Report on the Recommendations to Replace Pthalates in Hair Relaxers

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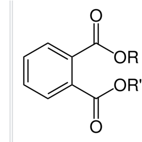
Introduction

Over the past few years, companies that make hair relaxers have come under fire through news articles and lawsuits because of the ability of their hair relaxers to cause cancer among women. Companies such as l'oreal, Dabur, and Godrej are all facing lawsuits as a result of their hair relaxer products. A class of chemicals that are often used in hair relaxers and are known to cause serious problems among women are phthalates. Phthalates are a group of chemicals with the chemical structure of two esters put in the ortho position of the benzene ring as shown in the image on the right.



Often referred to as the "everywhere chemical," phthalates are most widely used as plasticizers to help with the flexibility of plastics. Phthalates are used in hair relaxers due to their ability to stabilize fragrance and to be used as a solvent for nonpolar substances. In many hair products including hair relaxers, phthalates are often disguised in the ingredient list as "fragrance" or "parfum"; this is the case for many hair products including that of companies like the Big Sexy Hair company who are often known to have phthalates in their products. The presence of phthalates in cosmetic products including hair relaxers has become a health concern due to the potential to damage multiple organs and cause endocrine disorders. They can also harm the environment through contamination with leaching, migration and oxidation during product use and storage. Due to the hazards of phthalates, our goal was to find alternatives to phthalates in hair relaxers.

Since hair relaxers play a popular role amongst the African-American community, we partnered with Black Women for Wellness, a nonprofit looking to advocate safety among cosmetic products. By presenting our alternatives to phthalates in hair relaxers to Black Women for Wellness, we hope we can help them encourage companies who sell hair relaxers and target their products to black women to use safer alternatives so that women who feel like they need to use hair relaxers do not have to take unnecessary health risks.

	Solubility	Diffusion	Stability
Diethyl phthalate (DEP)	Insoluble in water Miscible in vegetable oil and most organic solvents	Boiling point:295 °C Vapor pressure : 0.0021 mm Hg at 25 °C	Half-life in Air : 22.2 Hours
Diethylhexyl phthalate (DEHP)	Slightly soluble in water Miscible in mineral oil	Boiling point: 384℃ Vapour pressure 10^{-7} mmHg	Evidence of time of degradation: 2 days

Table 1: Physical characteristics of predominant phthalates in hair products.
The two main phthalates found in hair products are DEP and DEHP. Both present low volatility (Observed in their low vapour pressure) which is favorable for stabilizing volatile particles.

Approach

The first step we took was to define the problem clearly: hair relaxers had unpleasant odors that needed to be addressed. Next, we set a specific goal for our project: to replace phthalates in the formulation of hair relaxers. Phthalates served multiple functions in the industry, but our primary focus was on their role as scent stabilizers and carriers. We wanted to find alternatives that could fulfill these functions effectively.

To tackle this problem, we devised two strategies. First, we aimed to find a complete replacement for phthalates by identifying a chemical compound capable of carrying a scent and prolonging its longevity. Second, we explored the possibility of eliminating the need for phthalates altogether by introducing stable fragrances into the formulation that did not require a stabilizer.

Our approach involved focusing on naturally occurring chemicals that could meet our requirements. For potential replacements of phthalates, we delved into the study of fixatives, which are a family of chemicals known to reduce the rate of evaporation[(1)]. Additionally, in our pursuit of stable fragrances, we searched for naturally derived scents that possessed long-lasting qualities. We discovered that these natural scents shared characteristics such as low volatility and high solubility.

With our criteria in mind, we proceeded to build a library of candidate chemicals that could fulfill either of the two approaches we had developed. We meticulously assessed each candidate for potential hazards, considering both their physical properties (volatility, solubility, molecule size) and their safety profiles using databases such as pharos. Additionally, we conducted a second assessment using greenscreen assessments to familiarize ourselves with how the hazards and safety of the candidates were evaluated.

During our investigation, we realized that the studies conducted on the candidates were based on concentrations higher than what we needed for our specific application. As a result, we established a range of concentrations for each candidate based on the weight percentage found in formulations of other hygiene products where they served similar roles as scents or scent stabilizers. We also determined a range of concentrations where there were no indications of hazards, ensuring safety in our formulation.[(2)(3)]

	Octyl alcohol	Tea tree oil
Weight % in formulation for other industries (skincare)	0.08% - 0.4%	1% - 40%
European cosmetic regulation (COLIPA)	2%	1%
Safe concentrations	4%	5%

Table 2: Concentrations of Octyl alcohol and Tea tree oil found in scented products.
The percent weight was determined using the information available on existing products. The following values are retrieved from COLIPA, and greenscreen assesments

Strategies and comparative assessment

Strategy 1: Octyl Alcohol

Technical Performance

Octyl alcohol belongs to the family of chemicals known as fatty alcohols. Positioned between short alcohols with oily and colorless characteristics and long-chain alcohols that function as emulsifiers, octyl alcohol possesses properties that bridge both subcategories. This compound is characterized by its non-volatile nature, allowing it to retain its scent for an extended period. In the past, octyl alcohol has found applications in the skincare and permufary industry.

The mechanism of action for octyl alcohol involves its interaction with scents through various intermolecular forces, such as hydrogen bonds, polar interactions, and van der Waals forces. The carbon chain present in the alcohol enhances the solubility of the scent and imparts stability to its molecular structure. As a result, the volatility of the scent is effectively regulated, ensuring a long-lasting aroma within the formulation. Octyl alcohol's unique properties make it suitable for achieving the desired longevity and scent profile in various products.

Additionally, it is important to note that the interaction between octyl alcohol and scents is highly dependent on the specific characteristics of the scent molecules themselves. Different scents may exhibit varying affinities for octyl alcohol or other fatty alcohols. Therefore, conducting studies to determine which scents work best in conjunction with octyl alcohol or other specific fatty alcohols is crucial.

	Solubility	Diffusion	Stability
Octyl Alcohol	Soluble in : Alcohol, fixed oils, propylene glycol, water, 814 mg/L @ 25 °C (est)	Boiling Point: 195°C Vapor pressure: 0.13 mm Hg (25C)	Shelf Life: 24 - 36 Months store below 25 C Scent life: 92 hours at 100.00 %

Table 3: Technical Performance for Octyl alcohol.
Octyl alcohol has good solubility in alcohol, fixed oils, propylene glycol, and water, with an estimated solubility of 814 mg/L at 25 °C. It has a boiling point of 195°C and a vapor pressure of 0.13 mm Hg at 25°C. The shelf life of octyl alcohol is 24-36 months when stored below 25°C. It has a scent life of 92 hours at 100.00%.

Considering the purpose of using octyl alcohol as a scent stabilizer, it can be noted that octyl alcohol possesses good solubility in various solvents, including alcohol and water. Its stability, as indicated by its boiling point, vapor pressure, and shelf life, suggests that it can effectively contribute to scent stability over an extended period. However, further evaluation is required to assess the specific role of octyl alcohol as a scent stabilizer and its compatibility with different fragrances.[4]

Health and Environmental Performance:

Improved Health and Safety:

Octyl alcohol, a long-chain fatty alcohol derived from vegetable sources, has the potential to improve the safety of hair relaxer products by replacing phthalates, which have been associated with various health concerns, such as endocrine disruption and reproductive issues. As a naturally derived compound and a long-chained fatty alcohol, octyl alcohol is generally considered to be safer and less toxic, offering a more sustainable and health-conscious alternative for scent stabilization.

Hazards Associated with Octyl Alcohol:

Health Hazards

Flammability (H227): Octyl alcohol is classified as a combustible liquid. 2-Ethylhexanol has a flashpoint between 73 and 82°C: following GHS criteria, chemicals with a flashpoint between 60 and 93°C are considered a Category 4 flammable liquid[(5)]. This means it can catch on fire at certain temperatures, posing a risk of burns or fire-related injuries if not properly handled. In the context of a salon setting, this poses a significant hazard due to the common use of high-heat appliances, such as hair straighteners and hair dryers. These devices can easily exceed the flashpoint of octyl alcohol, especially if the hair relaxer is still in liquid form on the hair. In addition, many salons are also relatively confined spaces, which can allow for the buildup of flammable vapors if there is inadequate ventilation. If a source of ignition (like a hot hair straightener or dryer) comes into contact with these vapors, it could potentially cause a fire.

Neurotoxicity, Single Exposure (H336): Octyl alcohol falls under the GHS Category 3 for single exposure neurotoxicity. This classification indicates that exposure to this substance may lead to neurological effects such as drowsiness or dizziness[(5)]. In the context of a salon setting, this represents a significant hazard. Salons are often enclosed spaces with limited ventilation, potentially leading to an accumulation of octyl alcohol vapors, especially during the application of hair relaxers or other products containing this substance. Salon workers and customers alike could inhale these vapors, leading to the aforementioned neurological effects.

Reproductive and Developmental Toxicity (H361): Octyl alcohol is suspected of damaging fertility or the unborn child, falling under the GHS H361 hazard category. This means there is evidence from animal studies that it could adversely affect reproduction or development, but there are currently no adequate and well-controlled studies in humans to confirm this risk[(5)]. In addition to this, octyl alcohol is categorized under Pregnancy Risk Group C. This classification indicates that risk cannot be ruled out; animal reproduction studies have shown an adverse effect on the fetus and there are no adequate and well-controlled studies in humans[(6)]. In a salon setting, this hazard might not be as prevalent as others since the main route of exposure that leads to this risk is through oral application, not topical. Topical application refers to application on the skin, whereas oral application refers to ingestion. Therefore, as long as salon workers and customers are not ingesting products containing octyl alcohol, the risk of reproductive and developmental toxicity should be minimal.

Systemic Toxicity (H371): Octyl alcohol is classified under the GHS H371 hazard category, indicating that it may cause damage to organs, particularly if ingested. Systemic toxicity refers to the potential for a substance to affect various body systems or organs when introduced into the body. The oral LD50 values for octyl alcohol fall between 300 and 2,000 mg/kg(7). LD50, or the lethal dose for 50% of the test population, is a measure used to assess the toxicity of a substance. These values indicate that this is the dose at which half of the test subjects would die if the substance were ingested. The fact that no effects have been reported within the 10 to 100 mg/kg guidance for skin formulation values suggests that the risk of systemic toxicity is moderate to low at these doses(5). In a salon setting, the risk of systemic toxicity due to octyl alcohol is primarily related to oral ingestion. Since salon products containing octyl alcohol are typically applied topically (on the skin) and not orally, the risk of systemic toxicity in this context should be minimal, provided that safety precautions are observed.

Skin Irritation/Corrosivity (H315): Octyl alcohol is classified under the GHS H315 hazard category(5). This indicates that it can cause skin irritation or burns, particularly at high concentrations. In the context of a salon setting, products containing octyl alcohol, such as certain hair relaxers or skin creams, may come into direct contact with the skin of both salon workers and customers. However, the current industry-approved concentration of octyl alcohol used in skin formulations is less than 4%, which is considered insignificant for causing skin irritation or burns(5). The reason it is considered safe to use octyl alcohol in skin products at lower concentrations is related to the principle of dose-response in toxicology, which essentially means that the effect of a substance on the body is related to the amount (or dose) of that substance. At lower concentrations, the dose of octyl alcohol that the skin is exposed to is reduced, thereby reducing the likelihood and severity of skin irritation or burns. This implies that while the potential for skin irritation or burns exists, the risk is relatively low provided that the concentration of octyl alcohol in the products used remains under 4%(5). This level has been deemed safe for topical use, suggesting that products containing octyl alcohol at these concentrations can be used without significant risk of skin irritation or burns.

Eye Irritation/Corrosivity (H319): Octyl alcohol is classified under the GHS H319 hazard category, indicating that it can cause serious eye irritation(5). This classification is based on experimental data, including an acute eye irritation/corrosion study (OECD 405) using rabbits(8). In this study, the compound demonstrated scores of 1.44 for corneal opacity and 2.56 for conjunctival redness. According to GHS criteria, a score above 1 for corneal opacity and above 2 for conjunctival redness classifies this chemical as a Category 2A eye irritant. These scores represent changes in the eye that were observed following exposure to octyl alcohol, with corneal opacity referring to cloudiness or loss of transparency of the cornea, and conjunctival redness referring to redness or inflammation of the conjunctiva, the mucous membrane that covers the front of the eye and lines the inside of the eyelids(9). This suggests that the substance has the potential to cause discomfort, redness, or even damage when it comes into contact with the eyes. In a salon setting, this risk could be present when salon workers handle products containing octyl alcohol or apply them to customers. In particular, activities such as mixing, pouring, or applying these products could potentially result in splashes or droplets that could reach the eyes. Similarly, customers could inadvertently touch their eyes with their hands after they've been in contact with these products.

Environmental Hazards

Acute Aquatic Toxicity (H401): Octyl alcohol has been classified as being toxic to aquatic life, scoring moderate (M) for acute aquatic toxicity. This classification is based on L/EC50 values (the concentration of the substance that is lethal or causes certain effects in 50% of the tested organisms) identified between 10 and 100 mg/L[5]. These values fall within the cutoffs for moderate acute aquatic toxicity. Multiple studies have indicated the toxic effects of octyl alcohol on various aquatic organisms, such as fish and algae[5]. These findings highlight the potential environmental hazard posed by octyl alcohol and the importance of proper disposal and containment measures to prevent the substance from entering aquatic environments. In a salon setting, this could involve ensuring that products containing octyl alcohol are not washed down the drain, and that any waste containing the substance is disposed of in a way that minimizes its potential to reach bodies of water. Training and education for staff about the potential environmental impacts of the substances they work with would also be beneficial.

Benefits Associated with Octyl Alcohol:

When comparing octyl alcohol and phthalates as ingredients in hair relaxers, there are several distinct advantages that favor the use of octyl alcohol.

Health Benefits

Safety is a paramount concern in any personal care product. Octyl alcohol excels in this area, especially when compared to phthalates. Unlike phthalates, octyl alcohol is not an endocrine disruptor and poses minimal systemic toxicity[10]. Furthermore, extensive research and literature suggest no potential for carcinogenicity or mutagenicity with octyl alcohol use[5].

The safety and effects of octyl alcohol have been extensively studied due to its widespread use in the cosmetic industry. Long-chain fatty alcohols, such as octyl alcohol, are known to have several caring benefits for hair and skin. Various concentrations have been observed and tested, from 1% to 15% of formulation weight, with the maximum reported concentration for 2-ethylhexyl esters in lotions and creams being 5%[11].

Acting as an emollient, octyl alcohol is beneficial for hair conditioning. Long-chain fatty alcohols like octyl alcohol interact with the hair surface, resulting in a hydrated, smooth, and soft hair feel[4]. As an emollient, it forms a protective film over the skin and hair, reducing water loss and helping to maintain hydration. Furthermore, its higher molecular weight means it does not easily penetrate the skin, thereby avoiding drying effects[12].

Environmental Benefits

Environmental considerations also favor octyl alcohol over phthalates. Although harmful to aquatic life, any release into the aquatic environment is anticipated to have a minimal effect, as the substance will degrade quickly and has a low potential for bioaccumulation[5]. The

LogKow value of 2.74, being less than 4, signifies a very low potential for bioaccumulation[6]. It has high solubility in water and, if accidentally released to soil or water, moderate volatilization to the atmosphere can be anticipated[6]. The substance is not considered to be persistent, bioaccumulating, and toxic (PBT) or very persistent and very bioaccumulating (vPvB)[5]. Phthalates, on the other hand, have been associated with environmental concerns, including highly adverse effects on wildlife and ecosystems[10].

Benefits of Technical Performance in Formulation

Octyl alcohol plays a crucial role in stabilizing hair products. Acting as a stabilizer, it ensures that beauty products do not spoil or separate between the time of production and their eventual purchase and use by the consumer[12]. This characteristic is particularly beneficial in products that comprise both water and oil, as octyl alcohol effectively prevents these from separating. Moreover, it mitigates the tendency of products to foam when shaken, providing a more consistent, reliable product[12].

Octyl alcohol enhances the texture of hair products. As a fatty alcohol, it possesses thickening properties that bestow upon products a rich and creamy consistency[12]. This property not only improves the tactile experience of using the product but can also facilitate more even application and better coverage[11].

Octyl alcohol also boasts broad applicability in the creation of numerous solvents, flavors, and fragrances. It is already manufactured on a vast scale for a variety of applications, with a group of 16 chemicals consisting of octyl alcohol esters of selected fatty acids which are widely used in cosmetics and domestic products available for consumers[11]. This extensive use and versatility further underscore the chemical's value as a scent stabilizer in hair relaxers.

Unknowns and Next Steps:

While there are several known benefits and characteristics of octyl alcohol that make it an attractive ingredient for use in hair relaxer formulations, there are still some areas that require further investigation and exploration. Based on our previous research, we recommend the following to be studied more closely for better confidence in the safety of octyl alcohol in formulation:

Dermal absorption at higher concentrations: While the low dermal absorption potential of octyl alcohol is well-documented at the concentrations currently used in cosmetics (no higher than 15%), more research is needed to understand the potential risks and effects of higher concentrations on the skin and systemic health.

Long-term exposure effects: Most of the available safety data are based on short-term or single exposure studies. Comprehensive long-term exposure studies, particularly with respect to repeated use in hair care products, are needed to fully understand any potential risks associated with chronic use.

Impact on sensitive populations: Additional research is needed to understand how octyl alcohol may affect sensitive populations, such as individuals with skin conditions, pregnant women, the elderly, and children.

Environmental impact: While octyl alcohol is readily biodegradable and not expected to be bioaccumulative, further study is needed to understand its full environmental impact, particularly in relation to its use in consumer products that are washed down drains and can enter aquatic ecosystems.

Formulation interactions: The intricacies of octyl alcohol's interactions within hair relaxer formulations merit further investigation. This includes understanding how octyl alcohol cooperates with other ingredients in these formulations. Of particular interest is the interplay between octyl alcohol and specific scent molecules. Each fragrance has its unique characteristics that could interact differently with octyl alcohol, underscoring the necessity for more comprehensive research to establish the compatibility between octyl alcohol and a wide array of fragrances. These complex interactions could have far-reaching implications, potentially influencing not just the safety profile of the product, but also its effectiveness and the overall user experience.

Strategy 2: Tea Tree Oil

Technical Performance

Table of the technical performance of tea tree oil

	Solubility	Diffusion	Stability
Tea tree oil	**Water soluble component:** terpinen-4-ol 387 mg/L soluble in water @ 25 °C[13]. **Components soluble in ethanol and fixed orders:** α-terpinene 100 mg/ml[14], γ-Terpinene is miscible in ethanol[15]. **To conclude:** Overall, tea tree oil is mostly insoluble in water and is soluble in 85 % ethanol[16].	**Boiling Point**: 211.00 to 213.00 °C for terpinen-4-ol[17]. **Vapor Pressure**:0.048mmHg @ 25.00 °C[17] for terpinen-4-ol[17]. **To Conclude:** -Terpenes in tea oil are known to be volatile but stable enough to produce lasting fragrance	-Shelf life: 1 - 3 years[18]. - Stored at stable temperature below 25 °C[18]. -Reactivity: require additional formulation tweaks to solubilize

Table 4: Technical Performance of Tea Tree Oil.
Tea tree oil is mostly insoluble in water but soluble in 85% ethanol. The water-soluble component, terpinen-4-ol, has a solubility of 387 mg/L in water at 25 °C. α-terpinene is soluble in ethanol at a concentration of 100 mg/ml, while γ-terpinene is miscible in ethanol. Tea tree oil has a boiling point range of 211.00 to 213.00 °C, and the vapor pressure of terpinen-4-ol is 0.048 mmHg at 25 °C. The shelf life of tea tree oil is typically 1-3 years when stored below 25 °C. The terpenes in tea tree oil are volatile but stable enough to produce a lasting fragrance. Additional formulation tweaks may be necessary to enhance solubility.

Summary of technical performance of tea tree oil

Overall, evaluating the technical performance of tea tree oil can be difficult because tea tree oil is composed of a lot of different chemicals and the percent composition of those chemicals in tea tree oil can vary. According to a paper that examined a large amount of tea tree oil, the main three components of tea tree oil are terpinen-4-ol, γ-Terpinene, and α-terpinene[19]. Therefore, when looking at solubility we examine the solubility of these three components. As shown above terpinen-4-ol is the water soluble component in tree oil but γ-Terpinene and α-Terpinene are considered to be insoluble in water and soluble in organic solvents like ethanol. Tea tree oil as whole is mostly sold in 85% ethanol and is mostly soluble in organic solvents like phthalates. However there is water soluble tree oil that is sold but involves a complex chemical process in its formulation. When examining the boiling point of tea tree oil we used terpinen-4-ol as an approximate value since it is the predominant component of tea tree oil and comprises about 40% of tree oil. The boiling point for tea tree oil is slightly lower than phthalates which have boiling points closer to 300 °C. This is mostly likely due to the fact that the terpinen-4-ol and the other terpenes in tea oil are slightly more volatile causing a decrease in the boiling point. Our goal is to have a fragrance that vaporizes at a slow rate so the scent can last longer which might be a concern for tea tree oil. However, the antioxidants especially of tea tree oil can prevent degradation of the scent by preventing radicals to be produced as a result of oxidation leading to a more lasting fragrance in the air[20]. Tea tree oil also has a high shelf life which is good but must be stored in stable conditions. Another concern from a technical perspective is that according to the head chemist in loreal Siva Muthukrishnan tea oil can be reactive to fatty acids which cause a problem in the production process. However it is important to mention that due to the fact that tea tree oil is composed of many chemicals, the % percent composition of those chemicals can be varied to best apply the oil in formulation.

Health and Environmental Performance

Health Hazards

Notable health hazards of tea tree oil are for skin sensitization and irritation (Skin irritation category 2) and eye irritation (Eye irritation category 2)[21]. Direct contact with pure tea tree oil to the skin can cause skin irritation, allergic skin rash (dermatitis), itching, stinging, burning, scaling, redness, and or dryness[22]. However, these hazards are a strong concern only at high concentrations, well above the expected amount to be used in personal care products. Only a small amount of tea tree oil is needed to perform its function in a hair relaxer, which is to impact a fragrance to the product. The irritation of tea tree oil in the concentrations found in personal care products can be comparable to mint oil in shampoos and other personal care products. It would be uncomfortable to get in the eyes, but should not cause damage as long as it is flushed with water or tears. Tea tree oil is already used in skin care, including skin care products for the face, so there is an expectation that some could get into or near the eyes.

Fragrances such as tea tree oil can trigger allergic reactions such as hives or ezcema[22]. People with sensitive skin or eczema prone skin are generally advised to avoid fragrances altogether. Oxidized tea tree oil and expired products containing tea tree oil should be discarded because oxidized tea tree oil is known to cause conditions such as contact dermatitis and skin irritation[20]. Tea tree oil has a shelf life of 1-2 years, and should be discarded if it smells off, since that is a sign that it is oxidized and may cause adverse reactions on contact. Otherwise, tea tree oil is generally well tolerated by most skin types[19], but one should patch test new products that will be on your skin because everyone is different.

Tea tree oil carries a moderate flammability risk of Flammable liquids category 3[21].

There is also the concern of the poisonous quality of tea tree oil when consumed orally, with the potential to cause developmental toxicity and acute toxicity[23]. Other possible effects of oral consumption are neurotoxic symptoms such as confusion, lack of muscle control or coordination of voluntary movements (ataxia), and decreasing levels of consciousness[22]. It is expected that since hair relaxers are for topical use along with the low concentrations expected to be used in the product, this hazard will not be as relevant. However this means tea tree oil and tea tree oil products should be kept away from young children who could accidentally ingest them. There is also a respiratory risk to inhaling tea tree oil for prolonged periods of time because tea tree oil is a volatile compound[(24)(25)]. It is relatively unknown how this characteristic would be like in a cream formulation, but tea tree oil should not be used in aerosol formulations to reduce the likelihood of inhaling large amounts of tea tree oil. This is especially pertinent for salon workers, who can work with hair products for hours at a time.

It is important to note that most of the studies done on the hazards of tea tree oil is performed on pure tea tree oil, a very concentrated substance compared to the amounts expected to be used in personal care and hygiene products. It is relatively unknown what the effects of tea tree oil would be in a 5% concentration in a product like shampoos and hair relaxers. For example, would the respiratory risk be to the same degree since the tea tree oil incorporated into a formulation as opposed to being in its pure form? Thus more research is needed on the hazards of tea tree oil in formulation.

Health Benefits

Studies have shown that tea tree oil can provide many benefits to the hair and scalp such as treating dandruff and improving scalp health[26]. Tea tree oil is also known to have antimicrobial, antibacterial, and anti-inflammatory properties.

Endocrine Disruptor Studies

The reccommendation that tea tree oil and products containing tea tree oil should not be used on children under 12 years of age[22] comes from a study in 2019 called “Lavender Products Associated With Premature Thelarche and Prepubertal Gynecomastia: Case Reports and Endocrine- Disrupting Chemical Activities”[27]. The study found that there may be a correlation between lavender oil and tea tree oil use with endocrine disorders in children, specifically male gynecomastia. A review in 2020 called “The relationship between lavender and tea tree essential oils and pediatric endocrine disorders: A systematic review of the literature” studied the incidences of endocrine disorders and tea tree and lavender oil use and found a total of 11 cases across 4 papers[28]. The review concluded that there was little to no evidence to substantiate the claims but more research needed on the topic. And so in 2021, a statistical study with a sample size of 556 children called “Prevalence of endocrine disorders among children exposed to Lavender Essential Oil and Tea Tree Essential Oils”[29]. The paper contradicted the claim of the 2019 paper and found little to no evidence for the claims of tea tree oil or lavender oil causing or increasing the incidence of endocrine disorders in children. Considering the large sample size compared to the original papers, it is unlikely that tea tree oil carries an endocrine risk, but further research should be conducted.

Environmental Hazards

Pure tea tree oil carries a high risk to both aquatic and terrestrial life. Ecotoxicity data available indicate that TTO is toxic to some insect species but more studies are required[23]. It is advised within essential oil circles to not dispose of pure essential oil down the drain due to its potential to cause harm to aquatic life. It should be either landfilled or disposed of as chemical waste[25]. A spill of pure tea tree oil in the quantities found in manufacturing would be a significant biohazard that would require intervention[25]. However, for consumers, there is a low probability of causing environmental damage when the product is washed down the drain due to the expected concentration to be used in hair products. Tea tree oil is generally thought to have a low risk of bioaccumulation. Tea tree oil is composed of many compounds, so it is difficult to obtain a comprehensive $\log K_{OW}$ value, but the average $\log K_{OW}$ of the components sits around 4 (Appendix 2)[19] so it is unlikely to cause any long term damage to the environment.

The production of tea tree oil is considered to be environmentally intensive due to the amount of plant matter needed to produce the oil. It is estimated that 100kg of leaves is needed to produce 1 liter of oil[30].

Unknowns and next steps

Tea tree oil is a very potent scent and any products with the compound will smell like it. This will restrict the creative freedom of product developers and the variety of scents on the market. More research should be done on other stable fragrances that can be used. More research must be done on the hazards of tea tree oil in formulation opposed to the pure essential oil form.

Recommendations: Summarize your final recommended solutions. Clearly present the advantages and disadvantages of each solution, along with the key remaining questions. We recommend that you create a summary chart or scorecard that shows relative feasibility and hazard of each solution relative to the baseline.

Summary of final recommended solution

Our final recommended solution was to move forward with octyl alcohol as a viable and effective substitute. Some popular uses for this solution center around the production of detergents and other cleaners. The primary reason octyl alcohol serves as a more suitable substitute is due to its flexibility. In addition, it provides stability to scent in a similar way to phthalates.

Advantages and Disadvantages

Octyl Alcohol:

Advantages: Works for stabilizing scents, Existing use in cosmetics, An emulsifier and solvent that gives many functions to replace phthalates.

Disadvantages: Harmful interactions with other chemicals.

Tea Tree Oil:

Advantages: Existing widespread use for cosmetics and personal care products, Historical use by the indigenous as an antiseptic, Used to help treat various conditions.

Disadvantages: Allergenic effects of oxidation products, Potential for skin irritation.

Phthalates:

Advantages: Can increase flexibility, transparency, durability, and longevity in plastics, Do not evaporate easily, Low temperature performance, Low-cost, Low Volatility, Heat resistant.

Disadvantages: Known endocrine disruptors, Known to cause breast cancer, Can damage the liver, kidneys, lungs, and reproductive system.

Comparison of technical performance

Octyl alcohol

Octyl alcohol exhibits good solubility in various solvents, including alcohol, fixed oils, propylene glycol, and water. Its stability, as indicated by its boiling point, vapor pressure, and shelf life, suggests that it can contribute to scent stability over an extended period. It is worth noting that the interaction between octyl alcohol and scents is influenced by the specific characteristics of the scent molecules, highlighting the need for further studies to determine the compatibility between different scents and octyl alcohol.

In contrast, when considering tea tree oil as a scent option, it presents challenges. While tea tree oil has antimicrobial and anti-inflammatory properties and can provide benefits for the hair and scalp, its technical performance as a scent stabilizer is limited. Tea tree oil is mostly insoluble in water and requires organic solvents like ethanol for solubility. Its boiling point is slightly lower than phthalates, indicating a potentially faster rate of scent vaporization. Moreover, tea tree oil has a high shelf life, but its volatile nature may limit its ability to maintain a long-lasting fragrance. Additionally, there are health concerns associated with tea tree oil, including skin sensitization, eye irritation, and potential allergic reactions. Its potential hazards when consumed orally and respiratory risks when inhaled for prolonged periods further raise concerns. The environmental impact of tea tree oil production and its strong, distinct scent that may limit fragrance variety are additional considerations.

Tea Tree Oil

When comparing tea tree oil to octyl alcohol it seems that octyl alcohol might provide a better one-one alternative considering that tea tree oil is a more complex system and it would be harder to apply it in the production process of tea tree oil. However the volatility of tea tree oil is more comparable to DEP ,which is used alot in cosmetics, compared to the higher volatility of octyl alcohol. We want a compound that is only moderately volatile so it can release fragrance for a longer period of time and not a molecule that is too voltitle. On the other hand, Octyl alcohol is also very comparable to phthalates in its uses since it is also used as a plasticizer whereas tea tree oil does not have the properties of a plasticizer. Currently it seems that octyl alcohol is the better alternative due to the fact that it is a simpler molecule that is better able function in the chemical system of the hair relaxer.

Hazards Summary

Common name or trade name	CAS Number	Group I Human Endpoints			Group II and Group II* Endpoints			Ecotoxicity	Fate	Physical Hazard
		Carcinogenicity / Mutagenicity	Developmental and Reproductive Toxicity	Endocrine Activity	Systemic Toxicity	Neurotoxicity	Skin, Eye, Respiratory Irritation/ Sensitization	Aquatic Toxicity Acute/chronic	Persistence Bioaccumulation	Reactivity, flammability / Other Pchem traits
Octyl alcohol (2-ethyl-1-hexanol)	104-76-7	Low: no evidence of carcinogenic effects following 2-year and 18 month carcinogenicity studies	Moderate: GHS Category 2 reproductive toxicant.	-	Moderate to low: oral LD50 values between 300 and 2,000 mg/kg, no effects reported within the 10 to 100 mg/kg recommended guidance values	-	High to moderate: corneal opacity and conjunctival redness, Category 2A eye irritant.	Moderate to low: L/EC50 values identified between 10 and 100 mg/L, readily biodegradable and not expected to bioaccumulate	Very low: readily biodegradable within a 10-day window, LogKow = 2.74 < 4	Moderate to low: Moderate for flammability (flashpoint between 73 and 82°C), no high energy bonds or oxidizing species
Tea Tree Oil (4-Terpineol)	562-74-3	Low: not genotoxic	pC: Potential to be developmentally toxic if ingested in high doses; Minimum oral POD: 20 mg/kg-day (developmental, oral)	-	Moderate: Harmful if inhaled (unverified); acutely toxic if ngested - Category · (high dose)	-	High: Causes skin irritation (unverified), Causes serious eye irritation (unverified); concentrated form	High: acute aquatic + terrestrial toxicity; can be used as pesticide in concentrated dose	LogKow = 3.16, <4, unlikely to bioaccumulate	Moderate: H227: Combustible liquid (Flammable)
Phthalates	117-81-7	High: CA EPA - Prop 65	High: May damage fertility. May damage the unborn child	High: endocrine disrupting properties cause serious effects to the environment or human health	High to moderate: May cause damage to organs through prolonged or repeated exposure	pC: neurotoxic	Moderate: Asthma - allergen, sensitizer - limited evidence, Causes serious eye irritation	Very high: Very toxic to aquatic life, Chronic aquatic toxicity - TSCA Criteria met	Very High: logKow = 7.53 >5.0	-

Figure 1: Summarized Hazard table for Octyl Alcohol, Tea Tree Oil, and Phtalates.
Octyl alcohol presents a safer alternative to phthalates in hair relaxers, particularly regarding health hazards. Unlike phthalates, which have been associated with endocrine disruption and reproductive issues, octyl alcohol derived from vegetable sources is considered less toxic and poses minimal systemic toxicity. It offers a more sustainable and health-conscious option for scent stabilization. On the other hand, tea tree oil carries potential risks of skin irritation, allergenic effects of oxidation products, and eye irritation. Octyl alcohol's lower health hazards make it a preferable choice for replacing phthalates in hair relaxers.

Financial Analysis

Production costs:

Octyl Alcohol: $7.00 per fl oz. to produce
Tea Tree Oil: $3.65 per fl oz. to produce

Current Company Examples:

Paul Mitchell Tea Tree Special Shampoo (6 on EWG)
Avalon Organics Scalp Treatment Tea Tree Shampoo (EWG Verified)

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Appendixes

Appendix 1: Complete Hazard Table

Common name or trade name	CAS Number	Group I Human Endpoints			Group II and Group II* Endpoints			Ecotoxicity	Fate	Physical Hazard
		Carcinogenicity / Mutagenicity	Developmental and Reproductive Toxicity	Endocrine Activity	Systemic Toxicity	Neurotoxicity	Skin, Eye, Respiratory Irritation/ Sensitization	Aquatic Toxicity Acute/chronic	Persistence Bioaccumulation	Reactivity, flammability / Other Pchem traits
Phthalates	117-81-7	High: CA EPA - Prop 65	High: May damage fertility. May damage the unborn child	High: endocrine disrupting properties cause serious effects to the environment or human health	High to moderate: May cause damage to organs through prolonged or repeated exposure	pC: neurotoxic	Moderate: Asthma - allergen, sensitizer - limited evidence, Causes serious eye irritation	Very high: Very toxic to aquatic life, Chronic aquatic toxicity - TSCA Criteria met	Very High: logKow = 7.53 >5.0	-
Glyoxylic acid	298-12-4	-	-	-	pC: Acute Mammalian Toxicity	-	Very high: Skin corrosion category 1C, Causes serious eye damage	Moderate: Harmful to aquatic life	U: Class 1 - Low Hazard to Waters	pC: May be corrosive to metals (unverified)
Eschscholzia californica (California poppy)	90028-46-9	-	-	-	-	-	-	-	-	-
TEC	77-93-0	pC: May cause cancer, May cause genetic defects	pC: Suspected of damaging fertility or the unborn child (modeled)	-	pC: Harmful if inhaled (unverified)	-	-	-	U: Class 1 - Low Hazard to Waters	pC: Extremely flammable gas (unverified)
DEHA, Diethylhexyl Adipate (bis(2-ethylhexyl) adipate)	103-23-1	Moderate: US EPA - IRIS Carcinogens (1986) Group C, Possible human Carcinogen	pC: Suspected of damaging fertility or the unborn child (modeled)	High to moderate: Potential Endocrine Disruptor	-	-	pC: Causes skin irritation (unverified), Causes serious eye irritation (unverified)	Very high: Hazardous to the aquatic environment, Inherently Toxic in the Environment (iTE)	pC: Low environmental persistence, Low bioaccumulation potential	-
Octyl alcohol (2-ethyl-1-hexanol)	104-76-7	Low: no evidence of carcinogenic effects following 2-year and 18 month carcinogenicity studies	Moderate: GHS Category 2 reproductive toxicant.	-	Moderate to low: oral LD50 values between 300 and 2,000 mg/kg, no effects reported within the 10 to 100 mg/kg recommended guidance values	-	High to moderate: corneal opacity and conjunctival redness, Category 2A eye irritant.	Moderate to low: L/EC50 values identified between 10 and 100 mg/L, readily biodegradable and not expected to bioaccumulate	Very low: readily biodegradable within a 10-day window, LogKow = 2.74 < 4	Moderate to low: Moderate for flammability (flashpoint between 73 and 82°C), no high energy bonds or oxidizing species
Tea Tree Oil	68647-73-4	Low: not genotoxic	pC: Potential to be developmentally toxic if ingested in high doses; Minimum oral POD: 20 mg/kg-day (developmental, oral)	-	Moderate: Harmful if inhaled (unverified); acutely toxic if ingested - Category 4 (high dose)	-	High: Causes skin irritation (unverified), Causes serious eye irritation (unverified); concentrated form	High: acute aquatic + terrestrial toxicity; can be used as pesticide in concentrated dose	LogKow = 3.16, <4, unlikely to bioaccumulate	Moderate: H227: Combustible liquid (Flammable)

Key:

- Very high
- High to moderate
- Moderate
- Moderate to low
- Low / Very low
- pC = potential concern, U = unspecified

Appendix 2: Log K_{ow} of TTO components

TABLE 2.

Properties of TTO components

Component	Type of compound	Chemical formula	Solubility (ppm)[a]	Log K_{OW}[b]
Terpinen-4-ol	Monocyclic terpene alcohol	$C_{10}H_{18}O$	1,491	3.26
γ-Terpinene	Monocyclic terpene	$C_{10}H_{16}$	1.0	4.36
α-Terpinene	Monocyclic terpene	$C_{10}H_{16}$	8.2	4.25
1,8-Cineole	Monocyclic terpene alcohol	$C_{10}H_{18}O$	907	2.84
α-Terpinolene	Monocyclic terpene	$C_{10}H_{16}$	4.3	4.24
ρ-Cymene	Monocyclic terpene	$C_{10}H_{14}$	6.2	
(+)-α-Pinene	Dicyclic terpene	$C_{10}H_{16}$	0.57	4.44
α-Terpineol	Monocyclic terpene alcohol	$C_{10}H_{18}O$	1,827	3.28
Aromadendrene	Sesquiterpene	$C_{15}H_{24}$		
δ-Cadinene	Sesquiterpene	$C_{15}H_{24}$		
(+)-Limonene	Monocyclic terpene	$C_{10}H_{16}$	1.0	4.38
Sabinene	Dicyclic monoterpene	$C_{10}H_{16}$		
Globulol	Sesquiterpene alcohol	$C_{15}H_{26}O$		

Open in a separate window

[a]From reference 63.

[b]K_{ow}, octanol-water partition coefficient, from reference 62.

Source: Carson, C. F., Hammer, K. A., & Riley, T. V. (2006). Melaleuca alternifolia (Tea Tree) oil: a review of antimicrobial and other medicinal properties. Clinical microbiology reviews, 19(1), 50–62. https://doi.org/10.1128/CMR.19.1.50-62.2006

Appendix 3: Comparison: Technical Performance - Octyl Alcohol vs Tea Tree Oil vs Phthalates

	Solubility	Diffusion	Stability
Diethyl phthalate (DEP)	Insoluble in water Miscible in vegetable oil and most organic solvents	Boiling point:295 °C Vapor pressure : .0021 mm Hg at 25 °C.	Half-life in Air : 22.2 Hours.
Diethylhexyl phthalate (DEHP)	Slightly soluble in water Miscible in mineral oil	Boiling point: 384℃ Vapour pressure 10^{-7} mmHg.	Evidence of time of degradation: 2 days.
Octyl Alcohol	Soluble in : Alcohol, fixed oils, propylene glycol, water, 814 mg/L @ 25 °C (est)	Boiling Point: 195°C Vapor pressure: 0.13 mm Hg (25C).	Shelf Life: 24 - 36 Months store < 25 C Scent life: 92 hours at 100.00 %
Tea tree oil	Tea tree oil is mostly insoluble in water and is soluble in 85 % ethanol[4].	Terpenes in tea oil are known to be volatile but stable enough to produce lasting fragrance.	Shelf life: 1-3 years, Stored at stable temperature < 25 °C, Reactivity: additional formulation tweaks to solubilize

Bio-sketches

KEY PERSONNEL:	
NAME & TITLE	**ROLE / RESPONSIBILITY**
Nassim Bishara- Chemical Analyst-	Nassim's job is to evaluate the chemical structures and interactions of phthalates as well as alternatives to phthalates to understand why phthalates are used in products, why phthalates are hazardous from a chemical perspective, and how the alternatives to phthalates could provide the same function chemically without having the same hazardous effects.
Lavanya- public health scientist/analyst- reference manager	Lavanya will analyze the public health impacts of phthalates and which groups of people that the hazards of phthalates impact the most. Lavanya can also evaluate possible public health policies that can be implemented to prevent the phthalates from being present in cosmetic products. She can also think of policies and possible strategies to encourage the companies to use our alternative to phthalates. She can help us figure out past chemicals that are known to be safer from a public health perspective. She will also be the reference manager.
Aditya- green economist-analyst of public perception	Since Aditya is an econ major, he will analyze why phthalates are used from an economic perspective. He will think of alternatives to phthalates that are not so pricey so that companies will be more inclined to use them. Aditya also majored in journalism, so he can investigate how phthalates are publicly perceived from articles like the New York times and from news reports. He can also help think of ways more people know about the dangers of phthalates and possible healthier alternatives.
Jiho- environmental scientist	Jiho will investigate the environmental impacts of phthalates and how phthalates can be detrimental to the environment. Jiho will also help us look for alternatives to phthalates that are environmentally safe and are decomposable so that they are not persistent in nature/wildlife.
Bruno- chemical engineer	Bruno is our chemical engineer which means he will take a deeper dive in the chemical processes and steps that are utilized in making chemical hair relaxers. From that knowledge he can understand how phthalates are made chemically and where in the production process they are used. This knowledge will be vital in understanding how our alternatives can be implemented into the production of relaxers. Since Bruno specializes in biotech, he can also think of unique and original ideas for alternatives of phthalates especially when considering bio inspired design ideas.