

**AUTHENTICATION OF ROMANIAN WINES AND COMPOSITION ANALYSIS OF  
ROMANIAN VEGETABLE OILS BY  
MODERN PHYSICAL METHODS (NMR, GC-MS)  
Project 240/01.10.2007, Cod. ID 928**

The aims of the first phase of this project regard:

**1. Creating a sample bank with Romanian wines from different varieties and vineyards harvest in 2007. Fermentation process study through compositional analyses using  $^1\text{H}$ -NMR method.**

*1.1. Must authentically sample collection from different varieties and vineyards*

In order to accomplish this objective sample of must were collected and used in fermentation studies. The fermentation occurs either under the influence of natural yeasts or under the influence of added yeasts.

*1.2 Recording of  $^1\text{H}$ -NMR spectra at 5 different fermentation periods*

In order to systematically monitor the alcoholic fermentation process of wine, we choose 5 distinctive moments for recording the  $^1\text{H}$ -NMR spectrum, depending on the changes which occurs in must composition, using the experience accumulated before.

The quantitative measurement of compounds during fermentation process was made using established markers for each compound. Because a more and more commune practice in wine making is the use of selected yeasts for wine fermentation, the must samples were also studied during fermentation process by adding yeasts.

*1.3 Data translations in terms of the compositional variation of products with known structure.*

Quantitative measurement of compounds was made using an internal standard added in the deuterated solvent in a known amount. In the must samples studied were measured the monosaccharide involved in fermentation process (glucose and fructose), and some other compounds identified during fermentation process using markers.

**2. Establish a method for the wine authentication of different varieties, vineyards (and crops, if available) by the original chemometric processing of the  $^1\text{H}$ -NMR data**

*2.1. Building up a bank of red wine samples and other varieties and vineyards.*

In order to create the samples bank of Romanian wines, we collected red and white wines produced in 2007.

In the figure below it is shown the general profile of a  $^1\text{H}$ -NMR spectrum for one of the wine sample studied.

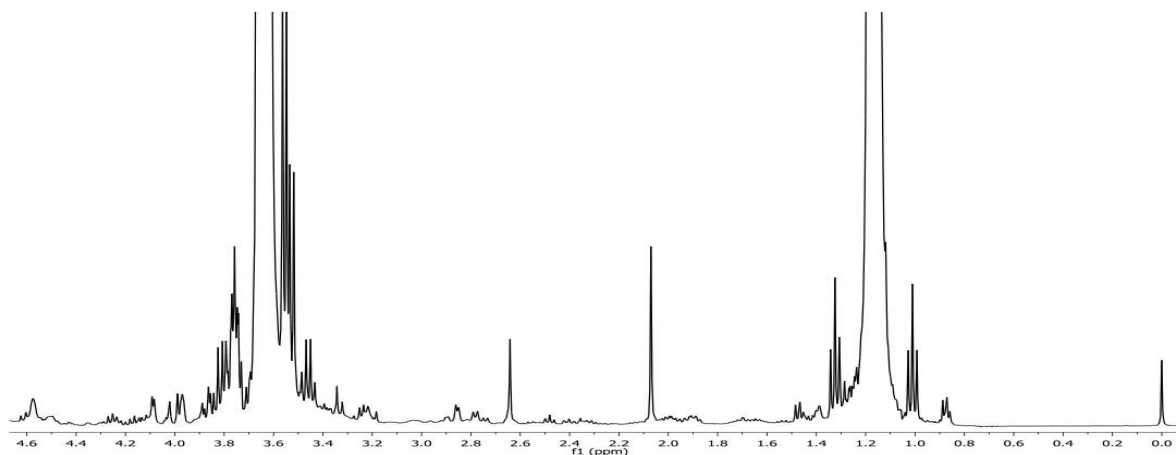


Figure 1. Area 0 – 4.6 ppm of  $^1\text{H}$ -NMR spectrum of a white wine sample

We could noticed that from one variety of wine to another the composition is similar, the general profile of the sample is comparable, but we could underline some small differences, especially in concentration level; those differences can be quantified and produce the “wine fingerprint” which can be used for wine authentication.

## *2.2. Chemometric data processing*

Chemometric data processing is the way used for quantification in a systematic manner the differences which occurs in  $^1\text{H-NMR}$  spectra for the wine varieties studied. In the chemometric data processing two important tracks where studied:

- the first one involves the use of the information regarding the concentration of different compounds identified and measured in each wine, obtained from each  $^1\text{H-NMR}$  spectrum.

- the second one involves the transformation of each  $^1\text{H-NMR}$  spectrum in a line of values obtained trough spectrum integration on small windows. This process permits obtaining 49 values for each  $^1\text{H-NMR}$  spectrum.

Chemometric data processing was made on two separate ways:

One of the approaches involves the using of PCA method. Following this route of data analyses we obtained a gathering of wine samples depending on the vineyard and as well one depending on the wine variety.

The second data analyses approach requires the use of an original computation method named “Sure area”. This method can differentiate the wine varieties two by two. The use of this method is important because it permits to distinguish between wines with similar composition.

### **NMR spectra recording**

NMR spectra were recorded using a Bruker Avance DRX 400 instrument, in pulses, with Fourier transformation, equipped with field gradients on the z axe; operates at 9.4 Tesla field, corresponding to 400 MHz for  $^1\text{H}$  nuclei and 100 MHz for  $^{13}\text{C}$  nuclei.

For this type of instrument we wised a multinuclear probe head with two channels and opposite detection.