

GC–MS-Based Identification of Bioactive Compounds and Evaluation of Antibacterial Activity in Medicinal Plant Essential Oils

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ABSTRACT

All around the world, plant-based medicine has been used to treat illnesses at a reasonable cost; medicinal plants are the main source of pharmaceuticals and the healthcare system. *Caesalpinia bonducella* seeds have long been used in traditional medicine to treat a wide range of illnesses and ailments, such as leprosy, fever, edema, colic, malaria, and stomach ache. Several ethnic groups have long utilized the kamala tree (*Mallotus philippensis*) to cure a wide range of illnesses and disorders; however, in order to generate medications from this tree, these traditional applications must be examined and verified by science researchers. Commonly referred to as "Sweta Arka," *Calotropis gigantea* (family Asclepiadaceae) is a highly therapeutic wild plant species found in the Indian Himalayan area that is resistant to drought and has a comparatively high degree of salt tolerance. The dried milky latex found in the stem of plants is used as a remedy for snake venom. On the other hand, the dried leaves of the *Calotropis* plant are used to treat rheumatic pain and paralysis as an expectorant and anti-inflammatory. The *Ulmaceae* family's *Holoptelea integrifolia* (Roxb.) is a beneficial medicinal plant with a variety of traditional medical applications linked to its possible phytochemical contents and antioxidant activity. The leaves, bark, and seeds of this plant are used by people to treat a variety of illnesses. A economically significant medicinal crop, *Emidesmus indicus* attracts interest from the food and flavoring industries as well as pharmaceutical companies. With regard to the morphologically different *H. indicus* plants, the present study aims to uncover the potentialities. Using extracts from the broad-leafed *H. indicus* fruits, GC-MS analysis identified different chemicals.

Keywords- *Emidesmus indicus*, *Caesalpinia bonducella*, *Ulmaceae*, *Calotropis* plant, *Holoptelea integrifolia*

Introduction

Over 80% of people worldwide rely on traditional medicine to meet their medical needs, according to the World Health Organization (WHO). With a reservoir of numerous unique phytoconstituents, medicinal plants have been an endless source of new medications and chemical compounds. Alkaloids, flavonoids, coumarins, glycosides, gums, phenols, tannins, terpenes, and terpenoids are among the many classes of compounds that have therapeutic potential, including immunomodulatory, antioxidant, anti-diabetic, and anticancer properties. This study uses GC-MS analysis to assess the chemical makeup of an ethanolic extract of the entire plant, *Chromolaena odorata*. Several phytoconstituents of chemical nature are being investigated in the current study. Terpenoids, phenols, flavonoids, coumarins, long-chain fatty acids, etc. were found. The most prevalent polyphenolic compounds found in plants are phenolic acids and flavonoid compounds. Numerous clinical studies have demonstrated a positive relationship between the consumption of polyphenolic compounds or flavonoids and a lower incidence of cancer. In chronic illnesses involving inflammation and metabolic disorders, long chain fatty acids are crucial. [1][2] Immunotherapy, radiotherapy, chemotherapy, and surgery are all part of the current interdisciplinary approach to treatment, which is customized based on the location and stage of the cancer. Due in large part to the decreased side effects of current medications, there is a growing interest in finding a naturally occurring bioactive, such as secondary metabolites, to treat cancers, including oral cancer. [3] Both targeted molecular therapy and traditional treatment methods for patients with oral squamous cell carcinoma continue to face numerous obstacles. Because phytochemical components have little to no toxicity to healthy tissues, they are excellent chemo preventive agents and have attracted a lot of attention for their potential use in cancer prevention. [4] observed a correlation between the presence of oral bacteria and oral squamous cell carcinoma. Acetaldehyde, nitrosamines, sulfides, and oxides are among the metabolites produced by microorganisms that have the potential to cause tumors. The oral microbiota affects oral squamous cell carcinoma in a number of ways, including its incidence, course, and prognosis. [5] The role of oral microbiota in the pathophysiology of cancer has been explained by three distinct mechanisms. The first factor is the start of persistent inflammation brought on by microbes, which results in the production of angiogenesis, mutagenesis, oncogene activation, and cell proliferation stimulated or induced by the inflammation-related substances. The activation of NF- κ B and the suppression of cellular apoptosis are two more processes associated with bacteria that may impact cell proliferation and ultimately contribute to the development of cancer. The third process involves the production of particular chemicals by cancer-causing bacteria. [6] Apricot is a little tree that grows to a height of 8 to 12 meters. It has a dense, spreading canopy and a trunk that may reach a diameter of 40 cm. The ovulation leaves have a rounded base, a pointed apex, and a serrated border. They are 5 cm long and 4–8 cm broad. The blossoms are produced singly or in pairs, and have five white to pinkish petals with a diameter of 2 to 4.5 cm. The fruit, which resembles a little peach and has a diameter of 1.5 to 2.5

cm, is yellow to orange in color and frequently has a red tint on the side that is exposed to the sun. Its surface can be smooth, glabrous, or velvety, with very short hairs, or pubescent. The meat is solid but not particularly juicy. Apricot is one of the most popular crops cultivated all over the world since it is high in vitamins and minerals. Certain areas with acceptable environmental conditions are home to apricot trees.[7] Because of its high phytochemical content, it is also a powerful source of antioxidants that limit the damaging effects of oxidant reactions brought on by free radicals. Butylated hydroxyl toluene (BHT), one of the many synthetic antioxidants used in industrial processing, has been linked to liver damage and carcinogenesis, which is a serious health risk.[8] The Bixaceae family includes the annatto plant (*Bixa orellana* L.), which is indigenous to tropical America and has spread widely from Brazil to the Guianas. Annatto seeds, which were once used by indigenous peoples to extract dyes, are now commercially used for the pigment bixin, with an estimated 14,500–17,000 tons produced worldwide each year. Bixin's substantial industrial and commercial importance is demonstrated by its widespread usage in the food, pharmaceutical, and cosmetic sectors. It also accounts for around 70% of the global market for natural colorants. The pigment is a crucial economic component since it is concentrated in the pericarp or aril, which makes about 5–10% of the seed's total weight. Depending on the cultivar, climate, and local soil properties, bixin concentration can range from 1% to 6%. However, it is essential for commercial viability, with a minimum threshold of 3% bixin required for successful production.[9] The current work explores a novel method for producing biodiesel from *Mallotus philippensis* seed oil using a green nanocatalyst made from the fruit extract of rotting fungus. The green nanocatalyst was made with sodium tungstate as a precursor. Sodium tungstate was selected because of its fascinating catalytic characteristics and promise for the production of nanomaterials. The rotting fungus fruit extract and sodium tungstate were combined to develop an eco-friendly catalyst that complied with green chemistry and sustainability standards. This unorthodox method demonstrates both the adaptability of renewable materials in catalysis and the utilization of unorthodox resources for the generation of sustainable energy.[10] The tropical plant species *Mallotus philippensis*, which is well-known for having a high oil content, shows promise as a feedstock for biodiesel since it is widely available and can be grown in a range of agroclimatic conditions. The synthesis of biodiesel from *Mallotus philippensis* seed oil has not been studied, as far as the authors are aware. Often referred to as "Kamala," it is a member of the Euphorbiaceae family of medicinal plants. It is indigenous to India, Nepal, and Bhutan in Asia.[11] Due to the careless usage of commercial antimicrobial drugs that are frequently used to treat infectious diseases, plant pathogenic bacteria have acquired diverse chemical resistance in recent years. Chemotherapy resistance has been seen in many types of microorganisms, including viruses, fungi, and bacteria. Using antibiotic inhibitors derived from plants is one way to lower antibiotic resistance. Strong natural, biologically active agents are found in compounds that have been extracted from culinary and medicinal plants.[12] Because they are more accessible and less expensive than contemporary medications, medicinal plants are still frequently utilized in nonindustrialized communities, such as many regions of Southeast Asia. Some of the most significant and well-known medicinal plants in the Philippines are members of the genus *Alstonia* in the Apocynaceae family. Of the five native species from the Philippines, two *Wall. ex G. Don*, *Alstonia macrophylla*, and *Alstonia scholaris* (L.)

R. Br. are significant regionally, and different parts of these plants are gathered to treat human illnesses naturally. Echitovenidine, echitamine, venenatine (an indole aloid), and anti-inflammatory triterpenoids have all been shown to be present in *A. macrophylla* and *A. scholaris*. [13][14] Fifteen of the 19 alkaloidal chemicals found in the aerial portions were identified. Alstomaline, 10,11-dimethoxynareline, alstohentine, alstomicine, 16-hydroxylalstonisine, 16-hydroxylalstonal, 16-hydroxy-N4-demethylalstophyllal oxindole, alstophyllal, 6-oxoalstophylline, and 6-oxoalstophyllal were among the 10 undiscovered indole alkaloids.[15] Fifteen of the 19 alkaloidal chemicals found in the aerial portions were identified. Alstomaline, 10,11-dimethoxynareline, alstohentine, alstomicine, 16-hydroxylalstonisine, 16-hydroxylalstonal, 16-hydroxy-N4-demethylalstophyllal oxindole, alstophyllal, 6-oxoalstophylline, and 6-oxoalstophyllal were among the 10 undiscovered indole alkaloids.[16] According to estimates from the World Health Organization, 80% of people in underdeveloped nations rely on herbal medicine to meet their basic medical needs. In many regions of the world, cancer is a major health concern. Abnormal cell growth that tends to spread to other places of the body is called cancer. There are two kinds of cancer: benign and malignant. While malignant tumors often spread, divide, and cause serious illnesses, benign tumors do not. Tobacco, obesity, excessive alcohol use, certain illnesses, poor nutrition, and inactivity are the main risk factors.

Escherichia coli and have shown excellent antibacterial and antioxidant properties. *Calotropis gigantea* was examined for anti-proliferative effect on colorectal cancer since it has demonstrated remarkable protective qualities and offers a variety of therapy options.[17] Determining the overall quality, stability, and effectiveness of the herbal product are the main issues in the field of herbal medicine. Most herbal medicines are known to be light-sensitive, and extracts from herbal plants may experience photodegradation responses when exposed to UV light, according to reports. Therefore, the purpose of this work was to assess the phytochemical and antibacterial activity of *Calotropis gigantea* leaf extract. In addition, we investigated the impact of light irradiation on the antimicrobial activity of *Calotropis gigantea* ethanolic leaf extract.[18] Chemotherapy, radiation, and surgical excision are the main methods used to treat cancer. These techniques do have some negative impacts, though. On the other hand, herbal remedies are increasingly being used to cure cancer. The traditional medicinal system makes extensive use of the herb *Calotropis gigantea*. There aren't any reports on its potential for managing cancer, though. Thus, we sought to investigate the phytochemical makeup and cytotoxic activity of *C. gigantea* methanolic leaf extract against three distinct cancer cell lines: A549 (lung), MCF7 (breast), and HeLa (cervical).[19] In addition to its medical properties, the plant produces helpful floss from the seeds and a robust fiber from the bark. According to certain findings, *C. gigantea* has an impact on agricultural crops' germination and seedling vigor. Because *C. gigantea* contains many cardiac glycosides (Cardenolides), all of its parts are poisonous. Cardenolides are found in plants, benzoylinesolone and benzoylisolinelone are found in the root bark, calotropin and calotropagenin are found in the leaves and stalk of the plant, uzarigenin and terpenol ester are found in the flower and latex, and so on. These phytochemical constituents are responsible for the medicinal qualities of *C. gigantea*. [20] A lot of individuals cure bacterial illnesses at random by using herbs, their leaves, roots, and/or seeds. However, understanding the particular pathogenic illnesses that these plants may treat as well as the phytoconstituents that are responsible for these actions is as essential. Additionally, several studies have shown the antibacterial efficiency of these plants; nevertheless, because of the emergence of drug resistance, it is necessary to continuously assess the performance of plant extracts as beneficial antimicrobial agents.[21] It may be found in both tropical and temperate regions of the northern hemispheres. It may be found in India up to 2000 feet in the outer Himalayan area. It is a huge, 30- to 35-meter-tall deciduous tree. The gray bark has slightly corky

scales. Alternating elliptic-ovate leaves are 5–13 cm long, acuminate, whole, sub-coreaceous, and pinnately veined. Flowers are greenish-yellow, typically male or hermaphrodite, monochlamydeous or sporadically polygamous, and typically occur between January and February. The suborbicular samara fruits, which typically appear in April or May, have membrane wings and a single tiny kidney-shaped seed.[22] Certain native plants are utilized as meals and spices in every part of the world, and studying their chemical makeup and bioactivities has emerged as an intriguing area of study. This is due to the fact that it highlights the nutritional worth and therapeutic potential of various dietary ingredients that are employed as treatments, particularly for stubborn infectious disorders brought on by food contamination. According to Corn et al. (1999), spices are ingredients that are typically derived from vegetables or various dried plant parts, such as barks, seeds, and leaves, that are added to food in nutritionally small amounts to enhance its color, taste, or flavor. They may also act as preservatives that prevent the growth of harmful bacteria.[23][24] Because they have fewer side effects and are less hazardous than synthetic medications, natural medicines are becoming more popular. Tyrosinase is a copper-containing oxidase enzyme that often starts the enzyme-mediated browning response in harvested fruits. This multifunctional enzyme is the cause of the unwanted overpigmentation of human skin, which is comparable to what happens when fruits brown. This enzyme catalyzes the first two stages of mammalian melanogenesis, thus researchers are interested in finding strong tyrosinase inhibitors, particularly ones that are safe to employ in foods and cosmetics.[25] The production of biofilms in flagellated *P. aeruginosa* PA01 is thought to begin with bacteria swimming, swarming, and colonizing surfaces. This bacteria can colonize surfaces and form biofilm communities by swimming toward surfaces with its flagella, then twitching and swarming.

Acetylcholine is normally broken down by a class of medications known as cholinesterase inhibitors. Dementia is linked to cholinergic insufficiency, which causes central nervous system deterioration and Alzheimer's disease (AD). Various cholinesterase inhibitors, including natural substances and extracts, synthetic counterparts, and their hybrids, are being used as a solution to this problem.[26]

Material and Methods

Collection of materials:-

Caesalpinia bonduc, *Mallotus philippensis*, *Holoptelea integrifolia* seed *Calotropis gigantea*, flower, and *Hemidesmus indicus* Root collected from the Rama University of Agriculture and Technology field in Kanpur is used in this research study. The seeds of the Solanaceae plant, *Caesalpinia bonduc*, *Mallotus philippensis*, *Calotropis gigantea*, *Holoptelea integrifolia*, and *Hemidesmus indicus*, will be available in March 2024. The plant material was found and confirmed by the Department of the Faculty of Engineering at Rama University in Mndhana Kanpur, Uttar Pradesh, India.

Oil Extraction using Soxhlet:-

The seeds were off-white in color and had a moisture content of 4%. Crushing the seeds prior to extraction makes oil extraction easier and more efficient. By rupturing the cell wall, this process effectively releases oil. The seeds were then haked at 105 OC for two hours. Heat treatment also makes it easier for oil to be released by eliminating moisture from the seeds. Pre-treating seeds prior to solvent extraction increases surface area and promotes solvent penetration, which results in effective extraction. Pre-treatment and heat treatment were followed by the setup of the solvent extraction assembly. Benzene, n-hexane, and a mixed solvent system were utilized to extract oil. Using a Soxhlet extractor, the extraction was carried out. use a petroleum ether solvent to extract seed oil. Following extraction, simple distillation was used to eliminate the solvent. In a desiccator, the oil was allowed to cool before being weighed. A dark brown glass bottle with a tight seal was used to keep the extracted oil for analysis. Determine the various characteristics and yield % of the oil. The solvent employed in the Soxhlet extractor to extract the oil was n-hexane.

Methanol extraction at a 1:2 feed to solvent ratio

To eliminate the moisture, dry 50 grams of *Caesalpinia bonduc*, *Mallotus philippensis*, *Calotropis gigantea*, *Holoptelea integrifolia*, and *Hemidesmus indicus*. in an oven or under the sun.

- Grind the date seeds into a powder.
- Use a 1:1:2 ratio of date seed powder to 100 milliliters of methanol.
- Take a cotton cloth or a piece of filter paper and fill it with date seed powder.
- Place the cloth or filter paper inside the Soxhlet extraction equipment thimble that holds the powdered seeds.
- Fill a Soxhlet flask with 100 ml of methanol as the solvent.
- Heat the mixture for two to three hours at 60 to 65 degrees Celsius (boiling point of the solvent).
- After extraction, remove the round-bottom flask from the Soxhlet apparatus.
- Use simple distillation to extract the date seed oil from the solvent.
- Simple distillation is done for separation at temperatures between 60 and 65 degrees Celsius.

- During the distillation process, oil collects at the bottom and petroleum ether rises to the top.

1. Preparation of Growth Media

- **Media Selection:** The selection of a suitable medium for growth should be made. Media such as Mueller Hinton Agar for the disk diffusion test or Mueller Hinton Broth for the dilution tests should be selected.
- **Sterilization:** The prepared media should be sterilized. This can be done by autoclaving the media at 121°C for 15 minutes.
- **Plate Preparation:** The sterilized media should be poured into sterile Petri dishes to a depth of 4 mm.

2. Inoculum Preparation:-

- **Selection:** 3 to 5 isolated colonies of the same type should be selected from a primary agar plate.
- **Suspension:** The isolated colonies should be transferred to a sterile tube containing saline or broth.
- **Standardisation:** The suspension should be standardized to the 0.5 McFarland standard. This is usually 1.5×10^8 CFU/mL.

3. Inoculation and Sample Application:-

- **Inoculating Plates:** A sterile cotton swab should be dipped into the standardized inoculum. The inoculum should be evenly distributed across the surface of the agar.
- **Applying Samples:-**
- **Disk Diffusion:** The disks should be placed on the surface of the inoculated agar.
- Wells should be made on the surface of the inoculated agar. The wells should then be filled with the drug.
- **E-test:** Well Diffusion: The strips should be applied to the surface of the inoculated agar.

4. Incubation and Observation:-

- **Incubation:** The inoculated agar should be incubated for a specified time. This is usually 16 to 24 hours. The temperature should be suitable for the microorganism. This is usually 35 to 37°C.

Reduction sugar

- Take Fehling's Solution A (Copper sulphate).
- Take Fehling's Solution B (Alkaline sodium potassium tartrate).
- Mix equal volumes (1 mL + 1 mL) just before the experiment.
- Take 2 mL of test solution (plant extract or sugar solution) in a test tube.
- Add the freshly prepared Fehling's mixture (2 mL) to the test sample.
- Place the test tube in a boiling water bath.
- Heat for 5–10 minutes.

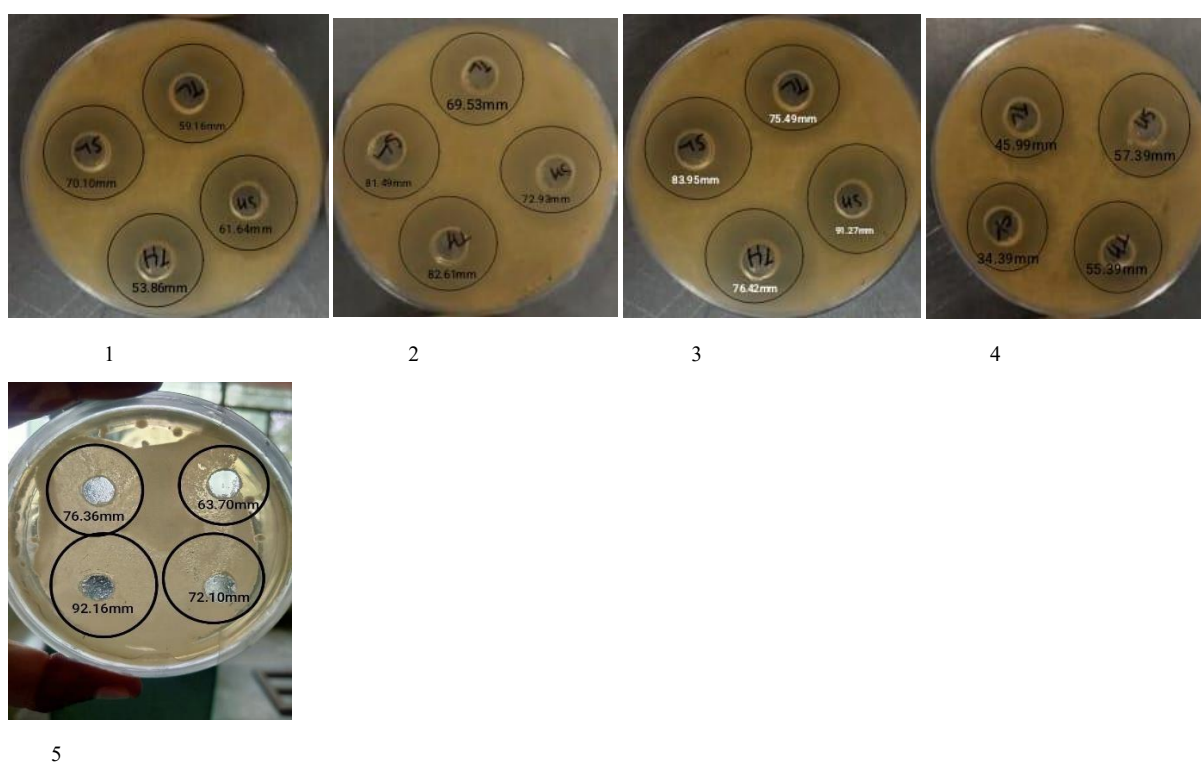
Gas chromatography mass spectrometry of *Caesalpinia bonduc*, *Mallotus philippensis*, *Calotropis gigantea*, *Holoptelea integrifolia*, and *Hemidesmus indicus*

- **GC-MS System:** The GC-MS system in this study is the GCMS-QP2010 model. This system combines gas chromatography (GC) and mass spectrometry (MS) to separate and identify compounds in a sample.
- **GC Column:** The chromatographic column used is an Rxi-1MS GC column, with a length of 30 m, an internal diameter of 0.25 mm, and a film thickness of 0.25 μ m. It is made entirely of 100% dimethyl polysiloxane and is manufactured by Restek in the United States. This column is commonly used for general-purpose GC separations.
- **Autosampler:** An AOC-20i autosampler from Shimadzu in Japan was used to introduce samples. The autosampler automates the injection of samples into the GC system, which improves efficiency and reproducibility.
- **Mass Range and Maximum Temperature:** The mass spectrometer can detect masses in the range of 45 to 500 g. The maximum temperature of the GC oven is 330°C, the highest temperature the GC column can withstand during analysis.
- **Carrier Gas:** Helium (He) serves as the carrier gas for the GC analysis. However, during the initial phase of the study, the split ratio and flow rate of the carrier gas were not optimized. These parameters are important as they affect the efficiency and resolution of the chromatographic separation.
- **Sample Preparation:** The test samples are diluted with dichloromethane to a specific concentration. The volume used for dilution is 1 L. Dichloromethane is a common solvent in GC-MS analysis due to its low polarity and volatility, making it suitable for dissolving a wide range of compounds.

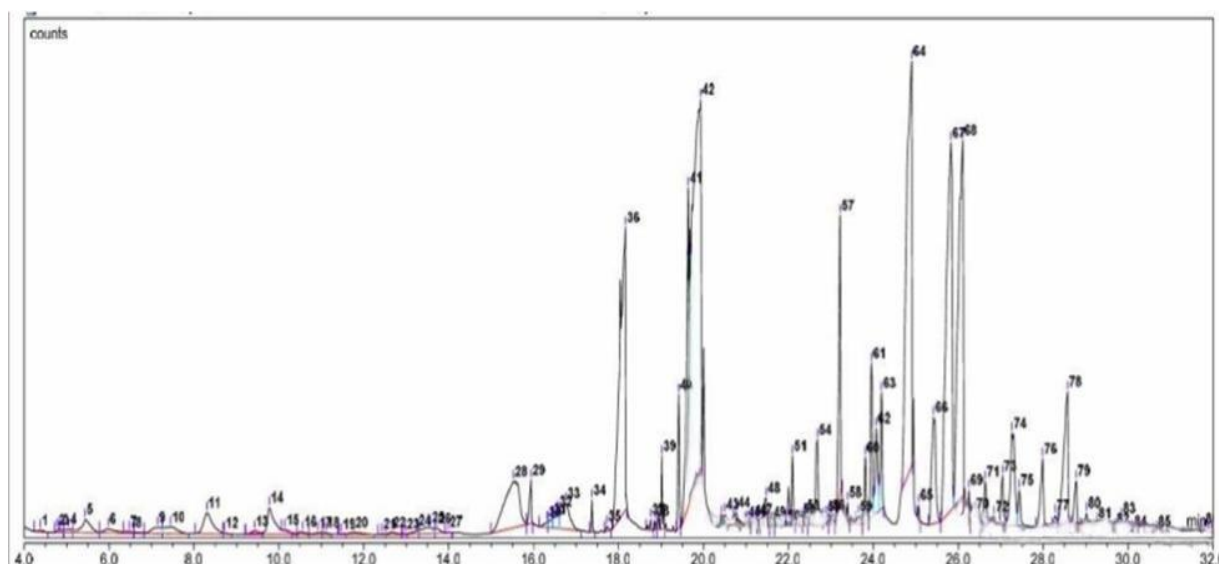
Results and Discussion

Antibacterial Activity:-

Antibacterial assay is an assay that tests the susceptibility of bacteria to different antibacterial agents or antibiotics. The antibacterial assay can be performed by using a Kirby-Bauer antibacterial assay. The formation of a zone of inhibition in the antibacterial assay indicates that the antibacterial agent or antibiotic is effective in inhibiting the growth of bacteria in the tested sample. For *E. coli* bacteria, the formation of a zone of inhibition in an antibacterial assay by an antibiotic disc indicates that the antibacterial agent or antibiotic is effective in inhibiting the development of *E. coli* bacteria. The level of susceptibility of bacteria in an antibacterial assay can be determined by the size of the inhibition zone. The agar well diffusion technique was used to assess the crude extracts' antibacterial activity. A Muller Hinton Agar (Hi-media) plate was covered with 200µl of standardized inoculums at a concentration of 108cfu/ml. A sterile cork borer with a diameter of 6 mm was used to punch wells into the Muller Hinton Agar plate. After adding 20 µl of the crude extracts at a concentration of 10 mg/ml to the well, it was left to stand at room temperature for around two hours before being incubated at 37 °C. The solvents used to reconstitute the extracts were employed to set up controls in parallel. After 24 hours, the plates were examined for the zone of inhibition. The extracts' activity was contrasted with streptomycin's. The diameter of the inhibitory zones' mean and standard error were computed.



Antibacterial activity use *S. aureus* 1. *Caesalpinia bonduc* 2. *Mallotus philippensis* 3. *Calotropis gigantea*, 4. *Holoptelea integrifolia* 5. *Hemidesmus indicus*

Graph 1. Gc-Ms of *Caesalpinia bonduc*

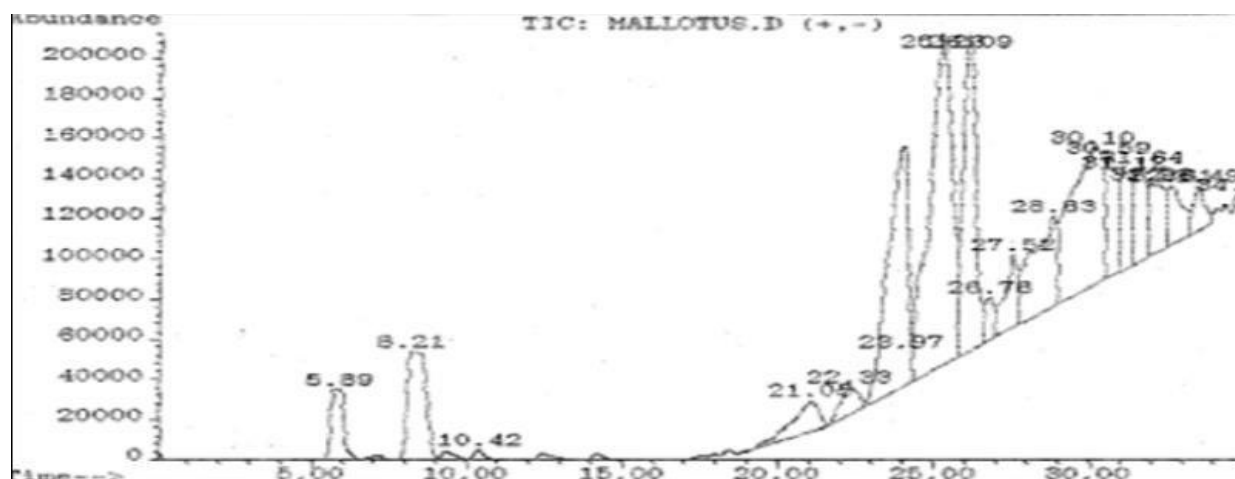
S. No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
1.	4.38	C ₄ H ₉ NO ₂	Sec-Butyl nitrite	63.3
2.	4.78	C ₄ H ₇ NO ₃	2-Nitro-1-buten-3-ol	66.4
3.	4.87	C ₇ H ₁₁ NO ₅	Isoxazolidine-3,5-dicarboxylic acid, dimethyl ester	104
4.	5.05	C ₁₀ H ₂₂ N ₂ O	N-Isopentyl-N-nitroso-pentylamine	32.34
5.	5.43	C ₇ H ₁₄ O ₃	Propanoic acid, 3-ethoxy-, ethyl ester	46.5
6.	5.98	C ₆ H ₁₂ O ₅	Alpha-l-rhamnopyranose	98
7.	6.47	C ₇ H ₁₄ O ₇	d-Glycero-d-ido-heptose	131
8.	6.59	C ₆ H ₁₂ O ₅	2-Deoxy-D-galactose	98
9.	7.14	C ₆ H ₈ N ₂ O ₈	Isosorbide Dinitrate	63.8
10.	7.45	C ₃ H ₈ O ₃	Glycerin	92.09
11.	8.30	C ₆ H ₈ O ₄	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	52.6
12.	8.71	C ₈ H ₁₅ NO ₆	α-D-Galactopyranose, 2-(acetylamino)-2-deoxy-	119
13.	9.42	C ₆ H ₈ N ₂ O ₈	Isosorbide Dinitrate	63.8
14.	9.77	C ₆ H ₆ O ₃	5-Hydroxymethylfurfural	58.5
15.	10.15	C ₈ H ₁₄ O ₇	6-Acetyl-B-d-mannose	116
16.	10.56	C ₁₀ H ₁₆ O ₃	Ascaridole epoxide	54.37
17.	10.92	C ₈ H ₁₄ O ₈	l-Gala-l-ido-octonic lactone	156
18.	11.10	C ₇ H ₁₃ NOS ₂	Dithiocarbamate, S-methyl-,N-(2-methyl-3-oxobutyl)-	80.7
19.	11.47	C ₁₈ H ₃₂ O ₁₆	Melezitose	268.68
20.	11.77	C ₁₈ H ₃₂ O ₁₆	Melezitose	268.68
21.	12.43	C ₁₇ H ₃₆ O	1-Hexadecanol, 2-methyl-	20.2
22.	12.66	C ₁₈ H ₃₂ O ₁₆	Melezitose	268.68
23.	12.98	C ₁₈ H ₃₂ O ₁₆	Melezitose	268.68
24.	13.25	C ₁₀ H ₁₇ NO ₆ S	Desulphosinigrin	148

S. No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
25.	13.56	C ₁₂ H ₂₄ O ₃	Dodecanoic acid, 3-hydroxy-	57.5
26.	13.72	C ₁₈ H ₃₂ O ₁₆	Melezitose	268.68
27.	13.99	C ₂₅ H ₄₄ N ₂ O ₅ S	2-Myristynoyl pantetheine	116
28.	15.52	C ₈ H ₁₆ O ₆	Ethyl α-d-glucopyranoside	99.4
29.	15.94	C ₁₄ H ₂₈ O ₂	Tetradecanoic acid	37.3
30.	16.32	C ₇ H ₁₄ O ₆	3-O-Methyl-d-glucose	99.4
31.	16.42	C ₇ H ₁₄ O ₆	3-O-Methyl-d-glucose	99.4
32.	16.57	C ₇ H ₁₄ O ₆	3-O-Methyl-d-glucose	99.4
33.	16.76	C ₇ H ₁₄ O ₆	3-O-Methyl-d-glucose	99.4
34.	17.37	C ₁₇ H ₃₄ O ₂	Hexadecanoic acid, methyl ester	26.3
35.	17.72	C ₁₆ H ₃₀ O ₂	9-Hexadecenoic acid	37.3
36.	18.16	C ₃₈ H ₆₈ O ₈	1-(+)-Ascorbic acid 2,6-dihexadecanoate	119
37.	18.75	C ₂₀ H ₄₀ O ₂	Ethanol, 2-(9-octadecenyl)-, (Z)-	37.3
38.	18.86	C ₁₆ H ₃₂ O ₂	n-Hexadecanoic acid	37.3
39.	19.02	C ₁₉ H ₃₄ O ₂	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	26.3
40.	19.41	C ₁₉ H ₂₆ O	Androsta-4,16-dien-3-one	17.1
41.	19.64	C ₂₀ H ₃₆ O ₂	9,12-Octadecadienoic acid, ethyl ester	26.3
42.	19.93	C ₁₈ H ₃₄ O ₂	6-Octadecenoic acid	37.3
43.	20.50	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
44.	20.77	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
45.	21.02	C ₂₅ H ₄₂ O ₂	Cyclopropanebutanoic acid, 2-[[2-[[2-(2-pentylcyclopropyl)methyl]cyclopropyl)methyl]cyclopropyl] methyl]-, methyl ester	37.3
46.	21.16	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
47.	21.29	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
48.	21.47	C ₂₀ H ₃₄ O ₂	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-	37.3
49.	21.60	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
50.	21.94	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
51.	22.09	C ₂₀ H ₂₂	2-Phenyl-4-tert-butyl-7-methylindene	
52.	22.30	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
53.	22.40	C ₁₉ H ₂₂ N ₂	Curan, 16,17,19,20-tetrahydro-	12.89
54.	22.68	C ₁₈ H ₃₀ S	2,4,6-Tri- <i>t</i> -butylbenzenethiol	1
55.	22.89	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
56.	23.00	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
57.	23.21	C ₂₁ H ₃₂ O	Pregna-5,17(20)-dien-3-ol, (36,17E)-	17.07

S. No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
58.	23.39	C ₃₅ H ₆₈ O ₅	Hexadecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	72.83
59.	23.64	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
60.	23.81	C ₂₀ H ₂₆ O ₅	Gibbane-1,10-dicarboxylic acid, 4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, 10-methyl ester, (1a,4aa,4bb,108)-	61.80
61.	23.95	C ₂₃ H ₂₈ O ₅	1,4,9(11)-Pregnatriene-3,20-dione, 21-acetoxy-17-hydroxy-	72.83
62.	24.07	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
63.	24.19	C ₂₂ H ₃₀ O ₄	17Alpha-ethynyl-17beta-hydroxy-6beta-methoxy-3alpha, 5-cyclo-5alpha-androstan-19-oic acid	77.75
64.	24.90	C ₂₁ H ₃₂ O ₂	Pregnenolone	37.3
65.	25.06	C ₂₀ H ₂₈ O ₃	68-Hydroxymethandienone	49.69
66.	25.42	C ₂₂ H ₂₈ O ₃	Norethindrone Acetate	43.40
67.	25.82	C ₂₈ H ₃₈ O ₉	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3- [(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1bb,4ab,5b,7aa,7ba,8a,9b,9aa)]-	20.23
68.	26.11	C ₂₈ H ₃₈ O ₉	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3- [(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1bb,4ab,5b,7aa,7ba,8a,9b,9aa)]-	20.23
69.	26.25	C ₂₈ H ₃₈ O ₉	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3- [(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1bb,4ab,5b,7aa,7ba,8a,9b,9aa)]-	20.23
70.	26.40	C ₂₅ H ₃₄ O ₄	5,16,20-Pregnatriene-3beta,20-diol diacetate	60.33
71.	26.63	C ₂₆ H ₃₆ O ₈	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3- [(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1bb,4ab,5b,7aa,7ba,8a,9b,9aa)]-	113.29
72.	26.84	C ₂₈ H ₃₈ O ₉	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3- [(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1bb,4ab,5b,7aa,7ba,8a,9b,9aa)]	113.29
73.	27.04	C ₂₈ H ₃₈ O ₉	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3- [(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1bb,4ab,5b,7aa,7ba,8a,9b,9aa)]-	20.23
74.	27.27	C ₂₆ H ₃₆ O ₈	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 1a,1b,4,4a,5,7a,8,9-octahydro-3-(hydroxymethyl)-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1bb,4ab,5b,7aa,7ba,8a,9b,9aa)]	113.29
75.	27.44	C ₂₅ H ₃₆ O ₇	4,13,20-Tri-O-methylphorbol 12-acetate	107.22

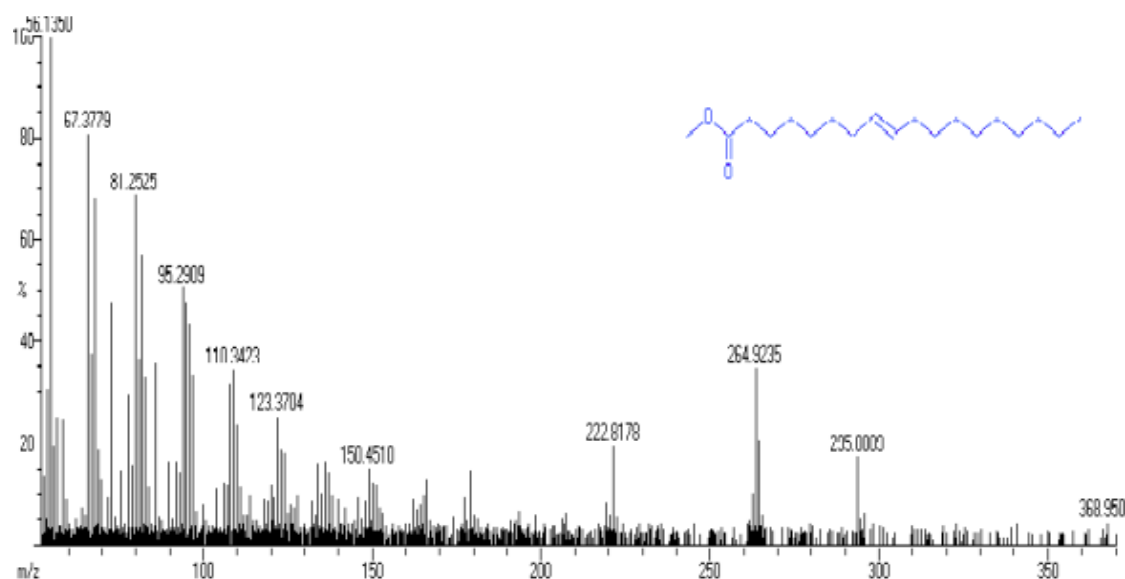
S. No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
76.	27.99	C ₂₆ H ₃₄ O ₉	Phorbol 12,13,20-triacetate	154
77.	28.28	C ₂₅ H ₃₄ O ₅	Acetic acid, 17-(1-acetoxy-ethyl)-10,13-dimethyl-3-oxo2,3,8,9,10,11,12,13,14,15,16,17-dodecahydro-1Hcyclopenta[a]phenanthren-11-yl (ester)	82.1
78.	28.57	C ₂₁ H ₃₀ O ₅	2-Cyclopenten-1-one, 3,4-dihydroxy-5-(3-methyl-2-butenyl)-2- (3-methyl-1-oxobutyl)-4-(4-methyl-1-oxo-3-pentenyl)-	94.8
79.	28.77	C ₃₂ H ₃₉ NO ₁₀	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo4a,7a-epoxy-5H-cyclopenta[a]cyclopropa[f]cycloundecen-11-yl ester,[1aR-(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-	144.13
80.	29.02	C ₂₄ H ₃₄ O ₇	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo4a,7a-epoxy-5H-cyclopenta[a]cyclopropa[f]cycloundecen-11-yl ester,[1aR-(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-	85.22
81.	29.27	C ₂₅ H ₃₄ O ₅	Acetic acid, 17-(1-acetoxy-ethyl)-10,13-dimethyl-3-oxo2,3,8,9,10,11,12,13,14,15,16,17-dodecahydro-1Hcyclopenta[a]phenanthren-11-yl (ester)	82.10
82.	29.69	C ₂₆ H ₄₄ O ₅	Ethyl iso-allocholate	87.0
83.	29.84	C ₂₈ H ₄₄ O ₇	Pregn-5-ene-3,11,12,14,20-pentol, 11-acetate 12-(3-methylbutanoate), (3B,11a,12B,14B)-	127
84.	30.11	C ₂₄ H ₃₄ O ₆	Butanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4- (hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester,[1aR- (1aa,2a,5B,5aB,6B,8aa,9a,10aa)]-	55.38
85.	30.67	C ₂₉ H ₄₈ O	Stigmasterol	20.23
86.	31.78	C ₂₉ H ₅₀ O	7-Sitosterol	40.46
87.	31.96	C ₂₈ H ₄₀ O ₄	9,12,15-Octadecatrienoic acid, 2-phenyl-1,3-dioxan-5-yl ester	60.33

: Compound of ethanol extract of *Caesalpinia bonduc* by GC-MS

Graph 2. Gc-Ms of *Mallotus philippensis*

S. No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
1.	21.03	C ₈ H ₆ O ₄	1, 2-benzenecarboxylic acid	74.6
2.	22.33	C ₂₄ H ₃₈ O ₄	Di-n-octyl phthalate	52.6
3.	25.23	C ₆ H ₄ (C ₈ H ₁₇ COO) ₂	Bis (2-ethyl hexyl) phthalate	52.6
4.	27.32	C ₆ H ₁₄ O ₆	d-mannitol, 1-0-heptyl	14.886
5.	28.83	C ₁₇ H ₃₂ O ₂	E-8-methyl-9-tetradecen-1-ol acetate	26.30
6.	30.10	C₅H₆O	3-methyl-2-(2-oxopropyl) furan	13.1
7.	30.59	C ₁₇ H ₃₄ O ₂	4-methyl-Z-4-hexadecen-1-ol	140
8.	31.12	C ₅₀ H ₁₀₂	Tetrapentacontane, 1,34-dibromo	2.00
9.	31.63	C ₁₈ H ₃₆ O ₂	Octadecanoic acid, 2-oxo	37.3
10.	31.96	C ₁₁ H ₃₄ O	4-methyl-dodecec-3-en-1-ol	9.23
11.	32.61	C ₁₅ H ₂₆ O	Longiborneol	20.23
12.	33.49	C ₁₀ H ₁₈ O	p-menth-8(10)-en-9-ol, cis	20.23
13.	34.73	C ₁₂ H ₂₄ Br ₂	Dodecane, 1, 2-dibromo	0

Chemical properties of Gc-Ms predicted compounds of *Mallotus philippensis*

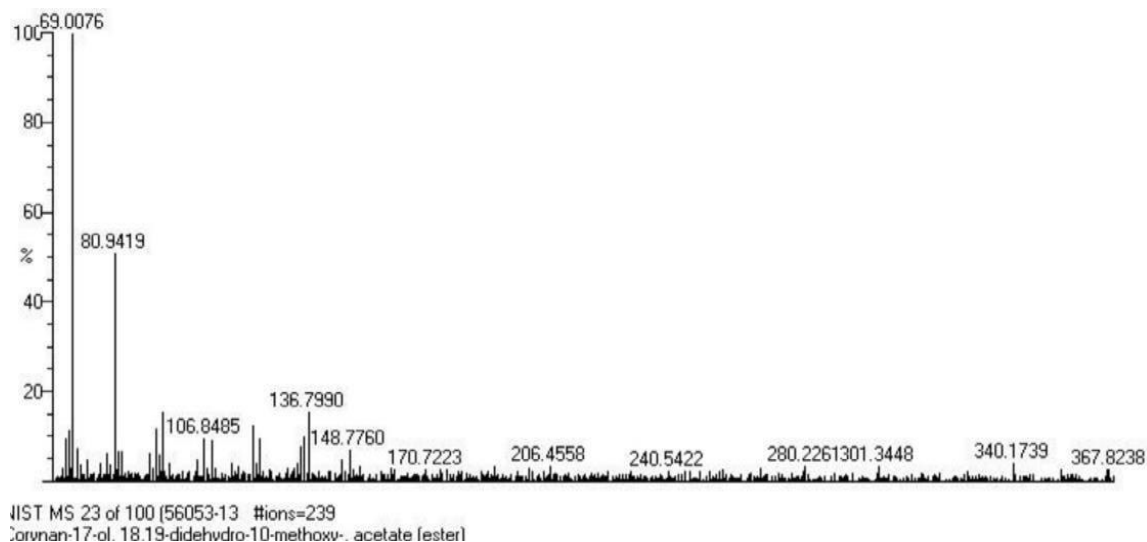


Graph 3. Gc-MS of Calotropis gigantea

S.No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
1.	22.78	C ₁₀ H ₂₂ O	1-Octanol-3,7-dimethyl	20.23
2.	53.21	C ₉ H ₁₀ O ₂	2- Methoxy 4-vinyl phenol ethenone	37.3
3.	4.34	C ₁₅ H ₁₃ N	Methyl-2-phenylindole	15.8
4.	33.40	C ₁₉ H ₃₈	5-Nonadecen-1-ol	0
5.	52.82	C ₁₉ H ₃₂ O ₂	9,12,15-Octadecatricenoic acid, methyl ester	26.30
6.	11.56	C ₁₀ H ₈	Azulene	0.0
7.	22.78	C ₂₀ H ₂₃ NO ₃	Benalaxyl	46.6
8.	50.19	BeH ₈ O ₈ S	Beryllium sulfate tetrahydrate	2
9.	3.44	C ₁₂ H ₁₀	Biphenyl	0.0
10.	6.66	C ₆ H ₁₄	Butane-2,2-dimethyl	0.0
11.	49.87	C ₂₈ H ₄₈ O	Campesterol	20.2
12.	41.79	C ₂₉ H ₄₈ O ₂	Cholest-5-en-3 ol, 24 Propylidene (3.beta.)	26.3
13.	22.78	C ₁₈ H ₃₄ O ₂	Cis-vaccenic acid	37.3
14.	3.46	C ₆ H ₁₂	Cyclohexane	0
15.	46.98	C ₁₀ H ₂₂	Decane	2
16.	6.66	C ₆ H ₁₃ O ₉ P	D-Mannose-1-phosphate sodium salt	157
17.	46.98	C ₂₀ H ₄₂	Eicosane	2
18.	53.21	C ₉ H ₂₂ O ₄ P ₂ S ₄	Ethion	152
19.	51.73	CH ₆ N ₄ O ₃	Guanidine nitriate	141
20.	49.87	C ₁₅ H ₂₆ O	Levomenol	20.23
21.	33.40	C ₂₅ H ₅₂	Pentacosane	0
22.	22.78	C ₁₁ H ₁₅ BrClO ₃ PS	Profenofos	60.8

S.No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
23.	22.78	C ₂₈ H ₄₈ O ₂	B-Tocopherol	29.5
24.	46.98	C ₂₉ H ₅₀ O	B-Sitosterol	20.23

Chemical properties of Gc-Ms predicted compounds of *Calotropis gigantea*

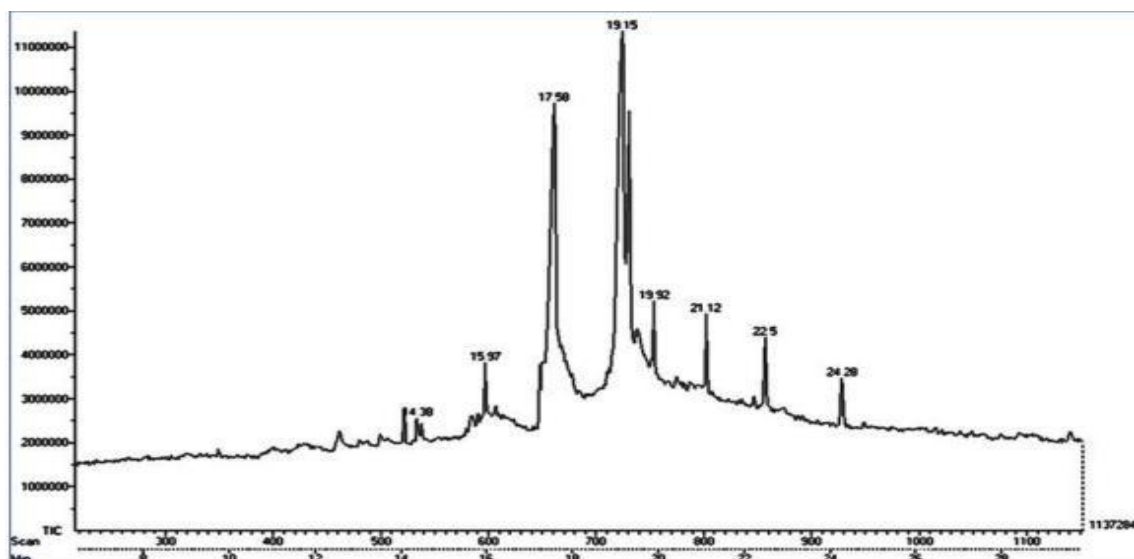


Graph 4. Gc-Ms of *holoptelea integrifolia*

S. No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
1.	6.309	C ₉ H ₁₅ NO ₂	Cyclohexenylalanine	49.3
2.	6.859	C ₂ HBrF ₂	1-bromo-1,2-difluoroethene	0
3.	8.3128	C ₃ H ₄ Cl ₂ O ₂	2,2-dichloropropanoic acid	37.3
4.	8.669	C ₁₃ H ₂₂ O ₂	3,7-dimethylocta-1,6-dien-3-yl propanoate	26.3
5.	47.52	C ₁₇ H ₂₄ O ₃	(4-methoxyphenyl)4-propylcyclohexane-1-carboxylate	46.5
6.	57.558	C ₁₄ H ₁₈ N ₂ O	2-methyl-1-(2-propan-2-ylpyrazolo[1,5-a]pyridin-3-yl)propan-1-one	23.6
7.	58.57	C ₁₉ H ₃₈ O ₂	2,6,10,14-Tetramethylpentadecanoic acid	26.3
8.	62.852	C ₁₈ H ₃₄ O ₄	Octadecane-1,18-dioic acid	52.6
9.	64.3	C ₁₄ H ₁₆ N ₂ O ₃	(3S,8aR)-3-benzyl-8a-hydroxy-3,6,7,8-tetrahydro-2H-pyrrolo(1,2-a)pyrazine-1,4-dione	73.4
10.	64.726	C ₂₁ H ₄₂ O ₂	18-Methyleicosanoic acid	37.3
11.	66.873	C ₂₀ H ₃₅ O ₂ ⁻	(8Z,11Z)-eicosa-8,11-dienoate	37.3
12.	67.499	C ₁₂ H ₂₄ O ₃	ethyl 5-hydroxy-4-keto-octadecanoate	57.5
13.	68.128	C ₂₀ H ₃₈ O ₂	cis-11-eicosenoic acid	37.3
14.	68.866	C ₂₃ H ₄₆ O ₂	n-Tricosanoic acid	37.3
15.	69.178	C ₂₄ H ₃₈ O ₄	di-N-Octyl Phthalate	37.3
16.	70.277	C ₁₆ H ₃₄ O	Hexadecan-1-ol	20.23
17.	70.605	C ₂₄ H ₄₈ O ₂	Tetracosanoic acid	37.3
18.	70.686	C ₂₆ H ₄₄ O ₅	ethyl 3,7,12-trihydroxy-5-cholan-24-oate.	86.7
19.	72.211	C ₂₅ H ₅₀ O ₂	Pentacosanoic acid	26.3

S. No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
20.	72.95	C ₂₂ H ₄₃ NO	Erucic acid amide	43.1
21.	77.077	C ₂₇ H ₄₀ O ₃	(5Z,7E,22E,24S)-24-cyclopropyl-9,10-secochola-5,7,10(19),22-tetraene-1 α ,3 β ,24-trio	43.37

Chemical properties of Gc-Ms predicted compounds of holoptelea integrifolia



Graph 5. Gc-Ms of Hemidesmus indicus

S. No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
1.	14.38	C ₁₀ H ₁₂ O	Trans-2-methyl-3-phenyl-2-propen-1-ol	9.23
2.	15.97	C ₁₄ H ₂₂ O	Dibutylphenol 2,3-dibutylphenol Phenol	20.23
3.	19.15	C ₁₆ H ₁₆ O ₃	Ethanone,1-[4-methoxy-3-(4-methylphenoxy)phenyl]-	38.69
4.	22.5	C ₁₈ H ₁₈ N ₂ O ₂	Piperazine-2,5-dione,1,4-(4-methylphenyl)-	12.03
5.	24.28	C ₂₁ H ₄₂ O ₂	Isopropyl stearate	37.3
6.	21.12	C ₁₉ H ₃₆ O	Z,E-2-Methyl-3,13-octadecadien-1-ol	17.07
7.	19.92	C ₁₁ H ₁₄ N ₄ O ₄	Butanal,3-methyl-[2,4-dinitrophenyl] hydrazone	76.9
8.	17.58	C ₁₅ H ₁₀ O ₂	Flavone	26.3

Chemical properties of Gc-Ms predicted

compounds of Hemidesmus indicus PubChem:-

It allows the possibility of one-to-one mapping of the chemical structure to its textual depiction, which is useful in indexing and duplicate removal for large chemical databases such as PubChem or ChEMBL. It is also known by the name of "Canonical SMILES" in certain cases. It depicts the core connectivity without any consideration for stereochemistry or isotopic information.

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
1.	Sec-Butyl nitrite	119	103.12	C ₄ H ₉ NO ₂	CCC(C(=O)O)N
2.	2-Nitro-1-buten-3-ol	10972	117.10	C ₄ H ₇ NO ₃	NC(=O)CCC(=O)O
3.	Isoxazolidine-3,5-dicarboxylic acid, dimethyl ester	70914	189.17	C ₇ H ₁₁ NO ₅	CC(=O)NCCC(C(=O)O)C(=O)O
4.	N-Isopentyl-N-nitroso-pentylamine	252237	186.29	C ₁₀ H ₂₂ N ₂ O	NCCCCCCCCNCO

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
5.	Propanoic acid, 3-ethoxy-, ethyl ester	11182677	146.18	C ₇ H ₁₄ O ₃	CCOC(=O)CCCCO
6.	Alpha-l-rhamnopyranose	108223	164.16	C ₆ H ₁₂ O ₅	CC1C(C(C(C(O1)O)O)O)O
7.	d-Glycero-d-ido-heptose	5459879	210.18	C ₇ H ₁₄ O ₇	OCC(O)C(O)C(O)C(O)C(=O)CO
8.	2-Deoxy-D-galactose	108223	164.16	C ₆ H ₁₂ O ₅	CC1C(C(C(C(O1)O)O)O)O
9.	Isosorbide Dinitrate	6883	236.14	C ₆ H ₈ N ₂ O ₈	O=N(=O)OC1COC2C(ON(=O)=O)COC12
10.	Glycerin	753	92.09	C ₃ H ₈ O ₃	OCC(O)CO
11.	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	911525	144.12	C ₆ H ₈ O ₄	O=C(O)CCCCC(=O)O
12.	a-D-Galactopyranose, 2-(acetylamino)-2-deoxy-	1738118	221.21	C ₈ H ₁₅ NO ₆	CC(=O)NC1C(C(C(C(O1)CO)O)O)O
13.	Isosorbide Dinitrate	6883	236.14	C ₆ H ₈ N ₂ O ₈	O=N(=O)OC1COC2C(ON(=O)=O)COC12
14.	5-Hydroxymethylfurfural	8369	126.11	C ₆ H ₆ O ₃	C1=CC(=C(C(=C1)O)O)O
15.	6-Acetyl-B-d-mannose	18392195	222.19	C ₈ H ₁₄ O ₇	CC(=O)OC1C(C(C(C(O1)CO)O)O)OC(=O)C
16.	Ascaridole epoxide	138243	184.23	C ₁₀ H ₁₆ O ₃	COC(=O)C1CCC(=O)C(C1)(C)C.
17.	1-Gala-l-ido-octonic lactone	22905610	238.19	C ₈ H ₁₄ O ₈	O=C(O)C(O)C(O)C(O)C(O)C(=O)O
18.	Dithiocarbamate, S-methyl-,N-(2-methyl-3-oxobutyl)-	206035	191.3	C ₇ H ₁₃ NOS ₂	CC(C)SSC(C(=O)N)CC
19.	Melezitose	440080	504.4	C ₁₈ H ₃₂ O ₁₆	OCC1OC(OC2C(OC3OC(CO)C(O)C(O)C3O)OC(CO)C(O)C2O)(CO)C(O)C1O
20.	1-Hexadecanol, 2-methyl-	15076	256.5	C ₁₇ H ₃₆ O	CCCCCCCCCCCCCCCC(O)
21.	Desulphosinigrin	24761678	279.31	C ₁₀ H ₁₇ NO ₆ S	O=C(O)CNC(=O)C(NC(=O)CC(C(N)C(=O)O)CS
22.	Dodecanoic acid, 3-hydroxy-	94216	216.32	C ₁₂ H ₂₄ O ₃	OCCCCCCCCCCCCC(=O)O
23.	2-Myristynoyl pantetheine	145865895	484.7	C ₂₅ H ₄₄ N ₂ O ₅ S	CCCCCCCCCCCCC#CC(=O)SCCNC(=O)CCNC(=O)C(C(C)(C)CO)O
24.	Ethyl a-d-glucopyranoside	121667	208.21	C ₈ H ₁₆ O ₆	CCOC1C(C(C(C(O1)CO)O)O)O
25.	Tetradecanoic acid	11005	228.37	C ₁₄ H ₂₈ O ₂	CCCCCCCCCCCCC(=O)O
26.	3-O-Methyl-d-glucose	64947	194.18	C ₇ H ₁₄ O ₆	OCC(O)C(O)C(O)C(O)CO
27.	Hexadecanoic acid, methyl ester	8042	270.5	C ₁₇ H ₃₄ O ₂	CCCCCCCCCCCCCCCC(=O)O
28.	9-Hexadecenoic acid	8906	254.41	C ₁₆ H ₃₀ O ₂	CCCCCCCC=CCCCCCC(=O)O

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
29.	1-(+)-Ascorbic acid 2,6-dihexadecanoate	54686917	652.9	C ₃₈ H ₆₈ O ₈	<chem>CCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCC)O</chem>
30.	Ethanol,2-(9-octadecenyoxy)-, (Z)-	21575642	312.5	C ₂₀ H ₄₀ O ₂	<chem>CCCCCCCCCCCCCCCCCCCC(=O)O</chem>
31.	n-Hexadecanoic acid	985	256.42	C ₁₆ H ₃₂ O ₂	<chem>CCCCCCCCCCCCCCCC(=O)O</chem>
32.	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	12921	294.5	C ₁₉ H ₃₄ O ₂	<chem>CCCCCCCC=CCCCCCCCC(=O)O</chem>
33.	Androsta-4,16-dien-3-one	71306304	270.4	C ₁₉ H ₂₆ O	<chem>O=C1C=C2CCC3C4CC=CC4(C)CCC3C2(C)CC1</chem>
34.	9,12-Octadecadienoic acid, ethyl ester	73114	308.5	C ₂₀ H ₃₆ O ₂	<chem>O=C(OCC)CCCCCCCC=CCCCCCCC</chem>
35.	6-Octadecenoic acid	56843142	282.5	C ₁₈ H ₃₄ O ₂	<chem>CCCCCCC/C=C\CCCCCCCC(=O)O</chem>
36.	1-Heptatriacotanol	537071	537.0	C ₃₇ H ₇₆ O	<chem>CCCO</chem>
37.	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl] methyl]-, methyl ester	554084	374.6	C ₂₅ H ₄₂ O ₂	<chem>CCCCC1CC1CC2CC2CC3CC3CC4CC4CCCC(=O)OC</chem>
38.	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-	15715159	306.5	C ₂₀ H ₃₄ O ₂	<chem>CC1=CC(O)CC(C)(O)C=CC(C(C)C)CCC(C)=CC1</chem>
39.	2-Phenyl-4-tret-butyl-7-methylindene	6425788	262.4	C ₂₀ H ₂₂	<chem>CC1=CC=C(C2=C1CC(=C2)C3=CC=CC=C3)C(C)(C)C</chem>
40.	Curan,16,17,19,20-tetrahydro-	5378056	278.4	C ₁₉ H ₂₂ N ₂	<chem>CC=C1CN2CCC34C2CC1=CC3NC5=CC=CC=C45</chem>
41.	2,4,6-Tri-t-butylbenzenethiol	12582791	278.5	C ₁₈ H ₃₀ S	<chem>CC(C)(C)C1=CC(=C(C(=C1)C(C)(C)C)S)C(C)(C)C</chem>
42.	Pregna-5,17(20)-dien-3-ol, (36,17E)-	235905	300.5	C ₂₁ H ₃₂ O	<chem>CC=C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C</chem>
43.	Hexadecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	99931	568.9	C ₃₅ H ₆₈ O ₅	<chem>CCCCCCCCCCCCCCCC(=O)OCC(CO)OC(=O)CCCCCCCCCCCCCCC</chem>
44.	Gibbane-1,10-dicarboxylic acid, 4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, 10-methyl ester, (1a,4aa,4bb,108)-	11725176	346.4	C ₂₀ H ₂₆ O ₅	<chem>CC12C(CCC34C1CC(C(=C)C3)O)C5(CCC(C5(C4)C(=O)OC)C2)OC(=O)</chem>
45.	1,4,9(11)-Pregnatriene-3,20-dione, 21-acetoxy-17-hydroxy-	454256	384.5	C ₂₃ H ₂₈ O ₅	<chem>CC(=O)OCC(=O)C1(CCC2C1(CCC3=C2C=CC4=CC(=O)C=CC43C)C)O</chem>
46.	17Alpha-ethynyl-17beta-hydroxy-6beta-methoxy-3alpha, 5-cyclo-5alpha-androstan-19-oic acid	624715	358.5	C ₂₂ H ₃₀ O ₄	<chem>CCC(C)CC(C)OC(=O)c1ccc(cc1)C(=O)OCC(C)CC</chem>

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
47.	Pregnenolone	92810	316.5	C ₂₁ H ₃₂ O ₂	<chem>CC(=O)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C</chem>
48.	68-Hydroxymethandienone	21726356	316.4	C ₂₀ H ₂₈ O ₃	<chem>CC12CCC3=C(C1CCC45C2CC(C(C4)C5(CO)O)C)C=CO3</chem>
49.	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3-[(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8-tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1bβ,4aβ,5β,7aa,7ba,8a,9β,9aa)]-	12443279	518.6	C ₂₈ H ₃₈ O ₉	<chem>CC(=CCC/C(=C/C(C/C(=C\CC/C(=C/OC(=O)C)/C=C/OC(=O)C)OC(=O)C)/C=O)OC(=O)C/C)C</chem>
50.	5,16,20-Pregnatriene-3beta,20-diol diacetate	11153754	398.5	C ₂₅ H ₃₄ O ₄	<chem>CC1=C(/C(=C/C(C)CCC/C(=C/CC/C(=C/CCC2=COC=C2)/C)/C)/OC1=O)O</chem>
51.	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3-[(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8-tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1bβ,4aβ,5β,7aa,7ba,8a,9β,9aa)]-	5281877	476.6	C ₂₆ H ₃₆ O ₈	<chem>CC1=C(C(CCC1)(C)C)C=CC(=CC=CC(=CC(=O)OC2C(C(C(C(O2)C(=O)O)O)O)O)C)C</chem>
52.	4,13,20-Tri-O-methylphorbol 12-acetate	21119912	448.5	C ₂₅ H ₃₆ O ₇	<chem>CC(=O)OCC1=CC2C(C(=O)C=C(C)C2(C)O)C3C(C(C1)O)C4(C(C)C)C43OC</chem>
53.	Phorbol 12,13,20-triacetate	14483909	490.5	C ₂₆ H ₃₄ O ₉	<chem>CC(=O)OC1CC(C2(C13C4C(C2)C5(CCC(C5(CC4OC3O)C)C6=COC(=O)C=C6)O)O)O</chem>
54.	Acetic acid, 17-(1-acetoxy-ethyl)-10,13-dimethyl-3-oxo2,3,8,9,10,11,12,13,14,15,16,17-dodecahydro-1Hcyclopenta[a]phenanthren-11-yl (ester)	77389706	414.5	C ₂₅ H ₃₄ O ₅	<chem>CC=C(C)C(=O)OC1C(=CC23C1(C(C(=CC(=O)C4C(C4(C)C)CC3C)C)O)O)C</chem>
55.	2-Cyclopenten-1-one, 3,4-dihydroxy-5-(3-methyl-2-butenyl)-2-(3-methyl-1-oxobutyl)-4-(4-methyl-1-oxo-3-pentenyl)-	58473839	362.5	C ₂₁ H ₃₀ O ₅	<chem>CC(C)=CCC1C(=O)C(=C(C1(C(=O)CC=C(C)C)O)O)C(=O)CC(C)C</chem>
56.	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo4a,7a-epoxy-5H-cyclopenta[a]cyclopropa[f]cycloundecen-11-yl ester,[1aR-(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-	5363175	597.7	C ₃₂ H ₃₉ NO ₁₀	<chem>CCC(=O)OCC1C(CCC2(C1CC(C3(C2C(C4=C(O3)C=C(OC4=O)C5=CN=CC=C5)O)C)OC(=O)C)OC(=O)C)C</chem>

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
57.	Ethyl iso-allocholate	6452096	436.6	C ₂₆ H ₄₄ O ₅	<chem>CCOC(=O)C1CCC2C3C(CC=C4C3(CCC5C4(CCC(C5)O)C)C)C2(C1)O</chem>
59.	Butanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester,[1aR-(1aa,2a,5β,5aβ,6β,8aa,9a,10aa)]-	539279	418.5	C ₂₄ H ₃₄ O ₆	<chem>CCCC(=O)OC1C(C)C2(O)C(C=C(CO)CC3(O)C2C=C(C)C3=O)C4C1(C)C4(C)C</chem>
60.	Stigmasterol	5280794	412.7	C ₂₉ H ₄₈ O	<chem>CCC(C=CC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C</chem>
61.	7-Sitosterol	5283634	412.7	C ₂₉ H ₅₀ O	<chem>OC1CC2=CC=C3C(CCC4(C)C3CCC4(C)CCC(CC)C(C)C)C2(C)CC1</chem>
62.	9,12,15-Octadecatrienoic acid, 2-phenyl-1,3-dioxan-5-yl ester	5367498	440.6	C ₂₈ H ₄₀ O ₄	<chem>CCC=CCC=CCC=CCCCCCCCC(C(=O)OC1COC(C2=CC=CC=C2)OC1</chem>

Table:- Pubchem CID M.W.g/mol M.F. Canonical smile Caesalpinia bonduc

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
1.	1, 2-benzenecarboxylic acid	181977	164.11	C ₈ H ₆ O ₄	<chem>C1=CC=C(C(=C1)C(=O)O)C(=O)O</chem>
2.	Di-n-octyl phthalate	8346	390.6	C ₂₄ H ₃₈ O ₄	<chem>CCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCC</chem>
3.	Bis (2-ethyl hexyl) phthalate	16213881	394.6	C ₆ H ₄ (C ₈ H ₁₇ CO) ₂	<chem>CCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC</chem>
4.	E-8-methyl-9-tetradecen-1-ol acetate	5363273	268.4	C ₁₇ H ₃₂ O ₂	<chem>CCCC/C=C/C(C)CCCCCCCCOC(=O)C</chem>
5.	3-methyl-2-(2-oxopropyl) furan	545772	138.16	C ₈ H ₆ O ₂	<chem>CC1=C(OC=C1)CC(=O)C</chem>
6.	4-methyl-Z-4-hexadecen-1-ol	5367910	254.5	C ₁₇ H ₃₄ O	<chem>CCCCCCCCCCC/C=C(/C)CCCCO</chem>
7.	Octadecanoic acid, 2-oxo	5281	284.5	C ₁₈ H ₃₆ O ₂	<chem>CCCCCCCCCCCCCCCCC(=O)O</chem>
8.	4-methyl-dodecec-3-en-1-ol	5364665	198.34	C ₁₁ H ₂₄ O	<chem>CCCCCCCC/C(=C/CCO)/C</chem>
9.	Longiborneol	11447401	222.37	C ₁₅ H ₂₆ O	<chem>CC1(CCCC2(C3C1C(C2(CC3)C)O)C)C</chem>
10.	p-menth-8(10)-en-9-ol, cis	543946	154.25	C ₁₀ H ₁₈ O	<chem>CC1CCC(CC1)C(=C)CO</chem>
11.	Dodecane, 1, 2-dibromo	18766	328.13	C ₁₂ H ₂₄ Br ₂	<chem>BrCCCCCCCCCCCCBr</chem>

Table:- Pubchem CID.M.W.g/mol M.F. Canonical smile *Mallotus philippensis*

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
1.	1-Octanol-3,7-dimethyl	7792	158.28	C ₁₀ H ₂₂ O	<chem>CC(C)CCCC(C)CCO</chem>
2.	2- Methoxy 4-vinyl phenol ethenone	332	150.17	C ₉ H ₁₀ O ₂	<chem>COC1CC(CCC1O)C=C</chem>
3.	Methyl-2-phenylindole	77095	207.27	C ₁₅ H ₁₃ N	<chem>CN1C2=CC=CC=C2C=C1C3=CC=CC=C3</chem>
4.	5-Nonadecen-1-ol	5367600	282.5	C ₁₉ H ₃₈	<chem>CCCCCCCCCCCCC/C=C/CCCCO</chem>
5.	9,12,15-Octadecatrienoic acid, methyl ester	5319706	292.5	C ₁₉ H ₃₂ O ₂	<chem>CCC=CCC=CCC=CCCCCCCCC(=O)OC</chem>
6.	Azulene	9231	128.17	C ₁₀ H ₈	<chem>C1=CC=C2C=CC=CC2=C1</chem>
7.	Benalaxyl	51369	325.4	C ₂₀ H ₂₃ NO ₃	<chem>CC1=C(C(=CC=C1)C)N(C(C)C(=O)OC)C(=O)CC2=CC=CC=C2</chem>
8.	Beryllium sulfate tetrahydrate	62672	177.14	BeH ₈ O ₈ S	<chem>O.O.O.O.[Be+2].[O-]S(=O)(=O)[O-]</chem>
9.	Biphenyl	7095	154.21	C ₁₂ H ₁₀	<chem>C1CCC(CC1)-C2CCCCC2</chem>
10.	Butane-2,2-dimethyl	6403	86.18	C ₆ H ₁₄	<chem>CCC(C)(C)C</chem>
11.	Campesterol	173183	400.7	C ₂₈ H ₄₈ O	<chem>CC(C)C(C)CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C</chem>
12.	Cholest-5-en-3 ol, 24 Propylidene (3.beta.)	222529	428.7	C ₂₉ H ₄₈ O ₂	<chem>CC(C)CCCC(C)C1CCC2C3CC=C4CC(CCC4(C)C3CCC12C)OC(=O)C</chem>
13.	Cis-vaccenic acid	5282761	282.5	C ₁₈ H ₃₄ O ₂	<chem>CCCCCCC/C=C\CCCCCCCCC(=O)O</chem>
14.	Cyclohexane	8078	84.16	C ₆ H ₁₂	<chem>C1CCCCC1</chem>
15.	Decane	15600	142.28	C ₁₀ H ₂₂	<chem>CCCCCCCCCC</chem>
16.	D-Mannose-1-phosphate sodium salt	23716114	260.14	C ₆ H ₁₃ O ₉ P	
17.	Eicosane	8222	282.5	C ₂₀ H ₄₂	<chem>CCCCCCCCCCCCCCCCCCCC</chem>
18.	Ethion	3286	384.5	C ₉ H ₂₂ O ₄ P ₂ S ₄	<chem>CCOP(=S)(OCC)SCSP(=S)(OCC)OCC</chem>
19.	Guanidine nitrate	10481	122.08	CH ₆ N ₄ O ₃	<chem>NC(N)=N.O[N+](=[O-])=O</chem>
20.	Levomenol	442343	222.37	C ₁₅ H ₂₆ O	<chem>CC1=CCC(CC1)C(C)(CCC=C(C)C)O</chem>
21.	Pentacosane	12406	352.7	C ₂₅ H ₅₂	<chem>CCCCCCCCCCCCCCCCCCCCCCCC</chem>
22.	Profenofos	38779	373.63	C ₁₁ H ₁₅ BrClO ₃ PS	<chem>CCCSP(=O)(OCC)OC1=C(C=C(C=C1)Br)Cl</chem>
23.	B-Tocopherol	6857447	416.7	C ₂₈ H ₄₈ O ₂	<chem>Cc1cc(O)c(C)c2c1OC(C)(CCCC(C)CCC(C)CCCC(C)C)CC2</chem>
24.	B-Sitosterol	57347730	421.7	C ₂₉ H ₅₀ O	<chem>CCC@HC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C</chem>

Table:- Pubchem CID M.W.g/mol M.F. Canonical smile Calotropis gigantea

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
1.	Cyclohexenylalanine	95475	171.24	C ₉ H ₁₅ NO ₂	C1CCC(CC1)CC(C(=O)O)N
2.	1-bromo-1,2-difluoroethene	588440	142.93	C ₂ HBrF ₂	C(=CF)(F)Br
3.	2,2-dichloropropanoic acid	6418	142.97	C ₃ H ₄ Cl ₂ O ₂	CC(C(=O)O)(Cl)Cl
4.	3,7-dimethylocta-1,6-dien-3-yl propanoate	61098	210.31	C ₁₃ H ₂₂ O ₂	CCC(=O)OC(C)(C=C)CCC=C(C)C
5.	(4-methoxyphenyl)4-propylcyclohexane-1-carboxylate	106715	276.4	C ₁₇ H ₂₄ O ₃	CCCC1CCC(CC1)C(=O)OC2=CC=C(C=C2)OC
6.	2-methyl-1-(2-propan-2-ylpyrazolo[1,5-a]pyridin-3-yl)propan-1-one	3671	230.31	C ₁₄ H ₁₈ N ₂ O	CC(C)C(=O)C1=C2C=CC=CN2N=C1C(C)C
7.	2,6,10,14-Tetramethylpentadecanoic acid	123929	298.50	C ₁₉ H ₃₈ O ₂	CCCCCCCC(C)CCCC(C)CCCC(C)CC(=O)O
8.	Octadecane-1,18-dioic acid	70095	314.5	C ₁₈ H ₃₄ O ₄	C(CCCCCCCC(=O)O)CCCCCCCC(=O)O
9.	(3S,8aR)-3-benzyl-8a-hydroxy-3,6,7,8-tetrahydro-2H-pyrrolo(1,2-a)pyrazine-1,4-dione	11673336	260.29	C ₁₄ H ₁₆ N ₂ O ₃	C1CC2C(=O)NC(C(=O)N2C1O)CC3=CC=CC=C3
10.	18-Methyleicosanoic acid	5282602	326.6	C ₂₁ H ₄₂ O ₂	CCC(C)CCCCCCCCCCCCCCCCC(=O)O
11.	(8Z,11Z)-eicosa-8,11-dienoate	86289633	307.5	C ₂₀ H ₃₅ O ₂ ⁻	CCCCCCCC=CCC=CCCCCCCC(=O)O
12.	ethyl 5-hydroxy-4-keto-octadecanoate	94216	216.32	C ₁₂ H ₂₄ O ₃	OCCCCCCCCCCCCC(O)=O
13.	cis-11-eicosenoic acid	5282768	310.5	C ₂₀ H ₃₈ O ₂	CCCCCCCC=CCCCCCCCC(=O)O
14.	n-Tricosanoic acid	17085	354.6	C ₂₃ H ₄₆ O ₂	CCCCCCCCCCCCCCCCCCCCC(=O)O
15.	di-N-Octyl Phthalate	8346	390.6	C ₂₄ H ₃₈ O ₄	CCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCC
16.	Hexadecan-1-ol	2682	242.44	C ₁₆ H ₃₄ O	CCCCCCCCCCCCCCCCCO
17.	Tetracosanoic acid	11197	368.6	C ₂₄ H ₄₈ O ₂	CCCCCCCCCCCCCCCCCCCCC(=O)O
18.	ethyl 3,7,12-trihydroxy-5-cholan-24-oate.	24853674	436.6	C ₂₆ H ₄₄ O ₅	CCOC(=O)CCC(C)C1CCC2C1(C(C3C2C(CC4C3(CCC(C4)O)C)O)O)C
19.	Pentacosanoic acid	10468	382.7	C ₂₅ H ₅₀ O ₂	CCCCCCCCCCCCCCCCCCCCC(=O)O
20.	Erucic acid amide	5365371	337.6	C ₂₂ H ₄₃ NO	CCCCCCCC=CCCCCCCCCCC(=O)N
21.	(5Z,7E,22E,24S)-24-cyclopropyl-9,10-secochola-5,7,10(19),22-tetraene-1α,3β,24-trio	6012	412.6	C ₂₇ H ₄₀ O ₃	CC12CCC(=O)C=C1CCC1C2CCC2(C)C(OC(=O)CCC3CCCC3)CCC12

Table:-Pubchem CID M.W.g/mol M.F. Canonical smile holoptelea integrifolia

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
1.	Trans-2-methyl-3-phenyl-2-propen-1-ol	6393846	148.2	C ₁₀ H ₁₂ O	<chem>CC(C)C(=O)C1=CC=CC=C1</chem>
2.	Dibutylphenol 2,3-dibutylphenol Phenol	3015343	206.32	C ₁₄ H ₂₂ O	<chem>C1=CC=C(C=C1)O</chem>
3.	Ethanone,1-[4-methoxy-3-(4-methylphenoxy)phenyl]-	617872	256.3	C ₁₆ H ₁₆ O ₃	<chem>CC1=CC=C(C=C1)OC2=C(C=C(C(=C2)C(=O)C)OC</chem>
4.	Piperazine-2,5-dione,1,4-(4-methylphenyl)-	576878	294.3	C ₁₈ H ₁₈ N ₂ O ₂	<chem>CC1=CC=C(C=C1)N2CC(=O)N(CC2=O)C3=CC=C(C=C3)C</chem>
5.	Isopropyl stearate	8162	326.6	C ₂₁ H ₄₂ O ₂	<chem>CCCCCCCCCCCCCCCCC(=O)OC(C)C</chem>
6.	Z,E-2-Methyl-3,13-octadecadien-1-ol	5364521	280.5	C ₁₉ H ₃₆ O	<chem>CCCCC=CCCCCCCCC=CC(C)CO</chem>
7.	Butanal,3-methyl-[2,4-dinitrophenyl] hydrazone	9569524	266.25	C ₁₁ H ₁₄ N ₄ O ₄	<chem>CC(C)CC=NNC1CCC(CC1[N+](=O)[O-])[N+](=O)[O-]</chem>
8.	Flavone	10680	222.24	C ₁₅ H ₁₀ O ₂	<chem>O=C1C=C(OC2=CC=CC=C2)C3=CC=CC=C3</chem>

Table:- Pubchem CID M.W.g/mol M.F. Canonical smile Hemidesmus indicus

Conclusions:

Bioactive Compounds :-

Identification of Bioactive Compounds The presence of alkaloids, flavonoids, terpenoids, phenolics, and other bioactive compounds is just a few of the many possibilities for what can be present in .GC-MS analysis on the extracts of *Caesalpinia bonduc*, *Mallotus philippensis*, *Calotropis gigantea*, *Holoptelea integrifolia*, and *Hemidesmus indicus*. The presence of these chemical compounds can contribute to the plants' antifungal and antibacterial effects.

Antibacterial Activity:-

Antibacterial Effect In their study on , the researchers find that extracts from *Caesalpinia bonduc*, *Mallotus philippensis*, *Calotropis gigantea*, *Holoptelea integrifolia*, and *Hemidesmus indicus* exhibit significant inhibition against several bacteria such as *Staphylococcus aureus* 2. The possible cause behind this antibacterial effect could be due to some of the compounds present identified using GC-MS analysis.

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