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"Docking Simulations and Phytochemical Study of Echinacea as an Antimicrobial Agent"

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ABSTRACT: -

Introduction The growth in antimicrobial resistance has fueled the hunt for innovative plant-based medicinal medicines. Echinacea purpurea, a popular medicinal herb, is recognized for its immunomodulatory and antibacterial effects. The purpose of this work was to assess the antibacterial activity of ethanolic extracts of Echinacea purpurea, identify its main phytochemical ingredients, and examine the molecular interactions of its bioactive chemicals using in silico docking analysis. Methodologically, the plant material was extracted with ethanol via Soxhlet. The agar well diffusion method was used to investigate antibiotic efficacy against a variety of microbiological species, including Staphylococcus aureus, Escherichia coli, Pseudomonas aeruginosa, and Candida albicans. Phytochemical screening showed the existence of flavonoids and terpenoids, as seen by distinct color changes in the Shinoda and Salkowski tests, respectively. According to the literature study, significant secondary metabolites include quercetin, kaempferol, luteolin, echinacoside, and cynarin. SwissDock was used to conduct molecular docking simulations targeting microbial protein 1KZN in order to determine the binding affinity and interaction stability of the chosen flavonoid, quercetin. The results showed that the ethanolic extract had moderate antibacterial activity, with the maximum zone of inhibition against Staphylococcus aureus (13 mm at 50 mg/mL). Docking experiments revealed that quercetin binds firmly to the target protein's active site. Cluster 0, Member 1 had the most stable binding, with a SwissParam score of -7.9313 kcal/mol and an AC score of -1.5921, indicating a very positive interaction. Conclusion, the antimicrobial effect of Echinacea purpurea appears to be linked to its flavonoid and terpenoid content. Quercetin's strong docking contacts support its function as a promising lead chemical in antibacterial medication development. This integrative approach combining experimental and computational analysis reinforces the therapeutic relevance of Echinacea purpurea and paves the way for further biological validation and pharmaceutical exploration.

Keywords: -*Echinacea purpurea*, Antimicrobial activity, Phytochemicals, Flavonoids, Terpenoids, Quercetin, Molecular docking, Swiss Dock, Secondary metabolites, DNA gyrase inhibition

Introduction

The growing challenge of antimicrobial resistance (AMR) has become a severe public health concern around the world, reducing the effectiveness of traditional antibiotics and necessitating the urgent identification of innovative therapeutic agents [1]. Medicinal plants have emerged as attractive sources of novel antimicrobial chemicals due to their structural variety and long-standing ethnopharmacological importance [2]. *Echinacea purpurea*, sometimes known as purple coneflower, has gained interest for its immunostimulant and antibacterial properties [3].

Phytochemical screening is an important first step in determining the bioactive elements that contribute to medicinal plants' therapeutic performance. *Echinacea purpurea* has a diverse range of secondary metabolites, including phenolic acids (such as cichoric and caftaric acid), flavonoids, alkamides, and polysaccharides, all of which are linked to its pharmacological characteristics [4]. These chemicals have been found to have antibacterial, antiviral, antifungal, and antioxidant properties [5].

Antimicrobial Agents

An antimicrobial agent is one that either kills or inhibits the growth of bacteria. Antimicrobial medications can be classified according to the type of microbes they target. Antibiotics are used to treat bacterial infections, while antifungal agents are employed against fungal infections. Additionally, they may be classified based on their purpose—antimicrobial chemotherapy is used to treat active infections, whereas antimicrobial prophylaxis aims to prevent infections [6].

There are three main types of antimicrobial agents: disinfectants, antiseptics, and antibiotics. Disinfectants, such as bleach, are non-selective agents that kill a wide range of microbes on surfaces to prevent the spread of disease. Antiseptics are applied to living tissue to minimize infection, particularly during surgical procedures. Antibiotics, initially defined as substances derived from living organisms such as bacteria or fungi, now include synthetic agents like sulfonamides and fluoroquinolones [7]. Although the term “antibiotic” originally referred only to antibacterials, its scope has broadened over time to include all classes of antimicrobial drugs.

They are classed as antibiotics, antifungals, antivirals, and antiparasitics based on the pathogen they target [8]. The principal modes of action include cell wall disintegration, protein synthesis inhibition, and nucleic acid replication interference [9].

Overuse and misuse of antimicrobial drugs in human, animal, and agricultural settings has resulted in the evolution of antimicrobial resistance (AMR), which poses a severe worldwide health concern. According to the World Health Organization [10], AMR undermines efficient prevention and treatment of diseases caused by resistant bacteria, resulting in millions of deaths each year. As a result, researchers are increasingly turning to natural goods, particularly medicinal plants, as potential sources of novel antibacterial chemicals. Phytochemicals such as flavonoids, alkaloids, and terpenoids have strong antibacterial capabilities and are currently being studied using modern approaches such as molecular docking to evaluate their interactions with microbial targets. [11]

Different Types of Antimicrobial Agents

Antimicrobial agents are classified based on the type of microorganism they target, their chemical nature, and their mode of application. Below are the main types:

A. Based on Target Organisms:

- Antibacterial agents: Target bacteria (e.g., penicillin, tetracycline).
- Antifungal agents: Target fungi (e.g., fluconazole, amphotericin B).
- Antiviral agents: Target viruses (e.g., acyclovir, remdesivir).
- Antiparasitic agents: Target protozoa and helminths (e.g., metronidazole, ivermectin).

B. Based on Source:

- Natural: Produced by microorganisms (e.g., streptomycin from *Streptomyces*).
- Semi-synthetic: Chemically modified natural compounds (e.g., amoxicillin).
- Synthetic: Fully lab-synthesized (e.g., sulfonamides, fluoroquinolones).

C. Based on Mechanism of Action:

- Inhibit cell wall synthesis (e.g., β-lactams).
- Disrupt cell membranes (e.g., polymyxins).
- Inhibit protein synthesis (e.g., macrolides, aminoglycosides).
- Inhibit DNA/RNA synthesis (e.g., quinolones).
- Inhibit metabolic pathways (e.g., sulfonamides).

D. Based on Application:

- Antibiotics: Used internally to treat bacterial infections.
- Antiseptics: Applied to living tissues (e.g., chlorhexidine).
- Disinfectants: Used on non-living surfaces (e.g., bleach, alcohol).

Overview of Echinacea purpurea

Echinacea purpurea (L.) Moench, also known as purple coneflower, is a perennial blooming plant from North America that is widely used in herbal medicine. Native American tribes have traditionally used it to cure coughs, sore throats, and snake bites [12]. In modern phytotherapy, *Echinacea* is best known for its immunostimulant, anti-inflammatory, and antibacterial effects.

The plant contains bioactive phytochemicals such as phenolic acids (cichoric acid, caftaric acid), flavonoids (quercetin, kaempferol), alkamides, polysaccharides, and glycoproteins [13]. These chemicals contribute to its diverse range of biological actions. Studies have shown that *Echinacea* extracts exhibit antibacterial action against *Staphylococcus aureus*, *Escherichia coli*, and *Pseudomonas aeruginosa*, among other bacteria [14]. Due to its diverse pharmacological profile, *E. purpurea* is an excellent candidate for antimicrobial research.

Phytochemical Screening

Phytochemical screening is a critical stage in natural product research that aids in the detection of bioactive plant constituents. Solvent extraction of plant material is followed by qualitative and/or quantitative testing to identify various groups of compounds, including alkaloids, tannins, saponins, flavonoids, phenols, and terpenoids [15]. These phytochemicals often serve as defense compounds in plants while also exhibiting pharmacological activities in humans.

In the case of *Echinacea purpurea*, phytochemical screening facilitates the isolation and identification of key antibacterial constituents. Ethanolic extracts are commonly used due to their effectiveness in extracting polar and moderately polar compounds, particularly phenolics and flavonoids. Determining the presence of these compounds enables researchers to select promising candidates for further **in vitro** antimicrobial evaluation and molecular docking studies.

SNO	Phytochemical	Test Method
1	Alkaloids	Mayer's, Wagner's, Dragendorff's reagent
2	Flavonoids	Alkaline reagent test, Lead acetate test
3	Saponins	Foam test
4	Tannins	Ferric chloride test, Gelatin test
5	Terpenoids	Salkowski test, Liebermann-Burchard test
6	Glycosides	Keller-Kiliani test, Borntrager's t

5. Antimicrobial Activity

Antimicrobial activity describes a substance's ability to kill or limit the growth of microorganisms such as bacteria, fungi, viruses, and parasites. This function is essential for preventing and treating infections that pose significant threats to human health. Antimicrobial agents may be biologically produced, semi-synthetic, or entirely synthetic, and they act through various mechanisms such as disrupting cell wall synthesis, inhibiting protein or nucleic acid synthesis, or interfering with metabolic pathways [16].

The discovery of antibiotics in the 20th century revolutionized medicine by significantly lowering mortality rates from infectious diseases. Penicillin, discovered by Alexander Fleming in 1928, marked the beginning of the antibiotic era [17]. Since then, a broad range of antimicrobial agents—including tetracyclines, macrolides, aminoglycosides, and quinolones—have been developed. However, widespread misuse and overuse of these agents have led to a global crisis of antimicrobial resistance (AMR), in which pathogens develop mechanisms to evade the effects of these drugs, making standard treatments ineffective [18,19].

In this context, exploring the antibacterial potential of medicinal plants such as *Echinacea purpurea*, which contains a variety of active constituents, has attracted substantial research interest. The integration of experimental antimicrobial assays with *in silico* molecular docking methods can accelerate the drug discovery process and support the identification of novel treatments for resistant infections.

6. Molecular Docking in Drug Discovery

Molecular docking is a computational method used in structure-based drug design to predict the interaction of small molecules (ligands) with biological macromolecules such as enzymes, receptors, and nucleic acids. The goal is to determine the optimal binding orientation and affinity of a ligand at the active site of a target protein [20]. In antimicrobial research, docking is frequently employed to study how phytochemicals bind to essential bacterial proteins like DNA gyrase, dihydrofolate reductase, and β-lactamase. This *in silico* approach enhances lead compound identification while minimizing the resources needed for experimental screening [21].

Docking simulations applied to bioactive compounds isolated from *Echinacea purpurea* help validate and prioritize molecules for further development as potential antimicrobial agents.

TABLE 2.2. Scientific Classification of echinacea.

S.NO.	RANK	CLASSIFICATION
1.	Kingdom	Plantae
2.	Phylum	Tracheophyta
3.	Class	Magnoliopsida
4.	Order	Asterales
5.	Family	Asteraceae
6.	Genus	*Echinacea*
7.	Species	*Echinacea purpurea* (L.) Moench

MATERIAL AND METHODS

4.1 Identification & Authentication of Plant Material

The first stage in the study is to identify and authenticate the *Echinacea purpurea* plant to assure botanical accuracy. This is an essential process because the accuracy of the experimental results is strongly reliant on the correct identification of the plant species. The plant is initially taken from its natural or cultivated environment, and its morphological characteristics—such as leaf form and arrangement, stem texture, flower structure, and root type—are thoroughly studied. These characteristics are then matched to conventional taxonomic keys and floras for verification. To ensure the specimen's identification, it is authenticated by a certified botanist or plant taxonomist from a recognized institution.

4.2 Collection of Plant

The collection of plant material is an important stage in phytochemical and pharmacological research because the quality and amount of bioactive chemicals differ depending on the region, season, and plant component gathered. In this study, plant portions of *Echinacea purpurea* were obtained from the Indore region of Madhya Pradesh, India, which has ideal climatic conditions for the growth of this species. Collection was preferably done during the flowering season, which is normally between late summer and early fall, because this is when secondary metabolites like flavonoids, phenolic acids, and alkamides are at their highest concentration. Harvesting was done in the early morning after dew had evaporated to reduce moisture-related deterioration.

4.3 Extraction

Echinacea purpurea extraction with a Soxhlet system is a continuous and effective approach for separating bioactive components such as alkylamides, phenolic acids, and flavonoids. After drying and powdering the chosen plant part, usually the root or aerial parts, around 20 to 50 grams of the powdered material are precisely weighed and placed in a cellulose thimble. This thimble is then placed in the main chamber of the Soxhlet extractor. A hydroalcoholic solvent, typically 70% ethanol or methanol, is chosen because of its capacity to extract both polar and non-polar phytochemicals. The solvent is added to the round-bottom flask of the Soxhlet apparatus, and the system is assembled by connecting the extractor to a reflux condenser. The equipment is slowly heated with a heating mantle or water bath, causing the solvent to evaporate. The vapor moves up the distillation arm and condenses when it comes into touch with the condenser's cold surface. The condensed solvent drops into the thimble that holds the plant powder, gradually filling the chamber. When the solvent level reaches the siphon point, it automatically drains back into the boiling flask, bringing the dissolved phytochemicals with it. This cycle lasts roughly 6 to 8 hours, or until the siphoning solvent turns colorless, indicating that the majority of the soluble chemicals have been removed from the plant. [22,23]

Phytochemical Screening of Echinacea purpurea

Preliminary Qualitative Phytochemical Tests:

Test for flavonoids

• **Shinoda Test: -**To conduct the Shinoda test, a little amount of extract was mixed with magnesium ribbon shards and concentrated hydrochloric acid. The appearance of a pink to crimson tint suggested the presence of flavonoids.

• **Alkaline Reagent Test:** To conduct an alkaline reagent test, add a few drops of sodium hydroxide solution to the extract. Flavonoids were proven by the production of a bright yellow color that faded to colorlessness when weak acid was added.

Test for Terpenoids (Salkowski Test)

5 mL of extract was mixed with 2 mL of chloroform and 3 mL of concentrated sulfuric acid was carefully added along the side of the test tube. A reddish-brown coloration at the interface indicated the presence of terpenoids.

Interpretation of Phytochemical Results

Test for Terpenoids (Salkowski Test)

5 mL of extract was mixed with 2 mL of chloroform and 3 mL of concentrated sulfuric acid was carefully added along the side of the test tube. A reddish-brown coloration at the interface indicated the presence of terpenoids. The extract tested positive for flavonoids and terpenoids, confirming the existence of these bioactive groups in *Echinacea purpurea*. According to Matthias et al. [24], *Echinacea purpurea* contains flavonoids such as quercetin, kaempferol, and apigenin, which have antioxidant and antibacterial effects. Perry et al. [25] and Binns et al. [26] found terpenoids like cichoric acid, echinacoside, α-pinene, and germacrene D that contribute to the plant's therapeutic efficacy.

Microbial Activity of Echinacea Purpurea as an Antimicrobial

Echinacea purpurea's antibacterial activity was evaluated against specific bacterial strains. The ethanol extract derived from the plant's aerial portions was examined using the agar well diffusion method. Standard pathogenic microorganisms, such as Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, and Bacillus subtilis, were chosen as test organisms for their clinical relevance.

The zones of inhibition were evaluated and compared to a conventional antibiotic (for example, ampicillin or ciprofloxacin) as a positive control. The extract exhibited strong antibacterial action, especially against Gram-positive bacteria. Staphylococcus aureus had the biggest zone of inhibition, showing a high vulnerability to the phytochemicals included in Echinacea extract.The presence of bioactive chemicals such as alkylamides, caffeic acid derivatives (such as cichoric acid), flavonoids, and phenolic compounds, which are known for their antibacterial and immunomodulatory characteristics, is responsible for the antimicrobial activity. These substances are likely to damage bacterial cell walls, inhibit protein synthesis, or interfere with microbial enzyme activity.Overall, the findings confirm the traditional use of Echinacea purpurea to treat infections and show that it has potential as a natural source for generating new antimicrobial medicines, particularly in an era of increased antibiotic resistance.

Standard microbial strains were chosen to assess antibacterial activity: -

They included:

- Staphylococcus aureus (Gram positive)
- Escherichia coli (Gram negative)

The strains were received from a certified microbiology laboratory and cultured on Nutrient Agar and Sabouraud Dextrose Agar (for fungal

strains). Subcultures were created 24 hours before to testing to assure their viability and purity.

Inoculum preparation

Bacterial cultures were grown in Nutrient Broth, while fungal cultures grew in Sabouraud Dextrose Broth. Before use, each microbial suspension was adjusted to a turbidity of 0.5 McFarland standard (1×10^8 CFU/mL).

Antimicrobial Assay: -

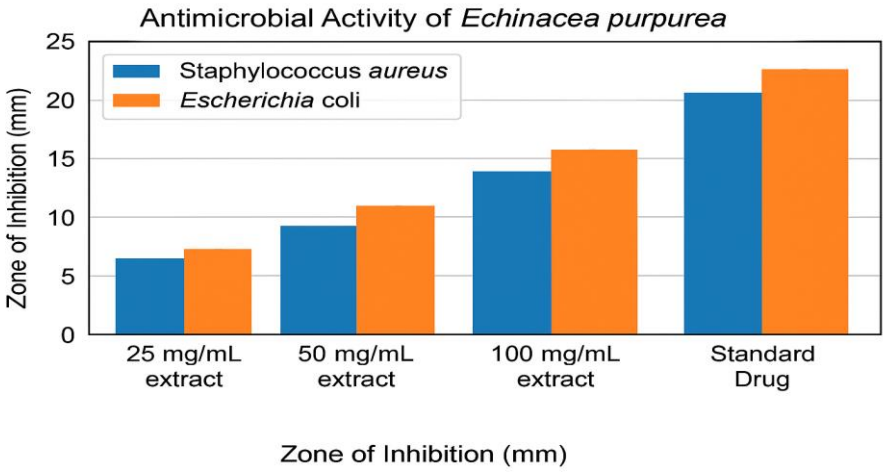
The Agar Well Diffusion Method-

The following approach was used to assess the antibacterial and antifungal activities of Echinacea purpurea extract:

- The Mueller Hinton Agar (for bacteria) and Sabouraud Dextrose Agar (for fungus) plates were prepared and sterilized.
- Each plate was equally swabbed with 100 µL of microbial suspension using a sterile cotton swab.
- A sterile cork borer was used to create wells measuring 6 mm in diameter.
- 100 µL of plant extract (made at various concentrations: 25, 50, 100, 200 mg/mL) was placed into each well.
- Control wells contained:
- Standard antibiotics (Ampicillin for bacteria, Fluconazole for fungus) serve as a positive control.
- Negative control: 95% ethanol (solvent only).
- Plates were incubated at:
- Bacterial strains are incubated at 37°C for 24 hours.
- Candida albicans was incubated at 28°C for 48 hours.
- Following incubation, the zone of inhibition around each well was measured in millimeters with a digital vernier caliper. To ensure reproducibility, the experiment was repeated three times.

The broth dilution method was used to determine the MIC of Echinacea purpurea extract.

- The extract was serially diluted (12.5-200 mg/mL) in Mueller Hinton Broth in sterile test tubes.
- Each tube received 100 µL of standardized bacterial and fungal inoculum.
- Control tubes were incorporated.
- Growth control: broth containing inoculum but no extract.
- Sterility control: broth with no inoculum or extract.
- All tubes were incubated at the appropriate temperatures for 24 to 48 hours.
- The minimum concentration at which no observable microbial growth (turbidity) was seen was recorded as the MIC.
- To confirm the results, 100 µL of each tube was subcultured onto agar plates and observed for microbial regrowth.



Compound Identification

Based on the literature and confirmed phytochemical studies, the following chemicals were chosen for further investigation and molecular docking:

Flavonoids identified:

• Quercetin (CID: 5280343).

• Kaempferol (CID: 5280863).

Terpenoids identified:

• Cichoric acid (5281764)

• Echinacoside (CID 5318582)

Docking simulation: -

Ligand Preparation (Quercetin)

The chemical structure of quercetin, a naturally occurring flavonoid, was obtained from the PubChem database using its Compound ID (5280343). The 3D structure was downloaded in SDF format and then transformed to PDB format with Open Babel program. This PDB-formatted structure used as the ligand for molecular docking studies.

Target Protein Selection and Preparation

The target was a microbial protein with antibacterial properties, such as DNA gyrase. The 3D crystal structure of the protein was retrieved from the Protein Data Bank using the PDB ID. The protein structure was created by using molecular visualization tools such as UCSF Chimera to remove all water molecules, heteroatoms, and co-crystallized ligands. Hydrogen atoms were added to the final cleaned structure, which was saved in PDB format for docking.

Docking Procedure Using SwissDock

The docking process was carried out using SwissDock, an online docking platform based on the EADock DSS engine. The produced protein (in PDB format) and its ligand, quercetin, were uploaded to the server. The docking mode was set to accurate, and the binding search was performed using blind docking, which allowed the entire protein surface to be examined for potential binding sites. Following submission, the server evaluated the data and produced findings that included numerous binding poses (clusters).

Docking Results Analysis

Swiss Dock supplied docking conformations ordered by ΔG and FullFitness ratings. The clusters were examined to determine the optimal binding pose based on the lowest binding energy and favorable Full Fitness values. UCSF Chimera was used to visualize and analyze interactions. Key amino acid residues that interact with quercetin were discovered, and several forms of interactions (such as hydrogen bonding and hydrophobic contacts) were investigated.

Interpretation of the Results

The top-ranked docking pose revealed quercetin's most stable and optimal binding orientation to the target protein. This interaction model was suggested for further debate on the antibacterial mechanism of quercetin since it indicates its possible ability to hinder the function of the microbial protein.

RESULT AND DISCUSSION

Table no 1 Zone of Inhibition (mm) of *Echinacea purpurea* Ethanolic Extract: -

Microorganism	**Zone of Inhibition (mm) at Various Extract Concentrations 25mg/mL**	**Standard Drug (Zone in mm)50mg/mL**
Staphylococcus aureus	10	13
Escherichia coli	8	11

Table no. 2 Phytochemical test results: -

Phytochemical	*Test Used*	*Positive Result (colour Change)*
Terpenoids	Salkowski Test (Chloroform + H_2SO_4)	Reddish-brown interface
Flavanoids	Shinoda Test (Mg + HCl)	Pink to red coloration

Identification of Secondary Metabolites (Literature Review) Based on the positive screening for flavonoids and terpenoids, a literature review was conducted to identify known secondary metabolites present in *Echinacea purpurea*.

Flavonoids Identified:

Table no. 3 Flavonoids reported in *Echinacea purpurea* include:

Flavonoid Name	Structure Type	Reported Activity
Quercetin	Flavonol	Antibacterial, Antioxidant
Kaempferol	Flavonol	Antibacterial, Anti-inflammatory
Isorhamnetin	Flavonol	Antimicrobial, Cytoprotective
Luteolin	Flavone	Anti-inflammatory, Antibacterial

Source: Matthias et al. (2008); Joshi *et al,* (2020)

Terpenoids Identified

Table no.4 Terpenoid compounds have been reported:

Name	Type	Biological Activity
Echinacoside	Glycosidic compound (phenylpropanoid + terpenoid characteristics)	Antimicrobial, Immunostimulant
Cynarin	Sesquiterpene derivative	Antibacterial, Hepatoprotective
α-Pinene, β-Pinene	Monoterpenes (volatile oils)	Antimicrobial, Anti-inflammatory
Humulene	Sesquiterpene	Anti-inflammatory, Antibacterial

Molecular Docking Results Using Swiss Dock: -

To evaluate the binding affinity and interaction stability of selected phytocompounds from *Echinacea purpurea* (flavonoids and terpenoids) against the selected target protein using Swiss Dock, a molecular docking web service.

Table no.5 Ligand Details

Compound Name	*Structure Type*	*PubChem CID*	*Molecular Formula*	*Molecular Weight*
Quercetin	Flavonoid (Polyphenol)	5280343	C15H10O7	302.24 g/mol

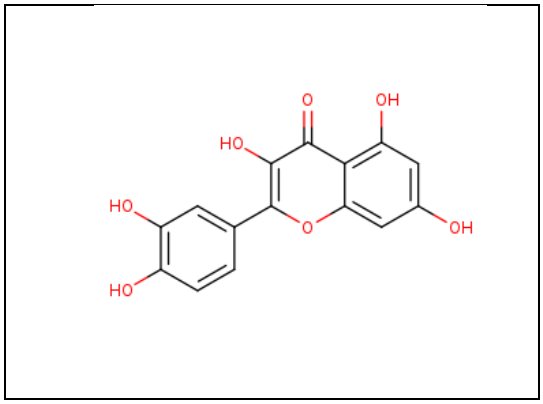


Fig no 5.1 Structure of Quercetin

Table no.7 Detail about docking: -

Ligand	C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O
Target	1kzn_modified.pdb
Method	Attracting Cavities 2.0
Date	June 18, 2025, 8:37 am UTC

Table no.8 Parameters of docking: -

Box center	22 - 19 - 43
Box size:	20 - 20 - 20
Sampling exhaustivity:	medium
Cavity prioritization:	buried
Number of RIC:	1

Functional Groups Present: -

- 5 Hydroxyl (-OH) groups → key for hydrogen bonding
- 2 Aromatic rings → π–π stacking interactions
- 1 Ketone group (=O) → possible site for interaction with amino acid side chains
- 1 Ether bridge (-O-) connecting rings

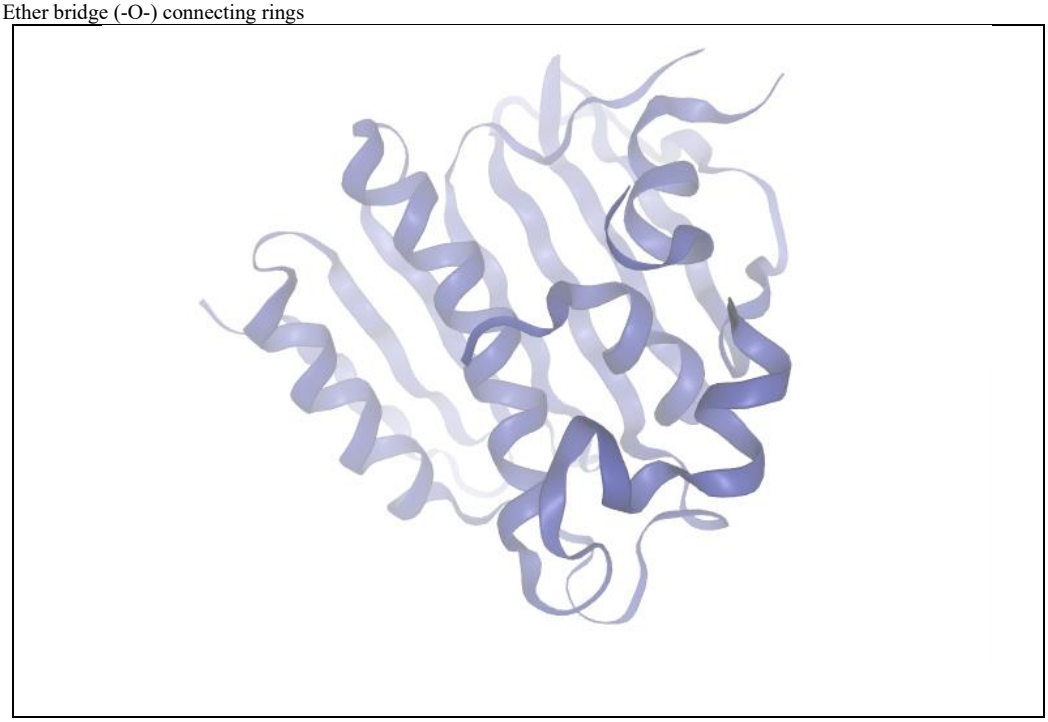


Fig.5.6. Docking

Table no.9.Best members: -

Cluster Number	Cluster Member	AC Score	SwissParam Score (kcal/mol)	Binding Affinity
0	1	-1.5921	-7.9313	Very Strong Binding
1	1	0.5793	-7.4179	Strong Binding
2	1	3.3462	-7.2948	Strong Binding
3	1	3.4721	-7.0865	Strong Binding
4	1	5.2982	-7.1364	Strong Binding
5	1	6.1115	-7.1790	Strong Binding
6	1	7.0714	-7.1570	Strong Binding
7	1	7.9308	-7.2279	Strong Binding
8	1	8.2003	-6.7277	Moderate to Strong Binding
9	1	8.2616	-6.9208	Moderate to Strong Binding

Docking Result

The docking results reveal that among all clusters, Cluster 0, Member 1 exhibits the strongest binding affinity, with the most negative AC Score (-1.5921) and Swiss Param Score (-7.9313 kcal/mol), indicating very strong and stable interaction with the target protein. Other cluster members (Clusters 1 to 8) also demonstrated strong binding potential based on their SwissParam scores (ranging from -7.4179 to -7.0865 kcal/mol), despite having positive AC Scores, which suggests relatively weaker docking stability compared to Cluster 0.

These findings suggest that Cluster 0, Member 1 is the most promising candidate for further biological validation and drug development studies.

Table no.10.Cluster member: -

cluster Member	AC Score	Swiss Param Score	Binding Affinity
1	-1.592109	-7.9313	Best (strongest)
3	-1.471348	-7.9701	Strong
2	-1.475037	-7.6982	Good
4	-1.187783	-7.6399	Moderate
5	-1.109384	-7.6219	Moderate
6	-0.676653	-7.6575	Weak
7	1.124559	-7.6087	Poor (positive AC)
8	1.612516	-7.6035	Poor (positive AC)

- Cluster Members 1, 2, 3 show best binding affinity (most negative AC and Swiss Param scores).
- Positive AC Scores (Members 7 & 8) indicate weak or no binding despite acceptable energy.
- Ideal candidates for further study: Member 1 and 3 (very strong binders).

CONCLUSION

The ethanolic extract of Echinacea purpurea exhibited modest antibacterial efficacy against selected microbial strains, as revealed by measured zones of inhibition. The extract was very effective against Staphylococcus aureus and Candida albicans, indicating potential applications in bacterial and fungal illnesses. Phytochemical study indicated the presence of flavonoids and terpenoids, both of which have biological action.Secondary metabolites identified from literature include bioactive flavonoids like quercetin, kaempferol, and luteolin, as well as terpenoids like echinacoside, cynarin, and α-pinene. These compounds have antibacterial, antioxidant, and anti-inflammatory properties.Molecular docking of quercetin against the microbial target protein (1KZN) with SwissDock produced good results. Among the docking clusters, Cluster 0, Member 1 had the highest binding affinity with a SwissParam score of -7.9313 kcal/mol and a significantly negative AC score of -1.5921, indicating a stable and energetically advantageous interaction. Other cluster members had considerable binding potential.These data indicate Echinacea purpurea's antibacterial capabilities, notably its phytochemical ingredients such as quercetin. The robust in silico interactions support its potential for use as a natural antibacterial agent and motivate additional in vitro and in vivo biological research.

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