

The Chemistry of Perfume

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Abstract

In order to understand the organic chemistry in perfume, our project was designed show the complexes of scent via a synthesis and extraction conducted in a semi-sterile lab. For this project, samples from three major brand cologne companies were extracted and then inserted in a Gas Chromatography Mass Spectrometry (GC/MS) instrument, giving us an data spectrum of substances detected within the solution of each sample.

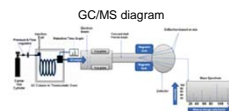
With this data, ingredients were determined and analyzed, the information provided gave us a spectrum of what molecules were used within each sample revealing the main ingredients utilized within main perfumery firms. Dior Homme cologne was selected as a sample to further conduct the research. Within the GC/MS data, approximately 40 substances were identified from the raw data.

From the 40 substances, eight of the major substances were selected. Within the raw data, several of the minute substances were found to not necessarily be essential to the structure of the perfume but rather factors more towards the scent component. Due to trademarks of the brand and high cost of each substance of the perfume, the replica was not conducted. This project was important to give a full understanding of aromatic chemistry, extraction and synthesizing of chemistry in a semi-sterile Junior College laboratory.

Materials & Methods

The GC/MS has been regarded as a gold standard" for forensic substance identification because it's used to perform a 100% specific test, which positively identifies the presence of a particular substance. It is used for the analysis of unknown organic compounds mixtures.

One critical use of this technology is to determine the composition of aromatic compounds, some naturally present in the raw materials and some forming during processing. GC-MS is extensively used for the analysis of these compounds which include esters, fatty acids, alcohols, aldehydes, and terpenes, which are found in perfumes and fragrances. The materials we used to run the solution through the GC/MS was Dior Homme (cologne) that has multiple polar compositions. The cologne was then diluted in a polar aprotic solution (acetone) which is a carbonyl. Acetone has a C=O group that can participate in hydrogen bonding allowing the solution to become miscible. Polar substance will dissolve in polar substance.



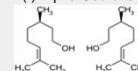
Introduction

After running the solution through the GC/MS, the graphical data showed that the cologne contains about 40 different compounds that indulges its rich fragrance.

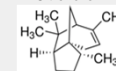
In the beginning, we were going to attempt to use 22 compounds that are listed in quantity of 80-100 to be able to mimic the fragrance. We realized that 22 compounds were too many, so we decreased the number to only 8 compounds. Due to trademark and high cost of the compounds, we were not able to afford the materials and mimic the fragrance. For example, 1 mL of (-)-Alpha-Cedrene is \$ 195.00, and 250 mg of Cis-Thujopsene is \$ 359.00.

We decided to do this project because we were inspired by one of our labs in Organic chemistry 12-A. The lab we worked on was to dissolve Aleve® (sodium naproxen). The sodium salt of the S-(+)-enantiomer smelled sweet like minty fresh, whereas the R-(-)-enantiomer smells like rye bread and it's also toxic. Both enantiomers have the same molecular formula, but they both have distinctive smells.

(-)-Alpha-Cedrene



Citronellol



Conclusion

The scent is one of the first sense, warning from dangerous substance, bringing cherished memory and attracting others. Knowing this huge effect of fragrance in modern culture the perfume industry has capitalized on it, yet perfume was dated far back to ancient Egypt where they used fragrance for health and worshipping the Gods.(Lisa,1999)

Most fragrances are aromatic; aromatic molecule has 5 to 6 ring carbon molecules with an odd number of the pi bond. The smell of this aromatic molecule is due to its structure, it relative conformation to other atoms, as well as the vibration of the molecule which get perceived by the olfactory neurons receptor. The receptor has shapes for the particular molecule where when molecule bind to the receptor. The neuron sends the signal. A human can smell up to trillion different scents (NIH,2017).

From the 40 trillion possible scent that can be detected by olfactory, a mixture of the particular compound in different ratio gives rise to a specific smell. In this experiment, we artificially try to identify the various aromatic molecule present in our colon through the use of Gas Chromatography-Mass Spectrometry GC-MS and will try to replicate the smell of the perfume through mixing particular ration of individual aromatic molecule detected by the machine.

Results

Cashmeran



Cis-Thujopsene



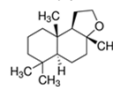
Cyclopentadecanone



The top image is the spectrum of data substances within the solution. Each peak is the relative abundance, therefore, the mass ratio of each ingredient within Dior Homme.

Each component is given a "library;" it identifies the components plausible molecular name, mass, as well as other information.

Ambrox



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Turin, Luca, and Turin Luca. "The Secret of Scent: Adventures in Perfume and the Science of Smell." *AbeBooks*. Harper Perennial, 01 Jan. 1970. Web. 05 May 2017.

MESA Program, Santa Rosa Junior College.

"Smell Disorders." *National Institutes of Health*. U.S. Department of Health and Human Services, 06 Mar. 2017. Web. 08 May 2017.

Manniche, Lisse. "Ancient Scent- An Evaluation of the Source [P1. I-II]." *Sacred Luxuries Fragrance Aromatherapy and Cosmetic in Ancient Egypt*. New York: Corner UP, 1999. 81-89. Print.