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Analysis of Fragrance Volatiles in Shampoos and Soaps using Thermal Desorption and GC/MS

The use of fragrances is prevalent in almost any of the multitude of "personal" care products. This includes cosmetics, soaps, oils, and perfumes. So called body fragrances number into the thou- sands and include colognes, perfumes, as well as toilet waters. These fragrances are now com- mon in a myriad of commercial products ranging from cleaning products to diapers.

Natural fragrances were once used extensively, but now a very large number of fragrances have been synthesized. It has been estimated that over 3000 synthetic organic compounds are used in the manufacture of fragrances. Analytically, it has been observed that a single fragrance can contain anywhere from ten to several hundred components. One qualitative study on thirty products showed the compounds ethanol, limonene, linalool, and myrcene to have commonality in all products.

Samples of bar soap, shampoo, and skin moisturizers (~100mg) were placed in individual test tubes (13mm x 100mm). Each sample tube was placed on a dynamic headspace station on the CDS TDA 9300 Thermal Desorber. The TDA 9300 was interfaced to a GC/MS. Figures 1,2, and 3 are respectively chromatograms of shampoo, bar soap, and hand cream volatiles. The terpene limonene as well as the unsaturated long chain alcohol linolool are present in all three samples. Acetate esters are observed in both the shampoo as well as the bar soap. The bar soap also contains the terpenes pinene and camphene.

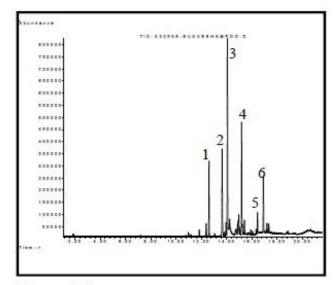


Figure 1 Shampoo

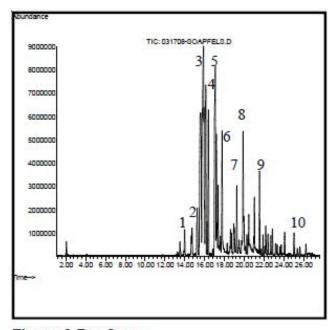


Figure 2 Bar Soap

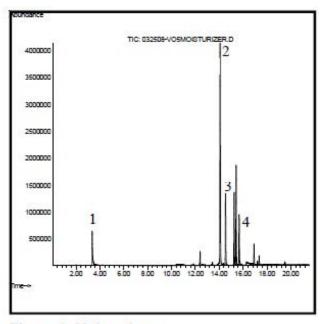


Figure 3 Moisturizer

CDS TDA 9300

Conditions

Valve Oven: 300°C
Transfer Line: 300°C 250°
Tube Heat: C/5min
Tube Cool: 0.50min
Trap Idle: 40°C 300°
Trap Heat: C/5min
Interconnect Line: 300°

C

GC/MS

Conditions

Carrier: Helium

Column: CP-Select 624

(30m x 0.25mm x

 $1.4\mu m$)

GC Program: 35°C/2min, 8°C/min

to 220°C, 5min

Figure 1 Shampoo Volatiles

- 1. Limonene
- 2. Dihydromyrcenol
- 3. Linalool
- 4. Benzyl Acetate
- 5. Benzyl Propionate
- 6. Tert-Butylcyclohexylacetate

Figure 2 Bar Soap Volatiles

- 1. Camphene
- 2. Pinene
- 3. Limonene
- 4. Eucalytptol
- 5. Terpinene
- 6. Linolool
- 7. Phenylmethyl Acetate
- 8. Terpenol
- 9. Chloroaniline
- 10. Butylated Hydroxytoluene

Figure 3 Skin Moisturizer Volatiles

- 1. Ethanol
- 2. Linalool
- 3. 1,2-Dihydrolinolool
- 4. Terpenol

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