinformatics like protein-ligand interaction [8] [23]. Both glycoprotein lead to viral entry and fusion with host cell that make them a possible targeting protein for therapeutic drug discovery and vaccine development [23].

### 2.4 Historical Aspect of '*Glycyrrhiza glabra*' Used as a Traditional Medicine

*Glycyrrhiza glabra*, a well known traditional herb and a natural product which used as a medicine with fewer side effect for diverse disease in different nation [24]. Historical documented evidence present that earliest used of licorice were written in The Code Humnubari 2100 BC, licorice effective remedy for control ulcer and quenching of thirst mentioned by 'father of medicine' Hippocrates, Theophrastus mention licorice use in cough and asthma, Abu Ali Sina mention use of licorice for respiratory tract disease, stomach, reduce voice hoarseness in his book 'The book of Healing' [25]. Recent decade, *Glycyrrhiza glabra* also known as mulaithi, licorice or sweetwood is small perennial herb, traditionally used in disease like respiratory disease, polydipsia, fits, fever, hyopsexuality, palsy, stomach ulcers, rheumatism, skin disease, hemorrhagic disease, and jaundice[13] [14] [24].

### 2.5 Pharmacology of *Glycyrrhiza glabra*

*Glycyrrhiza glabra* or licorice contains large number of Phytochemicals and exhibit many pharmacological action including estrogenic, aldosterone-like action, anti-

bacterial, antiviral, anti-inflammatory, anti-trichomonas, anti-convulsive, choleric, anticancer, and anti-tussive activities [26].

Some effect happen like sodium water retention, hypertension and hypokalemia due to regular use of licorice root or glycyrrhizin (more than 3 gram per day for more than 6 weeks) [26]. Licorice probable not recommends for patient which contains hypertension or renal failure [26]. Licorice root tea and syrup is recommended for coughs and licorice also increase the secretion of Bronchial glands [27].

## **2.6 Phytochemicals of *Glycyrrhiza glabra***

Licorice contains different types of bioactive compound compatible to human health and worldwide known as their nutrient and medicinal properties. Dry Licorice roots contains water-soluble metabolites, sugar, starch, glycyrrhizin, amines and sterols. Different parts of plant like roots, stems, and leaves contains different amount of their endogenous synthesis, concentration of phytochemicals depends upon their geographical region and their climate condition, and method of isolation, processing, storage [25]. Researcher still analyze licorice root and their new phytochemicals, till date all important class of phytochemicals identified such as coumarins, auronones, benzofurans, phenols, pterocarpanes, saponins, flavonoids, chalcones, stibenes, volatile oils, tannins, glycosides and other substances [14] [25]. Triterpenoid compound, Glycyrrhizin responsible for sweet-tastes of licorice root and flavonoid including liquiritin, isoliquiritin, and other compounds is responsible for yellow colour of licorice roots [14].

## **2.7 Molecular Docking : A Computational Technique for In-silico Study**

Molecular docking is type of computational technique which use to prediction binding affinity between suitable molecules one is ligand (small molecule) to another is macromolecules(Receptor) and one of important technique use in in-silico study [28]. Molecular docking calculate binding affinity score by three main types that is force-field based, Knowledge-based statistical function and Empirical scoring [29]. Scoring function used to estimate binding affinity and binding affinity is directly associated to the Gibbs energy of binding. Molecular docking is computation tool which use in drug development and biological research with some limitation [30].

In this modern era computer-aid drug design and discovery, Molecular docking is widely known and successful computational tool which make fast, saving time, cost saving and high-efficient in pharmacological activity in new drug research[31]. Different types tool which use in molecular docking example Autodock vina, PyRx widely use by academic student [31].

## **2.8 Curcumin as Control Compound Use in Molecular Docking Analysis**

In india, Turmeric use as spice in daily basis in cooked vegetable and other because of highly medicinal phytochemicals. Turmeric contains bioactive phytochemicals such as curcumin, its is lipohilic polyphenol and serve as anti-cancer, antibiotic, anti-inflammatory, anti-neurodegenerative and anti-aging. Several studies and clinical trials is going on for drug development[32] [33].

A library of 25 phytocompounds which found in *Glycyrrhiza glabra* compiled for the current experiment from a multiple sources, including IMPPAT database, research journals, scientific database and botanical references. A thorough literature review and investigation conduct for phytochemicals which present in '*Glycyrrhiza glabra*' with their structural properties and potential antiviral properties. *Glycyrrhiza glabra* and their phytochemicals present in their different parts (roots, stem, leaves), selection of plant and phytochemicals base on their medicinal properties and contains potential consider to develop antiviral drugs. This study conduct for investigation and interpretation of binding interaction and structure-activity relationship between phytochemicals of *Glycyrrhiza glabra* and Nipah virus fusion glycoprotein.

## CHAPTER 3

### Computational Tools and Database Used in Molecular Docking

For Current study and investigation we used computational software which is free available such as PyRx, Biovia Discovery Studio, SwissDock ADME and biological Database including IMPPAT, PubMed, Pubchem, and PDB.

1. **PyRx** - Computational software with search engine is Autodock-vina used to studies molecular docking and binding affinities between ligand and target protein based on protein-ligand interaction.
2. **Biovia Discovery Studio** - A computational toolkit programme used to modification of ligand and target proteins, visualization in 2D and 3D and analysis of interaction.
3. **IMPPAT** - IMPPAT is a database of collection of Indian traditional medicinal plant and their phytochemicals. Currently database store data of around 4000 Indian medicinal plant, 18000 phytochemicals and 1100 therapeutic application [34] [35].
4. **PubMed**- PubMed is database which contains large number of literature review and research articles, most use of PubMed for citations and review of publication.
5. **Pubchem**- Pubchem is world largest database in the field of chemicals sciences because it contains a vast number of chemicals information like physical properties, structure, biological activity, safety, toxicity, patient and literature citations.
6. **PDB**- Protein Data Bank is world-wide known as collection of large number of experimentally design three-dimensional structure of macro-molecules like protein, nucleic acid and complex structure.

## CHAPTER 4

### Methodology

#### 4.1 Data Collection

This project work contains In-silico investigation of potential therapeutic phytochemicals for antiviral or viral inhibition. For completing of this project, collection of data-set from different database such as phytochemicals identification from IMPPAT. Target protein from Protein Data Bank. Phytochemicals library which contain total 45 chemicals and 2 controls from Pubchem, which is one of the most famous database of small molecule, bioactive compound and chemical substances.

#### 4.2 Target Protein Selection and Modification

Selection of target protein on the basis of complete structure available on Protein Data Bank. The 3D crystal shape of Nipah Virus Fusion Glycoprotein (5EVM) in the pre-fusion State downloaded with resolution of 3.37Å from RCSB PDB [7]. Original protein structure contains five chain and 529 amino acid with mutation and molecule name is Fusion glycoprotein [7]. The protein classified as viral protein, organism of Henipavirus nipahense which expression shows in Homo sapiens [7]. Downloaded protein contains hetatm (Hetero-atom), protein group and ligand group (see figure 1). Hetero-atoms makes unfavourable for molecular docking and gives unreal results. Thus need to modified target protein (5EVM) by removing hetatm and add polar hydrogen atoms (see figure 2.), these process makes suitable for molecular docking with enhance electrostatic interaction. Now protein ready for docking and protein-ligand interaction.

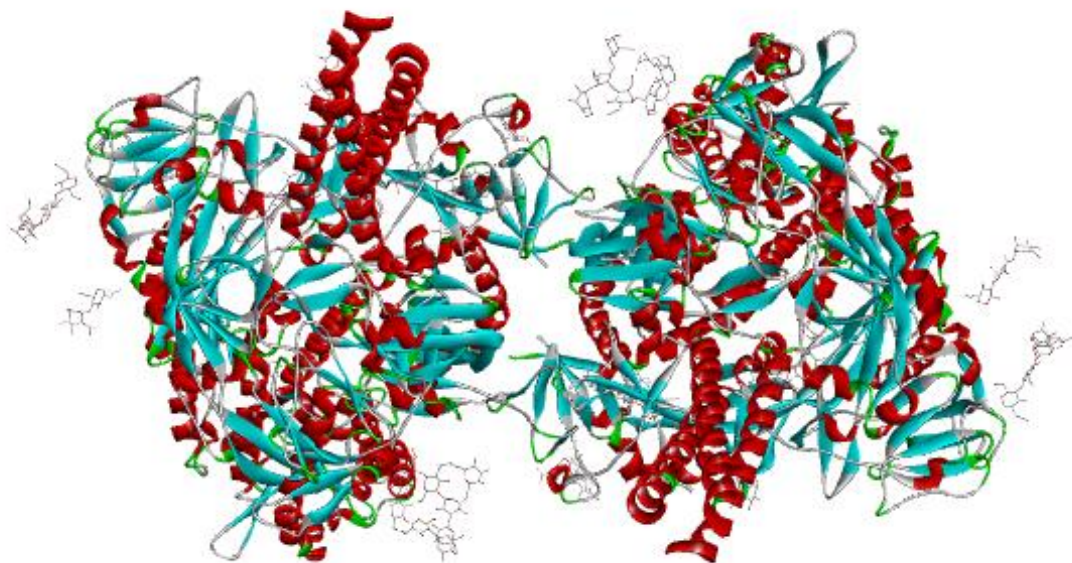


Figure 1.PDB downloaded three-dimensional structure of fusion glycoprotein (5EVM)

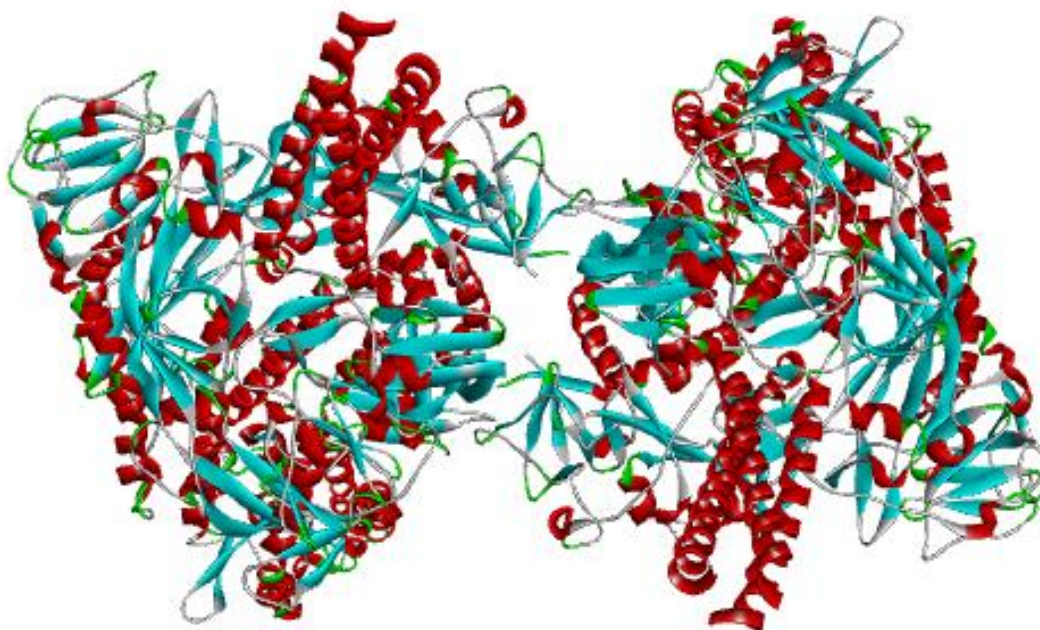


Figure 2. Modified PDB downloaded three-dimensional structure of fusion glycoprotein (5EVM).

#### 4.3 Selection and Preparation of Phytocompounds Library

*Glycyrrhiza glabra* one of the world wide known medicinal plant for cure different types of disease like asthma, Gastric Ulcers, Rheumatoid Arthritis, Herpes Simplex

Virus (HSV) and other. After an extensive review of scientific literature and phytochemicals database like IMPPAT, Pubchem, total 25 phytochemicals identify by IMPPAT and download in three-dimensional configuration by Pubchem[34] [35]. All bioactive compounds in SDF format (see table 1).

<b>Table 1. list of selected phytochemicals for library preparation with their Name, IMPPAT Id and Pubchem Id</b>		
<b>Phytochemicals Name</b>	<b>IMPPAT Id</b>	<b>Pubchem Id</b>
Hispaglabridin B	IMPHY001500	15228661
Glabrene	IMPHY000852	480774
Shinpterocarpin	IMPHY001239	10336244
3-Hydroxyglabrol	IMPHY000375	480854
Glychionide A	IMPHY001944	11597485
Licoflavone B	IMPHY000013	11349817
Glabranin	IMPHY010555	124049
Lutein	IMPHY011620	5281243
Glycyrrhisoflavone	IMPHY004988	5317764
Glabrocoumarin	IMPHY001798	11427657
Glabrol	IMPHY001866	11596309
Dehydroepiandrosterone	IMPHY016827	5881
Isoquercitrin	IMPHY012721	5280804
Licoricone	IMPHY004365	5319013
Isovitexin	IMPHY008689	162350
Hydroxywighteone	IMPHY005925	5378945
Galangin	IMPHY005434	5281616
Quercetin	IMPHY004619	5280343
Pratol	IMPHY004344	5320693
8-Prenlnaringenin	IMPHY000819	480764
beta-Sitosterol	IMPHY014836	222284
Glycyrin	IMPHY000864	480787
Kaempferol	IMPHY004388	5280863
Genistein	IMPHY004643	5280961
Glyzaglabrin	IMPHY005062	5317777

#### 4.4 Molecular Docking Studies

Molecular docking calculation was carried out on PyRx tool which run on the basis of AutoDock-Vina module available at (<https://pyrx.sourceforge.io/>). In PyRx programme, target protein in PDB format uploaded and make macro-molecule. Then we upload ligand in which download in 3D SDF, after uploading file minimize phytochemicals after that convert all to Autodock ligand in pdbqt format by Biovia discovery studio. Target protein 5EVM was docked with the Curcumin inhibitor as a control, run PyRx and calculate the binding energy. After few minutes process was completed and save the best best docking result in PDB at zero. Further, 25 Phytochemicals of *Glycyrrhiza glabra*, docked with target protein 5EVM. Docking results were evaluated based on binding affinity, interaction energy, and protein-ligand interactions, including different types of bond and their bond length like hydrogen bond, pi-pi interaction carbon- hydrogen bond[36].

In covalent docking, there are two method one is grid-based approach which determine a special map for the site of attaching covalent ligand and second one is modification of the flexible side chain method[37].

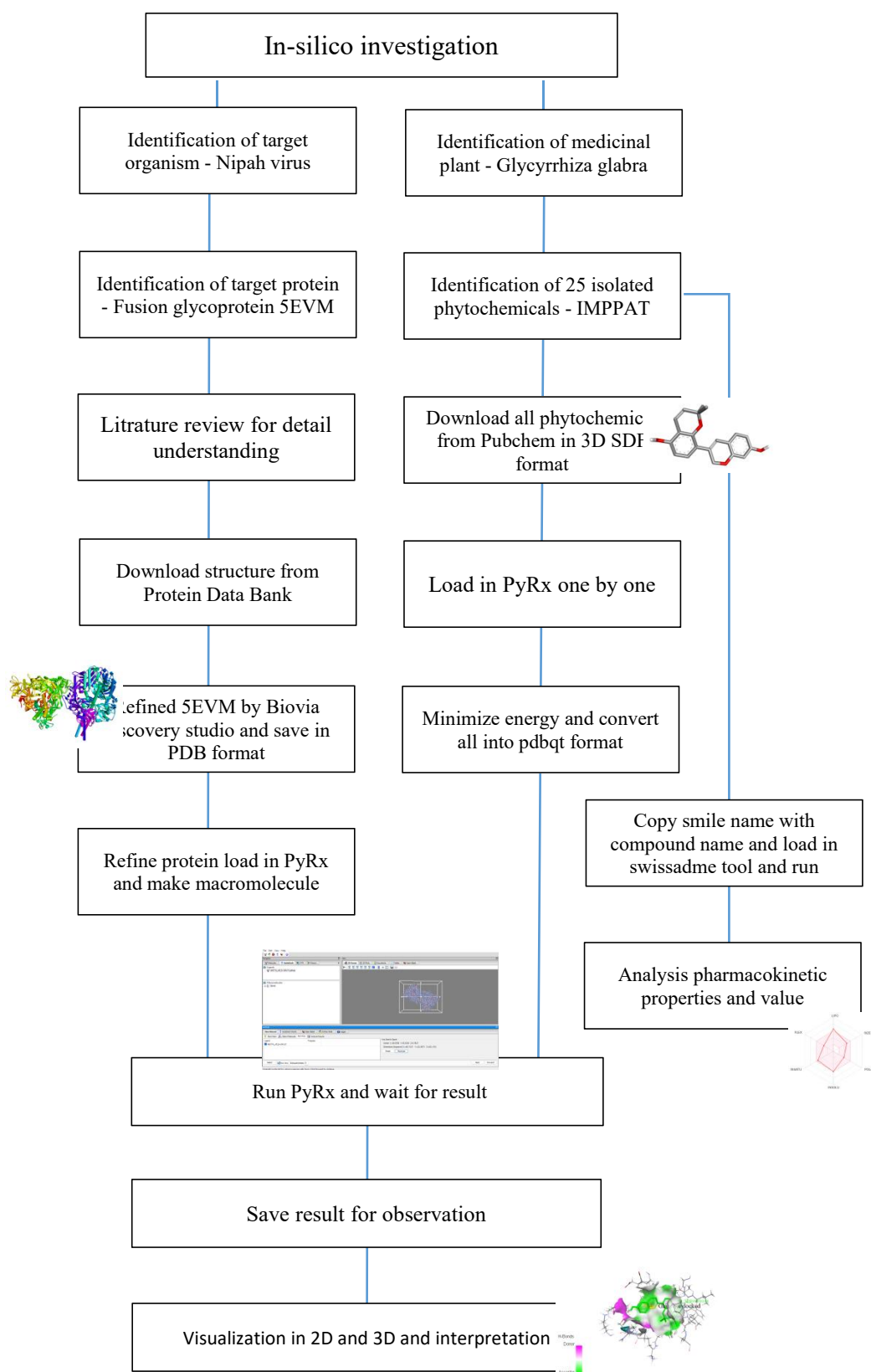
The result all ligand was loaded into Biovia discovery studio both target protein and ligand and these makes complex structure for visualization and analysis of receptor ligand interactions in 3D and 2D spaces.

#### 4.5 Docking Analysis

Different phytochemicals binding energy comparing with Curcumin and looking at the interaction between protein and ligand. Numerous of phytochemicals were studied. Some Curcumin equivalent, most of show higher binding affinity and some are low.

2D diagrams of the shortlisted five phytochemicals interactions with proteins as ligands. Hispaglabridin B, Glabrene, Shinpterocarpin, 3-Hydroxyglabrol and Glychionide A particular phytochemicals might make excellent candidates for pharmacological studies and further drugs trials. Other phytochemicals also shows good binding affinity with 5EVM.

## Overview of Methodology



## CHAPTER 5

### RESULT

#### 5.1 Binding Affinity and Scoring Analysis of Phytochemicals-5EVM Interactions

##### 5.1.1 Molecular Docking

The comparison of the docking result between the fusion glycoprotein (5EVM) of Nipah virus and conventional Coumarin as a control and 25 phytochemicals of *Glycyrrhiza glabra* was performed. Coumarin as control model, which demonstrate as

inhibitor of fusion glycoprotein with binding affinity of -7.9 Kcal/mol. Where as other 25 phytochemicals displaying good binding affinity [ Table 3 and figure 3]. out of 25 molecule, twenty molecule show very good binding affinity (-8.1 to 9.8 Kcal/mol) and other 10 molecule show little low binding affinity. Hispaglabridin B, Glabrene, Shinpterocarpin, 3-Hydroxyglabrol, Glychionide A showed significant inhibition with lower docking score as compared to control Coumarin.

Table 2. contains all analyzed Phytochemicals with their respective name and binding affinity at cluster RMSD vale is 0.

<b>Table 2. Estimated binding affinity of selected phytochemicals with fusion glycoprotein</b>	
<b>Ligands</b>	<b>Binding Affinity(kcl/mol)</b>
Hispaglabridin B	-9.8
Glabrene	-9.6
Shinpterocarpin	-9.5
3-Hydroxyglabrol	-9.4
Glychionide A	-9.4
Licoflavone B	-9.2
Glabranin	-9

Lutein	-9
Glycyrrhisoflavone	-9
Glabrocoumarin	-9
Glabrol	-9
Dehydroepiandrosterone	-8.8
Isoquercitrin	-8.7
Licoricone	-8.7
Isovitexin	-8.6
8-Prenlnaringenin	-8.6
Hydroxywighteone	-8.4
Galangin	-8.3
Quercetin	-8.1
Pratol	-8.1
beta-Sitosterol	-8
Glycyrin	-8
Kaempferol	-7.9
Genistein	-7.9
Glyzaglabrin	-7.9
Curcumin (control)	-7.9

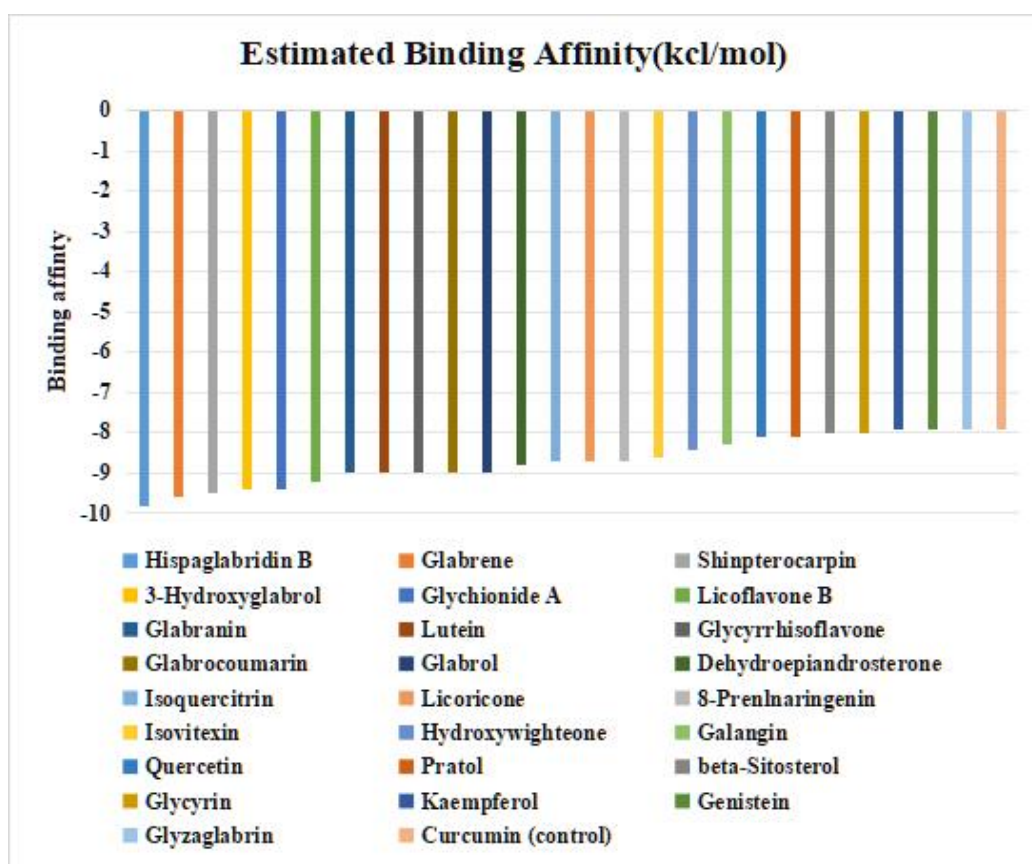


Figure 3. Graphical represent of binding affinity.

### 5.1.2 Molecular Visulization

In Figure 4(a). represent a 3D visualization which shows the cavities complex between Curcumin and fusion glycoprotein of Nipah virus and 4(b) display magnify version on 3D interaction with interacting atoms. Curcumin as a control model, It exhibits 4 Conventional Hydrogen Bond with Amino acid (Gln176, Asp177, Asn238 and Tyr178), 4 Pi-Alkyl Bonds with Amino acid (Ala202, Lys205, Leu and Tyr178), 1 carbon- hydrogen bond with amino acid Leu175, and 8 Van der Waals interaction with amino acid ( Lys205, Asp209, Tyr206, Gly236, Leu201, Leu175, Tyr178 and Ala174 {figure 4(c)}).

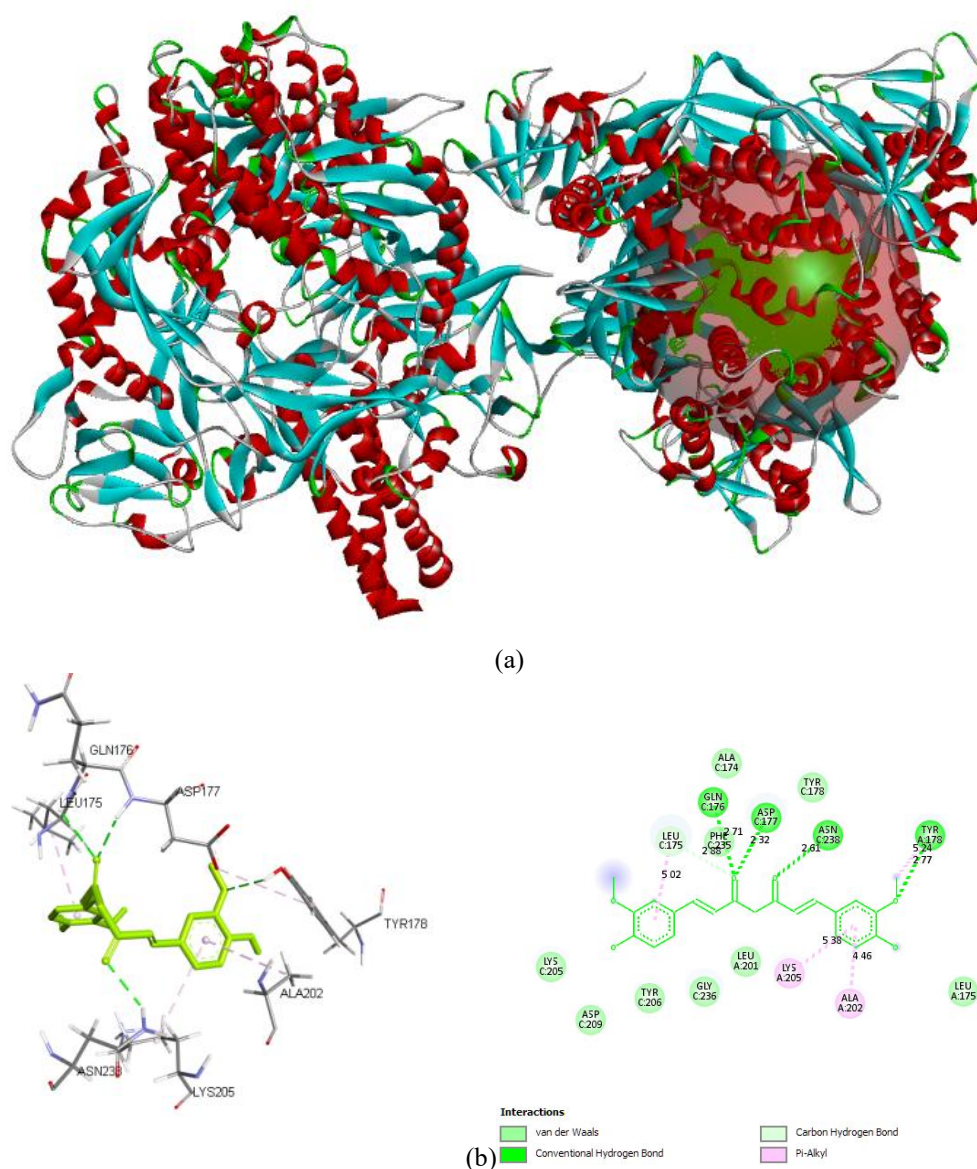
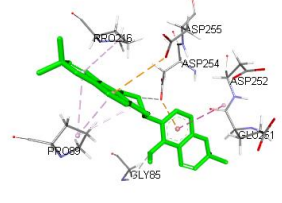
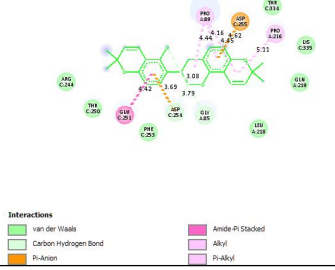
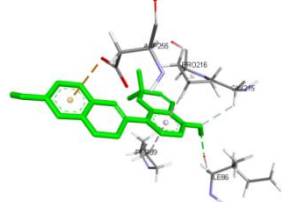
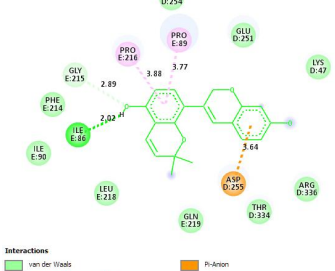
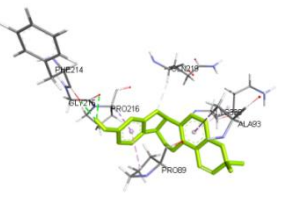
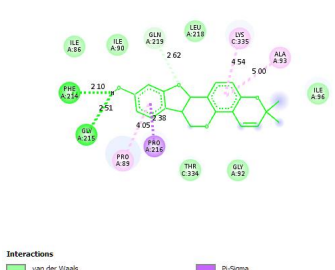
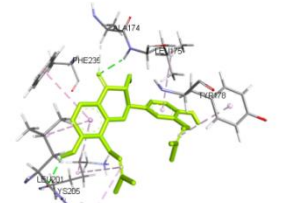
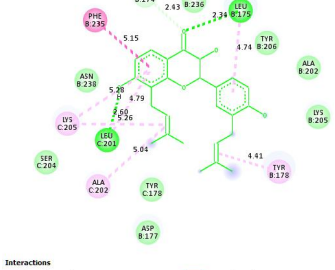
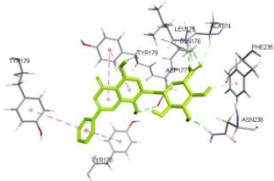
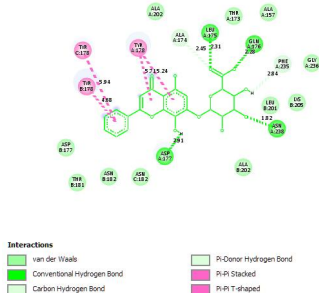
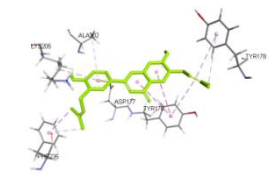
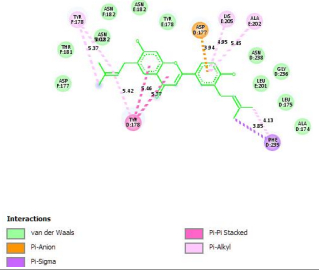
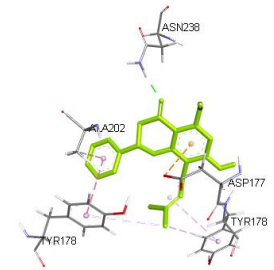
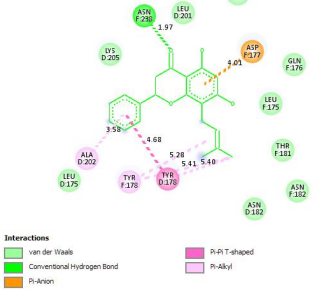
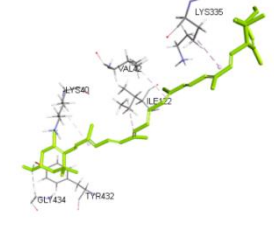
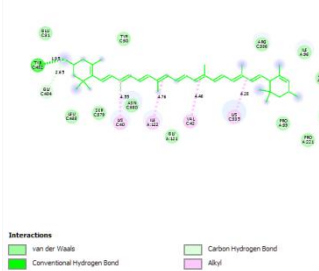
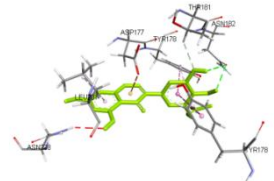
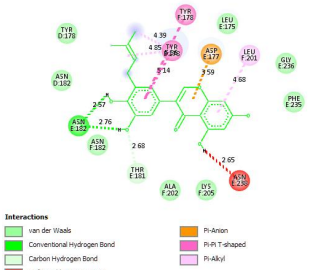


Figure 4. 2D and 3D visualization of control Curcumin with fusion glycoprotein( PBD ID; 5EVM) of Nipah virus via in-silico using Biovia discovery studio. (a) 3D visualization shows the cavities complex (b) 3D interaction with interacting atoms (c) 2D visualization of Curcumin complex with fusion glycoprotein.

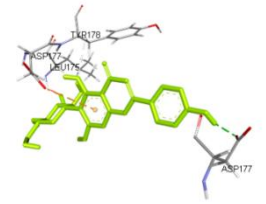
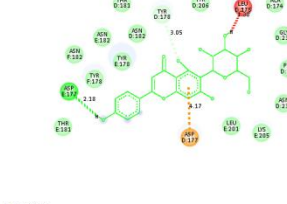
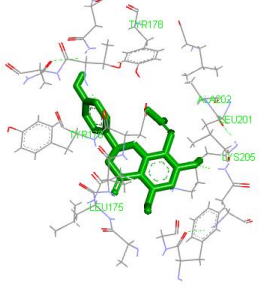
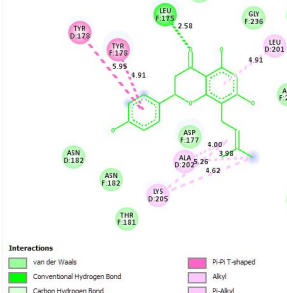
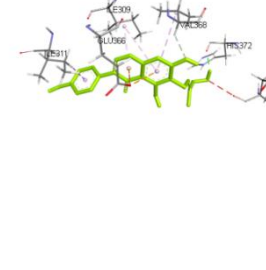
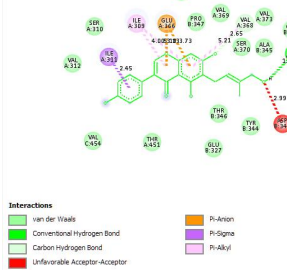
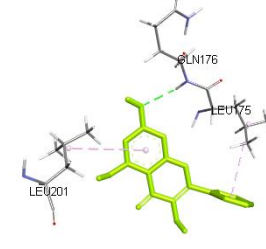
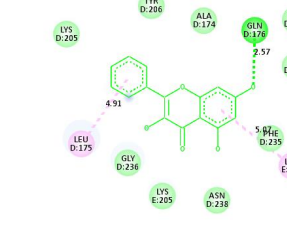
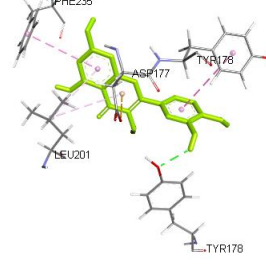
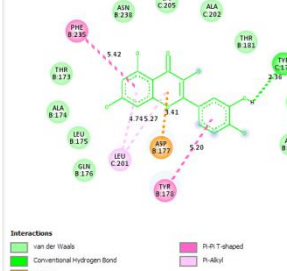
All the Phytochemicals successfully docked on Fusion glycoprotein of Nipah virus. Table 3 represents 3D and 2D images of post docking visualization all phytochemicals along with Active amino acid residues which involve in bond formation and number of hydrogen bond. 2D image contain ligand structure in green colour which enable us to identify groups and atoms involved in the bond formation with fusion glycoprotein.

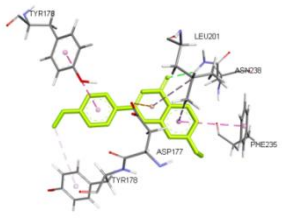
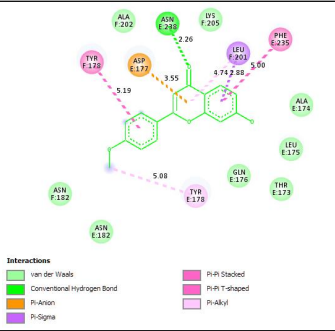
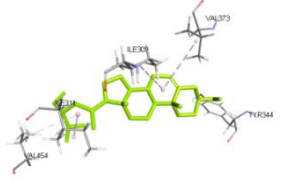
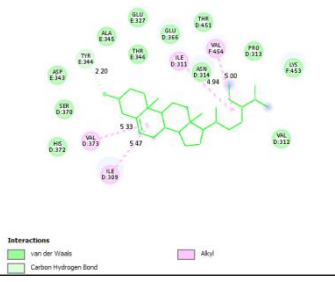
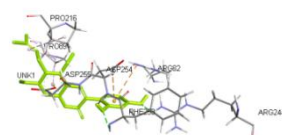
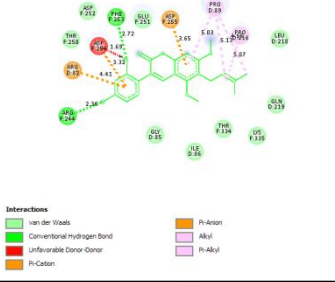
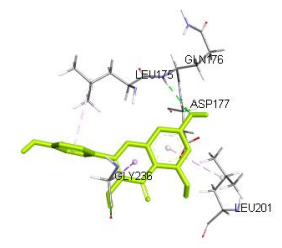
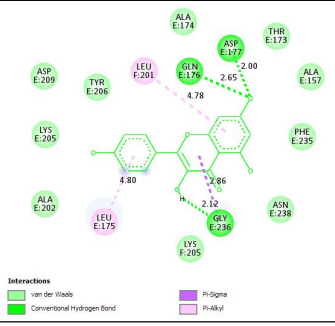
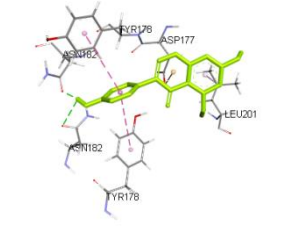
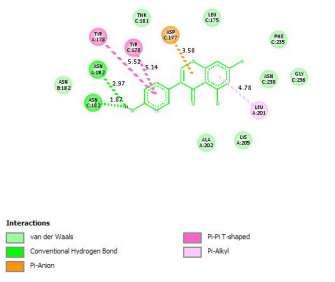
**Table 3. 2D and 3D visualization of all phytochemicals with their active amino acid residues and number of hydrogen bond**

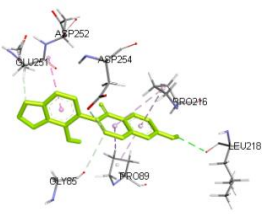
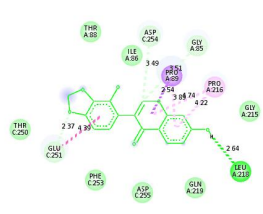
Molecule Name	3D interaction of phytochemicals (green in colour) and fusion glycoprotein (5evm) with their interacting atoms.	2D interaction of phytochemicals (green in colour) and fusion glycoprotein (5evm) with their interacting atom, ligand binding site atom, bond type and bond distance.	Active amino acid residues	Number of hydrogen bond (Figure 5.)
Hispaglabridin B			Pro89, Asp255, Thr334, Pro216, Lys355, Gln219, Leu218, Gly85, Asp254, Phe253, Glu251, Thr250, Arg244	0
Glabrene			Pro89, Pro216, Gly215, Ile86, Asp255, Asp254, Glu251, Lys47, Arg336, Thr334, Gln219, Leu218, Ile90, Phe214,	1
Shinpterocarpin			Pro216, Pro89, Lys355, Ala93, Gly215, Phe214, Ile86, Ile90, Ile96, Gly92, Thr334, Leu218	2
3-Hydroxyglabrol			Ala174, Leu175, Phe235, Lys205, Leu201, Ala201, Tyr178, Asp177, Lys205, Ala202, Ser204, Tyr206, Asn238, Gly336,	2

Glychionide A			Try178, Try178, Try178, Ala174, leu175, Gln176, Phe235, Asn338, Asp177, Ala20, Ala202, Ala157, Thr181, Asn182, Asn182, leu201, Gly236, Lys205	4
Licoflavone B			Thr178, Thr178, Asp177, Phe235, Lys205, Ala202, Asn182, Asn182 Asn178, Asn238, Try181, Try178, Leu201, Gly236, Ala174	0
Glabranin			Asn238, Asp177, Tyr178, Tyr178, Ala202, Lys205, Phe235, Ala157, Gln176, Leu175, Thr181, Asn182, Leu175	1
Lutein			Tyr432, Gly434, Lys40, Ile122, Val42, Lys335, Asn380, Glu81, Tyr90, Arg336, Ile96, Ala9, Glu121, Ile90, Pro89, Pro221, Asn380, Ser379, Leu433	1
Glycyrrhisoflavone			Tyr178, Pro178, Asp177, Leu201, Asn338, Asn238, Thr181, Asn182, Asn187, Asn182, Asp177, Leu175, Gly236, Phe235, Ala202, Lys205	2



Isovitexin		 <b>Interactions</b> van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Unfavorable Donor-Donor Pi-Alkyl	Asp177, Tyr206, Leu175, Asp177, Thr181, Tyr178, Tyr178, Asn182, Asn182, Thr181, Tyr206, Ala174, Gly174, Phe235, Asn238, Lys205, Leu201	1
8-Prenlnaringenin		 <b>Interactions</b> van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Pi T-shaped Alkyl Pi-Alkyl	Tyr178, try178, Leu175, Leu201, LYS205, Ala202, Asn182, Asn182, Asp177, Leu175, Asn238, Phe235, Gly236, Ala174, Gln176,	1
Hydroxywigteone		 <b>Interactions</b> van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Unfavorable Acceptor-Acceptor Pi-Alkyl	Ile311, Ile259, Glu366, Val368, His372, Asp343, Val454, Val312, Ser310, Leu367, Pro347, Val369, Val373, Ser370, Ala345, Gln342, Tyr344, Thr346, Glu327, Thr451,	1
Galangin		 <b>Interactions</b> van der Waals Conventional Hydrogen Bond Pi-Alkyl	Gln176, Leu201, Leu175, Lys205, Tyr206, Ala174, Thr173, Asp177, Ala157, Phe235, Asn238, Lys205, Gly236	1
Quercetin		 <b>Interactions</b> van der Waals Conventional Hydrogen Bond Pi-Alkyl Pi-Pi T-shaped	Phe235, Tyr178, Tyr178, Asp177, Leu201, Thr173, Asn238, Lys205, Ala202, Thr181, Asn182, Asn182, Gln176, Leu175, Ala174	1

Pratol		 <p><b>Interactions</b></p> <ul style="list-style-type: none"><li>van der Waals</li><li>Conventional Hydrogen Bond</li><li>Pi-Action</li><li>Pi-Sigma</li><li>Pi-Pi Stacked</li><li>Pi-Pi T-shaped</li><li>Pi-Alkyl</li></ul>	Tyr178, Asp177, Asn238, Leu201, Phe235, Tyr178, Ala202, Lys205, Ala174, Leu175, Gln176, Thr173, Asn182, Asn182	1
beta-Sitosterol		 <p><b>Interactions</b></p> <ul style="list-style-type: none"><li>van der Waals</li><li>Carbon Hydrogen Bond</li><li>Alkyl</li></ul>	Tyr344, Ile311, Asn314, Val454, Ile259, Val373, His372, Ser370, Asp343, Ala345, Thr346, Glu327, Glu366, Thr451, Asn314, Pro313, Lys453, Val312	0
Glycyrrin		 <p><b>Interactions</b></p> <ul style="list-style-type: none"><li>van der Waals</li><li>Conventional Hydrogen Bond</li><li>Unfavorable Donor-Donor</li><li>Pi-Cation</li><li>Pi-Action</li><li>Alkyl</li><li>Pi-Alkyl</li></ul>	Arg244, Arg82, Asp291, Phe253, Asp255, Pro89, Pro216, Asp252, Glu251, Leu218, Gln219, Lys335, Thr334, Ile86, Gly85, Thr250	2
Kaempferol		 <p><b>Interactions</b></p> <ul style="list-style-type: none"><li>van der Waals</li><li>Conventional Hydrogen Bond</li><li>Pi-Sigma</li><li>Pi-Alkyl</li></ul>	Leu201, Gln176, Asp177, Gly236, Leu175, Ala202, Lys205, Asp209, Tyr206, Ala174, Thr173, Ala157, Phe235, Asn238, Lys205	3
Genistein		 <p><b>Interactions</b></p> <ul style="list-style-type: none"><li>van der Waals</li><li>Conventional Hydrogen Bond</li><li>Pi-Action</li><li>Pi-Pi T-shaped</li><li>Pi-Alkyl</li></ul>	Asn182, Asn182, Tyr178, Asp177, Leu201, Asn182, Thr181, Leu175, Phe235, Asn238, Gly236, Lys205, Ala202	2

Glyzaglabrin			Glu251, Asp254, Pro89, Gly85, Pro216, Leu218, Thr88 Ile86, Gly215, Gln219, Asp255, Phe253, Thr250	1
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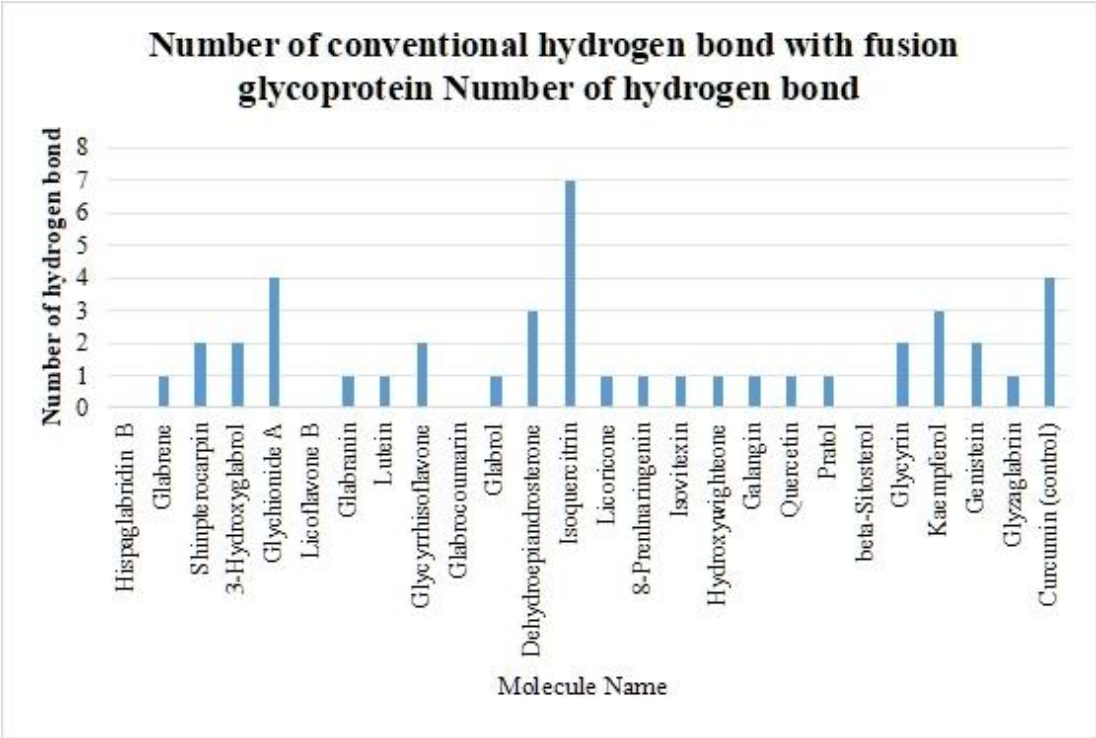


Figure 5. Number of conventional hydrogen bond with fusion glycoprotein Number of hydrogen bond

5.2 ADME ANALYSIS

The swiss ADME free web-based tool which help predict and estimate the value of physiochemical properties, lipo-philicity, water-solubility, pharmacokinetic, drug-likeness, medicinal chemistry of phytochemicals and pictorial representation of BOILED-Egg and Radar plot. Swiss ADME tool use to study and predict adsorption, distribution, metabolism and excretion in early stage of drugs development[38].

BOILED-Egg represent that number of molecule which cross the Blood Brain Barrier under the yellow and not cross Blood Brain Barrier beyond the yellow. Another molecular prediction to be PGP+ and PGP-marked with red, Pgp+ marked with blue dot indication that they may be effluxed from brain or gut and less effective. Whereas PGP- not pumped out by P-gp and higher chance to absorbed in Gastrointestine (figure 6.).

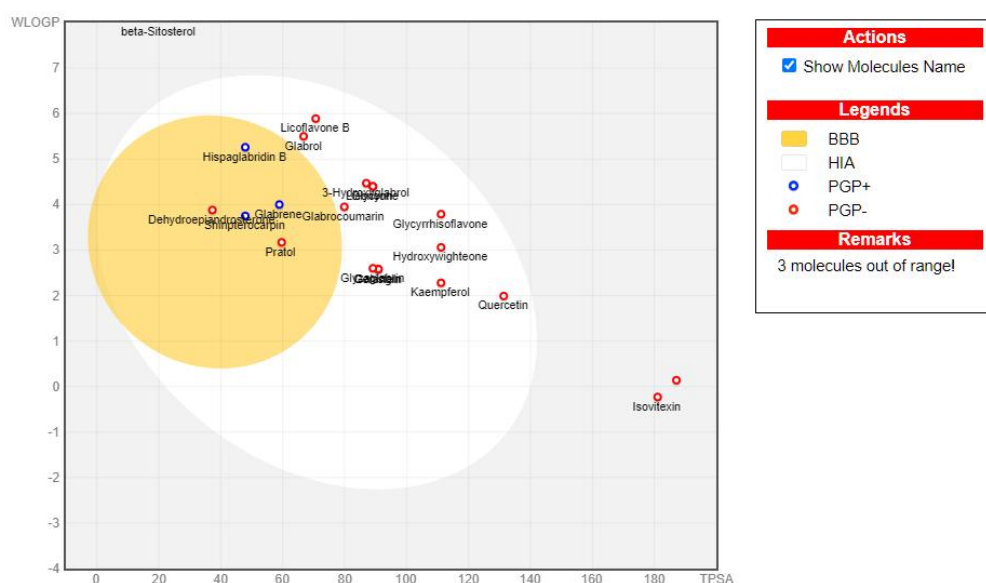


Figure 6. BOILED-Egg diagram of all phytochemicals

The analysis focused on molecular weight, consensus log P, Water solubility Class, gastrointestinal absorption, BBB permeability, P-glycoprotein (Pgp) substrate activity, skin permeability (log Kp), number of violations in Lipinski rule of five, value of bioavailability, violations of Lead-likeness, and synthetic accessibility which manifest that most of the phytochemicals under range demonstrated in Table 4.

All phytochemicals bioavailability under limit that is 0.55 excepted Glychionide A. Glychionide A, Isoquercitrin, Isoviteixin, beta-Sitosterol, Glycyrin, violate Lipinski rule of five (table 5.). whereas most of molecules shows high GI absorption and approx 50% molecule are BBB permeability.

Table 4. swiss ADME value of 25 phytochemicals and one control Curcumin with their respective molecular weight, consensus log P, Water solubility Class, gastrointestinal absorption, BBB permeability, P-glycoprotein (Pgp) substrate activity, skin permeability (log Kp), Lipinski rule of five's violations, bioavailability score, Lead-likeness violations, and synthetic accessibility.

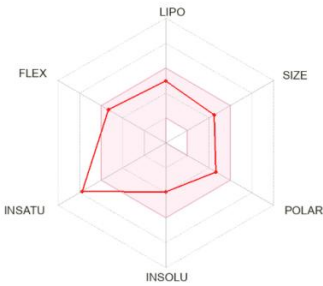
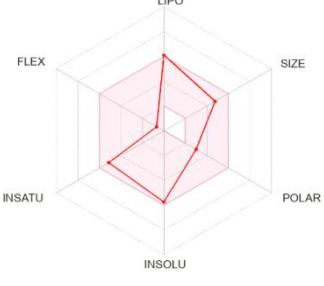
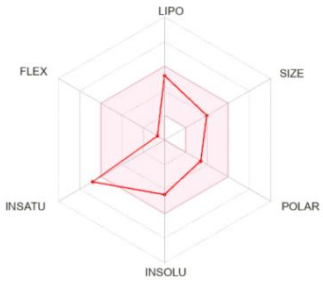
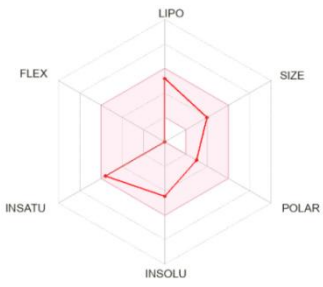
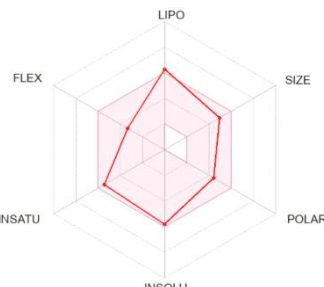
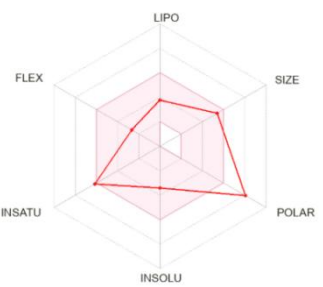

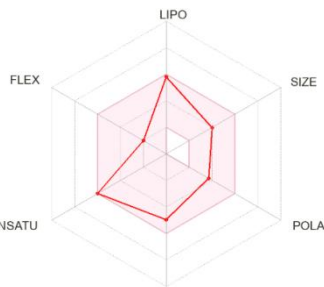


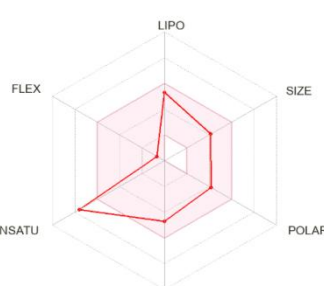
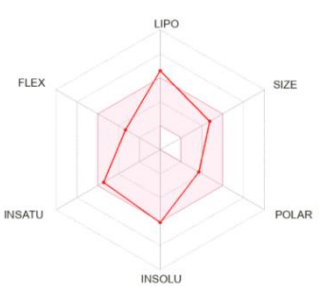
<b>Table 4. Pharmacokinetic of selected phytochemicals by swissadme</b>											
Molecule	MW (g/mol)	Consensus Log P	Water solubility (ESOL Class)	GI absorption	BBB permeant	Pgp substrate	log Kp (cm/s)	Violations of Lipinski rule	Bioavailability Score	Violations of Lead-likeness	Synthetic Accessibility
Control (Curcumin)	368.38	3.03	Soluble	High	No	No	-6.28	0	0.55	2	2.97
Hispaglabridin.B	390.47	4.69	Moderately soluble	High	Yes	Yes	-5.01	0	0.55	2	4.45
Glabrene	322.35	3.36	Moderately soluble	High	Yes	Yes	-5.68	0	0.55	1	3.54
Shinpterocarpin	322.35	3.37	Moderately soluble	High	Yes	Yes	-5.74	0	0.55	1	4.26
3-Hydroxy labrol	408.49	4.1	Moderately soluble	High	No	No	-4.89	0	0.55	2	4.51
Glychionide A	446.36	0.07	Soluble	Low	No	No	-8.23	2	0.11	1	5.12
LicoflavoneB	390.47	5.19	Poorly soluble	High	No	No	-4.19	0	0.55	2	3.93
Glabranin	324.37	3.67	Moderately soluble	High	Yes	No	-4.96	0	0.55	1	3.63
Lutein	568.87	3.67	Moderately soluble	High	Yes	No	-4.96	0	0.55	1	3.63
Glycyrrhiso flavone	354.35	3.08	Moderately soluble	High	No	No	-5.45	0	0.55	2	3.53
Glabroco umarin	336.34	3.33	Moderately soluble	High	No	No	-5.68	0	0.55	1	3.76
Glabrol	392.49	5	Poorly soluble	High	No	No	-4.4	0	0.55	2	4.15
Dehydroepiandrosterone	288.42	3.42	Soluble	High	Yes	No	-5.77	0	0.55	0	4.66
Isoquercitrin	464.38	-0.48	Soluble	Low	No	No	-8.88	2	0.17	1	5.32

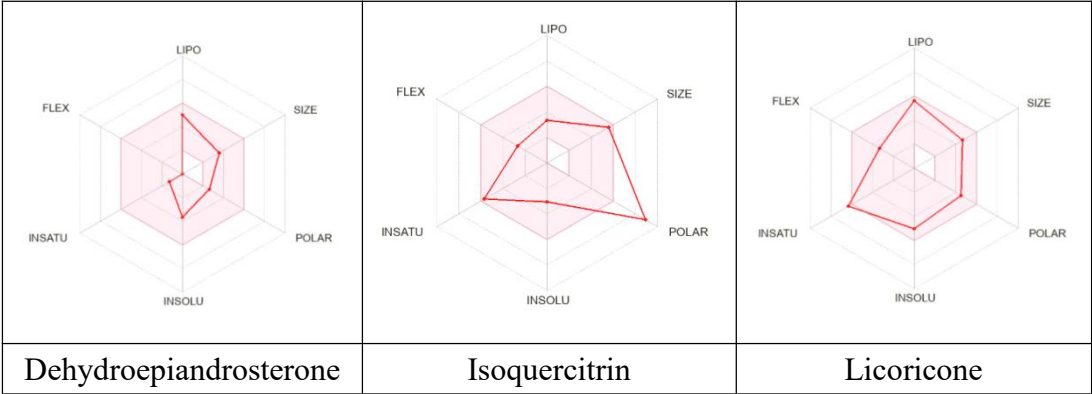
Licoricon e	382.4 1	3.67	Moderately soluble	High	No	No	-5.55	0	0.55	2	3.67
Isovitexin	432.3 8	-0.02	Soluble	Low	No	No	-8.79	1	0.55	1	4.99
Hydroxy wighteon e	354.3 5	2.64	Moderately soluble	High	No	No	-6.09	0	0.55	1	3.38
Galangin	270.2 4	1.99	Soluble	High	No	No	-6.35	0	0.55	0	3.12
Quercetin	252.2 4	1.23	Soluble	High	No	No	-7.05	0	0.55	0	3.23
Pratol	268.2 6	2.81	Moderately soluble	High	Yes	No	-5.39	0	0.55	1	2.92
8- Prenlnari ngenin	340.3 7	3.29	Moderately soluble	High	No	Yes	-5.22	0	0.55	0	3.67
beta- Sitosterol	414.7 1	7.24	Poorly soluble	Low	No	No	-2.2	1	0.55	2	6.3
Glycyrin	382.4 1	3.92	Moderately soluble	High	No	No	-5.3	0	0.55	2	3.66
Kaempfer ol	286.2 4	1.58	Soluble	High	No	No	-6.7	0	0.55	0	3.14
Genistein	270.2 4	2.04	Soluble	High	No	No	-6.05	0	0.55	0	2.87
Glyzagla brin	298.2 5	2.12	Soluble	High	No	No	-6.5	0	0.55	0	3.18

The RADAR plot integrated into swissadme web tool which represent novel graph of molecule to facilitate the rapid assessment of multiple physiochemical properties like lipophilicity, polarity, size, solubility, and flexibility onto a single radial graph. Each axis represent to one property and shape give overview of compound' ADME profile. Control Curcumin and Best 10 phytochemicals on the basis of their binding affinity compound Hispaglabridin B, Glabrene, Shinpterocarpin, 3-Hydroxyglabrol, Glychionide A, Licoflavone B, Glabranin, Lutein, Glycyrrhisoflavone, Glabrocoumarin RADAR plot (<http://www.swissadme.ch/index.php#>) represented in table 5.

The pink region represents the standard range for every characteristic.

**Table 5. RADAR plot of 14 phytochemicals with their name**

		
Curcumin (control)	Hispaglabridin B	Glabrene
		
Shinpterocarpin	Hydroxyglabrol	Glychionide A
		
Licoflavone B	Glabranin	Lutein
		
Glycyrrhisoflavone	Glabrocoumarin	Glabrol



## CHAPTER 6 CONCLUSION

In conclusion, in-silico drug design and discovery is one of suitable, cost reducing and minimum utilization of time and resources to discover novel therapeutic drugs. This study show that significant development in positive way to discover antiviral medication and a comprehensive literature review of medicinal value of plant *Glycyrrhiza glabra*, mechanism of cellular entry of Nipah Virus. Study also demonstrate that use of crystallographic structure of target protein, analysis of structure activity relationship and interpretation by molecular docking and visualization respectively and ADME analysis of phytochemicals.

On the base on result phytochemicals Hispaglabridin B, Glabrene, Shinpterocarpin, 3-Hydroxyglabrol, Glychionide A and Licoflavone B display very good binding affinity as compare to control that is more than -9 kcl/mol with target protein 5EVM ( fusion glycoprotein) which gives a positive signal to further in vivo experiment and antiviral drug against Nipah Virus. Whereas interpretation of two dimension and three dimension diagram, Isoquercitrin and Glychionide A formed highest conventional hydrogen bond with 5EVM that is 7 and 4 respectively as compare to control. Another aspect of this study is ADME, in ADME analysis most of molecule exhibit high GI absorption, few are BBB permanence and all phytochemicals shows 0.55 Bioavailability Score except Glychionide A and Isoquercitrin. Finally studies gives a good result in terms of binding affinity, hydrogen bond and ADMET, in aspect of binding affinity all phytochemical are good but top six Hispaglabridin B, Glabrene, Shinpterocarpin, 3-Hydroxyglabrol, Glychionide A and Licoflavone B potential inhibit Nipah Virus by blocking the activity of fusion glycoprotein. Further more studies required for antiviral medication like in-vivo experiments, clinical trails for complete understanding of their mechanism of action, effectiveness and safety.

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### Conference 1.

**Title of conference paper :** In-silico Investigation Of Phytocompounds From Polygonum cuspidatum As Therapeutic Drug Candidate For 1F9F Protein Of Human Papillomavirus (HPV)

**Name of Authors :** Ravishankar Kumar, Pinki and Navneeta Bharadvaja

**Name of conference:** Second International Conference on Emerging Technologies in Science and Engineering (ICETSE)

**Organizers details :** Akshaya Institute of Technology, Tumkur, Karnataka

**Status :** Accepted

**Date of Acceptance :** 6 May 2025

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International Conference on Emerging Technologies in Science and Engineering (ICETSE) to be held on 19-20 June 2025 at Akshaya Institute of Technology, Tumkur, Karnataka, Ravishankar kumar, Pinki and Navneeta Bharadvaja\* corresponding author in 'In-silico Investigation Of Phytocompounds From Polygonum cuspidatum As Therapeutic Drug Candidate For 1F9F Protein Of Human Papillomavirus (HPV)'

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 Likely AI-generated text that was likely revised using an AI-paraphrase tool or word spinner.

#### Disclaimer

Our AI writing assessment is designed to help educators identify text that might be prepared by a generative AI tool. Our AI writing assessment may not always be accurate (it may misidentify writing that is likely AI generated as AI generated and AI paraphrased or likely AI generated and AI paraphrased writing as only AI generated) so it should not be used as the sole basis for adverse actions against a student. It takes further scrutiny and human judgment in conjunction with an organization's application of its specific academic policies to determine whether any academic misconduct has occurred.

### Frequently Asked Questions

#### How should I interpret Turnitin's AI writing percentage and false positives?

The percentage shown in the AI writing report is the amount of qualifying text within the submission that Turnitin's AI writing detection model determines was either likely AI-generated text from a large-language model or likely AI-generated text that was likely revised using an AI-paraphrase tool or word spinner.

False positives (incorrectly flagging human-written text as AI-generated) are a possibility in AI models.

AI detection scores under 20%, which we do not surface in new reports, have a higher likelihood of false positives. To reduce the likelihood of misinterpretation, no score or highlights are attributed and are indicated with an asterisk in the report (\*%).

The AI writing percentage should not be the sole basis to determine whether misconduct has occurred. The reviewer/instructor should use the percentage as a means to start a formative conversation with their student and/or use it to examine the submitted assignment in accordance with their school's policies.

#### What does 'qualifying text' mean?

Our model only processes qualifying text in the form of long-form writing. Long-form writing means individual sentences contained in paragraphs that make up a longer piece of written work, such as an essay, a dissertation, or an article, etc. Qualifying text that has been determined to be likely AI-generated will be highlighted in cyan in the submission, and likely AI-generated and then likely AI-paraphrased will be highlighted purple.

Non-qualifying text, such as bullet points, annotated bibliographies, etc., will not be processed and can create disparity between the submission highlights and the percentage shown.



# Ravishankar Kumar

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Age :[24]

## Education

<b>Master of Science (Biotechnology)</b>	2023-25
Delhi Technological University	
<b>Bachelor of vocational studies (Biomedical sciences) with 70.1%</b>	2020-23
Central University of Haryana	
<b>Intermediate /10+2 (Science) with 80.40%</b>	2018-20
Nalanda College, Bihar sharif	
<b>Advance deploma in computer science with 78%</b>	2019-20
It vision, bihar sharif	
<b>10<sup>th</sup> with 74.2%</b>	2016-18
Nalanda collegiate, Bihar sharif	

## Experience

Molecular docking  
 Molecular Techniques (PCR, Electrophoresis, centrifugation, spectroscopy)  
 Quality control in API testing  
 Quality control in Biomedical devices  
 Analytical techniques for chemical testing  
 GLP AND GMP  
 SOP drafting by pharmacopeia  
 Validation and calibration  
 CAPA (corrective and preventive action)  
 Environmental and Biosafety, GMP, GLP

## Internship

Sterimed Surgical India Pvt Ltd (2023)  
 15-day internship in Handling of Biomedical Devices and Quality Assurance (Basic Pathology Lab)  
 Penam Laboratories Pvt Ltd (2022)  
 2-month internship in Quality Assurance and Quality Control

## Skills

**Technical Skills:** Basic understanding of medical/scientific equipment and their applications (By two types of internships), laboratory procedures, scientific data analysis.

### Soft Skills:

Communication: Excellent written and verbal communication skills, with the **ability to tailor presentations** to diverse audiences.

Teamwork: Proven ability to collaborate effectively within a team environment.

**Office skills:** Microsoft Office Suite (Word, Excel, PowerPoint), Basic of languages R and MySQL

**Certificate**

LSSSDC level 7 EHS manager certificate

LSSSDC level 6 licensing manager certificate

LSSSDC level 5 QC chemistry certificate

LSSSDC level 4 production/machine operator life science certificate