CASE STUDY

Cola

This study examines the olfactive information for full sugar and low calorie cola soft drinks from two different suppliers.

aryballe™

The potential for digital olfaction in R&D formulation for soft drinks

Traditional e-noses often struggle with samples that contain a high amount of water—making beverage comparison and discrimination a difficult use case to address. However, new bio-based methods like those from Aryballe allow not only the discrimination of beverages, but even those with extremely close odor profiles, like cola soft drinks.

Odor plays a strong role in the taste and experience of any beverage—and being able to capture and analyze the digital signature of formula candidates allow R&D to assess the character of new formulations between each other and against existing products so the best candidate can be selected.

This paper examines the use of digital olfaction tools from Aryballe to evaluate cola soft drinks from different brands and sweetener content to create a framework for integrating this data into existing R&D workflows.

Background

The popularity of reduced sugar soft drinks has shifted in the past years due to consumers' drive for natural ingredients and ever-growing suspicion of artificial ingredients—including sweeteners. However, the recent success of Coke Zero Sugar suggests that there is growth to be had when the taste of the low calorie version is close to the original.

The soft drink industry has been under regulatory pressures to reduce sugar content for over a decade—and consumer preferences have also moved toward reduced sugar beverages in recent years, with an increasing number choosing low- or no-sugar options. For example, the UK "Sugar Tax" saw a 50% decline in 'regular' soft drinks from 2015 to 2018, which sales of low- and zero-sugar soft drinks rose by 40%.

Sweeteners have a direct impact on sensory attributes of a beverage, including mouthfeel and taste, thus developing a low- or no-sugar formula can be complex and require multiple formulations and sensory panels.

Examination of Cola Soft Drink Samples

In this study, we examined commercially available samples of two brands of cola soft drinks, and of varying sweetener content. While generally cola flavoring is comprised of kola nuts, vanilla, citrus flavor, and spices like nutmeg, coriander, ginger or cinnamon, the specific composition of these flavors for each cola brand will vary. Although sugar does not have an odor alone, the interaction of these flavors and the sugar or sugar-substitute molecules can impact the overall aroma of the finished product.

Material & Method

This study used Aryballe's NeOse Advance connected to the Amplifier and a HeptaValve Mini. NeOse Advance is an instrument with embedded humidity and temperature sensors along with Aryballe's Core Sensor which captures odor signatures.

The Core Sensor is based on an array of Mach Zehnder Interferometers grafted with Aryballe's proprietary combination of biosensors. The signal detected from an odor depends on the interaction between VOCs from the samples and these biosensors. A different intensity signal is measured for each biosensor in link with the affinity between the VOCs and the biosensor. The pattern of the reaction for all the biosensors for one odor is called the "olfactive signature."

The olfactive signatures are compared and statistic methods are applied for analysis of the odors in the study using the software tools from Aryballe.

The Amplifier accessory enables detection of humid samples, such as beverages, for better discrimination than possible with the NeOse Advance alone. One valve on the Amplifier records the baseline (ambient air, dried air, Argon, etc), while the other is linked to a small Tenax column (20 mg).

When this valve is open, the sample from the headspace passes through the column. Some VOCs bind with the Tenax and are concentrated, while other small molecules (like water and ethanol) cannot bind and pass through the system.

After 40 sec of concentration, the column is heated to 250 °C and the VOCs are released due to the heat. These released VOCs are then analyzed with NeOse Advance.

The HeptaValve Mini is an automatic valve which enables analysis of seven samples in the same experiment set up to improve the repeatability of the results while optimizing workflow. Each sample collection tube is placed inside of the vials through the septum of the cap equipped with a vent system to avoid depressurizing the vial. Another tube connects the whole valve system to the Amplifier. The duration for analysis and between measurements is regulated to allow the headspace to adequately reform in the vials.

The experiment assembly used in this study can be seen in Figure 1.

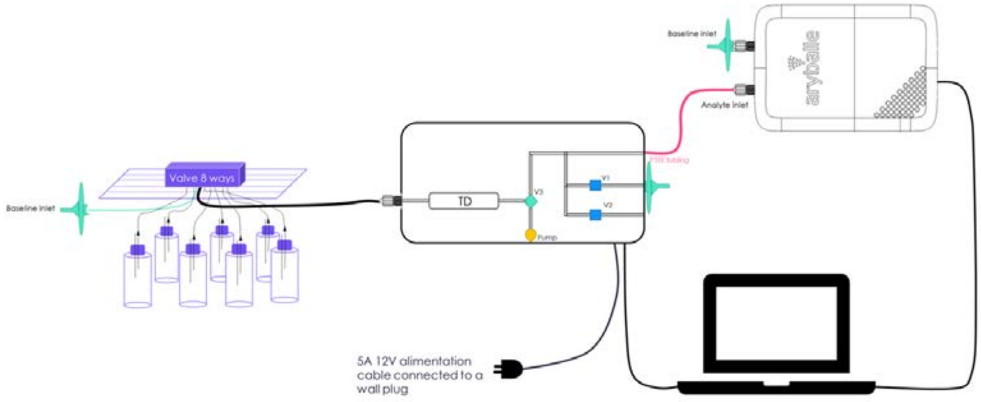

Figure 1 : *Illustration of the experimental set-up.*

This study used 100 ml vials with 10 ml of each sample as follows:

- Supplier 1 Cola
- Supplier 1 Cola Low Calorie 1
- Supplier 1 Cola Low Calorie 2
- Supplier 2 Cola
- Supplier 2 Cola Low Calorie

After sample preparation, the vials rested for 10 min to allow for adequate headspace generation. Each vial was measured at ambient temperature. The flowrate to concentrate the samples in the Amplifier accessory was set at 100 ml/min. During the thermodesorption measurement, the flowrate was set at 40 ml/min. The total duration for a single measurement using the NeOse Advanced associated with the Amplifier was approximately 6.5 minutes (Figure 2).

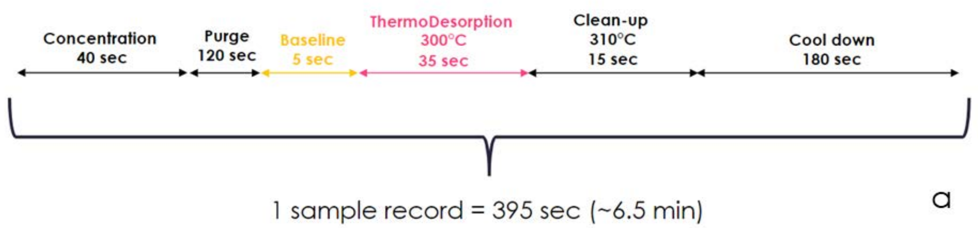

Figure 2a : *Description of the different steps of a single measurement done with NoA associated with the Amplifier.*

Figure 2b : *Example of one measurement visualization on the Live Data View of Aryballe's software.*

Five cycles were performed for a total of five replicates of each sample for the analysis. **One unique measure was performed in each vial, meaning 5 vials were used to obtain 5 replicates.**

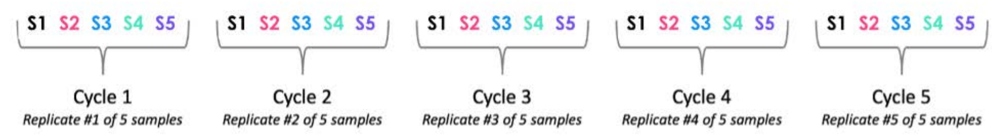

Figure 3 : *Five cycles were performed to achieve replicates for each of the samples.*

Results & Analysis

Normalized odor signatures are captured based on mapping the individual peptide response to an odor on a radar chart. The biosensor that reacts the most is normalized to one while the biosensor with smallest reaction is normalized to zero—and then all the other responses are mapped from 0 to 1. This gives us the unique fingerprint of the odor.

The signatures captured by the NeOse Advance (Figure 4) show a similar peptide response for many of the biosensors—as is to be expected as the odor profiles are very close for the human nose. But the comparison of the olfactive signature highlighted some specific differences between the full sugar and the low-calorie beverages. These differences are illustrated by the arrows on Figure 4.

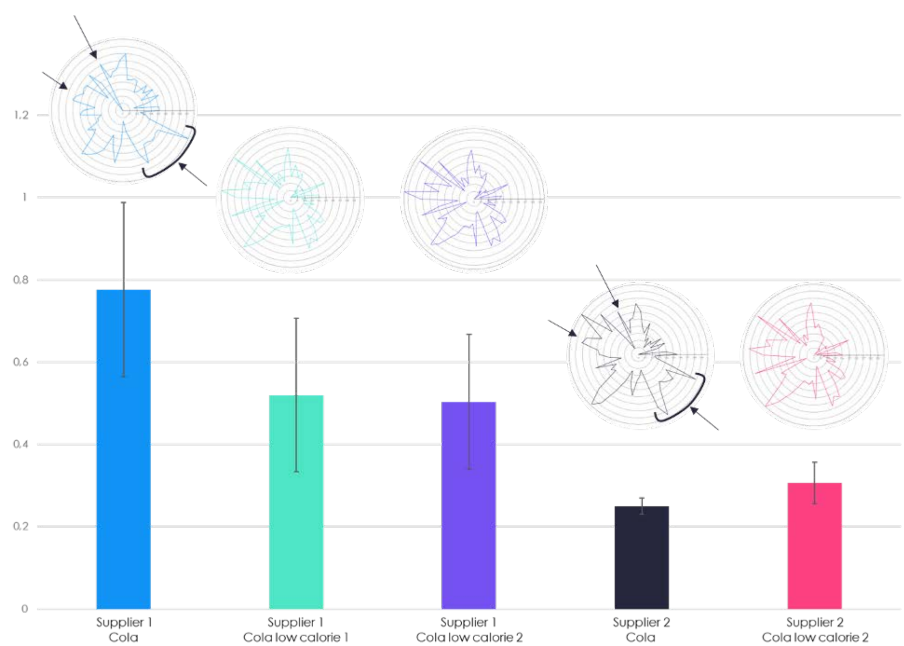

Figure 4 : *Average intensity for the measure of the 5 different beverages associated with their unique olfactive signature.*

Intensity: The intensity is based on the average of the reaction of all the peptides. On Figure 4, the samples from Supplier 2 have a significantly lower intensity—for both full sugar and low calorie—than the samples from Supplier 1. For the samples from Supplier 1, we observed a lower intensity for the two low calorie beverages.

Principal Component Analysis (PCA) is based on calculation of the distances between all biosensors. It is a graphic representation of the relative difference of odors. Datapoints located close to each other indicate a degree of odor proximity, while distant datapoints indicate different sample odors.

In this study, we see a global cluster including the 3 low calorie beverages from both suppliers on the left side of the PCA (Figure 5). The two full sugar beverages from each supplier are quite far apart on the right of the PCA.

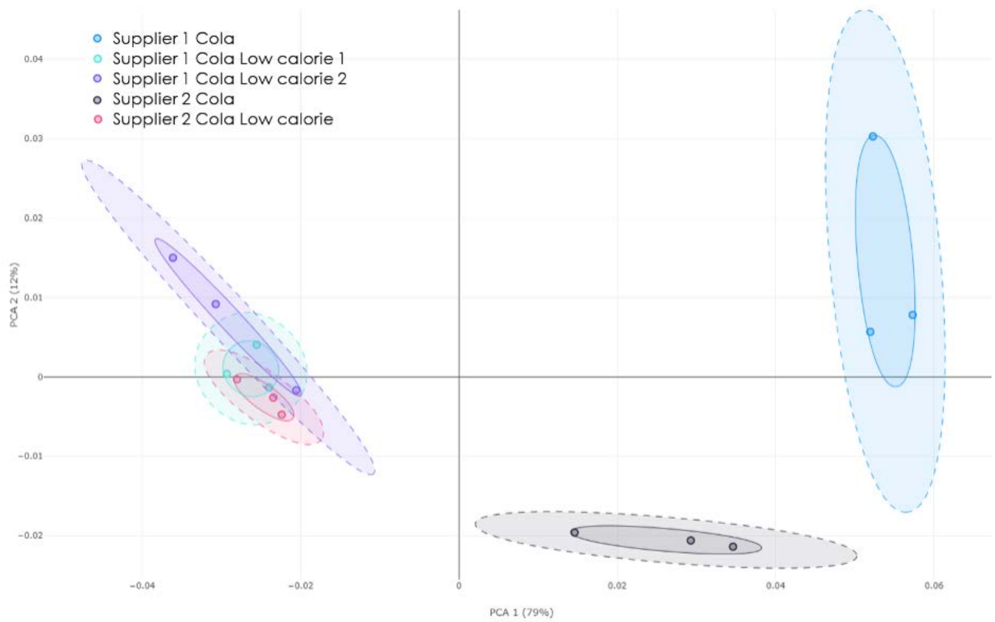

Figure 5 : *PCA analysis of 5 different Cola samples from 2 different supplier with various level of sweetener.*

Dendrogram: Hierarchical clustering is an unsupervised clustering algorithm that groups similar objects into groups called clusters. The endpoint is a set of clusters, where each cluster is distinct from each other cluster, and the objects within each cluster are broadly similar to each other. The hierarchy of clusters is often represented as a dendrogram (tree like structure as in Figure 6). The hierarchical clustering is based on the normalized olfactive signature.

The dendrogram confirms the clustering observed on the PCA with a global discrimination between the samples full sugar and low calorie, and also the discrimination of the two full sugar samples.

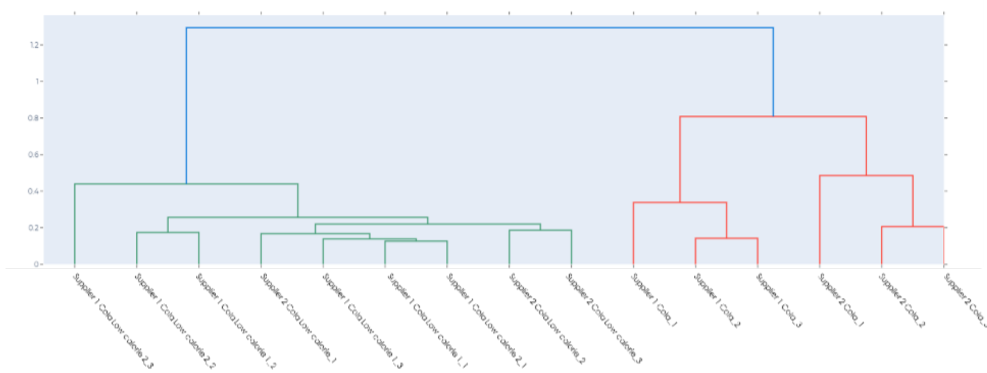

Figure 6 : *Dendrogram, hierarchical clustering based on the normalized olfactive signature for the 5 Cola samples analyzed in the study.*

This study shows an example of how manufacturers could use the olfactive data captured to compare a new formulation candidate against an existing portfolio and its intensity, olfactive signature and similarity to existing products.

R&D teams can use the analysis from digital olfaction tools from companies like Aryballe to inform formulation development with consistent, objective odor data. Although the instrument does not fully take the place of human panels for overall taste and mouthfeel of the product, this tool enables rapid screening of candidates against a target product or formula. Thus, bringing only high potential formulas to human panel for consideration.

About Aryballe

The best human noses can distinguish 10,000 odors. Unlike color and sound, smell does not fall along a clear spectrum, making it hard to compare various odors. But Aryballe is helping to change this by evaluating characteristics of individual scent molecules and testing them against a data-base of known smells using a combination of biochemistry, advance optics and machine learning.

Based in Grenoble, France and founded in 2014, Aryballe combines biochemistry, advanced optics and machine learning to mimic the human sense of smell. The company's premier product offering, NeOse Advance, uses silicon photonics technology to detect, record and recognize odor data, which powers improved decision making for R&D, quality control, manufacturing and end-user experiences. Aryballe Suite, the company's cloud-enabled software, enables customers to intuitively access and customize analysis of odors based on their unique needs. With operations in France, South Korea and the USA, Aryballe works with global leaders in automotive, consumer appliances, food manufacturing and flavor & fragrances.

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