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Molecular Docking and Antimicrobial Study of Selected Plant Extracts Against Pathogenic Bacteria Involved in Bedsore

Urooj Khalid
BS (Hons) Department of Botany, Government Post Graduate College Mandian, Abbottabad-22500, Pakistan. uroojkhalid381@gmail.com
Dr. Jawad Ahmed
Lecturer, Department of Botany, Government Post Graduate College Mandian, Abbottabad-22500, Pakistan. jawabotanist_atd@gmail.com
Syed Azhar Shah Kazmi
M.Phil. Scholar, Department of Botany, Hazara University, Mansehra-21300, Pakistan. azharshahkazmi@hu.edu.pk
Dr. Masab Saeed
PhD, Department of Chemistry, Hazara University, Mansehra-21300, Pakistan. masabsaeed@hu.edu.pk
Warda Ashfaq
BS (Hons) Department of Botany, Government Post Graduate College Mandian, Abbottabad-22500, Pakistan. wardaashfaq0@gmail.com
Muhammad Mudassar
BS (Hons) Department of Botany, Government Post Graduate College Mandian, Abbottabad-22500, Pakistan. muddasser888@gmail.com

Author Details

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Corresponding E-mails & Authors*:
Syed Azhar Shah Kazmi

Abstract

The increasing prevalence of antimicrobial resistance has necessitated the exploration of natural products as alternative therapeutic agents. In this study, the bark extracts of three Himalayan conifers—Pinus roxburghii, Cedrus deodara, and Abies pindrow—were evaluated for their antibacterial activity and molecular docking potential. Crude extracts were prepared using ethanol, methanol, and distilled water, and tested against Staphylococcus aureus and Pseudomonas aeruginosa through disc diffusion and

well diffusion methods. Results indicated moderate to strong inhibition, with *P. roxburghii* (methanolic extract) showing the highest zone of inhibition (21 mm) against *P. aeruginosa*, while *A. pindrow* and *C. deodara* also demonstrated measurable activity. In parallel, molecular docking studies were performed using MOE software to assess the interaction of selected phytochemicals with bacterial protein targets. Compounds such as apigenin, isovelleral, and phosphoamino-phosphonic acid-adenylate ester exhibited strong binding affinities (MOE scores up to –6.19), supported by stable ligand–protein interactions. Drug-likeness analysis using SwissADME confirmed compliance with Lipinski and related rules for several compounds, though variability in bioavailability was observed. Findings suggested that these Himalayan conifers are promising sources of bioactive compounds with potential antibacterial properties, supporting their ethnomedicinal use and highlighting candidates for further preclinical drug development.

1. INTRODUCTION

Medicinal plants have long been recognized as a cornerstone of traditional healing systems and continue to hold significant relevance in modern pharmacological research (Dhamodiran, Chinnaperumal, Venkatesan, Alshiekheid, & Suseem, 2024). Across cultures and continents, natural products derived from plants have served as the primary source of therapeutics for centuries, providing remedies for infections, inflammation, metabolic disorders, and other ailments (Bittner Fialová, Rendeková, Mučaji, Nagy, & Slobodníková, 2021). Even in contemporary medicine, where synthetic drug discovery has advanced tremendously, a considerable proportion of pharmaceuticals either originate directly from plant-derived compounds or are semi-synthetic derivatives inspired by natural molecules (Elbuckley, Sorour, Tayel, & Abbas,

2022). For instance, approximately 25% of prescribed drugs worldwide are derived from plant-based sources, underscoring the continued importance of ethnobotanical resources in modern drug discovery and development (Mashamba, Adeosun, Baloyi, Tshikalange, & Cosa, 2022).

One of the pressing global health concerns today is the rapid rise of antimicrobial resistance (AMR) (Kumar). The widespread and often indiscriminate use of antibiotics has led to the emergence of multidrug-resistant strains of bacteria, creating challenges in the management of infectious diseases. Common bacterial pathogens such as *Staphylococcus aureus*, *Pseudomonas aeruginosa*, and *Proteus mirabilis* have developed resistance to multiple antibiotic classes, including β-lactams, aminoglycosides, and fluoroquinolones (Gamedze, Mthiyane, Mavengahama, Singh, & Onwudiwe, 2024). This crisis has necessitated the exploration of alternative or complementary antimicrobial agents, particularly those derived from natural sources. Medicinal plants, owing to their chemical diversity and structural complexity, offer a reservoir of bioactive compounds that may provide novel scaffolds for drug development or synergistic effects with existing antibiotics (Abdelmoteleb et al., 2024).

In this context, plant secondary metabolites such as flavonoids, terpenoids, alkaloids, phenolics, and tannins have drawn extensive scientific interest (Abazari et al., 2022). These compounds not only exhibit broad-spectrum antimicrobial activity but also possess additional pharmacological properties including antioxidant, anti-inflammatory, anticancer, and immunomodulatory activities. Importantly, the structural novelty of plant-derived molecules often circumvents resistance mechanisms that render conventional antibiotics ineffective. Therefore, systematic evaluation of medicinal plants

for their phytochemical and antimicrobial potential represents a rational approach to address the growing AMR burden (Elbuckley et al., 2022).

In light of the above considerations, the present study was designed with two primary objectives. First, to evaluate the antibacterial activity of ethanolic, methanolic, and aqueous extracts of the bark of *Pinus roxburghii*, *Cedrus deodara*, and *Abies pindrow* against clinically relevant bacterial strains such as *Staphylococcus aureus* and *Pseudomonas aeruginosa* (Bhardwaj et al., 2021). The antibacterial activity was assessed using standardized disc diffusion and well diffusion methods, with zones of inhibition recorded for comparative analysis. Second, to conduct molecular docking studies of selected phytochemicals from these plants against bacterial protein targets using the MOE (Molecular Operating Environment) software. The docking results were complemented with drug-likeness and medicinal chemistry profiling using the SwissADME platform, thereby providing a comprehensive evaluation of both antimicrobial efficacy and pharmacological suitability.

2. LITERATURE REVIEW

The Himalayan region of South Asia, particularly northern Pakistan, harbors a rich diversity of medicinal plants that have been traditionally used by local communities for the treatment of infectious and non-infectious diseases (Deepthi, 2012). Among these, *Pinus roxburghii* (Chir pine), *Cedrus deodara* (Deodar cedar), and *Abies pindrow* (Silver fir) are notable coniferous species belonging to the family Pinaceae (Singh et al., 2019). These trees are widely distributed across the temperate forests of Khyber Pakhtunkhwa (KPK) and are valued not only for their timber but also for their medicinal and ethnobotanical applications (Anjali Sood, Krishna Khambra, & Rose, 2014).

Pinus roxburghii, commonly known as Chir pine, has been employed in traditional medicine for its antiseptic, anti-inflammatory, and wound-healing properties. Its bark and resin are particularly rich in terpenoids and phenolic compounds that exhibit antimicrobial and antioxidant effects. Previous studies have reported its potential against gram-positive and gram-negative bacteria, though systematic evaluations against resistant clinical isolates remain limited (Pattanayak, 2018).

Cedrus deodara, a culturally revered tree often referred to as the "wood of the gods," has also been extensively used in folk remedies (Kalam, Aqeel, Ahmad, Arzoo, & Mushtaq, 2023). Extracts of its bark and wood have been utilized for the treatment of skin infections, respiratory ailments, and joint pain (Pathak, Pathania, Metha, & Sharma, 2023). Phytochemical analyses have revealed the presence of flavonoids, lignans, and sesquiterpenes with reported antimicrobial and cytotoxic activities. However, its detailed molecular interactions with bacterial protein targets remain poorly understood (Chaudhary, Ahmad, & Mazumder, 2011).

Abies pindrow, known as Silver fir, is another important Himalayan conifer. Traditionally, its bark and needles are used in the treatment of asthma, bronchitis, and gastrointestinal disorders. It contains a rich composition of terpenoids and volatile oils with reported antibacterial and antifungal properties. Nevertheless, systematic studies integrating in-vitro antibacterial assays with in-silico molecular docking approaches remain scarce for this species (Deepthi, 2012).

The integration of computational methods such as molecular docking with experimental assays has become an indispensable strategy in modern drug discovery. Molecular docking provides insights into the binding affinity and interaction profiles of bioactive compounds with specific protein targets (Anjali Sood et al., 2014). By simulating

the binding conformations of ligands within the active sites of enzymes or receptors, docking studies predict potential mechanisms of action and allow prioritization of promising candidates for experimental validation. Importantly, such in-silico methods reduce the cost and time associated with conventional drug screening while enhancing the understanding of molecular pharmacology (Deepthi, 2012).

In the case of bacterial pathogens, docking studies often target essential proteins involved in DNA replication, protein synthesis, cell wall biosynthesis, and enzymatic resistance mechanisms. Ligands derived from medicinal plants, when shown to bind effectively to these proteins, may inhibit their function and thereby suppress bacterial growth. When combined with traditional antimicrobial susceptibility assays such as disc diffusion and well diffusion methods, docking analyses provide a powerful framework for evaluating the therapeutic potential of plant-derived compounds (Elbuckley et al., 2022).

Drug-likeness and medicinal chemistry profiling represent another critical step in rational drug discovery. Computational tools such as SwissADME facilitate the evaluation of pharmacokinetic and physicochemical properties, including Lipinski's rule of five, bioavailability, and toxicity alerts. These parameters help determine whether a compound is likely to exhibit desirable absorption, distribution, metabolism, and excretion (ADME) profiles in vivo. While many plant compounds demonstrate potent in-vitro activity, poor drug-likeness parameters often limit their clinical translation. Hence, coupling docking studies with ADME evaluation enhances the robustness of candidate selection.

In addition to their pharmacological promise, the exploration of *Pinus roxburghii*, *Cedrus deodara*, and *Abies pindrow* also carries ecological and socio-economic significance. These trees are integral components of the forest ecosystems of northern Pakistan, contributing to biodiversity, soil stabilization, and carbon sequestration.

Simultaneously, they are widely utilized by local populations for fuel, timber, and traditional medicine. By scientifically validating the therapeutic potential of these species, research can not only contribute to the discovery of novel drug candidates but also promote the sustainable use of natural resources and the preservation of indigenous knowledge.

Several studies from the Indian subcontinent and beyond have highlighted the antimicrobial potential of coniferous plants. For instance, essential oils extracted from pine and fir species have demonstrated inhibitory activity against *Escherichia coli*, *Bacillus subtilis*, and *Candida albicans*. Flavonoids such as apigenin and kaempferol, widely distributed in conifer bark, have been shown to disrupt bacterial cell wall integrity and interfere with quorum sensing pathways. Similarly, terpenoids and phenolic acids present in these plants exhibit strong radical-scavenging activity, contributing indirectly to antimicrobial defense by modulating host immune responses. However, despite these findings, systematic studies that couple computational docking with antimicrobial assays are still limited for Himalayan conifers.

By integrating in-vitro and in-silico approaches, this research aims to bridge the gap between traditional ethnomedicine and modern computational pharmacology. The findings are expected to contribute not only to the understanding of the antimicrobial potential of these conifers but also to the identification of promising lead compounds for further preclinical development. Ultimately, this study reinforces the value of medicinal plants as reservoirs of bioactive molecules and highlights the relevance of Himalayan biodiversity in addressing global challenges such as antimicrobial resistance.

3. MATERIALS AND METHODS

3.1 Plant Material and Extraction

The bark of *Pinus roxburghii*, *Abies pindrow*, and *Cedrus deodara* was collected from different locations in Abbottabad, Khyber Pakhtunkhwa (KPK). After washing with tap water, the samples were shade-dried for 15 days at 25 °C and ground into a fine powder. For extraction, 20 g of powdered plant material was soaked in 250 ml of 70% ethanol, 70% methanol, or distilled water. The mixture was stirred in a water bath at 45 °C for 10 h, filtered through Whatman No. 1 paper, and concentrated using a rotary evaporator at 40 °C. Extracts were lyophilized and stored at –20 °C until analysis. Extraction yield was calculated by mass balance.

3.2 Microorganisms and Culture Conditions

The bacterial strains used were:

- *Staphylococcus aureus*
- *Pseudomonas aeruginosa*
- *Proteus mirabilis*

Microbial cultures were maintained on nutrient agar and standardized in nutrient broth. Media were prepared, sterilized by autoclaving, and poured aseptically into Petri dishes. Cultures were refreshed by streaking on nutrient agar and incubated at 37 °C for 24 h, followed by subculturing in broth at 200 rpm for 18 h.

3.3 Antibacterial Activity Assays

Disc Diffusion Method:

Sterile filter paper discs (9 mm, Whatman No. 3) loaded with 2 mg of plant extracts were placed on Mueller-Hinton agar plates inoculated with test bacteria and incubated at 35 ± 2.5 °C for 18 h. Nitrofurantoin discs (0.03 mg) served as a positive control, while 70%

ethanol served as a negative control. Zones of inhibition were measured in mm. Minimum inhibitory concentration (MIC) was determined by two-fold serial dilutions (31.3–2000 mg/L) with final inocula of 10^4 CFU/mL (10^5 CFU/mL for ATCC 29212).

Well Diffusion Method

Wells (8 mm) were made in nutrient agar plates seeded with standardized bacterial inocula (1–2 × 10^7 CFU/mL; 0.5 McFarland). Plant extracts (24, 30, 36 µl corresponding to 4–6 mg) were added to wells. Antibiotic and DMSO served as positive and negative controls, respectively. Plates were incubated at 37 °C for 24 h, and inhibition zones were measured. All experiments were performed in triplicate.

3.4 Molecular Docking

Ligands (plant-derived compounds and acarbose) were retrieved from PubChem. Protein structures were obtained from the Protein Data Bank, water molecules removed, and energy minimized using the MOE software. Flexible docking was performed using MOE-Dock default settings, and ligand–protein interactions were analyzed.

3.5 Drug-Likeness Evaluation

Compounds with high binding scores were further assessed for drug-likeness using the SwissADME web tool, evaluating parameters such as lipophilicity, refractivity, molecular weight, atom count, and polar surface area.

4. RESULTS

4.1 Molecular Docking Of *Pinus Roxburghii*:

Molecular docking is carried out with selected phytochemicals of *Pinus Roxburghii* with proteins.

4.1.1 Interaction of Phosphoamino-Phosphonic Acid-Adenylate Ester with phosphorylated insulin receptor tyrosine kinase in complex with peptide substrate and ATP analog protein.

TABLE 1: SHOW THE MOE SCORE OF SELECTED LIGANDS WITH PROTEIN

S. No	S. Value
1.	-5.9404
2.	-5.3158

The phosphoamino phosphonic acid-adenylate ester compound was deeply bound into the binding cavity of IR3, making interactions with the residues. The docking studies indicate a good agreement between the ligand and protein.

4.1.2 Ligand Interaction

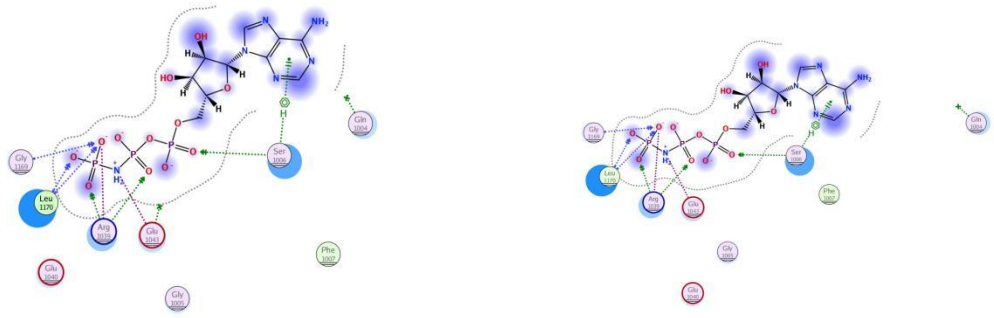

FIGURE 1: THE LIGAND PROTEIN INTERACTION OF TARGET PROTEIN

4.1.3 DRUG-LIKENESS AND MEDICINAL CHEMISTRY PARAMETERS OF THE SCREENED COMPOUNDS.

Lipinski	3
Ghose	2
Veber	1
Egan	1

Muegge	4
Bio-availability score	0.11
PAINS	0
Brenk	1
Leadlikeness	2
Synthetic accessibility	5.23

4.1.4 Interaction of UN608(3-(3-sulfoamino-phenyl)-propio-nylamino)-methyl)-phenyl-sulfamic acid with 2F70 protein

Table 2: show the MOE score of selected ligand with protein

S.no	S. value
1.	-3.6298
2.	-3.5125

UN608(3-(3-sulfoamino-phenyl)-propio-nylamino)-methyl)-phenyl-sulfamic acid show good interaction with 2F70 protein.

4.1.5 Ligand Interaction

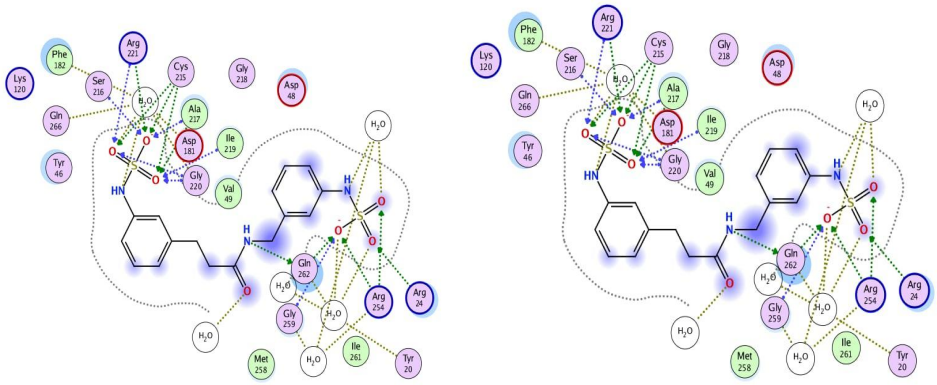

FIGURE 2: THE LIGAND PROTEIN INTERACTION OF TARGET PROTEIN

4.1.6 DRUG LIKENESS AND MEDICINAL CHEMISTRY OF SCREENED COMPOUND:

Lipinski	yes
Ghose	yes
Veber	no
Egan	no
Muegge	no
Bio-availability score	0
PAINS	0
Brenk	1
Leadlikeness	2
Synthetic accessibility	2.46

4.1.7 Interaction of (2-4-Bromo-2-Flouro-benzylthiocarbomyl-5-(Flouro-phenoxy)-acetic acid with 1USO protein:

TABLE 3: SHOW THE MOE SCORE OF SELECTED LIGAND WITH PROTEIN

S.no	S. value
1.	-3.1748
2.	-3.1617

(2-4-Bromo-2-Flouro-benzylthiocarbomyl-5-(Flouro-phenoxy)-acetic acid show goodinteraction with 1USO protein.

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4.1.8 Ligand Interaction

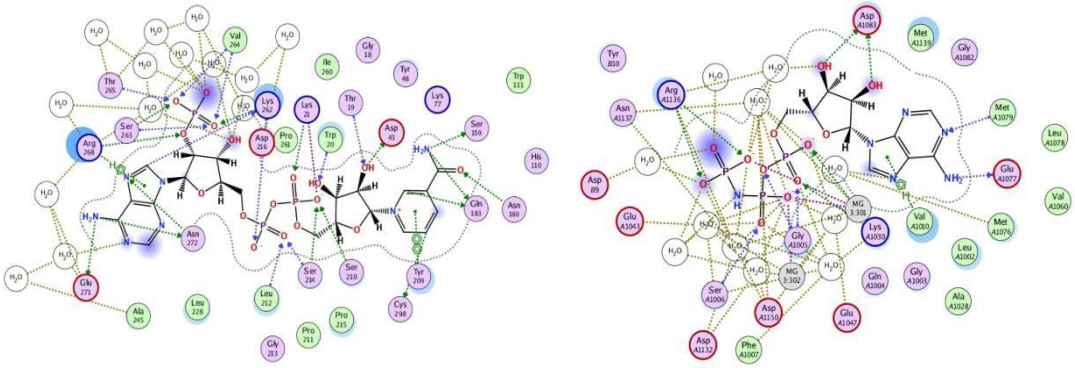

FIGURE 3: THE LIGAND PROTEIN INTERACTION OF TARGET PROTEIN

4.1.9 DRUG LIKENESS AND MEDICINAL CHEMISTRY OF SCREENED COMPOUND.

Lipinski	yes
Ghose	no
Veber	yes
Egan	yes
Muegge	yes
Bio-availability score	0.85
PAINS	0
Brenk	0
Leadlikeness	no
Synthetic accessibility	1.82

4.2 Molecular Docking of *Cedrus deodara*

Molecular docking is carried out by selected phytochemicals of *Cedrus deodara* with proteins.

4.2.1 Interaction of Apigenin with 6LU7 protein

TABLE 4: *SHOW THE MOE SCORE OF SELECTED LIGAND WITH PROTEIN*

S.no	S. value
1.	-5.3421
2.	-5.1191

Apigenin show good interaction with 6LU7 protein.

4.2.2 Ligand Interaction

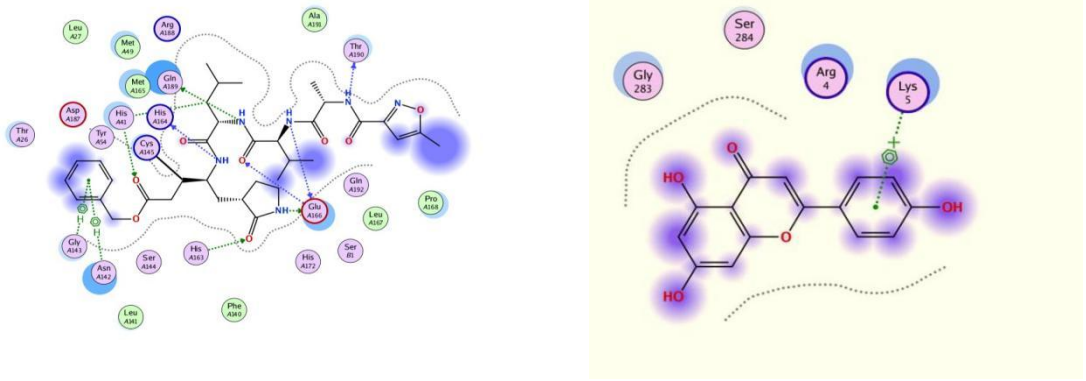

FIGURE 4: THE LIGAND PROTEIN INTERACTION OF TARGET PROTEIN

4.2.3 DRUG LIKENESS AND MEDICINAL CHEMISTRY OF SCREENED COMPOUND

Lipinski	yes
Ghose	yes
Veber	yes
Egan	yes
Muegge	yes

Bio-availability score	0.55
PAINS	0
Brenk	0
Leadlikeness	yes
Synthetic accessibility	2.96

4.2.4 Interaction of Isovelleral with 1YBV protein

TABLE 5: *SHOWS THE MOE SCORE OF SELECTED LIGAND WITH PROTEIN*

S.no	S. value
1.	-6.1996
2.	-5.8188

Isovelleral show good interaction with 1YBV.

4.2.5 Ligand Interaction

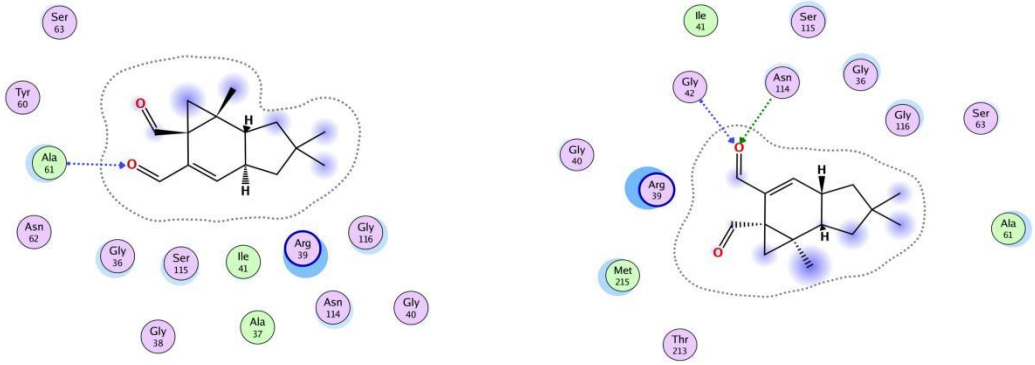

FIGURE 5: LIGAND INTERACTION OF TARGET PROTEIN

4.2.6 DRUG LIKENESS AND MEDICAL CHEMISTRY OF SCREENED COMPOUND

Lipinski	Yes
Ghose	Yes
Veber	Yes

Egan	Yes
Muegge	Yes
Bioavailability score	0.55
PAINS	0
Brenk	1
Leadlikeness	No
Synthetic Accessibility	4.53

4.2.7 Interaction of Melanin with 1YBV

TABLE 6: *SHOW THE MOE SCORE OF SELECTED LIGAND WITH 1YBV PROTEIN*

S.no	S. value
1.	-5.4502
2.	-4.8711

Melanin show high MOE score with 1YBV protein.

4.2.8 Ligand Interaction

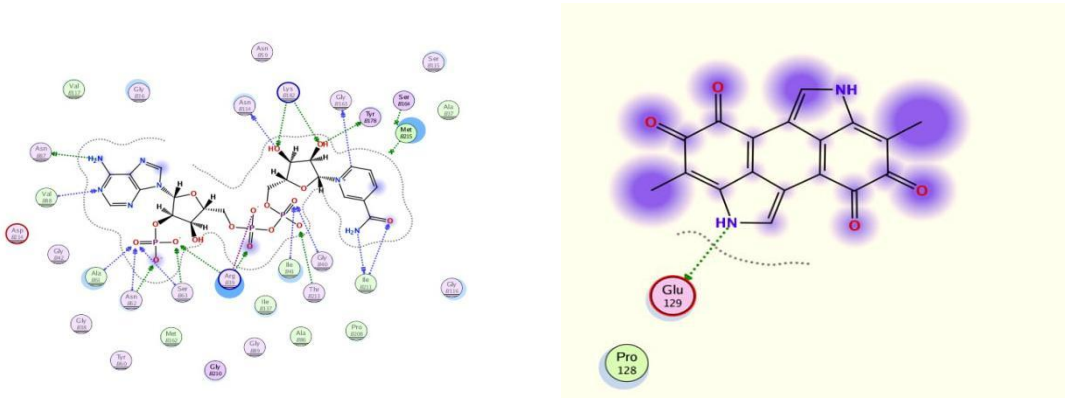

FIGURE 6: THE LIGAND PROTEIN INTERACTION OF TARGET PROTEIN

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4.2.9 DRUG LIKENESS AND MEDICAL CHEMISTRY OF SCREENED COMPOUND

Lipinski	Yes
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bio-availability score	0.55
PAINS	0
Brenk	2
Lead-likeness	yes
Synthetic accessibility	2.00

4.2.10 Interaction of kempferol with 6LU7 Protein

TABLE 7: *SHOWS THE MOE SCORE*

S.no	S. value
1.	-5.2239
2.	-4.6800

4.2.11 Ligand Interaction

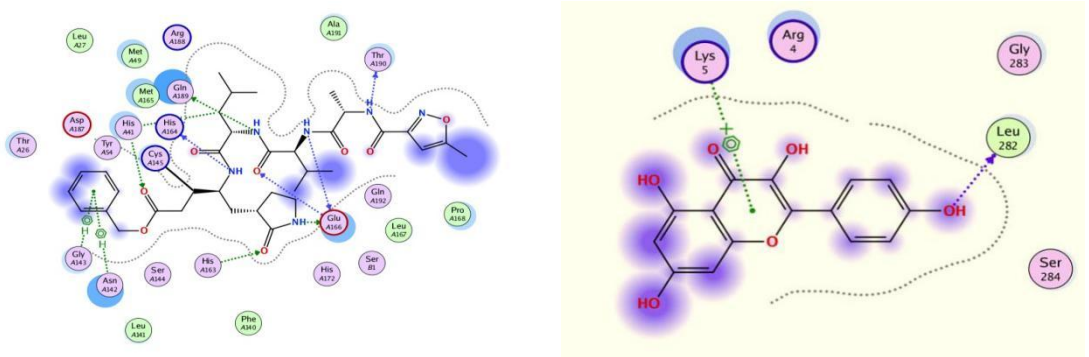

FIGURE 7: LIGAND INTERACTION OF TARGET PROTEIN

4.2.12 *DRUG LIKENESS AND MEDICAL CHEMISTRY OF SCREENED COMPOUND*

Lipinski	Yes
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailabilty score	0.55
PAINS	0
Brenk	0
Lead-likeness	Yes
Synthetic accessibility	3.14

4.3 Molecular Docking of *Abies Pindrow*.

4.3.1 Interaction of Tricyclene with Mpro protein

TABLE 8: SHOW THE MOE OF SELECTED LIGAND WITH PROTEIN

S.no	S. value
1.	-3.9752
2.	-3.9427

Tricyclene interact with mpro protein and show good interaction.

4.3.2 Ligand Interaction

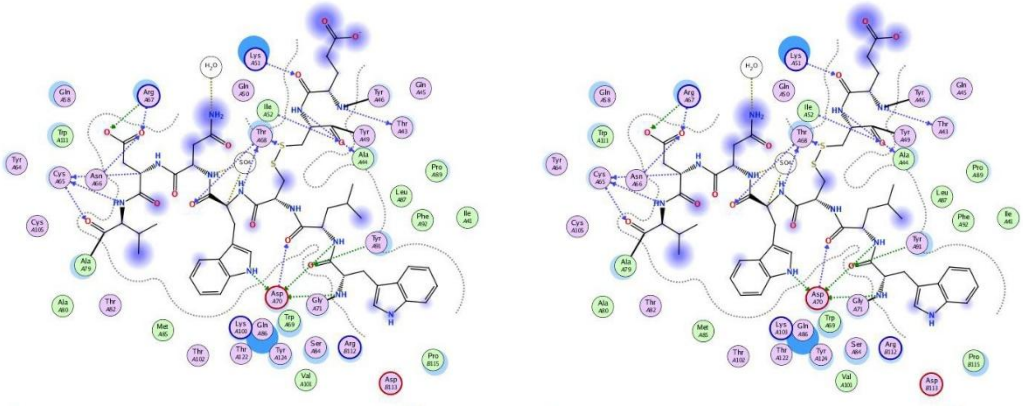

FIGURE 8: SHOW THE LIGAND PROTEIN INTERACTION OF TARGET PROTEIN

4.3.3 DRUG LIKENESS AND MEDICAL CHEMISTRY OF SCREENED COMPOUND

Lipinski	yes
Ghose	yes
Veber	yes
Egan	yes
Muegge	yes
Bioavailability score	0.55
PAINS	0
Brenk	2
Leadlikeness	yes
Synthetic accessibility	2.00

4.4 Antimicrobial Activity

In the antimicrobial assay, the crude extracts of *Pinus roxburghii*, *Cedrus deodara*, and *Abies pindrow* plant barks, dissolved in distal water, ethanol and methanol, were tested

against the bacterial strain *Staphylococcus aureus* and *psuedomonas aeruginosa*. The results are presented in the table.

TABLE 9: SHOWS THE ZONE OF INHIBITION BY DISC DIFFUSION METHOD

S.NO	Bacterial strains	solvent	Plant extract(ZOI)	Antibiotic disc (ZOI)	Distilled water disc (ZOI)
1.	*S.aureus*	*Abies Pindrow*(Ethanol)	1.9mm	-	-
2.	*S.aureus*	*Pinus Roxburghii*(Methanol)	2.3mm	2mm	3.3mm
3.	*S.aureus*	*Pinus Roxburghii*(Ethanol)	1.9mm	2.6mm	3mm
4.	*S.aureus*	*Cedrus deodara*(Methanol)	1.3mm	1.3mm	3mm
5.	*S.aureus*	*Abies Pindrow*(D.water)	1.3mm	1.5mm	2.7mm

TABLE 10: SHOW THE ZONE OF INHIBITION BY WELL DIFFUSION METHOD

S.NO	Bacterial strains	Solvent	Plant extract (ZOI)	Antibiotic disc (ZOI)	Distilled water disc(ZOI)
1.	*S.aureus*	*Abies Pindrow*(Ethanol)	2.8mm	-	-
2.	*S.aureus*	*Pinus Roxburghii*(Methanol)	1.5mm	-	-
3.	*S.aureus*	*Pinus Roxburghii*(Ethanol)	1.3mm	-	-
4.	*S.aureus*	*Cedrus deodara*(Methanol)	2.2mm	-	-
5.	*S.aureus*	*Abies Pindrow*(D.water)	2.6mm	-	-

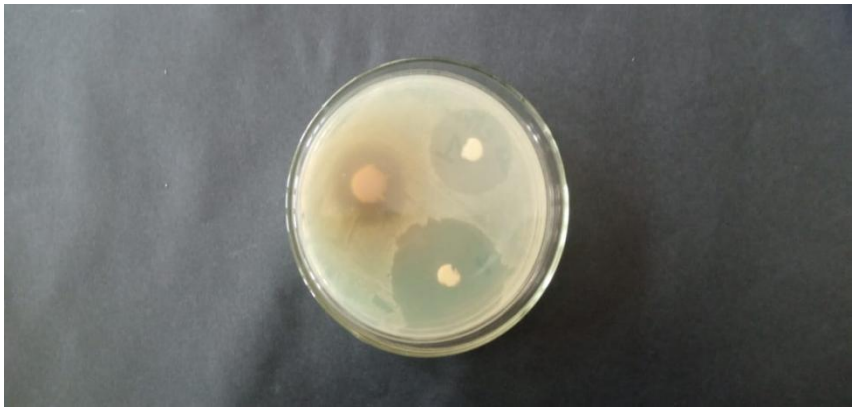

Figure 9: Zone of inhibition of Distilled water of *Pinus Roxburghii*(Ethanol) by disc diffusion method

TABLE 11: *SHOWS THE ZONE OF INHIBITION BY DISC DIFFUSION METHOD*

S.NO	Bacterial strain	solvent	Plant extract(ZOI)	Antibiotic disc(ZOI)	Solvent
1	*P.aruginosa*	*Pinus*(Ethanol)	20mm	-	-
2	*P.aruginosa*	*Pinus*(Methanol)	21mm	-	-
3	*P.aruginosa*	*Pinus*(D.water)	17mm	-	-
4	*P.aruginosa*	*Cedrus*(Methanol)	12mm	-	-
5	*P.aruginosa*	*Cedrus*(Ethanol)	12mm	-	-
6	*P.aruginosa*	*Abies*(Methanol)	13mm	-	-
7	*P.aruginosa*	*Abies*(D.water)	15mm	-	-
8	*P.aruginosa*	*Abies*(Ethanol)	18mm	-	-

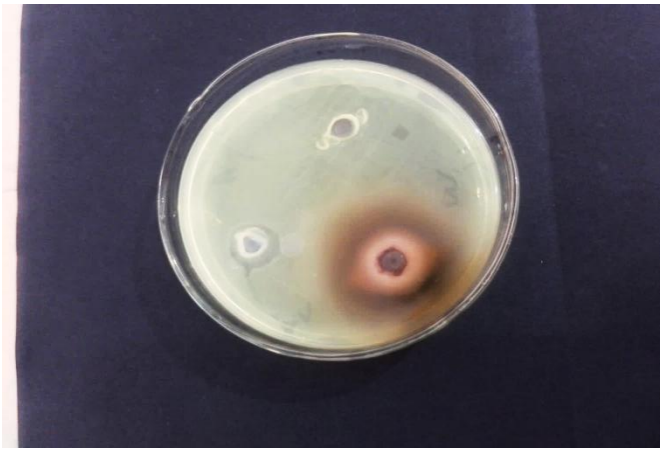

Figure 10: Zone of inhibition of Aqueous Ethanolic extract of *Pinus roxburghii* by well defusionn method

5. CONCLUSION

This study integrated experimental and computational approaches to evaluate the antimicrobial and pharmacological potential of three Himalayan conifers—*Pinus roxburghii*, *Cedrus deodara*, and *Abies pindrow*. Bark samples were shade-dried, powdered, and extracted using ethanol, methanol, and distilled water. Antibacterial activity was assessed through disc diffusion and well diffusion methods against *Staphylococcus aureus* and *Pseudomonas aeruginosa*, while molecular docking studies were conducted using MOE software to explore ligand–protein interactions. Drug-likeness and medicinal chemistry properties were further evaluated using the SwissADME platform. The results demonstrated that plant extracts exhibited measurable antibacterial activity, with solvent type significantly influencing efficacy. Methanolic extracts of *P. roxburghii* showed the highest inhibition zone (21 mm) against *P. aeruginosa*, while ethanol and aqueous extracts also produced moderate effects. *A. pindrow* and *C. deodara* displayed comparable though slightly lower activities. Molecular docking analyses revealed strong binding affinities of selected

phytochemicals, with isovelleral (–6.19), apigenin (–5.34), and phosphoamino-phosphonic acid-adenylate ester (–5.94) exhibiting the most favorable scores and stable interactions with target proteins. Drug-likeness profiling confirmed compliance with multiple filters for compounds such as apigenin and kaempferol, though some variability in bioavailability was observed. The findings highlight the dual significance of these conifers: their crude extracts possess promising antibacterial potential, and their phytochemicals exhibit favorable molecular interactions with bacterial proteins. This validates their ethnomedicinal relevance and identifies potential leads for further preclinical and pharmacological investigation, contributing toward the search for novel therapeutic agents against resistant pathogens.

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