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Original Research Article

GC-MS Fingerprint of *Mitracarpus hirtus* and *Commiphora africana:* Medicinal plants Used in the Treatment of Skin and Wound Infections in Bauchi Town

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Abstract

Purpose: *Mitracarpus hirtus* and *Commiphora africana* are two medicinal plants traditionally utilized in Bauchi town, Nigeria, for the treatment of skin and wound infections. However, the bioactive chemicals responsible for these effects have not been fully identified. On this basis, the current work employed GC-MS analysis in conjunction with computational prediction studies to investigate the presence of compounds in the aqueous extracts of these plants leaves, aiming to identify those with wound healing properties.

Methods: The Plants leaves were air-dried, pulverized into powdered form and extracted with aqueous. The extracts obtained were subjected to GC-MS analysis where the compounds identified were search both in the literature and in-silico for their wound healing characteristic. In-silico prediction for compounds' physiochemical properties, adsorption, distribution, metabolism, excretion, toxicity as well as drug-likeness properties and bioactive characteristics, including wound healing, anti-inflammatory, antioxidant, antibacterial, growth stimulation, and so on, were predicted using an online software such as activity spectra for biologically active substances (PASS) etc.

Results: The study's findings revealed various capacities of phytochemicals in *Mitracarpus hirtus* and *Commiphora africana* extracts for wound healing. Compounds in the extracts of *C. africana* were detected at retention times ranging from 2.6 to 16. 5 minutes. Pyranone has the largest percentage yield at 2.06%, whereas 4-acetoxy-3-methoxystyrene has a lower yield of 0.12%. In *M. hirtus* extracts, components were detected after a retention duration of 5-22 minutes, with Phenol, 2,5-bis(1,1-dimethylethyl)-, having a higher presence at 2.74%. Among the compounds identified and predicted to be responsible for the wound healing properties of the plants extracts were resorcinol, undecanoic acid, and tetradecanoic acid. Quantitative Estimate of Drug-likeness (QED) for the compounds indicates that the values fall within a desirable range, with 2,5-bis(1,1-Dimethylethyl)phenol exhibiting the most favorable QED at a value of 0.68.

Conclusion: *Mitracarpus hirtus* and *Commiphora africana* showed to possess compounds with good qualities for wound healing hence confirms their used in treating skin and wounds.

Keywords: *Mitracarpus hirtus, Commiphora africana,* GC-MS analysis, in-silico, Wound-healings.

INTRODUCTION

Mitracarpus hirtus (Tropical girdle pod), a tropical herb from the Rubiaceae family, is well-known for its several therapeutic properties. It has traditionally been used to treat various conditions, including skin disorders and infections. Recent investigations have revealed its antibacterial capabilities, particularly against microorganisms that cause skin infections. The plant contains several phytochemicals including flavonoids, phenolics, and alkaloids contributing to its biological activity.[1-2] *Commiphora africana* (African Myrrh) is another well-known plant utilized in traditional medicine due to its wound-healing abilities. It is frequently used topically to treat cuts and abrasions due to its antimicrobial properties. The plant contains resinous chemicals that are thought to help healing and prevent infection.[3]

Medicinal plants constitute an effective source of both traditional and modern medicine. Plants have been used as sources of remedies for the treatment of many diseases since ancient times and people of all continents especially Africa have this old tradition.[4] Traditional medicinal practices have a wide acceptability among the Nigerian people, probably because they believe in their effectiveness. Nigeria has a rich medicinal plant heritage, and numerous studies have been conducted to investigate the antibacterial properties of these plants.[5-6]

Plant components used for therapeutic purposes include leaves, roots, stems, bark, and fruits alone, or a combination of two or more within a species or with those of other species. However, research on plants used in traditional medicine is still scarce.[7] Furthermore, almost 80% of newly released pharmaceuticals are made from chemicals derived from natural materials.[9] In recent years, the use of plant remedies has grown significantly on a global scale, as has the search for novel phytochemicals that may one day be transformed into useful medications for the treatment of infectious diseases.[9]

Bauchi town, located in the Bauchi State of Nigeria, has a rich tradition of using medicinal plants for treating various ailments, particularly skin and wound infections. Recent studies have highlighted the effectiveness of several local plants in combating these health issues, emphasizing their antimicrobial properties.[10-11]The use of medicinal plants for treating skin and wound infections has gained attention in Bauchi town, Nigeria, particularly due to the increasing prevalence of antimicrobial resistance in the study area as reported by[28] and the quest for alternative therapies. However, several gaps have been identified in the current understanding and application of these traditional remedies. As such, there is a need for further investigation into the specific phytochemicals responsible for antimicrobial properties. Current research often highlights the effectiveness of certain plants but fails to isolate and identify these active constituents. *Mitracarpus hirtus* and *Commiphora africana* are two significant medicinal plants utilized in traditional medicine, particularly in Bauchi town, Nigeria. Both plants have been recognized for their therapeutic properties, especially in treating skin and wound infections. This study explores the chemical profiles of these plants through Gas Chromatography-Mass Spectrometry (GC-MS) fingerprinting, in order to determine and identify the bioactive components of the plants extracts and to highlight their medicinal applications.

MATERIALS AND METHODS

2.1. Plant collection and Identification

Fresh leaves of *Mitracarpus hirtus* and *Commiphora africana* were collected from Gubi Campus of Abubakar Tafawa Balewa University, located at near Gumi Dam (latitude 10°45′ N & longitude 9°82′ E) in Bauchi, Bauchi state. The plant samples were identified and authenticated by Musa Ibrahim of the Herbarium Unit, Department of Biological Science, Abubakar Tafawa Balewa University. Voucher specimens (voucher no: DBSH2572 and DBSH2574) were deposited in the herbarium of the Department.

2.2. Extraction of crude extracts

The leaves of the plants were air dried at room temperature (25°C) for about 3 days. The dried leaves were grounded using Ball Mill machine Model No. JT-ZM-1L (TMax Laboratory equipment, England). Ethyl acetate was used as solvent of extraction for *Mitracarpus hirtus* and Distilled water for the extraction of *Commiphora africana* at the ratio of 1:5 (w/v), powdered leaves to solvent. At this extraction ratio, 1 kg of the powdered leaves were extracted using 5,000 ml of solvent using a soxhlet extractor to get its product.[12-13] The extracts were evaporated to dryness using Rotary evaporator (Toption Instrument Co, Ltd, USA).

2.3. The GC–MS analysis

Analysis of extracts from *Commiphora africana* and *Mitracarpus hirtus* was done using Agilent

Tech's GC 7890B and MSD 5977A (USA). 1µL of the extracts' supernatant was introduced into the GC, and helium was used as the carrier gas at a flow rate of 1 ml/min. Starting at 80°C, the oven temperature was increased by 15°C per minute to 200°C, then by 5°C per minute to 280°C, ending in a 5-minute isothermal at 280°C. The ionization voltage was set at 70 eV, while the ion source was set at 230°C. The MS data was obtained and processed online using MassHunter software. The retention indices and mass spectra were compared to a spectrum of previously known components recorded in the National Institute of Standards and Technology database (http://chemdata.nist.gov).[12, 14 & 27]

2.4. In silico prediction of *Mitracarpus hirtus* and *Commiphora africana* GC-MS identified compounds

The bioactivities of chemicals identified via GC-MS analysis of *Mitracarpus hirtus* and *Commiphora africana* were predicted using a variety of applications. The substance's chemical features were obtained from the PubChem chemical data bank (https://pubchem.ncbi.nlm.nih.gov/), where chemical information, including canonical SMILES, were identified and obtained for each compound before being entered into the various predictions software. In addition, the compounds' physiochemical properties, adsorption, distribution, metabolism, excretion, and toxicity, as well as drug-likeness properties, were predicted using the Lipinski drug rule and other drug rule criteria enshrined in software called ADMET-lab 2.0 (Computational Biology & Drug Design Group (CBDD) Xiangya, China, 2011) at https://admetmesh.scbdd.com.

Compounds' bioactive characteristics, including wound healing, anti-inflammatory, antioxidant, antibacterial, growth stimulation, and so on, as described in the literature, were predicted using an online software called activity spectra for biologically active substances (PASS, Institute of Biomedical Chemistry (IBMC), Russia. 2011) at https://www.way2drug.com/passonline/predict.php.

RESULT AND DISCUSSION

3.1 GC-MS fingerprint of Aqueous extract of *Commiphora africana* leaves

Table 1 summarizes the numerous organic compounds found in the plant's leaf extract, along with their chemical formulae, precise masses, peak, retention period, and relative abundance. The relative quantities of chemical components in the extract were expressed as a percentage of the peak area in the chromatogram. Pyranone has the largest percentage yield, 2.06% whereas 4-acetoxy-3-methoxystyrene has a lower yield of 0.12%.

Figure 1 shows the GC-MS chromatogram for *Commiphora africana* leaf extracts. The components in the extract were found at retention times ranging from 2.6 to 16.5 minutes. The total number of components found fell into five categories: acyclic (open-chain) compounds, cyclic compounds, aromatic compounds, aliphatic compounds, and other complex organic structures.

3.2 GC-MS fingerprint of Aqueous extract of *Mitracarpus hirtus* leaves

Table 2 displays the results for the chemical components discovered in the *Mitracarpus hirtus* leaf extract. Similarly, this table outlines the extract's main components, which include two alcohols, five esters, two acids, two hydrocarbons, one siloxane molecule, and others. The percentage statistics showed that some compounds, such as Phenol, 2,5-bis(1,1-dimethylethyl)-, have a higher presence (2.74%), whereas others, such as Ethyl Acetate, are present in trace amounts (0.02%).The GC-MS chromatogram for this plant extract is presented in Figure 2 below. The extracts' components were detected after retention duration of 5-22 minutes.

3.3 Computational Predicted Bioactivity Properties of GC-MS Identified Compounds from *C. africana* and *M. hirtus* Leaves

The GC-MS analysis of *Commiphora africana* and *Mitracarpus hirtus* lea ves indicates a number of chemicals with potential wound healing effects. These plants' GC-MS examination revealed the presence of resorcinol, 2,5-bis(1,1-dimethylethyl) phenol, undecanoic, and tetradecanoic acids. These chemicals from literature have been shown to have remarkable wound healing effects. On that basis, the compounds were subjected to bioinformatics analysis to predict their potential bioactive capabilities in wound healing.

Table 1: GC-MS fingerprint of Aqueous extract of *Commiphora africana* leaves

S/N	Peak	R/T	Compound	Formula	Exact Mass	%
1	1	2.6	endo-2,3-O-Ethylidene-β-d-erythrofuranose	$C_6H_{10}O_4$	146.057909	0.49
2	4	4.3	N-(1-Methoxycarbonyl-1-methylethyl)-4-methyl-2-aza-1,3-dioxane	$C_9H_{17}NO_4$	203.115758	0.21
3	5	4.5	Pyranone	$C_6H_8O_4$	144.042258	2.06
4	7	5.3	2,6-Pyrazinediamine	$C_4H_6N_4$	110.059246	0.55
5	9	6.3	Resorcinol	$C_6H_6O_2$	110.0367794	0.39
6	10	6.8	4-Acetoxy-3-methoxystyrene	$C_{11}H_{12}O_3$	192.078644	0.12
7	11	7	Phymaspermone	$C_{15}H_{18}O_2$	230.13068	0.24
8	12	7.3	2H-Indeno[1,2-b]furan-2-one, 3,3a,4,5,6,7,8,8b-octahydro-8,8-dimethyl	$C_{13}H_{18}O_2$	206.13068	0.53
9	13	7.9	Cyclohexylthioglycolate	$C_8H_{14}O_2S$	174.07145	0.23
10	14	8.8	2-Hydroxy-3,5-dimethylcyclopent-2-en-1-one	$C_7H_{10}O_2$	126.0680795	0.14
11	15	9.6	2,6-Dimethyl-3-thioxo-5-oxo-2,3,4,5-tetrahydro-1,2,4-triazine	$C_5H_7N_3OS$	157.030983	0.16
12	16	9.8	1-Methyl-3,6-diazahomoadamantan-9-one	$C_{10}H_{16}N_2O$	180.126264	1.24
13	17	10	Spiro[androst-5-ene-17,1'-cyclobutan]-2'-one, 3-hydroxy-, (3β,17β)-	$C_{22}H_{32}O_2$	328.24023	0.13
14	21	12.8	2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl-	$C_7H_{10}O_2$	126.0680795	0.21
15	22	13.1	14-Heptadecenal	$C_{17}H_{32}O$	252.245316	0.26
16	23	13.6	Undecanoic acid	$C_{11}H_{22}O_2$	186.16198	0.12
17	25	14.2	Tetradecanoic acid, 10,13-dimethyl-, methyl ester	$C_{17}H_{34}O_2$	270.25588	0.13
18	26	14.4	10,10-Dimethyl-2,6-dimethylenebicyclo[7.2.0]undecan-5β-ol	$C_{15}H_{24}O$	220.182715	0.14
19	32	16.4	2-(3-Hydroxybutyl)cyclooctanone	$C_{12}H_{22}O_2$	198.16198	0.78
20	33	16.5	Photocitral B	$C_{10}H_{16}O$	152.120115	1.50

Table 2: GC-MS fingerprint of Aqueous extract of *Mitracarpus hirtus* leaves

S/No	Peak	R/T	Compound	Formula	Exact Mass	Percentage %
1	1	5.1	3-Undecene, 9-methyl-, (Z)-	$C_{12}H_{24}$	168.1878	0.67
2	2	2.6	Ethyl Acetate	$C_4H_8O_2$	88.052429	0.01
3	3	8.2	1-Dodecene	$C_{12}H_{24}$	168.1878	0.6
4	5	9.7	1-Octene, 3,7-dimethyl-	$C_{10}H_{20}$	140.156501	1.22
5	6	10.0	Phenol, 2,5-bis(1,1-dimethylethyl)-	$C_{19}H_{30}O_3$	306.219496	2.74
7	8	11.8	2,3,4-Trimethyl-1-pentanol	$C_8H_{18}O$	130.135765	0.41
8	9	11.9	1-Octene, 6-methyl-	C_9H_{18}	126.1408505	0.62
9	12	14.9	Acetic acid, trifluoro-, 3,7-dimethyloctyl ester	$C_{12}H_{21}F_3O_2$	254.149364	0.43
10	13	15.0	1,7-Dimethyl-4-(1-methylethyl)cyclodecane	$C_{15}H_{30}$	210.234751	0.13
11	14	15.4	3-Methyl-2-(2-oxopropyl)furan	$C_8H_{10}O_2$	138.06808	0.35
12	15	15.8	Ethylene diacrylate	$C_8H_{10}O_4$	170.057909	0.09
13	16	16.0	Z-2-Dodecenol	$C_{12}H_{24}O$	184.182715	0.13
14	17	16.7	Tetradecanoic acid, 12-methyl-, methyl ester, (S)-	$C_{16}H_{32}O_2$	256.24023	0.61
15	18	17.3	Oxalic acid, allylhexadecyl ester	$C_{21}H_{38}O_4$	354.27701	1.51
16	19	17.5	1-Nonadecene	$C_{19}H_{38}$	266.297352	0.51
17	20	18.8	Succinic acid, di(3,7-dimethyloct-6-en-1-yl) ester	$C_{24}H_{42}O_4$	394.30831	1.01
18	23	19.3	Heptacosanoic acid, 25-methyl-, methyl ester	$C_{29}H_{58}O_2$	438.443682	0.47
19	27	22.6	Trimethyl[4-(1,1,3,3,-tetramethylbutyl)phenoxy]silane	$C_{17}H_{30}OSi$	278.206593	2.15

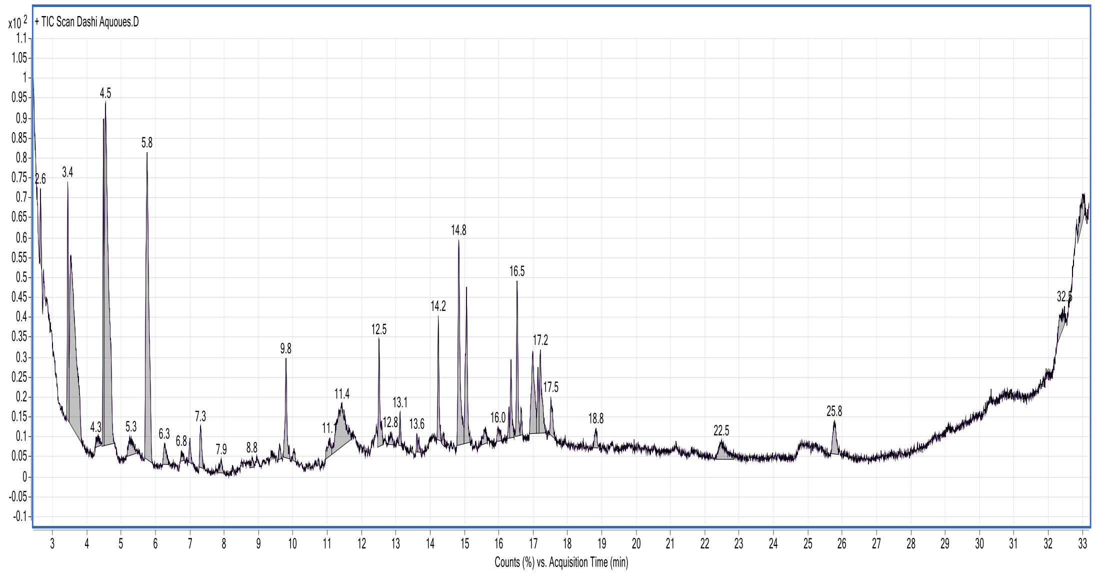

Figure 1: Chromatogram for the GC-MS analysis of aqueous extract of *C. African a* leaves

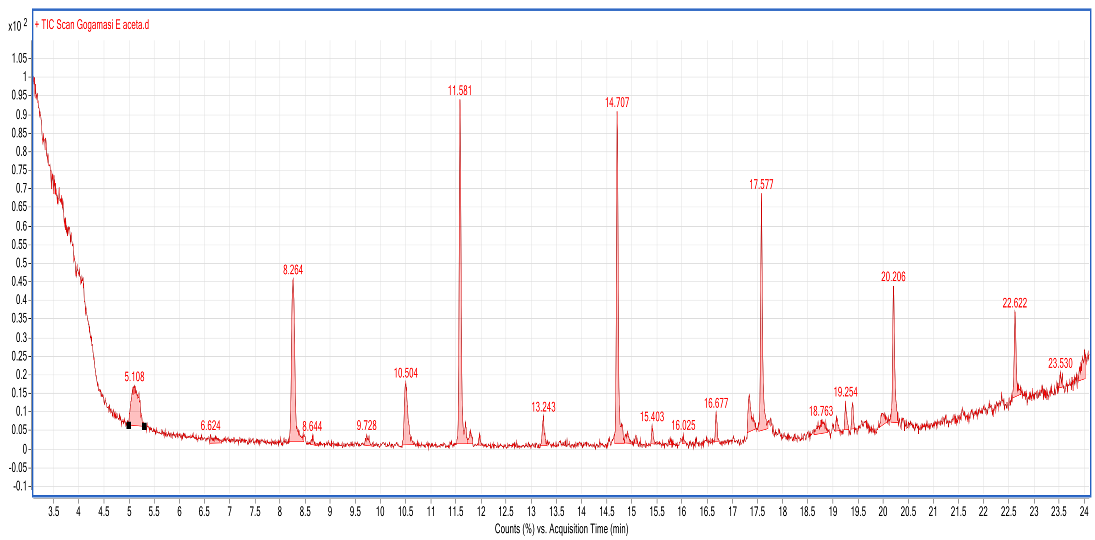

Figure 2: Chromatogram for the GC-MS analysis of aqueous extract of *M. hirtus* leaves

Table 3 shows the obtained chemical data for the *Commiphora africana* and *Mitracarpus hirtus* substance; resorcinol, 2,5-bis(1,1-Dimethylethyl) phenol, undecanoic acid and tetradecanoic acid, their probability of action as antiseptic, antio xidant, antiinflammatory, antibacterial, growthsti mulant, dermatologic and wound healing agent, etc., are found to be in a var iety of ranges with 2,5-bis(1,1-Dimethylethyl) phenol and tetradecanoic acids showing to have possess most of the predicted activities whereas only tetradecanoic acids and resorcinol compounds predicted as wound healing agents. Compounds physiochemical properties like molecular weight, volume, density, and so on for each of the compounds studied are presented in Table 4. The result for the drug-like properties of resorcinol, 2,5-bis(1,1-Dimethylethyl) phenol, undecanoic acid and tetradecanoic acid. predicted by the study seem to be suitable for drug development, with all the compounds having their Quantitative Estimate of Drug-likeness (QED) values of less than 0.67 which means they may have some undesirable properties but still have a chance of being developed in to drug, and value less than 0.34 is too complex. Based on this, 2, 5-bis (1, 1-Dimethylethyl) phenol acid with value of 0.68 is more attractive. All compounds had a value less than the minimum required medicinal chemistry evolution (MCV-18) value of ≥45.

Table 3: Computational Predicted Bioactivity of GC-MS Identified Compounds from the Leaves Extracts of *Commiphora africana* and *Mitracarpus hirtus*

	Phytochemicals			
Predicted Bioactivity	**Resorcinol**	**2,5-bis(1,1-Dimethylethyl)phenol**	**Undecanoic Acid**	**Tetradecanoic Acid**
Antiseptic	0.709	0.780**	0.573	0.366*
Anti-inflammatory	0.537	0.770**	0.515*	-
Antiviral	0.587**	0.177	0.186	0.176*
Antioxidant	0.486*	0.571**	-	-
Growth stimulant	0.311**	0.140*	-	0.203
Dermatologic	0.312*	0.527**	0.507	0.448
Macrophage colony stimulating factor agonist	0.746	0.655	0.891**	0.590*
Lipid metabolism regulator	0.586*	0.641	0.808**	0.740
Cytoprotectant	0.644	0.602*	0.712**	0.701
Antibacterial	0.310**	0.235*	0.300	0.263
Wound healing agent	0.288*	-	-	0.332**
Protein synthesis stimulant	0.276	0.260*	-	0.304**
Antibiotic	-	-	-	0.145
Antieczematic	-	-	0.920	

The larger the value of the score is, the higher is the probability that the particular molecule will be active. Score value with a double asterisks (**) along the column signifies the largest value of score while single asterisk (*) implies the less value of score and (---) means not available.

Compounds with higher activity, particularly thos e derived from natural sources, are constantly sought to cure wounds more successfully. Based on this, the current work used a GC-MS analysis to explore the presence of compounds in aqueous extracts of *Mitracarpus hirtus* and *Commiphora africana* leaves, intending to find those with wound-healing characteristics through a literature search and an in-silicon study. The study's findings revealed some relative capacities of phytochemicals in *Mitracarpus hirtus* and *Commiphora africana* extracts for wound healing.

Among the compounds predicted to be responsible for the wound healing abilities of *Mitracarpus hirtus* and *Commiphora africana* are resorcinol, undecanoic, and tetradecanoic acid. Resorcinol has been documented for its antimicrobial and anti-inflammatory effects, contributing to its wound-healing properties. According to Toppini *et al* [15], resorcinol was found to play a role in disinfecting wounds and preventing infections. Tetradecanoic acid, a fatty acid compound, has been associated with wound healing due to its roles in inflammation reduction and tissue repair mechanisms, thus maintaining skin integrity and promoting healing.[16] Tetradecanoic acid was found to exert its effects by enhancing collagen synthesis and promoting skin regeneration.[17-18] In addition, undecanoic acids were also found to be effective against skin pathogens, suggesting their utility in wound management.[19]

Table 4: Computational Details of GC-MS Identified Compounds from the Leaves Extracts of *Commiphora africana* and *Mitracarpus hirtus*

Property	Compounds				Interpretation
	Resorcinol	**2,5-bis(1,1-Dimethylethyl)phenol**	**Undecanoic Acid**	**Tetradecanoic Acid**	
Canonical SMILES	C1=CC(=CC(=C1)O)O	CC(C)(C)C1=CC(=C(C=C1)C(C)(C)C)O	CCCCCCCCCCC(=O)O	CCCCCCCCCCCCCC(=O)OC	
Molecular Weight	110.04	206.17	186.16	242.22	A molecular weight in the range:100~600 is accepted
Van der Waal Volume	113.45	243.03	213.76	282.94	A value between 300-800 Å is accepted
Density	0.97	0.85	0.87	0.86	Density = MW / Volume
No. of H Bond Acceptor	2	1	2	2	Hydrogen bond in the range 0~12 is accepted
No. of H Bond Donor	2	1	1	0	Hydrogen bond donor in the range 0~7 is accepted
No. of Rotatable Bonds	0	2	9	13	A compound with number of rotatable bonds in range of 0~11 is accepted.
No. of Rings	1	1	0	0	Number of rings for compounds should be between 0~6
No. of atoms in the biggest Ring	6	6	0	0	The biggest ring in a compound should have atoms between 0~18
No. of Heteroatoms	2	1	2	2	Compound with heteroatoms from 1~15 is accepted
Formal Charge	0	0	0	0	Compound formal charge from -4 ~ +4 is accepted
No. of Rigid Bonds	6	6	1	1	A rigid bonds above 0~30 is not accepted
Stereo Centers	0	0	0	0	Stereo centers for compound less or equal to 2 is accepted.
Topological Polar Surface Area	40.46	20.23	37.3	26.3	The topological polar surface area for compound above 0~140 is not accepted
Log of the Aqueous Solubility	-0.19	-4.35	-3.57	-6.14	Log of the aqueous solubility exceeding -4 ~ 0.5 log mol/L is not accepted
Log of the octanol/water Partition	0.98	3.66	2.96	3.97	The Log of the octanol/water partition coefficient of an accepted

Coefficient					compound should be between 0~3.0
LogP at Physiological pH 7.4	0.93	4.61	4.33	6.34	Compound with LogP at physiological pH 7.4 from 1~3 is accepted
QED[1]	0.525	0.68	0.558	0.361	Compound with values ofgreater than 0.34 is accepted
MCV-18	5	12	0	0	Compound with value of ≥45 is accepted
Lipinski	0	0	0	0	Score of 1 is accepted under the Lipinski's rule
Pfizer	0	1	1	1	Score of 1 is accepted under the Pfizer's rule
GSK	0	1	1	1	Score of 1 is accepted under the GSK's rule
Golden - Triangle	1	0	1	0	Score of 1 is accepted under the golden triangle's rule

The antiseptic properties predicted by those compounds identified in *Mitracarpus hirtus* and *Commiphora africana* shows that they could be used in formulations for disinfecting wounds and preventing infection, which is crucial in settings with limited access to advanced medical care. [20] Their effectiveness could help reduce the incidence of wound infections. [15] Other phytochemicals, such as the alcohols (2,3,4-trimethyl-1-pentanol and Z-2-dodecenol), can also serve as antiseptics for cleaning wounds. Using alcohol-based solutions to reduce microbial load on wounds has been encouraged in place of limited antiseptic medication.[21] Esters (acetic acid, trifluoro-, 3,7-dimethyloctyl ester, or tetradecanoic acid, 12-methyl-, methyl ester) have been used as emollients or skin protectants in wound care. They help maintain wound moisture and support the healing process by providing a barrier against pathogens.[22] Hydrocarbons (1, 7-Dimethyl-4-(1-methylethyl) cyclodecane) have also been effective in occlusive dressings where they protect wounds from external contaminants while allowing for moisture retention.[23]

Other phytochemicals, such as siloxanes (trimethyl [4-(1,1,3,3,-tetramethylbutyl) phenoxy] silane), may have applications in developing advanced wound dressings that provide antimicrobial properties and enhance healing through controlled moisture release. Their use could improve wound management strategies in resource-limited settings.[24] Pyranones (C6H8O4) were known for their antioxidant, antimicrobial, and anti-inflammatory properties and additionally exhibit anticancer effects, making them exceptional in drug discovery.[25] Moreover, resorcinol possesses remarkable dermatological applications, having marked anti-inflammatory activity.[26]

CONCLUSION

The leaves of *C. africana* and *M. hirtus* contain a variety of chemicals that may have medicinal uses in the treatment of wound and skin infections. In underdeveloped nations, these bioactive substances may be used as natural supplements or substitutes for traditional therapies, meeting the need for efficient cures as well as the problem of antibiotic resistance. The use of these substances in conventional medical systems may be improved by more investigation into their mechanisms of action and therapeutic uses. Further research into these compounds' mechanisms of action could facilitate their integration into modern therapeutic practices.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

AUTHORS DECLARATION

The authors hereby declare that the works presented in this article are original and that any liability for claims relating to the content of this article will be borne by them.

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