



## DISCRIMINATION BETWEEN CONVENTIONALLY AND ORGANICALLY FERTILIZED GRAINS BY FTIR AND <sup>1</sup>H NMR SPECTROSCOPY COMBINED WITH CHEMOMETRICS

In the last decade, the world has seen growth in interest about the food traceability. This includes not only origins of the food, but also, it's accordance to labelling [1]. In this study the authors researched the possibility of using FTIR and <sup>1</sup>H NMR spectroscopy in combination with chemometric approach to distinguish between conventionally and organically fertilized cereal grains.

Organically and conventionally fertilized barley and triticale grains were analysed in this study. The samples were obtained at Institute of Agricultural Resources and Economics, Priekuļi Research Centre. For both conventionally fertilized barley and triticale a complex synthetic fertilizer was used. And for biologically fertilized grains, green manure of peas and red clover (*T. pratense*) for barley and triticale, respectively, was incorporated into the soil.

Both FTIR and <sup>1</sup>H NMR spectra showed little or no significant difference between the organically and conventionally fertilized cereal grains. The FTIR spectra showed broad peaks, corresponding to the starch content in the grains. Also, several peaks at 1747 and 2888 cm<sup>-1</sup> were observed that correspond to the protein content in the grains. The main peak shifts in <sup>1</sup>H NMR spectra were observed at 3.69 ppm, 6.27 ppm, 6.90 ppm, 7.28 ppm, 7.52 ppm and are corresponding to ferulic acid. Less intense chemical shifts were observed also for cinnamic acid, p-coumaric acid, caffeic acid and sinapic acid.

For further analysis, the obtained data were investigated using chemometrics – principal component analysis (PCA). After applying the PCA to the data of FTIR spectra, it was concluded that a signal at 1738 cm<sup>-1</sup> and 1750 cm<sup>-1</sup> is specific only for the conventionally fertilized triticale and barley grains, respectively. This peak is characteristic for the amino acids in cereal grains and can be explained by the higher protein content in conventionally fertilized cereals. Regarding the treatment of <sup>1</sup>H NMR spectra with PCA, it was concluded that the chemical shifts of ferulic acid (in the organically grown barley and triticale grains) were more intense and could be used to discriminate between cereal grains from different fertilization regimes.

**Primary authors:** VIKSNA, Arturs (University of Latvia, Faculty of Chemistry); Ms TARANDA, Karina (University of Latvia, Faculty of Chemistry); BUŠA, Lauma (University of Latvia, Faculty of Chemistry); KLŪGA, Rihards (University of Latvia, Faculty of Chemistry)