Water molecular structure behind water activity: investigating on chemical modifications of rice germ during storage

Cristina Malegori[1], Paolo Oliveri[1], Roumiana Tsenkova[2], Carola Cappa[3], Mara Lucisano[3]

[1]*DIFAR Department of Pharmacy, University of Genova – Genova – Italy*
[2]*Bio Measurement Technology Lab, Kobe University – Kobe – Japan*
[3]*DeFENS Department of Food, Environmental and Nutritional Sciences, Università degli Studi di Milano – Milano – Italy*

The aim of this study is to investigate how different water activities affect rice germ shelf life. In fact, this matrix (a by-product of rice milling process) could be interesting for human nutrition but, for its composition characterized by unsaturated fatty acids, it undergoes rancidity during storage. Dried samples at different water activities (0.55, 0.45 and 0.36) were packed in three different modified atmosphere (air, nitrogen, vacuum) and stored at 27°C for 320 days (for a total of 7 sampling points). All the samples were analysed by FT-NIR spectroscopy in reflectance (in the 800 – 2780 nm spectral range) with a rotating sample holder, as a non-targeted analytical approach.
First of all, focusing on the Aquaphotomics approach, spectral analysis was done in the water first overtone range, 1300 and 1600 nm. Then an exploratory principal component analysis (PCA) was performed, followed by a partial least squares regression (PLSR) to understand the NIR spectral changes that characterize the differences caused by different water activity levels in rice germ during storage. In more depth, 12 wavelengths, essential for the description of this system, were found to define the WAter Spectral Patterns, WASP. The most important ones are: 1343 nm, associated with protonated water, 1392 nm, typical absorbance of trapped water, 1410 nm, the well-known band of free water and 1436 nm, the Zundel cation band ($H_5O_2^+$). Radial graphics of the normalised WAMACS absorbance values were built: such Aquagrams allow to understand the modification of different water molecular the structures along time, for each water activity under investigation.

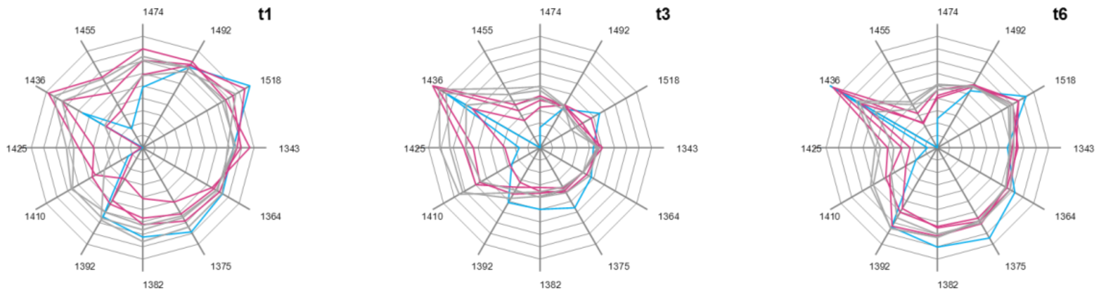

Figure 1: Aquagrams of rice germ samples during storage (from t0 to t6).

Thanks to this state-of-the-art approach, the water molecular conformation changes related to different water activities in rice germ along the storage seems to be a fundamental step for understanding the exponential nature of degradative process in biological matrices. These findings will open the venue of understanding the water molecular structure behind water activity in general.

Acknowledgment: the authors thank 'Rondolino - Società Cooperativa Agricola' for samples supply and economic support.