Investigation of near infrared characteristics of spring barley varieties

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Introduction

The constant good quality of malt is determined by the quality parameters of barley used as raw material. In addition to the size, moisture content, life activity, cleanliness and the composition (starch, protein, ß-glucan etc.) of the seed, the malting quality of barley depends on the variety. Sharp differences must be made between spring and winter barley in respect of brewing consumption. Due to higher protein content and thicker skin structure, winter barley is less valuable to the brewery as a raw material. The "brewing quality"is a new, commonly used, term in brewing practices and in malt production terminology. So-called "brewing quality"is an extremely complex property. It is composed of several non-additive properties as a result of mostly unexplored interactions. This is why "brewing quality"is just an approximate category, having many known constituents, but in the field of their judgement and weighting, the growers, traders and users could not make such a minimal compromise as in the case of wheat, where the commercial quality of the product can unambiguously be determined by measuring the falling number, farinographic value and the gluten content. The determination of the "brewing quality"requires a series of difficult measurements and long micro-malting procedures but these methods, due to their time and effort, can not be used as routine methods. From another aspect, it is an essential for plant breeders to determine whether the new lines derived from the hybridisation of spring and winter varieties (performed to enlarge the yield and crop stability of spring barley varieties) have "brewing quality"or are closer to the ones used for other purposes. The separation of winter and spring barley varieties, as well as tracking the changes of the inner components during germination and malt production caused by different enzymatic processes, have already been published in our previous paper.[1] The aim of this work is to present a feasible procedure for the prediction of quality parameters of barley samples from their near infrared (NIR) spectra in respect of their brewing consumption. The task is—in spite of the large variability caused by variety and harvest territory—to determine the joint features of brewing barley varieties so they can be separated from those spring varieties having lower quality which are used for animal feed.

Materials and methods

The samples were collected from the four most important Hungarian growing areas, (Táplánszentkereszt, Kornpolt, Putnok and Mosonmagyaróvár). Five different spring barley varieties were investigated. Three of them, having constant good brewing quality (Orbit, Jubilant and Maresi), cover 95% of Hungarian agricultural land used for barley cultivation, while Pannónia and Michka are also significant spring varieties used for animal feed. All the samples were analysed in their natural kernel form without milling in reflection mode. NIR is widely used in brewing and malting practices to determine the constituents of barley (starch, protein, moisture etc.)[2,3] as well as of malt (soluble N, starch extract, etc.).[4–8] During these measurements the device is calibrated by samples with well known composition before the analysis. During our measurements NIR was used for qualitative and not quantitative analysis for comparison of quality points derived from the spectra of barley samples. Based on the terms of PQS (polar qualification system) the so-called "quality points" of the samples were defined as the centre of the spectra represented in the polar co-ordinate system.[9–11] By representing the spectra in the polar co-ordinate system, the ranges affording the most significant differences can be found at 180°C of each other, balancing their shifting effect to the quality point. Using a wavelength range optimisation algorithm, the wavelength ranges providing the best classification result can be calculated. Although this data reduction method (750 data to 2 data, the *x y* co-ordinates of the quality point) causes a significant loss of information, in most cases it is suitable to determine the quality or quality differences without requiring analytical chemical analysis. The effectiveness of the classification can be expressed numerically by calculating the so-called normalised distance and sensitivity. The maximum value of the normalised distance (i.e. distance divided by the distance plus the sum of the standard deviations of the quality point co-ordinates of the two spectra groups) is 1, while the sensitivity (i.e. distance divided by the sum of the standard deviations) shows how much larger the distance is than the sum of the standard deviation of the groups. The smaller the deviation, the larger the selectivity. By optimising normalised distance, the calculated range provides the smallest standard deviations relative to the distance of the investigated groups. The non-selected points (the spectral values outside the selected range) can be omitted or set to zero. A Spectralyzer 1025 type spectrometer was used in the wavelength range of 1000 to 2500 nm with a spectral step of 2 nm. The recorded spectra were analysed with the help of PQS (Polar Qualification System) software.

Results and discussion

Figure 1 represents the location of the quality points of the Maresi variety which is known to be very sensitive to the cultivation conditions harvested in four different Hungarian agricultural territories in the wavelength range 1100–1850 nm. As can be seen, the effect of the properties of the different territories (soil, nutrition, weather condition, etc.) and the different agritechnical methods (manuring, soil preparation, time of sowing, etc.) can be well tracked with PQS.

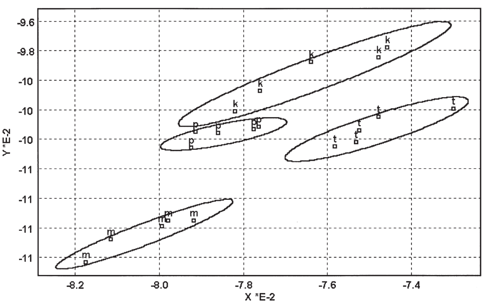

Figure 1. The location of the quality points of Maresi variety (1100–1850 nm, non selected points are zeros) harvested in four Hungarian agricultural territories k: Kompolt m: Mosonmagyaróvár, p. Putnok, t: Táplánszentkereszt).

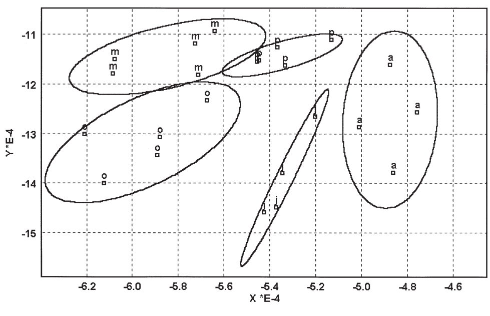

Figure 2. The location of the quality points of the investigated varieties (1762–1822nm, non selected points are omitted) harvested in Táplánszentkereszt (a: Maresi, m: Michka, j: Jubilant, p: Pannónia, o: Orbit)

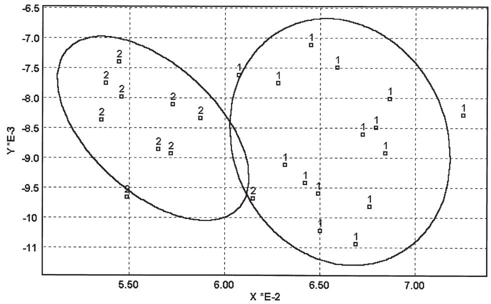

Figure 3. The location of the quality points of the investigated varieties (2nd der.,1728–1788nm, non selected points are zeros) harvested in Táplánszenkereszt (1: brewing quality, 2: crop quality).

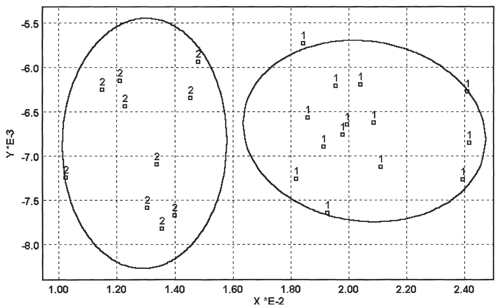

Figure 4. The location of the quality points of the investigated varieties (2nd der., 1736–1780 nm, non selected points are zeros) harvested in Kornpolt (1: brewing quality, 2: crop quality).

In the second part of our investigations (Figure 2) the five varieties harvested in Táplánszentkereszt were classified. As can be seen, although with the help of different agritechnical methods the physical and chemical parameters can be modified, they are basically determined genetically.

Finally, the joint features of varieties having been accepted as "brewing quality"were analysed. In the first step of this experiment, the effects of cultivation parameters were discriminated by investigating the samples grown and collected from the same territories (Figures 3 and 4). The samples were clustered in two quality groups, according to their brewing acceptance.

Figure 5 shows the classification result of the average of the samples, independent from the cultivation lands, while Figure 6 represents the same separation without averaging the samples.

A tendency can be observed but the separation is not as sharp as in the previous cases. The points in the overlapping region can be interpreted so that, in good conditions, the non-reliable samples can result in brewing quality while the accepted varieties can also produce lower quality. As is shown. using the wavelength range optimisation after the determination of the first range providing the best result, it

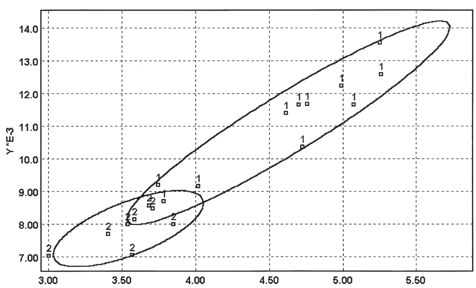

Figure 5. The location of the quality points of the investigated five varieties (average of the samples 1586–1638 nm and 1738–1784 nm, non selected points are zeros) harvested in the four territories (1: brewing quality, 2: crop quality).

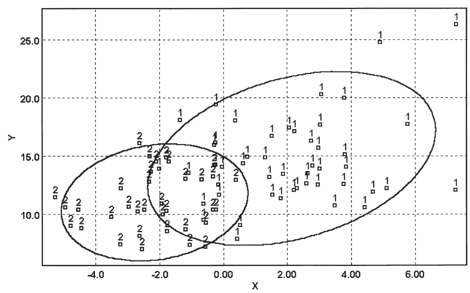

Figure 6 The location of the quality points of the investigated five varieties (1586–1638 nm and 1738–1784 nm, non selected points are zeros) harvested in the four territories (1: brewing quality, 2: crop quality).

is also possible to restart the algorithm so the best, second, third, etc. range can also be calculated. By omitting the spectral values between the selected ranges, the direction of the shifting effect of the absorption peaks to the quality points can be put together resulting in more efficient classification.

In all cases the ellipses surrounding the clusters were drawn by the double of the standard deviation. Namely, assuming a Gaussian distribution, 95% of the investigated population are inside the given area.

In all cases, the selected ranges providing the optimal result contain the absorption peak of starch, protein and oil, explaining the differences between the constituents of the brewing and fodder varieties.

Conclusions

In addition to the different calibration methods, near infrared spectroscopy, by using PQS techniques, is suitable as a quick, accurate, reagentless and non-destructive qualitative method, with no sample preparation, for the prediction of the quality of barley in respect of their brewing acceptance. By representing the spectrum in the polar co-ordinate system, the peaks are at the same wavelengths as in the rectangular co-ordinate system. So the method gives a good pictorial representation of the quality. Changes or differences in the composition of the samples show the quality points shifting parallel with the direction of the absorption peak of the changing or differing component and *vice versa*, from the direction of the quality point's shift conclusion can be drawn as regards which component had changed or are present in different quantities. If the given component has two or more peaks in the wavelength range used for producing the polar diagram, the direction of the shift is a result of two or more absorption peaks. Although it is a qualitative method, the effectiveness of the classification can be expressed numerically with the help of the normalised distance and the sensitivity so the different classification models are comparable. The feasibility of near infrared spectroscopy for the classification of spring barley related to brewing consumption ,as well as the investigation of the effect of cultivation and variety, were presented in this paper. Further investigations are planed to examine the effect of the harvest year.

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