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The NMR side of lentil: protein extraction and hydrolyzation, and a bit of data fusion

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In past years, the interest towards bioeconomy concepts has been considerably growing. In particular, the development of sustainable and renewable bio-based technologies for food production is becoming increasingly important. One of the most interesting applications of bioeconomy in the "food" area is the use of enzymes for the transformation of food materials [1], to improve food safety and optimize the overall food treatment process.
In this perspective, the present study is focused on the optimization of the parameters used for lentil flour treatment, which is known as a "functional food" in the field of food supplements. A sample of this grinded flour, after an initial extraction process at a fixed pH and temperature, was treated monitoring the addition of a protease enzyme, different stirring rate, and the effective treatment time in order to obtain a total amount of 32 different samples.
All samples were firstly analyzed with the solution ^{1}H-NMR spectroscopy, which is the main topic of this study, and then were also analyze with the NIR and the UV-Vis spectroscopies to compare and unite different characterization techniques.
All NMR spectra were imported into MATLAB software, which is used for the multivariate chemometrics analysis. With the principal component analysis (PCA) we explored similarities among the samples in order to find time dependent trend and discrepancies with respect to different treatment parameters (Figure 1). With the partial least square discriminant analysis (PLS-DA) we also created a model able to clearly distinguish the sample containing the protease enzyme from the others.
Finally, with the aim of improving the results we obtained, we also performed an early data fusion approach by merging spectroscopic data from NMR, NIR and Visible spectra. This kind of approach helped to explain some curious results observed in the scores plots from the PCA performed on NMR data.

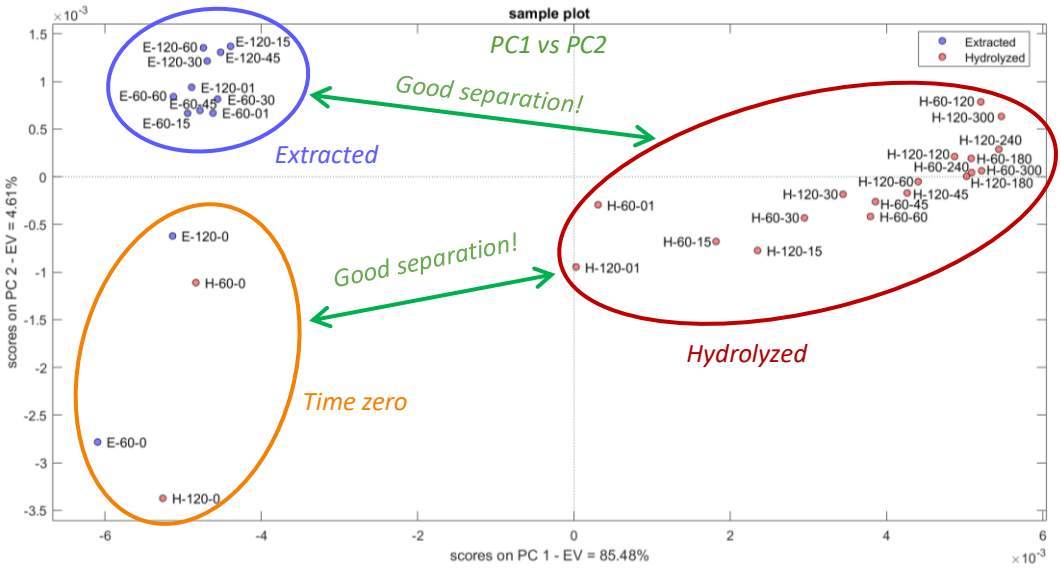

Figure 1 – PCA scores plot (PC1 vs PC2) obtained from all NMR spectra chemometrics analysis

References

[1] O. L. Tavano, *Journal of Molecular Catalysis B: Enzymatic,* **90** (2013) 1-11.