Enhanced Fragrance Release on Cotton Fabric Using β-Cyclodextrin Supported by Molecular Docking

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I. INTRODUCTION

Fragrance finishing in textiles has gained importance due to its sensory and therapeutic benefits. However, the volatility of essential oils and poor wash fastness limit the longevity of treated fabrics. β-cyclodextrin (β-CD) (Fig. 2) can form host guest inclusion complexes with essential oils (Fig. 1), enabling controlled release and enhanced retention [2]. Despite this, weak fixation to cotton fabrics reduces long term performance. Crosslinking agents and binders have been used to improve adhesion, but systematic studies combining these with molecular docking studies remain scarce [4]. This study aims to evaluate the effectiveness of citric acid as a crosslinker and polyvinyl alcohol (PVA) as a binder in retaining sandalwood oil β-CD inclusion complexes on cotton fabric, supported by molecular docking analysis to predict binding stability.

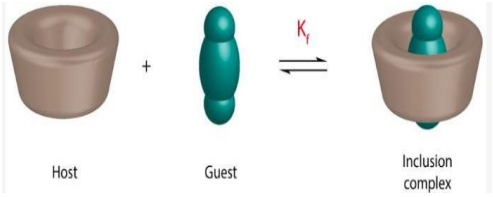

Fig. 1. Schematic representation of the formation of an inclusion complex between a β-CD (host) and a guest.

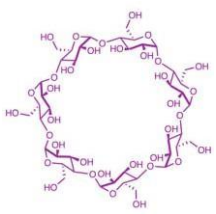

Fig. 2. Schematic representations of a general chemical structure of β-CD.

II. LITERATURE REVIEW

Fragrance retention is highly variable, dependent upon the type of essential oil used, the fabric substrate, and the application method employed [4]. Encapsulation of essential oils in β-CD has been widely studied for fragrance retention. Previous work shows fabrics can retain up to 35% of essential oils after 15 washes, though durability varies by oil type, fabric, and method [4]. Research confirms that fabrics treated with β-CD can retain up to 35% of the encapsulated oil after 15 washes and still maintain 25% retention after 25 washes [7]. Molecular docking has been employed to understand host guest interactions, providing insight into binding affinity and potential release mechanisms [2]. However, few studies integrate molecular docking results with wash durability testing [8]. This gap motivates the present study to quantify fragrance loss and validate β-CD complexation using computational and experimental approaches.

III. MATERIALS AND METHODS

A. Materials

Cotton fabric (plain-woven, 150 GSM), sandalwood essential oil (≥96% purity), β-CD (≥99% purity), citric acid (≥99% purity), PVA (≥99% purity), ethanol (≥95% purity) and distilled water (laboratory grade) were used.

B. Selection of Essential Oils

Through a literature review, lavender [1], jasmine [4], sandalwood [2], peppermint [6] and lemon [5] were shortlisted for their well documented fragrance longevity and compatibility with β-CD for sustained release. Molecular docking analysis was performed to assess the binding affinity of each selected essential oil with β-CD using the PyRx software [2]. Based on these results, one essential oil with the highest binding affinity was selected for further study.

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C. Fabric Treatment

β-CD-inclusion complexes with the selected essential oil were prepared using the co-precipitation method. Briefly, 5g of β-CD was dissolved in 100 ml of distilled water and stirred at 600 rpm at 40°C for four hours to ensure complete dissolution. The essential oil (5 ml) dissolved in 2 ml of ethanol was added dropwise under continuous stirring to form the host guest complex [3]. To enhance fixation to cotton fibers, 10% citric acid (10 g in 100 ml of β-CD-inclusion complex solution) was incorporated as a crosslinker and stirred at 500 rpm for 60 minutes at 40°C [5]. Cotton fabric samples were immersed in the prepared solution for 10 minutes, squeezed using a pad dry machine at 2 kg/cm² and cured at 80°C for 10 minutes [5]. A binder solution of 5% polyvinyl alcohol (5g in 100 ml distilled water) was prepared at 60°C under magnetic stirring and applied to the fabrics via screen printing [5]. Treated fabrics were air dried at room temperature for 1 hour and subsequently cured at 90°C for 15 minutes [5].

D. Durability Testing for Wash Fastness of Fragrance Finishes

The durability of the fragrance finishes was evaluated using a wash fastness test according to ISO 105-C06:2010, conducted on fabric samples after 5, 10, and 15 wash cycles [9].

E. Evaluating the Residual Amount of Essential Oil from Washed Samples

To quantify fragrance retention, each washed fabric sample was soaked in 30 ml of 95% ethanol for 6 hours to extract the residual essential oil, which was then measured using a UV-Vis spectrophotometer (model-DS5, Edinburgh Instruments, United Kingdom) [10]. A calibration curve was constructed from standard solutions of the essential oil (100–1000 ppm), prepared by diluting a 10000 ppm stock solution in 95% ethanol, with absorbance measured at 200–400 nm. Additionally, an olfactory test was conducted at Bureau Veritas Consumer Products Services Lanka (Pvt) Ltd by three trained sensory evaluators in a controlled, odor-free room. Each evaluator assessed the washed samples against unwashed references at 30-minute intervals to prevent olfactory fatigue, rating odor intensity on a 5-point scale (1 = no odor to 5 = very strong odor). The average score of the three evaluators represented the final fragrance retention for each sample.

IV. RESULTS AND DISCUSSION

A. Selection of Essential Oils

Molecular docking results summarized in Table I show sandalwood exhibited the highest binding affinity (-5 kcal/mol) due to strong interactions between α-santalol and β-CD, likely attributed to its larger molecular size and hydrogen bonding potential (Fig. 3). This enhanced affinity suggests improved encapsulation stability and prolonged fragrance retention.

TABLE I. BINDING AFFINITIES FOR INCLUSION COMPLEXES BETWEEN ESSENTIAL OILS AND B-CYCLODEXTRIN BASED ON MOLECULAR DOCKING RESULTS

Essential Oil	Chemical Compound	Highest Binding Affinity (kcal/mol)
Lavender	Linalyl Acetate	-4.1
Jasmine	Benzyl Acetate	-4.2
Sandalwood	Alpha Santalol	-5
Peppermint	Menthol	-4.5
Lemon	Limonene	-3.7

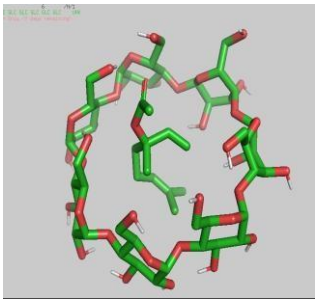

Fig. 3. Molecular Docking Simulation of β-CD and α-santalol

B. Evaluation of Residual Sandalwood Oil Concentration After Wash Cycles

Sandalwood essential oil concentrations in treated fabrics were quantified using a UV-Vis spectrophotometer with a calibration curve ($y = 0.0016x + 0.4413$, where y represents absorbance and x represents concentration in ppm, Table II).

TABLE II. UV-VIS PEAK ABSORBENCY VALUES FOR DIFFERENT CONCENTRATIONS OF SANDALWOOD ESSENTIAL OIL

Concentration(ppm)	UV-Vis Peak Absorbency Values
100	0.50944
250	0.75554
500	1.61816
750	1.58224
1000	1.99811

Residual essential oil concentrations decreased gradually with repeated washing, 925 ppm after 5 washes (2.73% reduction), 862 ppm after 10 washes (9.36% reduction), and 402 ppm after 15 washes (57.73% reduction) (Table III). These findings were consistent with the olfactory test, which indicated a slight odor but a perceptible fragrance even after 15 washes. This demonstrates the effectiveness of β-CD complexes combined with crosslinking agents and binders in enhancing fragrance durability on cotton fabrics. The molecular docking results correlated well with experimental observations, supporting the use of β-CD with sandalwood essential oil for controlled fragrance release and durable scent performance in practical textile applications.

TABLE III. THE PERCENTAGE REDUCTION OF RESIDUAL SANDALWOOD OIL CONCENTRATIONS AFTER WASH CYCLES

Wash Cycle	Before Washing Sandalwood Oil Concentration	After Wash Cycle-Residual Sandalwood Oil Concentration	Percentage Reduction
5	951ppm	925ppm	2.73%
10	951ppm	862ppm	9.36%
15	951ppm	402ppm	57.73%

V. CONCLUSION

Molecular docking confirmed that sandalwood essential oil (α-santalol) had the strongest affinity with β-CD (–5 kcal/mol). Application of citric acid and PVA enhanced fixation on cotton, improving wash durability. The treated fabric showed good durability, retaining fragrance even after 15 washes, with only a 57.73% reduction. Olfactory evaluation confirmed a slight odor, indicating prolonged fragrance retention. This study demonstrates the potential of β-CD inclusion complexes combined with crosslinkers and binders for durable fragrance finishing. Further optimization of crosslinkers and binders is required to improve long-term stability.

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