

**COMPARATIVE GC-MS AND FTIR PROFILING RESEARCH OF
ESSENTIAL OIL FROM *Ocimum gratissimum* HARVESTED FROM
DUMPSITES IN THREE LOCAL GOVERNMENT AREA IN EDO
STATE**



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BENIN CITY**

NOVEMBER, 2025.

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**A PROJECT WORK SUBMITTED TO THE DEPARTMENT OF SCIENCE
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CERTIFICATION

This is to certify that this project research titled “Comparative Gas Chromatograph-Mass Spectrometer and Fourier Transform Infrared Profiling of Essential Oil from *Ocimum gratissimum* Harvested from Dumpsites in Three Local Government Area in Edo State” was carried out by Rhoda Owenmen AJAYI with Matriculation number, LSC2010034 of the Department of Science Laboratory Technology, Faculty of Life Sciences, University of Benin, Benin City, under the supervision of PROF. EMMANUEL O. OSHOMOH.

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DEDICATION

This project research is dedicated to GOD ALMIGHTY, for his divine strength, inspiration and provision throughout the course of this project research.

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ABSTRACT

Ocimum gratissimum (scent leaf) is a medicinal herb renowned for its essential oils rich in antimicrobial and antioxidant constituents. This study evaluated the influence of dumpsite pollution on the phytochemical and functional composition of *O. gratissimum* essential oil obtained from Egor, Ovia North-East, and Oredo Local Government Areas of Edo State, Nigeria. Essential oils extracted using a Soxhlet apparatus were characterized by Gas Chromatography–Mass Spectrometry (GC–MS) and Fourier Transform Infrared (FTIR) spectroscopy. The GC–MS analysis revealed a predominance of hydrocarbons particularly decane and bis(2-ethylhexyl) phthalate suggesting petroleum- and plastic-derived contamination, while FTIR spectra identified nitrogenous, carbonyl, and halogenated functional groups absent in uncontaminated reference samples. These alterations indicate that dumpsite exposure disrupts the biosynthesis of natural oxygenated terpenes, thereby diminishing the therapeutic quality of the oil and introducing potential toxicants. The findings demonstrate that environmental pollution significantly affects the chemical integrity of *O. gratissimum* and hence, the need to restrict its cultivation near polluted environments.

CHAPTER ONE

INTRODUCTION

1.1 BACKGROUND OF STUDY

Humans have experienced several illnesses, discomforts and attempts to combat them in a variety of ways over the years (Ferronin *et al.*, 2018; Picard and McEwen, 2018). Of the many methods used to cure illnesses, the trend toward herbal medicine is growing because it uses medicinal plants as a complementary and alternative therapy in conjunction with other primary therapies to treat a variety of disorders (Kruk *et al.*, 2019; Lawal *et al.*, 2016). Despite growing worries about the growing toxicity of mainstream treatments (Akram *et al.*, 2021 ; Akram *et al.*, 2014 ; Khalid *et al.*, 2022). Other treatments have been used recently (Kawamura and Muraoka, 2018). Nowadays, plants used as medications to treat or prevent illnesses in order to preserve health and for other reasons are commonly referred to as medicinal and aromatic plants (MAPs). According to the World Health Organization (WHO, 2015), a greater understanding of natural plants completes a significant portion of medical and pharmacological findings, and many communities accept the natural products collected from ecosystems as reliable for cultural and medicinal purposes. Furthermore, according to WHO data, about 4 billion individuals worldwide now initially use herbal remedies to treat their medical issues.

Additionally, over the past ten years, a number of researchers have focused on medicinal plants and their bioactive compounds due to their potential for managing and preventing chronic and life-threatening diseases like cancer, diabetes, stroke, and arthritis (Sofowora *et al.*, 2013; WHO, 2019), treating psychiatric disorders as an alternative therapy (Venuprasad *et al.*, 2014), and meeting the health needs of the elderly (WHO, 2019). In addition to being used to cure a wide range of illnesses, these medicinal plants are currently being used to create new medications for conventional or traditional medicine. Medicinal herbs like *Cinchona officinalis*, *Digitalis purpurea*, *Saix alba*, and *Papaver somniferum* were used to make drugs

like quinine, digoxin, aspirin, and morphine (Mbanaso *et al.*, 2020). *Ocimum gratissimum* L., also referred to as scent leaf, is one of the newly found medicinal plants that may be used as a source of a new medication or as an alternative therapy for the treatment of a variety of illnesses. It is an aromatic perennial herbaceous plant that is widely grown and economically successful. It is widespread in Africa, Asia, and South America and is a member of the Lamiaceae family (Akara *et al.*, 2021 ; Tanko *et al.*, 2008). It can be added to fish, meat, soups, and stews as a natural flavoring ingredient, condiment, or vegetable. Several illnesses, including cough, pneumonia, fever, inflammation, anemia, diarrhea, aches, and bacterial and fungal infections, are also treated with it in traditional medicine (Akara *et al.*, 2021).

According to scientific sources, *O. gratissimum* has a variety of bioactive substances, including essential oils with a number of positive benefits (Benitez *et al.*, 2009 ; Melo *et al.*, 2019) and flavonoids and polyphenols (Ironi *et al.*, 2016 ; Venuprasad *et al.*, 2014). Major compound from *O. gratissimum* are Eugenol, limonene, myrcene, o cymene, p cymene, γ terpinene (from essential oil), and methyl chavicol, methyl cinnamate, and rosmarinic acid (from extract) are the main compounds found in *O. gratissimum*. According to a study by Yamani *et al.* (2016), of the 54 chemicals found in the leaves, flower spikes, or essential oil, camphor, eucalyptol, and eugenol are among those that have antibacterial activity against bacteria. Phenolic chemicals and a variety of other natural products, such as polyphenols like flavonoids and hydroxyl groups that exhibit antioxidant properties, are abundant in essential oils (Ijaz *et al.*, 2017). Polyphenols are secondary metabolites of plants that are highly significant since they are numerous and act as natural antioxidants. They have interesting qualities including scavenging free radicals and inhibiting several types of oxidative stress in the body (Maghsoudlou *et al.*, 2016).

Essential oils are naturally occurring compounds that have been exploited for their unique medicinal properties (Lesgard *et al.*, 2014). They are complex and multifunctional compounds

present in plants and used by plants for various roles including defence against herbivores, insects and microorganisms, and can be used in signalling communication between plants (Lesgard *et al.*, 2014). Each plant species has its own specific mix of essential oils (Blowman *et al.*, 2018). Essential oils have been documented to bear the scent or flavour of its parent plant (West *et al.*, 2023). The aromatic components of the compounds contained in the oil are responsible for the scent it bears (West *et al.*, 2023). The age of the plant affects its oil content, which increases as it becomes older (Orwa *et al.*, 2009).

1.2 AIM OF THE STUDY

The aim of this study is to evaluate GC-MS and FTIR studies in comparison with the chemical composition of essential oils from *Ocimum gratissimum* that were harvested near septic tanks and open dumpsites in the Edo State local government areas of Oredo, Egor, and Ovia North East.

1.3 SPECIFIC OBJECTIVES OF THE STUDY

The following are the objectives of this study which includes to;

1. extract essential oils from *Ocimum gratissimum* leaves that have been gathered in Edo State near septic tanks and open disposal sites.
2. identify the essential oils' phytochemical components with the use of Gas Chromatography–Mass Spectrometry (GC-MS).
3. use Fourier Transform Infrared Spectroscopy (FTIR) to describe the oils' functional groups and fingerprint regions.
4. evaluate the essential oil composition between environmental circumstances (Dumpsites) and localities (Oredo, Egor, and Ovia North East).
5. assess how exposure to environmental contaminants may affect the safety and therapeutic efficacy of *Ocimum gratissimum* essential oil.

CHAPTER TWO

LITERATURE REVIEW

2.1 *Ocimum gratissimum*

Members of the Lamiaceae family, *Ocimum gratissimum* (*O. gratissimum*) is a herbaceous plant that is also known as scent leaf, African basil, camphor basil, basil leaf, or ramtushi (Kalita and Narzary, 2023 ; Moneme *et al.*, 2024b). This specific tropical plant species is commonly referred to as "scent leaf," a name that Nigerians, especially those from the East and West, find charming (Moneme *et al.*, 2024a). In native Nigeria, it is referred to as "Nchanwu" in Igbo, "Daidoya" in Hausa, and "Efirin" in Yoruba (Chukwuma *et al.*, 2023 ; Moneme *et al.*, 2024a). It is a tiny to average sized plant with leaves that are comparable to cloves of similar flavor and aroma, making it a major herb in numerous cuisines (Puneet and Monika, 2022). In Nigeria, the plant is commonly grown for both culinary and medicinal reasons (Kalita and Narzary, 2023 ; Moneme and Nwaka, 2023), usually in gardens around communal huts. *O.gratissimum* is used as a culinary ingredient in salads, soups, pastas, vinegars and jellies in many parts of the world. Nutritionally, the plants have been documented to be rich in microelements sufficient for improved health and vitality (Moneme *et al.*, 2024a). It also contains several phytochemicals such as flavonoids and polyphenols (Ironi *et al.*, 2016 ; Melo *et al.*, 2019), responsible for its hypoglycemic (Shittu *et al.*, 2019), antiinflammatory (Ajayi *et al.*, 2017), antianaemic, hepatoprotective (Akara *et al.*, 2021), anti-hypertensive (Shaw *et al.*, 2017), antibacterial (Melo *et al.*, 2019), antifungal (Mohr *et al.*, 2017) as well as anti-hemorrhoidal activities (Moneme *et al.*, 2024a ; Moneme and Nwaka, 2023).

2.1.1 Botanical Description

Ocimum gratissimum is a herbaceous, fragrant shrub that is a member of the mint family (Lamiaceae). It is often referred to as scent leaf or African basil. It smells strong, unique, and a little camphoraceous. The eaves have serrated borders, are opposite, and are ovate to oblong

in form (Jahanger *et al.*, 2023). It is approximately 1-3 cm tall with an upright, branched stem that is round to slightly square and woody at the base, featuring slender, opposite leaves with toothed edges (Nweze and Eze, 2009). At elevations ranging from sea level to 2300 meters, *Ocimum Gratissimum* grows in disturbed areas around communities, along roadside and stream edges, savannas, coastal scrubland lake banks, and submontane forests. It is also grown as a hedge and ornamental plant in home gardens. In India, it usually grows in dry and wet deciduous woods, plains, and valleys. In the Lesser Antilles, it is categorized as a common and ubiquitous herb that often grows naturally in open, moist areas at lower and moderate elevations. It grows over Pacific islands as a weed of pastures, wastelands, and roadsides (Amadi *et al.*, 2010).

2.1.2 Classification

According to taxonomy, *Ocimum gratissimum* is a member of the genus *Ocimum*, which includes between 30 and 60 species of shrubs and herbs (Jahanger *et al.*, 2023). Other species in the genus, such as *Ocimum tenuiflorum* (holy basil) and *Ocimum basilicum* (sweet basil), are closely related to it. Along with a number of other plants that share a clove-like scent, *Ocimum gratissimum* is categorized in the genus under the section *Basilicum*. (Jahanger *et al.*, 2023).

According to the following taxonomic hierarchy, *Ocimum gratissimum* is categorized:

Kingdom: plantae

Division: Magnoliophyta

Class: Magnoliopsida

Order: Lamiales

Family: Lamiaceae

Genus: *Ocimum*

Specie: *Ocimum gratissimum* L.

(Ashokkumar *et al.*, 2020; Pandian *et al.*, 2021)



Plate 1: *Ocimum gratissimum*.

Source: Adebayo *et al.*, (2019).

2.2 ETHNOMEDICINAL AND TRADITIONAL USES OF *Ocimum gratissimum*

Many nations' traditional medical systems have made substantial use of *O. gratissimum*. It has culinary, medicinal, and condiment uses in north eastern Brazil. This plant is used to make teas and infusions because its leaves and blossoms are rich in essential oils (Rabelo *et al.*, 2003). The herb is used to cure diarrhea, high fever, and epilepsy in Nigeria's coastal regions (Effraim *et al.*, 2003). Leaf decoctions are used to treat mental disorders in the Savannah region (Akinmoladun *et al.*, 2007). The Ibo people of southeast Nigeria utilize *O. gratissimum* to treat the baby's cord and maintain the sterility of the wound surfaces. Additionally, it is used to treat fever, cold, catarrh, and fungal infections (Ijeh *et al.*, 2005). An infusion of *O. gratissimum* roots is used as a sedative for children by residents of Brazilian tropical forests (Cristiana *et al.*, 2006). This plant is used for a variety of uses by people in Kenya and sub-Saharan Africa, such as sniffing the leaves to clear clogged noses and rubbing them between hands. Along with regulating menstruation and treating prolapse of the rectum, they are also used to treat stomach aches, sore eyes, ear infections, coughs, barrenness, fever, convulsions, and tooth gargles (Matasyoh *et al.*, 2007). The entire plant has been utilized in India as a diaphoretic, antipyretic, and for its anti-inflammatory properties in the treatment of sunstroke, headaches, and influenza (Prajapati *et al.*, 2003 ; Ta[^]nia, 2006). Nigerian tribal people employ leaf extract to cure diarrhea, and cool leaf infusions are used to soothe upset stomachs and haemorrhoids (Kabif *et al.*, 2005). In traditional medicine, the plant is frequently used to treat a variety of illnesses, including upper respiratory tract infections, diarrhea, headaches, skin conditions, eye disorders, pneumonia, coughing, fever, and conjunctivitis (Adebolu and Salau, 2005). *O. gratissimum* leaves are employed as an antispasmodicum, antitussivum, and pulmonary antisepticum infusion (Ngassoum *et al.*, 2003).

Out of all the *Ocimum* species, *O. gratissimum* is widely used in clinical settings worldwide. Formulations of the medicinal essential oil of *O. gratissimum* (*Ocimum* oil) have been used in

a number of contexts as topical antiseptics and to treat pimples, boils, and minor wounds (Orafidiya *et al.*, 2001). *O. gratissimum* and *Xylopia aethiopica* are used together to make teas and potions for women during their puberty, according to (Ijeh *et al.*, 2005).

2.3 *Ocimum gratissimum* ESSENTIAL OIL

2.3.1 Essential Oil

Essential oils are naturally occurring compounds that have been exploited for their unique medicinal properties (Lesgard *et al.*, 2014). They are complex and multifunctional compounds present in plants and used by plants for various roles including defence against herbivores, insects and microorganisms, and can be used in signalling communication between plants (Lesgard *et al.*, 2014). The essential oil of *Ocimum gratissimum* has varying phytochemical constituents depending on geographical location from where the leaves were sourced and the time of the season. As the components vary in location, the medicinal uses also vary with locations since the medicinal properties are dependent on its phytochemical constituents (Sharma *et al.*, 2022).

2.3.2 Phytochemicals Constituents

Seasons and countries have different phytochemical compositions of *Ocimum gratissimum*. Joshi, (2021) explained how the components of *Ocimum gratissimum* collected in the summer and winter differed. Regardless of the season or the country of origin, tannins, flavonoids, and saponins are the main components of *Ocimum gratissimum* essential oil. The country of residence and the time of year when the leaves are harvested for the extraction of essential oils determine the other components. The literature search turned up findings primarily from Nigeria and India, despite the fact that this plant is common in the tropics. In contrast to extracts from Africa, plant extracts from the Indian subcontinent contain significant amounts of eugenol (Gilles *et al.*, 2023). Eugenol is an often colourless and sometimes yellow oily substance

extracted from essential oil of some plants like *Ocimum gratissimum*, clove and nutmeg. It is aromatic with a spicy scent. It has been used as antiseptics and flavourings.

Table 2.1: Some Components That Are Found In *Ocimum gratissimum* Essential Oil

S/N	Compound	Effect	Reference
1.	Sinapic acid	Exhibits antioxidant, antiinflammatory, anticancer, antimutagenic, antiglycemic, neuroprotective, and antibacterial activities.	(Chen. 2016)
2.	Thymol	Antiseptic, antibacterial, antifungal, anthelmintic, antiviral, antioxidant, diaphoretic, sedative, antirheumatic, and expectorant, antispasmodic, carminative, even anti-cancer, anti-hyperlipidemic and anti hyperglycemic action	(Codruta <i>et al.</i> 2020 ; Li <i>et al.</i> , 2017 ; Schnitzler. 2019 ; Salehi <i>et al.</i> , 2018 ; Tohidi <i>et al.</i> , 2020 ; Tariq <i>et al.</i> , 2019)
3.	Beta caryophyllene	Antioxidant, antiinflammatory, anticancer, cardioprotective, hepatoprotective, gastroprotective, nephroprotective, antimicrobial and immune-modulatory activity.	(Fidy <i>et al.</i> , 2016 ; Machado <i>et al.</i> , 2018)
4.	Eugenol	Analgesic, anti inflammatory, antioxidant, antimicrobial.	(Barboza <i>et al.</i> , 2018 ; Fujisawa and Murakami, 2016 ; Mohammadi <i>et al.</i> , 2017)
5.	p- Cymene:	Analgesic and anti-inflammatory properties	(Santana <i>et al.</i> , 2011)
6.	Rosmarinic acid	Antimicrobial, immunomodulatory, antidiabetic, anti-allergic, anti-inflammatory, hepato and renal protectant agent	(Alagawany <i>et al.</i> , 2017)
7.	Apigenin	Anti-inflammatory, antioxidant, antibacterial and antiviral activities and blood pressure reduction	(Yan <i>et al.</i> , 2017)
8.	Oleanolic acid	Antioxidant, anti-inflammatory, antiviral and. antidiabetic effects	(Sen, 2020)
9.	Beta-myrcene	Anti-inflammatory and anti-catabolic effects	(Rufino <i>et al.</i> , 2015)
10.	Luteolin	Antihypertension, anti-inflammatory and anticancer	(Lin <i>et al.</i> , 2008)

2.4. ENVIRONMENTAL INFLUENCE ON ESSENTIAL OIL

The yield and composition of essential oils (EOs) are strongly influenced by environmental factors such as soil conditions, climate, and cultivation practices. Plants grown in tropical regions generally have higher essential oil content compared to those in temperate zones. Even within a single plant, the type and concentration of EOs may vary depending on the organ (leaves, stems, roots, or flowers) from which they are extracted. Furthermore, the habitat in which a plant grows, alongside harvesting time, preservation, and extraction techniques, also determines both the quality and quantity of essential oils produced (Dao *et al.*, 2019a ; Dao *et al.*, 2019b ; Hien *et al.*, 2018 ; Mai *et al.*, 2019 ; Mai *et al.*, 2018 ; Nhan *et al.*, 2018 ; Thanh *et al.*, 2019 ; Tran *et al.*, 2019). However, when soils become contaminated particularly in regions adjacent to waste dumpsites, their favorable physicochemical conditions are compromised. A major contributor to soil contamination in developing countries is electronic waste (e-waste), also known as waste electrical and electronic equipment (WEEE). Electronic waste has emerged as a serious environmental concern due to inadequate disposal practices and the widespread occurrence of informal recycling activities (Perkins *et al.*, 2014). Over time, hazardous constituents from electronic waste leach into the surrounding soil and water bodies, resulting in extensive ecological contamination (Kiddee *et al.*, 2013).

Previous studies have demonstrated that improper recycling and disposal of e-waste release heavy metals and persistent organic pollutants (POPs) that exert deleterious effects on human health and the environment (Awasthi *et al.*, 2016). These contaminants include polybrominated diphenyl ethers (PBDEs), polychlorinated biphenyls (PCBs), dioxins, polycyclic aromatic hydrocarbons (PAHs), and tetrabromobisphenol A (Bhattacharya and Khare, 2016 ; Grant *et al.*, 2013). Such pollutants are highly toxic, chemically stable, and resistant to biodegradation, allowing them to persist in the environment and disrupt soil microbial community structures, ultimately impairing plant growth and metabolic activities (Zhang *et al.*, 2013). The

environmental implications of electronic waste contamination extend beyond soil degradation to affect agricultural crops and medicinal plants, including species cultivated for essential oil production. Elevated concentrations of polychlorinated biphenyls, polybrominated diphenyl ethers, and heavy metals such as lead (Pb) and cadmium (Cd) have been detected in crops and vegetables grown in proximity to electronic waste recycling areas (Cayumil *et al.*, 2016), because essential oil biosynthesis is closely associated with plant metabolic pathways and overall soil health, exposure to heavy metals and persistent organic pollutants may not only suppress plant productivity but also alter the phytochemical composition of essential oils thereby diminishing their therapeutic efficacy and commercial value.

2.5 ENVIRONMENTAL EFFECTS ON *Ocimum gratissimum* ESSENTIAL OIL

2.5.1 Changes in Essential Oil Yield and Chemical Profile

Dumpsites, and to a lesser extent septic tank leachates, serve as major sources of environmental contaminants, including heavy metals such as lead (Pb), cadmium (Cd), zinc (Zn), and copper (Cu). *Ocimum gratissimum* has been identified as a cadmium (Cd) accumulator, indicating its ability to uptake metals from contaminated soils (Rattanawat *et al.*, 2011). The exposure of medicinal plants to heavy metals has been shown to significantly influence both the yield and chemical composition of their essential oils. This effect is attributed to physiological stress responses that alter the expression of genes involved in essential oil biosynthesis (Hubai and Kovats, 2024). In related *Ocimum* species such as *O. basilicum*, cultivation in heavy metal contaminated soils markedly modifies the profile of key essential oil constituents. For instance, treatment with Cu and Pb resulted in an increase in linalool content and a reduction in methyl chavicol (estragole) levels (Kunwar *et al.*, 2015). Given that *O. gratissimum* commonly contains eugenol or thymol as its principal component, it is plausible that exposure to similar contamination stress may shift the relative concentrations of these dominant compounds and

other minor constituents. Also leachates originating from dumpsites and septic tanks are often enriched with organic matter and nutrients, particularly nitrogen (N) and phosphorus (P). Elevated levels of N and related nutrients have been shown to influence secondary metabolite production. Studies on other aromatic plants demonstrate that increased nitrogen availability enhances vegetative biomass but may simultaneously reduce essential oil concentration (expressed as yield, % w/w) or alter the relative proportions of terpenes and phenylpropenes (Kunwar *et al.*, 2015; Matasyoh *et al.*, 2007).

2.5.2 Bioaccumulation of Contaminants in the Essential Oil:

Although plants may accumulate heavy metals within their roots, stems, and leaves, previous studies on other aromatic species have demonstrated that the concentrations of heavy metals in the final essential oil are often below detectable limits (Kunwar *et al.*, 2015). This phenomenon is attributed to the physicochemical properties of essential oils, which consist primarily of volatile, lipophilic constituents such as terpenoids and phenylpropenes, whereas heavy metals are non-volatile inorganic ions that remain sequestered in nonvolatile plant tissues. The principal concern regarding essential oil quality, therefore, lies not in direct metal contamination but in the alteration of its chemical composition, which may consequently affect its aroma, flavor, and therapeutic attributes (e.g., antimicrobial and antioxidant activities). In the case of *Ocimum gratissimum* cultivated in soils contaminated with dumpsite the essential oil is expected to exhibit both a modified chemical profile and potentially reduced yield compared with plants from uncontaminated control sites. The physiological stress induced by heavy metals (e.g., Cd, Pb) and nutrient imbalance arising from such contamination can disrupt metabolic pathways, resulting in shifts in the relative proportions of key essential oil constituents such as eugenol, thymol, and β -caryophyllene (Hubai and Kovats, 2024 ; Kunwar *et al.*, 2015 ; Rattanawat *et al.*, 2011).

2.6 ANALYTICAL TECHNIQUE (GC-MS AND FTIR)

2.6.1 Overview of Gas Chromatography-Mass Spectrometry (GC-MS)

Gas chromatography–mass spectrometry (GC–MS) remains a fundamental analytical tool employed across diverse sectors, including food, environmental, forensic, and chemical analyses, owing to its robustness, precision, and adaptability (Wang *et al.*, 2020). The technique facilitates both qualitative and quantitative characterization of compounds through two principal approaches (Valdez, 2022).

2.6.2. Component Isolation and Structural Analysis

Compounds eluting from the gas chromatograph may be isolated and subjected to subsequent work-up procedures for structural elucidation. Once the chemical identity of specific compounds is established, unknown constituents within the same matrix can be characterized by comparing their fragment ion patterns with those of known reference compounds. In instances where reference standards are unavailable, spectral library matching provides a reliable alternative for compound identification (Teonata *et al.*, 2021).

2.6.3. Mass Spectral Characterization

Alternatively, chromatographically separated components can be introduced directly into the mass spectrometer for spectral analysis. This process yields essential information on molecular weight, fragmentation pathways, and isotopic distributions, which collectively facilitate the identification, authentication, and origin tracing of analytes (Shi *et al.*, 2020). Ongoing advancements in GC–MS instrumentation have significantly improved analytical sensitivity, spectral resolution, and the capacity to characterize an expanded range of chemical species. Gas chromatography serves as the pivotal separation stage in GC–MS, resolving individual components within a complex sample into discrete peaks based on their retention times. The efficiency of this separation is governed by the compounds' volatility and their

physicochemical interactions with the stationary phase of the chromatographic column (Meziani *et al.*, 2022).

2.7. FTIR SPECTROSCOPY OVERVIEW

Fourier Transform Infrared (FTIR) spectroscopy is a versatile and widely employed analytical technique used to investigate molecular vibrations and rotations (Hou *et al.*, 2018). The method detects molecules possessing a dipole moment and provides a distinctive “fingerprint” spectrum, as variations in atomic type, number, or arrangement generate unique spectral patterns. When infrared radiation of continuous wavelengths interacts with a molecule, specific wavenumbers are absorbed, corresponding to transitions between molecular energy levels. The resulting absorbance spectrum reflects the vibrational characteristics of the molecule’s chemical bonds and functional groups, allowing for detailed structural elucidation. Contemporary FTIR methodologies such as transmission, attenuated total reflection (ATR), and imaging have further expanded its analytical scope and practical applicability (Bunaciu *et al.*, 2010 ; Szentirmai *et al.*, 2020 ; Tiernan *et al.*, 2020).

CHAPTER THREE

MATERIALS AND METHODS

3.1 RESEARCH DESIGN/ STUDY AREA

The chemical composition of *Ocimum gratissimum* leaves collected from various habitats was examined in this study using an experimental and comparative design. Leaf samples were collected from Egor, Oredo and Ovia North East Local Government Areas (LGAs) of Edo State, in locations situated near dumpsites. The Essential oils were extracted from the leaves using solvent extraction, and their functional groups and constituents were determined using Fourier Transform Infrared Spectroscopy (FTIR) and Gas Chromatography–Mass Spectrometry (GC–MS). The identified constituents were quantified and compared based on their chemical components across the sampling sites. These analytical approaches provided insights into the environmental influences on the chemical composition of the plant.

3.2 PLANT COLLECTION

Fresh leaves of *Ocimum gratissimum* were harvested in July 2025 from three Local Government Areas (LGAs); Egor, Oredo, and Ovia North-East with their respective geographic coordinates presented in Table 3.1. In each LGA, samples were collected from sampling sites located near dumpsites to ensure consistency in environmental exposure.

Table 3.1: Sampling site and their various GPS

S/N	Sampling Sites	GPS
1.	Ovia North East	6.430163°N 5.616123°E
2.	Egor	6.380681°N 5.613125°E
3.	Oredo	6.33883°N 5.61722°E

3.3 PREPARATION OF SAMPLE

The leaves were dried away from direct sunlight for two weeks to prevent photodegradation of volatile compounds. Thereafter, they were oven-dried at 45 °C for 30 minutes to remove residual moisture. The dried samples were then blended into fine powder using an electrical blender. Each powdered sample was weighed using an analytical balance, and the results are presented in Table 3.2

Table 3.2: Samples and their various weight in kg

S/N	Samples	Weight (kg)
1.	Ovia North East	40.204
2.	Oredo	34.469
3.	Egor	18.664

3.4 EXTRACTION PROCESS

The extraction process was done with a Soxhlet apparatus and the solvent hexane was used for the extraction. The Soxhlet apparatus was assembled, and the powdered leaf samples were carefully placed inside a thimble and placed in the Soxhlet apparatus. A 125 ml volume of hexane was measured and poured into a round-bottom flask. The flask was positioned in the heating mantle, which was maintained at 100 °C for 2 hours. The extraction process was monitored until sufficient oil-solvent mixture was collected in the extraction chamber. The obtained extract was carefully transferred into clean jar bottles for further processing.

3.5 SOLVENT RECOVERY PROCESS

After extraction, the crude extract was subjected to rotary evaporation to remove and recover the hexane. The rotary evaporator was operated at 75 °C and 205 RPM for 45 minutes. After the solvent was completely recovered, the essential oil residues were obtained. The oil samples were stored in amber vials to protect them from light and oxidation until chemical analysis was performed.

3.6 GC-MS ANALYSIS

The Gas Chromatography–Mass Spectrometry (GC–MS) analysis of the essential oil extract was performed using an Agilent 5977B GC/MSD system coupled with an Agilent 8860 auto-sampler, interfaced with an Elite-5MS (5% diphenyl / 95% dimethyl polysiloxane) fused silica capillary column (30 m × 0.25 µm ID × 0.25 µm film thickness). The electron ionization system was operated in electron impact (EI) mode at 70 eV, with helium (99.999%) as the carrier gas at a constant flow rate of 1 mL/min. An injection volume of 1 µL was employed (split ratio 10:1). The injector temperature was maintained at 300 °C, ion-source temperature at 250 °C, and oven temperature programmed from 100 °C (isothermal for 0.5 min), increased at 20 °C/min to 280 °C, held for 2.5 min. Mass spectra were taken at 70 eV; a scanning interval of

0.5 s and fragments from 45 to 450 Da, the solvent delay was 0-3 min with a total run time of 21.33 minutes.

3.7 FTIR ANALYSIS

The Fourier Transform Infrared (FTIR) spectroscopy of the essential oil extract was carried out to identify the functional groups present in the essential oil. The analysis was conducted using a standard FTIR spectrometer, Samples were scanned within the mid-infrared range of 4000–400 cm^{-1} to identify functional groups present in the essential oil.

CHAPTER FOUR

RESULTS

4.1 PERCENTAGE YIELD OF *OCIMUM GRATISSIMUM* ESSENTIAL OIL

The percentage yield of *Ocimum gratissimum* essential oil for Ovia North East, Oredo and Egor are given in table 4.1

Table 4.1: Percentage yield of *Ocimum gratissimum* essential oil of the samples

S/N	Samples	Weight (kg)	Percentage yield
1.	Ovia North East	40.204	
2.	Oredo	34.469	
3.	Egor	18.664	

4.2 GC-MS ANALYSIS

This Gas Chromatography-Mass Spectrometry (GC-MS) analysis provides a detailed chemical profile of the sample analyzed. The Table 4.2, 4.3 and 4.4 lists 26, 30 and 32 compounds respectively separated by their Retention Time (RT), their relative abundance as a percentage of the total chromatographic area (Area %), and their identified names.

Table 4.2: GC-MS for *O. gratissimum* from Egor Local Government Area

PK#	RT(min)	Area %	Names Of chemical compounds
1.	3.145	4.66	Benzene 1-ethyl-4-methyl-
2.	3.185	2.79	(1S, 3R) - (f) - trans. - 2 - oxabicyclo [4.4.0] decane
3.	3.322	27.40	Decane
4.	3.459	1.21	Benzene, n-butyl-
5.	3.499	0.74	2- Tolyloxirane
6.	3.574	1.72	Decane, 4- methyl-
7.	3.631	1.46	p- Cymene
8.	3.671	7.86	o- Cymene
9.	3.734	1.96	Cyclohexane, butyl-
10.	3.768	0.70	Cyclopentane, (2-methylpropyl)-
11.	3.837	0.83	Benzene, 1-ethenyl-2-methyl-
12.	3.997	1.66	Benzene, 1-methyl-3-propyl
13.	4.089	5.01	Benzene, 1-ethyl-3, 5-dimethyl-
14.	4.329	0.80	o- Cymene
15.	4.358	0.96	o- Cymene
16.	4.438	1.34	p- Cymene
17.	4.552	3.03	Undecane

18.	4.981	0.66	Napthalene, decahydro- 2-methyl-
19.	5.771	0.59	Napthalene
20.	5.822	0.82	Dodecane
21.	7.104	10.26	Thymol
22.	7.230	0.80	Thymol
23.	8.529	1.23	Caryophyllene
24.	9.256	1.32	Napthalene, decahydro-4a-methyl-1- methylene-7-(1-methylethenyl)-,[4aR- (4a.alpha., 7. alpha.,8a.beta.)]
25.	16.328	3.75	Squalene
26.	19.212	16.42	Bis(2-ethylhexyl) phthalate

Table 4.3: GC-MS for *O. gratissimum* from Ovia North East Local Government Area

PK#	RT(min)	Area %	Names Of chemical compounds
1.	3.150	5.19	Benzene, 1-ethyl-4-methyl-
2.	3.185	2.62	1-Allylazetidine
3.	3.322	29.35	Decane
4.	3.459	1.21	Benzene, n-butyl-
5.	3.499	0.70	2- Tolyloxirane
6.	3.574	1.65	Decane, 4-methyl-
7.	3.631	1.47	o- Cymene
8.	3.671	7.80	Benzene, 1, 4-diethyl-
9.	3.734	1.94	Cyclohexane, butyl-
10.	3.768	0.72	Cyclopentane, (2-methylpropyl)-
11.	3.837	0.83	Benzene, 2-propenyl
12.	3.997	1.67	Benzene, 1-methyl-3-propyl-
13.	4.089	4.73	o- Cymene
14.	4.329	0.79	o- Cymene
15.	4.358	0.94	o- Cymene
16.	4.438	1.39	o- Cymene
17.	4.552	2.86	Undecane
18.	4.981	0.65	Napthalene, decahydro- 2-methyl-
19.	5.765	0.63	Napthalene
20.	5.822	0.92	Dodecane


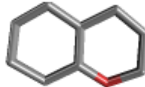
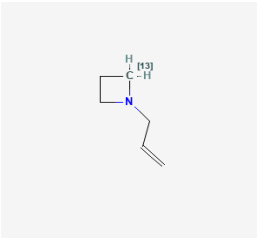
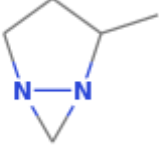
21.	5.902	0.76	Estragole
22.	7.110	4.19	Thymol
23.	8.529	1.68	Caryophyllene
24.	9.256	1.82	Napthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)-,[4aR-(4a.alpha., 7.alpha.,8a.beta.)]
25.	12.471	0.69	Neophytadiene
26.	14.737	0.72	Phytol
27.	16.311	1.42	Squalene
28.	16.345	1.64	Squalene
29.	18.966	1.61	Eicosane
30.	19.212	17.42	Bis (2-ethylhexyl) phthalate



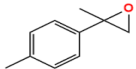
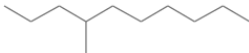

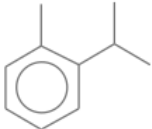
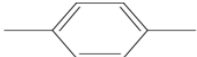
Table 4.4: GC-MS result for *O. gratissimum* from Oredo Local Government Area

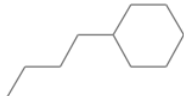
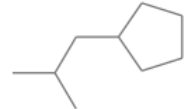
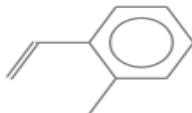

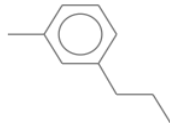
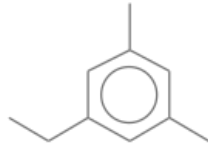

PK#	RT(min)	Area %	Names Of chemical compounds
1.	3.150	4.33	Benzene, 1-ethyl-4-methyl-
2.	3.184	2.31	2,4-Dimethyl-1, 5-diazabicyclo [3.1.0] hexane (cis)
3.	3.327	24.87	Decane
4.	3.465	1.10	Benzene, n-butyl-
5.	3.499	0.61	2- Tolyloxirane
6.	3.573	1.49	Decane, 4-methyl-
7.	3.631	1.20	p- Cymene
8.	3.671	5.99	Benzene, 1, 4-diethyl-
9.	3.739	1.58	Cyclohexane, butyl-
10.	3.768	0.68	Cyclopentane, (2-methylpropyl)-
11.	3.837	0.77	Benzene, 2-propenyl
12.	3.997	1.53	Benzene, 1-methyl-3-propyl-
13.	4.088	4.48	Benzene, 1-ethyl-3, 5-dimethyl-
14.	4.329	0.68	o- Cymene
15.	4.357	0.89	o- Cymene
16.	4.443	1.18	o- Cymene
17.	4.558	2.77	Undecane
18.	4.987	0.64	Napthalene, decahydro- 2-methyl-
19.	5.771	0.60	Napthalene
20.	5.822	0.76	Dodecane

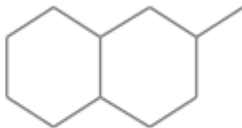



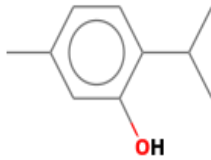
21.	7.110	9.47	Thymol
22.	7.230	0.85	Thymol
23.	8.529	1.29	Caryophyllene
24.	9.261	2.42	Napthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)-,[4aR-(4a.alpha., 7. alpha.,8a.beta.)]
25.	9.341	0.76	2- Isopropenyl -4a, 8-dimethyl-1,2,3,4,4a,5,6,7-octahydronapthalene
26.	10.280	0.54	Caryophyllene oxide
27.	12.471	0.68	Neophytadiene
28.	15.636	1.52	5-[3,5-Ditrifluoromethylphenoxy] -6 - methoxy- 4 - methyl- 8 - nitroquinone
29.	16.150	0.95	beta. -Sitosterol
30.	16.362	6.76	Squalene
31.	18.954	0.57	Octadecane
32.	19.223	15.74	Bis (2-ethylhexyl) phthalate

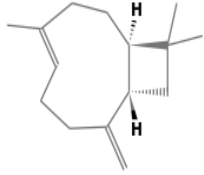
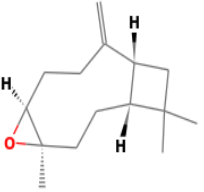
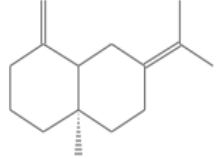


Table 4.5: Comparative GC-MS from the Three Local Government Areas

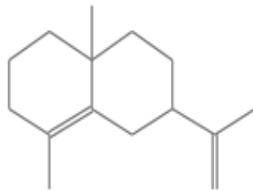
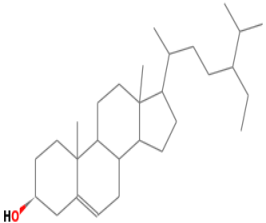



S/N	Name of Compound	Egor	Ovia North-East	Oredo	Class of Compound	Chemical Formular (g/mol)	Molecular Weight	Chemical Structure
1	Benzene, 1-ethyl-4-methyl-	4.66	5.19	4.33	Aromatic hydrocarbon	C ₉ H ₁₂	120.19	
2	(1S,3R)-(f)-trans-2-oxabicyclo[4.4.0]decane	2.79	–	–	Heterocyclic compound	C ₉ H ₁₆ O	140.22	
3	1-Allylazetidone	–	2.62	–	Heterocyclic compound	C ₆ H ₁₁ N	98.15	
4	2,4-Dimethyl-1,5-diazabicyclo[3.1.0]hexane (cis)	–	–	2.31	Heterocyclic compound	C ₅ H ₁₀ N ₂	98.146	

5	Decane	27.40	29.35	28.87	Alkane	C ₁₀ H ₂₂	142.28	
6	Benzene, n-butyl-	1.21	1.21	1.10	Aromatic hydrocarbon	C ₁₀ H ₁₄	134.22	
7	2-Tolyloxirane	0.74	0.70	0.61	Epoxide	C ₉ H ₁₀ O	134.19	
8	Decane, 4-methyl-	1.72	1.65	1.49	Alkane	C ₁₁ H ₂₄	156.31	
9	p-Cymene	2.80	–	1.20	Monoterpene hydrocarbon	C ₁₀ H ₁₄	134.22	
10	o-Cymene	9.62	9.32	2.75	Monoterpene hydrocarbon	C ₁₀ H ₁₄	134.22	
11	Benzene, 1, 4- dimethyl-	-	7.80	5.99	Aromatic hydrocarbon	C ₈ H ₁₀	106.16	

12	Cyclohexane, butyl-	1.96	1.94	1.58	Alkane	C ₁₀ H ₂₀	140.266	
13	Cyclopentane, (2-methylpropyl)-	0.70	0.72	0.68	Alkane	C ₉ H ₁₈	126.24	
14	Benzene, 1-ethenyl-2-methyl-	0.83	–	–	Aromatic hydrocarbon	C ₉ H ₁₀	118.176	
15	Benzene, 2-propenyl	–	0.83	0.77	Aromatic hydrocarbon	C ₉ H ₁₀	118.176	
16	Benzene, 1-methyl-3-propyl-	1.66	1.67	1.53	Aromatic hydrocarbon	C ₁₀ H ₁₄	134.22	
17	Benzene, 1-ethyl-3,5-dimethyl-	5.01	–	4.48	Aromatic hydrocarbon	C ₁₀ H ₁₄	134.22	
18	Undecane	3.03	2.86	2.77	Alkane	C ₁₁ H ₂₄	156.31	

19	Naphthalene, decahydro-2-methyl-	0.66	0.65	0.64	Terpene	$C_{11}H_{20}$	152.276	
20	Naphthalene	0.59	0.63	0.60	Polycyclic Aromatic hydrocarbon	$C_{10}H_8$	128.17	
21	Dodecane	0.82	0.92	0.76	Alkane	$C_{12}H_{26}$	170.33	
22	Estragole	–	0.76	–	Aromatic hydrocarbon	$C_{10}H_{12}O$	148.20	
23	Thymol	11.06	4.19	10.32	Oxygenated monoterpene	$C_{10}H_{14}O$	150.22	

24	Caryophyllene	1.23	1.68	1.29	Sesquiterpene hydrocarbon	$C_{15}H_{24}$	204.35	
25	Caryophyllene oxide	–	–	0.54	Oxygenated sesquiterpene	$C_{15}H_{24}O$	220.35	
26	Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)-[...]	1.32	1.82	2.42	Poly aromatic hydrocarbon	$C_{15}H_{24}O$	204.35	
27	Neophytadiene	–	0.69	0.68	Diterpene hydrocarbon	$C_{20}H_{38}$	278.51	
28	Phytol	–	0.72	–	Diterpene alcohol	$C_{20}H_{40}O$	296.53	

29	2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene	–	–	0.76	Sesquiterpene	$C_{15}H_{24}$	204.35	
30	β -Sitosterol	–	–	0.96	Triterpene (Sterol compound)	$C_{29}H_{50}O$	414.707	
31	Squalene	3.75	3.06	6.74	Triterpene hydrocarbon	$C_{30}H_{50}$	410.72	
32	Eicosane	–	1.61	–	Alkane	$C_{20}H_{42}$	282.55	
33	Octadecane	–	–	0.57	Alkane	$C_{18}H_{38}$	254.49	

34	Bis(2-ethylhexyl) phthalate	16.42	17.42	15.74	Phthalate ester	$C_{24}H_{38}O_4$	390.556
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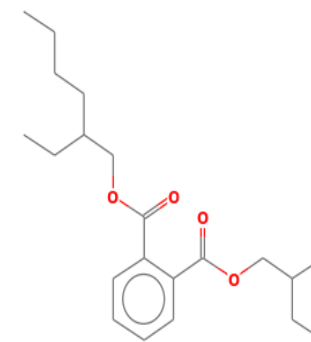


Table 4.6 : Summary of GC-MS from the Three Local Government Areas

Parameter		Egor	Ovia North-East	Oredo
Total Identified	Compounds	26	30	32
Major (Highest % Area)	Compound	Decane (27.40%)	Decane (29.35%)	Decane (24.87%)
Second Most Abundant Compound	Abundant	Bis(2-ethylhexyl) phthalate (16.42%)	Bis(2-ethylhexyl) phthalate (17.42%)	Bis(2-ethylhexyl) phthalate (15.74%)
Common Bioactive Compounds	Major	Thymol, Caryophyllene, Squalene, Decane, Bis(2-ethylhexyl) phthalate	Same as Egor	Same as Egor
Unique Compounds		(1S,3R)-trans-2-oxabicyclo[4.4.0]decane, Cyclopentane (2-methylpropyl)	1-Allylazetidine, Estragole, Phytol, Eicosane	Caryophyllene oxide, β -Sitosterol, Octadecane, Quinone derivative

4.3 FTIR ANALYSIS

Table 4.7: FTIR for *O. gratissimum* from Egor Local Government Area

S/N	Frequency	Appearance	Bond	Compound
1.	3440.57	Broad	NH- stretch	Heterocyclic amine
2.	2932.71	Medium Strong	Methylene CH- stretch	Alkyl group
3.	1642.84	Medium Strong	NH bend	Secondary amine
4.	1460.81	Medium Strong	Methyl CH bend	Alkyl group
5.	1378.73	Medium Strong	Methyl CH bend	Alkyl group
6.	727.59	Medium	Methylene rocking	Alkyl group
7.	692.13	Medium	C-Br stretch	Aliphatic organohalogen
8.	672.72	Medium	CH bend	Alkyne

Table 4.8: FTIR for *O. gratissimum* From Ovia North East Local Government Area

S/N	Frequency	Appearance	Bond	Compound
1.	3417.70	Broad	NH- stretch	Heterocyclic amine
2.	2930.59	Medium	Methylene CH- stretch	Alkyl group
3.	2872.31	Medium	Methyl CH- stretch	Alkyl group
4.	1643.52	Medium Strong	NH bend	Secondary amine
5.	1459.12	Medium Strong	Methyl CH- bend	Alkyl group
6.	727.51	Medium	Methylene rocking	Alkyne group
7.	692.29	Medium	C-Br stretch	Aliphatic organohalogen
8.	672.85	Medium	CH bend	Alkyne

Table 4.9: FTIR For *O. gratissimum* from Oredo Local Government Area

S/N	Frequency	Appearance	Bond	Compound
1.	3440.80	Broad	NH stretch	Heterocyclic amine
2.	3033.42	Medium	CH stretch	Olefinic/ Akene group
3.	2927.58	Medium Strong	Methylene stretch	Alkyl group
4.	1727.38	Strong	Aldehyde	Carbonyl group
5.	1644.63	Medium	NH bend	Secondary amine
6.	1460.87	Medium Strong	Methyl bend	CH- Alkyl group
7.	1379.55	Medium	Methyl bend	CH- Alkyl group
8.	1266.96	Medium	Organic nitrates	Hetero-oxy compound
9.	1115.70	Medium	Sulfate ion	Inorganic ion
10.	767.43	Medium	Phenyl	Aromatic ring
11.	728.00	Medium Strong	Methylene rocking	Alkyl group
12.	692.95	Medium	C- Br stretch	Aliphatic organohalogen
13.	673.58	Medium	CH bend	Alkyne

Table 4.10: Comparative FTIR from the Three Local Government Areas

S/N	Bond	Compound	Egor	Ovia North East	Oredo
1.	NH stretch	Heterocyclic amine	3440.57	3417.70	3440.80
2.	CH stretch	Olefinic/ Alkene group	-	-	3033.42
3.	Methylene CH stretch	Alkyl group	2932.71	2930.59	2927.58
4.	Aldehyde	Carbonyl group	-	-	1727.38
5.	NH bend	Secondary amine	1642.84	1643.52	1644.63
6.	Methyl bend	CH Alkyl group	1460.81	2872.31	1460.87
7.	Methyl bend	CH Alkyl group	1378.73	1459.12	1379.55
8.	Organic nitrates	Hetero-oxy compound	-	-	1266.96
9.	Methylene rocking	Alkyl group	727.59	727.51	728.00
10.	Sulfate ion	Inorganic ion	-	-	1115.70
11.	Phenyl	Aromatic ring	-	-	767.43
12.	C. Br stretch	Aliphatic organohalog en	692.13	692.29	692.95
13.	CH bend	Alkyne	672.72	672.85	673.58

CHAPTER FIVE

DISCUSSION OF RESULTS

5.1 OVERVIEW

This chapter presents the results of Gas Chromatography–Mass Spectrometry (GC–MS) and Fourier Transform Infrared Spectroscopy (FTIR) analyses of essential oils extracted from *Ocimum gratissimum* leaves collected from dumpsites in three Government Areas (LGAs) of Edo State: Oredo, Egor, and Ovia North-East. These LGAs represent distinct dumpsite environments. The aim is to compare the chemical compositions of the oils obtained from each location, evaluate the influence of the dumpsite environment on the oil profiles, and assess the implications of these variations for the purity and quality of the essential oils.

5.2 GC-MS ANALYSIS

The provided GC-MS data reveals a complex mixture of organic compounds present in samples from the three LGAs as seen in Table 4.5 above. The chemical profile is rich in thymol and varied, comprising several major classes of compounds, each with distinct chemical properties, natural origins, and industrial/biological importance. The compounds are grouped into alkanes (saturated hydrocarbons), aromatic hydrocarbons, terpenes and terpenoids, heterocyclic compounds and other miscellaneous compounds.

5.2.1 Alkanes (Saturated Hydrocarbons)

Alkanes are straight-chain, branched, or cyclic saturated hydrocarbons with a general formula of C_nH_{2n+2} . They are typically major components of fossil fuels like petroleum and natural gas.

Different Forms of Alkane

- Straight chain alkanes: Decane , Undecane, Dodecane, Eicosane, Octadecane .
- Branched alkane: Decane, 4-methyl- .

- Cycloalkanes with alkyl substituents: Cyclohexane, butyl-, Cyclopentane, (2-methylpropyl)-.

Uses and Importance:

- Fuel Source: Shorter-chain alkanes (C9-C16) are key components of gasoline, diesel, and jet fuel.
- Solvents: Used in industrial processes and in products like paint thinners.
- Lubricants: Longer-chain alkanes and cycloalkanes contribute to the lubricating properties of oils.
- Biomarkers: The specific profile and ratios of alkanes can serve as chemical fingerprints to identify the source of organic matter (e.g., petroleum vs. biological waxes).

5.2.2. Aromatic Hydrocarbons

These compounds contain one or more benzene rings. They are often derived from petroleum or formed during the incomplete combustion of organic matter.

Different Forms of Aromatic Hydrocarbon

- Alkylbenzenes: Benzene, 1-ethyl-4-methyl-; Benzene, n-butyl-; Benzene, 1,4-dimethyl-; Benzene, 1-ethenyl-2-methyl-; Benzene, 2-propenyl; Benzene, 1-methyl-3-propyl- ; Benzene, 1-ethyl-3,5-dimethyl-.
- Polycyclic Aromatic Hydrocarbons (PAHs): Naphthalene.
- Oxygenated Aromatics: 2-Tolyloxirane (an epoxide); Estragole (a phenylpropene);

Uses and Importance:

Industrial Solvents and Intermediates: Alkylbenzenes like p-Cymene are used in the production of fragrances, dyes, and resins.

- Pharmaceuticals and Fragrances: Thymol is a natural antiseptic used in mouthwashes and has a characteristic thyme scent. Estragole is found in tarragon and basil and is used in perfumery and flavoring.
- Petrochemical Indicators: The presence of a wide range of alkylbenzenes is a classic signature of petroleum-derived contamination or naturally occurring petroleum seeps.
- Concerns: Some lighter alkylbenzenes are volatile organic compounds (VOCs), and some PAHs like Naphthalene are considered pollutants and potential health hazards.

5.2.3. Terpenes and Terpenoids

This is a large and diverse class of naturally occurring organic chemicals derived from five-carbon isoprene units. Terpenes are hydrocarbons, while terpenoids contain additional functional groups (oxygen).

Different Forms of Terpenes and Terpenoids

- Monoterpenes: p-Cymene , o-Cymene .
- Sesquiterpenes: Caryophyllene , Caryophyllene oxide .
- Diterpenes: Phytol , Neophytadiene.
- Triterpenes: Squalene, β -Sitosterol (a sterol, which is a type of triterpenoid).
- Others: 2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene ,Naphthalene,decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)-[...].

Uses and Importance:

- Fragrances and Flavors: Terpenes are responsible for the scents of many plants (e.g., caryophyllene contributes to the spiciness of black pepper).
- Pharmaceuticals: Many terpenoids have significant biological activities. β -Sitosterol is known for its potential to lower cholesterol. Caryophyllene oxide has demonstrated antifungal properties.
- Essential Oils: This entire class is the primary constituent of plant essential oils.

- Biomarkers: Phytol is a breakdown product of chlorophyll, indicating plant-derived organic matter. The presence of these compounds strongly suggests a significant botanical source for the samples, especially in Ovia North-East and Oredo.
- Biological Role: Squalene is a vital biochemical precursor for the synthesis of all plant and animal sterols, including cholesterol and steroid hormones.

5.2.4. Heterocyclic Compounds

These compounds contain rings with at least two different elements as ring members, most commonly carbon with nitrogen, oxygen, or sulfur.

Different Forms of Heterocyclic compounds

- Oxygen-containing: (1S,3R)-(f)-trans-2-oxabicyclo[4.4.0]decane (an ether), 2-Tolyloxirane (an epoxide).
- Nitrogen-containing: 1-Allylazetidine (an azetidine), 2,4-Dimethyl-1,5-diazabicyclo[3.1.0]hexane (cis) (a diazabicyclo compound).

Uses and Importance:

- Pharmaceutical Intermediates: Heterocyclic structures are the backbone of a vast number of drugs. Azetidines and diazabicyclo compounds are important pharmacophores.
- Solvents and Intermediates: Cyclic ethers are used as solvents in organic chemistry.
- Flavor and Fragrance: Furans, like compound , are often found in roasted foods and are used in flavorings.
- High-Value Chemicals: Their presence, even in small amounts, can indicate complex chemical reactions or the presence of specific biological sources.

5.2.5. Other Miscellaneous Compounds

This category includes compounds that do not fit neatly into the above classes but are significant.

Compounds Found:

- Plasticizer: Bis(2-ethylhexyl) phthalate.
- Specialized Metabolite: 5-[3,5-Dinitrofluoromethylphenoxy]-6-methoxy-4-methyl-8-nitroquinone.

Uses and Importance:

- Bis(2-ethylhexyl) phthalate (DEHP): This is a very common plasticizer used to make plastics like PVC flexible. Its ubiquitous presence is a classic indicator of environmental plastic pollution or sample contamination from lab plastics.
- Complex Quinone: This is a highly specialized, synthetic-looking molecule. Its presence, unique to Oredo, is very unusual. It suggests a potential anthropogenic (human-made) pollutant, possibly from industrial waste, agricultural chemicals, or pharmaceutical contamination.

5.3 COMPARATIVE DISCUSSION AMONG THE THREE LGAs

Ocimum gratissimum leaves are rich in thymol, and the presence of compounds such as thymol, o-cymene, p-cymene and caryophyllene supports the plant's traditional medicinal uses. These compounds have been scientifically reported to possess the following biological activities:

- Antimicrobial Activity: Effective against bacteria, fungi, and viruses.
- Antioxidant Activity: Scavenging free radicals and preventing oxidative damage.
- Anti-inflammatory and Analgesic Properties: Helping to reduce pain and swelling.

Among the three sampling locations, Oredo LGA exhibited the highest number of identified compounds (32), followed by Ovia North-East (30) and Egor (26). This suggests that Oredo may have been more exposed to a diverse array of waste-derived chemicals, resulting in a more complex essential oil profile, as presented in Table 4.6.

The percentage composition of contaminants, such as Bis(2-ethylhexyl) phthalate and Decane, was highest in Ovia North-East (17.42% phthalate, 29.35% decane) and Oredo (15.74% phthalate, 24.87% decane) compared to Egor (16.42% phthalate, 27.40% decane), the presence of bis(2-ethylhexyl) phthalate suggests contamination from plastic materials, while the detection of decane may be attributed to incomplete recovery of hexane residues or contamination originating from petroleum-based products. This indicates that all sites exhibited notable levels of contamination, with Ovia North-East showing slightly elevated hydrocarbon concentrations. Also the compositional variation of *Ocimum gratissimum* essential oils harvested from dumpsite environments revealed site-dependent differences in monoterpenoid profiles. p-Cymene was highest in Egor (2.80%), moderately low in Oredo (1.20%), and undetected in Ovia North-East, suggesting inhibition of its biosynthetic pathway under elevated stress conditions. Conversely, o-cymene occurred at comparable levels in Egor (9.62%) and Ovia North-East (9.32%) but was markedly reduced in Oredo (2.75%), indicating enhanced oxidative stress response in the former sites. Thymol, a key oxygenated monoterpenoid, was most abundant in Egor (11.06%) and Oredo (10.32%), but notably lower in Ovia North-East (4.19%), reflecting potential suppression of enzymatic conversion in more contaminated soils. Collectively, these results suggest that the degree of dumpsite pollution modulates the biosynthesis of major terpenoid constituents, with Egor and Oredo exhibiting adaptive metabolic resilience, while Ovia North-East shows clear evidence of stress-induced metabolic inhibition. These findings are consistent with the hypothesis that dumpsite pollution influences the phytochemical composition of aromatic plants. The substantial presence of aromatic hydrocarbons and phthalates suggests the possible uptake of petroleum-derived contaminants through plant roots or their adsorption onto the plant surface.

5.4 GC–MS COMPARATIVE ANALYSIS OF OCIMUM GRATISSIMUM ESSENTIAL OIL FROM DUMPSITE AREAS AND THE REFERENCE STUDY BY ITAH AND AKINJOGUNLA (2024)

The Gas Chromatography–Mass Spectrometry (GC–MS) analysis of *Ocimum gratissimum* essential oil obtained from dumpsite environments in Egor, Ovia North-East, and Oredo Local Government Areas revealed pronounced qualitative and quantitative variations when compared with the findings of Itah and Akinjogunla (2024). These variations indicate that environmental exposure, particularly to dumpsite contaminants, exerts a measurable influence on the phytochemical composition of *Ocimum gratissimum*.

According to the reference study by Itah and Akinjogunla (2024), a total of 44 bioactive constituents were identified in the aqueous leaf extracts of *Ocimum gratissimum*. The predominant compounds included butanoic acid, 3-methyl- (13.89%), thymol (12.43%), butanoic acid, 2-methyl- (7.22%), and cis-thujopsene (7.10%). These compounds, primarily composed of carboxylic acids, oxygenated monoterpenes, and sesquiterpenes, are responsible for the plant's characteristic antimicrobial activity.

In contrast, essential oils extracted from *Ocimum gratissimum* plants collected from the Egor, Ovia North-East, and Oredo dumpsites contained 26, 30, and 32 compounds, respectively, with decane (27.40%, 29.35%, and 24.87%) and bis(2-ethylhexyl) phthalate (16.42%, 17.42%, and 15.74%) emerging as the dominant constituents, alongside notable benzene derivatives. This compositional shift suggests that environmental stress and pollutant exposure disrupt the plant's secondary metabolic pathways, promoting the accumulation of hydrocarbons and synthetic esters at the expense of naturally derived oxygenated metabolites.

Similarities Between Both Studies

Several key phytochemicals were consistently detected across both investigations. Thymol, a phenolic monoterpene renowned for its antimicrobial activity, was identified in all Local

Government Area (LGA) samples as well as in the reference report by Itah and Akinjogunla (2024). This persistent occurrence designates thymol as a potential chemotaxonomic marker for *Ocimum gratissimum*. Likewise, cis-thujopsene, caryophyllene, and caryophyllene oxide were observed in both datasets, reaffirming their stability as sesquiterpene hydrocarbons and oxygenated terpenes characteristic of the *Ocimum* genus. Additionally, aromatic hydrocarbons such as benzene, 1-ethyl-4-methyl-, and benzene, n-butyl-, appeared in both studies, suggesting that certain aromatic constituents are inherent components of the *Ocimum gratissimum* essential oil profile.

Differences in Chemical Composition and Relative Abundance

Pronounced variations were observed in the relative composition and abundance of the identified compounds. In the Itah and Akinjogunla (2024) study, oxygenated terpenes and organic acids predominated, reflecting normal biosynthetic activity under uncontaminated environmental conditions. In contrast, the essential oils obtained from dumpsite-grown samples were dominated by saturated alkanes such as decane, undecane, dodecane, octadecane, and eicosane, along with bis(2-ethylhexyl) phthalate; a plastic-derived phthalate ester, indicative of environmental contamination and pollutant uptake from surrounding waste materials. The absence of labile oxygenated compounds, including catechol, acexamic acid, nerolidol isobutyrate, and butyrolactone, detected in the uncontaminated reference samples suggests that oxidative stress and soil pollution may impair enzymatic pathways involved in terpene oxidation and organic acid biosynthesis. Collectively, these findings demonstrate that exposure to dumpsite-derived contaminants compromises the biosynthetic efficiency of *Ocimum gratissimum*, thereby altering its intrinsic phytochemical fingerprint.

5.5 ENVIRONMENTAL INFLUENCE OF DUMPSITE CONDITIONS

5.5.1 Modifies Soil Chemistry and Plant Metabolism

The altered phytochemical composition of *Ocimum gratissimum* grown in dumpsite environments can be attributed to exposure to heavy metals, hydrocarbons, and decomposing plastics, all of which modify soil chemistry and interfere with plant metabolic processes. Such contaminants alter nutrient availability, enzymatic activity, and secondary metabolite pathways, thereby reshaping the plant's biosynthetic profile.

5.5.2 Reduce the Therapeutic Quality and Fragrance of the Essential Oil

The substitution of bioactive terpenes and organic acids with hydrocarbons and phthalates reduces the antimicrobial efficacy and aromatic integrity of *Ocimum gratissimum* essential oils derived from dumpsite regions. While hydrocarbons and aromatic compounds may enhance volatility and fragrance, they are generally less biologically active than oxygenated terpenes such as thymol and caryophyllene oxide. The increased occurrence of synthetic esters like bis(2-ethylhexyl) phthalate further raises toxicological concerns, diminishing the suitability of such oils for therapeutic, pharmaceutical, or culinary applications.

5.5.3 Induction of Oxidative Stress

The accumulation of alkanes and aromatic hydrocarbons often produced as stress-response metabolites can trigger oxidative stress within plant tissues. These compounds interfere with enzymatic functions and disrupt redox homeostasis, ultimately impairing essential oil biosynthesis and altering the balance of key metabolites.

5.5.4 Environmental Effect on Humans

The contaminants identified present significant ecological and toxicological hazards. Bis(2-ethylhexyl) phthalate, a plasticizer commonly released from degraded waste materials, is a known endocrine disruptor, reproductive toxicant, and priority environmental pollutant. The presence of naphthalene, indicative of open-burning dumpsite activities, suggests potential

human carcinogenicity (Group 2B, IARC) and toxicity to aquatic organisms. Moreover, monoaromatic benzene derivatives although less toxic than benzene itself can induce narcotic effects and chronic health complications. The incorporation of such toxic residues into herbal preparations poses substantial health risks to consumers.

5.5.5 Affects the Quantity and Quality of the Essential Oil

The coexistence of natural bioactive terpenes with anthropogenic contaminants such as phthalates, alkanes, and polycyclic aromatic hydrocarbons (PAHs) provides clear evidence of biochemical interference induced by dumpsite exposure. Nutrient imbalances and pH fluctuations in contaminated soils further suppress the biosynthesis of oxygenated terpenes and organic acids. Consequently, the observed reduction in compound diversity (26, 30, and 32 compounds in polluted samples compared to 44 in the control) underscores the decline in secondary metabolite richness under pollution stress. The cultivation of *Ocimum gratissimum* or any medicinal plant in proximity to dumpsite environments is unsuitable for therapeutic or nutritional use. Persistent accumulation of pollutants may result in biomagnification through the food chain, thereby amplifying ecological and human health risks. This underscores the urgent need for effective waste management strategies and the adoption of phytoremediation practices to mitigate environmental contamination and safeguard medicinal plant integrity.

5.6 FOURIER TRANSFORM INFRARED (FTIR) ANALYSIS

The FTIR spectra of *Ocimum gratissimum* essential oils extracted from dumpsite environments in Oredo, Egor, and Ovia North-East Local Government Areas were examined to identify the characteristic functional groups present in the samples. The analysis provided valuable information on molecular vibrations, functional group interactions, and possible contamination resulting from exposure to pollutants commonly associated with dumpsites.

5.6.1 FTIR Interpretation for Egor LGA Sample

The FTIR spectrum of the Egor sample, as presented in Table 4.7, exhibited several distinct absorption bands indicative of various functional groups:

A broad absorption band at 3440.57 cm^{-1} corresponds to N–H stretching vibrations typical of heterocyclic amines, implying the presence of nitrogen-containing compounds that may originate from organic pollutants or the degradation of amino-based substances. Medium to strong peaks observed at 2932.71 cm^{-1} and 1642.84 cm^{-1} are attributed to C–H stretching vibrations of methylene groups and N–H bending of secondary amines, respectively. These signals suggest the presence of alkyl and amine functionalities, characteristic of naturally occurring phytochemicals such as terpenoids and alkaloids. Absorption bands at 1460.81 cm^{-1} and 1378.73 cm^{-1} correspond to C–H bending vibrations of methyl groups, further supporting the presence of alkane chains derived from essential oil constituents such as decane and cymene, as corroborated by the GC–MS results. A distinct band at 692.13 cm^{-1} is assigned to C–Br stretching vibrations associated with aliphatic organohalogens, indicating possible contamination from brominated or chlorinated hydrocarbons typical of dumpsite effluents. The minor absorption at 672.72 cm^{-1} corresponds to C–H bending vibrations of alkyne groups, which may be linked to unsaturated hydrocarbons within the volatile components of the essential oil. Overall, the spectral features indicate that while the intrinsic chemical profile of *O. gratissimum* essential oil remains discernible, the presence of halogenated compounds provides clear evidence of environmental contamination arising from dumpsite exposure.

5.6.2 FTIR Interpretation for Ovia North-East LGA Sample

The FTIR spectrum of the Ovia North-East sample, as presented in Table 4.8, exhibited several distinct absorption bands indicative of various functional groups.

A broad N–H stretching vibration observed at 3417.70 cm^{-1} confirmed the presence of heterocyclic amines, similar to the Egor sample, suggesting comparable environmental exposure. The absorption peaks at 2930.59 and 2872.31 cm^{-1} correspond to C–H stretching vibrations of methylene and methyl groups, which are characteristic of aliphatic chains and terpenoid structures commonly found in essential oils. An absorption band at 1643.52 cm^{-1} was attributed to N–H bending, signifying the presence of secondary amines that may be associated with alkaloid or amine-containing compounds, as also identified in the GC–MS analysis. The distinct C–Br stretching vibration at 692.29 cm^{-1} indicated possible organohalogen contamination, while the CH bending at 672.85 cm^{-1} confirmed the occurrence of alkyne moieties. Additionally, a methylene rocking band observed at 727.51 cm^{-1} supported the presence of long-chain hydrocarbons such as decane, which was identified as a major compound in the GC–MS profile of this sample. Overall, the FTIR spectrum of the Ovia North-East sample aligns with the GC–MS findings, revealing an alkane-rich hydrocarbon composition. The detection of halogen and nitrogen-containing functional groups further suggests mild environmental contamination resulting from dumpsite exposure.

5.6.3 FTIR Interpretation for Oredo LGA Sample

The FTIR spectrum of the Oredo sample, as shown in Table 4.9, displayed a more complex and diverse range of absorption bands, indicating a broader spectrum of chemical functionalities. A broad N–H stretching vibration at 3440.80 cm^{-1} signified the presence of heterocyclic amines, confirming nitrogenous phytochemicals or amine-based contaminants. A medium-intensity band at 3033.42 cm^{-1} was assigned to olefinic (C–H) stretching vibrations of alkenes, consistent with the presence of unsaturated compounds such as p-cymene and naphthalene derivatives identified in the GC–MS analysis. A strong absorption at 1727.38 cm^{-1} corresponded to C=O stretching of carbonyl or aldehydic compounds, which may arise from oxidized terpenoids or degradation products of organic matter. Peaks at 1266.96 cm^{-1} and

1115.70 cm^{-1} were attributed to organic nitrates and sulfate ions, respectively, indicating the presence of inorganic or anthropogenic contaminants likely derived from waste decomposition and combustion by-products at the dumpsite. The band observed at 767.43 cm^{-1} was characteristic of phenyl group absorption, corroborating the GC–MS detection of aromatic hydrocarbons such as benzene, 1-ethyl-4-methyl. Additional C–Br stretching at 692.95 cm^{-1} confirmed the occurrence of aliphatic organohalogens, while C–H bending at 673.58 cm^{-1} suggested alkyne linkages. Collectively, the FTIR results for the Oredo sample indicate a higher degree of chemical diversity and potential contamination relative to the Egor and Ovia North-East samples. The detection of carbonyl, nitrate, and sulfate functional groups substantiates the influence of anthropogenic pollutants, underscoring the significant environmental impact of dumpsite exposure on the essential oil's chemical profile.

5.7 Comparative Discussion of the FTIR Results

A comparative examination of the three spectra presented in Table 4.10 revealed that all samples shared common functional groups, including N–H stretch, methylene C–H stretch, N–H bend, methyl C–H bend, methylene rocking, C–H bend, and C–Br (organohalogen) vibrations. The presence of these consistent bands indicates a similar phytochemical framework among the *Ocimum gratissimum* essential oil samples. The uniform detection of C–Br stretching across all locations further suggests a common exposure to halogenated compounds at the dumpsite environments. Among the samples, the Oredo extract exhibited the highest degree of contamination, while those from Egor and Ovia North-East retained a comparatively purer essential oil profile, closer to the natural composition of *Ocimum gratissimum*.

5.8 FTIR COMPARATIVE ANALYSIS OF OCIMUM GRATISSIMUM ESSENTIAL OIL FROM DUMPSITE AREAS AND THE REFERENCE STUDY BY Arun *et al.*, (2022)

The FTIR spectra of *Ocimum gratissimum* essential oils from Egor, Oredo, and Ovia North-East LGAs, when compared with the reference study by Arun *et al.* (2022), revealed prominent aliphatic (C–H) stretching and methyl (–CH) bending vibrations in both datasets. This confirms that *O. gratissimum* essential oil characteristically possesses an aliphatic hydrocarbon backbone and methyl-substituted compounds.

Difference Between Studies

The reference study by Arun *et al.* (2022) exhibited a distinct O–H stretching band at 3319 cm^{-1} , indicative of higher free alcohol or phenolic content. In contrast, the dumpsite-derived samples lacked this O–H stretch but showed strong N–H stretching and bending vibrations (as detailed in Table 5.3). This shift implies an increased presence of nitrogenous or heterocyclic compounds, or conversely, a depletion of free alcohols potentially resulting from environmental stress, altered metabolic pathways, or pollutant-induced chemical transformations.

Furthermore, unique absorptions were observed in the dumpsite samples particularly in Oredo including carbonyl (1727.38 cm^{-1}), organic nitrate (1266.96 cm^{-1}), sulfate (1115.70 cm^{-1}), and organohalogen (692.13, 692.29, and 692.95 cm^{-1}) bands. These peaks were absent in the reference study and are suggestive of anthropogenic contamination processes such as oxidation, nitration, and halogenation, reflecting the influence of pollutant exposure within the dumpsite environments.

CONCLUSION

This study revealed that environmental contamination resulting from dumpsite exposure markedly influences the phytochemical and functional composition of *Ocimum gratissimum* essential oil. Samples obtained from Egor, Ovia North-East, and Oredo Local Government Areas exhibited a distinct shift from the predominance of naturally occurring oxygenated terpenes to profiles dominated by hydrocarbons and phthalates. Gas chromatography–mass spectrometry (GC–MS) analysis identified decane and bis(2-ethylhexyl) phthalate as major constituents, suggesting the absorption or surface adsorption of petroleum- and plastic-derived contaminants. Complementary Fourier-transform infrared (FTIR) analysis displayed characteristic N–H, C=O, and C–Br absorption bands, confirming the presence of nitrogenous, carbonyl, and halogenated compounds not observed in uncontaminated reference samples. These results indicate a perturbation of normal secondary metabolic pathways, likely induced by oxidative and chemical stress associated with polluted soil environments. Consequently, the biochemical modifications detected lead to a decline in the therapeutic efficacy, aromatic quality, and nutritional integrity of *Ocimum gratissimum* essential oils from dumpsite-impacted areas and may present potential toxicological hazards. It is therefore recommended that the cultivation and harvesting of medicinal plants in proximity to waste dumpsites be strictly avoided.

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APPENDIX I

Materials

1. Fresh leaves of *Ocimum gratissimum*
2. Hexane (99% HPLC grade)
3. Amber vial bottles
4. Jar bottles

Equipments

1. Analytical weighing balance
2. Electrical oven
3. Electrical blender
4. Soxhlet apparatus
5. Rotary evaporator
6. Gas Chromatography–Mass Spectrometry (GC–MS) machine
7. Fourier Transform Infrared Spectroscopy (FTIR) machine.

APPENDIX II



Plate 2: Grinding of *Ocimum gratissimum* samples using an electric blender

Photo credit: Rhoda Owenmen Ajayi

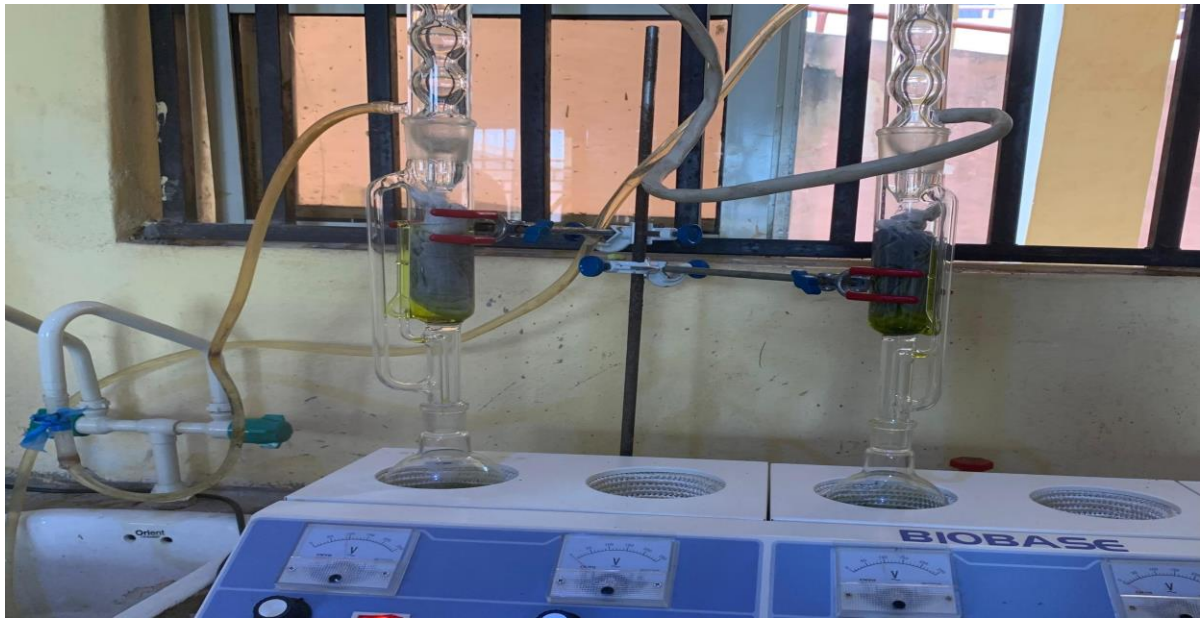


Plate 3: Extraction Process Using Soxhlet Apparatus

Photo credit: Rhoda Owenmen Ajayi



Plate 4: Rotary Evaporator for Recovery Process

Photo credit: Rhoda Owenmen Ajayi