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Abstract

Coupling of Sensors and Machine Learning Algorithms in the Qualitative Analysis of Wine †

Anna Herrera-Chacon [1], Inmaculada Campos [1], Andreu González-Calabuig [1], Mireia Torres [2] and Manel del Valle [1,*]

1. Sensors and Biosensors Group, Department of Chemistry, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain
2. Bodegas Miguel Torres, Miquel Torres i Carbó 6, 08720 Vilafranca del Penedés, Spain

* Correspondence: manel.delvalle@uab.es

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Abstract: This work attempts the identification of the production year, the cultivar's region and the aging method used in the elaboration of different Spanish red wines, all from the "tempranillo" grape variety. The identification of such characteristics relies on the use of a voltammetric Electronic Tongue (ET) system formed by modified graphite-epoxy electrodes (GEC) and metallic electrodes to collect a set of six voltammograms per sample, and different chemometric tools to accomplish the final identifications.A large sample set, that included 199 different wine samples from commercial and own elaboration origin were analysed with the electronic tongue system, using the cyclic voltammetry technique and without any sample pre-treatment. To process the extremely complex, and high dimensionality generated data, a compression strategy was used for the acquired voltammograms, using the Discrete Wavelet Transform (DWT). This treatment reduced the information to ca. 10%, preserving significant features from the voltammetric signals. Compressed data was evaluated firstly by unsupervised methods, i.e., Principal Component Analysis (PCA), without much success as it was found that such methods were unable to unravel the patterns contained within such complex data samples. Finally, the processed electrochemical information was evaluated by supervised methods to accomplish the proper identification, among those methods were Linear Discriminant Analysis (LDA), Supported Vector Machines (SVM) or Artificial Neural Networks (ANN). The best results were obtained using Artificial Neural Networks (ANNs) achieving 96.1% of correct classification for bottled year, 86.8% for elaboration region (protected designation of origin) and 98.6% for maturation type with or without use of wood barrel.

Keywords: voltammetry; multisensor array; electronic tongue; artificial neural networks; wines