



Study on phytochemical diversity of Lamiaceae: Promising leads in anti-malarial drug development

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Abstract

Malaria a health ailment primarily caused by *Plasmodium falciparum*, remains a global health challenge. The urgent need for new drugs and therapeutics has shifted the focus to natural products derived from medicinal plants. The Lamiaceae family is known for its wide ethno medicinal use and rich phytochemical diversity, holds a significant potential in anti-malarial research. This paper reviews the bioactive compounds of the Lamiaceae family. These compounds possess different mechanisms of action against *P. falciparum*, including destruction of parasite membranes, inducing oxidative stress, altering of heme detoxification, and interference with critical enzymes. Compounds like rosmarinic acid, thymol, carvacrol and essential oils from species such as *Ocimum gratissimum* and *Thymus vulgaris*, have shown significant anti-plasmodial properties *in vitro*. Also, the synergistic potential of these compounds with known anti-malarial drugs enhances their therapeutic value, potentially lowering resistance development. However, challenges such as difference in phytochemical composition, availability, and lesser *in vivo* and clinical studies must be addressed to fully recognise their potential. This review highlights the pharmaceutical promise of Lamiaceae derived compounds as anti-malarial agents. Bridging the gap between traditional medicinal knowledge and modern pharmacological practices could lead to innovative findings in the combat against malaria and drug resistance.

Keywords: Anti-malaria, lamiaceae, phytochemicals, natural products, anti-plasmodial, pharmacological, anti-oxidant

Introduction

Malaria is one among the oldest known infectious diseases. It is known to be a significant global health burden which is caused by the protozoan parasite *Plasmodium* (Carter & Mendis, 2002)^[1]. Malaria is the major cause for millions of cases and hundreds of thousands of deaths annually all around the globe (Joshi, *et al.*, 2024)^[3, 4]. *Plasmodium falciparum* is the most virulent and deadly among the five species of plasmodium which infects human health (Joshi, Pandey, *et al.*, 2024; Phillips *et al.*, 2017)^[3, 4, 8]. Natural products derived from medicinal plants have played a major role in discovery of anti-malarial drugs. From centuries traditional medicine has provided valuable insight into plant species with therapeutic properties out of which many are underexplored (Chaachouay & Zidane, 2024)^[2]. Lamiaceae family is one among the most useful family which is commonly known as the mint family. This family comprises genera like *Ocimum* (basil), *Rosmarinus* (rosemary), *Thymus* (thyme), and *Salvia* (sage) which are known for their diverse range of bioactive compounds such as essential oils, flavonoids, terpenoids, and polyphenols (Marchioni *et al.*, 2020)^[6].

The *Lamiaceae* family has a long history of utilisation in ethno medicine for its various pharmacological applications like anti-microbial, anti-inflammatory, and antispasmodic effects. Several species from this family are known for their promising anti-plasmodial activity, making them a potential source of novel anti-malarial agents. Rosmarinic acid, thymol, carvacrol, and essential oils have showed *in vitro* activity against *P. falciparum* (Zekar & Sharman, 2024)^[14]. This paper aims to provide a comprehensive review of the Lamiaceae family's phytochemical profile, highlighting its bioactive compounds and evaluating their pharmacological

potential against *Plasmodium falciparum*. By examining the mechanisms of action of these compounds, we aim to contribute to the ongoing search for novel, effective treatments for malaria. Given the growing challenge of drug resistance, tapping into the rich, untapped chemical diversity of Lamiaceae species offers a promising strategy to discover new leads for anti-malarial drug development.

Through this exploration, we hope to bridge the gap between traditional knowledge and modern pharmacology, fostering further research into the therapeutic applications of Lamiaceae-derived compounds.

Description of the family lamiaceae

Lamiaceae (mint family) is one of the largest and significant families of flowering plants of the order Lamiales. It comprises of over 250 genera and more than 7,000 species, this family is known for its ecological diversity, and economic importance (Uikey, 2024)^[12]. Members of the family *Lamiaceae* survive in a wide range of habitats, ranging from temperate to tropical regions, although they are particularly abundant and diverse in Mediterranean climates. The family is renowned for its aromatic plants, many of which have been utilized for centuries in field of culinary, medicinal, and ornamental applications (Uikey, 2024)^[12].

Members of *Lamiaceae* exhibit a remarkable variety of growth forms, including herbs, shrubs, subshrubs, and trees. Along with this they have several distinct morphological characteristics that facilitate identification, which includes opposite or whorled leaves, square stems, bilaterally symmetrical (zygomorphic) flowers, and fruits that often divides into four nutlets. Several members of this family produce essential oils, which contribute to their

characteristic aroma and therapeutic properties (Stankovic, 2020)^[11].

Numerous plants in the Lamiaceae family are studied for their antimalarial activities, particularly against *Plasmodium falciparum*, the causative agent of malaria. These studies highlight the potential of Lamiaceae plants as sources of antiplasmodial compounds.

Lamiaceae is of immense economical value. Various genera such as *Ocimum* (basil), *Mentha* (mint), *Salvia* (sage), *Rosmarinus* (rosemary), *Thymus* (thyme), and *Lavandula* (lavender) are cultivated worldwide for their different properties. They are also a major ingredient in traditional medicine systems, where they are utilised for their antimicrobial, antioxidant, and anti-inflammatory properties (Mamadaliyeva *et al.*, 2017)^[5]. The Lamiaceae family is a focal point of research in botany, agriculture, and pharmacology. Knowing the diversity, adaptations, and applications of *Lamiaceae* members offers insights into plant evolution, sustainable agriculture, and natural product development. This introduction sets the stage for a deeper exploration of this remarkable plant family.

1. Classification

Kingdom: Plantae

Division: Angiosperms

Class: Eudicots

Order: Lamiales

Family: Lamiaceae

2. Morphological Features of the family Lamiaceae:

The stem is typically quadrangular. Leaves are normally simple, opposite, or whorled, often have a characteristic aroma. Flowers are bisexual, zygomorphic, arranged in cymes or spikes, with a bilabiate (two-lipped) corolla. Fruits are mainly four nutlets enclosed in a persistent calyx.

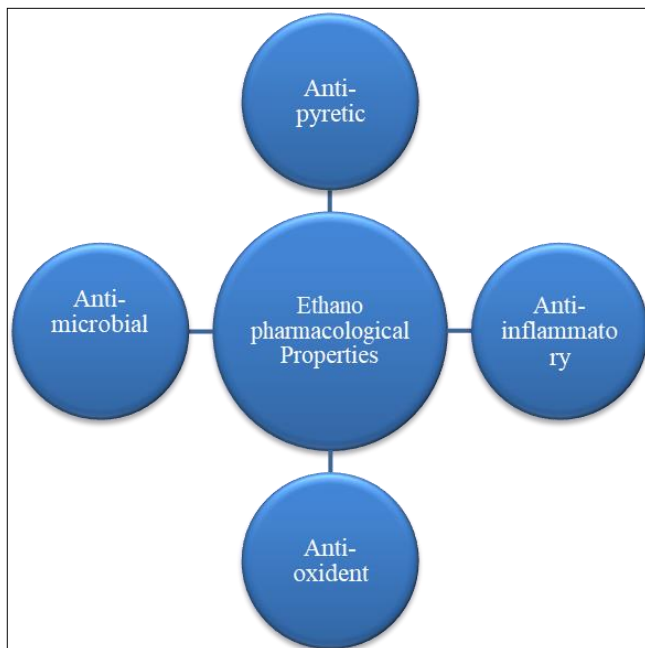


Fig 1: Ethno- pharmacological properties of the *Lamiaceae* family

Phytochemical constituent of *Lamiaceae*

Phyto-chemicals play crucial roles in defense mechanisms and therapeutic properties of the plants. The major classes of bioactive compounds in the *Lamiaceae* family include essential oils, phenolic compounds, flavonoids, terpenoids,

and alkaloids. Below is a detailed description of these constituents (Marchioni *et al.*, 2020)^[6].

1. Essential oils

Essential oils are one among the phytochemical constituents of the *Lamiaceae* family, known by their aromatic and volatile nature. Essential oils are concentrated plant extracts that comprises the natural aroma and beneficial properties of plants. They are obtained by using processes such as steam distillation or cold pressing. Essential oils have various applications, including aromatherapy, skincare, cleaning, and as natural remedies. Each essential oil constitutes a unique combination of volatile compounds, giving it its characteristic aroma and therapeutic effects (Ramos da Silva *et al.*, 2021)^[9]. Following are the major essential oils present in the members of the family *Lamiaceae*.

1.1. Monoterpenes: Menthol, thymol, carvacrol, limonene, linalool which are found in *Mentha* spp. (mint), *Thymus* spp. (thyme), and *Ocimum* spp. (basil).

1.2. Sesquiterpenes: β -caryophyllene, humulene which are found in *Rosmarinus officinalis* (rosemary), *Salvia* spp. (sage).

1.3. Phenolic Compounds in Essential Oils: Eugenol, cinnamaldehyde obtained from *Ocimum* spp., *Thymus vulgaris*.

2. Phenolic compounds

A type of chemical compound which contains a hydroxyl group (-OH) attached to an aromatic hydrocarbon ring. Phenolic compounds are found in plants, where they contribute to the colour, flavour, and resistance to pathogens. These compounds possess antioxidant properties, which protect cells from oxidative damage. Phenolic compounds can be divided into several subgroups, such as flavonoids, tannins, and lignans, each of which has different characteristics and health benefits. They are studied for their health promoting effects such as anti-inflammatory, antimicrobial, and anticancer activities. Phenolic compounds are abundant in *Lamiaceae* species and are a reason for their antioxidant and anti-inflammatory effects. Examples of phenolic compounds present in Lamiaceae members are Rosmarinic acid, caffeic acid, ferulic acid which are found in *Rosmarinus officinalis* (rosemary), *Salvia officinalis* (sage).

3. Flavonoids

Flavonoids are a group of naturally occurring plant compounds which are the member of the polyphenol class. They are characterized by a structure consisting two aromatic rings joined by a three-carbon bridge, along with various hydroxyl and other functional groups. Flavonoids are majorly distributed in the plant kingdom, primarily in fruits, vegetables, grains, and herbs. Flavonoids are known for their antioxidant properties, which help in protecting cells from oxidative stress. They also possess anti-inflammatory, antimicrobial, and anti-cancerous properties. In addition to this flavonoid also contributes to the color, flavor, and aroma in flowers, fruits, and vegetables. Certain flavonoids present in the members of *Lamiaceae* are Apigenin, luteolin, Quercetin, kaempferol which are found

in *Thymus vulgaris* (thyme), *Salvia officinalis* (sage), *Mentha* spp. (mint), *Ocimum basilicum* (basil).

4. Terpenoids

Another major class of compounds in Lamiaceae plants, with diverse therapeutic applications. Terpenoids are a large and diverse class of naturally occurring organic compounds which are derived from terpenes, made up of repeating units of isoprene (a five-carbon molecule). Terpenoids are found in a variety of plants, fungi, and some insects, and they are responsible for many of the distinctive aromas and flavours in plants. Terpenoids are known to have a wide range of biological activities which includes serving as plant defence compounds against various pathogens and animals. They also play a crucial role in growth and reproduction of the plants. Terpenoids can have various therapeutic effects, such as anti-inflammatory, antimicrobial, and anticancer properties. Major terpenoids which are found in *Lamiaceae* members are Camphor, borneol, Forskolin, Ursolic acid, oleanolic acid, *Rosmarinus officinalis* (rosemary), *Lavandula angustifolia* (lavender), *Coleus forskohlii*, *Salvia officinalis* (sage), *Ocimum sanctum* (holy basil).

5. Alkaloids

These are less common in the Lamiaceae family but are present in certain species. Alkaloids are a group of naturally occurring organic compounds that contain nitrogen atoms in a heterocyclic structure. These compounds are typically obtained from plants. They are also found in certain fungi, bacteria, and animals. Alkaloids are known for their physiological effects, which can be either beneficial or toxic, depending on the compound. Alkaloids can affect the nervous system, cardiovascular system, and other bodily functions, and are commonly used in medicine for their therapeutic properties.

6. Saponins

A class of naturally occurring compounds which are found in many plants. These are characterized by their ability to form soapy lathers when mixed with water. They are

glycosides, consisting of a sugar molecule linked to a non-sugar component, often a steroid or triterpene. These are found in species like *Ocimum sanctum*, contributing to immune-modulating effects.

7. Coumarins

A group of naturally occurring chemical compounds which are found in many plants. These are known by their fragrant, sweet aroma, often resembling the scent of freshly mowed hay or vanilla. They belong to the benzopyrone family and have a structure that contains a benzene ring fused to a pyrone ring.

Anti-plasmodial activity of Bio active compounds present in *Lamiaceae*

1. Flavonoids

Flavonoids possess antioxidant, anti-inflammatory, and enzyme-inhibitory properties, all of which contribute to their ability to inhibit the growth of the parasite. These interfere with the metabolism of parasite and can inhibit the formation of proteins and nucleic acids.

2. Terpenoids

These compounds have the ability to disrupt the integrity of cellular membranes in the parasite which affect mitochondrial function, and inhibit key enzymes involved in the parasite's metabolism.

3. Essential Oils

Essential oils derived from plants like basil and mint contain compounds like eugenol, menthol, and camphor, which possess direct toxicity against *Plasmodium* parasites. These oils can interfere with the ability of the parasite to penetrate and replicate within host cells.

4. Phenolic Acids

Rosmarinic acid, found in *Rosmarinus officinalis* (rosemary), acts as a potent antioxidant and also interferes with *Plasmodium* growth by inhibiting its metabolic pathways.

Table 1: Listing of Some phytochemicals.

Medicinal plant	Plant Part	IMPpAt ID	Phytochemical Name
<i>Ocimum tenuiflorum</i>		IMPHY002825	2-(4-Methylphenyl) propan-2-ol
<i>Ocimum tenuiflorum</i>		IMPHY003500	Citric acid
<i>Ocimum tenuiflorum</i>		IMPHY003657	Asiatic acid
<i>Ocimum tenuiflorum</i>		IMPHY003695	(-)-Germacrene A
<i>Ocimum tenuiflorum</i>		IMPHY003719	beta-Copaene
<i>Ocimum tenuiflorum</i>		IMPHY003999	d-Tartaric acid
<i>Ocimum tenuiflorum</i>		IMPHY004151	Geranyl formate
<i>Ocimum tenuiflorum</i>		IMPHY004597	Rosmarinic acid
<i>Ocimum tenuiflorum</i>		IMPHY004631	Stearic acid
<i>Ocimum tenuiflorum</i>		IMPHY004660	Luteolin
<i>Ocimum tenuiflorum</i>		IMPHY004783	Molludistin
<i>Ocimum tenuiflorum</i>		IMPHY006251	Guaiacylglycerol-beta-guaiacyl ether
<i>Ocimum tenuiflorum</i>		IMPHY006970	Decanal
<i>Ocimum tenuiflorum</i>		IMPHY007084	Vanillic acid
<i>Ocimum tenuiflorum</i>		IMPHY007182	1-Tetradecanol
<i>Ocimum tenuiflorum</i>		IMPHY007202	Nonane
<i>Ocimum tenuiflorum</i>		IMPHY007291	Heptane
<i>Ocimum tenuiflorum</i>		IMPHY007327	Palmitic acid
<i>Ocimum tenuiflorum</i>		IMPHY007366	alpha-Santalene
<i>Ocimum tenuiflorum</i>		IMPHY007528	Cadinane
<i>Ocimum tenuiflorum</i>		IMPHY009356	4-Hydroxybenzaldehyde
<i>Ocimum tenuiflorum</i>		IMPHY010083	4-Hydroxybenzoic acid

Ocimum tenuiflorum		IMPHY011588	cis-3-Hexen-1-ol
Ocimum tenuiflorum		IMPHY011659	alpha-Murolene
Ocimum tenuiflorum		IMPHY011660	(+)-alpha-Cadinene
Mentha piperita	aerial part	IMPHY000099	Myrtenol
Mentha piperita	aerial part	IMPHY000308	Hexadecane

Drug-likeness prediction of phytochemical library

Drug-likeness prediction evaluates whether a compound is suitable for use as an oral drug, based on its physicochemical and pharmacokinetic properties. For phytochemical libraries, in silico tools are widely used to streamline this process.

This analysis adhered to Lipinski's Rule of Five (RO5), which states that compounds with molecular weights below 500 Da, logP values under 5, no more than 10 hydrogen bond acceptors, and a maximum of 5 hydrogen bond donors

are likely to exhibit drug-like properties. Out of 1,458 phytochemicals, 500 met the RO5 criteria (Rawat *et al.*, 2024)^[10].

Among 500 further screened compounds, six exhibited violations of Lipinski's rules, primarily related to logP values and the number of hydrogen bond donors. Notably, L-DOPA demonstrated a violation due to an excess of hydrogen bond donors. Despite these exceptions, the majority of the 500 phytochemicals complied with Lipinski's Rule of Five, as summarized in the analysis table.

Table 2: The physicochemical properties of some screened phytochemicals by DruLiTo.

Title	MW	logp	Alogp	HBA	HBD	TPSA	AMR	nAtom	nHB
IMPHY000399	204.19	5.551	3.375	0	0	0	69.93	39	0
IMPHY003956	204.19	6.048	2.647	0	0	0	65.55	39	0
IMPHY004150	182.13	3.028	2.64	2	0	26.3	56.38	31	2
IMPHY007331	126.1	1.796	1.593	1	0	17.07	39.87	23	1
IMPHY007376	204.19	6.544	1.046	0	0	0	63.29	39	0
IMPHY007840	220.18	4.157	1.716	1	1	20.23	65.87	40	2
IMPHY010072	154.14	2.595	1.311	1	0	9.23	44.03	29	1
IMPHY011586	204.19	6.294	2.797	0	0	0	69.55	39	0
IMPHY011657	204.19	5.992	4.326	0	0	0	72.41	39	0
IMPHY011658	204.19	5.992	4.326	0	0	0	72.41	39	0
IMPHY011761	204.19	5.94	4.171	0	0	0	71.97	39	0
IMPHY011789	152.12	2.701	2.489	1	0	17.07	50.24	27	1
IMPHY011790	152.12	2.701	2.489	1	0	17.07	50.24	27	1
IMPHY012058	154.14	2.468	2.469	1	1	20.23	49.75	29	2
IMPHY012086	154.14	3.591	2.043	1	0	17.07	48.38	29	1
IMPHY012147	136.13	4.222	1.369	0	0	0	43.32	26	0
IMPHY012654	154.14	2.524	2.34	1	1	20.23	51.3	29	2
IMPHY012667	220.18	4.607	1.914	1	0	12.53	64.19	40	1
IMPHY014831	204.19	6.044	3.229	0	0	0	67.69	39	0
IMPHY014923	154.14	2.524	2.34	1	1	20.23	51.3	29	2
IMPHY014988	136.13	3.729	2.142	0	0	0	46.02	26	0
IMPHY015123	180	6.499	1.763	0	0	0	64.85	15	0

Mechanism of Anti plasmodial action

1. By inhibiting the erythrocytic cycle

The erythrocytic stage of the *Plasmodium* lifecycle is when the parasite infects the red blood cells of the host, leading to the symptoms of malaria. Several mechanisms of action from Lamiaceae-derived compounds inhibit parasite growth during this stage are as follows.

- **Disruption of Protein Synthesis:** Flavonoids such as luteolin and apigenin have been reported to inhibit the protein synthesis by interfering with the functions of ribosome's and enzymes within the parasite. This decreases the ability of the parasite to grow and reproduce.
- **Inhibiting the DNA and RNA Synthesis:** Many flavonoids also alter synthesis of the nucleic acids by inhibiting enzymes like DNA polymerase and topoisomerase. This prohibits the replication of the parasite's genetic material.
- **Impairment of Mitochondrial Function:** Terpenoids like thymol and carvacrol inhibits function of mitochondria in *Plasmodium* parasites. The parasite

depends on the mitochondria for the production of energy. This leads to death of cells due to energy loss. These compounds interfere with oxidative phosphorylation which in turn causes mitochondrial dysfunction and promotes apoptosis in the parasite.

- **Inhibition of Degradation of Haemoglobin:** *Plasmodium* parasites depend on the haemoglobin in red blood cells for its nutrition. Some compounds from Lamiaceae can inhibit the enzymes that degrades haemoglobin (e.g. *plasmepsin*), which is necessary for the nutrition of the plant. This inhibits the ability of the parasite to digest haemoglobin and lowers its ability to survive within red blood cells.

2. Effect on the gametocytic stage

Gametocytes are the reproductive or the sexual form of the *Plasmodium* parasite. This is responsible for transmission of parasite from humans to mosquitoes. Inhibition of the gametocyte stage is crucial in lowering malarial transmission. Various compounds from Lamiaceae plants, such as those present in *Ocimum* (basil) and *Mentha* (mint), have been shown to inhibit maturation of the gametocyte.

By disrupting the growth and development of gametocytes, these compounds reduce the chances of transmission to mosquitoes, therefore reducing the spread of malaria.

3. Anti-oxidant activity

Malarial infection induces the oxidative stress in both the parasite and the host. This stress is because of the metabolism of the parasite and the immune response of the host. Compounds like rosmarinic acid and other phenolic acids of the *Lamiaceae* plants have high antioxidant properties. They scavenge free radicals and reactive oxygen species (ROS), which in turn reduces the oxidative damage to the host's red blood cells and other tissues. By decreasing the oxidative damage caused by ROS the compounds help in preventing complications associated with malaria, such as anaemia, liver damage, and kidney failure (Ramos da Silva *et al.*, 2021)^[9].

4. Anti-inflammatory effects

Malaria triggers various inflammatory responses, especially in the liver and spleen, as a part of the immune defensive system of the host. However high inflammation can lead to the damage of the organs (Uritu *et al.*, 2018)^[13]. Some *Lamiaceae* plant extracts have anti-inflammatory effects that help in mitigating inflammatory responses:

- **Cytokine modulation:** Compounds, like those found in *Ocimum* and *Salvia* species, known to reduce the production of pro-inflammatory cytokines like TNF- α , IL-6, and IL-1 β , which are typically elevated in malarial infections. This helps in minimising tissue damage and improving the overall immune response.
- **Inhibition of NF- κ B signalling:** Some compounds can inhibit the NF- κ B pathway, which is mainly involved in activating the inflammatory cascade. By inhibiting this pathway, the compounds help in controlling the heavy inflammation caused by *Plasmodium* infection.

5. Immune system modulation

Other than the direct parasitocidal activities, various *Lamiaceae* derived compounds can enhance the activity of the host's immune system:

- **Activation of T-cell and macrophage responses:** Some essential oils and plant extracts proliferates the activity of immune cells, including T-cells and macrophages. This enhanced immune response helps the body to fight against the parasite more effectively.
- **Regulation of immune homeostasis:** By modulating the immune response, *Lamiaceae* plants help the body of the host to maintain immune homeostasis, thus reducing the risk of tissue damage (Nassar *et al.*, n.d.)^[7].

Conclusion

The *Lamiaceae* family offers a promising phytochemical source with significant anti-plasmodial potential. Species from this family, such as *Ocimum*, *Thymus*, *Rosmarinus*, and *Salvia*, have been used in traditional medicine because of their antimicrobial, anti-inflammatory, and anti-malarial activities. Phytochemical like terpenoids, flavonoids, polyphenols, and essential oils have a unique mechanism of action that interfere with the growth and development of the *Plasmodium falciparum*. These compounds have the effects

such as membrane disruption, oxidative stress induction, and inhibition of critical enzymes which are involved in parasitic metabolism.

Despite the promising *in vitro* and some *in vivo* findings the challenges remain in making these compounds into practical anti-malarial therapies. Concerns like difference in phytochemical composition, bioavailability and limited clinical data necessitate further studies and research. The potential for synergistic effects in which plant-based compounds increases the activity of existing anti-malarial drugs, is particularly exciting. Therefore, there is a need for comprehensive studies which focuses on the isolation, characterization, and optimization of these compounds in anti-malarial therapies.

The continued exploration of *Lamiaceae* species and their phytochemical diversity represents a notable direction in the discovery of novel anti-malarial agents, particularly in an era marked by increasing drug resistance. This work bridges the gap between traditional knowledge and modern drug discovery and opening the new avenues for the development of effective and herbal therapies in the anti-malarial programmes.

Summary

Malaria is a major health ailment, especially in regions where *Plasmodium falciparum* causes the majority of malaria-related fatalities. The increasing resistance to various current anti-malarial drugs highlights the need for new and effective treatments. The *Lamiaceae* family is known for its rich ethno-medicinal history, comprises of various bioactive compounds having potential anti-malarial properties. This paper reviews the phytochemistry of *Lamiaceae* family and their pharmacological activities against *P. falciparum*. Compounds like rosmarinic acid, thymol, and essential oils from species like *Rosmarinus officinalis*, *Thymus vulgaris*, and *Ocimum sanctum* have shown strong anti-plasmodial effects through various mechanisms.

The findings suggest that compounds from the *Lamiaceae* family could be important for the development of novel anti-malarial drugs. However, more research and clinical trials are needed to validate the efficacy and safety of these compounds in humans. As we move ahead, the addition of *Lamiaceae* based therapies into malarial treatment regimens could provide a better and much needed alternative to combat *Plasmodium falciparum* resistance.

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