IN SILICO APPROACH, TO STUDY THE PHYTOCHEMICALS PRESENT IN CAMELLIA SINENSIS AND WITHANIA SOMNIFERA TO TARGET MPXV VIRUS A42R FOR THE TREATMENT OF MONKEYPOX DISEASE

A Thesis Submitted

In Partial Fulfilment of the Requirements for the

Degree of

Master of Science in Biotechnology by

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2K23/MSCBIO/27

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CANDIDATE DECLARATION

I KHUSHI, Roll Number: 2K23/MSCBIO/27 hereby certify that the work which is being presented the thesis entitled- "in silico approach, to study the phytochemicals present in *caemllia sinensis* and *withania somnifera* to target MPXV A42R for the treatment of monkey pox disease" in partial fulfilment of the requirements for the award of Master of Science, submitted in the Department of Biotechnology, Delhi Technological University is an authentic record of my own work carried out during the period from january 2023 to May 2025 under the supervision of Dr. Navneeta Bharadvaja. The matter presented in the thesis has not been submitted by me for the award of any other degree of this or any other Institute.

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CERTIFICATE

Certified that KHUSHI (2K23/MSCBIO/27) has carried out their research work presented in this thesis entitled "in silico approach, to study the phytochemicals present in *camellia sinensis* and *withania somnifera* to target MPXV A42R for the treatment of monkey pox disease" for the award of Master of Science from Department of Biotechnology, Delhi Technological University, Delhi, under my supervision. The thesis embodies results of original work, and studies are carried out by the student herself, and the contents of the thesis do not form the basis for the award of any other degree to the candidate or to anybody else from this or any other University/Institution.

Place: Delhi
Date:

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ABSTRACT

The Human Monkeypox virus (hMPXV) causes a zoonotic disease and belongs to the Orthopoxvirus genus. In 2022, the largest outbreak of this disease led to an epidemic in various countries. As stated by the World Health Organisation (WHO), physical contact with affected animals, persons, or contaminated surfaces may serve as possible transmission routes for the virus infection. Symptoms may appear after about 7-14 days of infection, including myalgia, fever, fatigue, body aches, headaches, skin lesions, and lymphadenopathy.

JYNNEOS and ACAM2000 are both FDA-approved vaccines used to prevent Monkeypox disease however, the latter vaccine can cause severe conditions like pericarditis and myocarditis in immunocompromised vaccinated individuals. Thus, drugs that can target the virus are in high demand, according to current circumstances. Therefore, *Camellia sinensis,* a medical plant with active phytochemical compounds and *withania somnifera* is an herb traditionally have great use in ayurveda can serve as a potential source for synthesizing herbal drugs. In this research, using molecular docking, the leading active compounds observed in the plant showed remarkable interactions with suitable binding affinities. Barassinolide and teasterone from *camellia sinensis* have same binding energy whereas 27-Deoxy 14-hydroxywithaferin A from *withania somnifera* surpasses other phytochemicals regarding binding energy, i.e., -8.7 kcal/mol and –10 Kcal/mol making it the most promising phytochemical that can be used as a therapeutic target.

Keywords—*Camellia sinensis, withania somnifera,* Human Monkeypox virus, active phytochemical compounds, docking, in silico. ADMET analysis, therapeutic properties.

Acknowledgment

I would humbly convey my sincere thanks to the respected people who played an important part in making this thesis possible an immense support and guidance have been given throughout the year. I will humbly extend my gratitude towards my supervisor DR.**Navneeta Bharadvaja**, for regular guidance and support, her constant guidance and motivation were crucial throughout my journey. I am equally grateful to work under the guidance of my seniors in lab, Mr. Sidharth Sharma for his support. Finally, I would like to express my heartwarming thanks to my family and friend Eshita.

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CONTENT

Chapter 1

1 INTRODUCTION

1.1 Background

Mokey pox is a infectious disease spread from animals to humans (zoonotic). the virus of monkeypox is orthopoxvirus belongs to the poxoviradaceae family. the very first case of monkeypox has reported in the Democratic republic of Congo in 1970 in a small kid who was not vaccinated [1].there are 2 phases of this disease namely prodromal phase and the rash phase, the prodromal phase of around 7-21 days approximately includes fever, severe headache, muscle ache, fatigue, myalgia, malaise, and lymphadenopathy; subsequently, the rash phase appears, lasting about 7 to 21 days. Rash phase started within 1-5 days after patient got fever; during this phase there is high chances of transmission of virus. The rash appears mainly 95% on face, 75% on limbs, 30% on reproductive organs eyes and oral muscle are also affected. Due to rash plaque is formed further followed by formation of Paules, blisters, pustules, scab and eventually shedding. If there is a severe case, lesions are formed, and a large skin patch may fall off. The severity of MPX depends on the intensity of exposure to the virus and the health condition of the host, with a 1- 10% fatality rate [2]. The structure of virus has linear double stranded DNA with a length of about 197kb and enveloped in lipoprotein coat [3][4].hMPXV enters the host's cell by binding to glycosaminoglycans present on the human cell membrane [1]. The hMPXV can be classified mainly into 2 distinct genetic groups, such as the West African group (with a death rate of 0.1%) whereas Central African group (with a death rate of 1-12%), also known as the Congo Basin. The latter shows higher virulence activity compared to the former. Research showed that the Central African strain of monkeypox modulates T cell activation negatively and also prevents the release of cytokines, which are associated with inflammation in affected human cells and weaken the host's immunity by decreasing the apoptosis and preventing of transcription of genes related to the host's immunity [5].There are two transmission routes of this disease,1* transmission(interhuman)and 2*transmission route (zoonotic transmission).This involves injuries from infected animals, eating poorly cooked infected meat, exposure to infected blood or bodily fluids, and direct contact with

cutaneous/ mucosal lesions, sexual contact with infected humans, respiratory droplets, and contact with contaminated surfaces/objects. A few studies show that pregnancy during the infection can. In 2022, a surge in MPX infection cases affected nearly 88 nations, with continuously rising cases of infection via interhuman transmission. It was suspected that the men involved sexually with other infected men were the cause of the outbreak. In a recent scenario, there are three vaccines for Orthopoxvirus, for the treatment of the smallpox and monkeypox infection these drugs are FDA approved. However, there are no antiviral medications specifically for the monkeypox infection. However, a few medications used for smallpox, like tecovirimat, cidofovir, and immunoglobulin vaccinia, could be used to treat the infection [5]. Hence, there is an immediate need to investigate potential drug targets. In ancient times, herbal medicines were used to cure infections and diseases as they contained therapeutic bioactive substances that provided a framework for the development of herbal drug synthesis. *Camellia sinensis* is a therapeutic plant that belongs to Theaceae family. Studies show that the presence of the bioactive compounds in *Camellia sinensis* reduces cardiovascular diseases and cancer to some extent; it also improves oral health, exhibits neuroprotective power, antihypertension effect, anti-bacterial, aids body weight control, anti-viremic activity, increases bone mineral density, and antifibrotic properties [6-8]. Further analysis of the key phytochemicals of *Camellia sinensis* and *withania somnifera* on the Human Monkeypox Virus by molecular docking will enhance our knowledge about the basics of biochemical processes and the interaction of protein target (binding sites) with phytochemicals. By this approach, the most favorable binding of the receptor–ligand interaction will be determined. II.

1.2-PHYTOCHEMICALS AS THERAPEUTIC APPROACH TO TREAT MPOX

There are few convential drugs the treatment of monkeypox like tecovirimat work by inhibiting p37 viral protein and decrease the spread of virus particles. Brincidofovir and cidofovir drugs are also used, these drugs work by inhibiting viral replication. but all these conventional drugs have issues related to side effects on body.[7] thus, natural bioactive compounds have potential to treat viral and bacterial disease with less toxicity and side effects. Phytocompounds found in root, leaves, stem of plants have potential to treat various disease and shows potential to use as herbal drug.

There are number of different bioactive compounds like flavonoid, alkoids, steroids and polyphenols show antiviral properties against orthopoxvirus genus. Phytochemical can interfere with phases of life cycle of virus like entry into host cell, replication and maturation ad disrupting protein-protein connection require for viral assembly. Phytochemicals can also alter the host immune response so that body will eradicate infectious particles easily along with lowering oxidative stress and lowering inflammation by blocking inflammatory pathway NF-kB or cytokine production. Several bioactive compounds derive from plants has shown potential to eradicate certain viruses like variola and vaccinia from orthopoxvirus genus. Studies has shown curcumin a bioactive compound have good binding affinity of –37.43 kcal/mol for viral protein of monkeypox. Some other phytocompound are also tested for the same as gendunin, piperine and coumadin have binding affinity lower than curcumin.[8] phytochemical downregulate inflammatory pathway related to poxvirus infection. Another bioactive compound epigallocatechin gallate (EGCG) from *camellia sinensis* has shown virucidal properties by blocking DNA polymerase and protease activity and by destructing viral envelope.[9]. Few researchers have also worked to increase adsorption and targeted distribution of bioactive compound by linking phytochemicals with nanocarriers.

1.3OBJECTIVES

→ To identify potential phytochemicals, present in the *Camellia sinensis* and *withania somnifera* as potential herbal drugs against monkeypox.

→ To perform molecular docking by using auto dock tools to predict the interaction and binding affinity of phytocompounds against monkeypox viral protein A42R (MPXV).

→ To draw 2-D structure by using visualizing tool (BIOVIA DISCOVERY) to show interaction between A42R viral protein of monkey pox and potential phytochemicals of Camellia sinensis.

→ ADME analysis is done to check the Absorption, Distribution, Metabolism, and Excretion processes (abbreviated as ADME) of phytochemicals present in *Camellia sinensis* to evaluate their pharmacokinetic features for potential drug candidate.

Chapter 2

2 LITERATURE REVIEW

2.1 Overview of monkeypox

Monkeypox is an viral infectious disease spread from animals to humans. Monkeypox virus was first suspected in a unvaccinated kid in 1970 in the democratic Republic of congo. The lack of vaccination and in the attempt of eradication of smallpox monkeypox gets the clinical importance.[12] classification of monkeypox is as follow poxviridae is family, subfamily-chordopoxvirinae, genus-orthopoxvirus, species-mpox virus. Different cases has reported all over the world, In 2003 mpox spread in prairie dogs which were sold as pets in US due to these 53 human cases was repoted at that time[13] Another case of mpox was reported in 2018,2019 due to the infected man traveled from Nigeria to Singapore hence reveals humans to humans' transmission. In May 2022 there is an outbreak of this disease in multiple countries main cause for the spread was men sex with same gender resulted in genital lesions.[14], all these cases tells about transmission mode of disease which include transmission from infected animals through body fluids, skin lesion through breathing of infected droplet of infected animals also human to human transmission.

2.1.1-PATHPHYSIOLOGY- the virus may entre in body through the nasopharyngeal or through Guedel airway. Then it spread to nearby lymph nodes, the growth and spread of virus to other organ is initiated by formation of viremia. This is also called an incubation period which last for 21 days maximum. Symptoms like fever and lymphadenopathy is linked to the formation of secondary viremia, symptoms last for 1-2 days. Patients who have been infected maybe contagious by now. from the entry through oropharynx, lesions eventually spread all over skin and after lesions are formed antibodies may be detected in serum.[15].

2.1.2-LIFE CYCLE-there are 3 stages of virus infection and replication of monkeypox virus. First stage-virus invasion, second stage-virus synthesis and replication, third stage-assembly of virus and maturation.[16] For the invasion there are two infectious particles extracellular virions (EEV) and intracellular mature virions (IMV). The mode of entry of both infectious particles differs, EEV enter via membrane fusion, virus interact with GAGs and enter cell whereas IMV may enter through direct fusion or endocytosis. A29 viral protein helps in cellular entry process of IMV. A29 has similar heparin binding affinity like vaccinia virus. lipid rafts present in plasma membrane of host cell is utilized by pox virus to make entry into cell. there are several surface membrane proteins are present to facilitate entry like 15L, E8L and A43R. [17] After the entry of infectious particle into host cell second stage of virus life cycle begins, virus enter its core into the cytoplasm, here viral core has its genome and neucleocapsid envelope. The nucleocapsid uncoated itself by ubiquitination and degradation by protease of capsid proteins. Now after this virus begins to replicate its genome. Viral protein involve in replication are E9L, A20R, d5r this unwinds DNA, B1R and 13L. These all protein has different function to performed during replication.[18]. Immature virion particle of crescent shape is converted to mature virus particles after the condensation and proteolytic cleavage of core protein marking the beginning of stage three viral assembly and maturation.[19][20]. Host cell having these immature virions are released by lysis. These IMV escape the factory of through microtubule organizing center and enveloped into nuclear membrane. this will lead to the formation of intercellular enveloped virion. IEV will touch the periphery of host cell it will fuse to the membrane and by the process of exocytosis cell associated enveloped viruses will form.

For the assembly of virus particle on cellular plasma membrane two processes are their actin polymerization and microtubule transport. IEV employed microtubule transport system to reach the cell surface. A36R protein play vital role in viral particle transmission and the release of extracellular enveloped virions for infection in surrounding environment [21].

2.2 CAMELLIA SINENSIS

Camellia sinensis is a shrub or small tree native to Asia but it is now produced on large scale across the world. This species has two varieties one from China *(Camellia sinensis sinensis)* and other from assam *(Camellia sinensis assamica). camellia sinensis* belongs to theaceae family. The flowers of plant *Camellia sinensis)* are yellow- white in color diameter

ranging from 0.98-1.57 inches(4cm), it has tap roots with 7-8 petals, size of leaves are alternate, exstipulate lanceolate to obovate with around 4-15 cm long and 2-5 cm broad. [22]. From China green tea has gained huge popularity as one of the mostly consumed non-alcoholic beverages. It is reported that green tea has more than 500 chemical components including 400 organic compound and 40 inorganics compounds. Bioactive compounds of green tea include polyphenols, alkaloids, amino acids, vitamins and polysaccharides, several research shows their positive health benefits as anticancer, antidiabetic, anticataract, Anti Alzheimer and antioxidant [23].

2.2.1 PHYTOCOMPOUNDS OF *CAMELLIA SINENSIS*

Polyphenols; -include catechin, flavanols, phenolic acids, anthocyanin.

Polyphenols are most abundant and biologically active compound. Green tea has simple and complex polyphenols; simple polyphenol includes flavonoid present most abundantly which includes Catechins and flavanols. While flavanols such as quercetin, kaempferol, myristic were consider having therapeutic effects like antioxidant, anti-inflammatory, anti-allergic, antiviral and antibacterial properties. Catechins (tea tannins) another flavonoid monomer belongs to the flavan- 3-ol subclass of flavonoids. Catechins include epicatechin (EC), epigallocatechin (EGC), epicatechin gallate (ECG) and epigallocatechin gallate (EGCC). simple polyphenols include Gallic acid and its ester with quinic acid [24]. EGCC, ECG and EGC constitute 80% of total catechin. Catechin are found more dominantly in younger leaves. major beneficial effects of polyphenols include preventing tooth decay, controlling blood pressure also found to be antibacterial and antioxidant.

FLAVANOIDS-major flavonoid is glycosides which includes myricetin glycosides, quercitin glycosides and behenyl glycosides. Disaccharides and trisaccharide sugars are present in it. Anthocyanin is another flavonoid in green tea; it gives bitter taste to tea.

PHENOLIOC ACID-Phenolic acid is present in small amount and very less studies have done till now, according to few studies phenolic phytochemicals include gallic acid, p-coumaric acid and caffeic acid. It also has two derivatives the theogallin and chlorogenic acid [25].

ALKALOIDS-Purine alkaloids are some compound found in green tea. caffeine, theophylline and theobromine are purine alkaloid where caffeine is present most abundantly followed by theophylline and theobromine.

POLYSACCCHARIDES -Green tea polysaccharides are composed of heteropolysaccharides having monosaccharide units. green tea Polysaccharides can be divided into neutral and acidic polysaccharides; neutral polysaccharides have more neutral sugar as compared to uronic acid while acidic polysaccharides have high content of uronic acid whereas glucose, galactose, mannose are neutral sugar present in neutral polysaccharide while galacturonic, rhamnose, arabinose, xylose and galactose are Acidic polysaccharides[26].Plants use in folk medicine has contain polysaccharides which has various beneficial properties like anti-radiation,antiviral, antitumor, anti-inflammatory, anti-HIV and immunological responses.

2.3 WITHANIA SOMIFERA(L) DUNAL

Ashwagandha also *withania somnifera(L) dunal* which comes under solanaceae family.it is a medicinal plant with great health benefits and located in India sub-continent. The benefits of ashwagandha are well written in ayurveda. This plant is distributed in 84 genera and have 3,000 species around the world. Cultivated in tropical Africa, south Africa and the canary and cape island also grow in some countries of Asia on large scale [27]. This plant has great therapeutic values therefore count as good source of herbal drugs. traditionally has broad range of application in medicinal system include as an aphrodisiac, for treating health problems like constipation and anemia. Also been used to kill and remove intestinal worms, support liver health and manage cardiovascular system. Also found effective in treating conditions related to nervous system. the plant is rich in phytocompounds like alkaloid, steroids, saponins, phenolics in addition flavonoids, polyphenols and glycosides are there in plant.

ALKALOIDS- power and Salway extracted alkaloids from leaves and roots namely somiferine, somine,somniferininewithamine,withanmine,pseudowithamine and withanaminine.[28][29].these all are are found in alcoholic extract of leaves, in methanolic extract various other phytocompounds are found in leaves and roots, leaves phytochemical includes tisopelletierine, cuscohygrine, hygrine, withasomine and withania these all are alkaloid. Some other natural substances are also present in metholic extract.

STEROIDS- withanolides are steroidal lactones. Major steroids include withaferin A, withanaloid D, withanaloid C. Withanolide D an steroid has structural alikeness to withaferin A except the presence of hydroxyl group at C-20 rather than at C-27 on withanolide D. withanolide A is an alcoholic extract of roots. Other withanolide isloated from plant is withanoloide C. steroid contribute as antiinflammatory, anticancer, immunomodulatory and stress reducing properties. chemical structure of withanolides is similar to panax ginseng thus *withania somnifera* also knowns as “Indian ginseng”.[30].

SAPONINS-stoindoside VII, stoindoside VIII are two acylsterylglucoside prssent is withania also two glycowithanolides are also present.

Chapter 3

3 METHODOLOGY

Methodology use here for the study of potential phytochemicals of *camellia sinensis and withania somnifera against* monkeypox viral protein (A42R) is a combination of computational methods and molecular docking. Virtual screening tool PyRx is employed for testing binding affinities of phytochemicals as multiple ligands targeting viral protein of monkeypox. Visualizing tool Biovia Discovery Studio is employed for visualizing the interaction and retrieval of 2D structure of protein-ligand binding. ADME analysis is done to check efficiency and effectiveness of phytochemicals as potential herbal drug. Detailed methodology is discussed in Further section of methodology.

3.1. DATA COLLECTION

Different databases have come into use for retrieval of required data and structures. Databases like Google scholar, PubMed, IMPPAT, Research Collaboratory for structural bioinformatics protein data bank (RCSB) and PubChem are used for 3D structures of protein in PDB format and ligands structure in SDF format

3.2. BIOINFORMATICS TOOL

PyRx ,Biovia discovery tool, MGL tool and swiss ADME were use.

3.3. PREPARATION OF PROTEIN

To prepare protein, the 3D structure of protein is first downloaded with resolution of 1.52 Å from PCSB PDB in the format of PDB. By using Biovia Discovery Tool the heteroatoms, water molecules along with ligands were removed for making protein suitable for protein ligand interaction. Required Kolman charges were also added. To get better interaction results the side chains of protein were also removed, and only single A chain is considered. Such that our protein is prepared for docking.

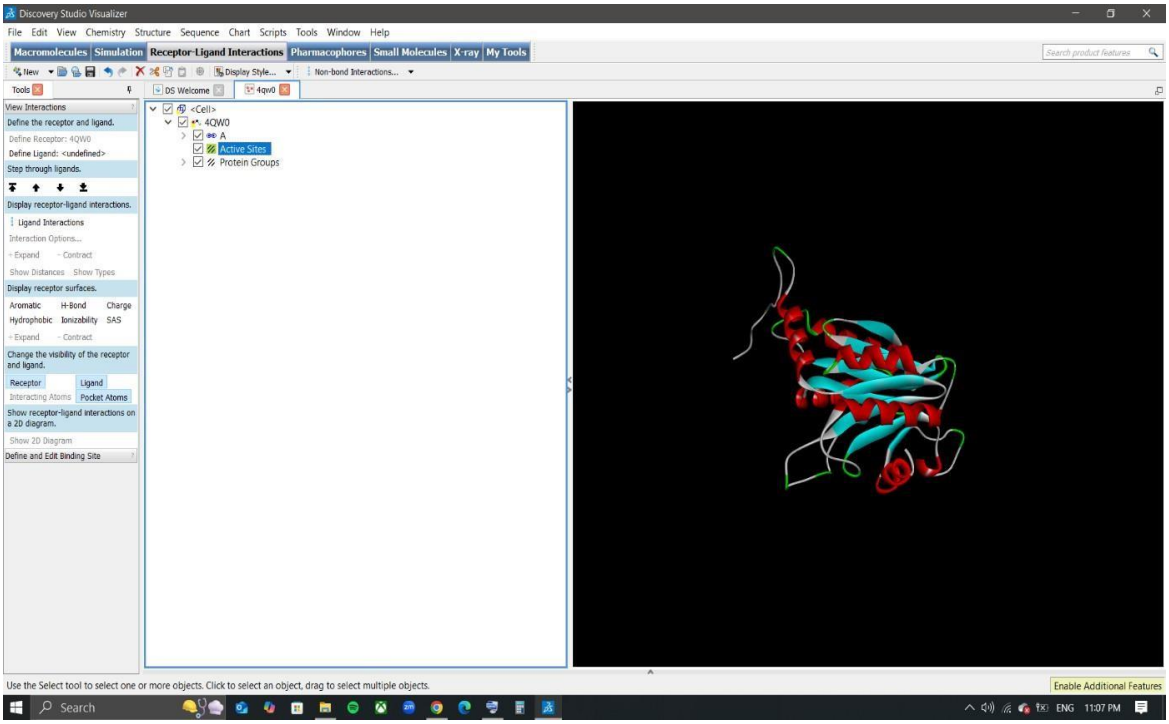


Figure 1- PROTEIN LOADED IN BIOVIA DISCOVERY STUDIO

3.4. RETRIEVING LIGANDS STUCTURE AND LOADING FOR DOCKING.

3.4.1-- The 16 phytochemicals from *camellia sinensis* and 6 from *withania somnifera* were downloaded in 3D SDF format from IMPPAT. The 3D structure of cidofovir is also downloaded from PubChem in the SDF format, here cidofovir will be used as negative control.

Phytochemicals from Camellia *Sinensis*	IMPPAT ID	Phytochemicals from *Withania Somnifera*	IMPPAT ID
Brassinolide	IMPHY003921	Withanolide Q	IMPHY002338
Teasterone	IMPHY003727	27-deoxy,14-hydroxy withaferin A	IMPHY005179
Typhesterol	IMPHY003725	27 deoxywithaferin A	IMPHY005187
Apigenin	IMPHY004661	17 alpha hydroxywithanolide D	IMPHY005227

Quercetin	IMPHY004619	pelletierine	IMPHY7448
kaempferol	IMPHY004388	Cuscohygrine	IMPHY12663
Gallocatechin	IMPHY011735		
Geranic acid	IMPHY004536		
Theobromine	IMPHY006394		
2,2trimethylcyclohexanone	IMPHY005364		
Myristic	IMPHY0060		
L+ (-) Arabinose	IMPHY004187		
2-Undecenal	IMPHY005526		
Riboflavin	IMPHY00846		
Theophylline	IMPHY005758		

TABLE 1- LIST OF ALL PHYTOCHEMICALS USED IN THIS STUDY FOR DOCKING WITH THEIR IMPPAT PHYTOCHEMICAL IDENTITY.

3.5. MOLECULAR DOCKING

- For the first step of molecular docking, the prepared protein(4QWO) in PDB format is loaded in pyRx a virtual screening tool that uses Autodock Vina tool and Vina algorithm for docking. The Protein can be loaded by going to the file menu and selecting “load molecule ".
- pdb format of protein is converted to pdbqt format and making it a macromolecule by clicking on protein(4QWO)->Autodock>macromolecule.

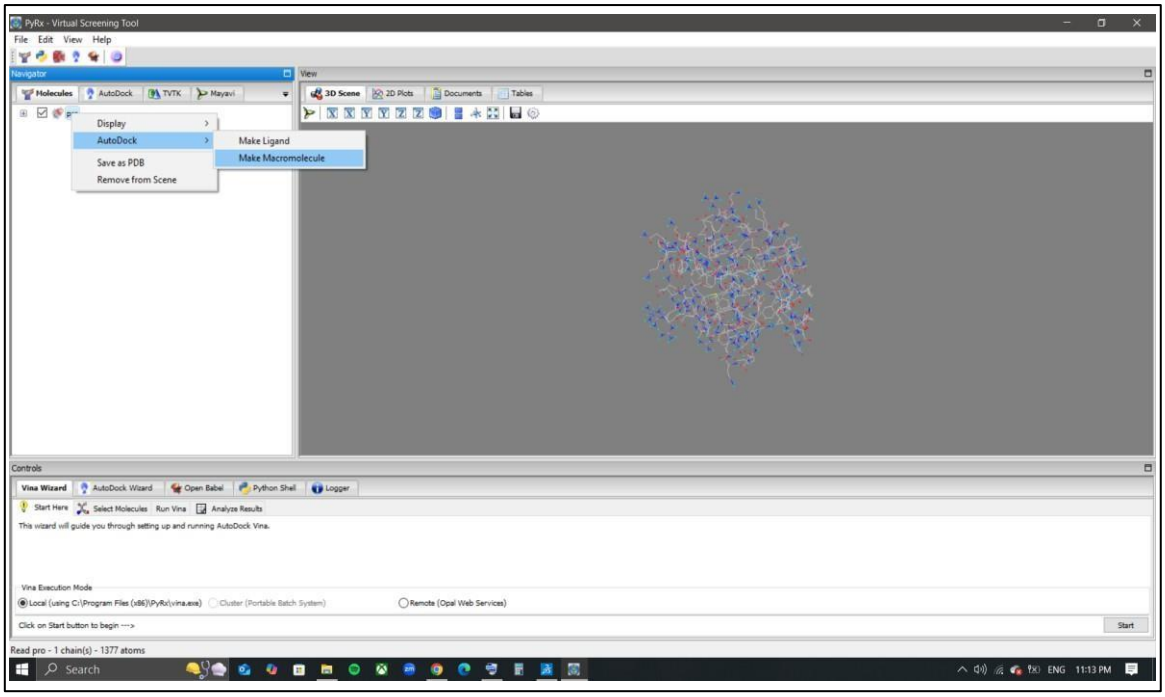


Figure 2- CONVERSION OF PROTEIN TO A MACROMOLECULE

- ligands are loaded into pyRx for docking by simply selecting OpenBable menu and clicking on insert new file, select all ligands one by one and upload it from files.
- After loading all the ligands are minimized to decrease their energies, after that again by right clicking all ligands were converted in pdbqt format.

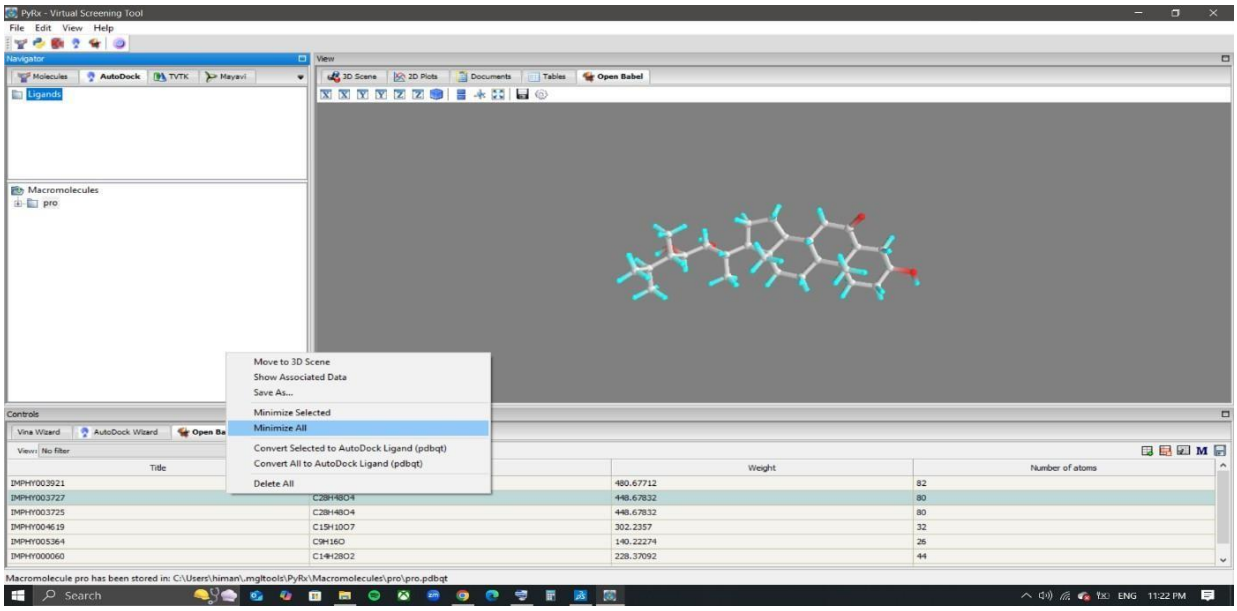


Figure 3 - step of minimization of ligands to decrease their energies.

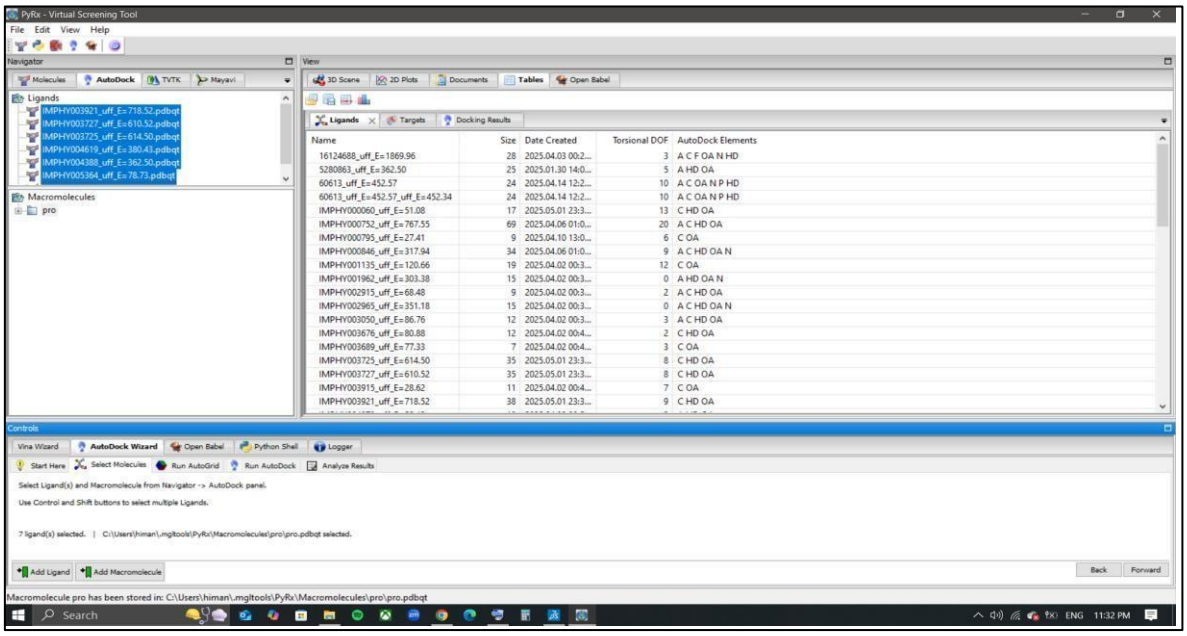


Figure 4- loading of protein in pyRx

- After loading both protein and ligands, define both by forming a grid box. To create a grid box, click on vina Wizard and by selecting start menu located on bottom right corner, select all protein and ligands from macromolecule section by pressing shift and control button.
- Click on forward and a grid box will appear, make sure all known binding sites are covered and if unknown try to consider broader region.
- Grid box dimension can also be included manually.
- Once the grid box is set press forward to start docking. Once the docking started the result will be shown on display.
- After all the ligands bind to protein marking completion of docking, the bottom region will list all the generated poses with their binding affinities and RMSD values.
- Save your result in an excel sheet, the ligand with highest negative binding energy is considered the best among results.
- All models of ligand with highest negative energy can be display by clicking on Auto dock and select macromolecule and select your ligand, right click on ligand and all models will be displayed and save it in pdb format to retrieve 2D model of interaction.

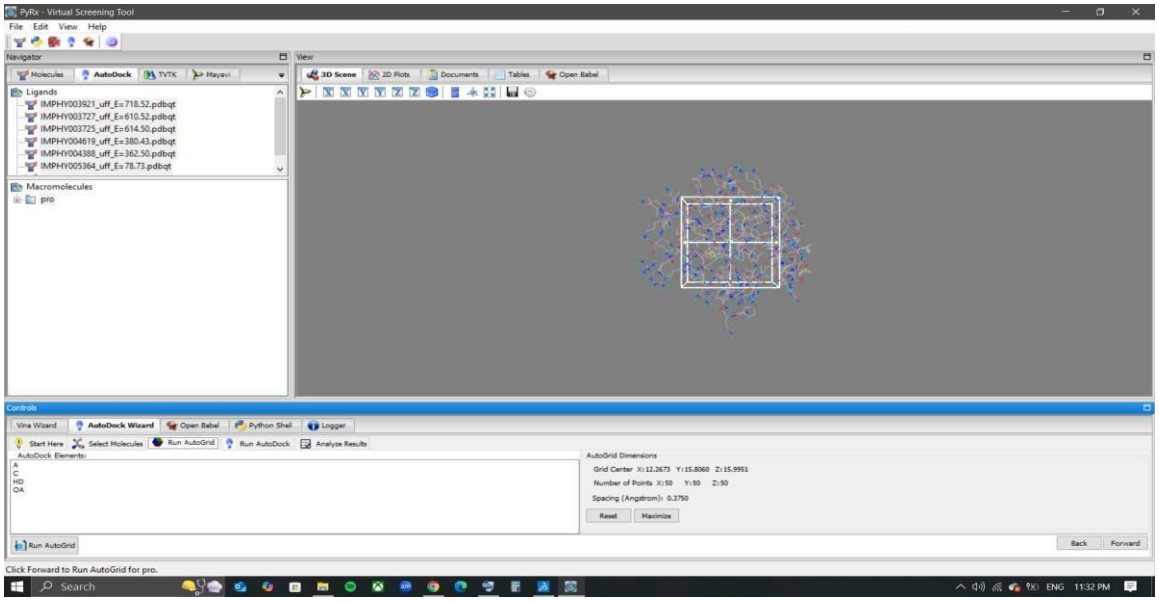


figure 5- showing grid box

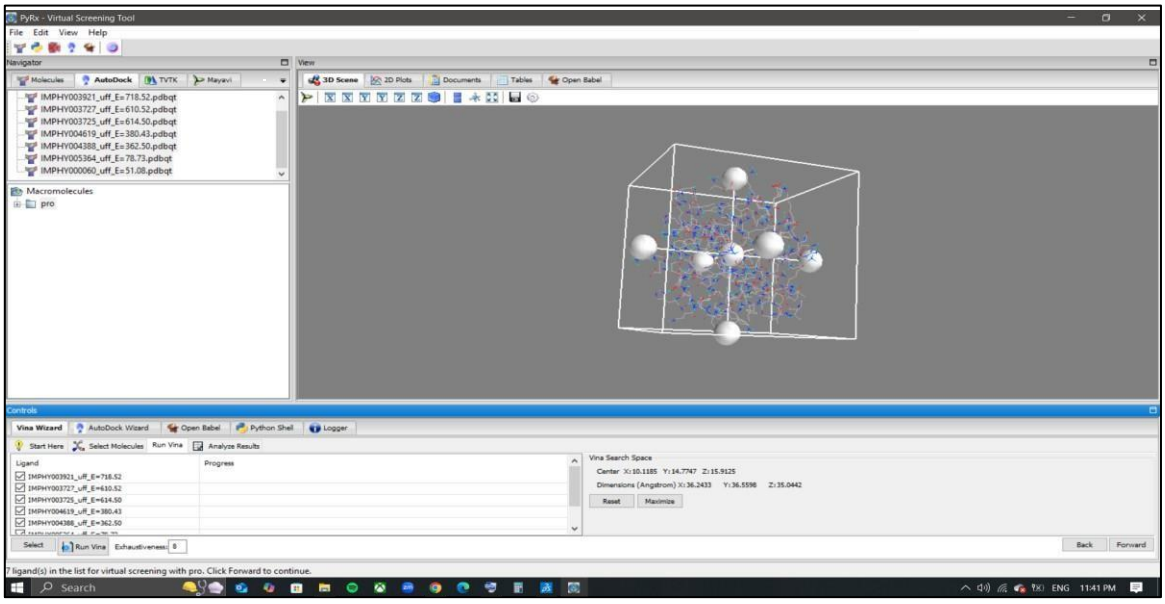


Figure 6- showing adjustment of grid box

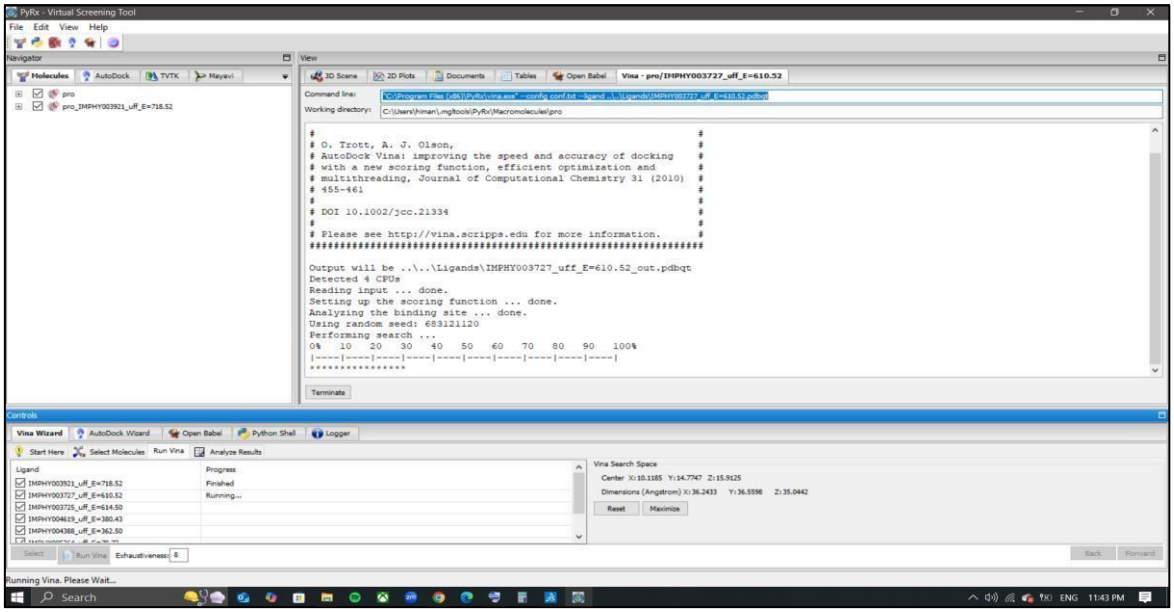


Figure 7- showing running docking in vina wizard

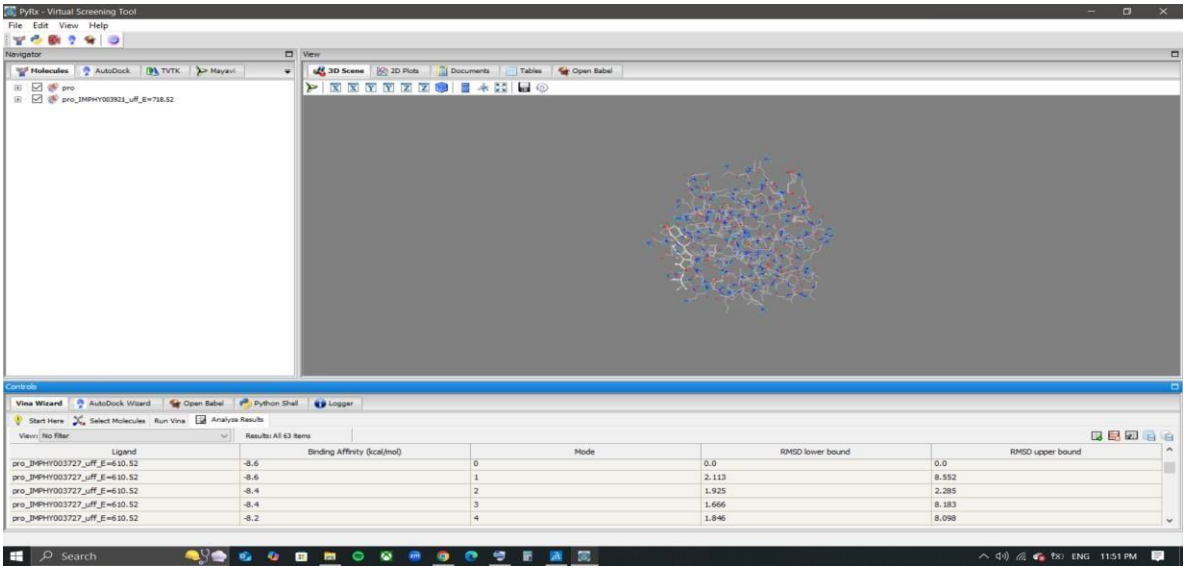


Figure 8- protein-ligand binding with their binding affinity

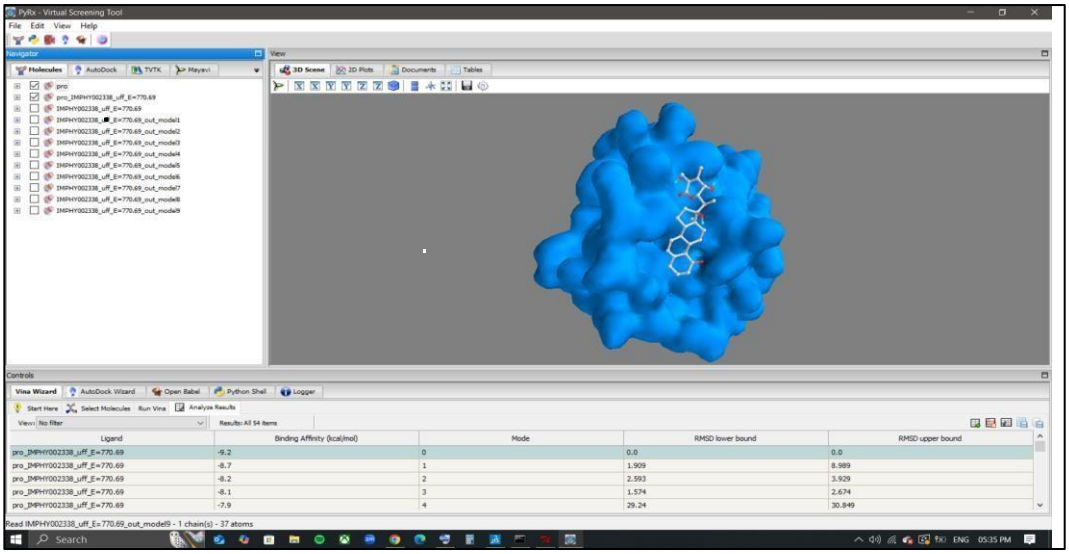


Figure 9- representation of protein-ligand binding in macromolecular display.

3. 6 VIZUALIZATION OF RESULTS.

- By using biovia discovery studio the docked protein-ligand interaction can be visualized. Open the visualizing tool and load your protein structure. To load protein, choose file>open and select your file.
- After that load the docked ligand in pdb format. Docked ligand confirmation can be loaded by following, file>open and select your ligand file.
- View both protein and ligand in hierarchy menu, Copy the ligand and paste it with protein by simply using ctrl+c > ctrl+p .
- Different display style is there to represent like stick, ball-stick or surface representation.
- To analyze interaction, use receptor-ligand interaction option located in the left vertical column.

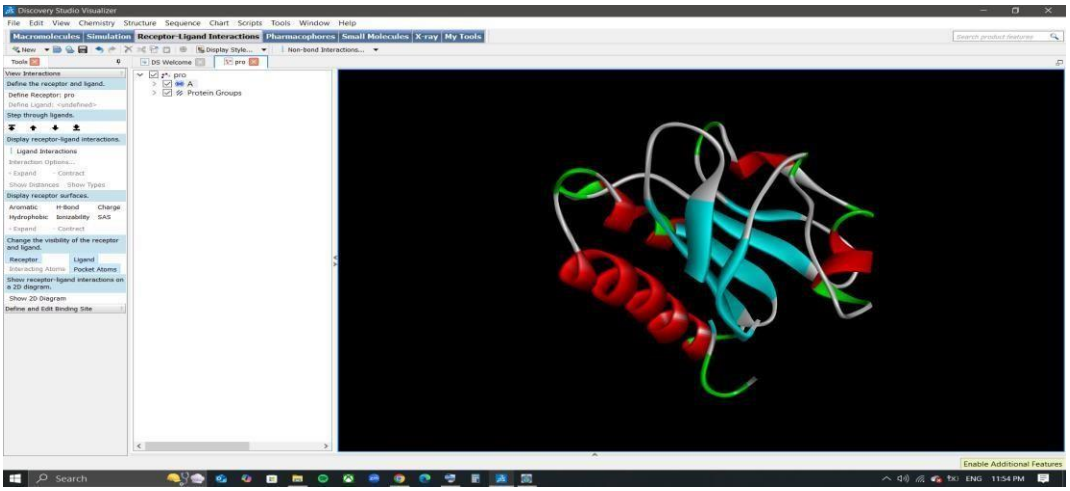


Figure 10-protein structure loaded in Biovia discovery.

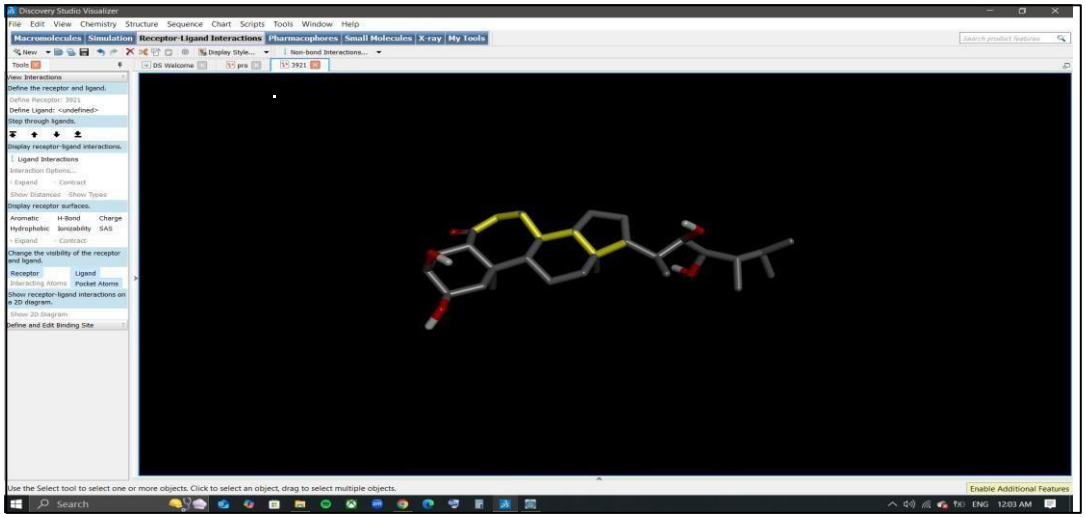


Figure 11-loading of docked ligand structure in Biovia discovery.

Chapter 4

4. RESULT

4.1. DOCKING RESULT

Molecular docking results shows different binding affinities of phytochemicals taken from two different plant *camellia sinensis* and *withania somniferra* with viral protein of monkey pox A42R (4QWO). Cidofovir is one of the antiviral medications which inhibit viral replication and slow down symptoms. Previous research has also shown that the binding energy of cidofovir ranges from (-6.0 Kcal/mol and -5.1 Kcal/mol) [32]. cidofovir are considered and results are concluded according to it. The interaction of cidofovir with viral protein of monkeypox A42R(4QWO) has 1 unfavourable electrostatic interaction,2 electrostatic (salt bridge) interactions,4 hydrogen bonds sharing and van der Waals interactions.

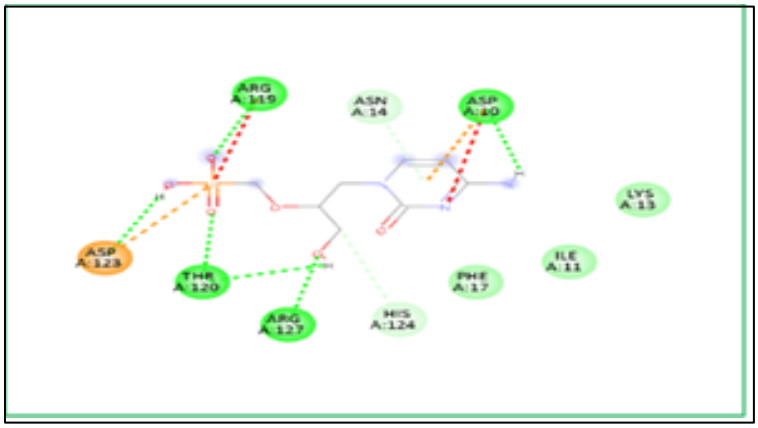


Figure 12- 2d interaction of cidofovir with protein A42R derived by using Biovia discovery studio showing all interactions.

According to analysis of the binding affinities of different phytochemicals of both plants and their interaction with target protein revealed Brassinolide from camellia sinensis with binding score of –8.7Kcal/mol and 27-deoxy 14- hydroxy withaferin A with binding score of –10 has highest binding score in negative hence, has better potential as an effective viral protein inhibitor, that will affect protein viral replication and entry into the body. Phytochemicals other than those with highest binding score may also serve as promising herbal drug candidate. Table 3 and 4 listed all phytochemicals binding affinities in decreasing order with protein. According the obtained 2-D structural interaction between protein and the ligand (Brassinolide). Hydrogen bonds forming between HIS A:5, SER A:12 and the ligand make this interaction more favourable making it more strong and stabilized structure. Further ILE:15 involved in hydrophobic interaction, increases binding affinity of ligand by stabilizing non-polar regions. As concluded, hydrogen bonds and hydrophobic interactions are key stabilizers in this interaction.

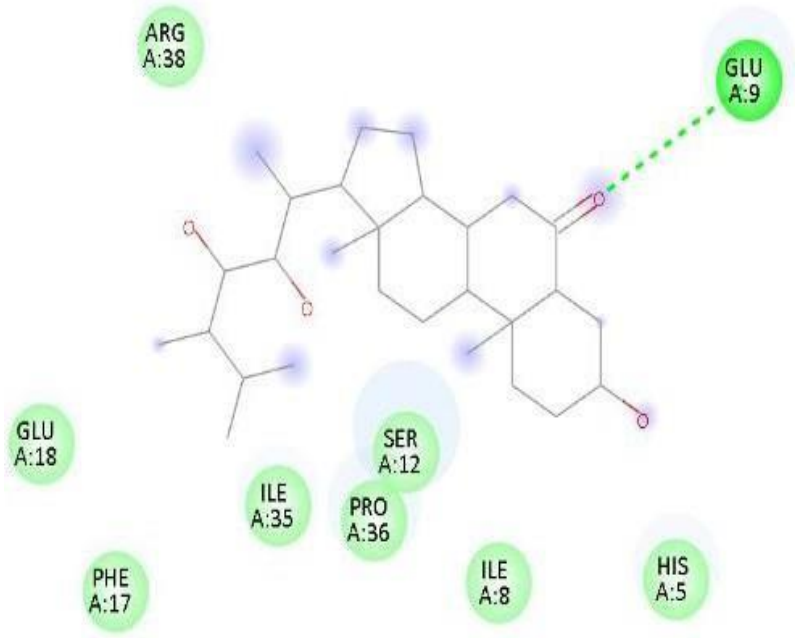
PHYTOCHEMICALS	BINDING AFFINITY (Kcal/mol)
Brassinolide	-8.7
Teasterone	-8.7
Typhasterol	-8.6
Apigenin	-8.1
Quercetin	-8.0
Kaempferol	-7.9
Gallocatechin	-7.5
Riboflavin	-7.0
theophylline	6.2
Glucuronic acid	-6.1
Geranic acid	-5.9
Theobromine	-5.9
2,2 Tri methylcyclohexanone	-5.5
Myristic	-5.4
L+(-) Arabinose	-5.0
2-udecenal	-5.0

Table 3- binding affinity of phytochemicals of *camellia sinensis* with target protein

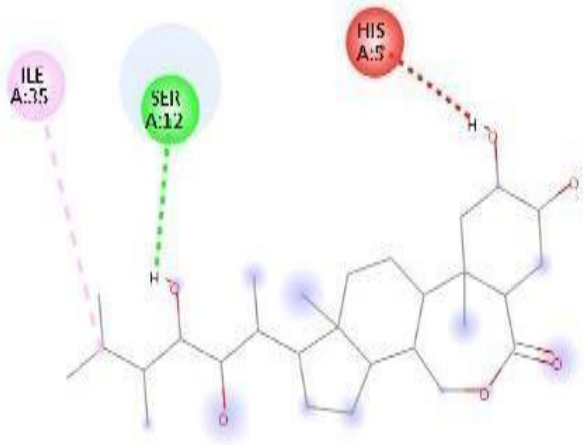
PHYTOCHEMICALS	BINDING AFFINITY (Kcal/mol)
27-Deoxy 14-hydroxywithaferin A	-10
27- deoxywithaferin A	-9.7
17 alpha hydroxywithanolide D	-9.3
Withanolide Q	-9.2
Pelletiere	-8.0
Cusco hygrine	-5.8

Table 4- binding affinity of phytochemicals of *withania somnifera with target protein.*

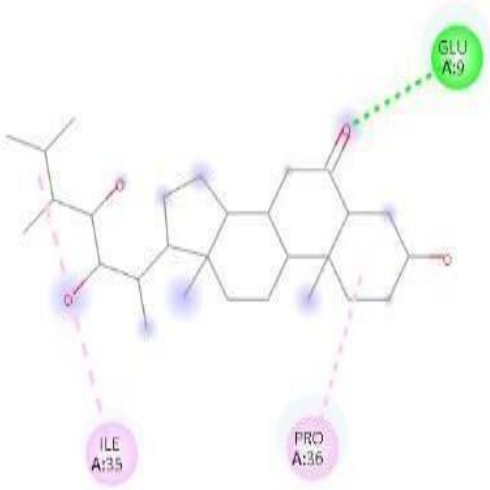
(a) Teasterone



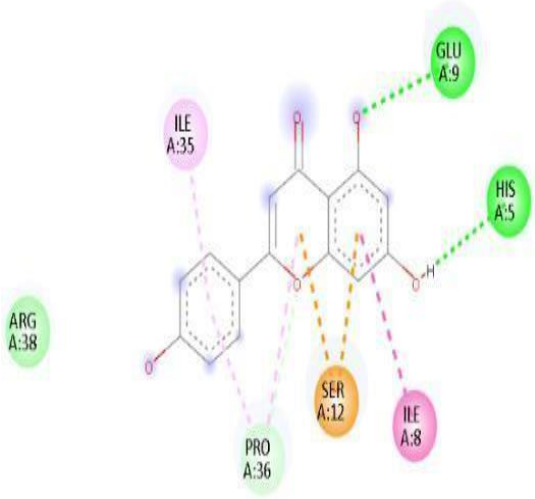
(b) brassinoloide



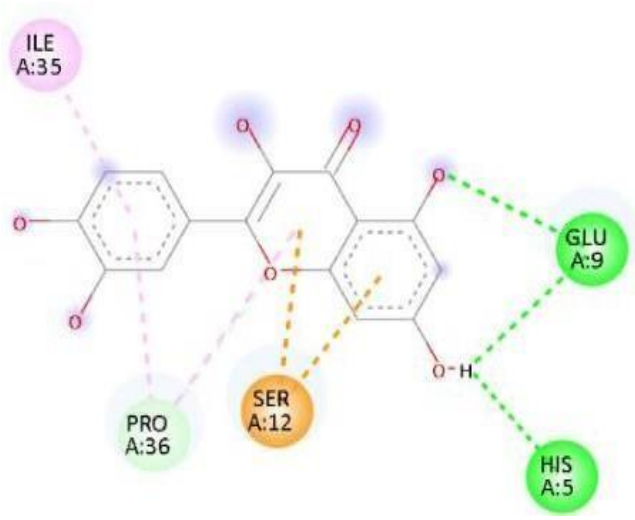
(c) Typhsterol



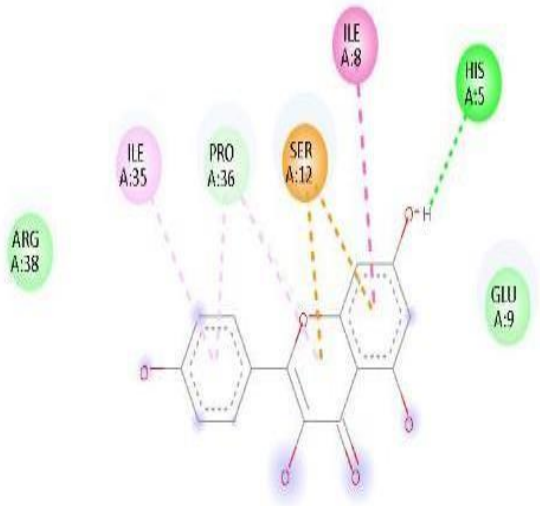
(d)apigenin



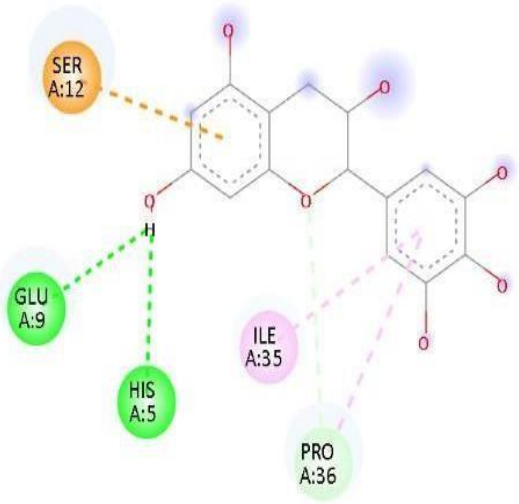
(e) quercitin



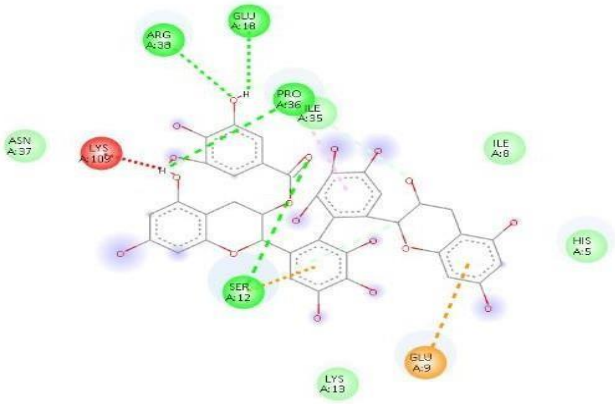
(f) kaempferol



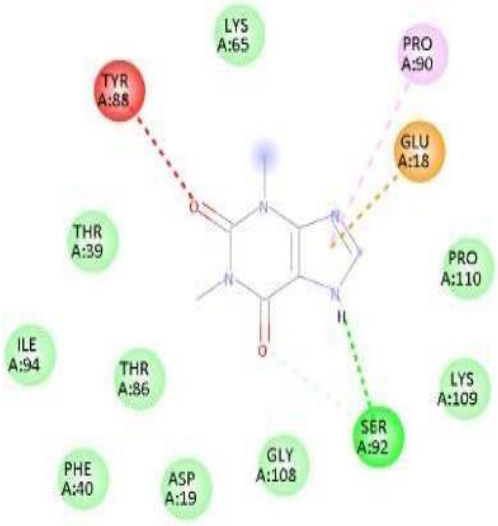
(g)gallocatechin



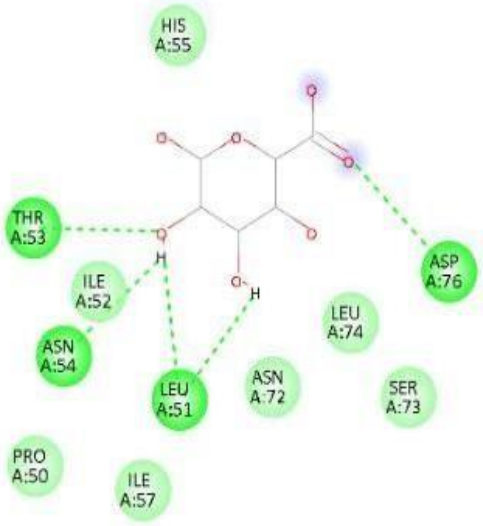
(h)riboflavin



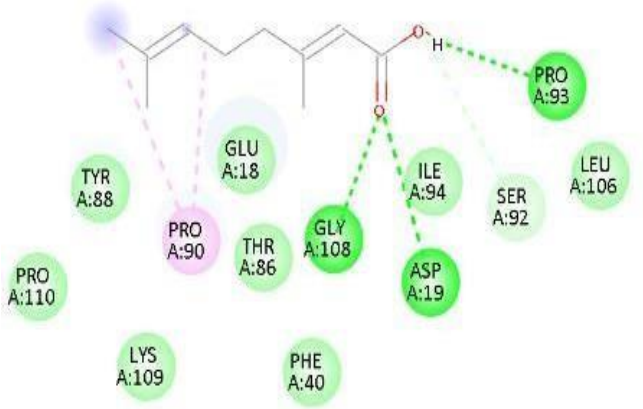
(i) Theophylline



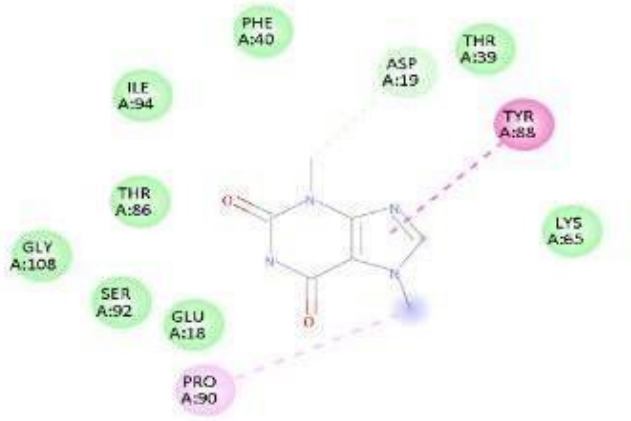
(j) glucuronic



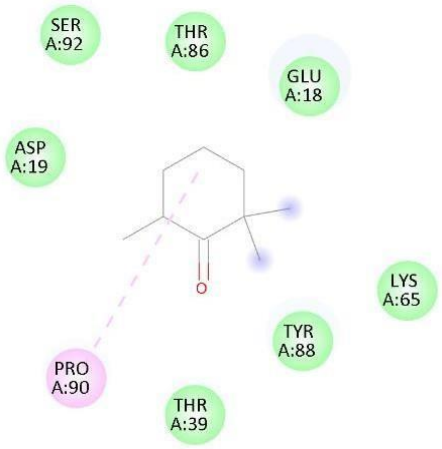
(k) Geranic acid



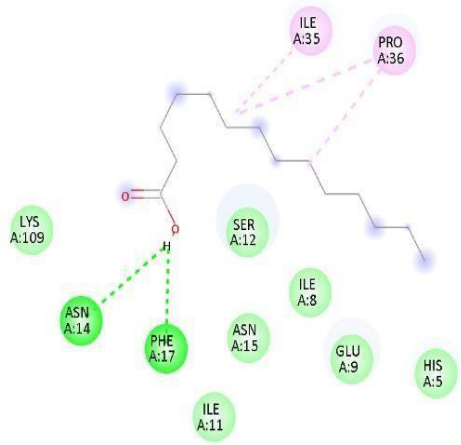
(l) theobromine



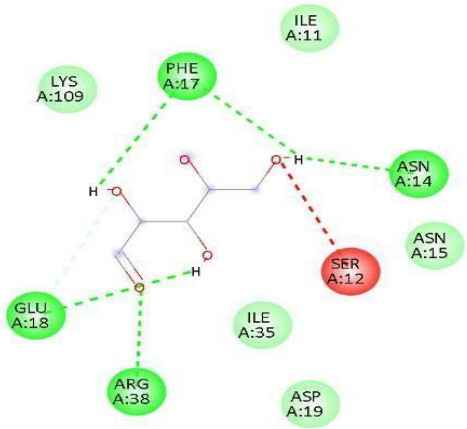
(m) 2,2,6-trimethyl cyclohexanone



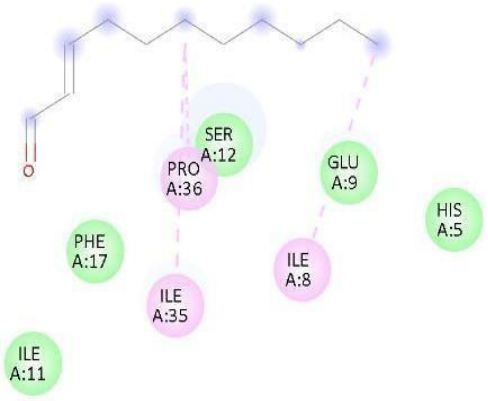
(n) myristic



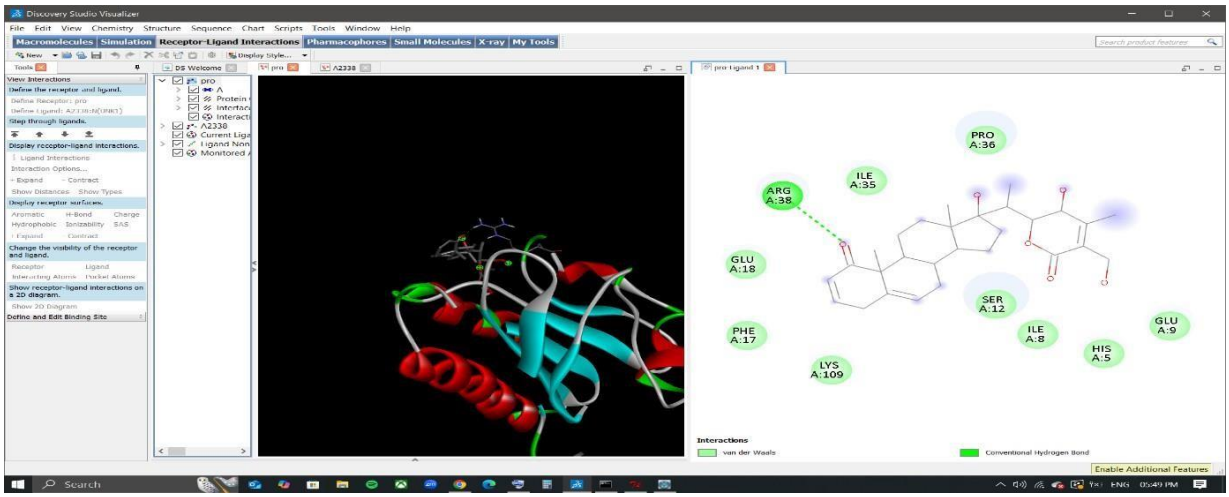
(o) Arabinose



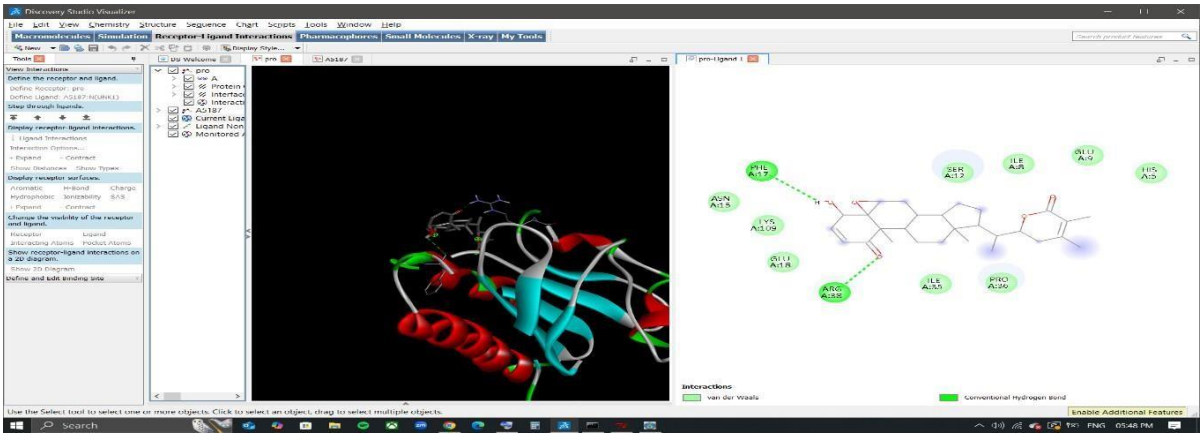
(p) 2-undecenal



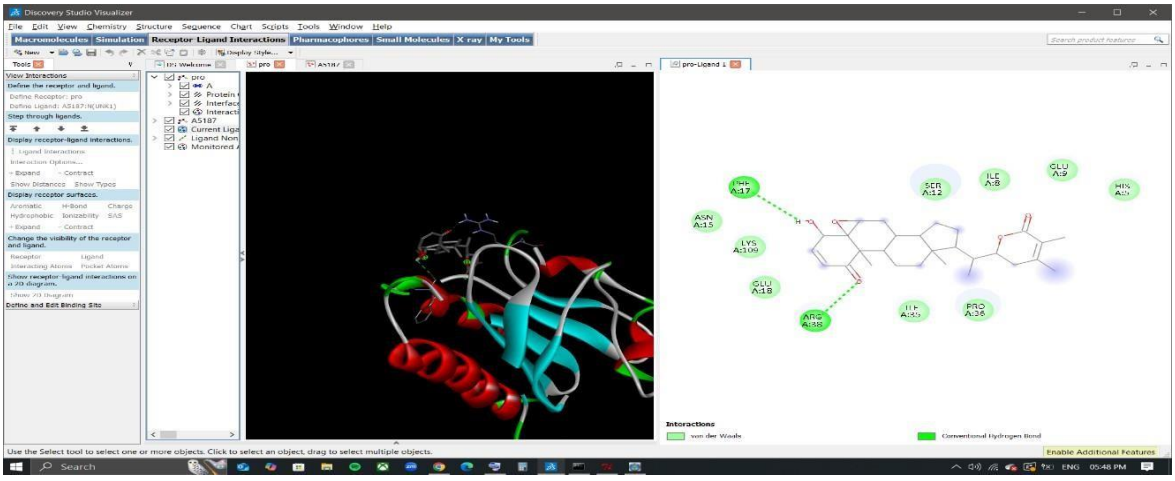
27-Deoxy 14-hydroxywithaferin A



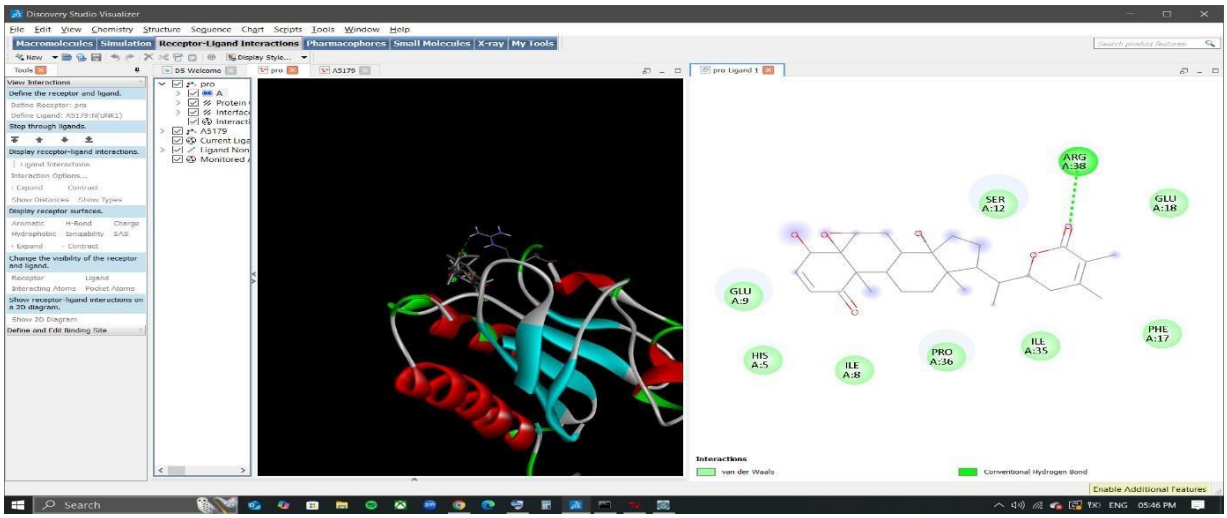
27- deoxywithaferin A



17 alpha hydroxywithanolide D



Withanolide Q



Cusco hygrine

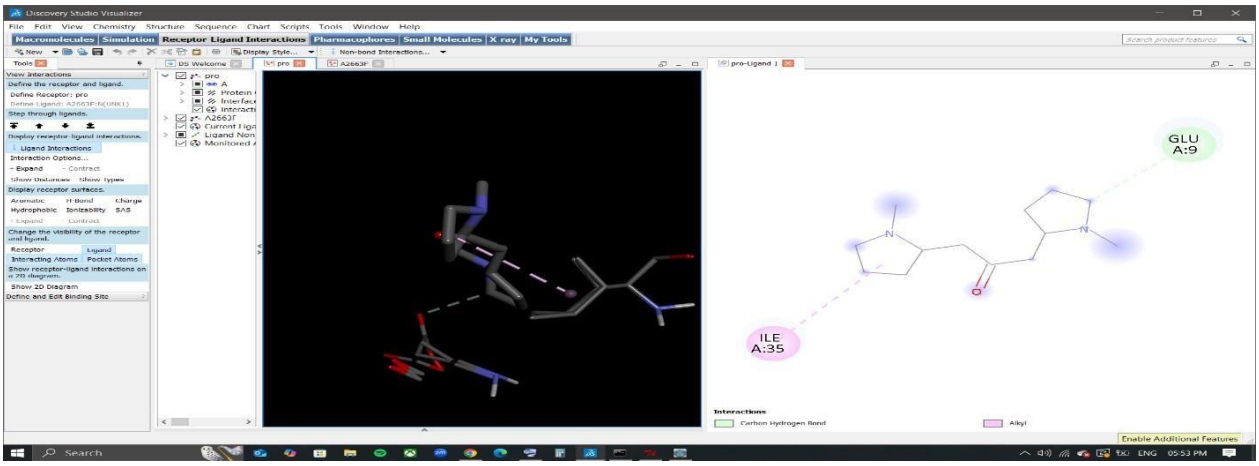


Figure- 13 screenshot showing 2D structure ligand (phytochemical of *withania somnifera* and *Camillia sinensis*) binding with target protein.

4.2. ADMET ANALYSIS

The analysis via SWISS ADME showed that most of the phytochemicals have appropriate bioavailability scores between 0.55 and 0.85. Evaluating the **A**bsorption, **D**istribution, **M**etabolism, **E**xcretion and Toxicity processes (abbreviated as

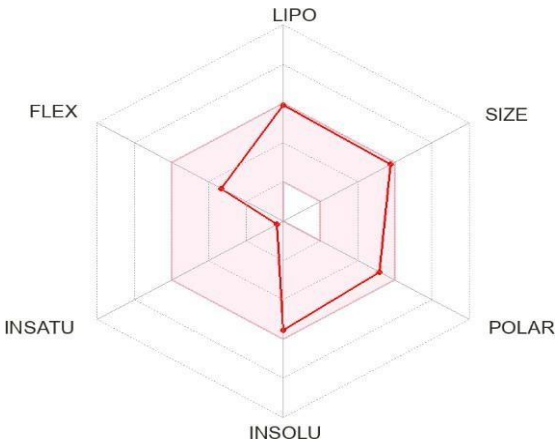
ADMET) of drugs in the body helps in defining the pharmacokinetic features of a particular drug. According to the Lipsik's rule of five drugs with molecular weights less than 500 g/mol can easily penetrate blood vessels and skin. Hence, selected phytochemicals have M.W. <500 g/mol.

In Fig. 14 the RADARS, i.e. Ranking Aggregated Drugs Attributes by Relevance and Similarity, demonstrating the bioavailability and pharmacological characteristics of phytochemical with highest binding energy, obtained using computational tools that account for several factors including polarity, saturation, flexibility, size, and lipophilicity, pink region in image shows the standard range for characteristics.

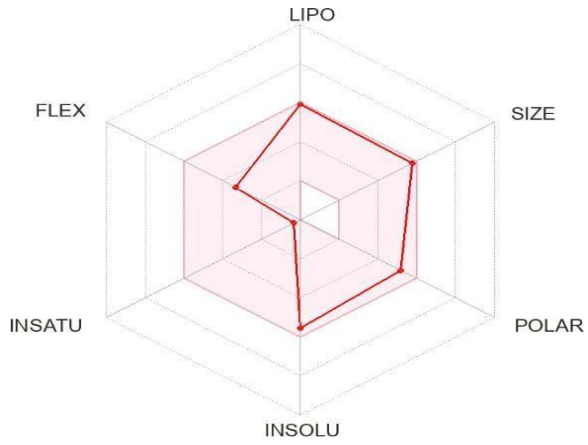
Phytochemical	Molecular weight	Hydrogen acceptors	Hydrogen donors	TPSA	logP
Brassinolide	480.68	6	4	107.2	3.53
Teasternone	448.68	4	3	77.76	3.87
27- deoxywithaferin A	470.60	6	2	96.36	3.74
17 alpha hydroxywithanolide D	488.61	7	4	119.75	2.93

Table 4 – ADMET results

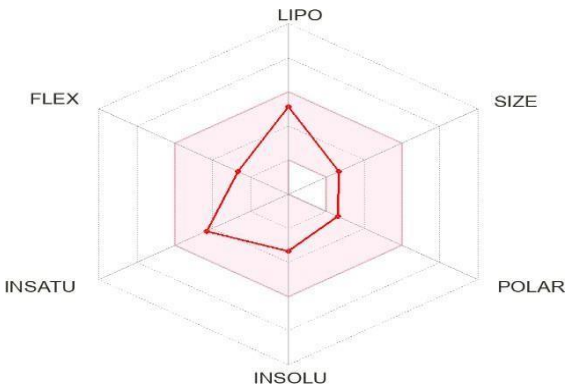
Brassinolide



teasterone



27- deoxywithaferin A



17 alphas hydroxy withanolide d

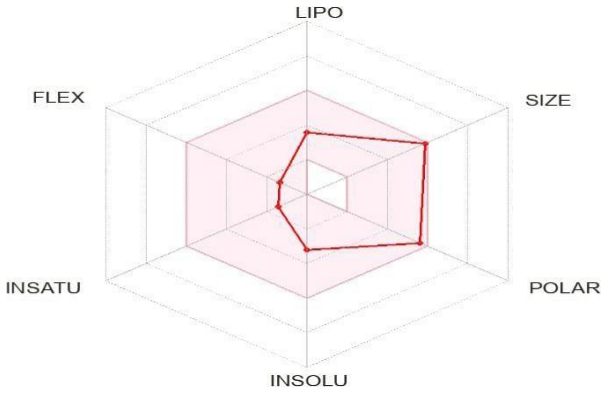


Figure 14 ADME analysis result of brassinolided

(a), teasterone(b),27 deoxywithaferin a (c), 17 alphas hydroxy withanolide d (d)

5 CONCLUSION

In this computational study docking simulation is tested to explore the use of phytochemicals present in plants for making herbal drug for the aim of management and treatment of monkeypox. Monkeypox virus is responsible for the zoonotic disease named monkeypox. The virus belongs to orthopoxvirus genus and parvoviridae family. This disease caused by zoonotic spread from animals to human or by human-to- human spread. Symptoms of the disease comes within 5-12 days, symptoms may include fever with headache, muscle pain, swollen lymph nodes rash and weakness. For the treatment, WHO approved drugs like tecovirimat, Brincidofovir are there and vaccines like JYNNEOS and ACAM200 is also there to prevent the disease, the vaccine and drug have some common side effects on body therefore, natural compound prsent plants are less toxic option for body. therefore, for this study in silico study is done to check natural compound present in two plants *camellis sinensis* and *withania somnifera* is tested for their potential as herbal drug. docking result showed blinding affinity and interactions by analysis binding score of phytocompounds with protein results are concluded. Typically, brassinolide and teasterone has same binding score of –8.7 Kcal/mol and 27- deoxy,14- hydroxywithaferin A has binding score of –10 Kcal/mol. Docking shows different docked pose and their score, lower binding score in negative is more favorable interaction. These phytochemicals will target protein A24R and restrict its function of viral replication. Some plants like amla, bitter leaf, holy basil, turmeric, etc has tested for for theri potential as herbal drugs Further ADME analysis is done by using computational tool to check Adsorption Distribution Metabolism Excretion of phytocompound in body. The result shows all phytochemicals having MW less then 500 so that herbal drug can easily get into blood vessel. Table 4 showing properties of phytochemicals like number of hydrogen atoms it donates or accept or topological polar surface area and logarithm of octanol-water partition coefficient (logP) all these properties define phytochemical compatibity as drug candidate.

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ANNEXURE-IV

DELHI TECHNOLOGICAL UNIVERSITY

(Formerly Delhi College of Engineering)
Shahbad Daulatpur, Main Bawana Road, Delhi-42

PLAGIARISM VERIFICATION

Title of the Thesis IN SILICO APPROACH TO STUDY THE PHYTOCHEMICALS PRESENT IN CAMELLIA SINENSIS AND WITHANIA SOMNIFERA TO TARGET MPXV VIRUS AMBR FOR THE TREATMENT OF MONKEYPOX DISEASE

Total Pages 51 Name of the Scholar Khushi

Supervisor (s)

(1) Dr. Navneeta bharadvaja

(2)

(3)

Department Biotechnology

This is to report that the above thesis was scanned for similarity detection. Process and outcome is given below:

Software used: Turnitin Similarity Index: 9% Total Word Count: 6,389

Date: 5-06-25

Candidate's Signature

5/6/25
Signature of Supervisor(s)

0% detected as AI

The percentage indicates the combined amount of likely AI-generated text as well as likely AI-generated text that was also likely AI-paraphrased.

Caution: Review required.

It is essential to understand the limitations of AI detection before making decisions about a student's work. We encourage you to learn more about Turnitin's AI detection capabilities before using the tool.

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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.

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9% Overall Similarity

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A Flag is not necessarily an indicator of a problem. However, we'd recommend you focus your attention there for further review.

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Gmail **Khushi <khushisingh251021@gmail.com>**

Re: submission of conference paper registration fees

5 messages

Khushi <khushisingh251021@gmail.com> 3 May 2025 at 12:34
To: ICETSE 2025 <icetse2025@gmail.com>

Respected conference chair
Registration step is done along with payment of required registration fees . Please find the attached payment slip.

PAPER ID -706

paper title:Structure-based computational investigation of Bioactive compounds from Camellia sinensis as a drug candidate for Human Monkeypox Virus.

On Wed, Apr 30, 2025, 8:11 AM ICETSE 2025 <icetse2025@gmail.com> wrote:

> Already deadline for paper submission completed through CMT... Anyway we are considering your paper for the conference...
>
> Your paper has been accepted with the paper ID 706. Please make the registeration within 5th May 2025 to consider your paper for the conference.
> Please visit the website www.ait-tumkur.ac.in for the payment process or do the payment to G pay or phone pay to the number 9902238768.
> Please send payment proof by mentioning paper ID to this Email ID.
>
> On Sun, 27 Apr, 2025, 11:21 pm Khushi, <khushisingh251021@gmail.com> wrote:
>
> > Respected conference chair,
> >
> > I am writing to respectfully request your consideration for the submission of my paper titled "Structure-based computational investigation of Bioactive compounds from Camellia sinensis as a drug candidate for Human Monkeypox Virus (MPXV)" in Second International Conference on Emerging Technologies in Science and Engineering (ICETSE) to be held on june 19-20,2025 at Akshaya institute of technology,tumkur karnataka. .
> >
> > I fully acknowledge the importance of deadlines and sincerely apologize for any inconvenience this may cause. The completed manuscript is attached herewith, and I would be most grateful if you could kindly consider it for review.
> >
> > Thank you very much for your time and understanding.
> >
> > warm regards,
> >
> > khushi
> >
> > Delhi technological university, Bawana Road,shahbad daulatpur village.

1000077184.jpg
211K

ICETSE 2025 <icetse2025@gmail.com> 17 May 2025 at 16:20

To: Khushi <khushisingh251021@gmail.com>

Dear Participants,

Regarding your ICETSE 2025 registration, we are pleased to confirm that your paper ID - 706 has been successfully registered. Further instructions will be communicated to you shortly.

Regards

ICETSE Team -2025

[Quoted text hidden]

ICETSE 2025 <icetse2025@gmail.com> 17 May 2025 at 16:21
To: Khushi <khushisingh251021@gmail.com>

Pls send your paper word file

Regards

ICETSE Team -2025

[Quoted text hidden]

Khushi <khushisingh251021@gmail.com> 17 May 2025 at 16:41
To: ICETSE 2025 <icetse2025@gmail.com>

paper id -706

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ICETSE 2025 <icetse2025@gmail.com> 20 May 2025 at 12:59
To: Khushi <khushisingh251021@gmail.com>

Dear Participants,

Regarding your ICETSE 2025 registration, we are pleased to confirm that your paper ID -706 has been successfully registered. Further instructions will be communicated to you shortly.

PUBLICATIONS

Title of Paper - “structure based computational investigation of Bioactive Compounds from camellia sinensis as drug candidate for human monkeypox virus (MPXV)”)

Author Names – Khushi, Eshita, Dr.Navneeta Bharadvaja

Name of Conference - second international conference on emerging technologies in science and engineering (ICETSE)2025.

Date of Conference – June 19-20, 2025

Indexing - Scopus Indexed

Status of Paper – Acceptance

Received Date of Acceptance-30/April/2025

Date of Camera-Ready Submission and Registration –20/May/2025