Characterization of Italian olive oils from different PDOs/regions based on ^{1}H-NMR data

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In the European Union quality products from agriculture, such as certain olive oil, can claim a Protected Denomination of Origin (PDO) based on geographical characteristics [(EEC) Regulation No 2081/92]. For this reason, the traceability of agricultural products is an important issue for both producers and consumers. In this context, analytical methods for the authentication of PDO olive oil are required. Thus, the aim of this study is to develop mathematical models in order to discriminate Italian olive oils belonging to a certain PDO/region from the rest of PDO olive oils produced in Italy. With this purpose, we analyzed 473 samples (2004/05 and 2005/06 harvests) of extra-virgin olive oils by ^{1}H-NMR produced in several Italian PDOs/regions. The ^{1}H-NMR spectra (7-0 ppm) obtained after signal processing (Fourier transformation on FID signal; line broadening, 0.3Hz, chemical shift alignment, and manual phase and baseline corrections) were bucketed, resulting in 342 buckets (width 0.02ppm). Multivariate data analysis was used in order to obtain binary classification methods: category 1, belonging to the PDO/region; category 2, not belonging to the PDO/region. The dataset (473 samples x 342 variables) was autoscaled and analysed by unsupervised and supervised pattern recognition techniques such as principal component analysis (PCA) and partial least square discriminant analysis (PLS-DA) respectively. The classification models obtained were evaluated by 3-fold cross-validation. Models were achieved for the PDOs: Riviera Ligure, Garda, Molise and Umbria; and for the regions: Siciliy, Puglia and Lazio. Recognition and prediction abilities were between 79-95% and 76-89% respectively for category 1; and 82-95% and 79-92% respectively for category 2. Samples from other PDOs/regions such as Campania, Calabria, Abruzzo, Toscana and Marche were also included, but classification models were not developed for them due to the small number of samples available. The results are encouraging but further studies with a larger sample set with representative olive oils of all PDOs are needed to achieve robust and stable models.