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INSILICO STUDIES OF *CENTELLA ASIATICA* PHYTOCONSTITUENTS ON ANTI-VIRAL ACTIVITY

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ABSTRACT

Objectives: A Virus is a tiny infectious agent that produces inside the cells of living hosts. The Present Study was designed to perform the Docking studies for various phytoconstituents present in *Centella asiatica* against viral protein using Argus lab and Auto dock tools and comparing its binding efficiency. **Materials and Methods:** Collection of chemical structure of phytoconstituents present in *Centella asiatica.* Downloading the following softwares such as Chemsketch, Argus lab 4.0.1, Autodock tools 1.5.4, discovery studio. Draw structures using chemsketch, docking studies using Argus and Auto dock tools, Selection of protein and preparation Selection of ligand and preparation, Docking and Analysis. **Results:** The following structures are drawn by chemsketch and Phytoconstituents of, *Centella asiatica*. Aminoacids involved in binding between protein (6LU7).The ligand protein interaction can be simply viewed by click the 'ligand interactions' in the discovery studio file and note the amino acid which were involved in the Hydrogen bond, Electrostatic bond and Hydrophobic bond. **Conclusion:** As the anti-viral agents are docked against anti-viral proteins, the docking scores were obtained. From the results we can concluded that best binding energy of the compound. The number of hydrogen bonds in the compound (weak electrostatic bonds between proton and electronegative of the compound) will estimate the better binding effects.

KEYWORDS

Virus, Anti-viral agent, *Centella asiatica* and Molecular docking.

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INTRODUCTION

A Virus is a tiny infectious agent that produces inside the cells of living hosts. When infected, the host cell is forced to rapidly produced thousands of identical copies of the original virus. Viruses are made of either two or three parts. All include genes. These genes contain the encoded biological

information of the virus and are built from either DNA or RNA. Viruses range in size from 20 to 300 nanometres; it would take 33,000 to 500,000 of them, side by side, to stretch to 1 centimetre (0.4in). Viral infections can cause disease in humans, animals and plants. In healthy humans and animals, infections are usually eliminated by the immune system, which can provide lifetime immunity to the host for that virus. Antibiotics, which work against bacteria, have no impact, but antiviral drugs can treat life-threatening infections. Those vaccines that produce lifelong immunity can prevent some infections. Currently, viral infection is the most serious health issue which causing unexpected higher rate of death globally. Many viruses are not yet curable, such as corona virus-2 (SARS-CoV-2), human immunodeficiency virus (HIV), hepatitis virus, human papilloma virus and so others

The development of antiviral agents is not trivial as viral replication is intricately linked with the host cell that any antiviral drug that interferes even to a lesser extent with host cell factors may be toxic to the host depending on the duration and dosage used. Available antiviral agents mainly target stages in the viral life cycle. The target stages in the viral life cycle are; viral attachment to host cell, uncoating, synthesis of viral mRNA, translation of mRNA, replication of viral RNA and DNA, maturation of new viral proteins, budding, release of newly synthesized virus, and free virus in body fluids. Antiviral agents used to treat viral diseases are currently limited, and at least half of the available agents are for the treatment of human immunodeficiency virus (HIV) infections.

MATERIAL AND METHODS

BOTANICAL INFORMATION OF *Centellaasiatica*

SCIENTIFIC CLASSIFICATION

Name : Centellaasiatica
Kingdom : Plantae
Division : Magnoliophyta
Class : Magnoliopsida
Order : Apiales
Family : Apiaceae
Genus : Centella
Species : Spade leaf

VERNACULAR NAME

Tamil : Vallarai
English : Indian pennywort
Hindi : Brahmi
Malayalam : Kudavan
Telegu : Saraswatiaku

CHEMICAL CONSTITUENTS

Centellaasiatica are widely reported for their high contents of amino acids, triterpene saponin, vitamins, minerals, sesquiterpene, flavonoids and polysaccharides. The main compounds among amino acids (Aspartic acid, glutamic acid, leucine, valine, etc), Triterpene saponin (Asiaticoside, brahmoside), Vitamins (Ascorbic acid, Nicotinic acid), Sesquiterpene (Spathulenol, viridifloral) Flavonoids (Quercetin, Kaempferol).

HEALTH BENEFITS

It is widely used in Anti-cancer activity.
It increases Anti- oxidant enzyme activities (catalase, GST)
It inhibits xanthine oxidase enzyme activity.
It reduces lipid peroxidation.
It is also used in wound healing properties, gastroprotective, memory enhancing, anti- viral and immunomodulatory.
This herb is also used in various skin conditions such as leprosy, lupus, eczema, psoriasis.
This herb also used to treat Diarrhoea, fever, amenorrhea diseases.

MOLECULAR DOCKING

Docking is a method which predicts the preferred orientation of one molecule to a second when bound to each other to form a stable complete knowledge of the preferred orientation in turn may be used to predict the strength of association or burning affinity between two molecules. Molecular docking is one of the most frequently used methods in structure-based drug design, due to its ability to predict the binding-conformation of such ligands to the appropriate target binding site. Characterisation of the binding behavior plays an important role in

rational design of drugs as well as to elucidate fundamental biochemical processes.

Applications of Molecular Docking

Lead optimization

Molecular docking can predict an optimized orientation of ligand on its target. It can predict different binding modes of ligand in the groove of target molecule. This can be used to develop more potent, selective and efficient drug candidates.

Hit identifications

Docking in combination with scoring function can be used to evaluate large databases for finding out potent drug candidate in silico, which can target the molecule of interest.

Drug-DNA interaction

Molecular docking plays a prominent role in the initial prediction of drug's binding properties to nucleic acid. This information establishes the correlation between drug's molecular structure and its cytotoxicity.

Bioremediation

Protein ligand docking can also be used to predict pollutants that can be degraded by enzymes. In silico stratergies and model applied to develop and design the drugs. Different softwares play a major role in these studies.

Software Used

Chem sketch
Argus 4.0.1
Discovery studio
Auto dock tools

Downloading websites

Chemsketch:
https://www.acdlabs.com/resources/freeware/chemsketch/index.php
Download Argus lab using following website:
http://www.arguslab.com/arguslab.com/ArgusLab.html
Download auto dock vina using following website:
http://vina.scripps.edu/download.html

STRUCTURESOFANTIVIRAL AGENTS

The following structures are drawn by chemsketch.

PROTEIN SELECTED FOR DOCKING STUDIES

Anti-viral proteins
6LU7
3S3Z

PROTEIN INFORMATION

6LU7
DOI : 10.2210/pdb6LU7/pdb
Classification : VIRALPROTEIN
Organism(s) : Severe acute respiratory syndrome coronavirus 2
Expression System: Escherichia coli BL21 (DE3)
Mutation(s) : No
Deposited : 2020-01-26
Released : 2020-02-05
Deposition Author(s): Liu X, Zhang B, Jin Z, Yang H, Rao Z.

Experimental Data Snapshot

Method : X-RAYDIFFRACTION
Resolution : 2.16Å
R-Value Free : 0.235
R-Value Work : 0.202
R-Value Observed : 0.204

3S3Z
DOI : 10.2210/pdb3S3Z/pdb
Classification : ANTIVIRALPROTEIN
Organism(s) : Nostocellipsosporum
Expression System : Escherichia coli
Mutation(s) : No
Deposited : 2011-05-18
Released : 2011-08-03
Deposition Author(s) : Keeffe J R, Bjorkman P J, Mayo S L.

Experimental Data Snapshot

Method : X-RAYDIFFRACTION
Resolution : 1.75Å
R-Value Free : 0.212
R-Value work : 0.188
R-Value Observed : 0.190

DOCKING PROCEDURE

ARGUS LAB TUTORIAL

Downloading websites

Download argus lab using following website: http://www.arguslab.com/arguslab.com/ArgusLab.ht

ml
Then download protein using following website: https://www.rcsb.org/.

AUTODOCKVINA TUTORIAL

Softwares to be downloaded

Download autodock vina using following website: http://vina.scripps.edu/download.html
Download discovery studio visualizer: https://www.3dsbiovia.com/products/co.
Download protein using following website: https://www.rcsb.org/

Ligand preparation

Draw chemical structure using following software: Chemsketch: https://www.acdlabs.com/resources/freeware/chemsketch/index.php
If the compound was already exixsting then, download chemical structure from following website,
Drug bank: https://go.drugbank.com/
Pub chem: https://pubchem.ncbi.nlm.nih.gov/
To complete the above procedure create a new folder then place a protein and ligand and vina files in a folder.

Protein Preparation

Open discovery studio

File open protein(the protein structure displayed in screen)
To remove water click water delete
Click ligand define and binding site click from current selection binding sphere was generated (red ball was formed surrounded the ligand)
The cursor was placed in red ball double click the color was changed red to yellow and right click check the attribute to note it down X, Y, Z values.
To remove the ligand select ligand delete.
Go to chemistry hydrogens add polar.
This is a prepared protein save it pdb format.
First copy program file
Local diskc program files the scripps research institute.
Vinafile open copythe3files pastein working folder.
To check the working folder containing prepared protein and ligand and vina file.
One another file create yourself to open note pad in your desk to pand type following content,
Configuration file format:
Receptor = protein.pdbqt
Ligand = choloro.pdbqt
Out = corona.pdbqt
Center_x = -10.71183
Center_y = 12.411388
Center_z = 68.831286
Size_x = 20.0
Size_y = 20.0
Size_z = 20.0
Exhaustiveness = 8
Saveconf.txt format.

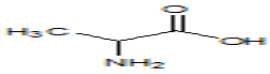
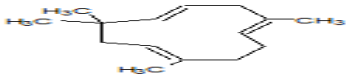
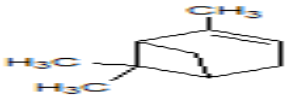
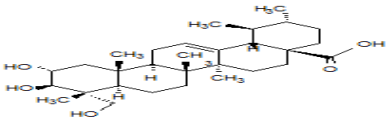
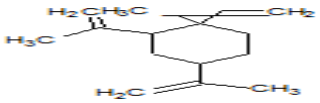
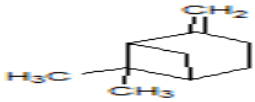
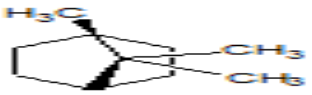
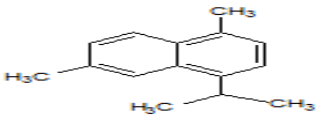
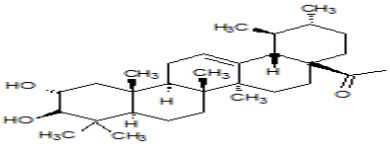
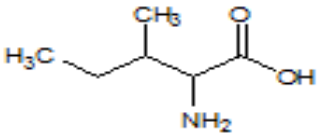
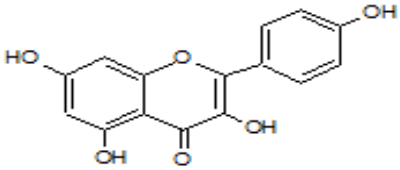
Then open autodock

File read molecule open prepared protein
The molecule viewed in the screen
Click grid macro molecule click choose select protein click select molecule (immediately warning was displayed non-bonded atoms click ok)
To save the protein in pdbqt format type protein.pdbqt.
Then prepare, Click ligand input open ligand (to appearing the summary of the ligand click ok)
Click ligand choose torsion tree done
Ligand output save as pdbqt file.
Then open command prompt.
Type the command.
Cd(space) paste the working folder pathway (click enter).
The path are changed type vina.exe(space)-help (click enter).
The help parameter are displayed, then type vina.exe(space)-config conf.txt(space)-log log.txt(enter)
The docking energy was displayed.
Then type, vina_split.exe(space)-Input out.pdbqt(click enter).
The splitting file create in the working folder.
Then the protein interaction are viewed in the discovery studio.
Open discovery studio copy paste the protein.pdbqt file and splitting file

RESULTS AND DISCUSSION

As the anti-viral agents are docked against anti-viral proteins, the docking scores were obtained. From the results we can concluded that best binding energy of the compound. However we can't say that only one drug out of these is the better one because the proteins are different and drugs are of natural origin. So the drugs possess different binding score with the different proteins.

Table No.1: Phyto constituents of *Centella asiatica*

S.No	-	-
1	**Alanine** 	**Alpha-humulene** 
2	**Alpha-pinene** 	**Ascorbic acid** 
3	**Asiatic acid** 	**Betaelemene** 
4	**Beta-pinene** 	**Camphane** 
5	**Candalane** 	**Corosolic acid** 
6	**Isoleucine** 	**Kaempferol** 

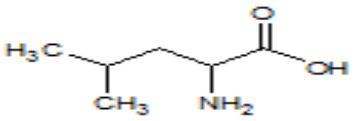
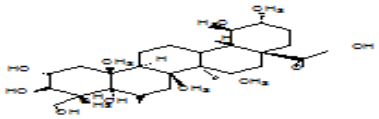
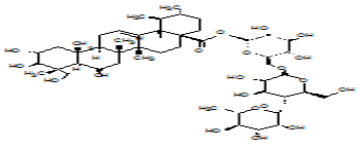
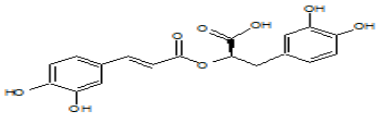
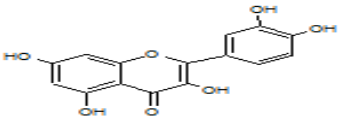
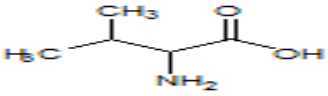
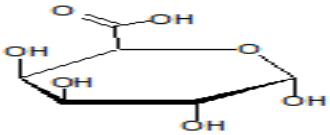
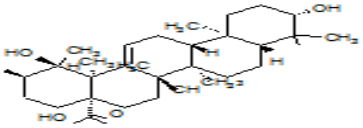
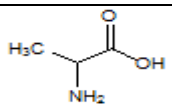
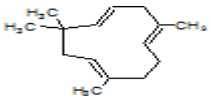
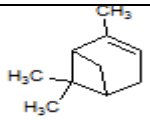
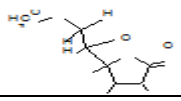
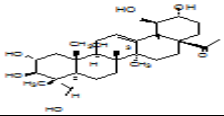
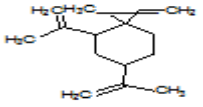
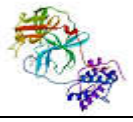
7	**Leucine** 	**Madecassic acid** 
8	**Madecassocide** 	**Rosamaricacid** 
9	**Quercetin** 	**Valine** 
10	**Pectin** 	**Pomolic acid** 

Table No.2: Binding energies of phytoconstituents of *Centella asiatica* with 6LU7

S.No	Protein name	Chemical name	Structure	Capture	Final energy
1	6lu7	Alanine			Arguslab: -7.3 Auto dock: -3.5
2	6lu7	Alpha-humulene			Arguslab: -10.8 Auto dock: -6.2
3	6lu7	Alphapinene			Arguslab: -8.5 Auto dock: -5.0
4	6lu7	Ascorbic acid			Argus lab: -5.1 Auto dock: -4.9
5	6lu7	Asiatic acid			Argus lab: -2.4 Auto dock: -7.0
6	6lu7	Betaelemene			Argus lab:-9.9 Auto dock:-5.0

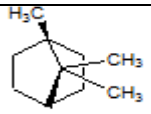
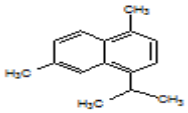
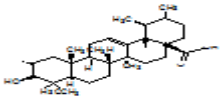
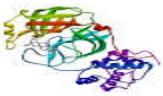
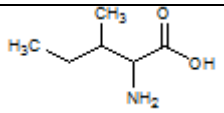
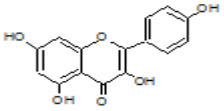
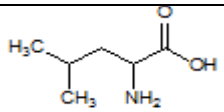
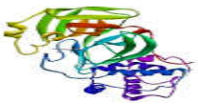
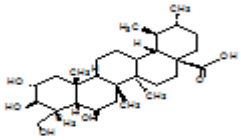
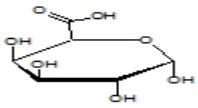
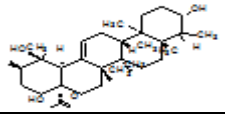
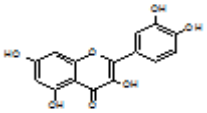
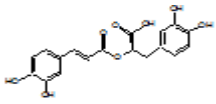
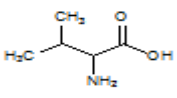
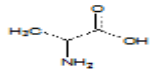
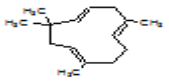
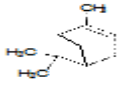
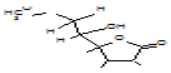
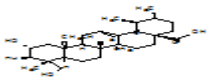
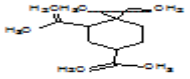
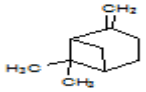
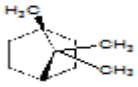
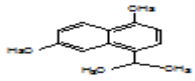
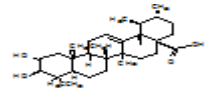
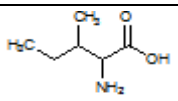
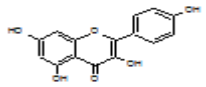
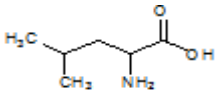
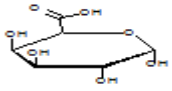
7	6lu7	Camphane			Argus lab:-8.7 Auto dock:-3.9
8	6lu7	Candalane			Argus lab:-9.8 Auto dock:-5.9
9	6lu7	Corosolic acid			Argus lab:-4.5 Auto dock:-7.6
10	6lu7	Isoleucine			Argus lab: -6.5 Auto dock: -4.1
11	6lu7	Kaempferol			Argus lab:-6.8 Auto dock:-7.4
12	6lu7	Leucine			Argus lab:-6.6 Auto dock:-4.3
13	6lu7	Madecassic acid			Argus lab:-8.9 Auto dock:-7.0
14	6lu7	Pectin			Argus lab: -5.0 Auto dock:-5.7
15	6lu7	Pomolic acid			Argus lab:-8.7 Auto dock:-7.9
16	6lu7	Quercetin			Argus lab: -6.4 Auto dock: -7.6
17	6lu7	Rosamarinic acid			Argus lab:-8.7 Auto dock:-7.1
18	6lu7	Valine			Argus lab:-5.9 Auto dock:-3.9

Table No.3: Binding energies of Phyto constituents of *Centella asiatica* with 3S3Z

S.No	Protein name	Chemical name	Structure		Final Energy
1	3S3Z	Alanine			Argus lab:-5.5 Auto dock:2.1
2	3S3Z	Alpha humulene			Argus lab:-11.0 Auto dock:-5.2
3	3S3Z	Alphapinene			Argus lab:-9.3 Auto dock:-4.4
4	3S3Z	Ascorbicacid			Argus lab: -5.2 Auto dock: -3.6
5	3S3Z	Asiaticacid			Argus lab:-7.2 Auto dock:-6.9
6	3S3Z	Betaelemene			Argus lab:-11.0 Auto dock:-4.5
7	3S3Z	Betapinene			Argus lab:-9.3 Auto dock:-3.7
8	3S3Z	Camphane			Argus lab:-9.1 Auto dock:-3.9
9	3S3Z	Candalane			Argus lab:-11.5 Auto dock:-5.7
10	3S3Z	Corosolic acid			Argus lab:-9.9 Auto dock:-6.3
11	3S3Z	Isoleucine			Argus lab:-6.8 Auto dock:-3.0
12	3S3Z	Kaempferol			Argus lab:-7.7 Auto dock:-5.5
13	3S3Z	Leucine			Argus lab:-6.9 Auto dock:-3.0
14	3S3Z	Pectin			Argus lab: -5.2 Auto dock: -3.5

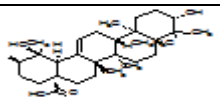
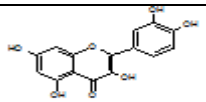
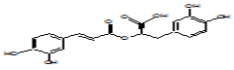
15	3S3Z	Pomolic acid			Argus lab:-13.6 Auto dock:-6.2
16	3S3Z	Quercetin			Argus lab:-7.4 Auto dock:-5.5
17	3S3Z	Rosamarinic acid			Argus lab: -8.8 Auto dock:-5.0

Table No.4: Aminoacids involved in binding between protein (6LU7) and phyto constituents present in *Centella asiatica*

S.No	Protein	Drugs	Hydrogen Bonds	Electrtostatic Bonds	Hydrophobi C Bonds
1	6LU7	Alanine	GLY143 SER 144 CYS 145 LEU141	-	ASN 142 SER 144 LEU141
2	6LU7	Alpha humulene	-	GLY143 ASN 53	CYS 145 GLY143 SER 144
3	6LU7	Alphapinene	-	-	HIS 163 CYS 145 GLN 189 LEU141
4	6LU7	Ascorbic acid	GLY143 CYS 145 SER 144 LEU141 HIS 163 GLU66	-	ASN 142 SER 144
5	6LU7	Asiatic acid	GLY143 GLN189 CYS 146 SER 144 HIS 163	LEU141	THR26 CYS 145
6	6LU7	Betaelemene	-	GLY143 SER 144 CYS 145	-
7	6LU7	Camphane	-	THR26 CYS 145	SER 144 GLY143 HIS 163
8	6LU7	Candalane	-	GLU166 THR190 SER 46	GLY143 LEU141
9	6LU7	Corosolic acid	ASN 142	ARG 188 CYS 145 CYS 145	ASN 142 LEU141

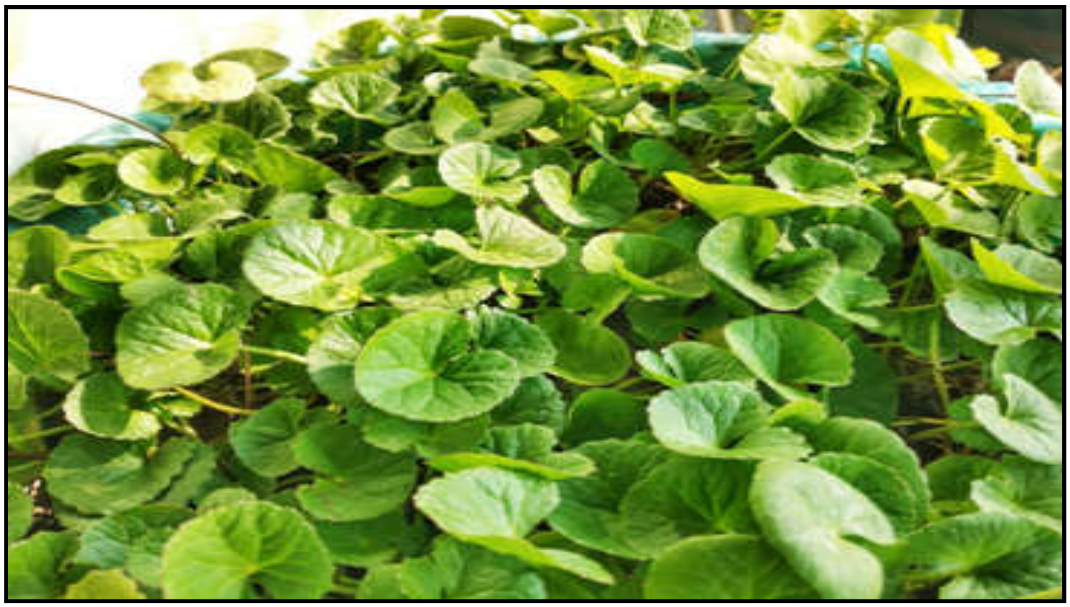
				HIS 163 SER 144	
10	6LU7	Isoleucine	LEU141 CYS 145 SER 144 GLY143	-	SER 144 HIS 163
11	6LU7	Kaempferol	SER 144 CYS 145 GLY143 THR26	-	-
12	6LU7	Leucine	LEU141 CYS 145 SER 144 GLY143	ASN 142 THR25 GLN189 MET 49	LEU141 CYS 145 SER 144
13	6LU7	Madecassic acid	LEU141 SER 144 GLY143 CYS 145	-	-
14	6LU7	Madecassoside	LEU141 HIS 163 SER 144 GLY143 CYS 145 ASN 142 THR25 GLN189 MET 49	LEU141 HIS 163 GLU166	-
15	6LU7	Valine	LEU141 CYS 145 SER 144 GLY143	LEU141 HIS 163 SER 144 GLY143 CYS 145	-
16	6LU7	Pectin	GLY143 SER 144 CYS 145 LEU141 HIS 163 GLU166	-	THR25 GLN189
17	6LU7	Pomolic acid	GLU166	ASN 142 THR25 GLN189	THR190 CYS 145
18	6LU7	Quercetin	THR190 ARG 188 GLU166 HIS163	-	SER 46 ASN 142

			CYS 145 LEU141 SER 144		
19	6LU7	Rosamarinic acid	SER46 GLY143 LEU141 CYS 145 SER 144	-	-
20	6LU7	Betapinene	-	GLU166 LEU141	GLY143 SER 144 THR190

Table No.5: Amino acids involved in binding between proteins (3S3Z) and phytoconstituents present in *Centella asiatica*

S.No	Protein	Drugs	Hydrogen Bonds	Electrostatic Bonds	Hydrophobic Bonds
1	3S3Z	Alanine	ILE55 PHE54	GLN50 ASN 42 SER 38	-
2	3S3Z	Alpha humulene	-	VAL39 GLN50 SER 38	-
3	3S3Z	Alphapinene	-	GLN50 ASN 53	TYR100 SER 38 ILE55
4	3S3Z	Ascorbic acid	GLN50 ASN 37 ASN 42	PRO 51 SER 38	VAL39 GLN50
5	3S3Z	Asiatic acid	ASN 37	ASN 37 ASN 53 SER 38 VAL39 GLN50	PHE54 PRO51
6	3S3Z	Betaelemene	-	ASN 37 GLN50 PHE54	-
7	3S3Z	Camphane	-	VAL39 PRO 51	ILE55 ASN 53 SER 52 GLN50
8	3S3Z	Candalane	-	GLU56	PRO 51 GLN50
9	3S3Z	Corosolic acid	SER 52 PHE54 TYR100	ASN 53	-
10	3S3Z	Isoleucine	ASN 53	ASN 42	GLN50

				THR100	SER 52
11	3S3Z	Kaempferol	GLN50 ASN 53	-	VAL39
12	3S3Z	Leucine	ASN 53	ASN 37	-
13	3S3Z	Madecassic acid	ASN 37	SER 38 PHE54 PRO 51	-
14	3S3Z	Madecassoside	PHE54 ASN 37 ASN 53 SER 38	-	
15	3S3Z	Valine	ASN 53	GLN50	GLU56 PHE54 ILE55
16	3S3Z	Pectin	ASN 53 GLU56 SER 52	ASN 42 ILE55	PHE54
17	3S3Z	Pomolic acid	GLN50 ASN 37	TYR100	ASN 53
18	3S3Z	Quercetin	PHE54 VAL39 GLN50 SER 38	-	SER 52 ASN 53
19	3S3Z	Rosamarinic acid	GLN50 SER 52 ASN 53 PRO 51	-	ILE55 PHE54
20	3S3Z	Betapinene	-	ASN 37	SER 52 GLN50 SER 38



Centellaasiatica

CONCLUSION

As the naturally screened derivatives were docked against the anti-viral proteins and the results were compared. This results shows that when the plant's constituents were used for anti-viral treatment which works better.

More than 70 compounds were docked with two major anti-viral protein (6LU7 and 3S3Z). Out of that, the compounds with least binding score was selected as the best anti-viral activity.

The constituents such as Pomolic acid [from *Centella asiatica*] were found best binding energy with the protein 6LU7 such as [-8.6, -6.4, -7.9, -9.8] respectively. Hence the further investigations on this particular constituents [viz., *in vitro* and *in vivo*] may give rise to better anti-viral agents among the synthetic drugs.

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CONFLICT OF INTEREST

We declare that we have no conflict of interest.

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