

NMR and Chemometric methods: A powerful combination for characterization of Balsamic and Traditional Balsamic Vinegar of Modena

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Abstract:

This work presents the capability of NMR spectroscopy combined with Chemometrics in predicting the ageing of Balsamic and Traditional Balsamic Vinegar of Modena. The need of an analytical method is an important requirement for both research oriented and commercial evaluation of these very valuable products. ¹H NMR spectroscopy, based on the advantage of rapid sample analysis without any manipulation or derivatization, is here proposed as a valid tool to describe Balsamic and Traditional Balsamic Vinegar of Modena. For this purpose, 72 reliable samples, were divided into three different groups according to their ageing process: young (<12 years), old (>12 and <25 years) and extra old (>25 years). Hierarchical Projection to Latent Structures Discriminant Analysis (PLS-DA) allowed us to characterize the ageing process. Variables showing the largest VIP (Variable Importance in the Projection) were extracted from PLS-DA model, thus shedding lights onto the role played by specific compounds in this complex ageing process. Two robust classification models, were built by PLS-DA and Naïve Bayes classifier and compared to prove the accuracy of the representation on both training and test sets. The predictions obtained for 41 “unknown” vinegar samples with these both methods gave more than 80% agreement among them.