

# Study on the Molecular Mechanism of the Effect of Surfactants on the Fragrance Retention of Spices

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**Abstract:** In this study, the effects of different concentrations of sodium dodecyl sulfate (SDS) on the fragrance retention of vanilla essential oil were discussed by olfactory sensory evaluation and infrared spectrum analysis. The results showed that the fragrance retention effect of vanilla essential oil decreased with time without SDS. 0.1 mM SDS slightly improved the fragrance retention ability, which was attributed to the enhancement of molecular dispersion; At the concentration of 0.5 mM to 1 mM SDS, the fragrance retention time was significantly prolonged, because SDS and vanilla essential oil formed a good balance; However, at the high concentration of 5 mM, although there is synergy, the fragrance retention performance is reduced due to excessive wrapping. Infrared spectrum analysis shows that low concentration SDS enhances stability through hydrogen bonding, while high concentration SDS enhances van der Waals force and hinders molecular release. The research provides new insights and theoretical guidance for understanding the role of surfactants in spices and their industrial application.

**Keywords:** Fragrance Retention; Spices; Molecular Mechanism; Surfactants.

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## 1. Introduction

Spice, as an important element to improve the quality of life, has been widely used in food, cosmetics, household items and other fields. Its unique aroma can not only bring people a pleasant sensory experience, but also be an important factor to attract consumers. However, the fragrance retention performance of spices during use, that is, the durability and stability of their fragrance, often becomes the key index to measure the quality of spices. With the improvement of consumers' requirements for product quality, how to improve the fragrance retention performance of spices has become a hot topic of current research.

Surfactants, as a kind of compounds with special structures and properties, can directionally arrange on the interface and reduce the interfacial tension, thus changing the physical and chemical properties of the system [1-2]. In the field of spices, surfactants are also widely used. They can not only improve the dispersion and stability of spices in aqueous or oily media, but also have a significant impact on the fragrance retention of spices. However, there is still a lack of in-depth and systematic research on the molecular mechanism of how surfactants specifically affect the fragrance retention properties of spices.

Therefore, the purpose of this study is to explore the influence of surfactants on the fragrance retention of spices and its molecular mechanism through experiments and theoretical analysis. By revealing the interaction between them, it can provide theoretical support and practical guidance for the formulation optimization and product innovation of perfume industry, and then promote the development of perfume technology and meet the market demand for high-quality spices.

## 2. Experimental Part

### 2.1. Experimental raw materials

Vanilla essential oil and sodium dodecyl sulfate (SDS) were selected as the research objects [3-4]. Vanilla essential oil was selected because of its unique aroma and wide

application in perfume industry. The main components of vanilla essential oil include vanillone, vanillinol and so on. These compounds not only give vanilla a unique fragrance, but also have certain stability, which is suitable for studying its fragrance retention performance under the action of different surfactants. As a typical anionic surfactant, SDS is widely used in cosmetics, detergents and other industries. The molecular structure of SDS enables it to form micelles in aqueous solution, thus changing the solubility and stability of perfume molecules, and it is an ideal choice to study the influence of surfactants on perfume retention performance.

### 2.2. Experimental design

In the experimental design, the control group used vanilla essential oil samples without SDS to evaluate its fragrance retention performance under natural conditions, while the experimental group added different concentrations of SDS (0.1 mM, 0.5 mM, 1 mM and 5 mM) to vanilla essential oil to explore the specific effects of different concentrations of SDS on the fragrance retention performance of vanilla essential oil.

Adding SDS into vanilla essential oil according to a predetermined concentration gradient, and ensuring full and uniform mixing, so as to prepare vanilla essential oil samples with different SDS concentrations; The fragrance retention performance of the samples in the control group and each experimental group was regularly detected and recorded by the olfactory evaluation method [5]; Finally, the data of fragrance retention performance of vanilla essential oil under different SDS concentrations were compared and analyzed to clarify the specific influence law of SDS concentration on its fragrance retention performance.

### 2.3. Molecular mechanism analysis

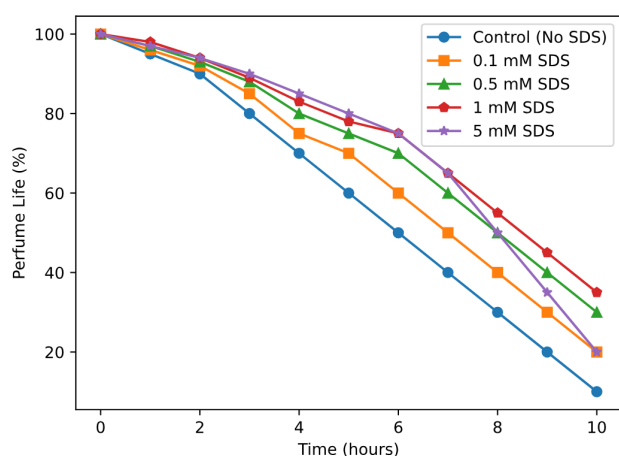
Infrared spectroscopy is a commonly used spectroscopic technique, which can provide information about the internal vibration and rotation modes of molecules, thus reflecting the molecular structure and their interactions. In this study, infrared spectroscopy was used to explore the interaction between vanilla essential oil molecules and SDS molecules.

Use infrared spectrometer to measure each sample and record spectral data. Special attention is paid to the position and intensity changes of characteristic peaks related to SDS and molecular functional groups of vanilla essential oil. By comparing the spectral data of SDS samples with different concentrations, the possible interactions between SDS and vanilla essential oil molecules, such as hydrogen bonds and van der Waals forces, and their effects on the fragrance retention of vanilla essential oil were analyzed.

### 3. Experimental Result

#### 3.1. Effect of surfactants on fragrance retention of spices

The fragrance retention performance of each group of samples was regularly detected and recorded by olfactory evaluation. The experimental results showed that the fragrance retention performance of vanilla essential oil in the control group gradually weakened with time (Figure 1). In the control group, in the absence of SDS, the fragrance retention effect of vanilla essential oil gradually decreased with time, showing its natural volatilization characteristics; However, at the concentration of 0.1 mM SDS, although the fragrance retention ability was only slightly improved, it has been shown that low concentration SDS is helpful to enhance the dispersion of vanilla essential oil molecules, thus promoting fragrance retention; When the concentration of SDS is increased to 0.5 mM to 1 mM, the effect of prolonging the fragrance retention time of vanilla essential oil is significantly enhanced, because there is a good balance between SDS and vanilla essential oil molecules, and the formed micelle can not only protect the vanilla essential oil molecules from rapid volatilization, but also ensure their moderate emission to achieve a more lasting fragrance retention effect; However, at the high concentration of 5 mM, although SDS can still play a certain synergistic role, the excessive micelle formation leads to the excessive encapsulation of vanilla essential oil molecules, which hinders its normal volatilization, making the fragrance retention performance slightly lower than the previous two concentration ranges.



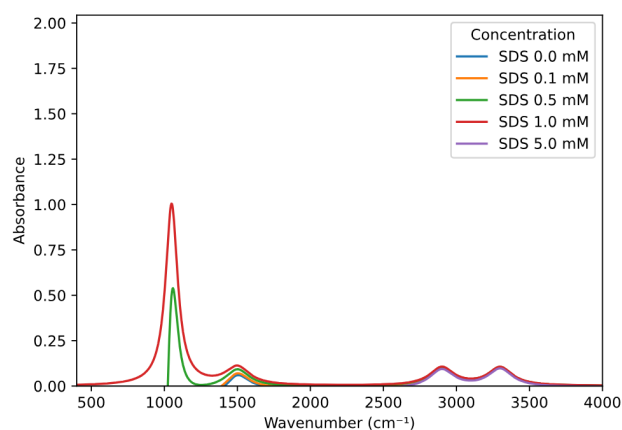
**Figure 1.** Fragrance retention time of spices at different SDS concentrations

The anionic head group of SDS may interact with polar groups in vanilla essential oil to form hydrogen bonds or other types of bonds, thus affecting the volatility and stability of vanilla essential oil. With the change of SDS concentration, the intensity and mode of this interaction may change, which

further affects the fragrance retention performance of vanilla essential oil.

#### 3.2. Molecular mechanism analysis results

Infrared spectrum analysis is used to explore the interaction mechanism between SDS and vanilla essential oil molecules. The experimental results showed that with the increase of SDS concentration, the position and intensity of characteristic peaks of vanilla essential oil molecules changed obviously. These changes are mainly reflected in the vibration modes related to functional groups (ketone groups, hydroxyl groups) in vanilla essential oil (Figure 2).



**Figure 2.** Infrared spectra of vanilla essential oil at different SDS concentrations

Through infrared spectroscopy, it can be observed that the changes in characteristic peaks and their intensities of vanilla essential oil under different SDS concentrations reveal the evolution of intermolecular interactions: at lower SDS concentrations (0.1 mM and 0.5 mM), the peak around 1050  $\text{cm}^{-1}$  is enhanced, indicating the formation of strong hydrogen bonds between the sulfate ions of SDS and polar groups such as hydroxyl groups in vanilla essential oil, which theoretically improves the stability and fragrance retention performance of vanilla essential oil molecules; as the SDS concentration increases to a moderate level (1 mM), the peak continues to enhance but begins to show a decreasing trend, indicating the gradual appearance of van der Waals forces; at higher SDS concentrations (5 mM), the hydrogen bond-related peak around 1050  $\text{cm}^{-1}$  weakens, and a new peak appears near 950  $\text{cm}^{-1}$ , suggesting an enhancement of van der Waals forces, which may be due to the formation of SDS micelles increasing the encapsulation of vanilla essential oil molecules, restricting their free movement and volatilization, and thus may have a negative impact on the fragrance retention effect.

Infrared spectrum data show that hydrogen bonds may be formed between sulfate ions of SDS and polar groups such as hydroxyl groups in vanilla essential oil. This interaction is particularly significant at low concentration of SDS, which helps to enhance the molecular stability of vanilla essential oil, thus improving its fragrance retention performance. With the increase of SDS concentration, the van der Waals force between SDS molecules and vanilla essential oil molecules is gradually enhanced. This non-specific interaction is particularly obvious when SDS forms micelles, which may hinder the release of vanilla essential oil molecules, and then affect its fragrance retention performance. Under the condition of low concentration SDS, hydrogen bonding is dominant, which is beneficial to the stable release of vanilla

essential oil molecules, thus prolonging the fragrance durability. However, under the condition of high concentration of SDS, the enhancement of van der Waals force may lead to excessive encapsulation of vanilla essential oil molecules by SDS micelles, which limits its volatilization and reduces its fragrance retention. This finding is consistent with the changing trend of fragrance retention obtained by olfactory sensory evaluation method.

#### 4. Discussion

The effect of SDS on the fragrance retention of vanilla essential oil in this study is different and consistent with previous studies on the interaction between surfactants and spices [6-7]. Previous studies mostly focused on the improvement of solubility and stability of spices by surfactants, but this study further explored the specific influence mechanism of different concentrations of SDS on the fragrance retention performance of vanilla essential oil. Through infrared spectrum analysis, it is found that low concentration SDS promotes the formation of hydrogen bonds and optimizes the fragrance retention performance, while high concentration leads to the dominance of van der Waals force and the decrease of fragrance retention performance. This discovery provides a new perspective for understanding the interaction between surfactants and spices.

In the experiment, the possible sources of errors include the mixing uniformity in the sample preparation process, the precise control of SDS concentration and the subjectivity of olfactory evaluation method. These errors may have some influence on the experimental results, for example, uneven mixing may lead to too high or too low local SDS concentration, thus affecting the evaluation of fragrance retention performance. In order to reduce the error, more accurate sample preparation method and objective flavor measurement technology can be adopted in the follow-up study.

The results of this study have important potential application value and practical significance for the formulation optimization and product development of perfume industry. By accurately controlling the concentration of surfactants such as SDS, the fragrance retention performance of spices such as vanilla essential oil can be finely regulated, thus meeting the needs of different application scenarios. For example, in cosmetics, detergents and other products, by optimizing the concentration of surfactants, the fragrance durability of products can be improved and the consumer experience can be improved.

#### 5. Conclusion

In this study, the effects of different concentrations of SDS on the fragrance retention of vanilla essential oil and its molecular mechanism were systematically explored by olfactory sensory evaluation and infrared spectrum analysis. The experimental results showed that low concentration SDS optimized the fragrance retention performance of vanilla essential oil by promoting the formation of hydrogen bonds, while high concentration SDS led to the predominance of Van der Waals force and the decrease of fragrance retention performance. This discovery reveals the complexity of the interaction between surfactants and perfume molecules and its important influence on perfume properties. This study not only provides new insights for understanding the role of surfactants in fragrance retention performance of spices, but also provides valuable theoretical guidance for the practical application of spice industry. Future research can be further extended to other types of surfactants and perfume systems to reveal the universality and regularity of this phenomenon more comprehensively.

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