5. CONCLUSIONS

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The aim of this work of thesis was that of approaching the task of food authentication, in the specific context of a chemical characterization of foodstuff through hyphenated analytical techniques or in general when multi-way data set are faced, with chemometrics, and to demonstrate its fundamental contribution. In particular two applications are analyzed: the quantification of specific compounds in a context of strong coelution of species solved by mathematical chromatography approach, and classification, through multi-set and multi-way methodologies of food products related to authentication and provenience identification.

For what concern the first application field, the quantification of several phenolic compounds in Lambrusco wine, by HPLC-DAD analysis and Multivariate curve resolution has permitted a perfect resolution of the signals and calibration curves were obtained for the target compounds. This study has permitted also an accurate application of constraints to solve problem of strict coelution. It was possible to quantify the analytes also in presence of interferents without the necessity of a perfect instrumental resolution.

For what concern the classification, three data sets were analyzed: the Lambrusco data set regarding an Italian DOP wine and the characterization of the three varieties, WINE data set which reports analysis of wines coming from geographical zone of the world (South America, Australia and South Africa), but of the same grape cultivar, and the EVOO data set which is related to the authentication of an important DOP olive oil produced in Liguria (Italy). As fingerprinting information secondary indicators were considered for this purpose, in particular phenolic fraction for Lambrusco and volatile fraction for WINE and EVOO. This comparison is made with a view on the different kinds the data can be arranged, namely considering multiset, multi-way and classical 2-way methods on unfolded data. The WINE and EVOO data sets were analyzed with GC-MS after sampling of the head-space fraction.

Here, the objective was evaluating the performances of the different methods used. Clearly each of them performs worst, equal or better depending on characteristics of the data set. In the case of Lambrusco data set, the strict coelution of the chromatographic peaks necessitates of the resolution step before the analysis and the alignment is troublesome, due to the complexity of the chromatogram and the consequent difficulty of identify in every chromatogram the maximum of the same compound in a cluster. Hence, the MCR resolution step, both for ALS-regression and PLS-DA classification, is more appropriate and gives excellent performance. In the other data sets, multi-way classification methods are a good solution. The multiset discriminant method ALS-regression provides an interesting interpretation of the data but not so high values in terms of discrimination.
In the WINE data set with strong classes overlap NPLS-DA performs much better than the NSIMCA class modeling approach. Both methods are instead suitable for EVOO data set and in this case, a one class problem, as in many authentication task class modeling may be preferred.

Clearly the methods proposed necessitate of being applied on a large number of data set to evaluate precisely their performance, and it will be part of future works, anyway the results obtained in this parallel were really interesting in the view of having developed mature multi-way and multiset classification and class-modeling tools which allows taking into account the truly multi-way structure of the data coming from the most advanced analytical platforms.