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"How Naturally Derived Ester CST Outperform Petroleum Derived Esters:

Pigment Dispersion and Coloring Properties of Novel Glycerol Succinate Fatty Acid Ester"

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1. Introduction

Predispersed pigment dispersions are widely used in industries such as coatings, inks, plastics, and cosmetics. In cosmetics, they are often used in makeup products, e.g., lipstick. Well-dispersed pigment dispersions are crucial because they directly impact the coloring performance, a key element of lipstick. Organic pigments are used for lipsticks that require particularly vivid colors. Several studies have explored methods to enhance chroma by complexing organic pigments with body pigments (1). Additionally, researchers are developing fine-particle organic pigments (2-3) and investigating rosin acid treatment to reduce color change in organic pigments (4). However, few studies to date have focused on the role of oils used as dispersants. Diisostearyl malate (DIM), a high-viscosity base oil, is commonly employed as a base oil for organic pigment dispersions owing to its excellent dispersibility and oxidation stability. However, the fact that it is a petroleum-derived oil does not align with the recent shift toward natural and sustainable sources. To date, no naturally derived base oil with performance equivalent to DIM has been developed, which presents a formidable challenge in finding a suitable alternative.

In this study, caprylic/capric/succinic triglyceride (CST, Figure 1) is investigated as a base oil for dispersing organic pigments. CST is a high-viscosity naturally derived oil originally developed to enhance the hardness stability of lipsticks (5). Dynamic viscoelasticity measurements, storage stability, and color development of the pigment dispersions were analyzed to evaluate the suitability of CST for organic pigment dispersion.

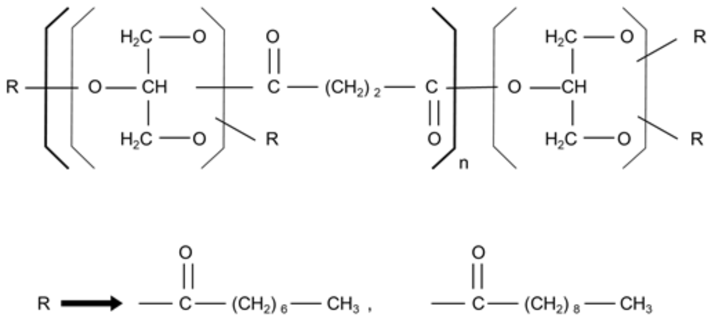

Figure 1. Structural formula of caprylic/capric/succinic triglyceride (CST).

2. Materials and Methods

Materials and preparation of pigment dispersions

CST was synthesized via the reaction of glycerin, caprylic, capric, and succinic acids. Untreated Red7 (CI 15850, Lithol Rubine BCA, Kishi Kasei), a red organic pigment most commonly used in lipsticks, was used as the organic pigment for evaluation. Six pigment dispersions were prepared by mixing 40 wt% Red7 pigment with 60 wt% of each oil listed in Table 1. Medium- to high-viscosity oils of natural origin were selected for evaluation. The mixtures were processed three times using a roll mill (BR-150HCVⅢ, IMEX). In the initial treatment, the roll clearance was set to 30 μm, rotational speed was 150 rpm, and the temperature was maintained at 25 °C. In the second treatment, the roll clearance was reduced to 10 μm, rotational speed was increased to 300 rpm, and the temperature was maintained at 25 °C. The same conditions were applied for the third treatment.

Table 1. List of oils used in this study and their viscosities.

No.	Oils	Abbreviated name	Natural origin index (ISO16128)	Viscosity of oils (20 °C, mPa・s)
1	Caprylic/capric/succinic triglyceride	CST	1	1,300
2	Diisostearyl malate	DIM	0	5,500
3	Ricinus communis (castor) seed oil	CAS	1	1,100
4	Polyglyceryl-2 tetraisostearate	PGTI	1	370
5	Polyglyceryl-2 triisostearate	PGTRI	1	450
6	Polyglyceryl-10 decaisostearate	PGDI	1	1,600

Dynamic viscoelasticity evaluation of pigment dispersions

The dynamic viscoelasticity was measured using a rotational rheometer (HAAKE MARS 40, Thermo Scientific™) with a cone plate (φ 35 mm, 2°) to assess the oscillatory stress and strain dependence. Conditions were measured at 1–1000 Pa, 1 Hz, and 25 °C.

Stability evaluation of pigment dispersion

Pigment dispersions were sealed in glass bottles and subjected to accelerated testing at 50 °C for one month, and a cycle test at 5°C to 40°C for one month. After testing, oil separation at the dispersion surface and within voids was visually assessed.

Coloring properties evaluation of pigment dispersion

Coloring properties were evaluated using a spectrophotometer (SE7700, NIPPON DENSHOKU INDUSTRIES) in the CIE 1976 (L*a*b*) system.

3. Results

Dynamic viscoelasticity evaluation of pigment dispersion

Figure 2(a) shows the results of viscoelasticity measurements of pigment dispersions prepared using CST, PGDI, and DIM. At low shear, the storage modulus (G'), which reflects elastic behavior, is higher than the loss modulus (G''), which reflects viscous behavior, for all pigment dispersions prepared with the texted oils. The results expressed as the loss factor (tan δ) for each sample are shown in Figure 2(b). Here, tan δ indicates the ratio of viscous to elastic behavior and is defined as tan δ = G''/G'. Structural strength was evaluated by measuring the shear stress at the G' and G"crossover point, defined as the point where tan δ exceeds one. The CST pigment dispersion exhibits the highest shear stress (351 Pa) at the G' and G'' crossover point, indicating superior structural strength compared to the other dispersions. This result suggests that CST pigment dispersion maintains elastic behavior more effectively under stress. The DIM pigment dispersion exhibits a shear stress of 305 Pa at the G' and G" crossover point, indicating lower structural strength than the CST pigment dispersion. In contrast, the G' and G" crossover point of the PGDI pigment dispersion is 50 Pa, clearly reflecting reduced structurally strength compared to the CST pigment dispersion. Notably, despite the CST oil having lower viscosity than PGDI, its correspoinding dispersion demonstrates higher structural strength. Among the remainging pigment dispersions—CAS, PGTI, and PGTRI—the shear stresses at the G' and G'' crossover point are 215, 163, and 66 Pa, respectively, all indicating lower structural strength than the CST pigment dispersion. Furthermore, no clear correlation is observed between oil viscosity and shear stress at the G' and G'' crossover point.

(a)

(b)

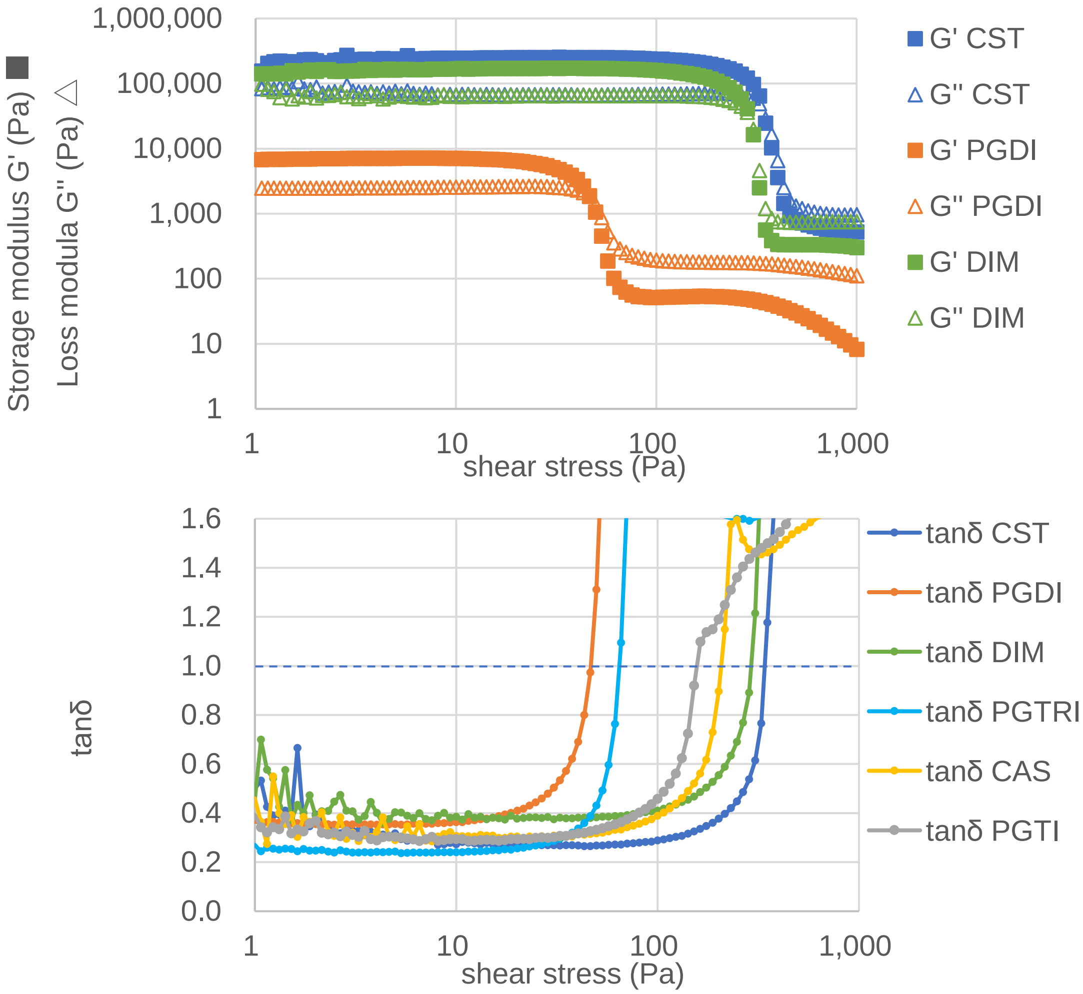

Figure 2. The oscillatory stress and strain dependence measurements of (a) storage modulus G’ and loss modulus G’’ and (b) tan δ.

Stability evaluation of pigment dispersion

Following accelerated testing, CST pigment dispersions did not show oil separation. Contrastingly, pigment dispersions prepared with the other oils showed visible oil separation into surface pores (Table 2).

Table 2. Stability test results of pigment dispersion (A: no visible oil separation, B: slight oil separation).

Pigment dispersion	Accelerated testing (50 °C)	Accelerated testing (cycle)
CST	A	A
DIM	B	B
CAS	A	B
PGTI	B	B
PGTRI	B	B

Evaluation of coloring properties of pigment dispersion

Color development was evaluated to determine the degree of pigment dispersion. Red7 is a bright red pigment that exhibits increased redness (higher a* value) as it becomes more finely dispersed. First, color development was measured before and after roll milling of the Red7 and CST mixture (Figure 3(a)). After the treatment, the a* value increased, indicating enhanced color intensity. Figure 3(b) compares the color of pigment dispersions prepared with various oils after roll milling. The CST pigment dispersion demonstrates the highest a* value, showing better color development than the other dispersions. DIM, PGTI, and CAS followed, while PGTRI and PGDI display lower a* values. These results suggest that the CST pigment dispersion achieves superior coloration performace owing to improved pigment dispersion.

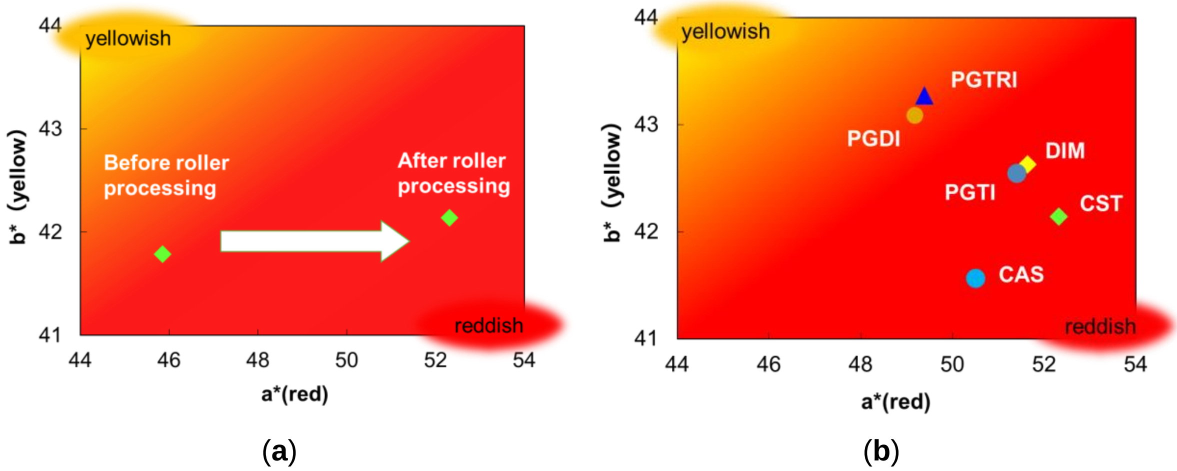

Figure 3. Evaluation of color properties of pigment dispersions: (a) Results before and after roll milling; (b) Results after roll milling for pigment dispersions prepared with various oils.

4. Discussion

This study revealed that CST can produce organic pigment dispersions with high stability and strong color rendering ability. The absence of oil separation is a crucial property that simplifies handling, as it eliminates the need for remixing before use. The viscoelastic behavior of CST pigment dispersion is similar to that of DIM pigment dispersion, indicating its suitability as a base oil for organic pigments. Furthermore, dynamic viscoelasticity measurements revealed that CST pigment dispersions had higher structural strength than those prepared with DIM. These results are consistent with the findings that CST pigment dispersions did not exhibit oil separation. Notably, no clear correlation was observed between the viscosity of the base oil and the shear stress at the G' and G” crossover point of the pigment dispersion. The results suggest that the shear stress at the G' and G” crossover point tends to be lower for partial esters in which the hydroxyl groups of the polyglycerol backbone remain, even when the oil viscosity is high. In the evaluation of color development, the CST pigment dispersion exhibited a more intense reddish hue compared to the DIM pigment dispersion. Generally, improved pigment dispersion enhances color strength. Therefore, the superior coloration of the CST pigment dispersion can be attributed to its higher dispersibility. In other words, CST exhibited the highest dispersibility of organic pigments among the oils tested.

The correlation between the viscoelasticity results and the coloration test results of pigment dispersions was examined (Figure 4). A strong positive correlation (R = 0.923) between a* values and the shear stresses at the G' and G” crossover points was confirmed. Additionally, the results were analyzed in relation to chroma (C*), which serves as a more effective indicator of pigment dispersibility (Figure 5). The chroma is calculated using the formula $\boldsymbol{C}^* = \sqrt{\boldsymbol{a}^{*2} + \boldsymbol{b}^{*2}}$. A correlation coefficient greater than 0.7 indicates a strong positive correlation between chroma and dispersibility.

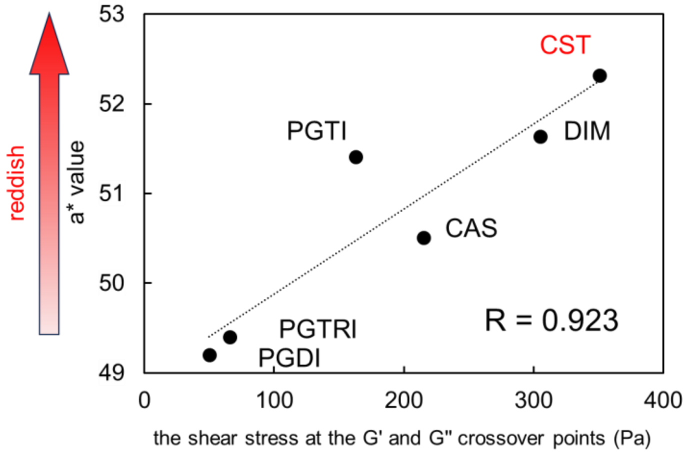

Figure 4. Correlation between rheological properties and a* values.

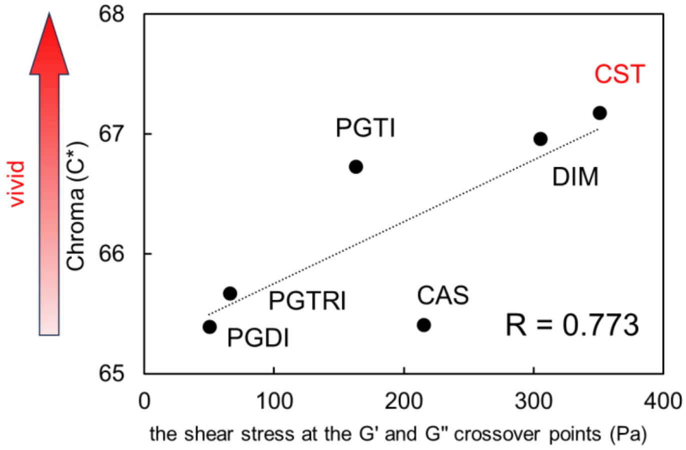

Figure 5. Correlation between rheological properties and chroma (C*) values.

5. Conclusion

This study demonstrated that naturally derived CST exhibits excellent functionality as a base oil for pigment dispersion. CST outperformed other tested oils in both structural strength and coloring properties. The higher a* value of the CST dispersion indicated enhanced pigment dispersibility. Interestingly, a correlation between color properties and viscoelastic behavior was observed. These results suggest that CST is a promising alternative to conventional petroleum-based oils in lipstick pigmentation applications.

Reference

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