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282

The effect of replacing fragrance compounds on emulsion rheology

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Introduction

Following nickel, fragrance compounds are the second leading cause of contact allergy in the European Union.

This study focuses on two common fragrance families, Florals and Musks, which contain ingredients likely to be banned due to more reported cases of skin sensitisation and contact allergy (Table 1). The aim of the study was to investigate whether and to what extent the proposed replacements Florol and Habanolide change the rheological properties of the original products, therefore, to determine whether they are suitable as direct replacements.

Table 1 Musk and Floral Fragrances Investigated in the study

INCI Name	Common name	Fragrance family
Hexamethylindanopyran	Galaxolide	Musk
Pentadecalactone	Habanolide	Musk
Musk Ketone	Musk Ketone	Musk
Butylphenyl methylpropional	Lilial	Floral
Hydroxyisohexyl-3-Cyclohexene carboxaldehyde	Lyral	Floral
Tetrahydro-methyl-methylpropy-pyran-4-ol	Florol	Floral

Materials & Methods

Emulsion formulations were kept simple in order to focus on the detection of fragrance-emulsion interaction. Each base formulation was an O/W emulsion with 25% oil phase. The manufacturing method used was a hot process.

In the base formulation, ingredient levels were kept at consistent levels for all the samples; the fatty alcohol components varied in their carbon chain length (C14, C16 and C18) and saturation level (Cis-C18), each used at 10% w/w (Table 2). Each fragrance sample was added at 0.5% w/w, which is the highest level deemed safe. These fragrances are normally base notes, hence unlikely to be used at their maximum allowed concentration. In total, 32 samples were formulated and analysed for this experiment – 16 samples for each fragrance family.

An air-bearing controlled-stress rheometer (Rheostress RS75, Haake™, Germany) with parallel-plate geometry (35mm diameter, 1.0mm gap) was used for rheological characterisation (Fig. 1). All results were recorded and analysed using the RheoWin 4.41. Each sample was analysed for its dynamic viscosity, level of thixotropy (time-dependent behavior) and viscoelasticity.

Table 2 Components of base emulsion

Phase	Ingredient (INCI name)	% w/w
A	Aqua	62.95
	Glycerin	5.00
B	Cetearyl Alcohol	5.00
	Isopropyl Myristate	10.0
	Sorbitan Monoleate	5.60
	Polysorbate 80	0.65
	Fatty Alcohol (Myristyl, Cetyl, Stearyl or Oleyl Alcohol)	10.0
C	Fragrance (Musk family: Galaxolide, Musk Ketone or Habanolide) (Floral family: Lyral, Lilial or Florol)	0.50
D	Methylparaben	0.40
	Propylparaben	0.40

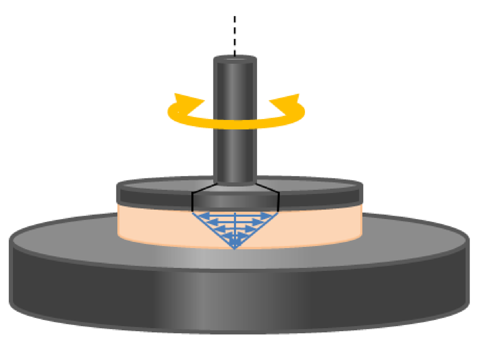

Figure 1 Visual representation of parallel plate rheometer configuration

Results & Discussion

The Musk family samples (specifically with Myristyl alcohol) with Habanolide and Galaxolide yielded viscosity curves that suggest considerable similarity in structure.

The Oleyl Alcohol Galaxolide and Habanolide samples had starting viscosities similar to the base (Fig. 2). Figures 2 and 4 demonstrate that unsaturated Oleyl Alcohol yielded more uniform viscosity and thixotropy curves compared to other alcohol families.

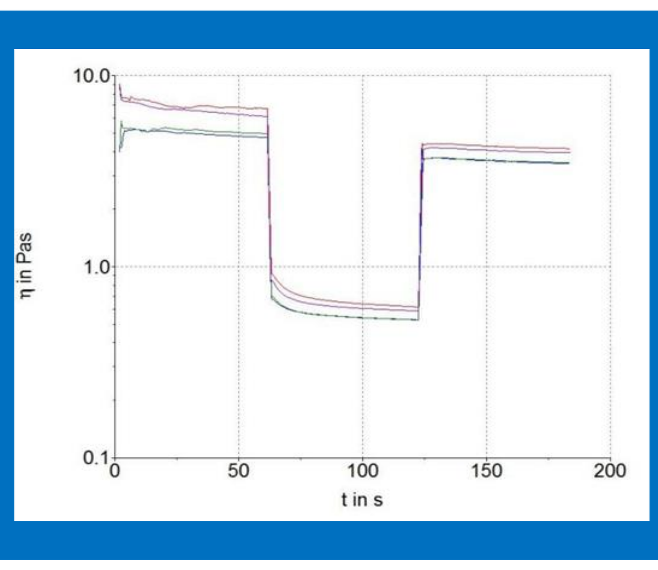

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Figure 2 Thixotropy curves for Musk family samples with Oleyl Alcohol

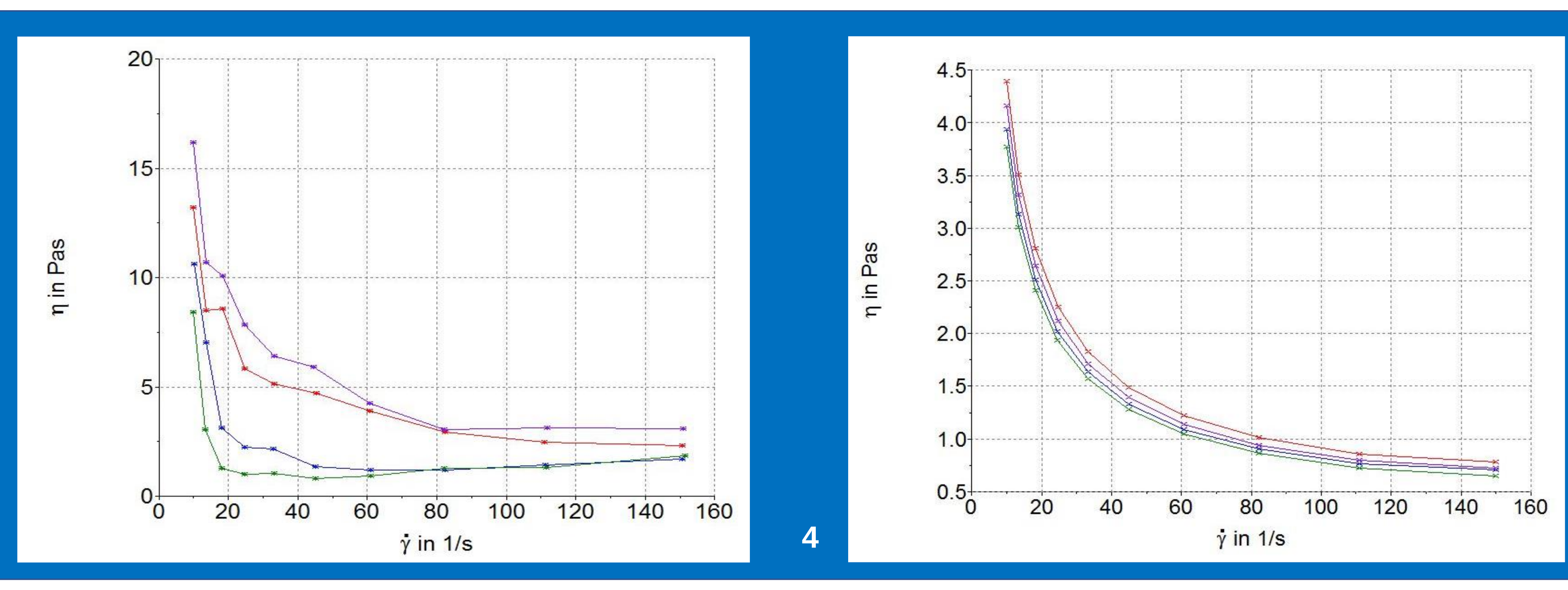

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Figure 3-4 Viscosity curves for Myristyl and Oleyl Alcohol Musk Family Samples

Three step thixotropy tests revealed that Oleyl alcohol samples from both fragrance families had the highest recovery rates, classifying them as the least thixotropic. Similarities between Galaxolide and Habanolide samples were highlighted amongst Stearyl and Cetyl Alcohol samples, while viscosity recovery rates amongst Floral family samples were generally inconsistent.

Table 3 Yield values (τ_y in Pa) obtained from the deflection of the complex modulus (rigidity)

Sample	C14	C16	C18	Cis-C18
Base	224.1	77.6	21.5	16.3
Galaxolide	247.8	101.6	22.0	5.3
Habanolide	247.8	101.6	10.9	5.3
Musk Ketone	302.8	65.5	21.5	12.3

Oscillatory Stress Sweep tests revealed that that the Myristyl Alcohol samples had much higher yield values than the other fatty alcohol samples (Fig. 5-7, Table 3). The Oleyl Alcohol samples required very little force to destroy their internal structure, which corresponds with the samples' low viscosity values, meaning that these samples can be described as having easy flow behaviour.

Habanolide and Galaxolide both produced the same yield values when used with Myristyl (Fig. 5-7), Cetyl (Fig. 8, 9) and Oleyl Alcohol (Table 3), which confirms the structural similarities between the samples, and suggests that Habanolide is a viable candidate for replacing Galaxolide in emulsion-based formulations.

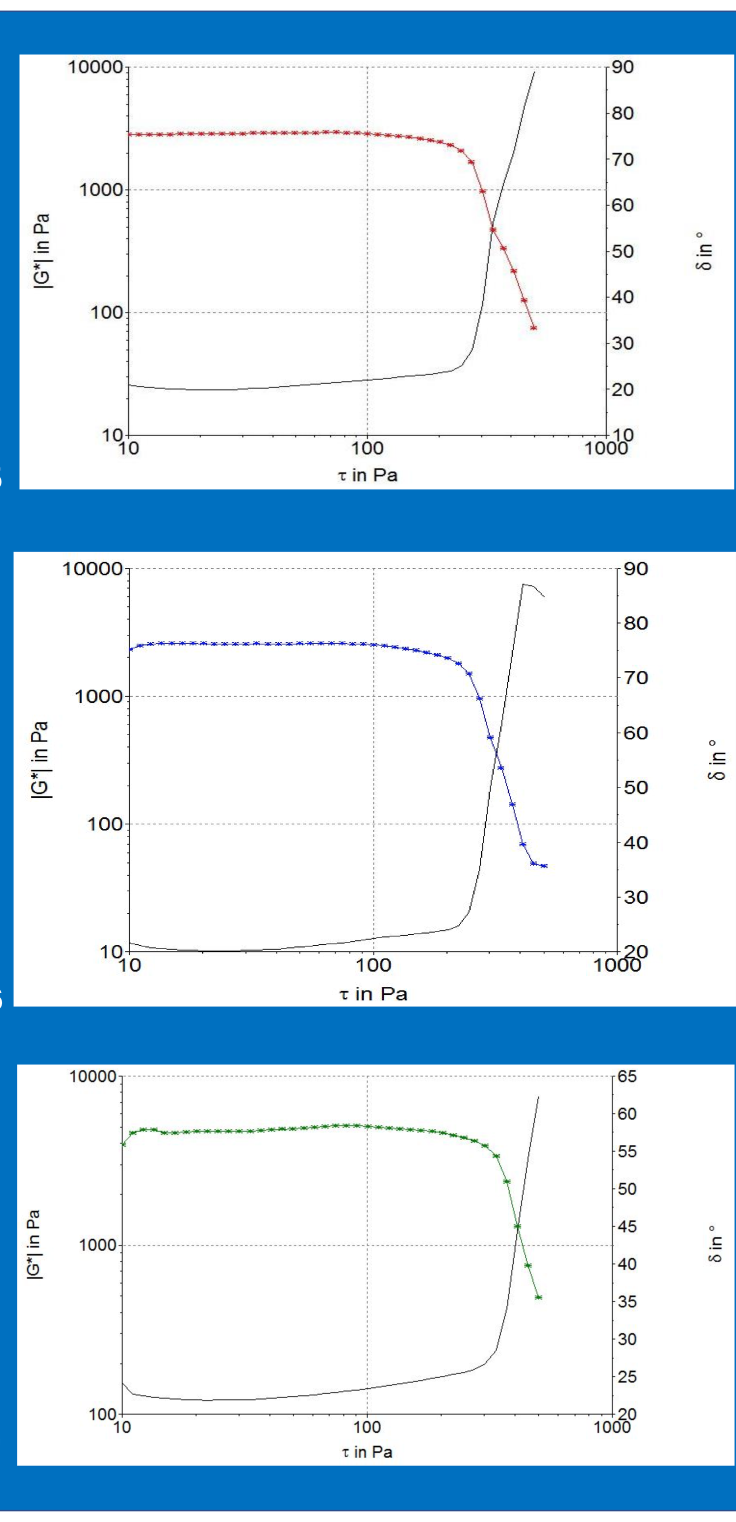

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Figure 5-7 Viscoelasticity graphs for the Base, Galaxolide and Habanolide Myristyl Alcohol samples (from top)

Conclusion

The results of this study show that there are promising replacement fragrances within both Musk and Floral families.

Based on its consistent rheological results, Habanolide would be an excellent candidate to replace Galaxolide.

The two musk fragrances shared the same textural and rheological properties when used in each emulsion, thus confirming that polycyclic musks are suitable replacement to nitro-musks, despite differences in chemical structure.

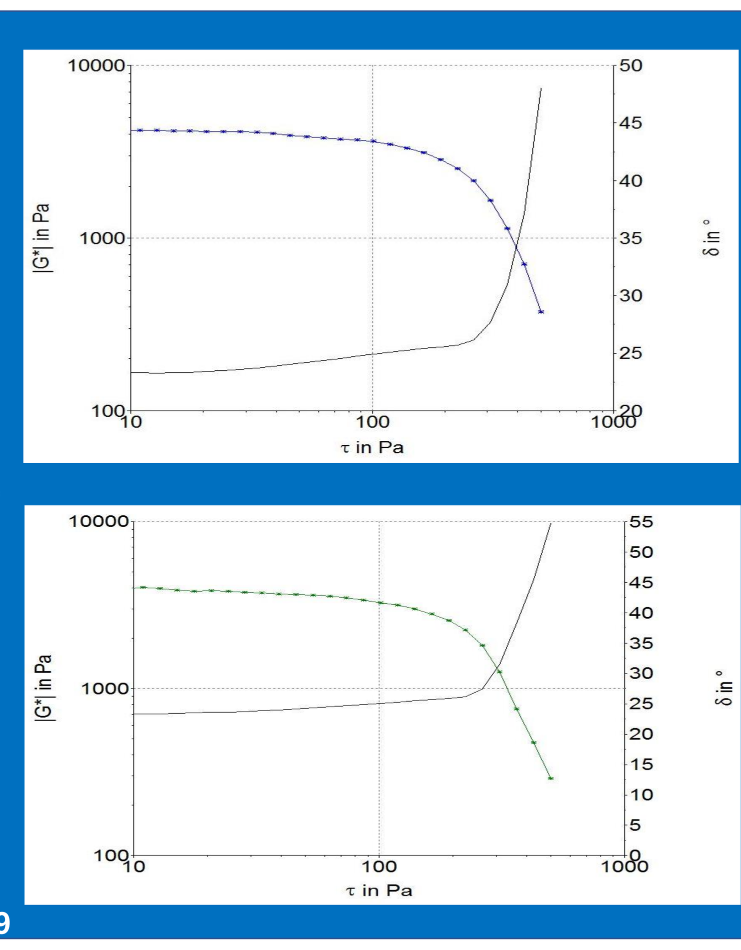

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Figure 8-9 Viscoelasticity graphs from Galaxolide and Habanolide Cetyl Alcohol samples (from top)

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