

## Chemometrical Evaluation of Different Brazilian Spirits by their Mineral Content Using ICP OES

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The developed work investigated the application of statistical and mathematical methods to Brazilian sugar cane spirits analysis. Sixty-seven samples of sugar cane spirit and twelve variables were analyzed by Principal Component Analysis (PCA) and Hierarchical Clusters Analysis (HCA). Data analysis was performed using the software Pirouette 2.7 (Infometrix, Seattle, WA).

Aluminum, Ca, Cu, Fe, K, Mg, Na, Pb, S, Se, Si, Sn, and Zn were determined in 67 samples of sugar cane spirits by axial viewing inductively coupled plasma optical emission spectrometry (ICP OES, Vista Varian, Mulgrave, Australia).

The recognition of the most important parameters for sample characterization using multivariate approaches allowed the differentiation between homemade and industrial Brazilian sugar cane spirits. The HCA analysis demonstrated two groups with similarity 0.2, showing a clear separation between them. Analysis of PCA yielded similar trends and characteristics shown by HCA, but with the advantage of identifying the main variables for the separation. The results showed that Cu, Se, Na, and Fe were the principal elements for discrimination among samples. Three PCs were accounted for explain 84.3% of the total data variance. The first PC encompasses 36.1% of variance in the data set and loadings indicate that it has significant contribution from Cu and Se concentrations. The second PC describes 29.4% of total variance and has high positive loadings for Cu and Fe concentrations. The third PC (18.0% of the total variance) was described by Cu and Na concentrations.

Copper was the major weight in all three components, being the principal analyte responsible for the discrimination between industrial and homemade sugar cane spirit. The latter presented a higher content of this element. Iron was also present in elevate concentration in homemade sugar cane spirits. The industrial sugar cane spirit presented higher amounts of Se and Na.