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Gas chromatography flame ionization detection of alkaloids, phytochemicals, antimicrobial and antifungal potential of *Ageratum conyzoides* leaf extract *in vitro* and in silico studies

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Abstract

Bacterial and fungal infections remain prevalent in the world especially African countries. Ageratum conyzoides is a plant with many medicinal uses found across many African countries. The aim of the present study was to evaluate the phytochemical, antibacterial, antifungal properties of methanolic extract of Ageratum conyzoides in vitro and molecular docking studies. Gas chromatographic flame ionization detection (GC-FID), spectrophotometric and antimicrobial assays were determined, also in silico methods were also carried out. The qualitative phytochemical results revealed the presence of tannins, saponins, alkaloids, phenols and flavonoids. Quantitative bioactives detected were tannins 10.76 ± 1.52 g/L, alkaloids 3.67 ± 1.07 %, phenols 39.42 ± 3.6 mg GAE/g, and flavonoids 24.34 ± 2.06 mg QE/g. The GC-FID analysis revealed many important alkaloids like camptothecin, jatrorrhizine, chelidonine, strychnine, stachdrine and leonurine which were docked against dihydrofolate reductase (PDB ID: 1AI9) and pectin lyase (PDB ID: 11DK).The extract (Ageratum conyzoides) inhibited Staph aureus, K. pneumoniae and P. aeruginosa at 100 mg/ml. A zone of inhibition of 11 mm, 8 mm and 7 mm respectively was recorded. The antifungal properties of Ageratum conyzoides revealed a zone of inhibition of 13 mm against Mucor sp at 100 mg/ml.Also the docking studies revealed high docking scores for leonurine −6.13 kcal/mol against pectin lyase, chelidonine −5.65 kcal/mol and Jatrorrhizine and camptothecin −6.81 and −6.40 kcal/mol respectively against dihydrofolate reductase. In conclusion, Ageratum conyzoides is a source of potential alkaloids useful as therapeutic agents against microbial infections.

Keywords: *Ageratum conyzoides, microbes, in silico analysis, bioactives and infection.*

Introduction

Infection caused by fungi is a growing public health concern especially in immune-compromised patients. The incidence of fungal infections is steadily increasing year after year [1]. About three hundred fungals cause devastating fungal infections in humans [2]. Fungal infections are grouped into superficial mycoses, opportunistic infections, and systemic infections. The fungal infections implicated in many clinical conditions are the general candida, penicillium and Aspergillus [1]. About 1.5 million deaths and 13 million fungal infections are recorded per year, especially in compromised immune individuals [3]. A major clinical factor contributing to the increase of fungal infections in patients is drug resistance, also anti-fungal therapies like azoles that inhibit 14-α-lanosterol demethylase (fluconazole) and polyenes that inhibits ergosterol from membrane formation (Amphotericine) have encountered some limitations due to off-target effect and the development of resistance strains [4]. Also long term ventilation in critically ill patients has a higher rate of fungal infections in hospital setting [5]. Additionally, fungal pathogens can thrive in an environment altered by antibiotics, making them an opportunistic to establish infections [6]. Various factors that increased fungal infection rate are organ transplantation, the use of anti-cancer drugs, parenteral nutrition, treatment with corticosteroids, dialysis, prolonged use of catheters and antibiotics [6].

Millions of individuals continue to die from bacterial infections every year despite the huge developmental strides in science and technology.

Due to poverty and ignorance leading to overuse and misuse of over the counter antimicrobial drugs, this has really led to the emergence of antimicrobial resistance, resulting in millions of deaths in 2019 [7,8]. Apart from antimicrobial resistance due to mutation also sepsis a life threatening condition in which there is an uncontrolled response of the immune system to infection leading to the malfunctioning of vital organs [8]. In the United States, about 1.7 million people develop sepsis due to prolonged usage of antibiotics, leading to thousands of deaths [9]. The burden of antimicrobial resistance is forecasted to rise to 1.91 million deaths and 8.22 million deaths by 2050 [9]. Therefore, there is a drastic need for a reduction in anti-bacterial mortality now.

Ageratum conyzoides also known as goat weed, belongs to the plant family Asteraceae. It is found in Central America, Africa, Asia and South Pacific Islands [10]. It grows up to about 1 meter high, with small flowers, it can quickly dominate the ecology as an aggressive weed and it also possess aromatic properties [11]. The plant contains bioactives ranging from flavonoids, coumarins, alkaloids, terpenoids, essential oils and minerals [12-16]. Due to the presence of these bioactives, Ageratum conyzoides is used traditionally for the treatment of wounds, diabetes, fever, and many infectious and inflammatory diseases [15,17, 18]. Ageratum conyzoides has also been reported for antioxidant and free radical scavenging ability [19]. It also has antiflammtory, antibacterial and antihyperglycemic properties [15, 14. 20]. Therefore, this study aims to evaluate the phytochemicals and antimicrobial of *Ageratum conyzoides* in vitro and *in silico*.

Materials and Method

Chemical/Reagents

Sodium hydroxide, $FeCl_3$, KI, iodine, lead acetate, $NaNO_2$, $AlCl_3$, Folin-Ciocalteu reagent, acetic acid, Sodium carbonate (Na_2CO_3), DMSO, methanol, ethanol, hydrochloric acid, normal saline, getamicin Injection, fluconazole, gallic acid, quercetin are all standard chemicals obtained from Fluka.

Plant collection and Identification

Fresh leaves of *Ageratum conyzoides L.* were collected from the Niger Delta University Botanical Garden. The plant was identified/authenticated and voucher specimen deposited at the Herbarium of the Department of Pharmacognosy and Herbal Medicine, Faculty of Pharmacy, Niger Delta University, Wilberforce Island, Bayelsa State, Nigeria, with Herbarium number NDUP/040.

Preparation of Plant Extract

The plant leaves were collected in large quantity, washed and left under shade at room temperature for two weeks to dry. Afterwards, they were ground into a fine powder. 500g of the powder was soaked in 1000ml of methanol and allowed to stand for 72 hours. The extract was filtered and centrifuged and the filtrate was evaporated in a water bath at 50 ^{0}C. The paste formed was stored in the refrigerator for further use.

Qualitative phytochemicals

The presence of tannins, saponins, alkaloids, phenols and flavonoids were detected in *Ageratum conyzoides* extract according to the method of Harbone, [21].

Analysis of condensed tannins

The presence of condensed tannins in *Ageratum conyzoides* was based on the fact that in acid medium, tannins are transformed into anthocyanins when heated [22].

Two sets of tubes labelled series 1 and 2, in each tube 3ml of methanolic extract of *Ageratum conyzoides* were added, and 3ml of conc. HCl. One set of tubes were heated in a water bath at 100°C for 30 mins, followed by cooling to room temperature.

The other set of tubes were placed at room temperature for 30mins. Later 0.5ml of ethanol was added to both sets of tubes and the absorbance was read at 550nm. The condensed tannins were detected through the following formular:

$CT = (OD_1 – OD_2) X 19.33 (g/L)$

Where:

CT = Condensed tannins

OD_1 = Optical density of tubes heated at 100°C

OD_2 = Optical density of tubes kept at room temperature

Flavonoid content

The total flavonoid content in *Ageratum conyzoides* was determined according to Zhishen et al., [23]. Exactly 0.5ml of distilled water was added to extract (1mg/ml) followed by the addition of 5% $NaNO_2$ (60 µL). This solution was kept at room temperature for 5 min. Thereafter 60 µl of 10% $AlCl_3$ was added and 400 µl of 1M NaOH and 450 µl of distilled water also added to the solution and was kept at room temperature for 30min. Later absorbance of the mixture was read at 510 nm. Quercetin served as reference compound and results were reported as quercetin equivalent per gram extract.

Phenol Content

The total content of phenol in *Ageratum conyzoides* was based on the Folin – Ciocalteu method of Singleton et al., [24] and Demiray et al., [25]. *Ageratum conyzoides* methanolic extracts (1ml) was mixed with 1ml of ten-fold diluted Folin–Ciocalteu reagent and was kept for 5 min. After that 1ml of sodium carbonate (0.7M) was added and the solution was kept at room temperature for 1hr with occasional shaking for the development of color. The absorbance was recorded at 765 nm, and gallic acid served as the standard. Total phenol was extrapolated and reported as gallic acid equivalent per gram extract.

Alkaloid Content

The total amount of alkaloids in *Ageratum conyzoides* was determined according to Unuofin et al., [26]. A weighed amount of 5g *Ageratum conyzoides* in triplicate was soaked in 100ml of 10 % acetic acid in ethanol. The solution was left standing for 4 hours at 25° C. Later the solution was filtered.

The filtrate was concentrated in a thermostat bath at 55^0 C to a quarter of its original volume. Thereafter concentrated ammonium hydroxide was added in drops to precipitate all the alkaloids. The solution was filtered, and the alkaloids were weighed and calculated as percentage.

Quantification of alkaloids by gas chromatography flame ionization detector

Exactly 0.2g of *Ageratum conyzoides* was added to a tube containing 15 ml ethanol and 10 ml 50% KOH. The tube was heated at 60°C in a water bath for 3hrs. Thereafter the extract was transported into a separating funnel and the extracted phytochemicals were solubilized in pyridine for alkaloid analysis. The GC-FID detection of alkaloid from *Ageratum conyzoides* was carried out using Agilent 6890 gas chromatography coupled with a flame ionization detector. Also a 15mm x 0.15mm MXT – 1 column was used. The injection temperature was 280°C and the carrier gas was helium with a flow speed of 40ml/min. Alkaloids were detected and expressed as ppm [27].

Antimicrobial activity of extract

Preparation of the extract concentrations: 100mg/ml, 50mg/ml and 25mg/ml concentrations were respectively prepared for each extract using 50% DMSO.

Preparation of Standard Microbial Inoculum: A standard inoculum of each of the isolate (*Staphylococcus aureus, Klebsiella pneumoniae, Pseudomonas aeruginosa, Candida albican, Aspergilus niger* and *Mucor* specie) was prepared by suspending few discrete colonies of the respective isolate into a sterile normal saline. The resultant turbidity for each suspension was matched/compared with that of 0.5M MacFarland standard.

Evaluation of Antimicrobial Activity of the Extracts against the Standardized Microbial Inocula: Antimicrobial activity of the extracts was assayed using the Agar Well Diffusion method with little modification. Mueller Hinton and Sabouraud Dextrose Agar media were prepared according to their manufacturer's instruction and poured into different sterile petri dishes to a depth of about 4mm and were allowed to set.

Thereafter, 0.2ml of each standardized inoculum was used to inoculate the appropriately labelled agar plate(s) surface(s) and spreading was done using the glass spreader. An 8mm sterile cork-borer was then used to make wells on the inoculated agar plates and the bottom of the wells were sealed with molten agar. Using a sterile glass pipette, a given volume of the prepared compounds' concentration were respectively added into the various wells and allowed to diffuse for one hour prior to incubation. Fluconazole antibiotics discs and Gentamicin injection solution where used as the standard drugs against the fungi and bacteria isolates. The agar plates were then incubated at 37^{0}C for 24hrs and the resulting zone diameters of inhibition were respectively measured around each of the extract concentration and recorded [28].

Molecular docking of *Ageratum conyzoides* bioactives

The molecular study of this work involves downloading the 3-D structures of the target proteins: Dihydrofolate reductase, PDB 1D, IAI9 and Pectin lyase, PDB 1D, 11DK from protein data bank (www.RCSBPDB.org). Also, the bioactives from *Ageratum conyzoides* methanolic extracts were camptothecin, jatrorrhizine, chelidonine, strychnine, leonurine and stachdrine were gotten from Pubchem. The downloaded proteins were prepared for docking studies by removing water and other group like the bound ligand, using the schrodinger suite. After this ligands (Ageratum conyzoides bioactives) were docked into the active site of dihydrofolate reductase and pectin lyase. Best docking poses were selected via 2-D visualization [29].

ADMET evaluation of *Ageratum conyzoides* bioactives

Absorption, distribution, metabolism, excretion, and toxicity of camptothecin, jatrorrhizine, chelidonine, strychnine, leonurine and stachdrine were predicted by ADMET lab 2.0. The parameters predicted were very important such as X log P, % human absorption and violation of Lipinski's rule [30].

Statistical analysis

All results were processed utilizing GraphPad prism and the mean ± SD (n =3) were presented.

Results

Percentage yield was 2.2g/50g x 100% = 4.4%

Table 1 Phytochemicals in *Ageratum conyzoides* methanolic extract

	Tannins	Saponins	Alkaloids	Phenols	Flavonoids
Qualitative	++	+	+	++	++
Quantitative	10.76±1.52g/L	N.A	3.67±1.07%	39.42±3.6mgGAE	24.34±2.06mgQE

Key + = present
GAE = gallic acid equivalent

QE = quercetin equivalent
N.A = not assayed

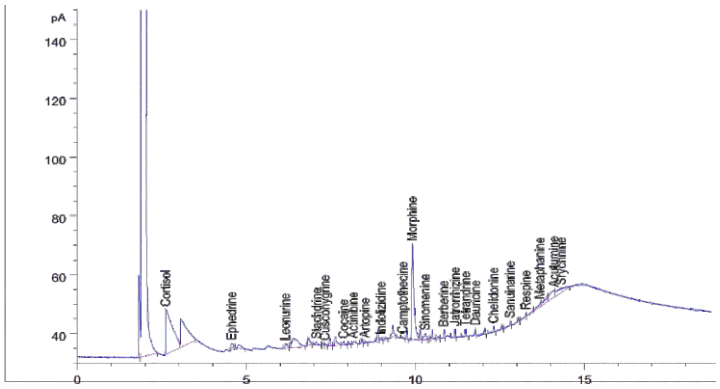

Fig 1: showing the GC-FID analysis of alkaloid in Ageratum conyzoides leave extract

Table 2: Showing retention time, amount and type of alkaloid detected in Ageratum conyzoides

S/N	RetTime (min)	Amount (ppm)	Compound
1	2.617	4.38452	Cortisol
2	4.567	1.24107	Ephedrine
3	6.160	1.54468	Leonurine
4	7.069	9.02883e-1	Stachdrine
5	7.334	2.65836e-1	Cuscohygrine
6	7.884	1.14995	Cocaine
7	8.174	9.05909e-1	Actinibine
8	8.517	2.19880e-1	Artopine
9	8.991	6.33522e-1	Indolizidine
10	9.618	1.76180e-1	Camptothecine
11	9.905	7.40094	Morphine
12	10.295	1.93921	Sinomenine
13	10.844	1.15437	Berberine
14	11.168	9.29261e-1	Jatrorrhizine
15	11.477	1.08953	Tetrandrine
16	11.769	5.66565e-1	Dauricine
17	12.310	6.88563e-1	Chelidonine
18	12.804	6.59585e-1	Sanguinarine
19	13.263	3.11100e-1	Respine
20	13.696	2.04746	Metaphanine
21	14.101	5.85880	Acutumine
22	14.310	6.01150	Strychnine
23	18.155	-	Nortopsentine

Table 3: Showing Antimicrobial effects of Ageratum conyzoides

	A. conyzoides			Gent
Isolate	100	50	25	25mg/ml
Staph aureus	11	0	0	26
K pneumonia	8	0	0	22
P aeruginosa	7	0	0	16

Fig 2: Antimicrobial effect of Ageratum conyzoides

The table shows the antimicrobial activity of Ageratum conyzoides against three bacterial isolates: Staphylococcus aureus, Klebsiella pneumoniae, and Pseudomonas aeruginosa. The effect is measured at different concentrations (100, 50 and 25 mg/ml), compared with standard antibiotics gentamicin respectively.

Table 4: Showing antifungal effects of Ageratum conyzoides

Isolate	A. conyzoides			FLU
	100	50	25	25mg/ml
C albican	0	0	0	0
A niger	0	0	0	0
Mucor sp	13	11	0	0

Fig 3: Antifungal effect of Ageratum conyzoides

The table presents the antifungal activity of *Ageratum conyzoides* against three fungal isolates: *Candida albicans*, *Aspergillus niger*, and *Mucor sp*. The effectiveness is measured at different concentrations: 100, 50 , and 25 mg/ml, compared with standard antifungal agent fluconazole at 25 mg/ml.

Table 5: Ligands and docking scores against dihydrofolate reductase PDB ID: 1AI9

	ligand name	Pubchem ID	1AI9 (kcal/mol)
1	Camptothecin	24360	-6.40
2	Jatrorrhizine	72323	-6.81
3	Chelidonine	197810	-6.34
4	Strychnine	441071	-5.04

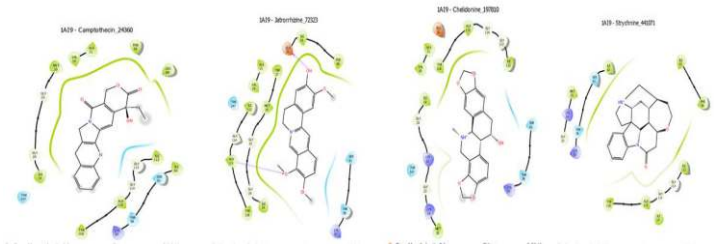

Figure 4: Docking poses of camptothecin, Jatrorrhizine, chelidonine and strychnine bound to the active site of dihydrofolate reductase PDB ID: 1AI9

Table 6. Ligands and amino acids interactions with 1AI9

S/N	Ligand name	Type of amino acid interaction with ligand		
		Hydrogen	Hydrophobic	Polar
1	**Camptothecin**		ILE-112, ALA-115, TYR-118, LEU-69, MET-25,	THR-147, SER-67, THR-58
2	Jatrorrhizine	ALA-115, GLU-32	ILE-19, MET-25, VAL-10, ILE-33	THR-147, SER-61, THR-58
3	Chelidonine	-	ILE-112, TYR-118, ILE-19, MET-25	THR-147, SER-61, THR-58
4	Strychnine	-	ILE-112, ALA-115, TYR-118, MET-25	SER-61, THR-58

Table 7: Ligands and docking scores against pectin lyase PDB ID: 11DK

1.	Ligand name	Pubchem ID	1IDK (kcal/mol)
2.	Leonurine	161464	**-6.13**
3.	Stachdrine	554	**-5.01**
4.	Jatrorrhizine	72323	**-4.74**
5.	Chelidonine	197810	**-5.65**

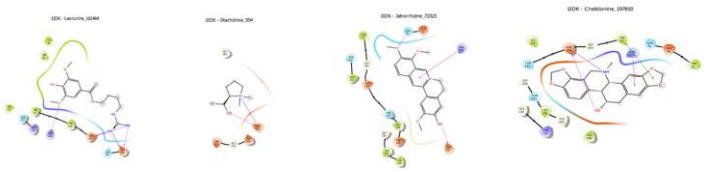

Figure 5: Docking poses of leonurine, stachdrine, Jatrorrhizine and chelidonine bound to the active site of pectin lyase PDB ID: 11DK

Table 7: Ligand interactions with 1IDK

S/N	Ligand Name	Type of amino acid interaction with ligand				
		Hydrogen	Hydrophobic	Polar	Salt bridge	Pi-cation
1.	Leonurine	ARG-236, ASP-242, ASP-217	TYR-215, TRP-212, TRP-151, TRP-81	GLN-177, GLN-241	-	-
2.	Stachdrine	ASP-242	-	-	ASP-242	-
3.	Jatrorrhizine	ASP-217	-	-	-	ARG-176
4.	Chelidonine	ASP-154,	VAL-180, LEU-102, ILE-145, TRP-151	THR-101, THR-157, GLN-78	ASP-154	ARG-176

Table 8: Drug Likeness – ADMET parameters predictions

Parameters/Sample ID	Leonurine	Stachdrine	Camptothecin	Jatrorrhizine	Chelidonine	Strychnine	Standard Ranges
Molecular Weight (g/mol)	311.33	143.18	348.35	338.4	353.4	334.41	130.0 / 725.0
Rotatable Bonds	9	1	1	1	2	0	0.0 / 15.0
H-Bond Donors	4	0	1	1	0	0	0.0 / 6.0
H-Bond Acceptors	7	2	5	4	5	4	2.0 / 20.0
TPSA (Ã…Â²)	103	34	79.7	44	66	32.8	7.0 / 200.0
XLogP (est)	-0.5	-2	1	1.6	2	0.6	-0.307692308
logS (est)	-1	-0.5	-4	-3.5	-3	-1.5	6.5 / 0.5
Lipinski violations	0	0	1	0	0	0	max 4
% Human Oral Absorption (est)	60% (moderate)	80% (high)	<25% (poor)	30-50% (low-moderate)	40-60% (moderate)	>80% (high)	<25% poor ; >80% high
Caco-2 (nm/s)	<25 (poor)	<25 (poor)	<25 (poor)	25-200 (low-mod)	50-300 (mod)	>500 (good)	<25 poor ; >500 great
MDCK (nm/s)	<25 (poor)	<25 (poor)	<25 (poor)	25-200 (low-mod)	50-300 (mod)		<25 poor ; >500 great
HERG concern	no (>-5)	No	possible (near -5)	possible	unlikely	no	concern if log IC50 < -5
logBB (est)	-1.5	-2.5	-1	-1.2	-0.9	0.5	-2.5
No. Primary Metabolites (est)	3	1	4	4	3	3	1.0 / 8.0
Globularity (est)	0.8	0.9	0.78	0.75	0.74	0.92	0.75 / 0.95
QP Polarizability (Ã…Â³, est)	25	8	32	31	34	22	13.0 / 70.0

Discussion

Preliminary phytochemical analysis of the methanolic extract of *Ageratum conyzoides* revealed the presence of tannins, saponins, alkaloids, phenols and flavonoid as depicted in table 1. The presence of these secondary metabolites are useful as antioxidant, anti-inflammatory, antimicrobial, immunomodulatory and metal ion chelating properties [31].

Also quantitative evaluation of phytochemicals in methanolic extract of *Ageratum conyzoides* shows the presence of tannins 10.76 ± 1.52 g/l, alkaloids 3.67 ± 1.07 %, phenol 39.42 ± 3.6 GAE/g and flavonoids 24.34 ± 2.06 mg QE/g.

Tannins are polyphenolics existing as hydrolysable and condensed the presence of the above secondary metabolites have various effects against many diseases related free radicals and possess neuroactive, astringent, anti-inflammatory and antimicrobial properties. Our results are similar to the findings of Habu and Ibeh [32] who also reported the presence of secondary metabolites in *Newbouldia laevis*.

The antimicrobial and antifungal activity of *Ageratum conyzoides* was tested against many isolates including C. albicans, A. niger, Mucor sp., S. aureus, K. pneumoniae and P. aeruginosa.

The results showed in table 3 and 4 revealed that *Ageratum conyzoides* methanolic extract at concentrations of 100, 50 and 25 mg/ml inhibited S. aureus, K. pneumoniae and P. aeruginosa with a zone of inhibition of 11mm for S. aureus at 100 mg/ml, 8mm and 7mm for K. pneumonia and P. aeruginosa respectively. Also gentamicin at 25mg/ml inhibited all three isolates that is S. aureus, K. pneumonia and P. aeruginosa at 26, 22, and 16mm respectively. The extract inhibition at 25 and 50mg/ml concentrations were not significant. This report is in line with the report of Eboh et al., and Mir et al., [33, 34]

The antifungal ability of fluconazole (standard) shows no inhibition against C. albicans, A. niger and Mucor sp at 25mg/ml. However methanolic extract of *Ageratum conyzoides* at 50mg/ml and 100mg/ml inhibited only Mucor sp with a zone of inhibition of 11mm and 13mm respectively. Therefore the antimicrobial and antifungal activities of Ageratum conyzoides could be partly due to the presence of a wide range of secondary metabolites detected in the extract qualitatively and quantitatively [35].

The docking results of the selected compounds against dihydrofolate reductase and pectin lyase were depicted in table 5. Camptothecin, Jatrorrhizine, chelidonine and strychnine were docked against dihydrofolate reductase (PDB: 1AI9) and the result revealed Jatrorrhizine as having the highest docking score of -6.81, and least score was strychnine -5.04 kcal/mol. The scores of camptothecin and chelidonine were -6.40 and - 6-34 kcal/mol respectively. Jatrorrhizine made good interactions with the amino acid of dihydrofolate reductase for example H-bonding between ALA-115, GLU-32 and functional groups of Jatrorrhizine like -OH and phenolic groups. Also there were hydrophobic Interactions between ILE-19, MET-25, VAL-10 and ILE-33 and the hydrophobic regions of Jatrorrhizine (benzene rings). Polar interactions also strengthen the binding affinity between Jatrorrhizine and PDB:1AI9 due to the polar interactions of THR-147, SER-61 and THR-58. Therefore, camptothecin, Jatrorrhizine, chelidonine and Strychnine made interactions with dihydrofolate reductase ranging from H-bond,hydrophobic and polar interactions hence the higher docking scores Also selected phytocompounds docked against pectin lyase were leonurine, starchdrine, Jatrorrhizine and chelidonine. The result revealed leonurine has the highest docking score of -6.13 kcal/mol and the least was Jatrorrhizine -4.74 kcal/mol. Leonurine made H-bonds:ARG-236,ASP-242 and ASP-217, hydrophobic interactions of TYR-215,TRP-212,TRP-151 and TRP-81 and also a polar bonding of GLN-177 and GLN-241 and the functional groups of leonurine such as -OH groups. Also stachdrine, Jatrorrhizine and chelidonine made favorable interactions too [34, 36, 37]. Therefore the compounds to a greater extend inhibited the activity of these microbial and fungal enzymes. Also the ADMET parameters revealed that leonurine, stachdrine, camptothecin, Jatrorrhizine, chelidonine and strychnine do not violate lipinski rule of 5. Also the percentage human oral absorption was higher in stachdrine and strychnine.

The number of primary metabolites of these phytocompounds were also in the standard range of 1-8 metabolites [34,36].

Conclusion

This study shows that *Ageratum conyzoides* has antimicrobial and antifungal activity against pathogenic isolates. Molecular binding interaction shows that leonurine, camptothecin, jatrorrhizine, strychnine, chelidonine and stachdrine, have binding potential against dihydrofolate reductase and pectin lyase. Therefore these compounds can be exploited as antimicrobial.

References

1. Brown, G. D., Denning, D. W., Gow, N. A. R. Levitz, S. M. Netea, M. G. White, T. C. (2012). Hidden killers: Human fungal infections. Science and Translational Medicine 4, 165-13.
2. Wall, G., Lopez-Ribot, J.L. (2020). Current antimycotics, new prospects, and future approaches to antifungal therapy. Antibiotics. https://doi.org/10.3390/antibiotics9080445.
3. Rayens, E., Norris, K.A., 2022. Prevalence and Healthcare Burden of Fungal Infections in the United States, 2018. Open Forum Infectious Diseases, 9. https://doi.org/10.1093/ofid/ofab593.
4. Odds, F. C., Brown, A. J. Gow, N. A. (2003). Antifungal agents: Mechanisms of action. Trends in Microbiology, 11, 272–279.
5. Jaiswal, N., Kumar, A. (2024). Modulators of Candida albicans Membrane Drug Transporters: A Lucrative Portfolio for the Development of Effective Antifungals. Molecular Biotechnolology 66, 960–974. https://doi.org/10.1007/s12033-023-01017-1
6. Dos Santos Ramos, M.A., Da Silva, P.B., Spósito, L., De Toledo, L.G., Bonifácio, B. vidal, Rodero, C.F., Dos Santos, K.C., Chorilli, M., Bauab, T.M., 2018. Nanotechnologybased drug delivery systems for control of microbial biofilms: A review. International Journal of Nanomedicine, 13, 1179–1213. https://doi.org/10.2147/IJN.S146195
7. Sharma, S.; Mohler, J.; Mahajan, S.D.; Schwartz, S.A.; Bruggemann, L.; Aalinkeel, R. (2023). Microbial Biofilm: A Review on Formation, Infection, Antibiotic Resistance, Control Measures, and Innovative Treatment. Microorganisms, 11, 1614. https://doi.org/10.3390/microorganisms11061614
8. Cesar, O, A., Hoffman, S.C., Das, P., Fuente-Nunez, C. (2025). Challenges and applications of artificial intelligence in infectious diseases and antimicrobial resistance. Antimicrobial and Resistance 3:2.
9. Soni, J., Sinha, S and Pandey, R. (2024) Understanding bacterial pathogenicity: a closer look at the journey of harmful microbes. Frontiers in Microbiology. 15:1370818. doi: 10.3389/fmicb.2024.1370818.
10. Paul, S., Datta, B., Ratnaparkhe, M., & Dholakia, B. (2021). Turning waste into beneficial resource: Implication of Ageratum conyzoides L. in sustainable agriculture, environment and biopharma sectors. Molecular Biotechnology, 64(3), 221–244. https://doi.org/10.1007/s12033-021-00409-5
11. Yadav, N., Ganie, S., Singh, B., Chhillar, A., & Yadav, S. (2019). Phytochemical constituents and ethnopharmacological properties of ageratum conyzoides. Phytotherapy Research, 33(9), 2163-2178. https://doi.org/10.1002/ptr.6405

12. Dogra, R. (2014). Therapeutic effects of flavonoids in Ageratum conyzoides: A review. International Journal of Pharmaceutical Sciences and Research, 5(5), 1985-1990. https://doi.org/10.13040/IJPSR.0975-8232.5(5).1985-90
13. Kamboj, A., & Saluja, A. (2008). Medicinal uses of Ageratum conyzoides: A comprehensive review. Pharmacognosy Reviews, 2(4), 485-493.https://doi.org/10.4103/0973-7847.50749
14. Satyal, P., Kaphle, A., & Weathers, P. J. (2018). Essential oils from Ageratum conyzoides: Extraction and antimicrobial properties. Natural Products Journal, 8(3), 151-157. https://doi.org/10.2174/2210291510666180307110022
15. Kotta, S., Khandare, R. A., & Tare, S. D. (2020). Exploration of anti-inflammatory properties of Ageratum conyzoides through its bioactive compounds. European Journal of Pharmaceutical Sciences, 143, 105183. https://doi.org/10.1016/j.ejps.2019.105183
16. Onwudinjo, F. C., & Nnoli, E. J. (2024). The nutritional and medicinal value of Ageratum conyzoides: Elemental analysis. Journal of Food Science and Technology, 61(3), 400-408. https://doi.org/10.1007/s11483-023-05910-1
17. Rajput, S. K., Singh, A., & Kumar, S. (2022). Evaluating the therapeutic potentials of Ageratum conyzoides: A comprehensive review. Journal of Ethnopharmacology, 278, 114-123. https://doi.org/10.1016/j.jep.2021.114123
18. Chabi-Sika, K., Sina, H., Boya, B., Salami, H., Dossou, G., Mama-Sirou, I., & Baba-Moussa, L. (2023). Ethnobotanical survey and some biological activities of Ageratum conyzoides collected in southern Benin. International Journal of Biochemistry Research & Review, 9, 25. https://doi.org/10.9734/ijbcrr/2023/v32i1793
19. Abiodun, O. M., Akinmoladun, O. F., & Olawuyi, O. (2020). Antioxidant properties of Ageratum conyzoides and its potential biomedical applications. Journal of Medicinal Plants Research, 14(2), 15-23. https://doi.org/10.5897/JMPR2019.5123
20. Nyunaï, N., Njikam, N., Abdenneb, E., Mbafor, J., & Lamnaouer, D. (2010). Hypoglycaemic and antihyperglycaemic activity of Ageratum conyzoides L. in rats. African Journal of Traditional, Complementary and Alternative Medicines, 6(2). https://doi.org/10.4314/ajtcam.v6i2.57083
21. Harborne JB (1998) Textbook of Phytochemical Methods. A Guide to Modern Techniques of Plant Analysis. 5th Edition, Chapman and Hall Ltd, London, 21-72.
22. Bahorun, T.; Gressier, B.; Trotin, F.; Brunet, C.; Dine, T.; Luyckx, M.; Vasseur, J.; Cazin, M.; Cazin, J.C.; Pinkas, M. (1996). Oxygen species scavenging activity of phenolic extracts from hawthorn fresh plant organs and pharmaceutical preparations. Arzneimittelforschung, 46, 1086–1089.
23. Zhishen, Y, Meugcheng, T, Jianming, W. (1999). Determination of flavonoids content in mulberry and their scavenging effect on superoxide radicals. Food Chemistry, 64:555–9.
24. Singleton, V.L., Orthofer, R., Lamuela-Raventos, R.M. (1999). Analysis of total phenols and other oxidation substrates and antioxidants by means of Folin-Ciocalteu reagent. Methods in Enzymolology. 299: 152-179.
25. Demiray, S, Pintado, M.E., Castro, P.M. (2009). Evaluation of phenolic profiles and antioxidant activities of Turkish medicinal plants: Tiliaargentea, Crataegi folium leaves and Polygonum bistorta roots. World Academic Science and Engineering Technolology, 54:312–17.
26. Unuofin, J.O., Otunola, G.A., Afolayan, J.A. (2017). Phytochemical Screening and in vitro evaluation of antioxidants and Antimicrobial activities of kedrostis africana (L.) cogn. Asian Pacific Journal of Tropical Biomedical Science, 7(10): 901-908.
27. Esther Lydia, D., Khusro, A., Immanuel, P., Esmail, G.A., Al-Dhabi, N.A., Arasu, M.V. (2020). Photo-activated synthesis and characterization of gold nanoparticles from Punica granatum L. seed oil: An assessment on antioxidant and anticancer properties for functional yoghurt nutraceuticals. Journal of Photochemistry and Photobiology B: Biology. 206, 111868. https://doi.org/10.1016/j.jphotobiol.2020.111868.
28. Dalir, S., bakht Djahaniani, H., & Nabati, F. (2020). Characterization and the evaluation of antimicrobial activities of silver nanoparticles biosynthesized from Carya illinoinensis leaf extract. Heliyon, 6(3), Article e03624.
29. Enyiekere, V.J., Asanga, E.E., Okokon, J.E., Ekeleme, C.M., Anagboso, M.O., Uduak, I.P. (2024). Fatty acid esters and acyclic monoterpenoid from Justicia insularis leaf fractions, attenuated malaria pathogenesis through docking with plasmodium falciparum serine hydroxymethyl transferase and plasmodium falciparum erythrocyte membrane protein 1 proteins. National Product Communication, 19(7): 1-14.
30. Diana, A., Michielin, O., Zoete, V. (2019). Swiss target prediction: updated data and new features for efficient prediction of protein targets of small molecules. Nucleic Acid Research. 47(1): 57-64.
31. Farombi, E.O (2003). African indigenous plants with chemotherapeutic potentials and biotechnological plants with production of bioactive prophylactic agents. African Journal of Biotechnology. 2(12):662-7.
32. Habu, J.B and Ibeh, B.O. (2015). In vitro antioxidant capacity and free radical scavenging evaluation of active metabolic constituents of Newbouldia laeves ethanolic leaf extract. Biological Research, 48:16.
33. Eboh, A.S., Wodu, E., Eboh, D.D., Azibanasamesa D.C. Owaba, A.D.C., Toby, T.D and Sogo, B.P. (2025). Chromatographic, Antimicrobial and Antioxidant efficacy of Acmella caulirhiza. Sokoto Journal of Medical Laboratory Science, 10(2):112 – 124.
34. Mir, W. R., Bhat, B. A., Almilaibary, A., Asdaq, S. M. B. & Mir, M. A. (2022). Evaluation of the in vitro antimicrobial activities of Delphinium roylei: An insight from molecular docking and MD-simulation studies. Medicinal Chemistry. https://doi.org/10.2174/1573406418666220429093956.
35. Belmekki, N., Bendimerad, N. & Bekhechi, C. Chemical analysis and antimicrobial activity of Teucrium polium L. essential oil from Western Algeria. Journal of Medicinal Plants Research. 7, 897–902 (2013).
36. Singh, K., Coopoosamy, R. M., Gumede, N. J. & Sabiu, S. Computational insights and in vitro validation of antibacterial potential of Shikimate pathway-derived phenolic acids as NorA efflux pump inhibitors. Molecules, 27, 2601 (2022).
37. Maulidya, S., Nuari, D., Suryana, S., & Almarifah, S. (2020). Antibacterial activity of Ageratum conyzoides L. leaves extracts against methicillin-resistant Staphylococcus aureus. Borneo Journal of Pharmacy, 3(4), 243–248. https://doi.org/10.33084/bjop.v3i4.1552