Near-Infrared Reflectance Estimates of Malt Extract[1]

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ABSTRACT

Traditional laboratory methods used to test malting quality of barley are poorly adapted to rapid screening of early generation breeding lines in a plant-breeding program. Selection of lines that are potentially high in malt extract would help to eliminate undesirable genotypes, preventing the need for expensive and time-consuming laboratory testing. New near-infrared reflectance (NIR) technology may provide the means to speed the development of malting barley by eliminating poor-quality lines as early as the F_3 generation. Use of traditional laboratory tests could then be used on the more promising selections. We selected 54 barley genotypes having known malt extract (ME) values for use in calibration of a Technicon 400-R InfraAlyzer. The calibration techniques recommended by the equipment manufacturer were followed to obtain necessary regression coefficients. These were b = −600.2 for F_{10} and b = 594.9 for F_{14} with the intercept F_{00} = 58.03. With these values entered in the electronic NIR system, we measured the malt extract values of the barley samples used in the calibration procedure. The correlation coefficient between laboratory (Lab) ME values and NIR ME values was r = 0.95**, standard deviation from regression 0.833, and the regression coefficient of b = 1.00. One hundred thirty-three samples of known Lab ME not used in the calibration were analyzed for NIR ME. The correlation coefficient between Lab ME and NIR ME was r = 0.98**, the regression coefficient b = 1.00, and the standard deviation from regression 1.43. On 199 selected F_3 experimental lines, the range of Lab ME was 74.1–79.2. The NIR ME values were highly correlated with Lab ME value (r = 0.36**), with a regression coefficient b = 0.38 and the standard error from regression 0.78.

Malting barley cultivar development requires extensive traditional testing. The specified testing techniques for micro malt and wort production require several days to complete (Peterson and Foster 1973). Such procedures are poorly adaptable to rapid screening of early generation breeding lines in a plant-breeding program because they require lengthy procedures on a limited number of samples. Tests such as sedimentation (Palmer 1975), malt β-glucanase activity (Bendelow 1976a), polyphenol content (Bendelow 1976b), wort viscosity (Bendelow 1977), β-glucan content (Allison et al 1978), viscosity of barley extracts (Bendelow 1977, Greenberg and Whitmore 1974), mash filtration rate, and reducing sugar content (Bendelow 1976b) help to predict malt quality. Some tests require malted grain, whereas others use sound barley. The ideal test would predict malting quality from sound grain with sufficient reliability that only the best experimental lines would be selected in early generations. By reducing the test materials to only the most promising lines, more time could be spent on more rigorous testing of them. The ideal test may be beyond our grasp, but the potential rewards make its pursuit desirable.

Recent research on near-infrared reflectance (NIR) spectroscopy shows that it has some potential for important advancements in early generation screening techniques for cereal breeders. NIR users have expanded the technology to measure starch and insoluble pentosans (Law and Tkachuk 1977), soluble β-glucan content of barley (Allison et al 1978), and malt hot-water extracts (Morgan and Gothard 1979).

A major objective of these studies was to investigate various absorption bands in the NIR region and to attempt to relate these to the malt extract potential of barley. With this information, the NIR machine could be programmed to rapidly screen for this important quality factor of barley from sound grain.

MATERIALS AND METHODS

All barley samples used in this study were of spring growth habit and grew in Montana yield nurseries in the years 1970–1979. These nurseries included a wide range of genotypes, mostly two-row barleys. The 54 samples used for calibrating the NIR included 20 from 11 named cultivars and 34 samples from 32 experimental lines. These experimental lines came from Oregon, Idaho, Washington, California, and Montana breeding programs. A second set of 133 samples used to evaluate the NIR ME calibration came from the same nurseries. These included 75 from experimental lines and 58 from 22 named cultivars.

The F_3 lines studied came from a total of 11 crosses among eight parents, all two-row cultivars. At least one parent in each cross was an accepted malting cultivar. These lines were grown at Bozeman, MT, in 1979. The malting barley Klages served as the nursery check.

Malt extract (Lab ME) data for all samples came from the Barley and Malt Laboratory at Madison, WI. The standard method of the American Society of Brewing Chemists (1976) was used to obtain Lab ME data. These data were used to determine regression coefficients for NIR calibrations. A total of 54 samples with a range of 74.0–82.9% Lab ME was selected. Samples were evenly distributed over this range. The NIR equipment used was the Technicon InfraAlyzer 400-R. Regression coefficients for the calibration equation were estimated using a backward elimination multiple regression procedure of Lab ME against filter reflectance values. The procedure followed to select wavelengths for estimating malt extract was that presented by the equipment manufacturer.

Ten randomly selected barley samples were used to measure the reproducibility of NIR ME estimates. Each of the 10 samples was divided equally into two parts. One set of these 10 subsamples was ground and analyzed five times for NIR ME. After each analysis, the sample in the NIR sample holder was returned to the container and mixed thoroughly before being packed into the NIR sample holder for the subsequent analysis. The other set from each of the 10 original samples was divided into five subsamples, each of which was ground and analyzed for NIR ME. Data from these two sets of 10 samples were analyzed to determine the variability of the NIR among repeated readings.

All samples used throughout the research were ground in a Udy Cyclone mill equipped with a 1.0-mm screen.

RESULTS

The range of Lab ME and the distribution of samples in the calibration set are shown in Table I. By using this set of samples and following the recommended calibration procedure, regression coefficients were obtained from multiple regression analysis for log of reflectance values for filters 10 (2,180 nm) and 14 (2,100 nm). The regression equation was $y = 58.03 - 600.2(X_{2,180}) + 594.9(X_{2,100})$ with a coefficient of determination of 0.95.

The validity of estimating malt extract percent by NIR of samples not included in the calibration set was determined next.

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TABLE I
Calibration Samples Showing the Number in Each Class According to Lab ME[a] and NIR ME[b]

Classification (% ME)	Distribution of Samples	
	Lab ME	NIR ME
74.0–74.9	5	4
75.0–75.9	7	4
76.0–76.9	6	8
77.0–77.9	6	7
78.0–78.9	7	7
79.0–79.9	6	9
80.0–80.9	5	3
81.0–81.9	7	9
82.0–82.9	5	3
Mean	78.4	78.4

[a] Lab ME = laboratory malt extract.
[b] NIR ME = near-infrared reflectance malt extract.

TABLE II
Distribution of Malt Extract (ME) Values from 133 Barley Samples Grown in Nurseries at Ft. Ellis and Bozeman, MT During 1970–76

Classification (% ME)	Distribution of Samples		Classification (% ME)	Distribution of Samples	
	Lab ME[a]	NIR ME[b]		Lab ME	NIR ME
67.0–67.9	2	0	76.0–76.9	32	46
68.0–68.9	2	0	77.0–77.9	31	23
69.0–69.9	1	0	78.0–78.9	24	14
70.0–70.9	1	0	79.0–79.9	15	3
71.0–71.9	0	3	80.0–80.9	7	13
72.0–72.9	2	1	81.0–81.9	1	3
73.0–73.9	0	2	82.0–82.9	0	2
74.0–74.9	2	3	83.0–83.9	1	1
75.0–75.9	11	19	84.0–84.9	1	0

[a] Lab ME = laboratory malt extract.
[b] NIR ME = near-infrared reflectance malt extract.

TABLE III
Distribution of Malt Extract (ME) Values from 199 Selected F_3 Lines Grown at Bozeman in 1979 and Related Statistics

Classification (% ME)	Distribution of Samples	
	Lab ME[a]	NIR ME[b]
74.0–74.9	3	0
75.0–75.9	12	2
76.0–76.9	72	43
77.0–77.9	85	84
78.0–78.9	24	63
79.0–79.9	3	7

Lab ME $\bar{X}$, 77.07
NIR ME $\bar{X}$, 77.57
$\bar{X}$ of Klages NIR ME, 78.2
r^2, .126

[a] Lab ME = laboratory malt extract.
[b] NIR ME = near-infrared reflectance malt extract.

TABLE IV
Near-Infrared Reflectance (NIR) Estimates of Repeatability for Malt Extract of Barley

Sample No.	Lab ME[a] (%)	NIR ME[b] (Repack) (%)	CV[c] (%)	NIR ME[d] (Separate Grind) (%)	CV[c] (%)
1	76.3	76.7	.39	76.4	.30
2	77.9	78.0	.19	77.6	.74
3	75.2	77.2	.34	77.0	.70
4	78.3	77.2	.15	77.3	.29
5	79.0	78.2	.37	78.0	.42
6	75.1	77.1	.37	77.0	.15
7	77.5	78.0	.25	77.6	.72
8	77.4	77.6	.43	77.5	.49
9	77.5	78.6	.27	79.4	1.10
10	77.6	77.7	.17	77.7	.82

[a] Lab ME = laboratory malt extract.
[b] Mean of five repacks.
[c] CV = coefficient of variation.
[d] Mean of five separate grinds.

One hundred thirty-three barley samples grown in the same nurseries and in the same years as the calibration set were analyzed for NIR ME. Data from this set of samples are in Table II. The Lab ME values ranged from 67.1 to 84.6%. The mean of NIR ME was 76.6, and that of Lab ME was 76.7. The correlation between Lab ME and NIR ME values was 0.96**. These data suggest that Lab ME is predicted by NIR ME.

One test of NIR ME prediction was as a screening tool among F_3 lines. Approximately 1,500 of these were submitted for NIR testing, so that only those most likely to have good malting potential would be malted experimentally. NIR ME values on 199 F_3 lines that equalled or exceeded Klages NIR ME were analyzed for Lab ME. The NIR ME values initially determined on these 199 F_3 lines were correlated with Lab ME values. These data showing the range and distribution of ME values are in Table III. The correlation coefficient for these data was r = 0.36**, highly significant statistically. The narrow range of malt extract values, from 74.1 to 79.2, had some bearing on the magnitude of the r value. Deviations of NIR ME estimates were no greater than in previous experiments.

Coefficients of variation in the repack data (Table IV) range from 0.15% for sample 4 to 0.43% for sample 8, showing less variability in successive readings of certain samples than in others. These values, however, would all be within acceptable limits for routine screening work. Coefficients of variation in the separate grind data ranged from 0.15% for sample 6 to 1.10% for sample 9, suggesting a range in sampling and/or grinding variation. These two sets of data show that the NIR has good repeatability in estimating this important malt quality characteristic.

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