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"Biodegradable Fragrance Design: Scents That Disappear, Not the Planet."

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1. Introduction

Pharmaceuticals and personal care products as pollutants (PPCPs) refer to various types of chemical products intended for personal health, hygiene, and beauty. These chemical components present in PPCPs are emerging as a global problem because they can cause temporary or long-term toxicity to aquatic life. In particular, among PPCPs, musk-based ingredients (synthetic musk) are recognized as representative fragrance components with an appealing scent and high durability. PPcPs chemicals, such as Musk components, dissolve in water and accumulate in the adipose tissue of aquatic organisms. In addition, due to their impact on the aquatic environment, these chemicals cause malformations in aquatic organisms and disturbances in the ecosystem. Conversely, research on perfumes concerning their impact on the aquatic ecosystem is insufficient and there is a lack of biodegradability data in water environments for all fragrance components. Therefore, there is a need for tools that can predict this and the development of althernative fragrance compositions with high biodegradability.

2. Materials and Methods

In this study, biodegradability data of fragrance raw materials decomposing in aquatic environments were screened and biodegradable fragrance compounds were formulated.

A. Selection of biodegradable fragrance materials according to OECD guidelines

In order to screen raw materials with high biodegradability, values derived from experiments based on The Organisation for Economic Co-operation and Development (OECD) guidelines were used for 121 frequently used fragrance ingredients (92 chemical raw materials and 29 natural raw materials). The OECD guideline for biodegradability measurement primarily uses the 301 (Ready Biodegradability) method, and there are few biodegradability values measured through the 310 (Ready Biodegradability) and 302 (Inherent Biodegradaility Test) methods.

OECD screening tests for evaluating ready biodegradability are valuable and necessary tools for assessing a chemical's potential to biodegrade in the environments. The types of test

methods for 301 (Ready Biodegradability) of the OECD guideline and their characteristics are as follows:
301A: Similar to the ISO standard 7827-1984, modified version of the AFNOR (Association Francaise de Normalisations)
301B: A method that measures the CO_2 produced as the substance decomposes
301C: A method used by MITI (Japanese Ministry of International Trade and Industry)
301D: A method using a closed bottle, representing the most simplified version
301E: A modified version of the OECD guildeline adopted in 1981
301F: Manometric respirometry, the most recently devised and currently the most widely used version.

The principle of the test methods involves quantifying the biodegradability of a substance by measuring the amount of CO_2 produced in methods B, D and E, and the amount of O_2 consumed in methods C and F. Since these techniques fundamentally rely on measuring changes in CO_2 and O_2 as microorganisms decompose the substance, the biodegradability can vary within a certain range even when the same method is used on the same substance. Therefore, when dealing with biodegradability internationally, values obtained from experiments adhering to OECD guidelines are accepted. Substances with a biodegradability score of 60% or higher are considered readily biodegradable.

B. Formulation of fragrance compounds with high biodegradability
To develop fragrance compounds that are readily biodegradable, we selected fragrance raw materials that have a naturally appealing herbal scent, which is highly favored. Additionally, the fragrance ingredients were chosen with consideration for their biodegradability. Based on the biodegradability data for each material according to these criteria, 10 types for synthetic raw materials were selected as primary fragrances: cis-3-hexenol, allyl heptanoate, nerolidol, hedione, 3-hexen-1-yl methyl carbonate, linalyl acetate, ethyl linalool, citronellyl acetate, sandalore and vanillin. The formaulation of the fragrance compounds was performed twice in accordance with the results of sensory evaluations.

C. Sensory Evaluation
Twenty subjects were healthy adults between the ages of 20 and 45. For the sensory evaluation, the following 5 fragrance compound formulas were adopted and evaluated on a 5-point scale (1 to 5): natural-unnatural, pleasant-unpleasant.

3. Results & Discussion

A. 1st Formulation
Using the selected synthetic fragrance materials, fragrance formulas #1 to #3 (Table 1) were prepared. For the purpose of creating biodegradable fragrance compounds, fragrance ingredients with green, herbal, fruity, floral, and woody odors were primarily selected. These ingredients are highly preferred and are intended to create a natural-friendly scent. Unless otherwise stated herein, the content is in weight percent (wt%).

Table 1. Formulation of Biodegradable Fragrance Compounds.

Fragrance Composition (%)	Formula #1	Formula #2	Formula #3	Formula #4	Formula #5
cis-3-Hexenol	2.5	1.5	0.5	0.49	0.49
Allyl heptanoate	0.7	0.7	0.7	0.69	0.69

Nerolidol	2	1	1	0.98	0.98
Hedione	20	31.5	31.5	30.87	30.87
3-Hexen-1-yl methyl carbonate	0.3	0.25	0.25	0.24	0.24
Linalyl acetate	35.5	42.05	42.55	41.7	41.7
Ethyl linalool	30	16.5	16.5	16.17	16.17
Citronellyl acetate	5	2	2	1.96	1.96
Sandalore	1	2	2.5	2.45	2.45
Vanillin	3	2.5	2.5	2.45	2.45
Grapefruit oil	-	-	-	0.5	1
Geranium oil	-	-	-	0.5	0.5
Clary sage oil	-	-	-	1	0.5
Total (%)	100	100	100	100	100

As a result of the sensory evaluation (formulas #1 to #3), there was an opinion that these fragrances do not blend smoothly when used only with chemicals. In the case of formulas #1 and #2, prepared only with synthetic fragrances, there were many opinions that they had a chemical sensation. Specifically, many felt that the synthetic raw materials didn’t harmonize and there was an overwhelming harsh green scent. On the other hand, in the case of formula #3, in which the green fragrance was reduced and the cozy floral and woody-based fragrance ingredients were adjusted upwards, it felt relatively fresh, and the chemical sensation was also reduced. However, there were still opinions that it felt like it originated from synthetic fragrances and that certain chemical ingredients seemed predominant.

B. 2nd Formulation

For the 2nd formulation, while the high biodegradability of the fragrance compounds is essential, consumer preference remains a critical factor in evaluating a fragrance’s functionality. Formula #3 displayed a generally favorable preference with its natural essence; however, there was feedback indicating a lack of scent harmony. To address this, efforts were directed towards enhancing the fragrance’s palatability and its natural and luxurious appeal. Screening essential oils to diminish the chemical odors from synthetic fragrances and to achieve a harmonious blend was prioritized. To create a natural and fresh herbal feeling, citrus grapefruit oil, floral geranium oil, and herbal clary sage oil were selected, and fragrance compounds wre reformulated as fornulas #4 and #5 (Table 1).

Key conponents of natural fragrance were integrated to complement formula #3 while yielding a luxurious sensation. Theses were added at approximately 2% of the total fragrance composition to preserve the existing scent while enhancing its natural appeal. Specifically, to infuse a more vivid herbal sensation, grapefruit oil, a component of the citrus family known for its refreshing aroma, geranium oil, adding a fresh floral touch, and clary sage oil, known for its rustic herbal feel, were chosen to create formulas #4 and #5. In the composition fo formula #4, 1% clary sage oil was used to emphasize the herbal aspect, but this resulted in a pronounced rustic sensation. To counterbalance this, formula #5 was modified by reducing the clary sage oil content and increasing the grapefruit oil ratio, thereby enhancing the fresh scent derived from citrus peels.

4. Conclusion

Despite the increasing awareness of the social impact of PPCPs on the aquatic environment, research on the biodegradability of fragrance ingredients remains insufficient, especially given their prevalent use in wash-off formulations driven by consumer demand. Our study highlights the utility of the OECD guideline tool in predicting the biodegradability of fragrance ingredients, thereby aiding the development of alternative fragrance compositions with enhanced biodegradability.

From our experiments, it is evident that while synthetic fragrance materials can achieve high biodegradability, they often lack the olfactory satisfaction needed for wider consumer acceptance. The first formulation indicated a disconnect between synthetic fragrance compositions and olfactory harmony, with many synthetic ingredients failing to blend smoothly, resulting overpowering harsh green scents. This was particularly evident in formulas #1 and #2.

To address these concerns, the second formulation employed a strategic integration of natural ingredients like grapefruit oil, geranium oil, and clary sage oil, which significantly enhanced the fragrance compounds in formulas #4 and #5. These adjustments not only improved the fragrance's palatability and luxurious appeal but balanced the rustic herbal impressions with fresh citrus notes.

Overall, while biodegradability remains a priority, our findings underscore the importance of achieving a harmonious blend and consumer satisfaction in fragrance compositions. Future developments should continue to balance these aspects by exploring innovative combinations of natural and synthetic ingredients to ensure both eco-friendliness and consumer appeal. The significance of our research lies in improving the preference for eco-friendly biodegradable fragrance compositions, enhancing both their environmental impact and consumer receptivity.