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Phytochemical Profiling and In-Silico Investigations of *Cyperus Rotundus* Essential Oil for Targeting Fungal Pathogens

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KEYWORDS

Cyperus rotundus, Insilico studies, Candida albicans, Trichophyton rubrum, phytochemical profiling

ABSTRACT:

Background: Essential oil (EOs) obtained from the rhizomes of Cyperus rotundus is composed of numerous volatile phytochemicals belonging mainly to monoterpene and sesquiterpene groups and responsible for various pharmacological activities.

Aim: The primary objective of our work was the insilico evaluation of the antifungal effectiveness of an essential oil of Cyperus rotundus against the strains of fungus "Candida albicans" and "Trichophyton rubrum."

Material and Methods: Hydrodistillation performed for essential oil extraction, and the combined GCMS and GLC evaluation verified that the primary composition was cyperene. FTIR confirm the presence of active components by functional group detection. To validate the in vitro test, an in computational investigation using docking molecules and MM-GBSA was also carried out.

Results: According to molecular findings, an essential oil component does, in fact, act as a strong inhibitor of pathogenic strains. Rotundene had the greatest docking grade between the components (−4.262 kcal/mol), followed by copaene and longiverbenone, suggesting moderate binding affinity toward the target protein in Trochophytum rubrum. In case of Candida albicans, rotundene demonstrated a more favourable docking score (−7.276 kcal/mol) than fluconazole (−6.204 kcal/mol), indicating a stronger predicted binding affinity at the active site.

Conclusion: Study confirm that essential oil of Cyperus rotundus can be effective against pathogenic fungus in in-vivo studies.

INTRODUCTION

Having been used for thousands of years, Ayurveda is the most well-known conventional healthcare in India. Because of its in-depth knowledge about alternative remedies, Ayurveda has greatly influenced modern study. In addition to being crucial for numerous biological activities, essential oil compounds are sometimes referred to as natural antibacterial substances. Their wide range of antimicrobial properties renders them a suitable option. It does not support resistance-building due to its special function. In today's scientific industry, essential oils are crucial.[1] Often referred to as nut grass, Nagarmotha is a perennial single-celled plant that is a member of the Cyperaceae family (*Cyperus rotundus*). Its capacity to adapt to many conditions is responsible for its wide dissemination; it spreads mainly via its rhizomes, which may expand in all directions upward, or downward. This plant's calming, pain reliever, and antispasmodic qualities make it a popular herbal treatment.[2]

Essential oil (EOs) obtained from the rhizomes of *Cyperus rotundus* is composed of numerous volatile phytochemicals belonging mainly to monoterpene and sesquiterpene groups. Identified components include α-pinene, sabinene, β-pinene, p-cymene, limonene, cineole, terpinen-4-ol, citronellal, α-terpineol, myrtenol, verbenone, carvone, carveol derivatives, and dihydrocarvone. In addition, several sesquiterpenoid compounds such as α-cubebene, α-copaene, isolongifoline, cyperene, trans-caryophyllene, aromadendrene derivatives, selinene, calamenene isomers, caryophyllene oxide, cyperone derivatives, aristolone, vulgarol, vellerdiol, ledenoxide, longiverbenone, longifolinaldehyde, and longipinocarvone have also been reported. Other minor constituents, including bicyclic ketones, alcohols, and

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oxygenated terpenoids, further contribute to the complex chemical profile of the rhizome essential oil (Fig. 1).[3,4]

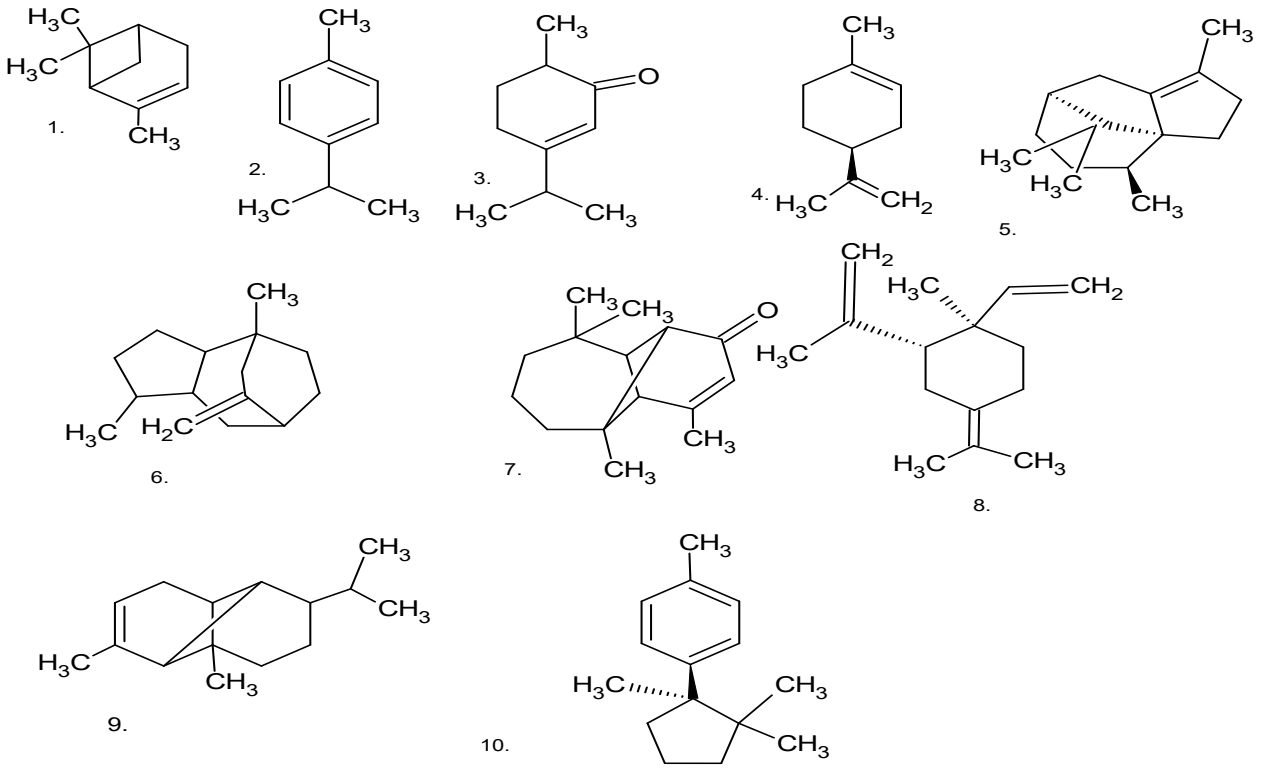

Figure 1: (1) 2,6,6-trimethylbicyclo[3.1.1]hept-2-ene (or α-pinene), (2) 1-methyl-4-propan-2-ylbenzene (or p-cymene), (3) 6-methyl-3-propan-2-ylcyclohex-2-en-1-one (or Carvenone), (4) (4S)-1-methyl-4-prop-1-en-2-ylcyclohexene (or (-) Limonene), (5) (1*S*,7*S*,10*S*)-4,10,11,11-tetramethyltricyclo[5.3.1.0[1,5]]undec-4-ene (or α-cyperene) (6) 1,5-dimethyl-9-methylidenetricyclo[6.2.2.02,6]dodecane (or Rotundene), (7) 2,6,6,11-tetramethyltricyclo[5.4.0.02,8]undec-10-en-9-one (or longiverberone), (8) (1S,2S,4S)-1-methyl-2-(1-methylethenyl)-4-(prop-1-en-2-yl)cyclohexene (gamma elemene), (9) Tricyclo[4.4.0.02,7]dec-3-ene (or α-copaene), (10) 1-methyl-4-[(1R)-1,2,2-trimethylcyclopentyl]benzene (or Cuparene).

Fungal infections are often classified into four main groups: regional mycoses, dermal mycoses, dermatology, and miscellaneous mycoses. These organisms, which infest and proliferate on decomposing bovine connective tissue, cause a disease known as dermatophytosis, or skin peeling. The three principal genera related to epidermal microalgae are Epidermal algae, Microsporum, which stands for and Trichophyton, among other genera.[5] *Candida albicans* is the most often involved type in candidiasis, a term used to describe bacterial infections caused by *Candida* spp. Although both itraconazole and fluconazole are frequently employed to treat these infections, they have resulted in azole resistance in Candida species. With a focus on concentration dependency, we currently know very little about the exact mechanisms that govern the action of EOs. Loss of membrane integrity, decreased ergosterol levels, suppression of transmembrane ATPases and cytokine interactions, a decrease in wall construction, and inhibition of transcription are often some of the apparent consequences of EOs. Therefore, it is thought that the characteristics of the corresponding main component are related to the efficiency of the antifungal features; nevertheless, consistency of evaluation methods and measuring subunits is crucial for future comparability and research.[6]

To streamline lead identification and reduce experimental attrition, a rational target-based strategy was employed in the present study. First, in order to anticipate binding affinities and important interactions

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between molecules, simulated silico testing was performed against certain fungus protein targets that were retrieved through the Protein Information Bank. Compounds exhibit better docking scores and favorable binding profiles than the standard drug. Based on these results, the oil was subsequently subjected to in vitro antifungal evaluation to validate their biological efficacy and to establish a correlation between computational predictions and experimental outcomes.

MATERIAL AND METHODS

Extraction of *Cyperus rotundus* essential oil & its yield determination:

To reduce the size of the cleaned rhizome, they were smashed. The following shows how the essential oil was extracted from the crushed samples using hydrodistillation. 750 milliliters of purified water were added to a 1000 ml bottomed round flask containing crushed rhizome segments. After the boiling potatoes were added, the flask was warmed for three to four hours. In the Clevenger apparatus, the distillate separates into two layers, with water vapour at the bottom and molecules of organic matter at the top. The anhydrous form of sodium sulphate was used to dry the organic component after it had been collected in tiny vials. The essential oil's weight was determined, and the resulting oil yield % was computed.[7,8]

The formula that was used for calculating percentage oil yield is

$$\% \ yield = mass of oil \ / mass of sample used x \ 100$$

Physiochemcial Characterization of extracted oil:

Odor

A little quantity of the volatile oils was placed on a piece of paper towel, and the paper towels then gently waved under the nose to detect the odor. A number of common terms—floral, woody, citrus, medicinal, hot, spicy, minty, aromatic pine, and vanilla-like—as well as separate categories of each—soft, dominant, soothing, energetic, pleasant, fruity, soft, smooth, icy, acidic, bitter acidic, sweet, full, and flat—were used to convey the fragrance of essential oils.[9]

Specific gravity, Optical rotation and Refractive index

Using the particular gravity bottle, the oil's specific gravity was ascertained. When calculating optic movement, a 10-milliliter oil-filled polarizing tube was put into the device's trough between the polarizer and analyser. The conduit is carefully filled to prevent air bubbles from entering and tampering with the light's spin. Slowly rotating the analyzer allowed the observatory to examine both half of the field. The rotation was found to be levo (-) if clockwise and dextro (+) if reversed. The detector was rotated counterclockwise from the point where it stopped to get the final measurement. With Abbe's refractometer the oil's refraction coefficient was measured at 34 °C.[10]

Gas Liquid Chromatography

Gas Liquid Chromatography (GLC) instrument (Alginate Technology) equipped with FID detector at 40 ℃ temperature in packed column was used in analyzing the volatile constituents of the essential oil.

Fourier Transform Infrared Spectroscopy

Fourier Transform Infrared Spectroscopy was used for the detection of active function groups present in the essential oil. The spectra were recorded in the range of 4000-650 cm^{-1}.[11]

Gas Chromatography Mass Spectroscopy

The molecular composition of the material was ascertained by means of gas chromatography coupled with mass spectrometry (GC–MS)vital oil of Nagarmotha (*Cyperus rotundus*).[12] Assuming ideal circumstances, an automatic fluid sampler was used to inject the collected material. To guarantee constant sampling uptake, the plunger speed was kept high throughout both evacuation and injection, with a viscous compensatory time of 0.2 s. To improve sample homogeneity, five hammering strokes were used before injection, and the syringe inserting speed was modified to high.No terminal air gap was used. The syringe was washed at high plunger speed using a washing volume of 6 µL, employing solvents A, B, and C to prevent sample carryover.

A column oven's temperature was originally kept at 40.0 °C for the separation chromatography process. To provide improved sensitivity for volatile substances below the trace level, the sample was injected in splitless mode and the injector temperatures was adjusted to 250.0 °C. A divided sample duration of one minute continued to be used. With an intake pressure of

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49.5 kPa, flow control was run in pressure mode using helium as the carrier gas. A linear speed of 36.1 cm/s was attained by maintaining the column's rate of flow at 1.0 mL/min. After the splitless time, a purging velocity of three mL/min was given, with the overall flow rate being 14.0 mL/min. Standard ionization electron (EI) settings (70 eV) were used for mass spectrometric detection. Individual components of the essential oil were identified by examining their retention behavior and comparing mass spectra to those found in the NIST mass spectral collection. Reliable quantitative characterization of the volatile along with semi-volatile components found in Nagarmotha essential oil was made possible by the GC–MS investigation.

Insilico studies:

Ligand Preparation

Using ChemDraw 22.2.0 64-bit, the structures of cyperene, cuparene, rotundene, longiberverone, copaene, gamma-elemene and the standard drug fluconazole were drawn and saved in sdf format. Then the LigPrep module of Schrödinger Maestro (Version 12.5) was employed to prepare the test ligands and standard by generating energy-minimized 3D structures, appropriate tautomers, and correct protonation states. This ensures that all the ligands were in their most stable forms for subsequent molecular docking studies.

Preparation of Protein

The experimentally determined three-dimensional (3D) crystal structure of *Candida albicans* (PDB ID: 5V5Z), and *Tryphophyton rubrum* (PDB ID: 7P1R), were retrived from the RCSB Protein Data Bank. These structures, with resolutions of 2.90 Å and 1.75 Å, respectively, were employed for molecular docking studies. Both structures of proteins were prepared using Schrödinger Maestro's Proteins Prep Wizard (version 12.5) before docking.To guarantee the stability of the structure, the process included allocating appropriate bond arrangement, eliminating unnecessary side chains or remains of heteroatoms in particular and unneeded molecular water molecules, and then optimizing and minimizing energy applying the OPLS4 electrostatic force field.Subsequently, receptor grids were generated using the Schrödinger receptor grid generating tool's default parameters. The grid was formed by picking a particular active site segment on the respective protein chains to localize the docking site.

Protein-ligand docking

Molecular docking of the test ligands and the standard drug fluconazole into both the target proteins (PDB IDs: 5V5Z, and 7P1R) was performed using the Glide module of Schrödinger Maestro (version 12.5) under the OPLS3e force field, employing the Standard Precision (SP) mode with default parameter using the procedure reported by Gupta *et al*.[13] Docking poses and protein–ligand interactions were visualized and analyzed using Schrödinger Maestro Version 12.5. The docking outcomes were assessed according to the docking rating (kcal/mol) and various chemical connections to enzymes (pi-pi interactions, bonds of hydrogen, bridges of salt, etc.).

MM-GBSA Analysis

The Molecular Dynamics Generalized Born Surface Model (MM-GBSA) can be used to compute the liberated energy of binding for molecular compounds. The MM-GBSA analysis of the under consideration ligands was conducted with the primary instrument of Heisenberg Suite 12.8, employing the VSBG expulsion model with the OPLS4 force field. To further refine the experiment's compounds and validate the docking results, the released binding strengths (ΔG bind) associated with the receptor-ligand complex were calculated using MM-GBSA as the basis. The methodology outlined by Parveen et al. [14] was adhered to.

RESULTS AND DISCUSSION

Extraction of *Cyperus rotundus* oil and its yield determination:

The essential oil of *Cyperus rotundus* was extracted by using the Clevenger apparatus.

Weight of oil obtained = 1.4 gm

Weight of plant material taken = 100 gm

Yield value = weight of oil obtained/ weight of plant sample taken * 100

= 1.4/100* 100

= 1.4%

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Physiochemical analysis of *Cyperus rotundus* essential oil:

The results of physiochemical analysis represented in Table 1. The extracted oil was evaluated at 27 °C temperature.

Table 1: Physiochemical analysis of *Cyperus rotundus* essential oil

S. No.	Parameter	Results
1.	**Color**	Amber
2.	**Odor**	Woody type
3.	**Optical Rotation (**at 27 °C)	-2.0
4.	**Specific gravity (**at 27 °C)	0.960
5.	**Refractive index (**at 27 °C)	1.510
6.	**Yield value**	1.4%

GLC

Cyprene was identified as the main constituent present in the nagarmotha oil at the concentration of about 26.94% which is highest among all present constituents. Different peaks at different time intervals signify the presence of different components (Fig. 2).

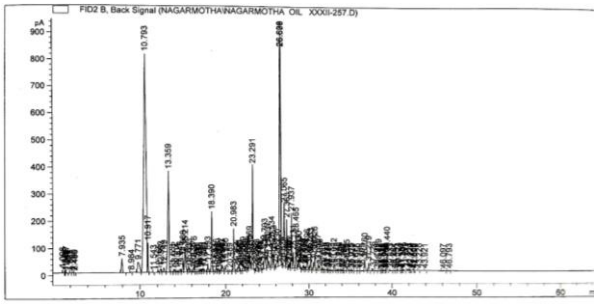

Figure 2: GLC of *Cyperus rotundus* oil

FTIR

Typically, peaks belonging to different functional groups were seen in the essential oil of *Cyperus rotundus*, also known as nutgrass or nagarmotha. This plant is rich in a variety of sesquiterpenes and other chemical substances.The oil is typically rich in sesquiterpenes such as cyperene, cyperotundone, α-cyperone, and rotundone. These components contribute to many of the functional groups mentioned above.

- **Sesquiterpenes**: Expect strong C–H stretches (2800–3000 cm^{-1}) and C=C stretches (1600–1680 cm^{-1}). In the graph peak at 3474.16 and 2925.71 cm^{-1} revealed the peak of C-H stretching. C=C stretching was observed through the peak 1661 cm^{-1}
- **Oxygenated Sesquiterpenes** (like cyperone or rotundone): Could contribute to C=O or C–O stretches, though these are often weaker in intensity. The peak at 1706.76 cm^{-1} detects the presence of carbonyl group in the essential oil.[15]
- The peaks at fingerprint region i.e., at 886.53 cm^{-1}, 751.02 cm^{-1}, 601.72 cm^{-1} confirms the overlapping peak of C-C and C-H bonding (Table 2, Fig. 3).

Table 2: FTIR peaks of *Cyperus rotundus* oil

Peak Number	X (cm-1)	Y (%T)	Functional group identified
1.	2921.73	70.35	C–H stretches (Strong)
2.	2868.37	78.39	C–H stretches (Strong)
3.	1706.79	78.65	Carbonyl group (C=O or C–O stretches)
4.	1664.87	80.08	C=C stretches
5.	1460.95	80	C-H bending vibrations
6.	1374.18	81.52	These peaks due to the C-O stretching (generally due to the esters, ethers, alcohols).
7.	1327.69	89.74	
8.	1275.99	89.98	
9.	1158.81	89.25	
10.	1065.69	87.74	C-O stretching v
11.	982.57	89.26	C-H bending

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12.	886.17	84.59	C-C & C-H bonding
13.	542.69	90.88	C-C & C-H bonding
14.	455.74	89.37	C-C & C-H bonding

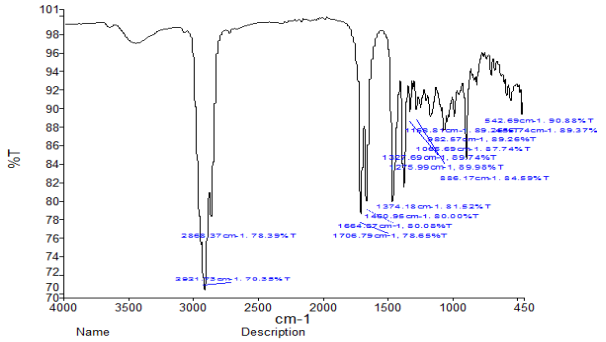

Figure 3: FTIR peaks of *Cyperus rotundus* oil

GCMS

GCMS data identifies the major active constituents present in the essential oil through the NIST library **(Table 3).**

Table 3*:* GCMS of *Cyperus rotundus* essential oil

S. No.	Constituents	Retention Index
1.	Isolaricriesinol	3844
2.	Cuparene	1556
3.	Copaene	1221
4.	Curcumene	1524
5.	Cyperene	1432
5.	Rotundene	1450
6.	Gamma-Elemene	1431
7.	Longibervenone	1574

Docking and MM-GBSA Analysis of constituents with Protein 5v5z:

The molecular docking and MM-GBSA binding free energy analysis against *Candida albicans* PDB ID 5V5Zrevealed that several constituents exhibited comparable or superior binding interactions with the target protein when compared to the reference drug fluconazole. Notably, rotundene demonstrated a more favourable docking score (−7.276 kcal/mol) than fluconazole (−6.204 kcal/mol), indicating a stronger predicted binding affinity at the active site. Similarly, copaene (−7.050 kcal/mol), cuparene (−6.497 kcal/mol), longiverbenone (−6.268 kcal/mol), and γ-elemene (−6.267 kcal/mol) also showed docking scores equal to or better than fluconazole.

MM-GBSA binding free energy calculations further supported these findings. While fluconazole exhibited the most negative ΔG_bind value (−37.99 kcal/mol), rotundene (−36.71 kcal/mol) and copaene (−35.20 kcal/mol) showed closely comparable binding free energies, suggesting stable protein–ligand complexes. These results indicate that certain constituents, particularly rotundene, possess binding affinities and interaction stability comparable to or exceeding that of the standard antifungal agent.The docking scores and MM-GBSA obtained binding free energiesof all the constituents and fluconazole are reported in Table 4.

Overall, the combined docking and MM-GBSA analyses suggest that selected constituents may serve as promising lead molecules with potential antifungal activity against the target protein.

Table 4: Docking scores of Nagarmotha oil constituents against *Candida albicans* and their

MM-GBSA binding free energies (ΔG bind)

Compound	Docking Score (kcal/mol)	MM-GBSA (dG Bind)
Rotundene	-7.276	-36.71
Copaene	-7.050	-35.20
Cuparene	-6.497	-30.24
Longiverbenone	-6.268	-31.46
Gamma elemene	-6.267	-34.97
Cyprene	-5.905	-31.77
Fluconazole	-6.204	-37.99

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Docking and MM-GBSA Analysis of constituents with Protein 7P1S:

Docking analysis against *Trichophyton rubrum* (PDB ID: 7P1S) revealed that fluconazole exhibited a more favorable docking score (−5.601 kcal/mol) compared to all the tested constituents, indicating stronger predicted binding at the docking stage. Among the constituents, rotundene showed the best docking score (−4.262 kcal/mol), followed by copaene and longiverbenone, suggesting moderate binding affinity toward the target protein.

Interestingly, MM-GBSA binding free energy calculations presented a different trend. Several constituents demonstrated more negative ΔG_bind values than fluconazole (−9.31 kcal/mol), indicating enhanced complex stability after binding. Notably, γ-elemene (−16.94 kcal/mol), cuparene (−15.78 kcal/mol), and rotundene (−14.67 kcal/mol) showed substantially more favorable binding free energies, suggesting stronger and more stable protein–ligand interactions than the reference drug.The docking scores and MM-GBSA obtained binding free energiesof all the constituents and fluconazole are reported in Table 5**.**

The observed discrepancy between docking scores and MM-GBSA results highlights the importance of post-docking free energy calculations, as MM-GBSA accounts for solvation effects and interaction energies that are not fully captured during docking. Overall, although fluconazole exhibited superior docking performance, several constituents—particularly γ-elemene, cuparene, and rotundene—demonstrated improved binding stability, supporting their potential as promising antifungal lead compounds.

Table 5: Docking scores of Nagarmotha oil constituents against *Trichophyton rubrum*

and their MM-GBSA binding free energies (ΔG bind)

Compound	Docking Score (kcal/mol)	MM-GBSA (dG Bind)
Rotundene	-4.262	-14.67
Copaene	-3.809	-10.58
Longiverbenone	-3.739	-12.17
Gamma elemene	-3.356	-16.94
Cuparene	-3.293	-15.78
Cyprene	-2.590	-8.92
Fluconazole	-5.601	-9.31

CONCLUSION

The treatment of diseases gets more difficult as microorganisms become resistant to different medications, which raises mortality rates, lengthens illness, makes infections more severe, and raises healthcare expenses. Research on new antimicrobial agents has focused on essential oils, which are volatile and lipophilic combinations of chemicals and can be serve as the new therapeutic agents against the pathogenic strain. The phytochemical profiling of the extracted oil revealed that the extracted oil was of highest quality with good extractive value. Insilico analysis revealed the potency of *Cyperus rotundus* essential oil against the *Candida albicans* and *Trichophyton rubrum*. The results indicate that certain constituents, particularly rotundene, possess binding affinities and interaction stability comparable to or exceeding that of the standard antifungal agent when evaluated against the *Candida albicans* while in case of *Trichophyton rubrum*, fluconazole (standard drug) was found to be more superior. GCMS and GLC revealed the cyperene as the main constituents while insilico studies depicted the importance of rotundene in the antifungal potential.

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