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Original Article

GC-MS/FTIR Profiling, Wound-Healing Potential, and *In-Silico* Dermal Toxicity Assessment of *Archachatina marginata* Shell Extract

[*1]Abalaka, M. E., [2,1*]Attah, F.,[1]Auta, S. H., [1]Bala, J. D., [3]Chinma, C. E. and [1]Tauheed, F. L.

[1]Department of Microbiology, Federal University of Technology, Minna, Nigeria
[2]Department of Microbiology, Confluence University of Science and Technology, Osara, Kogi State, Nigeria
[3]Department of Food Science and Technology, Federal University of Technology, Minna, Nigeria

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ABSTRACT

Background: The shell of *Archachatina marginata* has drawn interest because to its potential for medical use, especially in the treatment of wounds. This work used GC–MS, FTIR, and in silico studies to assess the methanol shell extract's potential for wound healing and computational dermal toxicity. *A. marginata* shell methanol extract was examined using GC-MS for bioactive substances and FTIR for functional groups. ADMETLAB 3.0, pkCSM, and StopTox were used for silico toxicity and skin permeability evaluations. The most prevalent of the seven bioactive substances found was Erythro cis-4,5-Dimethyl-2-undecene (27.30%). Functional groups connected to antibacterial, antioxidant, and anti-inflammatory properties were identified by FTIR analysis. All the compounds were predicted to be non-mutagenic, non-haematotoxic, and to have minimal acute cutaneous toxicity, however several indicated potential for skin sensitization. Skin permeability was poor for the majority of substances. The potential application of *A. marginata's* methanol shell extract in topical wound care is supported by the presence of bioactive substances with encouraging wound healing qualities and comparatively safe skin toxicity profiles.

Keywords: Bio-constituents, GC-MS/FTIR, Wound healing, snail shell, *in-silico, A. marginata*
*Corresponding author's email: attahf@custech.edu.ng. Phone no: 08075425472

INTRODUCTION

Traditional healing methods have greatly aided in the discovery and development of numerous contemporary medications, and nature has long been one of the most major sources of medicine. Communities have learned a great deal about the medicinal application of natural materials throughout centuries of ongoing observation and experimentation [1- 3]. Currently, bioactive substances produced from plants and animals account for around 60% of pharmaceuticals that are sold commercially [4]. Zootherapy, the term for the medical use of animals and animal-derived products, has gained

widespread recognition throughout the world [5].

Snails, an invertebrate belonging to the phylum Mollusca and class Gastropoda, are among the animals utilized medicinally. Snails have soft bodies surrounded by a hard protective shell primarily made of calcium carbonate, while the body itself is high in protein and water. In many species, the shell constitutes almost one-third of the snail's total body weight. Snails are widely spread throughout Africa, with the most frequent species being *Achatina achatina, Archachatin marginata*, and *Achatina fulica* [6].

After an injury, injured skin and bodily tissues recover through a complicated biological process called wound healing [7]. Normally, the dermis and epidermis serve as barriers that shield the body from outside influences [8]. The body starts a coordinated sequence of cellular and metabolic processes to restore tissue integrity as soon as this barrier is compromised. Haemostasis, inflammation, tissue proliferation, and remodeling are some of the overlapping stages of the healing process that are controlled by resident cells, migrating cells, extracellular matrix proteins, and signaling molecules [9-10]. Therefore, maintaining skin function and avoiding infection depend on effective wound healing.

The identification and characterization of bioactive chemicals derived from natural sources have been improved by recent developments in analytical techniques. Among these methods, Fourier Transform Infrared Spectroscopy (FT–IR) and Gas Chromatography–Mass Spectrometry (GC–MS) have emerged as crucial instruments in natural product and pharmaceutical research [11]. While GC-MS provides extremely sensitive chemical constituent detection, even at very low concentrations, FT-IR spectroscopy has been widely used in the investigation of natural tissues and biomolecules [12]. These analytical techniques offer important information about the chemical makeup and potential medical benefits of natural items.

Moreover, drug discovery and skin-related therapeutic research are increasingly using computational methods as in silico ADMET and cutaneous investigations [13]. Before in vitro and in vivo studies were carried out, these techniques offer quick and affordable first evaluations of the pharmacological and toxicological characteristics of bioactive substances. Natural compounds have been effectively screened for antibacterial, anti-inflammatory, and wound-healing properties using silico approaches [14].

There is still little information connecting GC-MS-identified bioactive chemicals with computational dermal analysis and antimicrobial evaluation, despite the increased interest in the therapeutic uses of *Archachatina marginata*. Therefore, this study aims to investigate the wound healing and antimicrobial potentials of GC–MS-identified bioactive compounds from *Archachatina marginata* using *In-silico* dermal approaches.

MATERIALS AND METHODS

Identification and Processing of Snail Shell

The snail specimen was identified and authenticated as *Archachatina marginata* by Professor Omowaye Stephen, a zoologist at the Federal University of Lokoja. The shells were processed using a

slightly modified method described by Abdul-Khaliq [15]. The shells were broken with a small hammer, and the edible tissues were carefully separated from the shell material. The shells were then cleansed, cleaned, dried in an incubator at 55°C, and crushed. A commercial milling machine was then used to grind the shells into a fine powder, which was then kept in a dry container until needed.

Extraction of *Archachatina marginata* Shell powder

Archachatina marginata shell powder weighing 100 grams was steeped in 500 mm of methanol. To achieve adequate extraction, the mixture was left at room temperature (28 ± 2°C) for three (3) days, shaken occasionally. The extract was then sieved using a muslin cloth and filtered through Whatman No. 1 filter paper. The beaker containing the extract was placed on a water bath until a greasy residue was produced, which concentrated the filtrate. The finished oily extract was put into appropriately labelled screw-cap vials and kept in the refrigerator until needed.

GC-MS Analysis of Snail Shell Extract

Gas Chromatography-Mass Spectrometry analysis was performed on a GCMS-QP 2010 PLUS SHIMADZU instrument [16]. A 95% dimethyl polysiloxane-based Perkin Elmer Elite-5 capillary column (30 m × 0.25 mm, 0.25 µm film thickness) was used for separation. Helium was used as the carrier gas at a flow rate of 0.5 mL/min. The injection volume was kept at 1 µL. The injector temperature remained steady at 250°C.

The oven temperature program was originally set at 80°C for 4 minutes, then increased to 200°C, and finally elevated to 280°C at a rate of 20°C/min for 5 minutes, for a total run duration of 25 minutes. The MS transfer line temperature was kept at 200°C, while the ion source temperature remained at 180°C. The GC-MS data were collected using electron impact ionization at 70 eV, and the total ion chromatogram (TIC) was utilized to identify and quantify the compounds [16].

Identification of Components

The GC-MS mass spectra were interpreted using the National Institute of Standards and Technology's (NIST) database, which includes approximately 62,000 spectral patterns. The spectra of unknown chemicals were matched to recognized compounds found in the NIST collection. The detected compounds were characterized by their molecular weight, structure, and compound name, and the resulting data were assembled appropriately, as stated by Kavitha and Nadu [17].

FTIR Spectroscopic Analysis

One of the best analytical methods for determining the kinds of chemical bonds and functional groups found in substances is FTIR spectroscopy [18]. Ten milligrams of the powdered dried extract were combined with one hundred milligrams of KBr pellet to create the translucent sample disc. An FTIR spectroscope (Shimadzu IR Affinity-1, Japan) was then used to evaluate the powdered material at a resolution of 4 cm^{-1} throughout the 400–4000 cm^{-1} scan range.

In-silico Dermal Toxicity and Skin Permeability Study of Snail Shell Extract

To predict toxicity, the following skin-based characteristics were measured: skin sensitization, acute dermal toxicity, ocular irritation and corrosion, mutagenicity, haematoxicity, and skin permeability. StopTox was chosen as the primary software because it is new and simple to use, as well as because it implements QSAR

models established utilizing standard procedures for validation and development mandated by the Organisation for Economic Cooperation and Development (OECD) [19].The SMILES strings for each GC-MS-identified molecule were collected from chemSpider (https://www.chemspider.com/) and then imported into pkCSM) (https://biosig.lab.uq.edu.au/pkcsm/prediction), ADMETLAB 3.0 ((https://admetlab3.scbdd.com/), and StopTox (https://stoptox.mml.unc.edu/) for endpoint-specific analysis.

RESULTS

GC-MS Analysis of the Methanol Extract of *A. Marginata* shell Powder

A total of seven chemicals discovered from the GC-MS analysis of the methanol extract of *A. Marginata* shell exhibited varying bioactive properties. Figure 1 depicts the chromatogram, while Table 1 lists the chemical contents of the extract, including their retention time (RT), molecular formula, molecular weight (MW), and concentration. The GC-MS study of shell extract contained the following bioactive compounds: Erythro cis-4,5-Dimethyl-2-undecene (27.30%) was the most abundant substance found in the extract, followed by 2-Butyl-1-octanol (18.64%) and Decanoic acid, methyl ester (16.75%). Trans-2-Tridecen-1-ol (14.07%) and 9,12-Octadecadienoic acid, methyl ester (12.46%) was detected in considerable amounts, but 2-Methyldecane (8.37%) was less abundant. The least prevalent chemical found was 1-Tridecyne (2.41%).

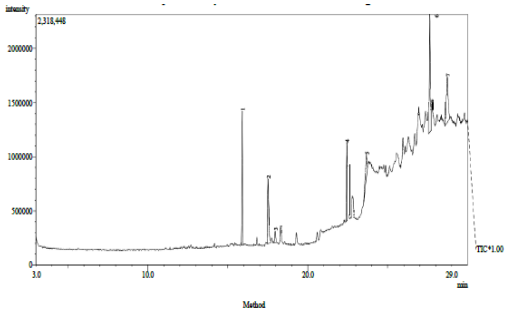

Figure 1: the Chromatogram of GC-MS analysis of the methanol extract of *A. Marginata* shell

Table 1: GC-MS Analysis of the Methanol Extract of *A Marginata* shell Powder

Peak	Retention Time	Compounds	MF	Area%	MW
1	15.899	Decanoic acid, methyl ester	$C_{11}H_{22}O_2$	16.75	186
2	17.518	trans-2-Tridecen-1-ol	$C_{13}H_{26}O$	14.07	198
3	17.963	1-Tridecyne	$C_{13}H_{24}$	2.41	180
4	22.444	9,12-Octadecadienoic acid, methyl ester,	$C_{19}H_{34}O_2$	12.46	294
5	23.667	2-Methyldecane	$C_{11}H_{24}$	8.37	156
6	27.634	Erythro cis-4,5-Dimethyl-2-undecene	$C_{13}H_{26}$	27.30	182
7	28.721	2-Butyl-1-octanol	$C_{12}H_{26}O$	18.64	186

The Result of FTIR Characterization of Functional Groups Present in the Methanol Extract of *A. marginata* Shell Extract

The Fourier Transform Infrared (FTIR) spectroscopic analysis of the methanol extract of *A. marginata* shell extract, revealing the presence of several important functional groups and chemical bonds. The absorption frequencies obtained ranged from 879.57 cm^{-1} to 2974.33 cm^{-1} as shown in Table 2 and FTIR spectra in Figure 2. The FTIR spectrum showed characteristic peaks

associated with aromatic compounds, alcohols, ethers, alkanes, aldehydes, nitro compounds, and amines. Peaks observed at 879.57 cm^{-1}, 1421.58 cm^{-1}, and 1584.08 cm^{-1} corresponded to aromatic compounds, suggesting the presence of aromatic ring structures through C–H bending and C=C stretching vibrations. The strong peaks at 1045.45 cm^{-1} and 1085.45 cm^{-1} indicated C–O stretching vibrations typical of alcohols and ethers, while the absorption band at 1276.92 cm^{-1} showed the presence of aromatic ethers through Ar–O stretching. Also, the peak at 1327.07 cm^{-1} suggested the occurrence of nitro compounds or amines due to N–O and C–N stretching vibrations. The bands at 1384.94 cm^{-1}, 1458.30 cm^{-1}, 2887.53 cm^{-1}, and 2974.33 cm^{-1} were attributed to alkanes, indicating CH_3 bending and C–H stretching vibrations. A notable absorption peak at 2827.74 cm^{-1} corresponded to aldehydic C–H stretching, confirming the presence of aldehyde functional groups. Lastly, the peak at 1923.09 cm^{-1} represented aromatic overtone or combination bands, which are commonly associated with substituted aromatic systems.

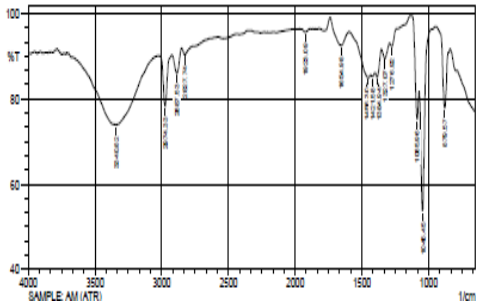

Figure 2: FTIR spectra of Methanol Extract of A. marginata Shell Extract

Table 2: Various Functional Groups/Chemical Bonds Present in the Methanol Extract of A. Marginata shell extract Identified by FTIR Analysis

S/No	Frequency (cm^{-1})	Types of Compounds	Bond Responsible	Intensity
1	879.57	Aromatic compounds	C–H bending	87.87
2	1045.45	Alcohols / Ethers	C–O stretching	53.86
3	1085.45	Alcohols / Ethers	C–O stretching	75.26
4	1276.92	Aromatic ethers	Ar–O stretching	92.38
5	1327.07	Nitro compounds / Amines	N–O stretching / C–N stretching	95.13
6	1384.94	Alkanes	CH_3 bending	95.13
7	1421.58	Aromatic compounds	C=C stretching	95.25
8	1458.30	Alkanes	C–H bending	95.09
9	1584.08	Aromatic compounds	C=C stretching	92.56
10	1923.09	Aromatic overtones	Combination bands	95.71
11	2827.74	Aldehydes	C–H stretching	80.42
12	2887.53	Alkanes	C–H stretching	85.01

13	2974.33	Alkanes	C–H asymmetric stretching	81.31
14	879.57	Aromatic compounds	C–H bending	87.87

The Computational Toxicity and Skin Permeability Evaluation of the Identified Compounds

The computational toxicity evaluation of the identified compounds revealed that all compounds showed negative acute dermal toxicity (ADT), Haematotoxicity (HMT) and AMES toxicity (AMT) while most of the compounds, including Decanoic acid methyl ester, trans-2-Tridecen-1-ol, 1-Tridecyne, 9,12-Octadecadienoic acid methyl ester, 2-Methyldecane, and Erythro cis-4,5-Dimethyl-2-undecene, showed positive skin sensitization (SS), suggesting possible allergic or sensitizing effects on the skin. Eye irritation and corrosion (EIC) potential was observed only in Decanoic acid methyl ester and 2-Butyl-1-octanol, while the remaining compounds were negative. The skin permeability (SP) values showed that most compounds had logKp values greater than -2.5, indicating relatively low skin permeability and limited dermal absorption except 9,12-Octadecadienoic acid methyl ester, with an SP value of -2.719, may exhibit comparatively higher skin permeability than the other compounds as shown in Table 3

Table 3: The Computational Toxicity and Skin Permeability Study of the Compounds

Peak	compounds	Area%	ADT	SS	EIC	SP	AMT	HMT
1	Decanoic acid, methyl ester	16.75	-	+	+	-1.597	No	-
2	trans-2-Tridecen-1-ol	14.07	-	+	-	-1.723	No	-
3	1-Tridecyne	2.41	-	+	-	-1.451	No	-
4	9,12-Octadecadienoic acid, methyl ester,	12.46	-	+	-	-2.719	No	-
5	2-Methyldecane	8.37	-	+	-	-1.091	No	-
6	Erythro cis-4,5-Dimethyl-2-undecene	27.30	-	+	-	-1.117	No	-
7	2-Butyl-1-octanol	18.64	-	-	+	-1.700	No	-

Keys: SP = Skin Permeability, SS= Skin Sensitization, ADT = Acute dermal toxicity, EIC = Eye Irritation and Corrosion, AMT = AMES toxicity, HMT = Haematotoxicity, - = Negative, + = Positive and No = No AMES toxicity

A compound is considered to have a relatively low skin permeability if it has a logKp >- 2.5.

DISCUSSION

Gas Chromatography-Mass Spectrometry analysis is one of the first steps towards understanding the nature of active principles in medicinal and to decide whether the plant species has any individual compound or group of compounds [20] In this study, the GC–MS analysis of the methanol shell extract of *A. marginata* revealed the presence of seven bioactive compounds with varying concentrations of the extract possessing chemically active constituents that may contribute to wound healing activity. The predominance of Erythro cis-4,5-Dimethyl-2-undecene (27.30%), unsaturated hydrocarbon compounds which constitute a significant proportion of the extract. Hydrocarbon derivatives and unsaturated aliphatic compounds

have been reported to exhibit membrane stabilization, antimicrobial, and anti-inflammatory activities, which are important biological processes involved in tissue repair and wound contraction [21].

The presence of 2-Butyl-1-octanol (18.64%) and trans-2-Tridecen-1-ol (14.07%) further strengthens the possible wound healing properties of the extract because long-chain alcohols are known to possess antimicrobial and anti-inflammatory activities capable of preventing microbial colonization at wound sites and promoting tissue regeneration [22]. Fatty alcohols can disrupt microbial membrane integrity and reduce oxidative stress, thereby enhancing the healing environment necessary for rapid epithelialization [23]. In wound management, compounds with antimicrobial activity are particularly important because microbial infection remains one of the major causes of delayed wound healing [24].

Decanoic acid methyl ester (16.75%) and 9,12-Octadecadienoic acid methyl ester (12.46%) identified in the extract are fatty acid methyl esters that have been associated with antioxidant, anti-inflammatory, and antimicrobial activities [25]. Unsaturated fatty acid esters, especially linoleic acid derivatives such as 9,12-Octadecadienoic acid methyl ester, are known to modulate inflammatory pathways, promote fibroblast proliferation, and support collagen synthesis during wound repair [26].

The detection of 1-Tridecyne and 2-Methyldecane, Alkyne and alkane derivatives, although in relatively lower abundance have been implicated in hydrophobic interactions that contribute to antimicrobial activity and structural stabilization of bioactive compounds [27]. The broad spectrum of compounds identified in this study supports the assertion that the methanol shell extract of *A. marginata* contains multiple bioactive constituents capable of acting synergistically to enhance wound healing processes.

The FTIR characterization of the methanol shell extract further confirmed the occurrence of several biologically relevant functional groups associated with wound healing activity. The absorption frequencies observed between 879.57 cm^{-1} and 2974.33 cm^{-1} indicated the presence of aromatic compounds, alcohols, ethers, aldehydes, alkanes, nitro compounds, and amines. Functional groups identified by FTIR spectroscopy are important indicators of the biochemical properties and therapeutic potential of natural extracts because they determine molecular interactions and biological functionality [28].

The peaks detected at 879.57 cm^{-1}, 1421.58 cm^{-1}, and 1584.08 cm^{-1} corresponded to aromatic compounds characterized by C–H bending and C=C stretching vibrations. Aromatic compounds are widely recognized for their antioxidant activities because of their electron-rich structures [29], which enable stabilization of reactive oxygen species generated during inflammatory responses at wound sites. Antioxidant activity is essential in wound healing because excessive oxidative stress can impair fibroblast proliferation and collagen deposition [30].

The strong absorption bands observed at 1045.45 cm^{-1} and 1085.45 cm^{-1} confirmed the presence of alcohols and ethers through C–O stretching vibrations.

Alcohol-containing compounds are important in wound management because they contribute to antimicrobial activity and facilitate interactions with biological membranes through hydrogen bonding [31-32]. Similarly, the absorption band at 1276.92 cm^{-1} indicated aromatic ethers through Ar–O stretching, while the peak at 1327.07 cm^{-1} suggested nitro compounds or amines resulting from N–O and C–N stretching vibrations. Nitrogen-containing compounds are frequently associated with antimicrobial and anti-inflammatory properties capable of enhancing tissue regeneration and reducing microbial contamination in wounds [33].

The alkane-related peaks observed at 1384.94 cm^{-1}, 1458.30 cm^{-1}, 2887.53 cm^{-1}, and 2974.33 cm^{-1} indicated CH_3 bending and C–H stretching vibrations associated with lipid-derived compounds. Lipid-associated molecules play essential roles in maintaining skin barrier integrity and promoting cellular repair mechanisms during wound healing [34]. The aldehydic peak observed at 2827.74 cm^{-1} further suggests the presence of aldehyde-containing compounds, which may contribute to antimicrobial effects through interactions with microbial proteins and enzymes [35].

The computational dermal toxicity assessment of the identified compounds demonstrated generally favourable safety characteristics for potential topical application. All compounds were predicted to be negative for acute dermal toxicity, haematotoxicity, and AMES toxicity, signifying low risks of systemic toxicity, mutagenicity, and blood-related adverse effects. The absence of predicted mutagenicity is particularly important because AMES-negative compounds are generally considered less likely to induce carcinogenic or genotoxic effects during therapeutic application [36]. Despite the favourable toxicity profile, most of the compounds exhibited positive skin sensitization potential, except 2-Butyl-1-octanol, which showed negative sensitization activity. Positive skin sensitization predictions indicate the possibility of allergic or inflammatory reactions following repeated dermal exposure [37].

Eye irritation and corrosion potential were predicted only for Decanoic acid methyl ester and 2-Butyl-1-octanol. Alcohol-containing compounds are known to alter membrane permeability and may induce irritation in sensitive tissues such as the eye and mucosal surfaces [23]. However, the absence of eye irritation potential in most of the compounds further supports the relatively safe toxicological profile of the extract.

The skin permeability analysis revealed that most compounds possessed logKp values greater than −2.5, indicating relatively low dermal permeability and limited systemic absorption through the skin barrier. Low skin permeability is advantageous in topical wound healing formulations because it allows localized activity at the wound surface while reducing systemic toxicity risk [38-39]. Interestingly, 9,12-Octadecadienoic acid methyl ester exhibited a comparatively lower logKp value (−2.719). Unsaturated fatty acid esters are known to exhibit enhanced membrane penetration due to their lipophilic nature and structural flexibility, which may improve bioavailability at the wound site [40]

CONCLUSION

The study revealed that the methanol shell extract of *Archachatina marginata*

contains several bioactive compounds with potential wound healing properties. Gas Chromatography-Mass Spectrometry and FTIR analyses confirmed the presence of biologically active constituents and functional groups associated with antimicrobial, antioxidant, and anti-inflammatory activities. Computational toxicity evaluation further showed low acute dermal toxicity, absence of mutagenicity, and relatively low skin permeability of the identified compounds, suggesting possible safety for topical application. The findings confirmed the therapeutic capacity of *A. marginata* shell used in traditional wound healing. Therefore, further experimental and clinical studies are necessary to validate its efficacy and safety.

Authors' Contribution

AME and AF conceptualized the study. AF prepared the first draft of the manuscript and performed in-silico analysis. AME, ASH, BJD, CCE and TFL reviewed the manuscript. All authors contributed to the development of the final manuscript and approved its submission.

Conflict of interest: The authors declare that there is no conflict of interest.

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