

Publications

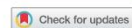
Research publications

- [1] Singha, J., Dutta, N., and Saikia, J.P. A novel method to produce maximum ajoene and vinyl dithiin during garlic mustard oil macerate preparation. *Journal of Sulfur Chemistry*: 1-13, 2025.
- [2] Singha, J., Dutta, N., and Saikia, J.P. A novel volatile staphyloxanthin biosynthesis inhibitor against *Staphylococcus aureus*. *Microbial Pathogenesis*: 107489, 2025.
- [3] Singha, J., and Saikia, J.P. Optimisation of garlic mustard oil macerate with respect to its antifungal activity against *Candida albicans* MTCC 183 and in-silico molecular docking of the volatile compounds with N-myristoyltransferase. *Natural Product Research*: 1-8, 2024.
- [4] Roy, B., Singha, J., Goswami, S., and Saikia, J.P. Spectral Change of Curcumin in DMSO–NaOH Solution after Exposure to Air. *Russian Journal of General Chemistry*, 93(10): 2672-2676, 2023.

List of presentations in conferences/ workshops

- 1. Presented Poster at the International Conference on Environment and sustainable development (ICESD 2022) organized by Biotech KISAN Hub, NEHU, Tura Campus, funded by DBT, New Delhi, India on November 24-25, 2022.
- 2. Presented poster in the National Seminar on “Advances in Basic and Translational Research in Biology (ABTRiB)” organized by the Department of Molecular Biology and Biotechnology, Tezpur University from 11-12 March 2022.
- 3. Presented Poster in the national level seminar titled “Biology is fascinating” organized by the Department of Molecular Biology and Biotechnology in association with inSCIgnis’22 on 1st March 2022.

RAPID COMMUNICATION

**A novel method to produce maximum ajoene and vinyl dithiin during garlic mustard oil macerate preparation**Joydeep Singha^a, Nipu Dutta^b and Jyoti Prasad Saikia^a^aDepartment of Molecular Biology and Biotechnology, Tezpur University, Tezpur, Assam, India; ^bDepartment of Chemical Sciences, Tezpur University, Tezpur, Assam, India**ABSTRACT**

Garlic mustard oil macerate is a traditional medicine used as a nasal decongestant by the people of northeast India. In this study, a unique preparation technique that maximized the yield of organosulfur compounds in GMM was developed at the lowest preparation temperature and time duration compared to existing preparation methods. Liquid chromatography-mass spectrometry (LCMS), central composite design (CCD) and high-performance liquid chromatography (HPLC) were used for compound identification, experimental design, and quantification of the organosulfur compounds (OSCs), respectively. Through LCMS analysis, ajoene and 2-vinyl-4H-1,3-dithiin were detected as the major OSCs. CCD analysis suggested 17 experiments for HPLC analysis, after which the quantity of mustard oil and heating temperature were found to be the significant parameters for optimum OSCs formation. Based on this, the optimized conditions to maximize the yield of ajoene ((garlic: oil (1:2.00), 55.00°C, 4 $\frac{1}{2}$ h)) and 2-vinyl-4H-1,3-dithiin ((garlic: oil (1:2.20), 77.51°C, 2 $\frac{1}{2}$ h)) were achieved.

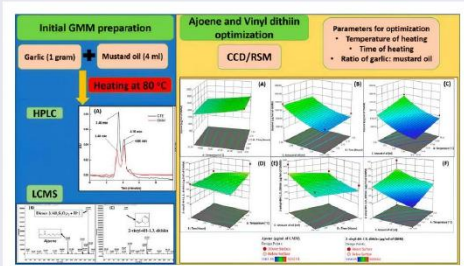
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A novel volatile staphyloxanthin biosynthesis inhibitor against *Staphylococcus aureus*

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ABSTRACT

In the present research, volatile organic compounds (VOCs) of garlic/mustard oil macerate (GMM) (garlic clove and mustard oil in the ratio of 1:4, heated at 80 °C for 4 h) were found to enhance the antibacterial activity of antibiotics (gentamycin, 41.17 %; kanamycin, 38.89 %, and streptomycin, 43.75 %) against *S. aureus*. The mechanism behind the enhancement of *S. aureus*'s sensitivity to antibiotics may be due to the reduction of antibiotic resistance. On evaluating one of the well-known antibiotic resistance mechanisms of *S. aureus*, the ability to produce staphyloxanthin, it has been observed that the VOCs of GMM alone can decrease staphyloxanthin (44.23 ± 0.14 %) production. This decrease in staphyloxanthin production thereby increasing sensitivity to antibiotics, may be assigned to the compounds present in the VOCs of GMM. The major VOCs present in the GMM were identified as allicin, ajoene, vinyl dithiin, allyl isothiocyanate (AITC) and sinigrin. The order of binding of VOCs with dehydroxysqualene synthase (crtM) protein, which is important in staphyloxanthin production of *S. aureus*, was found to be sinigrin > ajoene > allicin > dithiin > AITC. Further, a decrease in staphyloxanthin production was found to increase the membrane fluidity of *S. aureus* as validated by Fourier-transformed infrared spectroscopy and scanning electron microscopy and this may allow antibiotics to enter inside the bacterial cell more rapidly. Thus, our research indicates that the VOCs in GMM may serve as a potential adjuvant when treating *S. aureus* infection.

1. Introduction

About 30 % of the world's population is colonised by a significant human pathogen *S. aureus*, which is known to cause infection of skin, nasopharyngeal mucosal linings and lungs leading to pneumonia [1–4]. In the case of nasopharyngeal and lung infection cases, a drug which can be delivered through inhalation is preferred compared to oral or intra-venous drugs [5]. A drug which can be delivered through inhalation can give better results with low drug doses in respiratory infections and therefore impart low adverse effects in non-targeted tissues [6,7]. Staphyloxanthin (an orange carotenoid pigment) of *S. aureus* provides three-way protection against: antibiotics (by enhancing membrane integrity), host neutrophil-based attack and oxidative damage to the bacterial cells [8,9]. Non-volatile compounds (25°C) such as phosphonoacetamides, rhodomyrtone, and eugenyl acetate are reported to inhibit the synthesis of staphyloxanthin in *S. aureus* and subsequently increase antibiotic susceptibility [10–12]. Drug delivery using the inhalation route is not possible using the above-mentioned compounds

in the treatment of *S. aureus* infection in organs like the nasopharynx and lungs. Therefore, VOCs having the capacity to decrease staphyloxanthin production in *S. aureus* will be of great interest in controlling the bacteria in respiratory diseases. The adverse effect during the use of such VOCs may be further less if the compound is from edible spices and oils [13]. In northeast India, traditionally garlic cloves are crushed and heated in boiled mustard oil for a few minutes and the oil is used for treating the symptoms related to the common cold.

Garlic (*A. sativum*) when crushed, alliinase enzyme comes in contact and converts alliin to allicin and is reported to remain stable in polar solvents like alcohol and water. In non-polar solvents and vegetable oils, allicin gets converted to ajoene and vinyl dithiin [14–16] (Fig. 1). Mustard (*B. nigra*) seed oil is a vegetable oil which is used for cooking in India. Mustard oil which is used in the macerate is reported to have sinigrin and allyl isothiocyanate [17]. The compounds allicin, ajoene, dithiin, sinigrin and allyl isothiocyanate are known for their antibacterial, antifungal, and anti-inflammatory properties [18–20]. As these VOCs are volatile in nature, therefore, they can be delivered to the

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Optimisation of garlic mustard oil macerate with respect to its antifungal activity against *Candida albicans* MTCC 183 and *in-silico* molecular docking of the volatile compounds with N-myristoyltransferase

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ABSTRACT

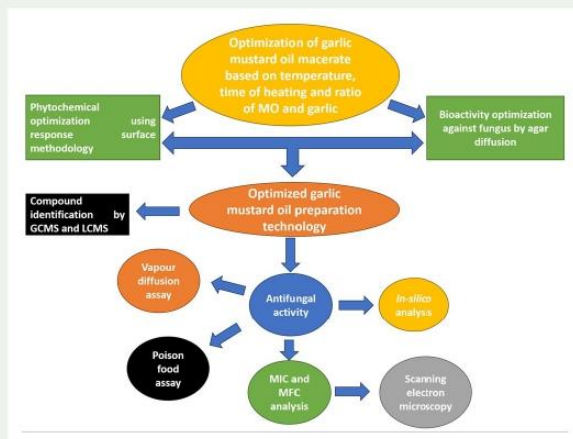
Candida albicans infections are widespread in people and cause cutaneous and systemic infections. Optimisation of garlic mustard oil macerate (GMM) based on antifungal activity against *C. albicans* was done using agar diffusion method. Upon vapour diffusion assay, the volatile organic compounds of both GMM and MO were found to eradicate *C. albicans*. During agar diffusion, MO did not inhibit fungal growth, while undiluted GMM oil demonstrated a 26.33 ± 0.33 mm zone of inhibition. The minimum inhibitory concentration and minimum fungicidal concentration against *C. albicans* were 12.5%, v/v of GMM oil and 25%, v/v of GMM oil, respectively. Scanning electron microscopy analysis showed cell membrane disintegration of fungal cells by 50%, v/v of GMM oil, and MO caused no cell wall damage. *In-silico* analysis revealed strong binding affinity of sinigrin, ajoene, dithiin with N-myristoyltransferase. In conclusion, the optimised GMM preparation can be a potential antifungal agent against tropical *C. albicans* infections.

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This article has been corrected with minor changes. These changes do not impact the academic content of the article.

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Spectral Change of Curcumin in DMSO–NaOH Solution after Exposure to Air

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Abstract—Curcumin (CurH_3) forms a blue derivative (CurH^{2-}) when it combines with superoxide radicals. The blue coloring is caused by the proton loss of curcumin to the superoxide radicals. In DMSO, in the presence of excess NaOH and dissolved oxygen, superoxide radicals are produced by consuming the hydroxyl ion which causes the deprotonation of curcumin (Cur^{3-}) and gives the corresponding orange color. The production of superoxide radicals increased as it was more exposed to air (maybe oxygen). As a result, the pH drops, and the orange derivative is protonated by one H^+ ion, producing the corresponding blue color derivative (CurH^{2-}). The conversion of the orange derivative to the blue derivative may suggest the presence of oxygen in the surrounding atmosphere, allowing the feasibility of a novel oxygen sensor. The physicochemical characteristics and stability of this blue-colored curcumin derivative are investigated. The distinct color shifts of curcumin upon the addition of different volumes of NaOH were also investigated. The UV-Vis and FTIR analyses were used to study the stability of the blue curcumin derivative.

Keywords: curcumin, DMSO, air sensor, blue-derivative, orange-derivative

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INTRODUCTION

Curcumin [1,7-bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione] is one of the bioactive compounds found in the widely used condiment *Curcuma longa* [1]. It is an unstable compound and degrades into different compounds under different physiological conditions [2]. Curcumin combines with superoxide to produce a blue color derivative [3]. Qiao and his colleagues discovered that DMSO generates superoxide during its interaction with NaOH (Sodium hydroxide) [4]. According to the research by Tsaplev et al., curcumin has three hydrogen-donating groups (CurH_3), and deprotonation accordingly rises with alkalinity, going from one proton loss (CurH_2) to two proton losses (CurH^{2-}) to three proton losses (Cur^{3-}) [5]. The color likewise shifts in relation to that, going from yellow (CurH_3) to green (CurH_2) and from blue (CurH^{2-}) to orange (Cur^{3-}), respectively [5]. The change in color forms of curcumin are mainly due to its deprotonated forms [5]. Curcumin is resistant to auto oxidation in DMSO [5].

Here in the present investigation, we have examined the physicochemical properties as well the stability of the various colored derivatives of curcumin in DMSO. Curcumin solution in DMSO gives rise to blue color derivative when a particular alkali condition is maintained. The reaction escalates in the presence of excess oxygen [3]. The presence of oxygen can turn the curcumin solution blue which might be used as a potential sensor of oxygen. The concentration of curcumin and amount of NaOH to reproduce the blue form of curcumin only in the presence of oxygen/air was optimized. The UV-visible spectrum of the blue colored derivative of curcumin was also seen.

RESULT AND DISCUSSION

Curcumin degradation in alkaline condition. Curcumin solution in DMSO gives the maximum absorbance λ_{max} at 432 nm (Fig. 1a, DC). In addition of 5 μL NaOH (0.1 M), curcumin readily changes the color into a blue color derivative and shifts the absorbance λ_{max} to 614 nm (Fig. 1a, DCN5). However, on the addition of 40 μL of NaOH (0.1 M) the yellow color of curcumin