Smells Like Teen Shampoo

Abstract
Shampoos are an important part of our daily lives and they vary in terms of their smells and cleaning actions. This project involved making shampoo using distillation to extract the key ingredient of a fragrance, essential oil. A variety of plants were used to extract the oils. To understand the chemical ingredients of the oils, two methods of analysis were performed: a process called thin layer chromatography, conducted in-class; and another called gas chromatography-mass spectrometry which was conducted by the Scotch Whisky Research Institute. Both tests revealed the chemicals present in the oils, the latter with a much higher accuracy. Once the shampoo was made, it was tested for pH, ability to clean and the all important ability to foam. To test if the shampoos could clean, horse hair and dolls’ hair were used. Afterwards, the shampoo work was presented in a Dragon’s Den style poster session to other students, teachers and a professional scientist who was as a partner in our project. Overall the shampoos all worked well and a greater understanding and enthusiasm for chemistry was gained.

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Introduction
This project studied the chemistry of the production of essential oils, the making of commercial shampoos, what chemicals are in shampoos and how to find out what chemicals are in shampoos. The school project at Dornoch Academy was performed in partnership with Whyte and Mackay, which allowed a professional scientist to give advice, look at our work and do chemical analysis that would otherwise be too expensive or difficult for our school to do. James Pryde is the chief chemist at Whyte and Mackay and has published a paper in which he analysed whisky taken to the South Pole by the explorer Ernest Shackleton and used chemical techniques such as gas chromatography, mass spectrometry and gas chromatography (GC) olfactrometry to identify the whisky and its components.1

Steam distillation was used to separate the essential oil from plants. This works by heating the mixture above the boiling point of the essential oil allowing the components to evaporate into the condenser. The condenser permits the distillate to condense and run off into the collection flask. Thin layer chromatography (TLC) was then carried out on the distillate and pure essential oils, to allow separation of the components of each essential oil and identification. TLC separates mixtures of substances into their component parts, allowing the distillate to be separated into the compounds it is composed of, and by comparison with the known pure compounds, the separate components can be identified. Different components separate due to them travelling different distances on the chromatography plate.

The emulsifier (in this case polysorbate-20) bonds with a polar water molecule on the left and the non-polar limonene from citrus oils on the right. This allows oil and water to mix and form a shampoo emulsion.
“Two important ingredients for shampoo: emulsifier to blend the oil and water; foaming agent to form the bubbles”

The distillate was then mixed along with the emulsifier (polysorbate-20) to allow the oils and the water to form an emulsion. The oils do not mix with water normally because the oils are non-polar and the water is polar. The emulsifier is able to bind to both the water and the oils due to it having a long non-polar tail and a polar head, this forms a stable emulsion (figure 1).

Sodium laureth sulfate was the foaming agent we used; its purpose is to give the shampoo the bubbles that are seen when shampoo is used and also to give the impression that it is thoroughly cleaning.

Method

The main outline of the task was to extract essential oils from various materials and use them in the production of a shampoo. This involved blending and testing the shampoo to see how it performed and acted.

Preparation for distillation:

Firstly the plants were chosen for the distillations to extract the essential oils. This included ginger, pine needles and citrus fruits such as lemon, orange and grapefruit. These were all obtained from local shops except pine needles, which came from a pine tree in the school. These plants needed to be cut or grated into smaller pieces to achieve a sufficient yield due to the increase in surface area. Water and a few anti-bumping granules were added to the plant matter. These granules are made from aluminium oxide and help ensure smooth boiling.

Carrying out the distillation of plant matter:

A heating plate combined with a sand basin provided a consistent and gentle heat. This meant that the plant matter’s extract could be collected efficiently by condensing the rising steam and to not char the plant matter. The sand is also a safety precaution to prevent the glass from shattering. The essential oil would gather in the collecting basin (figure 2).

Forming the Shampoo:

The essential oil extract (which provides the scent) was added to a 250cm³ beaker to which 5cm³ of water was added. The next chemical added was 30cm³ of sodium laureth sulphate (this is the foaming agent in shampoo) which works by encapsulating the dirt molecules by folding itself around it. It needed to be stirred in well so a magnetic stirrer was used for a consistent and thorough stir. Then 10cm³ of coco betaine was added and stirred in to the existing mixture; this was added to reduce irritation to the skin. 2cm³ of polysorbate-20 was added and stirred in. Polysorbate-20 is an emulsifier and which makes it useful in binding other components together. Coco Betaine is a surfactant, along with polysorbate-20, which bonds the water and oil molecules and reduces potential irritation by the sodium laureth sulfate. This is in the soap as it suspends the dirt molecules in the water to make it easier to wash away. Next the essential oils were added, only 0.5cm³ was needed due to the intensity of the fragrances. The mixture was then stirred to ensure total blending of all the components involved.

Thin Layer Chromatography:

One drop of the essential oil dissolved in 1 ml hexane – along with two pure sample terpenes that were believed to be present in the essential oil – was spotted onto TLC paper and put it in a glass jar with 0.5 ml of solvent (Figure 3). After the solvent had run to 1cm from the top of the TLC paper, the TLC was removed and soaked in p-anisaldehyde solution or a permanganate dip. This procedure was a modified version of a published one. The TLC strip was then gently heated on a heating mantle to evaporate the solvent and reveal the terpenes present in the essential oil. Thin layer chromatography was
attempted on the distillates but the yields of oils appeared to be too low for detection. Commercially bought essential oils were used for the thin layer chromatography analysis instead and the steam distillates were used for the shampoo.

**Results**

Various fragrances of distillate were created, such as: lemon, lime and ginger. The distillations were a success, all groups produced a good product. However the distillates by themselves proved not to be concentrated enough and so essential oils were bought commercially and also added in tiny quantities, such as ylang ylang and pine oil.

“red would mean it was acidic and so possibly irritant but would make the outer layer of hair lay flat and so make hair seem smoother”

There were several tests done to analyze the shampoo based on published methods\(^1\), they are as follows: the pH test, which was done in order to see if the shampoo was safe enough for even the most sensitive of scalps, it was done using pH paper strips and universal indicator, red would mean it was acidic and so possibly irritant but would make the outer layer of hair lay flat and so make hair seem smoother, blue/purple would mean alkali and so possibly irritant but would make the outer layer of hair open up and swell making the hair frizzier. What was looked for was a nice shade of green meaning it was neutral and so would cause no harm and not be irritant in the slightest. All the shampoos produced green using the pH test.

The next test was the dirt test, or rather ink test as ink was used instead of dirt. This involved putting 2 drops of shampoo and one drop of ink into 10 ml of distilled water in a test tube then shaken vigorously and left to settle.

This would produce foam. The ideal outcome is for there to be no ink/dirt in the foam, for it is meant to be in the water so that when you wash your hair it easily runs off your head. If it stayed in the foam, it could easily be redistributed into your hair as foam is harder to wash out than water (Figure 4). The final tests were an analysis of the foam produced upon vigorous shaking. 50 ml of 1% shampoo was put into a 250 ml graduated cylinder and shaken 10 times, the volume of the foam was then recorded as was the size of the bubbles, they could be either small, medium or large. A good shampoo should produce a foam volume of around twice the original volume of the shampoo, which our shampoo did\(^3\). The bubbles of the foam should also be small as it means the retention time of the foam will be longer. At the same time as measuring the volume of foam the time of retention was also measured, a good shampoo will keep the same volume for around 5 minutes. Our shampoos managed to do this. To test if the shampoos could clean, horse hair and dolls’ hair were used.

The results from the TLC experiments are summarised in the table: the table shows the terpenes present in each essential oil that were detected. Example TLCs are shown in figures 5 and 6.

The essential oil distillates were sent off for GC-MS analysis at the Scotch Whisky Research Institute. Gas chromatography allows separation of the
chemical components and mass spectrometry allows identification of the components. The results were sent back to the class to analyse the data, with the conclusions shown in the table.

Pinene and myrcene were expected to be in the pine oil but were not detected, although limonene was. It is possible that heat damaged the pinene and myrcene but not the limonene.

**Shampoo Project – Poster Presentation**

Once the shampoo had been made, a presentation was done, showing how effective the shampoo was.

Since there were three groups, it was decided that there would be a competition for best presentation and results. Posters were produced and explained to James Pryde from White and Mackay, Katie Elder (Science Curriculum Development Officer for the region) and pupils from the Advanced Higher chemistry class. The processes of steam distillation, TLC and the making of the shampoo were explained. Demonstrations were then done to show that the shampoo lathered, that it removed dirt, and that it was suitable for use on skin. At the end of the presentation, questions were asked and satisfactorily answered. This project was very beneficial, as the information involved had to be learnt for the Higher
Chemistry exam. It was easier to understand the theory behind the shampoo production because it was actually concocted. Making it a competition motivated the class to work to a high standard. Presenting the shampoo to professionals meant that the information had to be thoroughly learnt, to avoid severe embarrassment!

Summary
This was an enjoyable project which seemed to make chemistry more relevant as we all use shampoos in our daily lives. Essential oils were extracted,

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