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Influence of minerals on the taste of bottled and tap water: A chemometric approach

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ABSTRACT

Chemometric analysis was performed on two sets of sensory data obtained from two separate studies. Twenty commercially-available bottled mineral water samples (from the first study) and twenty-five drinking tap and bottled water samples (from the second study) were blind tasted by trained panelists. The panelists expressed their overall liking of the water samples by rating from 0 (worst flavor) to 10 (best flavor). The mean overall score was compared to the physicochemical properties of the samples. Thirteen different physicochemical parameters were considered in both studies and, additionally, residual chlorine levels were assessed in the second study. Principal component analysis performed on the physicochemical parameters and the panelists' mean scores generated models that explain most of the total data variance. Moreover, partial least squares regression of the panelists' sensory evaluations of the physicochemical data helped elucidate the main features underlying the panelists' ratings. The preferred bottled and tap water samples were associated with moderate (relatively to the parameters mean values) contents of total dissolved solids and with relatively high concentrations of HCO_3^-, SO_4^{2-}, Ca^{2+} and Mg^{2+} as well as with relatively high pH values. High concentrations of Na^+, K^+ and Cl^- were scored low by many of the panelists, while residual chlorine did not affect the ratings, but did enable the panel to distinguish between bottled mineral water and tap water samples.

1. Introduction

It is well known that the taste of water depends on the chemical composition of the salt content, with both cations and anions contributing in different ways and interacting through synergism and antagonism (Burlingame et al., 2007). In addition to the dissolved inorganic salts (total dissolved solids, TDS), some volatile organic compounds can be detected through retro-nasal mechanisms when drinking water (Dietrich, 2009). Therefore, the global perception of water is considered more of a flavor than a taste (Dietrich, 2006).

The mineral and chemical contents of bottled natural mineral water are determined by the composition of the rocks from which it is extracted and by geochemical processes (van der Aa, 2003). Moreover, potable tap water is also characterized by its specific chemical (mineral and organic) content (Meng and Suffet, 1997) in relation to the incoming raw water and the disinfection procedures implemented. The latter may

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add other chemical compounds at significant concentrations (such as residual chlorine), which also contribute to the final flavor of drinking water.

Traditionally, water distribution companies have tried to improve the flavor of water through conventional water treatment procedures. Their efforts have focused on producing water with low organic matter content and minimum levels of residual disinfectants that are just enough to sanitize water. With the introduction of membrane technologies, it is now possible to significantly reduce organic matter levels and water mineralization (Bruchet and Lainé, 2005), thus improving flavor. The remineralization stage, which is commonly applied to treated water, also plays an important role in final taste (Devesa et al., 2010).

The assessment of improvements in the flavor of drinking (tap) and bottled water needs sensory experiments in which water samples are systematically presented to trained panelists or random consumers, who test them in various ways (Naes and Risvik, 1996). Recent studies by Teillet et al. (2010a,b) confirmed that water flavor assessments are complex and should be performed very carefully. Using a free sorting task technique, these authors concluded that consumer acceptance of water was mostly driven by the mineral content and that medium-mineralized water was preferred by regular consumers; however, no conclusions were reached about what specific components were responsible for their preferences. The use of a trained panel of assessors is appropriate for a reliable sensory description and assessment of unknown water sample preferences.

Carefully-designed experiments and analysis of variance (ANOVA) are the starting steps in sensory studies (Hibbert, 2009). Data sets are usually multivariate and multiway, having as dimensions the number of samples multiplied by the number of sensory attributes, multiplied by the number of panelists. Usually, sensory data are noisy (between people and along time for the same person) (Hibbert, 2009). The application of ANOVA is extremely useful in studying the sources of data variance. It helps to test the panelist's performance and statistically evaluate all factors that influence responses to the sensory attributes, i.e., the physicochemical parameters in our case studies (Naes and Risvik, 1996). Since these responses can be influenced by two or more factors as well as their interactions, the proper methodology in this case is a two-way ANOVA or, when more than two factors are simultaneously tested, an N-way ANOVA (Peña Sánchez, 1994).

Principal component analysis (PCA) has already been shown to be useful for correlating chemical and sensory data in drinking water samples from a distribution system (Meng and Suffet, 1997). PCA (Jolliffe, 2002) has been applied to reveal the most important patterns in the physicochemical parameters that correlate with the panelists' ratings. Mallevialle and Suffet (1987) introduced background information on chemical/sensory correlation methods and showed general results from correlation studies. Suffet et al. (1989) used a similar statistical method, factorial correspondence analysis, to link chemical and sensory data. Generally, the choice of method depends on the type of sensory data, e.g., whether the data are of a ranking or rating (giving evaluation scores) type, a categorical or continuous character, or even concatenated in multiblocks (Stanimirova et al., 2011).

Partial least squares regression (PLS) is a well-known and useful tool in consumer preference analysis (Lengard and Kermit, 2006). The complex relationship between the sensory panel rates and the physicochemical parameters of the mineral and tap water will be discovered using PLS (Geladi and Kowalski, 1986). Recently, the variable importance in projection (VIP) scores has been proposed as useful tool for interpreting PLS models (built from several latent variables) (Chong and Jun, 2005). The interpretation of VIP scores can be employed to evaluate the importance of each water physicochemical parameter in the final PLS projection.

This paper aims to discover the most influential physicochemical parameters associated with the overall score of water flavor in two separate sensory studies performed using selected bottled mineral and tap water samples with different mineral contents and origins.

2. Material and methods

2.1. Water samples

In the first study (A), 11 bottled mineral water samples, commercially available in Spain, were collected. In addition, 9 new samples were obtained by blending two water samples or by diluting with purified water. Therefore, this study was performed with 20 water samples. The high number of samples considered, and the process of blending and diluting were decided in order to cover a broad range of TDS and mineral composition, as well as the percentages of the different cations and anions. Therefore, the study included water samples with very different mineralization levels and percentages of sodium, calcium, magnesium, chloride, bicarbonate and sulfate, i.e., the most relevant species driving the taste of water.

In the second study (B), 25 water samples were considered: 12 bottled waters selected from the first study and another 13 tap water samples from different resources and networks in Catalonia, northwest Spain. The tap water samples were selected with the same intent as in the first study: covering a wide range of mineralization and chemical composition types.

The results of the physicochemical compositions of the water samples used in the studies A and B are presented in Tables 1 and 2, respectively. Analytical analyses of the samples were made in the accredited laboratory of the Aigües de Barcelona Company. Water blends and dilutions were allowed for 48 h of equilibration before analysis. Sodium, potassium, calcium, magnesium and silica levels were analyzed by inductively coupled plasma optical emission spectrometry (ICP-OES) (Perkin Elmer Optima 4300 DV). Conductivity at 20 °C, pH and bicarbonate levels were determined by a robotic titrosampler (Metröhm modules 855 and 856). Chloride, nitrate and sulfate concentrations were analyzed by ionic chromatography (Dionex ICS-2000). TDS (dry residue at 180 °C) levels were measured by gravimetry. Free residual chlorine was analyzed by the classical DPD colorimetric method. All these analytical determinations, except for the bicarbonates and TDS that are not included in