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Molecular Docking and Drug-Likeness Analysis of Oxalis corniculata Phytochemicals for Antifungal Therapy

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ABSTRACT

Leucorrhea is a common gynecological condition characterized by excessive vaginal discharge caused by physiological imbalance, microbial infections, poor hygiene, hormonal disturbances, and inflammatory disorders. Medicinal plants are widely explored as alternative therapeutic agents because of their bioactive compounds and reduced side effects. Oxalis corniculata is a medicinal herb rich in flavonoids, phenolic compounds, organic acids, and other phytoconstituents with reported antimicrobial properties. The present study aimed to evaluate the binding interaction of phytoconstituents from Oxalis corniculata against Lanosterol 14α-demethylase, a key enzyme involved in fungal ergosterol biosynthesis and an important target for antifungal therapy. Molecular docking and virtual screening studies were carried out using PyRx and Discovery Studio software. The three-dimensional protein structure was obtained from the Protein Data Bank, while phytochemical data were collected from PubChem. Binding affinity, 2D and 3D molecular interactions, and ADMET properties of selected phytoconstituents were analyzed. The docking results revealed favorable interactions between the phytoconstituents and the active site of CYP51, indicating possible antifungal potential. ADMET analysis also demonstrated acceptable pharmacokinetic and drug-likeness properties of the selected compounds. The findings suggest that phytoconstituents of Oxalis corniculata may serve as promising natural candidates for the management of leucorrhea-associated fungal infections and support further experimental and clinical studies.

Keywords: Leucorrhea; Oxalis corniculata, Molecular Docking , ADMET Analysis.

INTRODUCTION

Leukorrhea disease

Leucorrhea, also called white discharge or vaginal discharge, is a condition in which women experience a white or yellowish fluid coming from the vagina. The discharge is usually mild, clear or milky in color, and may not have a strong smell..[1] Vaginal discharge is a normal part of female health. Changes in the discharge can occur due to infections, hormonal changes, or certain diseases. In some girls, vaginal discharge may appear before the first menstrual period and is considered a normal sign of puberty [2] Leucorrhea is also commonly called “whites,” and in rural areas it is often known as “Safed Pani.” It can be diagnosed by examining vaginal fluid under a microscope, where more than 10 white blood cells per high power field may be seen [3] Adolescence is the stage of life between childhood and adulthood, usually between 11 and 20 years of age. During this period, physical, emotional, and psychological changes take place. Teenagers begin to develop their own identity, become more independent, and try to gain the trust of their parents. Adolescence is commonly divided into three stages: early adolescence, middle adolescence, and late adolescence. [4] Leucorrhoea is a condition in which women experience a thick white or yellowish discharge from the vagina. It commonly occurs during puberty when the reproductive organs are developing. The discharge may be thin and watery or thick and sticky. A small amount of vaginal discharge is normal and healthy because it helps remove dead cells and harmful microorganisms from the reproductive system. In healthy women, the discharge is usually milky white in color. [5,6]. Abnormal vaginal

Relevant conflicts of interest/financial disclosures: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

discharge may appear white, yellow, red, brown, or blackish in color. If the discharge is thick, sticky, excessive, or causes irritation and itching, it may need medical attention. Discharge that is grayish white, yellow, greenish-brown, or rusty in color can indicate infection or another health problem. When the discharge is heavy, continuous, foul-smelling, or associated with itching and discomfort, immediate treatment may be required. [5,6].Every woman normally experiences vaginal discharge from time to time. It helps maintain the chemical balance of the vagina, keeps the vaginal tissues flexible, and acts as a natural defense against infection. When the discharge becomes excessive, thick, white or yellowish, and has a bad smell, the condition is called leucorrhea. [5]

Types of leucorrhea.

1.Physiological Leucorrhea

Physiological leucorrhea is a normal vaginal discharge that is clear or milky white, thin, odorless, and does not cause irritation or itching. It commonly occurs during puberty, pregnancy, and other times when estrogen levels increase. During pregnancy, increased blood flow and hormonal changes lead to more vaginal discharge. In young girls after puberty, clear discharge without itching, pain, or bad smell is usually normal and does not require treatment. This discharge helps maintain the natural balance of the vagina and keeps the tissues healthy and flexible. It occurs due to hormonal stimulation, especially by estrogen, which causes changes in the vaginal lining, normal bacteria, and pH. On examination, there are no signs of redness, injury, or infection, and only a few white blood cells are present. [7, 8,9,10]

2.Pathological Leucorrhea

Vaginal discharge may increase because of vaginal infections or sexually transmitted infections (STIs). Different microorganisms such as Neisseria gonorrhoeae, Candida albicans, Chlamydia trachomatis, Ureaplasma urealyticum, streptococci, and Trichomonas vaginalis can cause leucorrhoea. These infections may lead to inflammation of the vaginal lining, producing yellowish and foul-smelling discharge. Common symptoms include itching, burning sensation, irritation, and thick, foamy white or yellow discharge. Leucorrhoea may also occur due to poor nutrition, weakness, reproductive tract disorders, or other gynecological problems. [7,10,11]

3.Inflammatory Leucorrhea

Leucorrhoea can also occur due to inflammation or congestion of the vaginal lining. If the discharge becomes yellowish or develops a bad smell, medical advice should be taken because it may indicate bacterial infection or sexually transmitted diseases (STDs). After childbirth, foul-smelling discharge along with back pain may suggest infection. To diagnose the condition, doctors may perform tests such as wet smear examination, Gram staining, culture tests, cervical smear, and biopsy. In many cases, bacterial infection causes inflammation of the vaginal tissues, leading to yellow and foul-smelling discharge [7,11]

Causes of leucorrhea

Leucorrhoea mainly occurs due to hormonal imbalance, particularly changes in estrogen levels. Estrogen is an important female hormone that helps in the growth and proper functioning of the reproductive system.

• Pregnancy, menstruation, perimenopause, and congestion in the uterus may increase vaginal discharge. Infections or inflammation of the reproductive organs can also cause leucorrhoea.

• The use of chemical contraceptives, intrauterine devices (IUDs), and other physical factors may result in irritation, itching, or infection.

• Mental and emotional factors such as stress, anxiety, depression, and emotional pressure may also play a role in the development of leucorrhoea

Unhealthy eating habits and excessive use of tranquilizers or sedative medicines may contribute to leucorrhoea.

• Poor personal hygiene, especially during menstruation, can increase the risk of infection.

• Diseases such as tuberculosis, anemia, gout, arthritis, typhoid, and diabetes may weaken immunity and make infections more likely.

• Urinary tract infections that spread upward may also cause vaginal discharge.

• Inflammation or infection of the uterus can lead to leucorrhoea.

• Bacterial and fungal infections are common causes of abnormal discharge.

• Pregnancy at a very young age may increase the risk of this condition.

• Injury to the vagina, uterus, or cervix may also result in abnormal discharge.

• Allergies or contact dermatitis can cause irritation and discharge.

• Pelvic inflammatory disease (PID) and sexually transmitted diseases (STDs) are important causes of leucorrhoea.

• Infections such as gonorrhea and syphilis may lead to abnormal vaginal discharge.

• Fungal infections, especially yeast infections, can affect the reproductive organs and cause itching and discharge.

• Swelling or sores near the cervix may produce excessive gray-colored discharge that can resemble coagulated blood [6.7.12,14]

Leucorrhea Symptoms

Leucorrhoea commonly causes excessive vaginal discharge along with burning while passing urine and pain in the thighs or calf muscles. The discharge may be white, yellow, red, or dark in color and can sometimes have an unpleasant smell, itching, or irritation.

Other possible symptoms include:

• Lower abdominal or pelvic pain

• Constipation

• Weakness and anemia

• Lower back pain

• Fatigue and discomfort

• Difficulty in breathing

• Headache and dizziness

• Poor digestion and reduced appetite

• Pale appearance

• Frequent urination

• Itching in the genital region

• Painful or difficult urination

• Pain during sexual activity

• Bleeding after intercourse

• Bleeding between menstrual cycles

• Unusual growths around the vaginal area

• Swelling or inflammation of the vagina.[6,7,13,14,]

Pathophysiology

Normal vaginal discharge mainly depends on the level of estrogen hormone in the body. When estrogen levels increase, the glands produce more secretions and the vaginal lining becomes rich in glycogen. The mucus produced by the cervical glands is usually small in amount. The carbohydrates present in the mucus are converted into lactic acid, which helps maintain the normal vaginal environment. When the secretion becomes excessive, it may appear outside the vulva as discharge. Excessive discharge may occur due to:

• Normal physiological changes

• Problems related to the cervix

• Conditions affecting the vagina [5,6,12]

***Oxalis corniculata Linn*. Plant**

Natural resources have played an important role in the development of many modern medicines. Ancient systems of medicine such as Ayurveda and Unani contain valuable knowledge about the use of

medicinal plants. The ancient Indian text Charaka Samhita (around 1000 BC) describes the medicinal use of more than 2,000 herbs. Research on plant chemicals and their pharmacological activities helps in discovering new active compounds from plants. Herbal medicines continue to be important in modern healthcare because many effective and life-saving drugs have been developed from natural sources. [15] Medicinal plants are studied in laboratories around the world because they may contain useful compounds with therapeutic effects. Herbal medicines are often considered safer and to have fewer side effects than synthetic drugs. In traditional Indian medicine, many herbs are used for the treatment of different diseases and health problems. [16,17] Oxalis corniculata is a small herb belonging to the Oxalidaceae family. The word Oxalis originates from the Greek term "Oxys," meaning sour, which refers to the sour taste of the plant. It is a delicate, spreading herb that grows close to the ground and is known for its many medicinal and biological properties. [18] Oxalis corniculata grows commonly in human surroundings such as roadsides, parks, gardens, and courtyards, especially in warm regions of India. It is also found in the Himalayan areas up to an altitude of about 2500 meters. This herb usually grows well in moist and shady places. The plant is widely known in India and is valued for its medicinal importance. It contains several phytonutrients that support normal health and body functions. [19,20]

TAXONOMICAL CLASSIFICATION [21]

Taxonomic Rank	Classification
Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Oxalidales
Family	Oxalidaceae
Genus	Oxalis
Species	corniculata
Botanical Name	*Oxalis corniculata* Linn.

VERNACULAR NAMES [21]

Language	Name
Sanskrit	Ambashta, Amlapatrika, Amlika, Amlotaja, Cangeri
Hindi	Seh-patti, Tinpatiya, Anboti, Bhilmori, Khatari
English	Indian sorrel
Urdu	Khatt-i-buti
Assamese	Changeritenga, Sarutengesi
Bengali	Amrul-sak, Amrulshak, Amrul, Amrool
Kannada	Huli-huniche, Hulihunice, Teltuppi
Tamil	Palaikiri, Puliyarail
Telugu	Ambotikura, Pulichintha, Pallachintha
Marathi	Ambali, Chicha, Umbuti, Ambuti, Bhinsarpati, Ambatachukaa
Malayalam	Poliyarala, Puliyaral, Puliyarala, Pullampurachi

Distributions

Oxalis corniculata Linn.is a herbaceous medicinal plant and it is low in growing habit and fragile. It is widely distributed in roadside, yards, gardens, parks, human settled areas and nearly all warmer parts of India and it grows up to a height of 2500 m of the Himalayas. Throughout the temperate and tropical regions of West Indies, South, Central and North America it is found widely. All over in Florida these

medicinal plants are found, it is a cosmopolitan weed occurs in the old world as well. It is also spread in the eastern seaport town of the United States and in Ontario and Texas states [21,22]

Morphological Descriptions

Oxalis corniculata is a bushy herb that spreads over the ground and forms a mat-like growth pattern. The upper parts of the plant are weakly upright and may appear smooth or slightly hairy. The plant produces many branches from the base, and roots can develop at the nodes where the stem touches the soil. [22]

Leaves:

Oxalis corniculata has trifoliate leaves, meaning each leaf is made up of three small leaflets. The leaves are thin and heart-shaped with a small notch at the tip. They are arranged alternately along the stem, and the leaflets show a reticulate or net-like vein pattern. [22]



Stem: Oxalis corniculata has a thin and slender stem covered with soft, short hairs. The internodes are usually about 5–9 cm long. The plant has a sour taste and gives an acidic smell. [23]

Root: Oxalis corniculata has thin, soft, and branched roots that are dark brown in color. The roots do not have any noticeable smell or taste. [21]



Flowers: Oxalis corniculata produces small flowers that are about 6–12 mm wide and contain five yellow petals. [22]



Fruits: Oxalis corniculata produces capsule-type fruits that are cylindrical, pointed, and ridged in shape. The fruits are usually about 1–1.5 cm long. [24]



Seeds: Oxalis corniculata has oval-shaped seeds that are rounded with a pointed base. The seeds are flat, light brown in color, and have a clearly ridged surface. The plant also produces stolons, which help it spread along the ground [22]



***Oxalis corniculata Linn*. Plant**

Phytochemical Profile

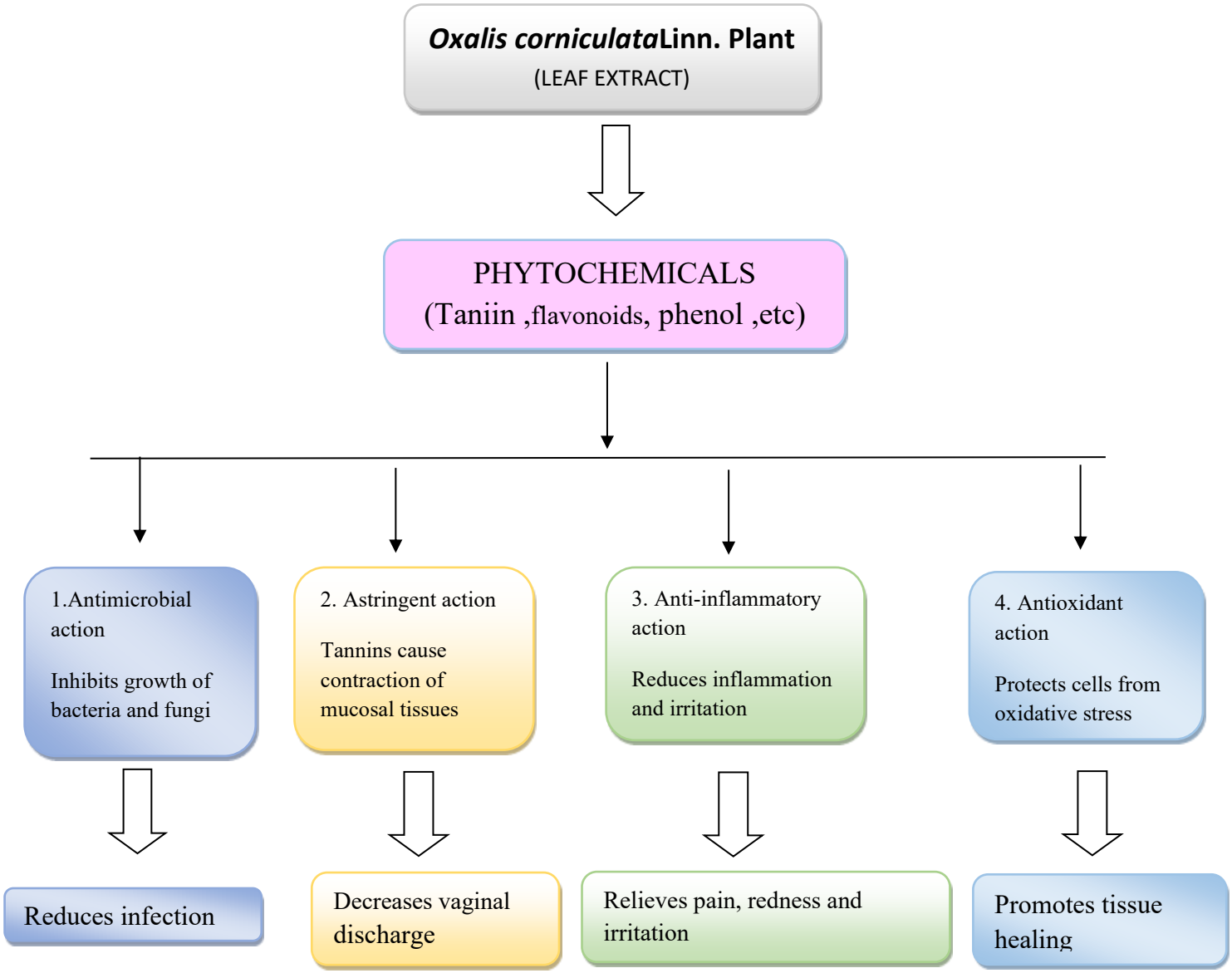
OC contains a rich amount of secondary metabolites. In many studies, water and alcohol extracts prepared from the leaves, roots, and whole plant were analyzed to identify its phytochemical constituents. Liquid–liquid fractionation was commonly used to isolate and purify these bioactive compounds.The plant is also consumed as a food source in different regions of the world, and nutritional studies have shown that it possesses a diverse nutrient composition. One important characteristic of the plant is its ability to survive and grow in saline conditions, tolerating nearly 70–90% salinity levels, which highlights its strong adaptability. In addition, the plant contains high levels of soluble salts and minerals that may provide therapeutic benefits. The total phenolic content was reported as 7.76 mg gallic acid equivalents per serving, while the flavonoid content was measured at 6.92 mg rutin equivalents per serving. [25, 26] OC water extracts were found to contain high levels of tannins, palmitic acid, and fatty acids such as oleic, linoleic, linolenic, and stearic acids. In contrast, alcoholic extracts showed the presence of carbohydrates, glycosides, phytosterols, phenolic compounds, amino acids, and stearic acid. Research studies also reported the presence of calcium, dietary fiber, and tannins in the plant.The plant is rich in bioactive compounds including flavones, flavonoids, volatile oils, and proteins associated with organic acids. The leaves specifically contain flavones, flavanols, and phenolic acids such as syringic acid and p-hydroxybenzoic acid. Organic acids including tartaric acid and citric acid have also been identified.Nutritional analysis revealed that the plant contains approximately 86.8% water, 0.8 g fat, and 8.2% carbohydrates. It also provides important minerals and nutrients, including 150 mg calcium, 78 mg phosphorus, 8 mg iron, and 6,050 µg beta carotene. However, the plant contains about 7–12% oxalates, which may contribute to the formation of kidney stones when consumed in excess. [27,28,29] OC contains several important phytochemicals and flavonoid compounds. Researchers isolated a novel flavonoid glucoside known as corniculatin A from the ethyl acetate–soluble fraction of the whole plant. Other compounds identified from the plant include luteolin, luteolin-7-O-β-D-glucoside, and sitosterol-3-O-β-D-glucoside. Studies by Zeb A and Imran M also reported the presence of kaempferol-3-sophorotrioside, quercetin-3-(caffeoyldiglucoside)-7-glucoside, isorhamnetin-3-caffeoyl-7-glucoside, and p-coumaric acid in the plant. The stems and leaves are rich sources of citric acid and tartaric acid, while the stem additionally contains malic acid. Different parts of the plant also provide vitamin C and carotene, contributing to their nutritional value. The plant is naturally rich in oxalates, and the acidic taste of the leaves and stems is mainly due to the presence of these acidic phytochemical compounds. [31,32]

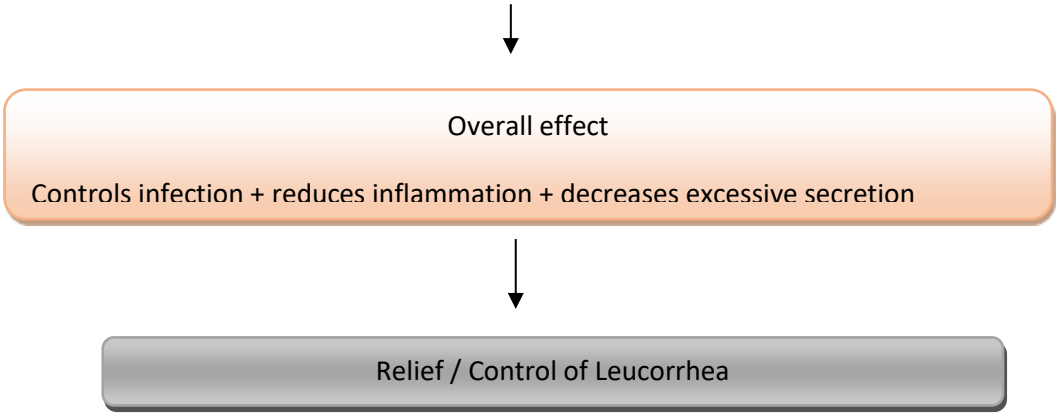
Lanosterol 14α-demethylase (CYP51)

Lanosterol 14α-demethylase, also known as CYP51, P45014DM, or Erg11, belongs to the cytochrome P450 superfamily of enzymes. It plays an important role in ergosterol biosynthesis by catalyzing the oxidative removal of the 14α-methyl group (C-32) from lanosterol. This reaction produces Δ14,15-desaturated intermediates that are essential for the formation of ergosterol, a major component of fungal cell membranes. [33] . During the catalytic cycle of Lanosterol 14α-demethylase, the substrate undergoes three sequential monooxygenation reactions. These reactions lead to the formation of 14-hydroxymethyl, 14-carboxaldehyde, and 14-formyl intermediates. Subsequently, formic acid is eliminated, accompanied by the formation of a double bond between carbon atoms C-14 and C-15.CYP51 is considered one of the essential enzymes involved in sterol biosynthesis across various biological kingdoms, including fungi, higher plants, and mammals. Despite differences among organisms, the enzyme performs common metabolic function, which is the removal of the 14-methyl group from sterol precursors such as lanosterol during sterol synthesis. [35] Lanosterol 14α-demethylase is part of the cytochrome P450 family of monooxygenase enzymes. Its primary function is to remove the 14-methyl group (C-32) from lanosterol through an oxidative reaction, producing 14,15-desaturated compounds that are required for ergosterol formation in fungi.The enzyme has a major role in sterol biosynthesis and is important in many living organisms. Sterols produced through this pathway help maintain cell membrane structure and function. They contribute to membrane permeability and fluidity, support enzyme activity, help preserve

cell shape, and assist in regulating the cell cycle and cellular growth. [36,37]

Lanosterol 14α-demethylase is present in all eukaryotic organisms, including humans. Azole compounds target this enzyme to inhibit sterol biosynthesis, particularly in fungi. However, azoles may also affect other cytochrome P450-dependent enzymes such as CYP3A4. Therefore, selective inhibition of CYP51 is important to achieve better therapeutic effectiveness while minimizing unwanted side effects and improving the therapeutic index. [38,39] , The interaction of azole antifungal agents with Lanosterol 14α-demethylase depends on both hydrophilic and hydrophobic interactions within the enzyme's active site. The binding strength is mainly influenced by the coordination between the nitrogen atom of the azole ring and the heme iron present in the active center of CYP51. In triazoles, the N-4 nitrogen participates in this interaction, whereas in imidazoles the N-3 nitrogen is involved. In addition, the N-1 substituent of the azole compound interacts with the apoprotein region of the enzyme. The remaining portion of the antifungal molecule fits into the hydrophobic groove of CYP51 in a manner similar to the natural substrate, lanosterol, which enhances binding affinity and antifungal activity. 1,2,4-Triazine and its derivatives are important heterocyclic compounds widely recognized for their diverse pharmacological properties. These compounds serve as a common structural framework in many biologically active molecules and have demonstrated significant antifungal and antibacterial activities along with other therapeutic applications.[42]





DRUG DISCOVERY STUDIO

The development of modern computational software and bioinformatics tools has greatly simplified the process of drug discovery and development. Computer-assisted methods are widely used for virtual screening, structure-based drug design, ligand-based drug design, and lead optimization. These approaches help researchers identify and modify potential drug candidates more efficiently and accurately.Several computational platforms are also available to evaluate structural affinity and optimize physicochemical properties, which contribute to improving drug efficacy, selectivity, and safety. Modern drug discovery integrates multiple scientific approaches, including combinatorial chemistry, molecular biology, high-throughput screening, and studies related to absorption, distribution, metabolism, and excretion (ADME). Together, these interconnected techniques support the identification and development of effective therapeutic agents. [43,44]

PyRx software

PyRx is a user-friendly and multi-platform computational tool commonly used in drug discovery and molecular docking studies. It integrates several open-source applications, including Auto Dock Vina, Auto Dock, and Open Babel, allowing smooth performance of database-based virtual screening (DBVS).The software helps researchers identify potential bioactive compounds for further laboratory evaluation. Using PyRx, database compounds can be screened efficiently against specific biological targets such as Vps34, an important autophagy-related protein. Step-by-step virtual screening procedures with PyRx assist in selecting promising molecules for experimental drug development studies. [45]

Protein Data Bank

Protein Data Bank is a global repository that stores experimentally determined three-dimensional structures of biological macromolecules at the atomic level. These macromolecules include proteins, DNA, and RNA, which are essential for understanding biological processes and drug interactions. The PDB archive is maintained and managed by the Worldwide Protein Data Bank, an international organization responsible for collecting, validating, and distributing structural biology data to researchers worldwide.

Pub Chem

It including Substance, Compound, BioAssay, Protein, Gene, Pathway, Cell Line, Taxonomy and Patent. Substance archives chemical descriptions submitted by individual data depositors and Compound stores unique chemical structures extracted from Substance through chemical structure standardization

Autodock is a molecular modeling simulation software. It is effective for protein- ligand docking. Autogrid for pre- calculating grids around the active site. Autodock is for docking of the ligand into the grids describing the target active site

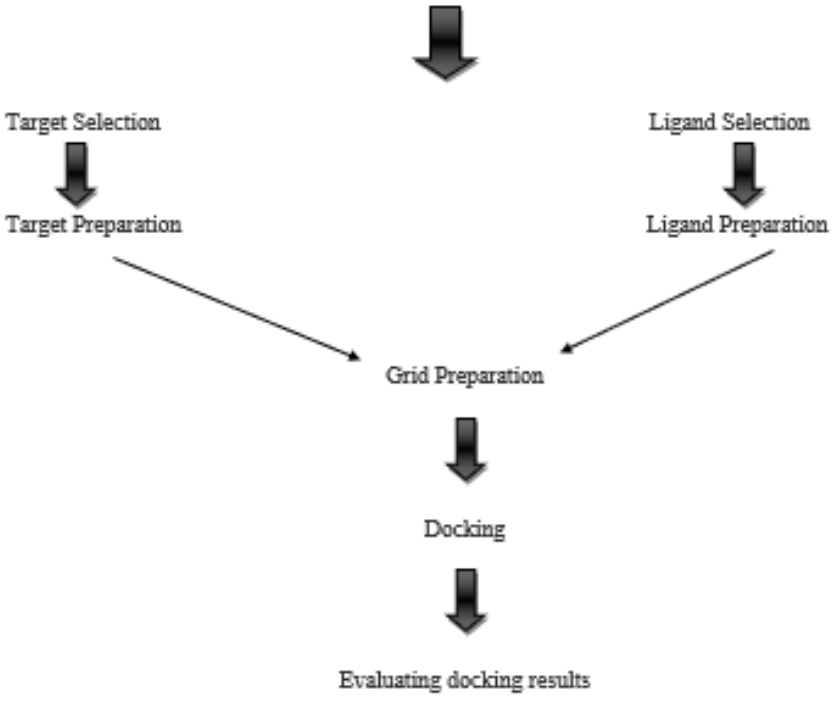
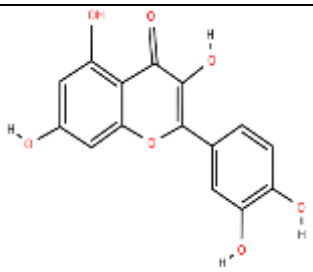
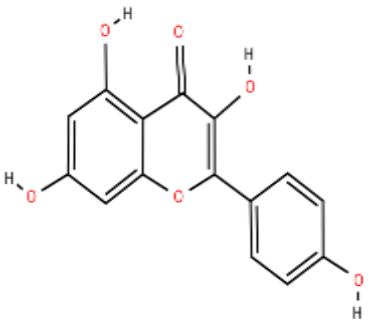
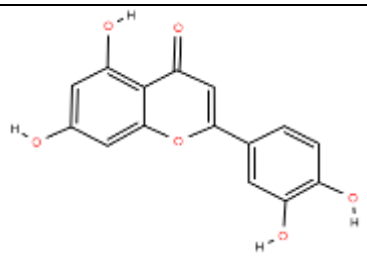
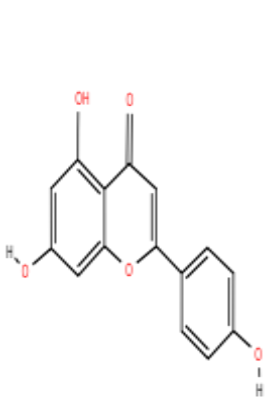
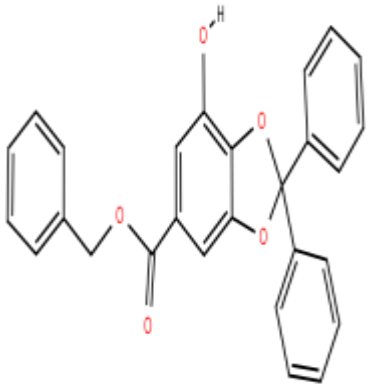
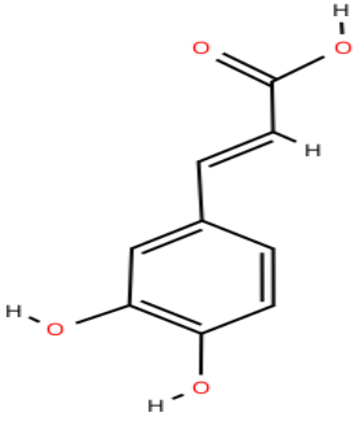
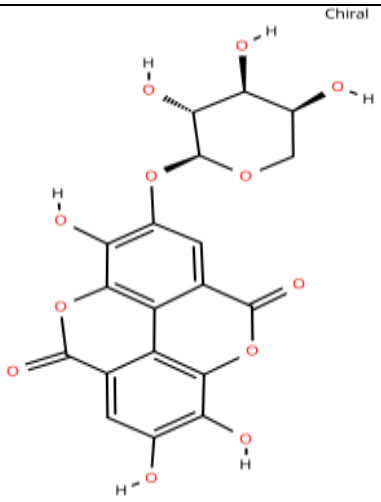
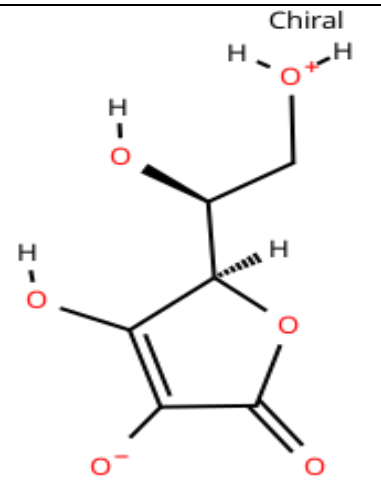
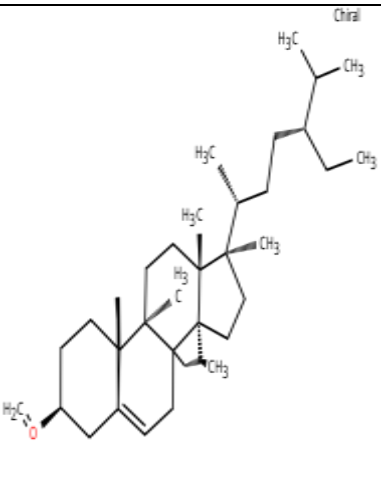


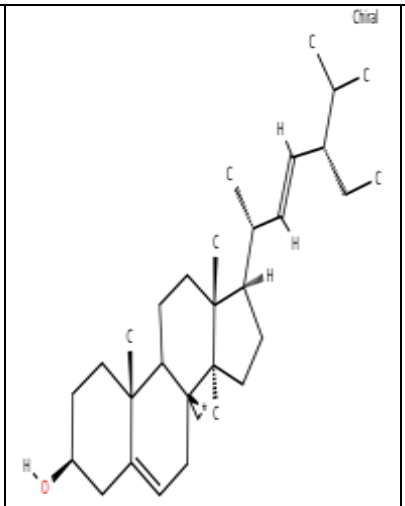
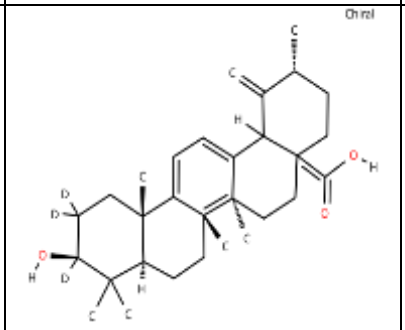
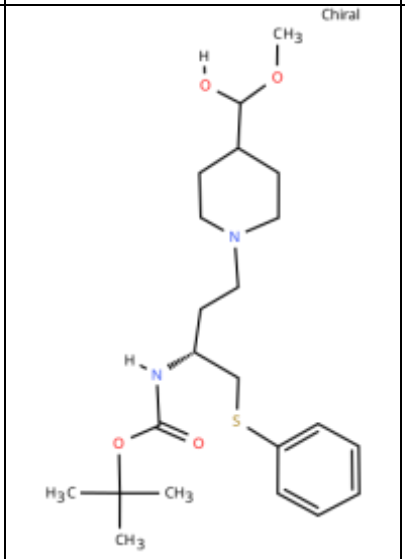
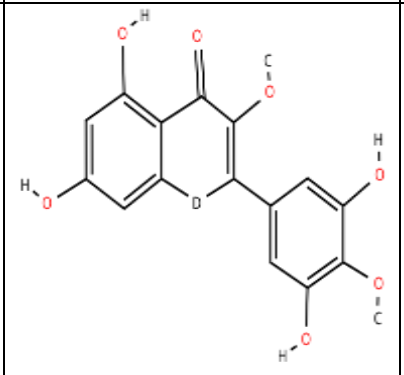
Fig docking procedure chart

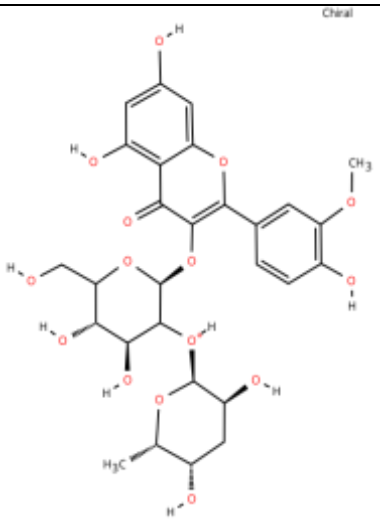
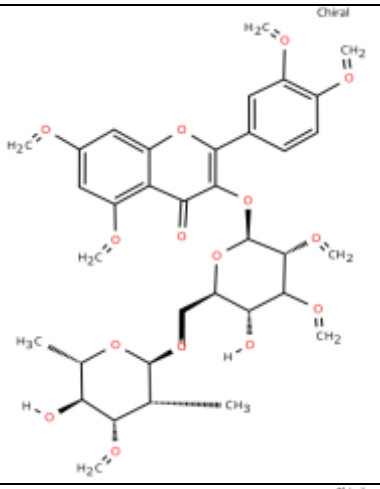
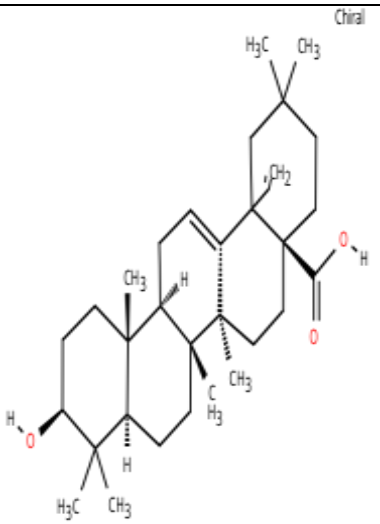
Binding Affinity of phytoconstituent against target receptor

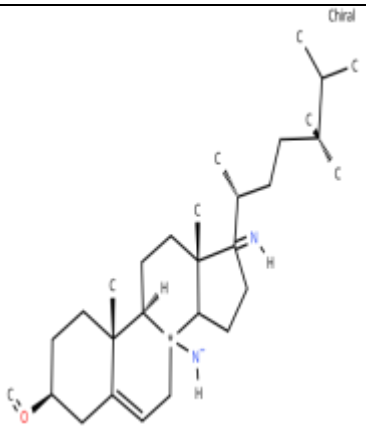
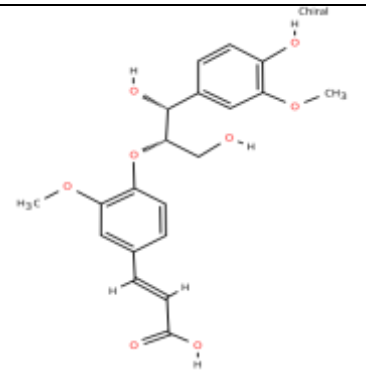
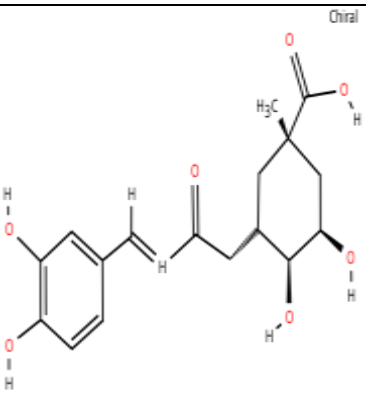
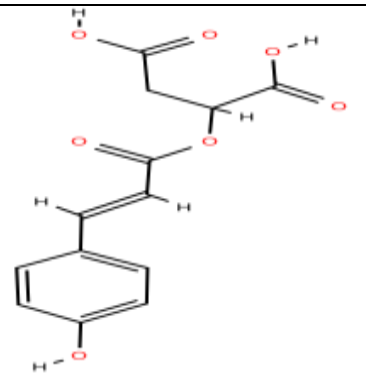
Phytoconstituents name	Structure of phytoconstituents	CID NO of phytoconstituents	Affinity of phytoconstituents
Quercetin		5280343	**-10.2**
Kaempferol		5280863	**-8.1**

Luteolin		5280445	**-10.5**
Apigenin		5280443	**-9.3**
Gallic acid		370	**-7.9**
Caffeic acid		689043	**-7.6**

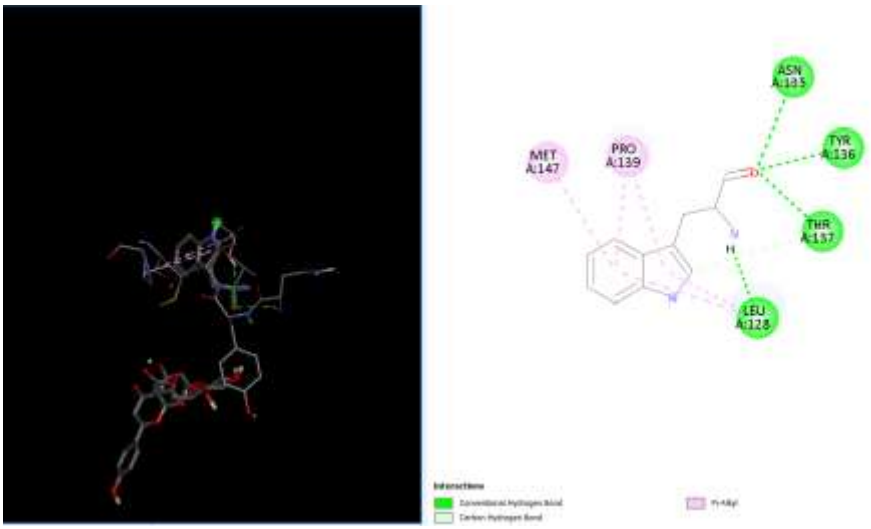
Ellagic acid		5281855	**-9.7**
Ascorbic acid		54670067	**-5.9**
β-Sitosterol		222284	**-7.6**

Stigmasterol		5280794	**-7.4**
Ursolic acid		64945	**-8.6**
Oxalic acid		971	**-5.5**
Myricetin		5281672	**-7.7**

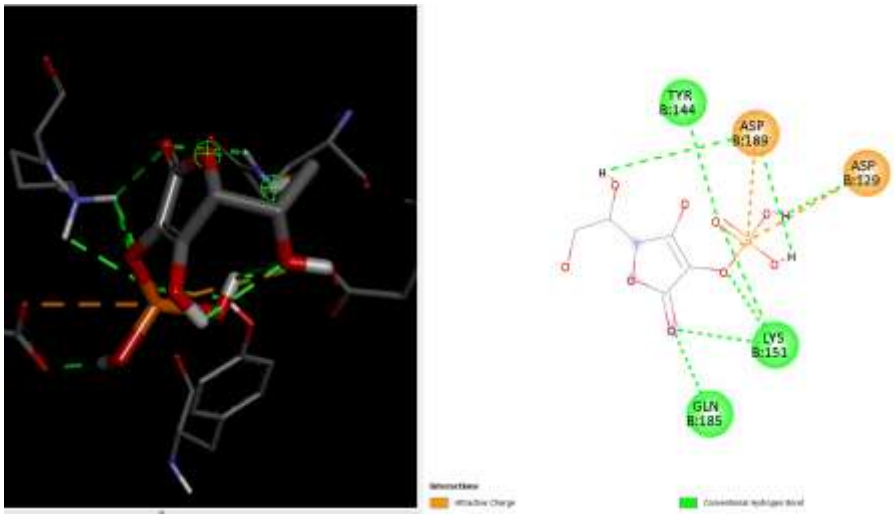
Isorhamnetin		5281654	**-9.1**
Rutin		5280805	**-9.3**
Oleanolic acid		10494	**-7.6**

Campesterol		173183	**-7.6**
Ferulic acid		445858	**-7.5**
chlorogenic acid		1794427	**-7.7**
p-Coumaric acid		637542	**-6.2**

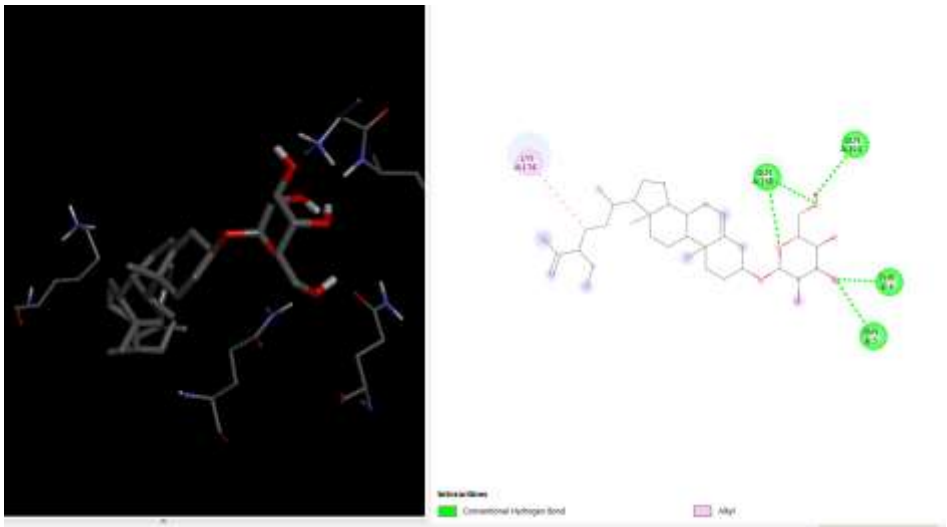
2D and 3D binding Interaction



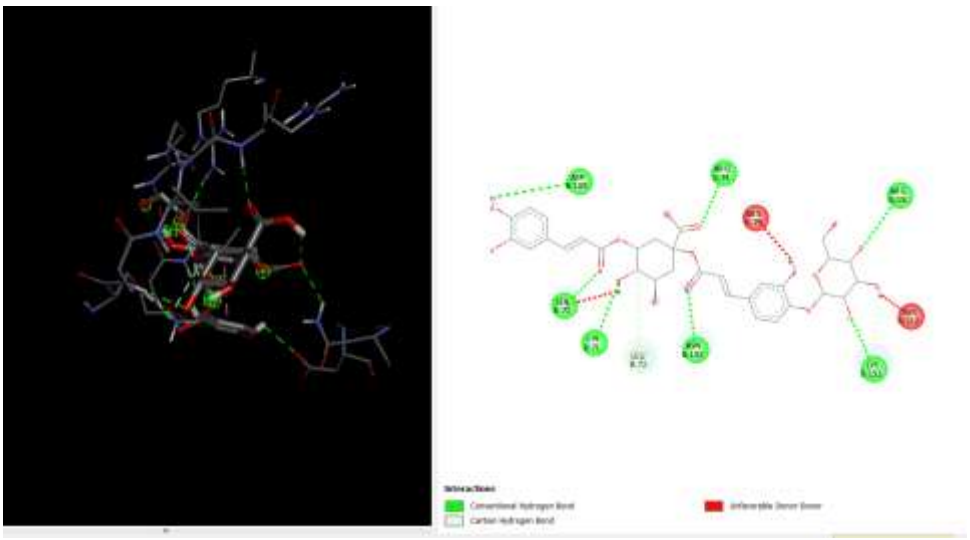
1. Apigenin



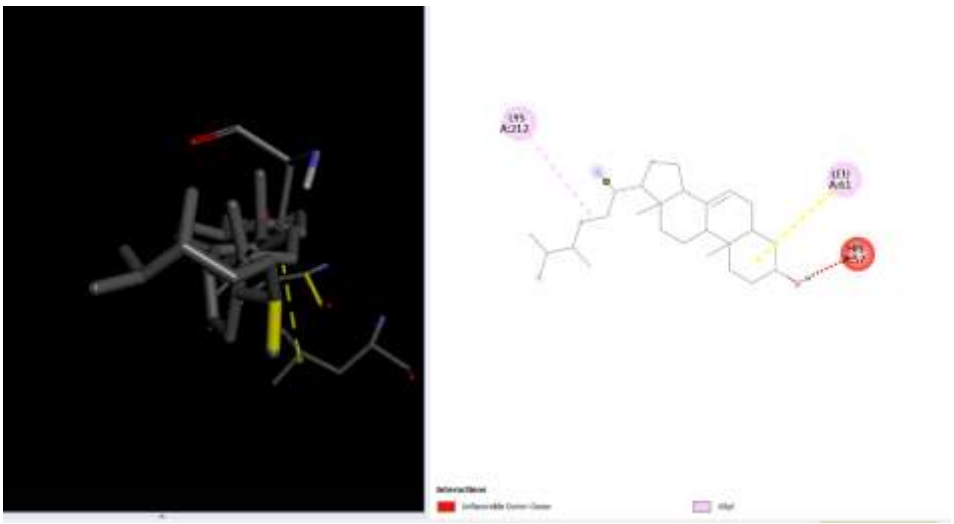
2.Ascorbic Acid



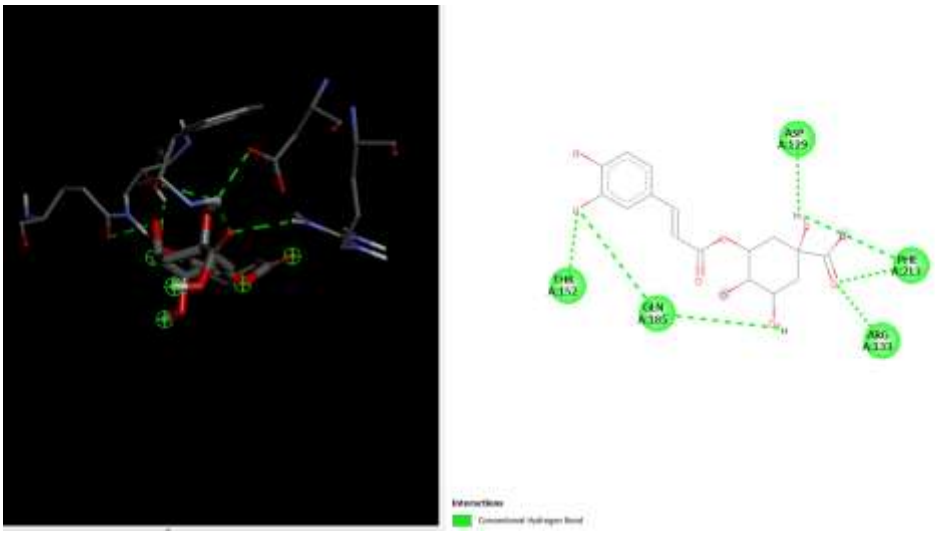
3.β-Sitosterol



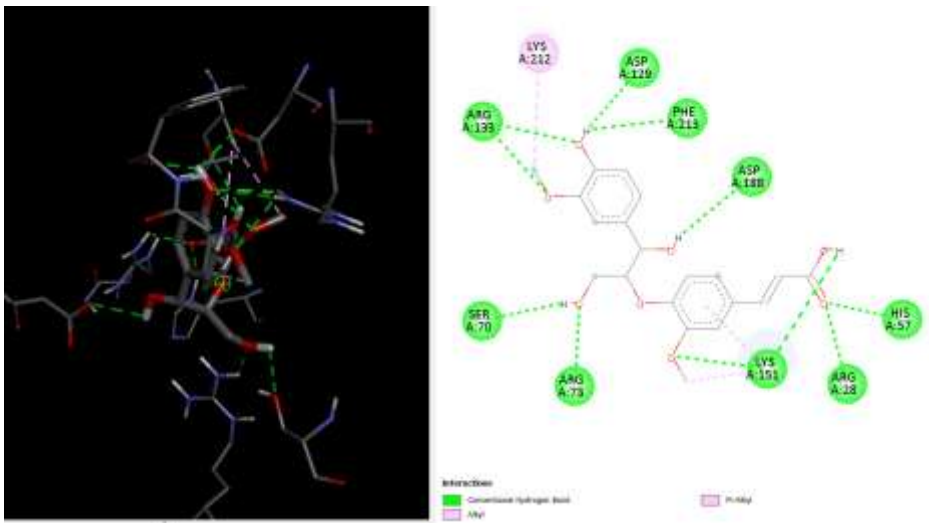
4.Caffeic acid



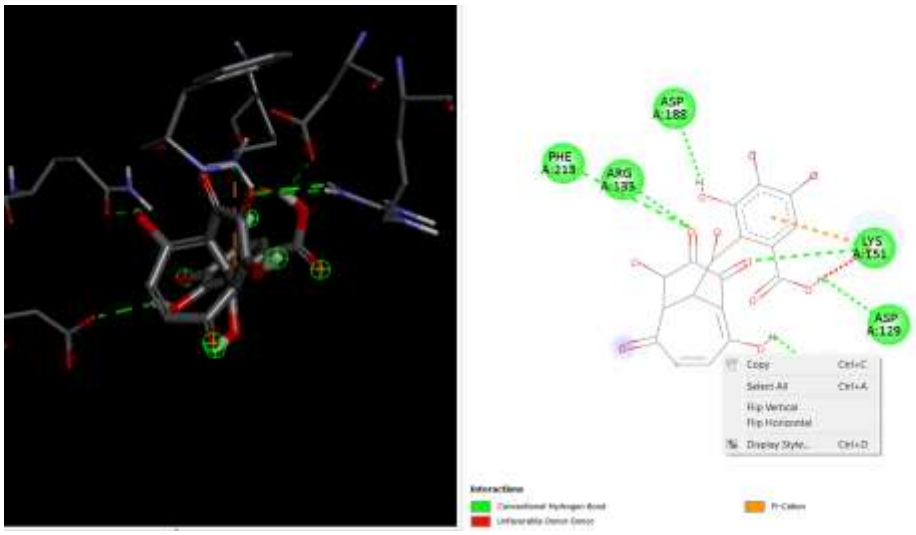
5.Campesterol



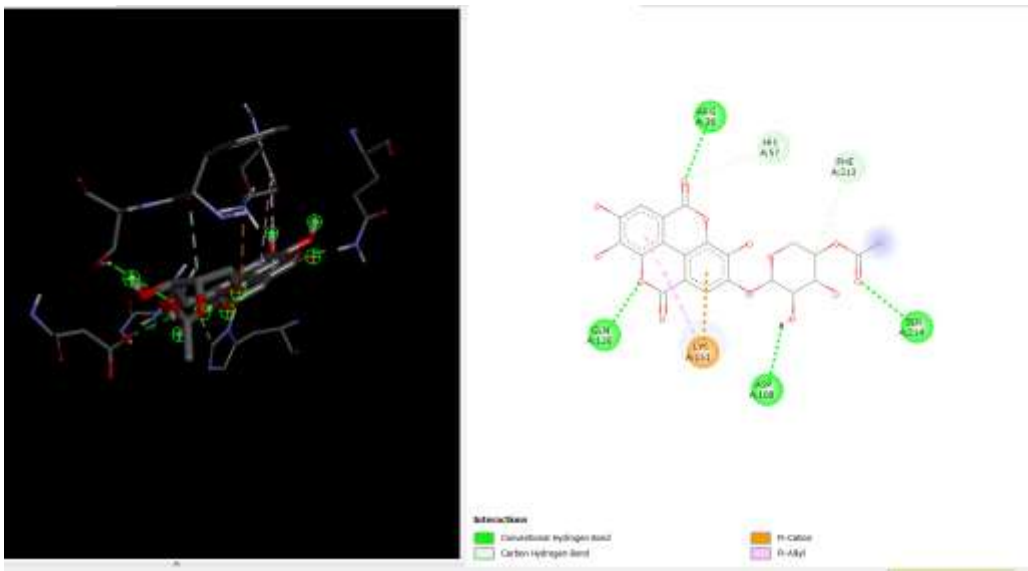
6.Chlorogenic acid



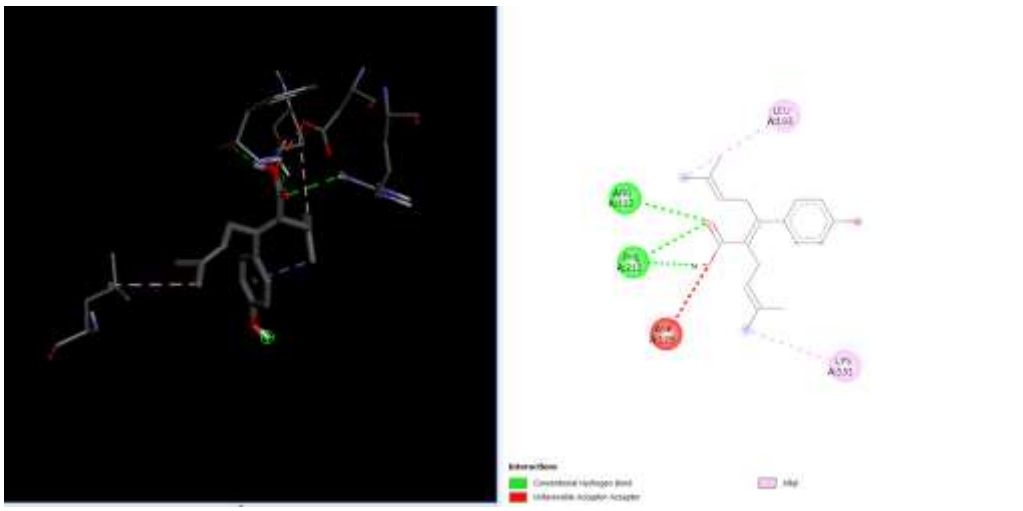
7. Ferulic acid



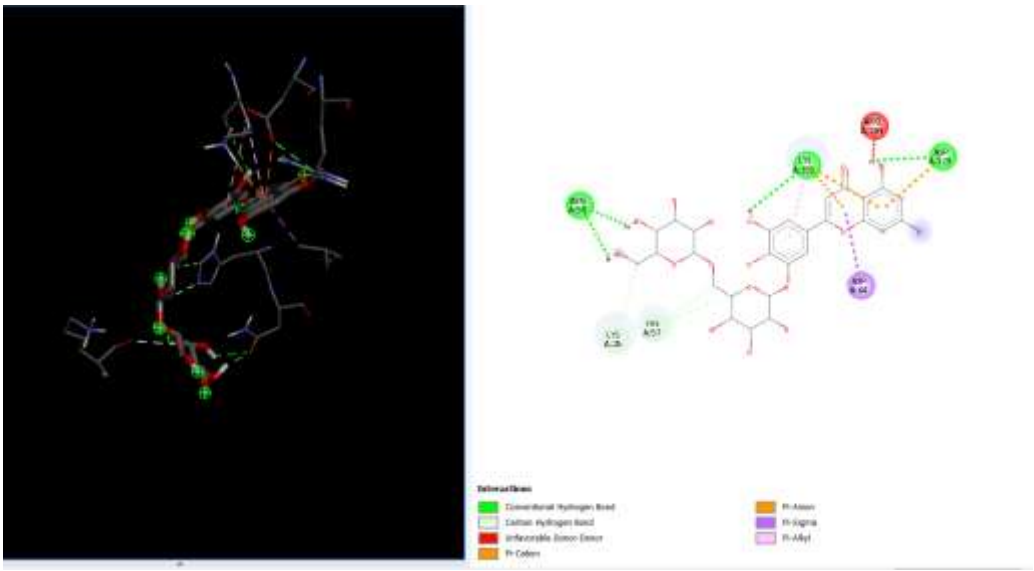
8. Gallic acid



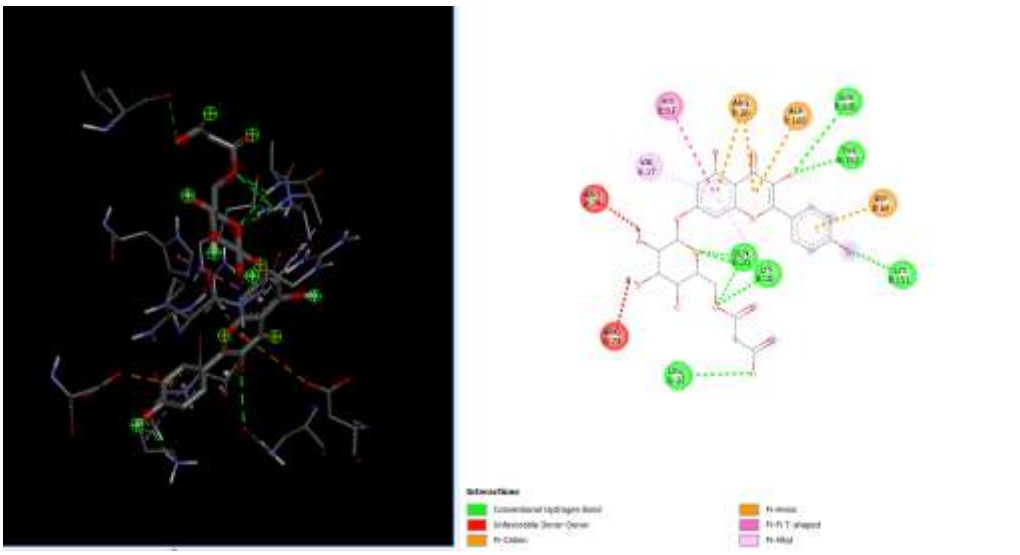
9.Ellagic acid



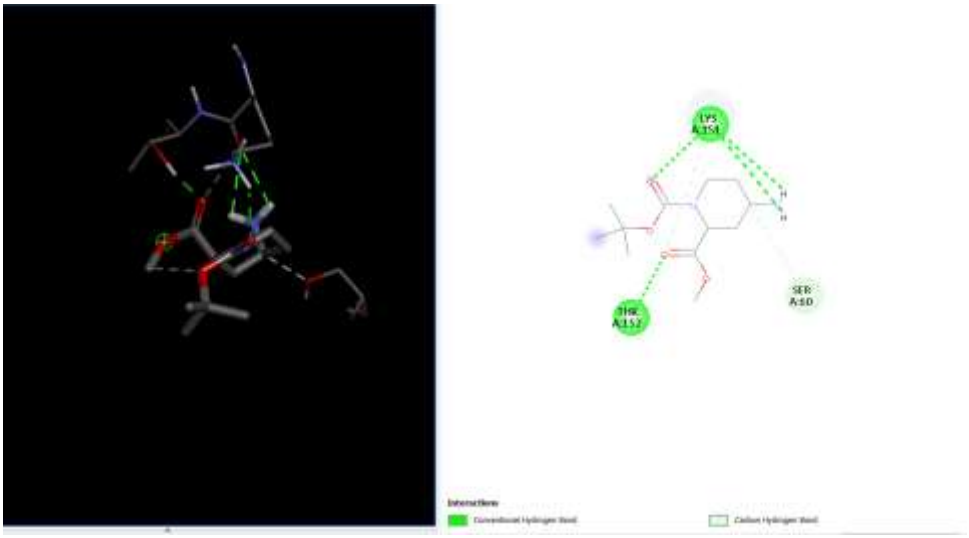
10. p-Coumaric acid



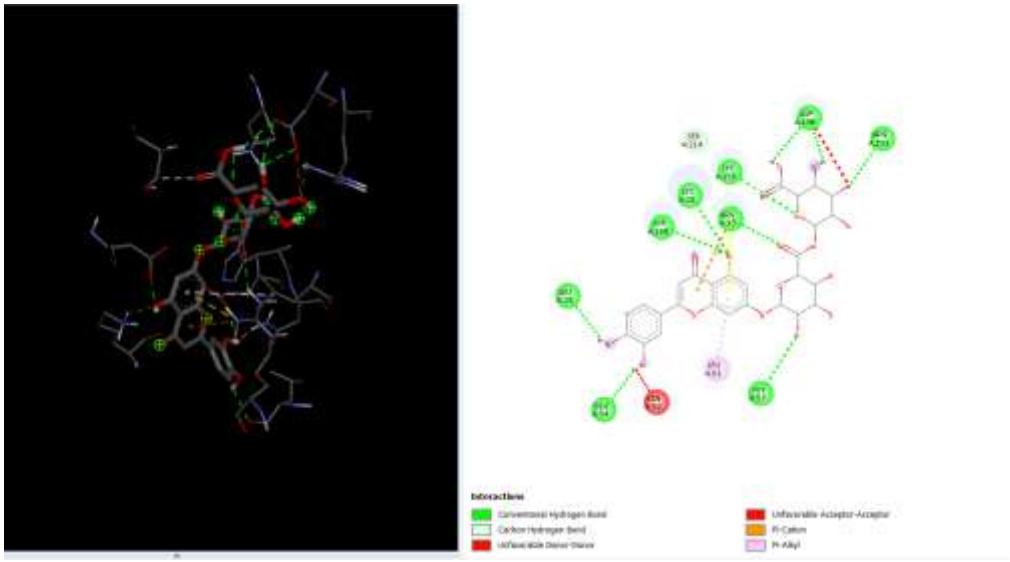
11.Quercetin



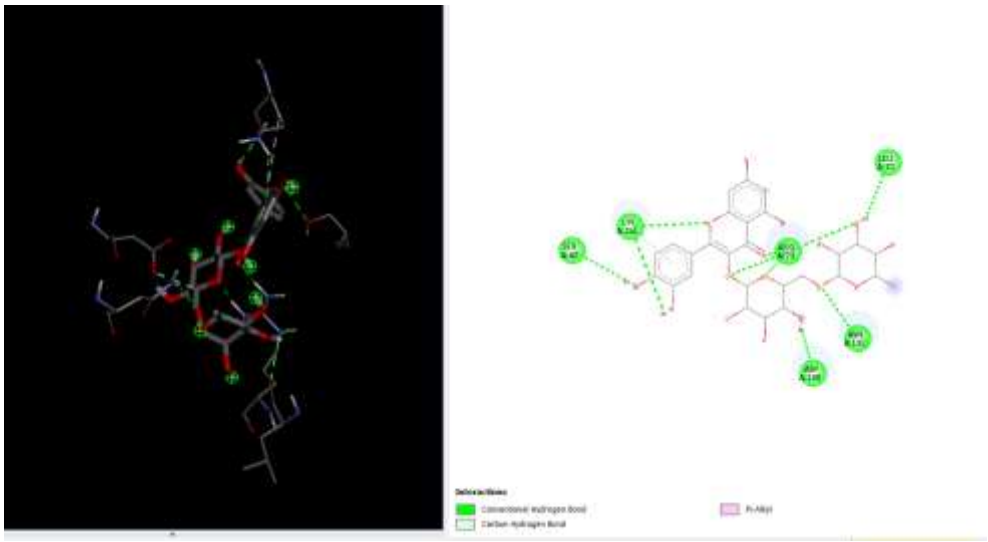
12. Kaempferol



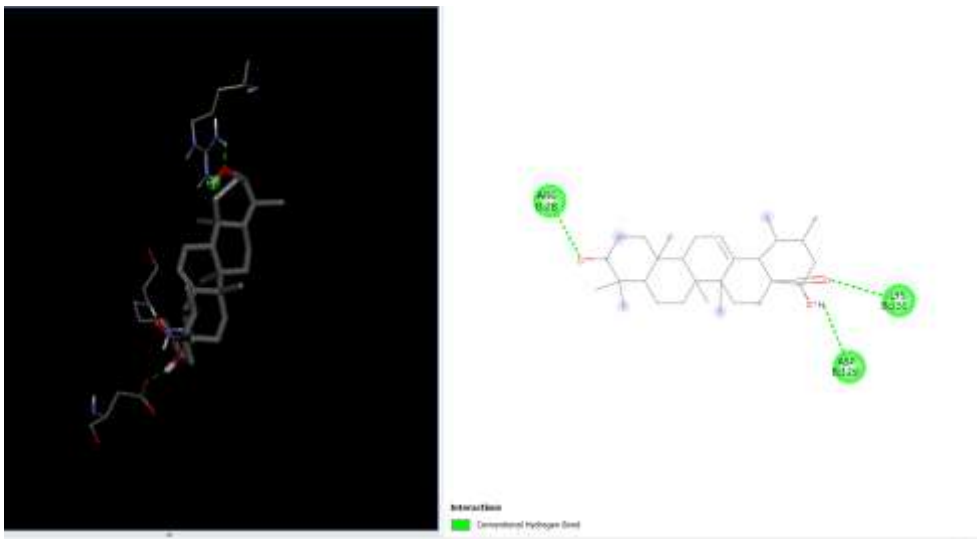
13.Oxalic acid



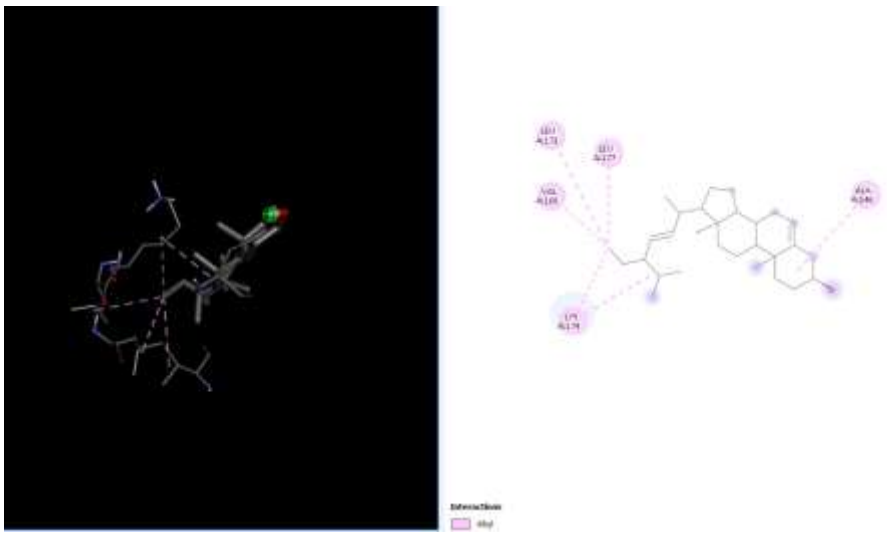
14.Luteolin



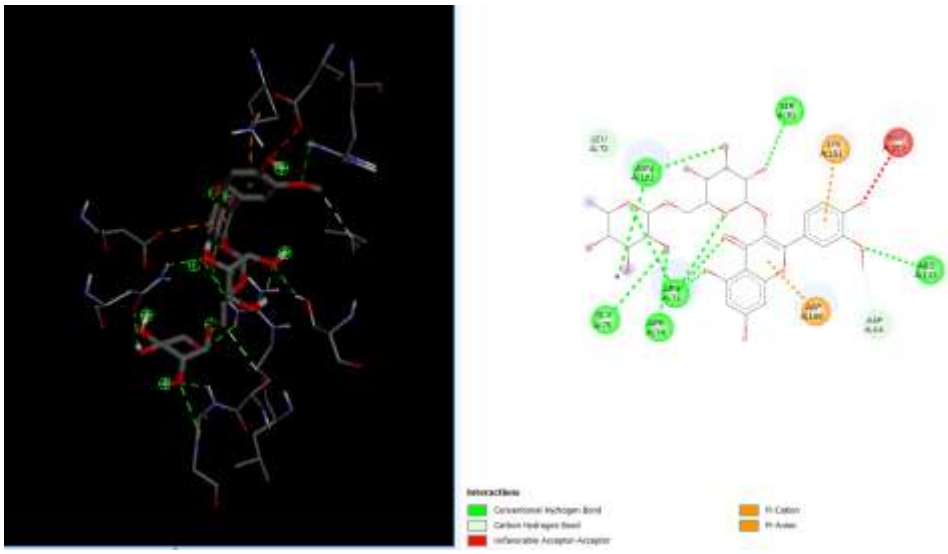
15.Rutin



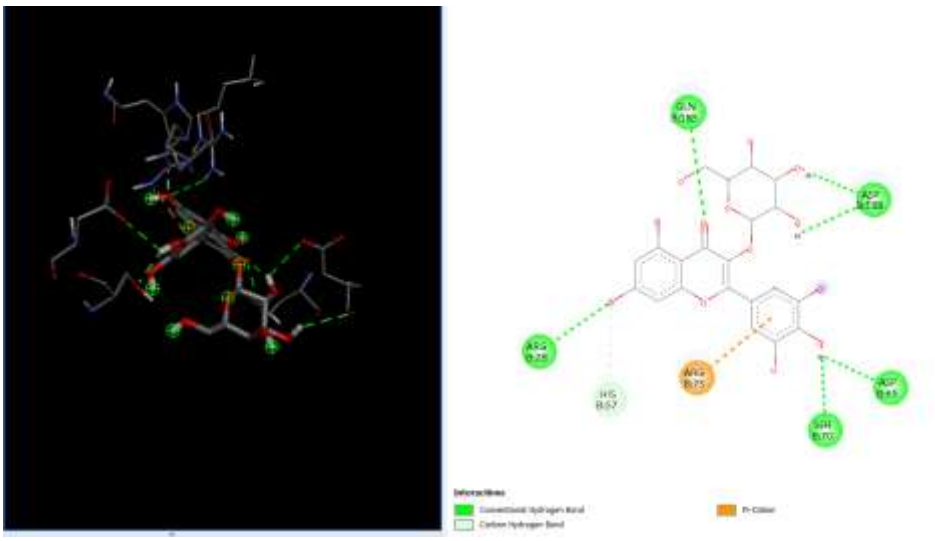
16.Ursolic acid



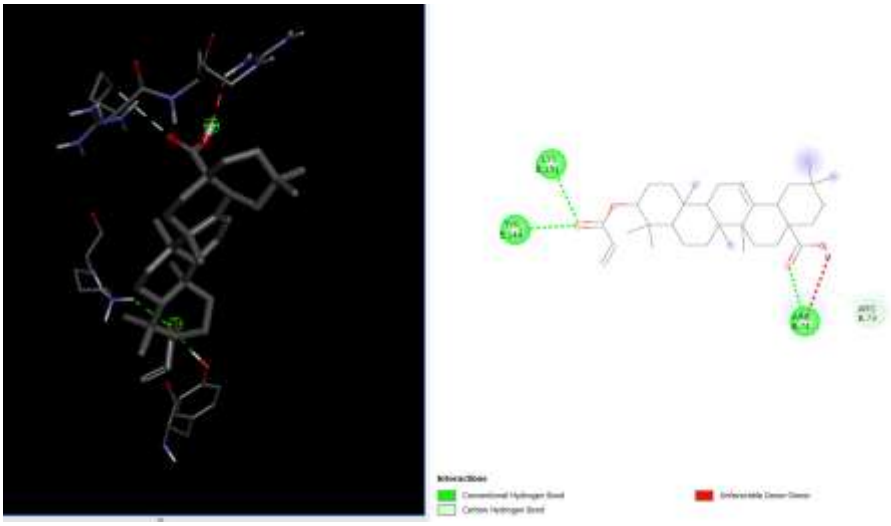
17.Stigmasterol



18. Isorhamnetin



19.Myricetin



20.Oleanolic acid

ADMET STUDY

Compound Name	MW (Da)	MLogP	HBA(H-Bond Acceptors)	HBD(H-Bond Donors)	MR(Molar Refractivity)	Lipinski Violations	Lipinski Result
Quercetin	302.24	1.5	7	5	74.0	0	Passed
Kaempferol	286.24	1.9	6	4	72.4	0	Passed
Luteolin	286.24	2.1	6	4	72.0	0	Passed
Apigenin	270.24	2.5	5	3	70.0	0	Passed
Gallic acid	170.12	0.7	5	4	33.5	0	Passed
Caffeic acid	180.16	1.2	4	3	45.2	0	Passed
Ellagic acid	302.19	1.3	8	4	71.3	0	Passed
Ascorbic acid	176.12	-1.8	6	4	33.2	0	Passed
β-Sitosterol	414.71	8.0	1	1	131.2	1	Failed
Stigmasterol	412.69	7.8	1	1	129.8	1	Failed
Ursolic acid	456.70	6.4	3	2	124.5	1	Failed

Oxalic acid	90.03	-0.8	4	2	13.3	0	Passed
Myricetin	318.24	1.2	8	6	75.5	1	Failed
Isorhamnetin	316.26	2.3	7	4	78.0	0	Passed
Rutin	610.52	-1.3	16	10	135.0	3	Failed
Oleanolic acid	456.70	6.2	3	2	123.7	1	Failed
Campesterol	400.68	7.1	1	1	126.4	1	Failed
Ferulic acid	194.18	1.5	4	2	49.8	0	Passed
Chlorogenic acid	354.31	-0.4	9	6	82.6	1	Failed
p-Coumaric acid	164.16	1.4	3	2	42.1	0	Passed

BINDING INTERACTION OF PHYTOCONSTITUENTS

Sr no	Phytoconstituent name	Interacting Residue	Interaction Type
1	Quercetin	ASN A 58 ,LYS A 25 ,HIS A 57 , LYS A 151 , ASP A 64 ,ASP A 129 ARG A 133 LYS A 151	Conventional hydrogen bond, pi alkyl , Carbon hydrogen bond , pi cation , pi anion , pi sigma , pi alkyl
2	Kaempferol	ARG B 74, ARG B 73 LEU B 20, LYS B 25 , GLN B 26 , LYS B 151 , ASP B 64 , THR B 152 , GLN B 185 , ASP B 188 , ARG B 28 HIS B 57 , VAL B 27	Conventional hydrogen bond , unfavorable donor donor , pi cation , pi anion ,pi pi T – shaped , pi alkyl
3	Luteolin	LEU A 20 , GLU A 54 ASN A 58 , LEU A 61 , HIS A 57 ARG A 133 ,ASP A 129 , LYS A51 , ARG A 73 ,SER A 214 , LYS A 25 ,ASP A 188	Conventional hydrogen bond , Carbon hydrogen bon unfavorable donor donor , pi alkyl , pi cation , unfavorable acceptor acceptor
4	Apigenin	MET A147 , PRO A 139 , ASN A135 ,TRY A136 ,THR A137 , LEU A128	Conventional hydrogen bond, pi alkyl , Carbon hydrogen bond
5	Gallic acid	PHE A 213 , ARG A 133 , ASP A 188 ,LYS A 151 ,ASP A 129	Conventional hydrogen bond , unfavorable donor , pi cation
6	Caffeic acid	ASP B 189 ,SER B 70 ,LYS B 71 , LEU B 72 , ASN B 192 ,LYS B 151 , THR B 152, ARG B 28 , ARG B 73	Conventional hydrogen bond , Carbon hydrogen bond, unfavorable donor donor
7	Ellagic acid	ARG A28, GLN A126,LYS A151ASP A 188,SER A 214 ,PHE A 213 , HIS 57	Conventional hydrogen bond, pi alkyl , Carbon hydrogen bond , pi cation
8	Ascorbic acid	TYR B 144 ,ASP B 189 , ASP B 129 , LYS B 151 ,GLN B 185	Attractive charge , Conventional hydrogen bond
9	β-Sitosterol	LYS A174 ,GLN A 150 ,GLN A124 , THR B 4 , GLN B 5	Conventional hydrogen bond , alky

10	Stigmasterol	LEUA 173 , VAL A 160 , LYS A 174 , LEU A 177 , ALA A 146	Alky l
11	Ursolic acid	ARG B 28 , ASP B 129 , LYS B 151	Conventional hydrogen bond
12	Oxalic acid	THR A 152 , LYS A 151 SER A 60	Conventional hydrogen bond , Carbon hydrogen bond
13	Myricetin	ARG B 28 , HIS B 57 , ARG B 73 , SER B 70 , ASP B 70 ,ASP B 65 ,ASP B 188 ,GLN B 185	Conventional hydrogen bond , Carbon hydrogen bond, pi cation
14	Isorhamnetin	GLY A 75 , ARG A 74 , ARG A73 , ASP A 188 , ASP A 64 ARG A 133 , ASP A 129 , LYS A 151 ,SER A 70 , ASN A 192 , LEU A 72	Conventional hydrogen bond , Carbon hydrogen bond, unfavorable acceptor acceptor , pi cation, pi anion
15	Rutin	SER A60 , LYS A 151 , ARG A 73 ,ASP A 188 ,ASN A 192 , ARG A 73 , LEU A 72	Convent Carbon hydrogen bond, pi alkyl
16	Oleanolic acid	TYR B 144 , LYSB 151 ,ARG B 74 , ARG B 73	Conventional hydrogen bond , Carbon hydrogen bond, unfavorable donor donor
17	Campesterol	LYS A 212 ,LEU A 61,HIS A 57	unfavorable donor donor , alky , pi alkyl
18	Ferulic acid	SER A70 , ARG A 73 , LYS A 151 , ARG A 28 ,HIS A57 ,ASP A 188 , PHE A 213 , ASP A 129 , LYS A212ARG A 133	Conventional hydrogen bond , alky
19	Chlorogenic acid	THR A152 , GLN A 185 , ARG A 133 , PHE A 213 ,ASP A 129	Conventional hydrogen bond
20	p-Coumaric acid	ARG A 133 , PHE A 213 , ASP A 129 , LYS A 151 , LEU A 193	Conventional hydrogen bond, unfavorable acceptor acceptor , alky

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