RESEARCH ARTICLE

Preformulation: Development of Solubility, UV and FTIR estimation of Phytobioactive Antifungal Compounds Allicin

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ABSTRACT
When developing new dosage forms, compatibility tests between excipients and active pharmaceutical ingredients (API) are essential for preformulation. An API’s chemical composition, stability, and bioavailability, as well as its safety and therapeutic efficacy, can all be affected by possible physical and chemical interactions with its excipients. Solid dosage forms are typically less stable than the constituents of their API. Even though testing for API-excipient compatibility is important, there isn’t a universally accepted method for assessing these kinds of interactions. The oily, yellow material that gives garlic its distinct smell is called allicin. It’s a thioester of sulfenic acid. Another name for it is allyl thiosulfinate. Its interaction with proteins containing thiols and antioxidant activity are what give it its biological activity. In the present work various preformulation parameters of allicin was estimated and reported.

Keywords: Allicin, Preformulation, Phytobioactive Compounds


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Conflict of interest: None

INTRODUCTION
The stability, chemical structure, and bioavailability of the API are all affected by interactions with the excipients. Treatment safety and efficacy are reduced by these alterations. Generally speaking, separate API is more stable than solid dosage formulations. There is still disagreement on the test to be utilized, despite the fact that it is acknowledged that API excipient compatibility testing must always be carried out when developing new dosage forms. The most common signs of API deterioration include changes in color, taste, odor, polymorphic form, or crystallization (pharmaceutical incompatibility). The degradation of the API is brought about by chemical interactions with the excipient. Allicin is an organosulfur compound found in garlic. The smell of fresh garlic is caused by the enzyme alliinase, which changes alliin into allicin when fresh garlic is chopped or crushed. Allicin is a very unstable molecule that breaks down quickly into many distinct chemicals that include sulfur, including diallyl disulfide. As of 2016, it remained unknown whether allicin was safe and effective for treating infections in humans, despite studies on the herb’s potential to treat a number of drug-resistant bacterial, viral, and fungal illnesses in-vitro.

MATERIAL AND METHODS
For this study, the anti-fungal phytobioactive chemicals allicin (diallyl thiosulfinate) was chosen. The pharmacy facility in Indore provided the sample as a gift.

Preformulation Studies
To guarantee the development of a stable, therapeutically effective, and safe dosage form, pre-formulation studies are required. This phase of development involves the physical chemist describing the physical and chemical characteristics of the drug substance and how it interacts with various stimulant constituents.

Organoleptic Properties
The drug’s visual appearance was used to record its organoleptic qualities.

Solubility Studies
Based on the drug’s solubility data in various fluids, the dissolution and diffusion fluids for drug release and pharmaceutical research, respectively, were selected. By gradually adding 100 mg of the drug sample as a c-solvent to various fluids, the solubility of the sample was ascertained. A variety of solvents, including distilled water, methanol, ethanol, chloroform, 0.1 N HCl, PBS, and DMSO, were used to assess the solubility of allicin.

Determination of Partition Coefficient
Bach’s method was used to determine the partition coefficients of allicin in phospholipids, octanol, and hexadecane. In summary, 0.5 M Na phosphate buffer (pH 6.5) containing 6.5 mM allicin was added to either solvent (10 μL) or dry lipid (10 mg). The homogenization of the allicin/lipid dispersions
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was achieved using vortexing and shaking for 1-hour at 37°C (for phospholipid) or room temperature (for solvents). HPLC was used to calculate the amount of allicin that was still present in the water phase. The following is the definition of the partition coefficient (Kp) of allicin (solvent/water or lipid/water): (1) \( K_p = \text{lipid} \times \frac{[\text{allicin}]_{\text{lipid}}}{V_{\text{lipid}}} \times \frac{[\text{allicin}]_{\text{water}}}{V_{\text{water}}} \), where \( V_{\text{water}} \) and \( V_{\text{lipid}} \) are the volumes of the lipid or solvent phase and the water phase, respectively, and \( [\text{allicin}]_{\text{lipid}} = [\text{allicin}]_{\text{total}} - [\text{allicin}]_{\text{water}} \).

**Determination of \( \lambda_{\text{max}} \)**

Using a UV-visible spectrophotometer (Model-1800, Shimadzu, Japan), the UV spectrum of medicines was recorded. A stock solution was prepared by dissolving 100 mg of the medication in 100 mL of methanol. 10 mL of this was extracted, and 100 mL of methanol was used to dilute it once more. The sample containing 10 µg/mL was scanned at 200–400 wavelengths using a UV–visible spectrophotometer.

**IR Spectroscopy of Drug**

The pure drug sample was subjected to infrared spectroscopy in order to identify the drug. The ATR sampling technique was employed in the FTIR experiments, which were conducted using an FTIR spectrophotometer (Model-8400 S, Shimadzu, Japan).

**RESULTS AND DISCUSSION**

To ensure the legitimacy of the sample medicine and determine certain parameters for the development of the simulator, a preliminary investigation was conducted. Allicin’s preliminary investigations, which included the drug’s solubility profile, partition coefficient, UV absorption maxima, and drug sample identification using FTIR spectroscopy, were completed and the results were given. The findings of determining the organoleptic quality of the phytobioactive components allicin are displayed in Table 1. Drug sample’s solubility, or the presence of phytobioactive substances To ascertain the type of solvent in which the medication is soluble, allicin was used. The drug sample’s solubility was assessed for the purpose of selecting a dispersing and diffusing medium in several solvents at room temperature. The volume of solvent needed to dissolve the medication was noted in Table 2. Allicin, one of the phytobioactive chemicals in the medication sample, had its partition coefficient value calculated and noted. Table 3 presents the findings. Through UV scanning, phytoactive chemicals, such as allicin (diallyl thiosulfinate), were detected (Model-1800, Shimadzu, Japan). The highest absorbance of allicin in methanol was ascertained. With a concentration of 10µg/mL in methanol, the standard stock solution of allicin was scanned in a UV-visible spectrometer (Model-1800, Shimadzu, Japan) between 200 and 400 nm. At 240 nm, the maximum absorption (\( \lambda_{\text{max}} \)) was measured. (Figure 1). A FTIR spectroscopic examination was done to evaluate the medication. The resulting FTIR spectrum was contrasted with the pharmacopoeia’s spectrum. Fingerprint regions and diagnostic peaks were determined to be identical. These peaks in the features are helpful in identifying the substance (Figure 2).

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<td>Phospholipid</td>
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**Table 1: Organoleptic properties of allicin**

**Table 2: Solubility of allicin**

**Table 3: Determination of partition coefficient of allicin**

![Figure 1: UV spectrum of allicin in methanol](image1)

![Figure 2: FTIR spectra of allicin](image2)
CONCLUSION
From the results obtained it was concluded that all the preformulation parameters were evaluated and reported. Also solubility parameters, UV spectral studies and FTIR were determined so as to ascertain the purity of the drug.

REFERENCES