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Chemometric Expertise of Bulgarian Mineral Waters

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Abstract

Five brands of Bulgarian bottled mineral waters are subjected to chemometric expertise using cluster analysis. The waters are classified into several patterns depending on their chemical composition and are related to the specificity of their local origin. The obtained results point to the stability of the chemical composition of the bottled mineral waters in examination even for a prolonged period of storage (within 2.5 years after bottling).

Introduction

Bulgaria is one of the countries in the world richest in mineral waters (more than 850 springs and boreholes), both with respect to its surface area and per capita [1]. This natural richness has been known and exploited since antiquity. Nowadays, more than 50 brands of bottled mineral and spring waters are offered on the Bulgarian market. The quality of the waters, including their macro- and microelement content, as well as their stability during storage, is of paramount importance for the consumers. The great variety of mineral water springs with respect to their location and chemical composition often requires a specific approach for expert assessment of mineral water origin and quality. Since careful monitoring of the chemical content of different mineral, spring and table waters creates large data sets, chemometric data classification, modelling and interpretation seems to be the most reliable assessment procedure. Subject of the present work was the chemometric assessment of Bulgarian potable waters of several brands using cluster analysis. It was also of substantial interest to compare the water quality during a prolonged period after bottling.

Materials & Methods

The microelement composition of the waters was determined in former works of the authors using total reflection X-ray fluorescence spectrometry (TXRF) on a S2 PICOFOX (BRUKER AXS GmbH Karlsruhe, Germany) [2,3]. The data for the microelement composition of the waters were treated in the present chemometric study [4,5] (applying the STATISTICA 7.0 software) in order to:

• find out groups of similarity between the chemical components of the waters, to which the local specificity of the potable waters may be related;

• find out groups of similarity between the different types of potable waters;

• find out the specific indicators for the separate groups of waters.

Results

A data set (10×12) was treated including the waters the following brands: „Gorna Banya“ (samples 1,6), „Kom“ (samples 2,7), „Thorn Springs“ (samples 3,8), „Devin“ (samples 4,9) and „Mihalkovo“ (samples 5,10), analyzed in the year of bottling and 2.5 years after bottling for 12 chemical parameters (As, Zn, Cu, Ba, Fe, Ni, Ca, Br, Mn, Rb, K, Cl). Fig. 1 presents the hierarchic dendrogram for clustering of the 12 variables from the data set (10×12). As can be seen, three clusters (denoted as K1, K2 and K3, respectively) are formed at the significance level of 33.3 % Dmax: K1 (As, Zn); K2 (Cu, Ba, Fe) and K3 (Ni, Ca, Br, Mn, Rb, K, Cl). It follows from the results shown in Fig. 1

that three main sources form the composition of all examined waters, two of them being related to the microcomponents in the mineral waters (K1 and K2), and the third one (K3) – mainly to the major components and the microcomponents Mn, Rb, Br, and Ni.

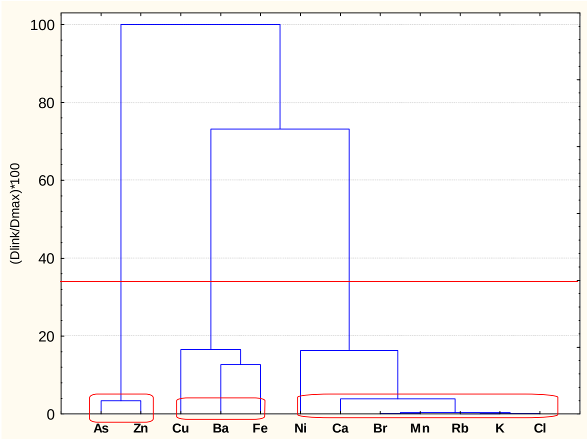

Fig. 1. Hierarchic dendrogram for clustering of 12 variables

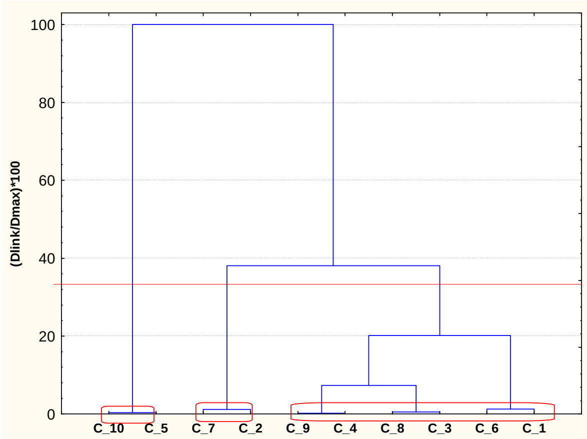

Fig. 2. Hierarchic dendrogram for clustering of the types of mineral waters analyzed in the year of bottling (samples 1-5) and about 2.5 years after bottling (samples 6-10)

Fig. 2. presents the hierarchic dendrogram for clustering of the mineral waters (firstly in the year of bottling and secondly – about 2.5 years later). Three clusters can be distinguished; there is a good correlation (grouping) between the results in the year of bottling and those about 2.5 years after bottling (samples 1 and 6; 2 and 7; 3 and 8; 4 and 9; and 5 and 10, respectively). This points to the stability of the chemical composition of all examined mineral waters even 2.5 years after bottling.

The five brands of mineral waters included in the data set (10×12) ("Gorna Banya", "Kom", "Thorn Springs", "Devin" and "Mihalkovo") form three groups of similarity:

• „Mihalkovo": highest values of all major components (strong mineralization) and of the microcomponents manganese, nickel, copper, bromine and rubidium.

• „Kom": highest values of zinc and arsenic (specific As-Zn mineralization) and lowest values of chlorides and calcium.

• „Gorna Banya", „Thorn Spring" and „Devin": mineral waters with similar chemical composition – lowest potassium content, significant content of calcium and iron.

Conclusions

The present study has indicated that the brands of Bulgarian potable waters in consideration could be classified into several patterns depending on their chemical composition. The separation is obviously related to the specificity of the local origin of the waters, e.g. crustal and soil properties and composition. The results of the cluster analysis point to the stability of the chemical composition of the bottled mineral waters even for a prolonged period of storage (2.5 years after bottling).

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