RESEARCH ARTICLE

Preformulation Studies, UV Spectral and FTIR Analysis of Allicin

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Received: 25th March, 2024; Revised: 08th July, 2024; Accepted: 04th August, 2024; Available Online: 31st August, 2024

ABSTRACT

Allicin is chemically known as 3-prop-2-enylsulfinylsulfanylprop-1-ene. It is a volatile compound and poorly soluble in water. With a molecular weight is 162.3 g/mol, it is also known as diallyldisulfi-S-oxide, S-allyl-prop-2-ene-1-sulfinothionate and diallyl thiosulfinate. In the present study pre-formulation studies, UV spectral and fourier-transform infrared (FTIR) analysis of allicin was reported.

Keywords: Allicin, Preformulation, UV, FTIR, Analysis.

International Journal of Pharmaceutical Quality Assurance (2024); DOI: 10.25258/ijpqa.15.3.11

How to cite this article: Chauhan S, Dwivedi A. Preformulation Studies, UV Spectral and FTIR Analysis of Allicin. International Journal of Pharmaceutical Quality Assurance. 2024;15(3):1168-1170.

Source of support: Nil.

Conflict of interest: None

INTRODUCTION

Physicochemical characteristics of any drug are essential to knowing the growth of final products and are very crucial in the drug development process. Preformulation investigation parameters help in drug development and stability of final preparation and help in the determination of the shelf and half life of all the marketed products.[1] Allicin (Figure 1) is a sulfur-containing compound commonly present in garlic as a defense molecule. Along with other useful pharmacological activities, allicin was found to be a potent antifungal agent against *Candida* infections.[2] A group of researchers used pure allicin derived from garlic and confirmed its activity against dermatophytes.[3] Another research demonstrated the antifungal effects of allicin against phytopathogenic fungi, such as *Fusarium oxysporum, Phytophthora casici, Verticilium dahlia* and *Botrytis cinerea*.[4] Allicin was found to be responsible for the accumulation of reactive oxygen species and disturbing biosynthesis of cell walls of fungal species, thus showing a cidal effect.[4,5]

METHODOLOGY

Preformulation Studies

Preformulation studies are an important component of drug or therapeutics development. It ensures the safety, effectiveness and stability of the developing formulation. In pre-formulation studies, physical pharmacists characterize the developing therapeutics based on physicochemical properties, along with the interaction of drug with the excipients environment.[6-11]

Identification of Drug

Physical appearance

The physical appearance of the API was visualized by taking guidance from IP.

UV absorption

It was done using UV-visible spectrophotometer Model 1800. 100 mg of drug dissolved in 100 ml of methanol and from it various dilutions were made and 10 µg/mL sample was scanned at 200 to 400 nm

FTIR spectroscopy

FTIR was done using FTIR spectrophotometer (Model – 8400 S, Shimadzu, Japan), by using ATR sampling technique.

Determination of solubility

Solubilities of the drug in various solvents were determined by simply adding 100mg of sample drug into various solvents with increasing the solvent volume until the drug was fully dissolved. This allowed an understanding the properties of different co-solvents for the solubility of drug. The solubility of allicin were investigated in different solvents, including ethanol, methanol, water, 0.1N HCl, PBS and DMSO.

Determination of partition coefficient

N-octanol is a phase of non-aqueous and a phosphate buffer solution of pH 74 is taken. To determine the partition coefficient of a drug, equal volumes of both phases were taken and 10 mg drug was placed in the solvent system and was remained untouched for 30 minutes. A separating funnel was used for

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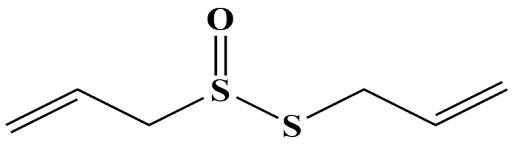

3-prop-2-enylsulfinylsulfanylprop-1-ene

Figure 1: Molecular structure of allicin

the process. The aqueous phase was than separated using Whatmann filter paper by filtration technique. Spectrometric analysis was performed for the determination of the amount of drug present in each phase. The wavelength chosen for the study was 267 nm. The phosphate buffer solution was chosen as a blank sample.

Preparation of standard curve

For obtaining a stock solution of 1000 µg/mL, 50 mg of accurately weighed allicin was dissolved in 25 mL of DMSO and then filled to brim with phosphate buffer pH 7.5 in 50 mL volumetric flask. For obtaining 100 µg/mL solutions, 5 ml of stock solution was pipetted out and subsequently diluted with buffer to make 50 ml. For getting a concentration range of 2 to 10 **µg**/mL, dilutions of 2, 4, 6, 8, 10 & 12 mL were taken out and diluted to 10 mL with buffer. 5 ml was taken from the 100 µg/mL solution and diluted to 50 mL to get 10 µg/mL solution. Using a UV-vis spectrophotometer, the absorbances of the solutions were determined at 240 nm. Concentration versus absorbance was put on a graph.

RESULTS AND DISCUSSION

Preformulation studies are an important component of the drug or therapeutics development. It ensures safety, effectiveness and stability of the developing formulation. In pre-formulation studies, physical pharmacists characterize the developing therapeutics based on physical and chemical properties, along with the interaction of drug with the excipients environment. The result obtains from the characterization of allicin are reported in Table 1. Powder of Allicin was reported as colorless, having a characteristic odor and pungent in taste.

A standard stock solution of allicin with a concentration of 10 µg/mL prepared in methanol was scanned by employing a UV-vis spectrophotometer at 200 and 400 nm wavelengths. Maximum absorption was recorded at a wavelength of 240 nm, as shown in Figure 2.

FTIR was done and spectra were recorded. An IR spectrum (KBr) showed characteristic bands of allicin at 3423, 1655, and 1590 cm^{-1} (Figure 3).

Solubility studies were conducted for the determination of solvents that can facilitate the dissolution of API.[12] The

Table 1: Allicin: Organoleptic properties

Test	*Observations*
Colour	Colorless
Odor	Characteristics
Taste	Pungent

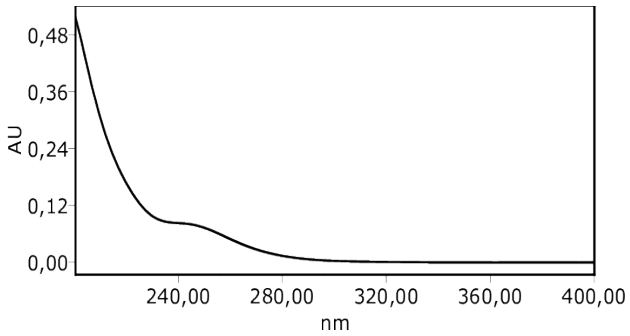

Figure 2: UV spectrum of allicin in methanol

study also evaluated the nature of solvent that can dissolve the API. The volume of solvents required for dissolving allicin completely is presented in Table 2. The partition coefficient was assessed and recorded and was found to be 10.92. At 240 nm, the absorbance was measured in relation to a blank. Table 3 contains the data for the standard curve of allicin, and Figure 4 highlights the standard curve.

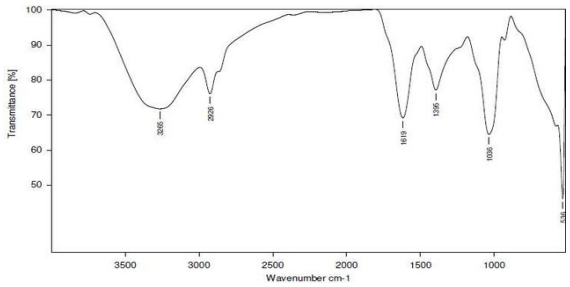

Figure 3: FTIR spectra of allicin

Table 2: Solubility profile of allicin

Solvents	*Solubility*
MeOH	Soluble
EtOH	Soluble
$CHCl_3$	Soluble
Ether	Soluble
DW	Sparingly soluble
PBS	Soluble
DMSO	soluble

Table 3: Absorbance of different dilutions of allicin

Conc	*Abs*
2	0
4	0.212
5	0.329
6	0.486
8	0.592
10	0.718
12	0.882

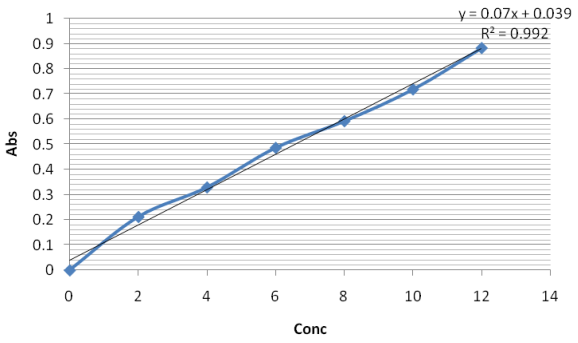

Figure 4: Calibration curve of allicin

CONCLUSION

The pre-formulation studies of allicin were investigated and it was concluded that the drug is soluble in various solvents. The maximum wavelength was recorded to be 240 nm.

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