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Chemistry of Perfume and Fragrance: Aroma Molecules, Extraction Techniques, Formulation and Emerging Sustainable Approaches

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A B S T R A C T

The field of fragrance chemistry is multidisciplinary and involves organic chemistry, natural product chemistry, formulation science, analytical chemistry, and olfactory perception. Fragrances available today consist of perfume and aroma combinations that are made of synthetic and botanical raw materials and solvents, carriers and additives for obtaining a typical scent, diffusion, stability, and pervasiveness. The current paper looks into the fundamental aspects of perfume and fragrance creation, with a focus on odorants, their functional groups, structure-odor relationships and natural and synthetic raw materials, working methods, formulations, volatility, stability, and innovation. The organic compounds used in perfumes, such as alcohols, aldehydes, ketones, esters, ethers, terpenes, and carboxylic acids, are characterized by different olfactory abilities determined by the stereochemical arrangement of atoms and their structure. Natural raw materials are obtained through steam distillation, cold pressing, and extraction as well as using supercritical carbon dioxide, while synthetics produce odorants with defined chemical composition. Essential oils are ingredients of complex mixtures and fixatives affect the volatility and durability of the product. The current paper discusses the functioning of olfactory receptors, skin interaction, and importance of stability in relation to quality control of perfumes. Special attention is paid to sustainability, including studies of biotechnology, biocatalysis, metabolic disturbances, renewables, and eco-friendly synthetic methods of obtaining aroma substances. Computational approaches and artificial intelligence may support the tardy approach. Overall, the field of perfumery involves integration of different branches of science, which simplifies production and makes it environment-friendly.

Introduction

Perfume is a created combination of volatile and non-volatile essential ingredients made to yield a nice and easy-to-recognize smell. A typical perfume consists of fragrant components, a solvent and other compounds that affect thie stability, diffusion, evaporation, and persistence of the solution. Natural oils, absolutes, resins, and balsams can be blended with synthetic components, thus creating both simple and complicated mixtures. Ethanol is usually used as the main solvent, since this component can dissolve majority of odorous elements and quickly disappear from the skin. Modern science of perfumes is a highly developed field of science that has been developing as a part of research into structures and activities where chemical alterations lead to changes in smell. Thus, structure–odor relationships have gained a lot of scientific interest (Rossiter, 1996; Armanino *et al*., 2020, Sharma, 2025).

In order to reach the smell receptors, aroma molecules need to have certain physicochemical properties. It is especially important to have volatility which allows a compound to evaporate. Nonetheless, this characteristic alone cannot explain the smelling properties. Size, form, functional groups, stereochemistry, polarity, flexibility, and influence on smell receptors will influence the smell properties of a substance. Even the components with very similar structure and properties might have different smells (Rossiter, 1996; Kraft *et al*., 2000, Yadav & Kamal, 2025). As the result, modern science combines the knowledge of organic chemistry with modeling and sensory evaluation as well as receptor biology. The use of natural ingredients is still important because essential oils and plant extracts contain a lot of substances which form the overall smell profile. Their composition might depend on many factors such as oils, the conditions under which they were produced, and harvesting methods. Hence, in this present work we will analyze perfume chemistry from different perspectives including its chemical, technological, sensory, and sustainable aspects.

Chemistry and Classification of Fragrance Molecules- Fragrance molecules cover a wide range of volatile organic compounds belonging to different classes such as alcohols, aldehydes, ketones, esters, ethers, terpenes, lactones, and carboxylic acids. Notably, it is the functional group responsible for polarity of the molecule, its chemical reactivity, volatility and other phenomena, and that has an impact on its odor properties. Thus, while linalool corresponds to floral notes of the lavender, geraniol has sweet notes that smell like roses. Aldehydes are another class with different characteristics depending on their molecular structure. For instance, while cinnamaldehyde is known for its specific warm cinnamon scent, aliphatic aldehydes and their peculiarities may form fresh or waxy odors. Ketones are also important materials for perfumery and include such substances as ionones and muscone. Ionones are associated with violet and woody scents, whereas muscone is a classic musk substance. Esters usually have sweet or floral feelings. For example, isoamyl acetate is well known for its strong fruity flavor, while benzyl acetate and methyl anthranilate are used to create floral and sweet flavors. Ethers like anethole help get sweet, anisic and spicy scents. Short carboxylic acids can be sour, rancid or sweaty, which means they are not very pleasant. In their respective concentrations, though, they might produce interesting combinations. However, establishing how the molecular structure relates to the produced odor is difficult. According to Rossiter (1996), understanding this connection requires knowing the 3D structure of the molecule. Changes in the length and thickness of the chain, the presence of branches, rings, or specific stereochemistry will lead to different odor formation. The above allows saying that modern fragrance chemistry has created various families of fruity, marine, musky, and woody odors (Kraft *et al*., 2000; Armanino *et al*., 2020, Singh, 2025). At the same time, stereochemistry is of utmost importance. Enantiomers have the same molecular formula and other properties but interact with the receptors in different ways. It is obvious that the studies of rose scents confirm the above assumption. Thus, it is important to say that fragrance chemistry is not a simple process of identifying smells by their chemical composition. It is more complex and relies not only on chemistry of the substance but on the physicochemical properties of the odorant itself, its concentration, how it will be perceived by the receptor, etc.

Natural and Synthetic Fragrance Materials- Natural fragrance ingredients obtain their source primarily from flowers, leaves, fruits, seeds, roots, woods, barks, and resins. Many compounds can constitute several essential oils and extracts together, which leads to complicated sensory properties. Important natural materials include such products, as rose, jasmine, lavender, bergamot, sandal, patchouli, frankincense, benzoin, and myrrh. The resinous materials contribute such characteristics, as balsamic, woody, sweet, and earthy. People appreciate natural materials, because complex mixtures produce multidimensional smells that cannot be reached by an ordinary molecule. However, natural origin does not mean high quality, safety, and sustainability. Besides, natural materials may vary due to batch-to-batch utilization, difficulty of obtaining enough amount, oxidation effectiveness, allergen potential, and ecological issues related to intensive harvesting. Synthetic fragrance chemistry solves many of the problems. Synthetic materials can reproduce some molecules from nature, and there is an opportunity of developing novel molecular structures with new smells. The good sides of such materials include the control over purity, steadiness of composition, possibility of scalability, and optimization of volatility and diffusion. New synthetic chemistry has significantly increased the number of materials perfumers may rely on and their exploration of new olfactory architecture.

Extraction and Isolation of Natural Fragrance Compounds- Natural fragrance raw materials' quality is directly aligned with the method by which it was extracted. Fragrance molecules contain numerous components of botanical origins, which means that it is necessary to choose the extraction method wisely taking into account the volatility, thermal instability, polarity, plant material used, and the quality of final product.

Steam Distillation- Steam distillation still is widely known as an essential technology for producing essential oils. This technique employs steam which passes through plant stock causing the aromatic components to vaporize. Steam is later cooled down and the oil can be separated from the liquid. This technology works well with the volatile substances that can endure the temperature effects. Water distillation is also called steam distillation and is well known for extracting oils from the fragrant plants. The only drawback is that heat, moisture and time can change the composition of the compounds that are thermally unstable or hydrolyzed.

Cold Pressing and Solvent Extraction- The cold pressing process, or expression, is very significant in the case of citrus peels, as it makes it possible to release fragrant oils by mechanical means without heating. The volatile components remain preserved in the extraction process as well as pigments, waxes, and other non-volatile materials. The solvent extraction method is suitable for fragile flowers whose components cannot survive steam distillation. When using organic solvents, the aromatic and semi-volatile components are dissolved and concentrated for further refinement. The solvent extraction method allows obtaining a variety of odors but requires careful management of solvent recovery, residues, environmental issues, and process safety. Enfleurage is an ancient method that is now rarely used in practice; in this technique, floral volatiles are absorbed in a fatty medium. Despite this method being useful in extracting the essences of fragile flowers, a large amount of time it requires and its low effectiveness do not allow to use this method in the industry.

Supercritical CO_2 Extraction- Extraction via supercritical fluids, especially CO_2 extraction, represents a well-known alternative technique. Under its critical conditions, CO_2 has important solvent properties that can be modified in terms of pressure and temperature. CO_2 operates under low pressure and temperature and it does not leave residual elements that conventional organic solvents do (Fornari *et al*., 2012, Sah, 2025). The authors consider supercritical CO_2 extraction a new method of extraction that permits the selective extraction of oils due to various factors including temperature, pressure, and co-solvent conditions used. Later studies point out similar advantages of supercritical CO_2 in aroma extraction namely tunable selectivity, mild conditions, and decreased toxicity. Thus, extraction should be seen as not rather as a separation process but as very important process determining the chemical as well as olfactory nature of the extracted compound.

Essential Oils, Fixatives and Fragrance Architecture-Essential oils are combinations of volatile plant substances in concentrated form. The compositions of oil usually involve monoterpenes, sesquiterpenes, terpene alcohols, aldehydes, ketones, esters, phenylpropanoids, and other nearby oxygenated objects. Also, the chemical structure of each oil enables them to produce different smells. According to the traditional fragrance description, the development of a perfume can be illustrated by a pyramid, which consists of three elements: top notes, heart notes, and base notes. Top notes can be perceived immediately after application and consist of very volatile ingredients including citrus and fresh green ingredients. Heart notes come into being when very volatile elements fade away, usually characterized by a floral, fruity, or spicy smell. Base notes are made up of more stable elements such as wood, resins or musks. Despite the simplicity of the matter, real evaporation of a perfume takes place continuously complexly. Rodrigues *et al*. (2021) claim that the process can be studied using vapor – liquid equilibrium techniques, diffusion, and matrix effects, because evaporation and transportation phenomena are directly involved in forming a fragrance. Fixatives are used in perfuming to affect the stability and time process of the perfume. Natural classical materials can be resins and balsams. Recently developed chemicals can include synthetic long-life musks or woody ingredients. The fixation process cannot be understood as the act of merely locking the volatile components. The process consists of many factors such as vapor pressure, intermolecular interaction, nature of the mixture, as well as vapor effect.

Volatility, Longevity and Stability- Volatility is indicative of how easily a scent component escapes from a formula or skin into the surrounding air. Although highly volatile components play a key role in the first few minutes, they are quickly used up. Lower-volatility materials dominate over a longer period. The process depends on fragrance concentration, type of solvent, temperature, substrate, and the way different components interact. Fragrance products in the market are often categorized according to the approximate amount of aromatic materials. An equally important concept is the chemical stability of the perfume. Effects of light, moisture, oxygen and elevated temperature can change perfume composition. Esters may undergo hydrolysis, aldehydes may be oxidized and unsaturated terpenes are especially likely to autoxidize.

The project focuses on oxidation of limonene, pinene and linalool, and mentions some main degrading factors, such as light, moisture, temperature and oxygen. The oxidation of the fragrance industry's terpenes is significant from the point of view of safety and sensory properties. For instance, linalool and limonene may autoxidize upon contact with air, resulting in the formation of hydroperoxides and other products causing contact allergy in some people (Sköld *et al*., 2002; Christensson *et al*., 2009; Ogueta *et al*., 2022, Chahar, 2025). The stability can be increased by proper packaging, addition of antioxidants, light and oxygen protection, formulation improvement and proper storage.

Olfaction and Structure–Odor Perception

A smell does not have sensory meaning until the molecules are able to interact with the sense of smell. The process begins when the odor molecules reach the olfactory epithelium and a reaction occurs with the sensory neurons' odorant receptors. The first discovery of odorant receptors by Buck and Axel (1991) helped understand the molecular processes of smell recognition. The olfactory receptors belong to the superfamily of G-protein-coupled receptors. The olfactory system does not have dedicated receptors for each smell that could be experienced. Rather, the system uses the technique of combinatorial coding, whereby every molecule of odor interacts with various receptors and every receptor reacts to various odorants. The information is sent to the glomeruli of the olfactory bulb and processed in the higher centers of the brain (Buck, 2004; Antunes & Simoes de Souza, 2016). Genomic studies revealed hundreds of intact genes responsible for the olfactory receptors in humans, thus showing the huge molecular diversity of the human sense of smell (Malnic *et al*., 2004, Kumar, 2025). The mere two-dimensional molecular structure of a particular odor cannot provide any prediction for the odor. There are various factors that could influence the smell perception: molecular conformation, stereochemistry, receptor specificity, concentration, and individual biological variation (Young *et al*., 2020).

Skin Chemistry and Perfume Performance- The skin can alter the way scent works compared to the blotting paper where it has been applied or in the bottle. When perfume is put on skin, it interacts with surfaces characterized by a heterogeneous chemical composition, including sebum, sweat, lipids, proteins, water, and metabolites of microbe activity. Temperature and skin moistness can also influence processes of evaporation and diffusion. These data confirm the general idea of chemical engineering that the substrate and matrix play a significant role in fragrance evaporation and diffusion (Rodrigues *et al*., 2021). Some hydrophobic fragrance molecules can become part of skin lipids in the course of diffusion, which may delay their arrival to the receptors. Higher temperature can increase vapor pressure and diffusion. Certain individual differences in the composition of skin and microbiota can also lead to differences in the smell felt after applying the fragrance. Thus, one cannot expect to understand how the perfume works solely relying on the liquid formulation.

Perfume Formulation and Analytical Quality Control- Perfume formulation integrates chemical knowledge and sensory imagination. A perfumer chooses particular materials based on different parameters such as odor quality, intensity, volatility, persistency, stability etc. Also, the individual materials are combined into accords to create some impactful smells that differ from the smell of the ingredients individually. Analytical chemistry is crucial for this process. GC-MS allows identifying volatile components and is useful in cases such as identification of raw materials, analysis of compositions, study of degradation, etc.

Safety and Environmental Considerations- In order to evaluate the safety of fragrances, it is necessary to look at each component and its concentration levels instead of simply making a distinction between what is considered “natural” and “synthetic.” Natural plant materials may have certain irritants in them, whereas synthetic substances may need to be limited based on the toxicity profile and environmental impact of the chemical compounds. One example of why this is important is oxidation. Linalool may be a very mild allergen, but being exposed to the air leads it to cause other chemicals that are much more irritating (Sköld *et al*., 2002). The same has been recorded in literature regarding contact allergy to oxidized linalool and limonene (Christensson *et al*., 2016; Ogueta *et al*., 2022). Considering the environment here includes renewable resource consumption, land use, biodiversity, use of solvents, energy involved in the production process, waste created, the biodegradability of the product, and how long it lasts in the environment. Natural substances are not always good for the environment since the use of a lot of plant biomass or aromatic plants that have been harvested too much may produce excess waste. In turn, making synthetic production may help save the environment; however, it can also rely on the use of petrochemicals or energy using processes.

Green Chemistry, Biotechnology and Future Perspectives- Sustainability represents a new trend in fragrance chemistry research. Some current methods include using renewable raw materials, catalytic and biocatalytic reactions, fermentation, metabolic engineering, and synthetic biology. Antoniotti *et al*. (2021) demonstrated that enzymatic processing is capable of selective modifications of essential oils leading to alterations in odor and safety while promoting sustainability. The field of industrial biotechnology has developed the idea further. Michailidou (2023) considers fermentation, biocatalysis, and genetic engineering to be effective methods for reducing the environmental impact of fragrance production while maintaining high uniformity and quality. The field of biotechnology is of great interest due to the possibility of working with high-value terpenoids, which often demand a lot of efforts and resources for extraction or synthesis. Modern approaches to creating microbial factories, applying metabolic engineering and enzyme modification, pathway regulation, and synthetic biology are creating multiple ways of producing terpenoid-based aromatics. At the same time, hybrid approaches are believed to be efficient. For example, Ceccoli *et al*. (2023) proposed using both chemical and biocatalytic methods for producing rose-scented aromas and demonstrated the interconnection between conventional chemistry and biotechnology. Yet, the shift towards renewable and biodegradable fragrance chemistry is a challenging task due to the fact that sustainability differs among various fragrance families. Some substances have effective renewable routes, while others still pose significant financial challenges (Elterlein, 2024). Moreover, computational chemistry and artificial intelligence contribute to the development of fragrance products. Machine learning is supposed to connect molecular descriptors and smell properties, make suggestions on the candidate odorants, optimize compositions, and find methods for sustainable synthesis. Although it is tough to predict odor from the molecular structure because of the complexity of olfactory perception, new modeling techniques, and advances in the field of receptor biology and data science allow better predictions in this area over the course of time.

Conclusion

Perfume chemistry can be defined as an interdisciplinary field in which molecular structure, volatility, extraction and formulation, stability, and human smell all affect how a fragrance works. The role of various compounds of perfume is also essential as alcohols, aldehydes, ketones, esters, terpenes, musks, and other elements create cosmetic characteristics, nevertheless, the odor cannot be defined with the help of only functional groups. The three-dimensional molecular structure, stereochemistry, concentration, and interaction with receptors are rather important too. At the same time, natural substances include complicated and specific profiles while synthetic chemistry guarantees reproducibility of production, the scalability of techniques, and the larger olfactory palette. The methods of extraction, such as traditional distillation or supercritical CO_2, significantly impact the composition and quality of raw materials. Then, the formulation combines the ingredients into an updating system where processes of volatility, diffusion, fixation, matrix influences, and skin impact make the gradual development of scent in time. Stability and safety take the vital importance as the fragrance could undergo the process of oxidation, hydrolysis, or photochemistry. Thus, the role of such analytical techniques, as GC–MS is crucial for control. The future improvements are characterized by the development of green chemistry, renewable raw materials, biocatalysis, metabolic engineering, and computational perfume design

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