## P-002: NIRS prediction of the ethanol content in various rose oil samples from Bulgaria

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Essential oils have been widely used all over the world in the flavor and fragrance industry, cosmetics, and in the health industry with aromatherapy and phytomedicine. Essential oil *(rose otto, attar of roses*) obtained from *Rosa damascena* Mill. (Damask rose), which has been traditionally cultivated in Bulgaria, is considered as superior in terms of the essential oil quality. Bulgarian rose oil is recognized as one of the world most sought-after products for its fine aroma and has a status of a protected geographic indication since 2014. Geographic and botanical origin, environmental conditions, production method [1] and storage of the raw materials (fresh rose petals) are among the factors, affecting the chemical composition and quality of essential oil. Oil composition is also influenced by the flower stages, flower parts, and the harvesting period.

According to the international standard (*ISO 9842*), only fresh flowers are used for oil production. However, at the peak of the harvesting season large amount of rose flowers are collected and are not able to be processed all together in the distilleries. As a result some parts of the petals undergo various degrees of fermentation prior to distillation. Both, the amount and the quality of essential oil are affected significantly and negatively by the fermentation process. Although ethyl alcohol is a natural occurring component of the rose oil, its content increases due to the fermentation process and, therefore, could be used as a marker for this undesired process. The quantitation of ethanol content in the rose oil is usually performed by GC-FID. But the price of the equipment is substantial, analyses and the interpretation are time- and effort-consuming, and high qualification of the staff is needed. At the same time the spectroscopic methods, based on near infrared (NIR), mid infrared (MIR) and Raman spectroscopy can provide a fast and non-destructive alternative [2,3].

The aim of the current study is to test an alternative approach applying a simple, fast and non-destructive NIRS method for quantification of ethyl alcohol. For this purpose, quantitative analysis of ethanol content in various rose oil samples from Bulgaria was performed by means of GC-FID (for reference data) and followed by NIR-spectral measurements. Calibration of NIR spectra with partial least squares algorithm (PLS) results in a suitable model for this purpose (Figure 1). The applicability of the model is proven by a comparatively high coefficient of determination ($R^2$ = 95.27 %) and a low root mean square error of cross validation (RMSECV = 0.405 % ethanol).

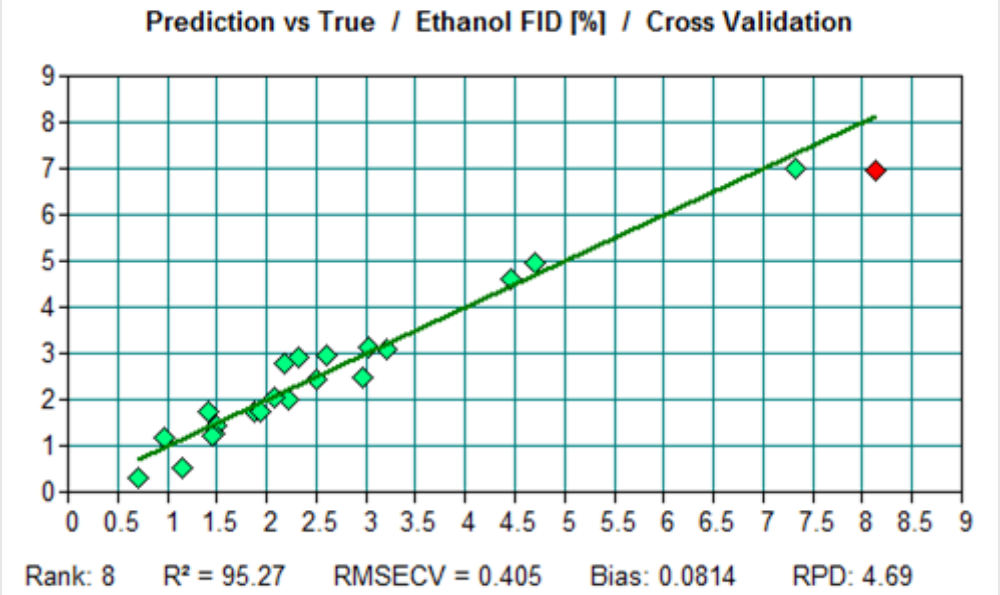


Figure 1: Cross validation of NIRS predicted alcohol content in rose oil from Bulgaria. The regression model was performed with PLS algorithm and validated by leave one out cross validation on 22 samples

**References**

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