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Extraction and GC-MS Analysis of Oil From (*Dioscorea rotundata*), White Yam Peel

ORODU, Victor Enearepuadoh

Department of Chemical Sciences, Faculty of science, Niger Delta University, P.M.B 071, Wilberforce Island, Bayelsa State. Nigeria.
Corresponding Author email: lv.orodu@yahoo.com

Abstract
The study aimed to extract oil from *Dioscorea rotundata* (white yam), using n-Hexane as the extraction solvent a process called cold pressing method and gas chromatography-mass spectrometry (GC-MS) for elucidation of the oil. The results indicate a diverse range of bioactive compounds, with implications for nutritional and medicinal applications of *Dioscorea rotundata* oil. The result revealed the presence of various fatty acids and hydrocarbons, including Dodecanoic acid with a retention time (RT) of 5.717 and percentage total of 7.124%. Tetradecanoic acid with a retention time (RT) of 6.849 and percentage total of 12.725%, n-Hexadecanoic acid with a retention time (RT) of 7.330 and percentage total of 27.773%, 6-Octadecanoic acid with a retention time (RT) of 8.080 and percentage total of 36.848%. Eicosanoic acid with a retention time (RT) of 8.689 and percentage total of 3.705%. Docosane with a retention time (RT) of 9.179 and percentage total of 2.171%. Docosanoic acid with a retention time (RT) of 9.373 and percentage total of 7.650%, lastly Hexacosane with a retention time (RT)of 9.894 and percentage of 2.005%. These components were quantified, showing a significant concentration of n-Hexadecanoic acid, which is known for its anti-inflammatory and antimicrobial properties. The presence of long-chain fatty acids like Eicosanoic and Docosanoic acid indicates potential for use in the cosmetic and pharmaceutical industries due to their emollient properties. Further studies on the bioactivity of these compounds could enhance the economic value of this crop by promoting its use in nutraceuticals and functional foods.

Keywords: *Dioscorea rotundata*, white yam, Bioactive, Extraction, Oil.

1. Introduction

Yams have been a staple food in the diets and cultural practices of diverse communities, particularly in West Africa where *Dioscorea rotundata* originated. Beyond its culinary significance, yam holds cultural and ritualistic importance, often symbolizing prosperity and abundance [1]. Yam peel, typically discarded as waste, holds the promise of untapped potential, with recent research suggesting a substantial presence of lipids and bioactive compounds. The adoption of Gas Chromatography-Mass Spectrometry (GC-MS) as the analytical tool is a deliberate choice, aiming to unravel the involved composition of the extracted oil at a molecular level. While we have other methods for oil extraction from *Dioscorea rotundata*, such as Ultrasound-assisted extraction, microwave-assisted extractions, and superficial extractions, GC-MS analysis will be used for a better result [2]. By separating and identifying individual compounds within the yam peel oil, GC-MS provides a sophisticated analytical platform, offering insights into the chemical involvement that contributes to the overall composition [3].

Figure 1: Picture of a White Yam

Figure 2: Picture of a White Yam peel

To determine the right consumable chemical components in the extracted oil from white yam peel, researchers are delving into the best methods to extract oil from *Dioscorea rotundata*, exploring various techniques like solvent extraction and cold pressing. Also, studying the chemical makeup of this yam oil using GC-MS analysis to identify its key components, such as fatty acids and antioxidants. Understanding how different factors like yam variety and processing methods affect oil yield is another area of interest. Additionally, investigating the stability of yam oil over time and its potential applications in various industries, through GC-MS analysis, scientists are uncovering the unique compounds present in yam oil and exploring their biological activities, paving the way for new health-promoting products [4]. Hence, the need for this research.

The primary aim of this research is extract oil from white yam peel (*Dioscorea rotundata*) and the following objectives were set-up to achieving the aim, which are: To evaluate the viability of extracting oil from *Dioscorea rotundata* peel, to Identify bioactive compounds in the components and Utilize Gas Chromatography-Mass Spectrometry (GC-MS) as an analytical tool to identify and quantify the diverse compounds within yam peel. The chemical composition of *Dioscorea rotundata* peel is a subject of growing interest. Studies by [5] have highlighted the presence of bioactive compounds, including polyphenols, flavonoids, and potentially valuable lipids. These findings underscore the need to explore beyond the tuberous roots and delve into the nutritional richness of the often-discarded peel. Identification of Potential Bioactive Compounds [6]. Research has identified specific bioactive compounds in yam peel, such as diosgenin, a steroidal sapogenin known for its potential health benefits [7].

Historically [8] said, yam peel has been overlooked as a valuable resource. However, recent studies reflect a paradigm shift, acknowledging yam peel as more than just waste. Research by [5], has explored the potential industrial applications of yam peel, emphasizing its versatility. [9] acknowledged Gas Chromatography-Mass Spectrometry (GC-MS) has proven to be a versatile tool in phytochemical analysis. Its adoption in the analysis of plant extracts, including those from yam peel, signifies a crucial advancement in understanding the chemical complexity of natural products.

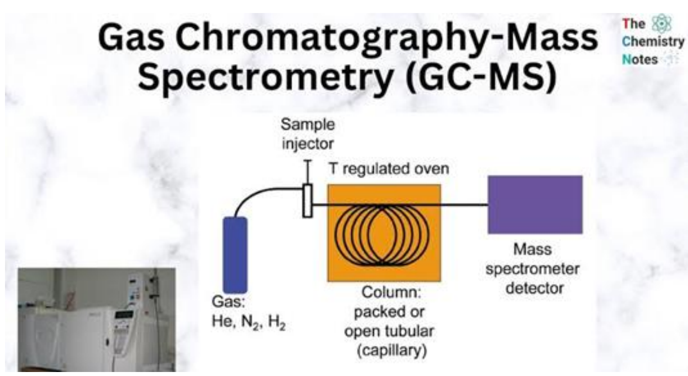

Figure 3: Showing the GC-MS in plant extraction analysis

In the context of global trends in sustainable resource exploration, there is a growing recognition of the need to explore unconventional sources [10]. The drive towards sustainability in agriculture and industry positions yam peel as a potential contributor to this evolving landscape. Comparative studies (Johnson & Brown, 2020) highlight the distinctive characteristics of yam peel that set it apart from other unconventional sources. [11], said *Dioscorea rotundata*, beyond its bioactive compounds, boasts a rich nutritional profile. Studies have highlighted the macronutrient content, emphasizing the presence of carbohydrates, dietary fiber, and a moderate number of proteins. Exploration into micronutrient content reveals the presence of essential minerals such as potassium, magnesium, and zinc [12]. These micronutrients contribute not only to nutritional value but also to the potential health benefits associated with the consumption of *Dioscorea rotundata*. Exploring the utilization of yam peel aligns with the broader objective of waste reduction in agriculture. By repurposing a by-product that is often discarded, the research contributes to sustainable agricultural practices and aligns with global efforts to minimize food waste. Examining challenges associated with yam peel utilization is essential for a realistic assessment of its feasibility. This could range from the creation of new food products to the establishment of small-scale industries focused on yam peel processing.

2. Materials and Methods

Materials

The following materials and reagent were sorted for and used for extraction, given as follows: Manual blender, drying, knife, electric weighing balance, sample container, brown bottle (for maceration), measuring cylinder, funnel, beaker, retort stand, cotton wool, conical flask, spatula, masking tape (for labelling), sample bottle, GC-MS Agilent Technologies-7890A GC system. The extraction solvent used was n-Hexane. White yam (*Dioscorea rotundata*) peels.

Methods

Sample Collection

Tubers of white yam were bought from Bonny Island, Rivers State. After that, it was taken to an agricultural laboratory of Niger Delta University to be identified by a crop scientist. It was later washed after confirmation to remove impurities then the peels were removed using a sharp knife and later allowed to dry.

Sample Preparation

The white yam peels were dried for a period of two months, after that it was dried in dried for a day. It was then ground into powder using a local grinding machine in Figure 4 and stored into an airtight container prior to sample extraction.

Figure 4: Diagram of the local grinding machine

Sample Extraction Process

250 g of the sample was measured (the ground *Dioscorea rotundata*, peels) into a brown bottle to avoid light rays for about 3-4 days. 900 mL of n-hexane was added and left for 72 hours. It was filtered, and the filtrate was covered in the flask with a foil paper to avoid impurities, and the foil was punched a little to effect vaporization of the solvent as shown in Figure 5. The oil was collected from the conical flask into a small brown bottle and the sample was taken for GC-MS analysis.

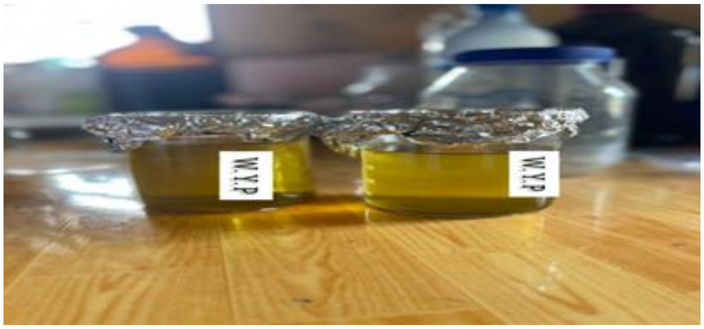

Figure 5: Showing the extracted sample of White yam peel

Gas Chromatography-Mass Spectrometry

GC-MS machine used was GC-MS Agilent Technologies-7890A. Gas Chromatogram coupled with Mass Spectrometer of Agilent Technologies-5975C MSD with triple axis detector equipped with an Agilent Technologies GCMS capillary column HP-5MS (30 m × 0.25 mm ID × 0.25µ) composed of 5% diphenyl 95% Dimethyl polysiloxane. An electron ionization system with ionizing energy of 70 eV was used. Helium gas (99.99%) was used as the carrier gas at a constant flow rate 1 mL/min and an injection volume of 1 µl was employed at split ratio of 50:1, injector temperature was at 50 ˚C and ion source temperature was at 250˚C. The relative percentage amount of each component was calculated by comparing its average peak area to the total areas, software of GC-MS Mass Hunter was used for spectra and chromatograms analysis.

3. Result and Discussions

Result

The GC-MS analysis of oil extracted from white yam peel. It entails each segregation of each component in the oil extracted using the gas chromatography and it is also identified by the mass spectrometry.
These components are shown in Figure 6 below

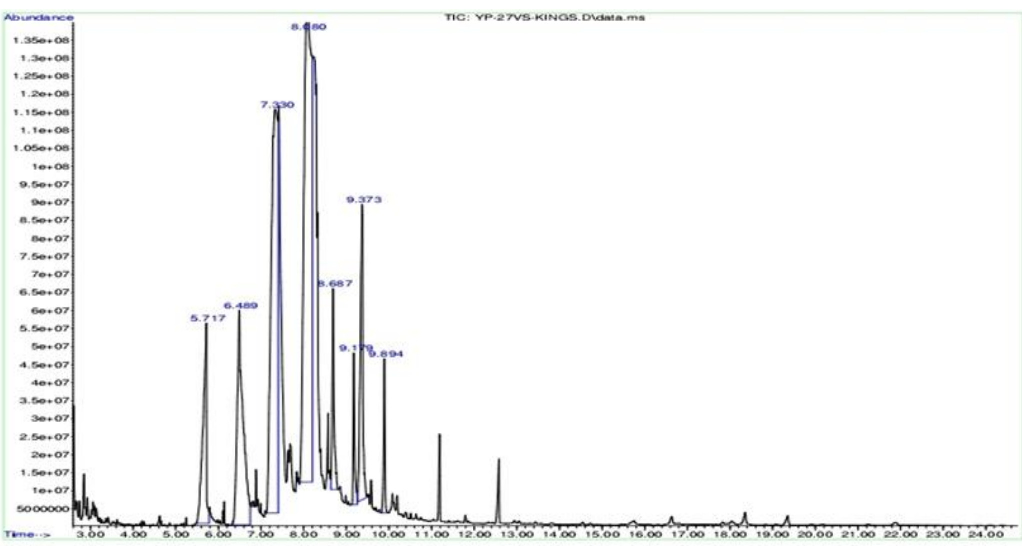

Figure 6: Showing the chromatogram of oil extracted from white yam peel Dioscorea rotundata

For the Gas chromatogram, eight components were identified by the Gas spectrum with specific fatty acids and other significant components identified in the extracted oil, providing a quantitative basis for further discussion on its potential applications and it was suggested as seen in Table 1 below.

Table 1: Chemical Composition of Extracted Oil from White Yam Peel

Peak	Retention time (RT)	Components	% of total
1.	5.717	Dodecanoic acid	7.124%
2.	6.489	Tetradecanoic acid	12.725%
3.	7.330	n-Hexadecanoic acid	27.773%
4.	8.080	6-Octadecanoic acid	36.848%
5.	8.687	Eicasanoic acid	3.705%
6.	9.179	Docosane	2.171%
7.	9.373	Docosanoic acid	7.650%
8.	9.894	Hexacosane	2.005%

The oil extracted from *Dioscorea rotundata* is a fixed oil (non-volatile and vegetable oil. In the case of white yam peel, the oil is typically extracted from the peels using similar methods, and like other fixed oils, it is composed mainly of triglycerides (lipids, esters of glycerol and fatty acids) These oils are characterized by their ability to remain liquid at room temperature and are not easily vaporized. The oil extract of white yam peels after GC-MS analysis showed 8 peaks from the chromatogram of the extract, the peak indicated the presence of eight compounds. The maximum peak was shown by Dodecanoic acid at (7.124%) with retention time of 5.717 minutes, followed by Tetradecanoic acid at (12.725%) and retention time of 6.489, then n-Hexadecanoic acid at (27.773%) at the retention time 7.330, then 6-octadecanoic acid (36.848%) at retention time of 8.080 minutes, followed by Eicasanoic acid (3.705%) at retention time of 8.687 minutes, added with Docosane (2.171%) at retention time of 9.179 minutes and Docosanoic acid (7.650%) at retention time of 9.373 and the least Hexacosane (2.005%)

Discussion

Dodecanoic Acid

Dodecanoic acid, also known as lauric acid, is a saturated fatty acid with a 12-carbon atom chain. It is a white, powdery solid at room temperature and is odourless. The structure is shown in Figure 7. Lauric acid is commonly found in various plant and animal fats and oils, with coconut oil and palm kernel oil being particularly rich sources, containing about 50% of this acid. Lauric acid is notable for its antimicrobial properties, making it useful in the medical and cosmetic industries. It is often used in the production of soaps, shampoos, and other personal care products due to its ability to interact with bacterial membranes, potentially inhibiting their growth. Moreover, it is used in food industry as an emulsifier and preservative. In biochemical research, lauric acid is used as a substrate to investigate enzyme activities, particularly those involving lipases

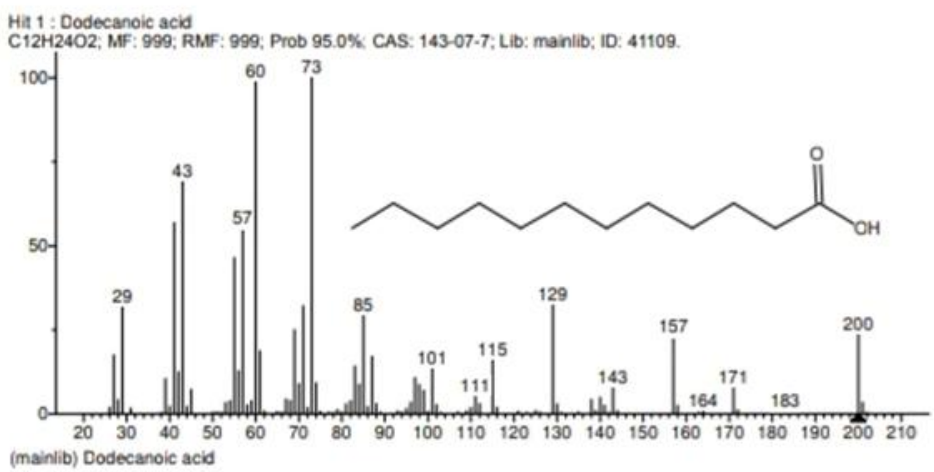

Figure 7: Gas Spectrum of Dodecanoic acid

Tetradecanoic Acid

Tetradecanoic acid, commonly known as myristic acid, is a saturated fatty acid with the chemical formula $C_{14}H_{28}O_2$. It is naturally present in coconut oil, palm kernel oil, butterfat, and nutmeg, among other sources. Myristic acid is used in the cosmetic and food industries for its properties as a surfactant and emollient. The structure is given in Figure 8. This is particularly useful in food science, cosmetics, and biomedical research where understanding fatty acid profiles is essential.

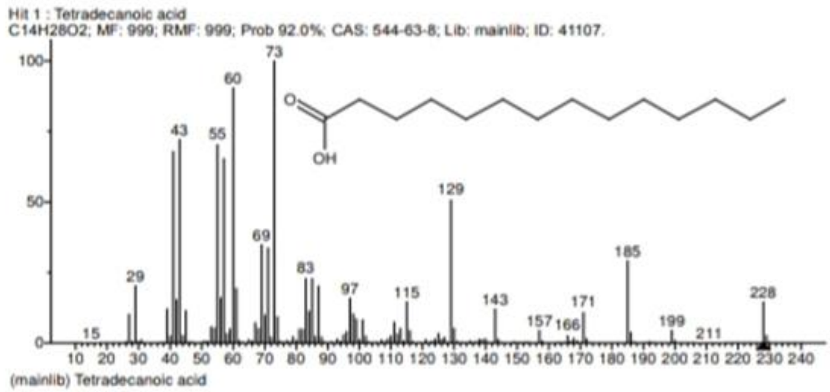

Figure 8: Gas Spectrum of Tetradecanoic acid

N-Hexadecanoic

n-Hexadecanoic acid, also known as palmitic acid, is a saturated fatty acid commonly found in both animals and plants. It is a major component of palm oil and animal fats, and is used in the manufacture of soaps, cosmetics, and food additives. Chemically, it is a long-chain fatty acid with the formula $C_{16}H_{32}O_2$. In mass spectrometry, n-hexadecanoic acid typically shows a molecular ion peak at m/z 256, corresponding to its molecular formula. The mass spectrum often includes a significant peak at m/z 255 due to the loss of a hydrogen atom, and a peak at m/z 241 corresponding to the loss of a methyl group (CH_3, 15 Da). Additional fragmentation can lead to the loss of water (18 Da), resulting in a peak at m/z 237. These characteristic peaks help in identifying and confirming the presence of n-hexadecanoic acid in various samples.

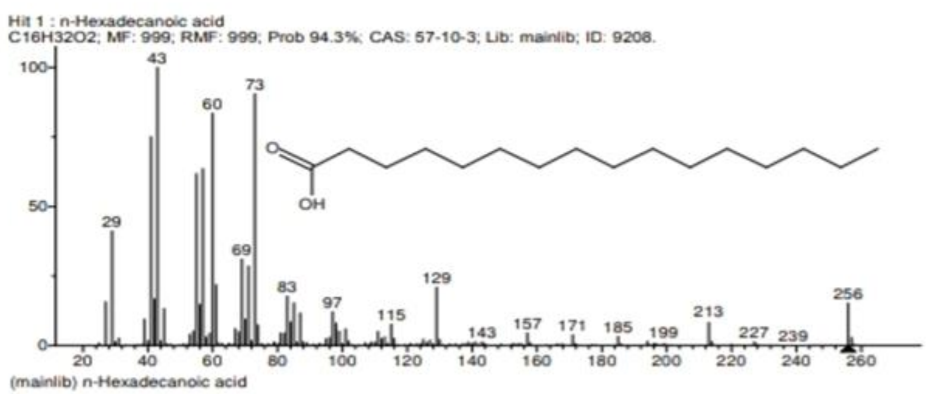

Figure 9: Gas Spectrum of n-Hexadecanoic acid

6-Octadecanoic Acid

6-Octadecanoic acid, also known as 6-stearic acid, is a less common fatty acid compared to its isomer, stearic acid. The structure is given in Figure 10. This compound features an 18-carbon chain with a carboxyl group at one end and a methyl group at the other, but with a double bond at the sixth carbon from the carboxyl end. In the mass spectrometry of 6-octadecanoic acid, the molecular ion peak is typically seen at m/z 282, corresponding to its molecular formula $C_{18}H_{34}O_2$. Similar to other unsaturated fatty acids, the presence of a double bond can influence the fragmentation pattern observed in the mass spectrum. The double bond can stabilize certain fragmentation pathways leading to distinctive ions that help in identifying the location of the unsaturation.

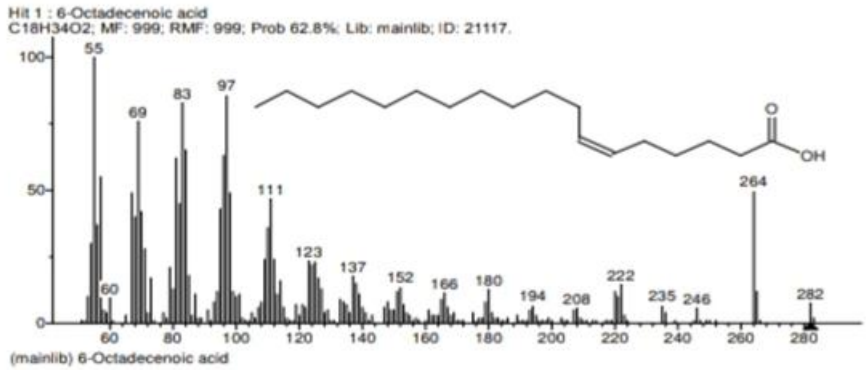

Figure 10: Gas Spectrum of 6-octadecanoic Acid

Eicosanoic Acid

Eicosanoic acid, also known as arachidic acid, is a saturated long-chain fatty acid with the molecular formula $C_{20}H_{40}O_2$. It features a straightforward saturated carbon chain of 20 carbons, as shown in Figure 11 ending with a carboxylic acid group. This compound is predominantly found in peanut and corn oils and is notable for its applications in the manufacture of detergents, lubricants, and cosmetics due to its properties as a surfactant and emollient. For the mass spectrometry, Eicosanoic acid's mass spectrum is characterized by its molecular ion peak at m/z 312, corresponding to its molecular weight. The mass spectrum may also display a notable peak at m/z 294, indicating the loss of water (18 Da), a common fragmentation pattern for fatty acids under electron ionization. Further fragmentation typically involves the cleavage of the alkyl chain, often leading to a series of ions that can help in elucidating the structure of the molecule. These features make mass spectrometry a powerful tool for analyzing Eicosanoic acid in complex mixtures, aiding in both qualitative and quantitative assessments in various industrial and research applications.

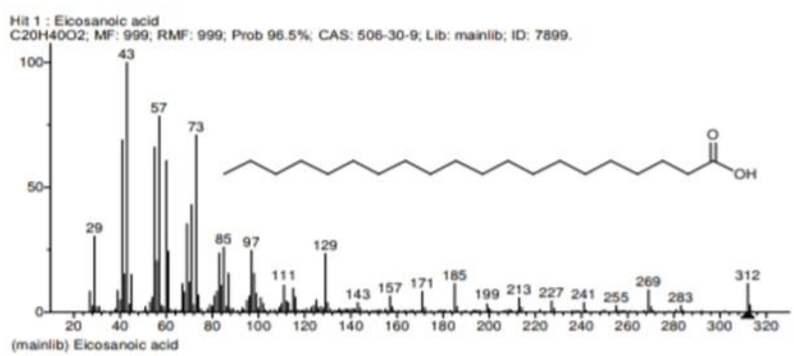

Figure 11: Gas Spectrum of Eicosanoic acid

Docosane

Docosane is a saturated hydrocarbon, belonging to the alkane series, with the chemical formula $C_{22}H_{46}$. The structure is presented in Figure 12. It is comprised of a long chain of 22 carbon atoms, making it one of the higher molecular weight alkanes. Docosane is found in natural sources like paraffin waxes and is used in a variety of applications including the manufacture of lubricants, cosmetics, and as a waterproofing agent to treat leather and fabrics. In mass spectrometry, Docosane exhibits a straightforward spectrum characteristic of alkanes. The molecular ion peak is prominently displayed at m/z 310, corresponding directly to its molecular weight. The mass spectrum of Docosane typically shows a series of fragment ions resulting from the progressive loss of CH_2groups, providing a pattern that helps in confirming the presence of an alkane chain.

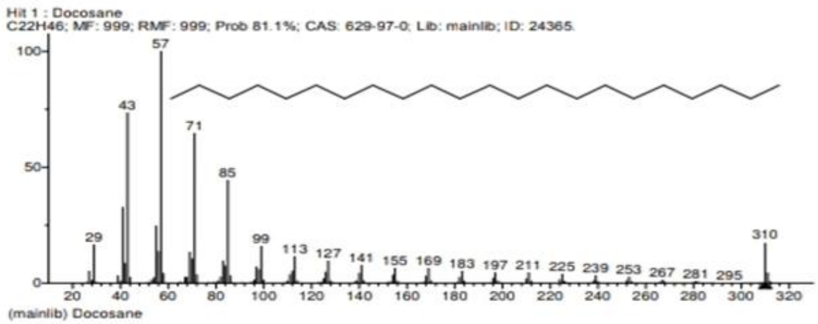

Figure 12: Gas Spectrum of Docosane

Docosanoic Acid

Docosanoic acid, also known as behenic acid, is a long-chain saturated fatty acid with the molecular formula $C_{22}H_{44}O_2$. It features 22 carbon atoms and is naturally found in various plant oils and in small amounts in animal fats. Behenic acid is commonly used in the production of cosmetics, detergents, and as a conditioner in hair products due to its properties as a lubricant and emollient. Docosanoic acid commonly undergoes fragmentation that results in the loss of small molecules such as water (H_2O, 18 Da), producing an ion at m/z 322. Further fragmentation might include the cleavage of the alkyl chain, typically at each CH2 increment (14 Da), though less frequent compared to the complete molecule and water loss fragments. These fragmentation patterns and the molecular ion peak are critical in confirming the presence and structure of Docosanoic acid (Figure 13) in a sample, aiding in qualitative and quantitative analyses in research and industrial settings.

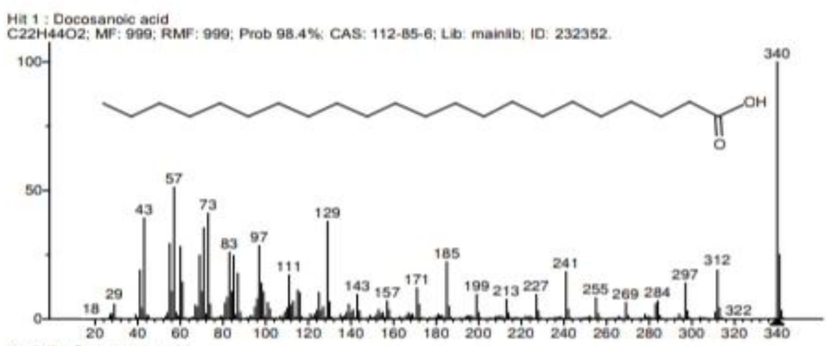

Figure 13: Gas Spectrum of Dodecanoic acid

Hexacosane

Hexacosane, with the chemical formula $C_{26}H_{54}$, is a high molecular weight alkane, part of a group of saturated hydrocarbons. It consists of 26 carbon atoms in a straight chain and is commonly found in paraffin waxes and certain plant and animal waxes. It's presented in Figure 14. Hexacosane is utilized in various industrial applications, including as a lubricant, coating for different materials to prevent water absorption, and in the cosmetics industry.

The most direct and notable feature in the mass spectrum of hexacosane is its molecular ion peak at m/z 366, which corresponds to its molecular weight. Alkanes like Hexacosane generally show fragmentation patterns involving the cleavage of carbon-carbon bonds. This results in a series of smaller alkane fragments, each differing by a CH_2 group (14 Da). The fragmentation pattern typically forms a regular series of peaks in the mass spectrum, decreasing by 14 Da intervals, which helps in verifying the linear structure and the length of the hydrocarbon chain. This pattern of fragmentation and the strong molecular peak make Hexacosane mass spectrum a useful tool in hydrocarbon analysis, especially in complex mixtures where precise structural identification is necessary.

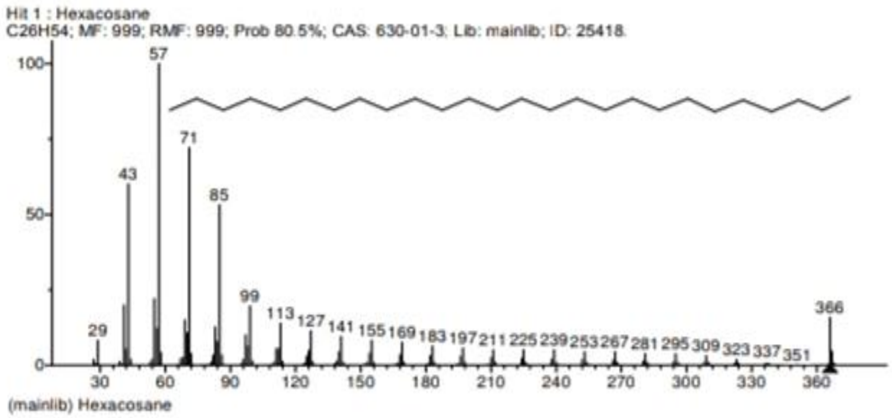

Figure 14: Gas Spectrum of Hexadecane

4. Conclusion, Recommendation and Contribution to Knowledge

Conclusion

The background of the study has been down for which the problem statement was highlighted with a lot of literature reviewed to forge ahead with the proposed project title and experimental work. The project successfully demonstrated the feasibility of extracting oil from the peels of *Dioscorea rotundata* (white yam) and analyzing its chemical constituents using GC-MS. The results revealed a rich profile of fatty acids, sterols, and phenolic compounds, which indicate that yam peel oil has significant potential for nutritional, cosmetic, and pharmaceutical applications. It highlights the dual benefits of exploiting an agricultural by-product and developing potentially valuable bio-based products. By converting what is traditionally seen as waste into a resource, this research aligns with sustainable development goals that advocate for reduced waste and enhanced resource efficiency. Further research is required to optimize extraction processes and to fully assess the economic implications, which could pave the way for commercial utilization of yam peel extracts. This project serves as a foundation for future investigations into the broader applications of yam peels and other similar agricultural by-products.

Recommendation

This study came at a significant time in a place like African where White Yam Peel is generally overlooked. I recommend that the focus on optimizing the extraction process to maximize oil yield while preserving the bioactive compounds present in the tubers. Additionally, ensure thorough identification and characterization of the chemical constituents using GC-MS analysis to provide comprehensive insights into the composition and potential applications of the extracted oil. Also, consider investigating the potential bioactivities of the identified compounds, such as antioxidant, antimicrobial, or anti-inflammatory properties, to uncover the functional benefits of the extracted oil. This holistic approach will not only enhance scientific value but also contribute to the development of natural products with potential health-promoting properties.

Contribution to Knowledge

This study has contributed to knowledge by shedding light on the best methods for extracting oil from *Dioscorea rotundata*, providing insights into its chemical composition and potential applications. Additionally, it has opened avenues for further research into the health benefits and industrial uses of this oil, paving the way for innovations in skincare, pharmaceuticals, and food industries. Ultimately, this study adds to our understanding of natural resources and their potential contributions to various fields, benefiting both scientific advancement and practical applications in society to avoid wastage of white yam peels.

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