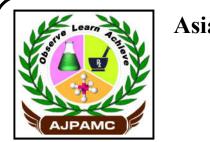
Nagavalli D. et al. /Asian Journal of Pharmaceutical Analysis and Medicinal Chemistry. 11(1), 2023, 15-28.

Research Article

CODEN: AJPAD7

ISSN: 2321 - 0923



Asian Journal of Pharmaceutical Analysis

and

Medicinal Chemistry Journal home page: www.ajpamc.com

https://doi.org/10.36673/AJPAMC.2023.v11.i01.A03



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

January – March

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 for the treatment agents are of human immunodeficiency virus (HIV) infections.

MATERIAL AND METHODS BOTANICAL **INFORMATION** OF *Centellaasiatica* SCIENTIFIC CLASSIFICATION : Centellaasiatica Name Kingdom : Plantae Division : Magnoliophyta : Magnoliopsida Class Order : Apiales : Apiaceae Family Genus : Centella

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Species

: Spade leaf

VERNACULAR NAME

Tamil: VallaraiEnglish: Indian pennywortHindi: BrahmiMalayalam: KudavanTelegu: 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 January – March 16 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/chems ketch/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.

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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 : Nostocellipsosporum Organism(s) 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 : Х-RAYDIFFRACTION · 1 75Å Resolution **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 January – March 17

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/chemsk etch/index.php

If the compound was already existing 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 \Box open \Box protein(the protein structure displayed in screen) \Box

To remove water click water delete

Click ligand \Box define and binding site \Box click from current selection \Box 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 \Box hydrogens \Box add polar.

This is a prepared protein save it pdb format. First copy program file

Local diskc \Box program files \Box the scripps research institute.

Vinafile open \Box copythe3 files \Box pastein working folder.

To check the working folder containing prepared protein and ligand and vina file.

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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 \Box input \Box open ligand (to appearing the summary of the ligand click ok) Click ligand \Box choose torsion tree \Box done

Ligand \Box output \Box 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.

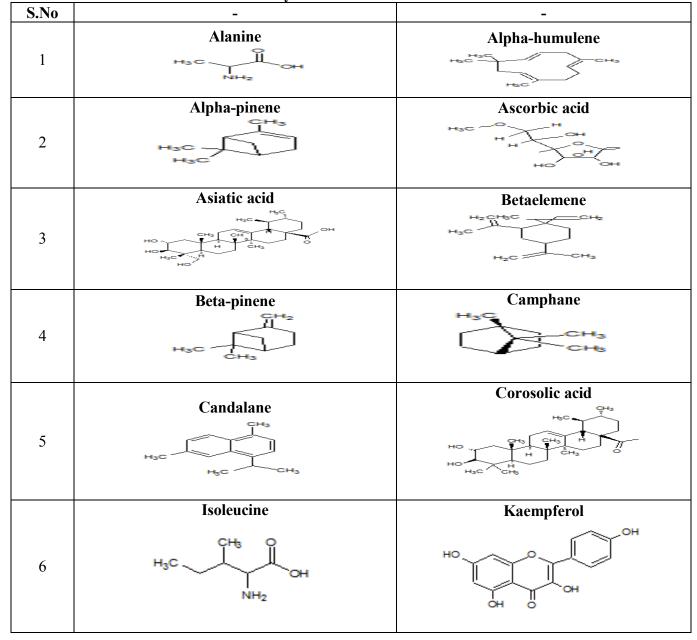


Table No.1: Phyto constituents of Centella asiatica

		Leucine		Madecass	sic acid	
7			ц он			
8		Madecassocide Rosamaricacid Image: State of the sta			ricacid	
9		Quercetin	рн	Valin ньс Ц NH	Он	
10		Pectin OH OH OH	Эн	Pomolic acid		
	Table No.2 Protein		of phytoconstituents of			
S.No		: Binding energies Chemical name	of phytoconstituents of Structure	of <i>Centella asiatica</i> Capture	Final energy	
S.No	Protein					
	Protein name	Chemical name Alanine	Structure $H_3C \xrightarrow[NH_2]{} OH$		Final energy Arguslab: -7.3 Auto dock: -3.5	
	Protein name	Chemical name	Structure $\begin{array}{c} \downarrow \\ \downarrow $		Final energy Arguslab: -7.3	
1	Protein name 6lu7 6lu7	Chemical name Alanine Alpha- humulene	Structure $H_3C \xrightarrow{O}_{H_3C} OH$ $H_3C \xrightarrow{O}_{H_3C} OH$		Final energy Arguslab: -7.3 Auto dock: -3.5 Arguslab: -10.8	
1	Protein name 6lu7	Chemical name Alanine Alpha-	Structure $\begin{array}{c} \downarrow \\ \downarrow $		Final energyArguslab: -7.3Auto dock: -3.5Arguslab: -10.8Auto dock: -6.2Arguslab: -8.5Auto dock: -5.0	
1	Protein name 6lu7 6lu7	Chemical name Alanine Alpha- humulene	Structure $H_{S}C \xrightarrow{O} H_{S}$ $H_{S}C \xrightarrow{O} H_{S}$ $H_{S}C \xrightarrow{H_{S}C} H_{S}$ $H_{S}C \xrightarrow{CH_{S}}$		Final energyArguslab: -7.3Auto dock: -3.5Arguslab: -10.8Auto dock: -6.2Arguslab: -8.5Auto dock: -5.0Argus lab: -5.1	
1 2 3	Protein name 6lu7 6lu7 6lu7	Chemical name Alanine Alpha- humulene Alphapinene	Structure $H_{S}C \xrightarrow{O} H_{S}$ $H_{S}C \xrightarrow{O} H_{S}$ $H_{S}C \xrightarrow{H_{S}C} H_{S}$ $H_{S}C \xrightarrow{CH_{S}}$		Final energyArguslab: -7.3Auto dock: -3.5Arguslab: -10.8Auto dock: -6.2Arguslab: -8.5Auto dock: -5.0Argus lab: -5.1Auto dock: -4.9	
1 2 3	Protein name 6lu7 6lu7 6lu7	Chemical name Alanine Alpha- humulene Alphapinene	Structure $H_{S}C \xrightarrow{O} H_{S}$ $H_{S}C \xrightarrow{O} H_{S}$ $H_{S}C \xrightarrow{H_{S}C} H_{S}$ $H_{S}C \xrightarrow{CH_{S}}$		Final energyArguslab: -7.3Auto dock: -3.5Arguslab: -10.8Auto dock: -6.2Arguslab: -8.5Auto dock: -5.0Argus lab: -5.1	
1 2 3 4	Protein name 6lu7 6lu7 6lu7 6lu7	Chemical name Alanine Alpha- humulene Alphapinene Ascorbic acid	Structure $H_{S}C \xrightarrow{O} H_{S}$ $H_{S}C \xrightarrow{O} H_{S}$ $H_{S}C \xrightarrow{H_{S}C} H_{S}$ $H_{S}C \xrightarrow{CH_{S}}$		Final energyArguslab: -7.3Auto dock: -3.5Arguslab: -10.8Auto dock: -6.2Arguslab: -8.5Auto dock: -5.0Argus lab: -5.1Auto dock: -4.9Argus lab: -2.4	

_			H ₃ C		Argus lab:-8.7
7	6lu7	Camphane	СНа		Auto dock:-3.9
8	6lu7	Candalane	i de la companya de l		Argus lab:-9.8
8	0107	Candalane		and the second s	Auto dock:-5.9
9	6lu7	Corosolic acid			Argus lab:-4.5
,	0107				Auto dock:-7.6
10	6lu7	Isoleucine			Argus lab: -6.5
10	0107	Isoleucille	NH ₂		Auto dock: -4.1
11			P P	A CONTRACTOR	Argus lab:-6.8
11	6lu7	Kaempferol		A A A A A A A A A A A A A A A A A A A	Auto dock:-7.4
10	(1.7	т.:	H ₃ C ₂	-	Argus lab:-6.6
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15	6lu7	Pomolic acid			Argus lab:-8.7
15	0107	Pomone acid			Auto dock:-7.9
16	(1.7			-	Argus lab: -6.4
16	6lu7	Quercetin			Auto dock: -7.6
17	6lu7	Rosamarinic	~uró	-0000	Argus lab:-8.7
1/	0107	acid	~~	Ser Ser	Auto dock:-7.1
18	6lu7	Valine	c∺, o ↓ ↓		Argus lab:-5.9
10	0107	v anne	H ₂ C VH		Auto dock:-3.9

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5383ZAsiaticacidAsiaticacidAuto dock:-6.96383ZBetaelemeneArgus lab:-11.0Auto dock:-4.57383ZBetapineneArgus lab:-9.3Auto dock:-4.57383ZCamphaneArgus lab:-9.1Auto dock:-3.78383ZCamphaneArgus lab:-9.1Auto dock:-3.99383ZCandalaneArgus lab:-9.1Auto dock:-3.99383ZCorosolic acidArgus lab:-9.1Auto dock:-3.910383ZCorosolic acidArgus lab:-9.9Auto dock:-6.311383ZIsoleucineArgus lab:-9.9Auto dock:-6.312383ZKaempferolIf a constraintArgus lab:-7.713383ZLeucineIf a constraintArgus lab:-7.714383ZPectinIf a constraintArgus lab:-5.214383ZPectinIf a constraintArgus lab:-5.2	-				K	Auto dock: -3.6	
63S3ZBetaelemeneArgus lab:-11.073S3ZBetapinene 4 regus lab:-9.373S3ZCamphane 4 regus lab:-9.383S3ZCamphane 4 regus lab:-9.193S3ZCandalane 4 regus lab:-9.193S3ZCandalane 4 regus lab:-9.1103S3ZCorosolic acid 4 regus lab:-9.9113S3ZCorosolic acid 4 regus lab:-9.9113S3ZIsoleucine 4 regus lab:-6.8123S3ZKaempferol 4 regus lab:-7.7133S3ZLeucine 4 regus lab:-6.9143S3ZPectin 4 regus lab:-6.9143S3ZPectin 4 regus lab:-5.2	5	3S3Z	Asiaticacid		A A A	Argus lab:-7.2	
63532Betalelentene $4uto dock:-4.5$ 7383ZBetapinene $4uto dock:-4.5$ 8383ZCamphane $4uto dock:-3.7$ 9383ZCandalane $4uto dock:-3.9$ 9383ZCandalane $4uto dock:-5.7$ 10383ZCorosolic acid $4uto dock:-6.3$ 11383ZIsoleucine $4uto dock:-6.3$ 12383ZKaempferol $4uto dock:-5.5$ 13383ZLeucine $4uto dock:-5.7$ 14383ZPectin $4uto dock:-6.3$ 14383ZPectin $4uto dock:-3.0$ 14383ZPectin $4uto dock:-5.2$				~~~~~	20	Auto dock:-6.9	
7383ZBetapinene $\mathbf{Argus lab:-9.3}$ Auto dock:-3.78383ZCamphane $\mathbf{Argus lab:-9.1}$ Auto dock:-3.99383ZCandalane $\mathbf{Argus lab:-9.1}$ Auto dock:-3.99383ZCandalane $\mathbf{Argus lab:-11.5}$ Auto dock:-5.710383ZCorosolic acid $\mathbf{Argus lab:-9.9}$ Auto dock:-6.311383ZIsoleucine $\mathbf{argus lab:-9.9}$ Auto dock:-6.312383ZKaempferol $\mathbf{argus lab:-6.8}$ Auto dock:-5.513383ZLeucine $\mathbf{argus lab:-6.9}$ Auto dock:-5.514383ZPectin $\mathbf{argus lab:-6.9}$ Argus lab:-6.9	6	3S3Z	Betaelemene	He Contraction	A.	Argus lab:-11.0	
7 $3S3Z$ Betapinene $4uo$ Auto dock:-3.78 $3S3Z$ Camphane $4io$ $4rgus lab:-9.1$ 9 $3S3Z$ Candalane $4rgus lab:-11.5$ Auto dock:-3.99 $3S3Z$ Candalane $4rgus lab:-11.5$ Auto dock:-5.710 $3S3Z$ Corosolic acid $4rgus lab:-9.9$ Auto dock:-6.311 $3S3Z$ Isoleucine $4eo ff f f f f f f f f f f f f f f f f f $				H20 55 0 H2	~	Auto dock:-4.5	
83S3ZCamphane $Hach CarrentCarrentArgus lab:-9.1Auto dock:-3.793S3ZCandalaneMait odock:-3.993S3ZCandalaneMait odock:-5.7103S3ZCorosolic acidMait odock:-6.3113S3ZIsoleucineHach CarrentMait odock:-6.3Argus lab:-9.9123S3ZKaempferolMait odock:-5.5133S3ZLeucineHach CarrentMait odock:-3.0Argus lab:-6.9143S3ZPectinMait odock:-5.2$	7	3S3Z	Betapinene		St	Argus lab:-9.3	
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93S3ZCandalane \checkmark Auto dock:-3.993S3ZCandalane \checkmark \checkmark Argus lab:-11.5103S3ZCorosolic acid \checkmark \checkmark Argus lab:-9.9103S3ZCorosolic acid \checkmark \checkmark Argus lab:-9.9113S3ZIsoleucine \checkmark \checkmark \land 123S3ZKaempferol \checkmark \checkmark \land 133S3ZLeucine \checkmark \checkmark \checkmark 143S3ZPectin \checkmark \checkmark \checkmark 143S3ZPectin \checkmark \checkmark \checkmark	o	2527	Comphana	H ₃ C	14	Argus lab:-9.1	
9 $3S3Z$ Candalane $4uto dock:-5.7$ 10 $3S3Z$ Corosolic acid $4rgus lab:-9.9$ 11 $3S3Z$ Isoleucine $4rgus lab:-6.8$ 11 $3S3Z$ Isoleucine $4rgus lab:-6.8$ 12 $3S3Z$ Kaempferol $4rgus lab:-7.7$ 13 $3S3Z$ Leucine $4rgus lab:-6.9$ 14 $3S3Z$ Pectin $4rgus lab:-6.9$	0	383L	Camphane	С	the state of the s	Auto dock:-3.9	
103S3ZCorosolic acid $\mathbf{Auto dock:-5.7}$ 103S3ZCorosolic acid $\mathbf{Argus lab:-9.9}$ 113S3ZIsoleucine $\mathbf{Argus lab:-6.8}$ 113S3ZIsoleucine $\mathbf{Argus lab:-6.8}$ 123S3ZKaempferol $\mathbf{argus lab:-7.7}$ 133S3ZLeucine $\mathbf{argus lab:-6.9}$ 143S3ZPectin $\mathbf{argus lab:-6.9}$ 143S3ZPectin $\mathbf{argus lab:-6.9}$	0	2827	Candalana	<u> </u>		Argus lab:-11.5	
103S3ZCorosolic acidAuto dock:-6.3113S3ZIsoleucine $H = \int_{H_2} \int_{H_2$	9	383Z	Candalane	HO YOH	ý	Auto dock:-5.7	
113S3ZIsoleucine $HachingAuto dock:-6.3113S3ZIsoleucineHachingHachingArgus lab:-6.8123S3ZKaempferolHachingHachingArgus lab:-7.7133S3ZLeucineHachingHachingArgus lab:-6.9143S3ZPectinHachingHachingArgus lab:-5.2$	10	2527	Concellinguid	, A	C.	Argus lab:-9.9	
113S3ZIsoleucine $HechinghordArgus lab:-6.8123S3ZKaempferolHechinghordArgus lab:-7.7123S3ZKaempferolHechinghordArgus lab:-7.7133S3ZLeucineHechinghordArgus lab:-6.9143S3ZPectinHechinghordArgus lab:-5.2$	10	222 222	Corosonic acid	The	2 Contraction	Auto dock:-6.3	
InterpretInterpretInterpretAuto dock:-3.0123S3ZKaempferolInterpretInterpretInterpret133S3ZLeucineInterpretInterpretInterpret143S3ZPectinInterpretInterpretInterpret143S3ZPectinInterpretInterpretInterpret	11	2827	Icoloucino	1 1	A.	Argus lab:-6.8	
123S3ZKaempierol $1 \leq r \leq r$ Auto dock:-5.5133S3ZLeucine $H_2 \subset \downarrow \downarrow \downarrow \cup H$ $3 \leq r \leq r$ Argus lab:-6.9143S3ZPectin $3 \leq r \leq r$ $3 \leq r \leq r$ Argus lab: -5.2	11	383Z	Isoleucine	NH ₂	and a start	Auto dock:-3.0	
13383ZLeucine $H_2 C \rightarrow C H_2$ Auto dock:-5.514383ZPectin $H_2 C \rightarrow C H_2$ Auto dock:-3.0	12	3S3Z	Kaempferol	*****	No. 1	-	
133S3ZLeucine H_2 H_2 $Auto dock:-3.0$ 143S3ZPectin H_2 $Argus lab: -5.2$			•	J. J. CH	and the second s	Auto dock:-5.5	
Image: Letting of the section of t	13	3837	Leucine	н₂сон	5.1	Argus lab:-6.9	
14 3S3Z Pectin	1.5	5552		CH3 NH2	J.	Auto dock:-3.0	
Auto dock: -3.5	14	3837	Pectin		5 2 1	Argus lab: -5.2	
	17	JUJL	reetin	J. J.	Y	Auto dock: -3.5	

Table No.3: Binding ene	rgies of Phyto constituent	ts of <i>Centella asiatica</i> with 3S3Z

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15	3S3Z	Pomolic acid	THE PARTY OF	2 St	Argus lab:-13.6
			د بلغی م		Auto dock:-6.2
16	3S3Z	Quaraatin	*	A	Argus lab:-7.4
10	202Z	Quercetin	ŢŢ.	and and a second	Auto dock:-5.5
17	3S3Z	Rosamarinic acid	an YÖ	A	Argus lab: -8.8
1/	363Z		4	and and a second	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	<u>Hydrogen</u> 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	
			LEU141		
10		т 1 .	CYS 145		CED 144
10	6LU7	Isoleucine	SER 144	-	SER 144
			GLY143		HIS 163
			SER 144		
11			CYS 145		
11	6LU7	Kaempferol	GLY143	-	-
			THR26		
			LEU141	ASN 142	
10		т ·	CYS 145	THR25	LEU141
12	6LU7	Leucine	SER 144	GLN189	CYS 145
			GLY143	MET 49	SER 144
			LEU141		
10			SER 144		
13	6LU7	Madecassic acid	GLY143	-	-
			CYS 145		
			LEU141		
			HIS 163		
			SER 144		
			GLY143		
14	6LU7	Madecassoside	CYS 145	LEU141	
			ASN 142	HIS 163	
			THR25	GLU166	-
			GLN189		
			MET 49		
				LEU141	
			LEU141 CYS 145	HIS 163	
15	6LU7	Valine	SER 144	SER 144	
			GLY143	GLY143	-
			UL1143	CYS 145	
			GLY143		
			SER 144		
16	6LU7	Pectin	CYS 145		THR25
10	ULU/	i octili	LEU141		GLN189
			HIS 163	-	
			GLU166		
				ASN 142	THR190
17	6LU7	Pomolic acid	GLU166	THR25	CYS 145
				GLN189	010145
			THR190		
18	6LU7	Quercetin	ARG 188		SER 46
10	ULU/	Quereetiii	GLU166	_	ASN 142
			HIS163	-	

19	6LU7	Rosamarinic acid	GLY143 LEU141 CYS 145 SER 144	-	- GL V143
20	6LU7	Betapinene	CYS 145	- GLU166	- GLY143 SER 144

 Table No.5: Amino acids involved in binding between proteins (383Z) and phytoconstituents present in

 Centella asiatica

Centella asiatica						
S.No	Protein	Drugs	Hydrogen Bonds	Electrostatic Bonds	Hydrophobic Bonds	
1	383Z	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	383Z	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	383Z	Kaempferol	GLN50 ASN 53	-	VAL39
12	3S3Z	Leucine	ASN 53	ASN 37	-
13	383Z	Madecassic acid	ASN 37	SER 38 PHE54 PRO 51	-
14	383Z	Madecassoside	PHE54 ASN 37 ASN 53 SER 38	-	
15	383Z	Valine	ASN 53	GLN50	GLU56 PHE54 ILE55
16	383Z	Pectin	ASN 53 GLU56 SER 52	ASN 42 ILE55	PHE54
17	383Z	Pomolic acid	GLN50 ASN 37	TYR100	ASN 53
18	383Z	Quercetin	PHE54 VAL39 GLN50 SER 38	-	SER 52 ASN 53
19	3S3Z	Rosamarinic acid	GLN50 SER 52 ASN 53 PRO 51	-	ILE55 PHE54
20	383Z	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.

ACKNOWLEDGEMENT

I'm very thankful to Department of pharmaceutical chemistry, Adhiparsakthi College of Pharmacy, Melmaruvathur. I would also like to thank the Management, for providing the necessary facilities to carry out this work.

CONFLICT OF INTEREST

We declare that we have no conflict of interest.

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Please cite this article in press as: Nagavalli D *et al.* Insilico studies of *centella asiatica* phytoconstituents on antiviral activity, *Asian Journal of Pharmaceutical Analysis and Medicinal Chemistry*, 11(1), 2023, 15-28.