## Discriminating Between Energy Drinks and Sports Drinks Based on Their Chemical Properties Using Chemometric Methods

Authors: Robert Cazar, Nathaly Maza

Abstract: Energy drinks and sports drinks are quite popular among young adults and teenagers worldwide. Some concerns regarding their health effects - particularly those of the energy drinks - have been raised based on scientific findings. Differentiating between these two types of drinks by means of their chemical properties seems to be an instructive task. Chemometrics provides the most appropriate strategy to do so. In this study, a discrimination analysis of the energy and sports drinks has been carried out applying chemometric methods. A set of eleven samples of available commercial brands of drinks seven energy drinks and four sports drinks - were collected. Each sample was characterized by eight chemical variables (carbohydrates, energy, sugar, sodium, pH, degrees Brix, density, and citric acid). The data set was standardized and examined by exploratory chemometric techniques such as clustering and principal component analysis. As a preliminary step, a variable selection was carried out by inspecting the variable correlation matrix. It was detected that some variables are redundant, so they can be safely removed, leaving only five variables that are sufficient for this analysis. They are sugar, sodium, pH, density, and citric acid. Then, a hierarchical clustering `employing the average - linkage criterion and using the Euclidian distance metrics was performed. It perfectly separates the two types of drinks since the resultant dendogram, cut at the 25% similarity level, assorts the samples in two well defined groups, one of them containing the energy drinks and the other one the sports drinks. Further assurance of the complete discrimination is provided by the principal component analysis. The projection of the data set on the first two principal components - which retain the 71% of the data information - permits to visualize the distribution of the samples in the two groups identified in the clustering stage. Since the first principal component is the discriminating one, the inspection of its loadings consents to characterize such groups. The energy drinks group possesses medium to high values of density, citric acid, and sugar. The sports drinks group, on the other hand, exhibits low values of those variables. In conclusion, the application of chemometric methods on a data set that features some chemical properties of a number of energy and sports drinks provides an accurate, dependable way to discriminate between these two types of

Keywords: chemometrics, clustering, energy drinks, principal component analysis, sports drinks

Conference Title: ICC 2023: International Conference on Chemistry

Conference Location: Montevideo, Uruguay Conference Dates: January 09-10, 2023