

Comparison of Three Whole Seed Near-Infrared Analyzers for Measuring Quality Components of Canola Seed¹

James K. Daun*, Kathleen M. Clear and Phil Williams

Canadian Grain Commission, Grain Research Laboratory, Winnipeg, Manitoba R3C 3G8, Canada

Whole seed near-infrared (NIR) analyzers are capable of high-speed compositional analysis of oilseed commodities. This study compared the PerCon Inframatic 8144 (Perten Instruments, North America Inc., Reno, NV), the Tecator Infratec 1225 (Tecator AB, Hoganas, Sweden) and the NIR-Systems 6500 (NIR Systems, Inc., Silver Spring, MD) analyzers for measurement of oil, protein, chlorophyll and glucosinolates in intact canola seed of composite samples from the Grain Research Laboratory's (Winnipeg, Manitoba, Canada) annual Western Canada Harvest Surveys (1985-1989) for assembly of calibration and prediction sets. No significant differences were found between the three instruments for oil [standard error of prediction (SEP 0.43-0.55%)], protein (SEP 0.35-0.42%) and glucosinolates (SEP 2.4-3.8 mM/g). Neither the Tecator nor the PerCon instruments were effective for determining chlorophyll. By combining oil content and fatty acid composition data to give an estimate of the total level of each fatty acid in the sample, high correlations were obtained for total saturates, linolenic acid, and linoleic acid although the RPD (ratio of the S.E. of prediction to the S.D. of the original data) values were not high enough to enable routine use of the method to predict results.

KEY WORDS: Canola, chlorophyll, fatty acids, NIR, NIR analysis, oil content, protein, rapeseed.

Near-infrared reflectance (NIR) spectroscopy instruments are widely used to determine quality components in cereal grains (1). Early instruments called for the seed to be finely and uniformly ground. It is difficult to obtain a uniform and consistent grind of soft oilseeds, such as canola. Also, oil is expressed on grinding, and loading the sample cell may contaminate the optical surface of sample cells making it necessary to clean the window between samples or to use an open cell. NIR analysis of canola was reviewed by McGregor (2), who concluded that the technique, especially with whole seeds, had potential for use in varietal selection programs for some components, but that traditional methods of analysis gave better results, and was sometimes just as rapid. NIR instrumentation has been used for the determination of chlorophyll in canola (3), and also of glucosinolates in whole seed (4,5). Williams and Sobering (6) compared transmittance and reflectance modes of analysis and found, for a limited number of samples, that oil, protein, chlorophyll and glucosinolates could be determined with reasonable success by either method.

The American Oil Chemists' Society (AOCS) recommends a procedure for determining oil, moisture and protein in oilseeds by NIR (7). The procedure, which requires that samples be ground, suggests that correlations greater than 0.8 and standard error of prediction (SEP) values of not more than 0.3% for oil and 0.4% for protein be obtained. Although these levels may be achieved for soybeans (8), the literature

suggests that these levels of precision often cannot be met for rapeseed. For ground samples of rapeseed or crambe, SEPs have been reported of about 0.8% for either oil or protein (%N \times 6.25) (9-12). McGregor (2) obtained a SEP of 0.43% for protein, and Panford *et al.* (13), working with a scanning instrument, reported SEPs of about 0.1% for both oil and protein in ground rapeseed. Ribailier and Maviel (14) considered that oil could be determined with an SEP of better than 0.5% on three instruments if the samples were dried before analysis. Results for whole seed analysis of canola have shown SEPs greater than 0.8% for oil and protein (2,6,15-17).

The near-infrared instruments, capable of working with large, whole seed samples, have made it possible to avoid some of the problems associated with grinding. The objectives of this work were to compare the performance of three instruments in measuring oil and protein content and to determine the extent to which chlorophyll and glucosinolates could be determined in whole canola seed. The NIRSystems Model 6500 (NIRSystems, Inc., Silver Spring, MD) was also used to develop calibrations for estimating individual fatty acids in whole canola seeds. Composite samples, representative of canola grown in western Canada between 1985 and 1989, were used to assemble calibration and prediction sets.

MATERIALS AND METHODS

NIRSystems 6500 (NIRSystems, Inc.) Primarily designed as a research instrument for near-infrared studies, this instrument is microcomputer-controlled and operated. The instrument can operate in either transmittance or reflectance mode, and log 1/R spectra can be converted to first- and second-derivative form for calibrations. The coarse sample cell holds about 120 g and presents about 60 cm² of surface for analysis. The coarse sample cell can be used with 3/4, 1/2 and 1/4 cell loading depths as well as full.

Calibrations can be developed with partial least squares (PLS) or multiple linear regression (MLR) by using the NSAS software (NIRSystems), which also controls the instrument. The present studies were carried out with the instrument in reflectance mode. Both PLS or MLR were used in developing calibrations from the second derivative of the log 1/R spectra.

Tecator Infratec 1225 (Tecator AB, Hoganas, Sweden). The Tecator Infratec 1225 is a near-infrared transmittance instrument. The instrument scans between 850 and 1050 nm. It has a built-in computer and uses PLS regression based on "Unscrambler" for development of calibration equations. Spectra can also be down-loaded to a personal computer (PC) for further data processing and expanded calibration development. For this study, the instrument was set at 10 scans per sample. The sample cell has a surface area of about 22.5 cm². Canola seed requires a 6-mm path length, and cereals require 18 mm.

PerCon Inframatic 8144 (Perten Instruments, North America, Inc., Reno, NV). The Inframatic 8144 is a reflectance unit equipped with an array of 44 discrete interference filters (from 540 to 2345 nm). The instrument has no true sample cell; the sample is poured into a sample

¹Presented at the 84th AOCS Annual Meeting & Expo, April 27, 1993, Anaheim, California.

*To whom correspondence should be addressed at Canadian Grain Commission, Grain Research Laboratory, 1404-303 Main St., Winnipeg, Manitoba R3C 3G8, Canada.

compartment and packed with a spring-loaded device. After analysis it is dropped into a hopper.

Samples. Composite samples used in the study closely represent the railway carlot and cargo increment samples normally analyzed at terminal elevators. The 215 samples were compiled from the Grain Research Laboratory's (Winnipeg, Manitoba, Canada) annual canola harvest surveys from 1985 to 1989 (17). Newly harvested samples are received from country stations across the growing area. After cleaning and grading, composite samples were prepared by grade and by crop district. Each composite contained from fifteen to several hundred samples. They included grades from No. 1 Canada to No. 3 Canada and species from predominantly *Brassica rapa* varieties to predominantly *B. napus* varieties, depending on the year and location. Composite samples display less individual spectral diversity than individual farm-grown samples but are more characteristic of "real-world" commercial material. The calibration and prediction samples (Tables 1 and 2), respectively, represented a wide range of qualities and varieties of canola seed grown over a 5-year period. They were drawn from southeastern Manitoba to the Peace River Region in British Columbia. This region covers 7° latitude and 25° longitude, ranges in altitude from 600 to 1000 M, and includes prairie, parkland and semi-arid regions under irrigation. Weather conditions covered ranged from wet (1985) to dry (drought) (1988–1989) and from cool (early frost) (1986) to extreme heat (1989). Samples included 123 of Grade No. 1, 78 of No. 2 and 16 of No. 3 Canada Western Canola.

The predominant varieties grown in the period 1985–1989 were *B. napus* cv. Westar (ca. 50% of acres sown) and *B. rapa* cv. Tbbin (ca. 40% of acres sown). No distinction was made between varieties in the sampling procedures, but the earlier-maturing *B. rapa* varieties tended to pre-

dominate in the northern and western growing regions. *Brassica rapa* varieties had mainly yellow-colored seed coats and less oil, protein and chlorophyll but more glucosinolates than the larger-seeded, later-maturing *B. napus* varieties, which have dark-colored seed coats.

Analytical Methods. Samples were analyzed before commencing the NIR study with the following analytical methods: oil content by nuclear magnetic resonance according to the Federation of Oil Seeds and Fats Associations (FOSFA) method (18); protein content by Kjeldahl (19) and combustion analysis (20); chlorophyll by extraction and spectrophotometry (21); glucosinolates by gas-liquid chromatography (GLC) (22) (aliphatic) and high-performance liquid chromatography (HPLC) (23) (total); fatty acid composition by gas-liquid chromatography (GLC) (24); and moisture by gravimetric analysis (25).

Because the samples had equilibrated to the same moisture level (about 7%) in dry air, it was not possible to calibrate for moisture content. All chemical results were converted to moisture-free bases before use in calibrations.

Calibration (150 samples) and prediction (54 samples) sets were prepared by ranking the samples according to component and randomly selecting samples across the range of composition. The Tecator software restricts calibration sets to 100 samples (in this study 94 were used). The Tecator Infracalc PLS program uses 100 wavelength points and generates factors (loadings) rather than regression statistics at discrete wavelengths.

The instruments were calibrated for each constituent by scanning each sample in the calibration set and then computing the optimum equations. The prediction sets were then scanned, and the predicted values were compared with the reference values to evaluate accuracy and precision.

TABLE 1

Reference Method Summary for Calibration and Prediction Samples^a

Factor	Mean	Standard deviation	Minimum	Maximum	Range
All samples					
Oil (% dry basis)	45.6	2.3	39.8	49.9	10.2
Protein (Kjeldahl N × 6.25%, dry basis)	23.8	2.5	19.7	29.8	10.2
Protein (combustion N × 6.25%, dry basis)	24.4	3.9	20.0	30.9	10.9
Total glucosinolates (mMwg, whole seed)	17.9	4.6	9.7	30.0	20.3
Aliphatic glucosinolates (mM/g, whole seed)	12.5	3.9	5.6	25.3	19.7
Chlorophyll (mg/kg)	18.6	9.4	6.0	64.0	58.0
Calibration					
Oil (% dry basis)	45.8	2.3	39.8	49.9	10.2
Protein (N × 6.25%, dry basis)	23.7	2.4	19.8	29.8	10.0
Protein (combustion N × 6.25%, dry basis)	24.1	2.6	20.0	30.9	10.9
Total glucosinolates (mM/g, whole seed)	17.8	4.8	9.7	30.0	20.3
Glucosinolates (mM/g, whole seed basis)	12.4	4.1	5.6	25.3	19.7
Chlorophyll (mg/kg)	18.3	8.8	6.0	64.0	58.0
Prediction					
Oil (% dry basis)	44.9	2.3	40.4	49.2	8.7
Protein (N × 6.25%, dry basis)	24.3	2.6	19.7	29.5	9.8
Protein (combustion N × 6.25%, dry basis)	25.0	2.8	20.0	30.0	10.8
Total glucosinolates (mM/g, whole seed)	18.3	3.9	10.7	28.5	17.8
Glucosinolates (mM/g, whole seed basis)	12.7	3.4	6.6	22.5	15.9
Chlorophyll (mg/kg)	19.7	10.7	7.0	59.0	52.0

^aAll samples were equilibrated to a moisture content of about 7% (±0.3%). Glucosinolates are on an 8.5% moisture basis and chlorophyll on a *tel quel* basis.

COMPARISON OF THREE WHOLE SEED NEAR-INFRARED ANALYZERS

TABLE 2

NIR Calibration and Prediction Data for Quality Factors for Canola

Component	Instrument ^a	Calibration			Prediction			
		R ^{2b}	SEE ^c	Factors	R ²	SEP ^d	R/SE ^e	RPD ^f
Oil (%)	PerCon Inframatic 8144	0.972	0.49		0.963	0.55	15.8	4.18
	Tecator Infracorec 1225	NA	NA	13	0.964	0.55	15.8	4.18
	NIRSystems 6500 1	0.982	0.41		0.967	0.54	16.1	4.25
	NIRSystems 6500 2	0.979	0.43		0.979	0.43	20.2	5.34
Protein (%) Kjeldahl	PerCon Inframatic 8144	0.981	0.48		0.99	0.38	25.8	6.84
	Tecator Infracorec 1225	NA	NA	11	0.987	0.42	23.3	6.19
	NIRSystems 6500 1	0.987	0.40		0.984	0.48	20.4	5.41
	NIRSystems 6500 2	0.991	0.35		0.992	0.33	26.7	7.87
Protein (%) combustion	NIRSystems 6500 1	0.984	0.34		0.989	0.43	25.1	6.51
	NIRSystems 6500 2 ^g	0.985	0.48	8	0.988	0.43	25.1	6.51
Chlorophyll (mg/kg)	PerCon Inframatic 8144	0.850	4.8		0.901	5.2	10	2.05
	Tecator Infracorec 1225	NA	NA	12	0.576	9.0	5.8	1.18
	NIRSystems 6500 1	0.942	3.0		0.939	3.9	13.3	2.74
	NIRSystems 6500 2	0.951	3.4		0.958	3.2	16.3	3.34
Glucosinolates mM/g oil free aliphatic	PerCon Inframatic 8144	0.860	3.6		0.812	3.6	4.9	1.08
	Tecator Infracorec 1225	NA	NA	11	0.827	3.8	4.6	1.02
	NIRSystems 6500 1	0.929	2.6		0.899	2.7	6.6	1.44
	NIRSystems 6500 2	0.858	1.8	13	0.857	1.7	10.5	2.29
Glucosinolates mM/g in seed total	NIRSystems 6500 2	0.900	2.1	13	0.823	2.5	6.4	1.36

^aPerCon Inframatic 8144 from Perten Instruments, North America Inc. (Reno, NV); Tecator Infracorec 1225 from Tecator AB (Hoganas, Sweden); and NIRSystems 6500 1 and 2 from NIR Systems, Inc. (Silver Spring, MD).

^bR², coefficient of determination.

^cSEE, standard error of estimate.

^dSEP, standard error of prediction.

^eRatio of the range as determined by the reference chemical method to the SPE.

^fRatio of the SPE to the standard deviation of the prediction set data as determined by the reference chemical method.

^gNo math, 1100–2500 nm.

RESULTS AND DISCUSSION

For the NIRSystems 6500 applications, results from PLS regression (which are presented here) gave better SEPs than did those from MLR.

Oil and Protein. For oil determination, SEPs were about 0.5% for all three instruments, and SEPs for protein were about 0.4%. The ratio of the SEP to the standard deviation of the prediction set reference data is known as the ratio of the S.E. of prediction to S.D. of the original data (RPD) (6). RPD values for oil (4–5) and protein (5–8) sug-

gested that all of the instruments would be suitable for quality control purposes. The R/SE (range/standard error, also known as RER) values of 15–20 for oil and 20–26 for protein were significantly higher than those reported by McGregor (2) or Starr *et al.* (9).

The wavelengths chosen for calibration of oil and protein (Table 3) included wavelengths previously associated with oil and protein (26). A strong negative correlation exists between oil and protein in canola ($r =$ about 0.9), and it was not surprising to find protein bands appearing in the oil calibration.

TABLE 3

Principle Wavelengths Used in Developing Calibrations for Oil, Protein, Chlorophyll and Glucosinolates

Component	Instrument ^a	Wavelengths					
Oil	NIRSystems 6500	1274	1284	1772 ^b	2136 ^b		
	PerCon Inframatic 8144	1318	1410 ^b	1510	1790	2245	2250
Protein	NIRSystems 6500	1282 ^b	2110	2388 ^b	2442 ^b		
	PerCon Inframatic 8144	1680 ^b	1709	2083 ^b	2139 ^b	2180 ^b	2190
Chlorophyll	NIRSystems 6500	662 ^c	686 ^c	1534	17532		
	PerCon Inframatic 8144	675 ^c	696 ^c	2050	2130	2139	2230
Glucosinolate	NIRSystems 6500	890	1016	1614 ^d	1776	2139	2230
	PerCon Inframatic 8144	696	1360	1644 ^d	1680 ^d	1759	1778

^aCompany sources as in Table 3.

^bWavelengths close to absorbers identified as due to oil or protein (Ref. 21).

^cWavelengths close to absorbers identified as due to chlorophyll (Ref. 22).

^dWavelengths close to absorbers identified as due to glucosinolates (Ref. 23).

Glucosinolates. Glucosinolates are relatively minor components in canola. Much previous NIR work on this seed (4-6,18,24,27,28) has dealt with determining glucosinolates over a wide range (20-200 mM/g), but this study dealt with the range encountered in Canada, where virtually all seed planted is low-glucosinolate or canola quality. Earlier studies concentrated only on the aliphatic glucosinolates as defined in the current canola definition. By the time results for total glucosinolates by HPLC were available, it was not possible to carry out re-calibration and analysis with the Tecator or PerCon instruments. For aliphatic glucosinolates, the SEPs found for all three instruments were acceptable and comparable to SEPs from studies with ground seed. The best result was obtained from the NIRSystems instrument where the SEP was 2.7 mM/g. This is lower than SEPs reported in the other studies. The results for total glucosinolates determined by HPLC were even more promising, with a SEP of 1.89 mM/g. Wavelengths chosen for calibration of glucosinolates (Table 3) included wavelengths previously assigned to bands associated with glucosinolates (29).

Chlorophyll. An instrument must be capable of detecting absorption maxima near 670 nm (30) to predict chlorophyll. The Tecator instrument has a minimum wavelength of only 800 nm and was not able to successfully determine chlorophyll. This deficiency hopefully may be remedied in future models. The SEP of 3.4 mg/kg for the NIRSystems instrument was higher than the 2.5 mg/kg reported by Williams and Sobering (6), but only slightly higher than 3.0 reported for ground seed instruments (29). The RPD for chlorophyll was in the range of 2 to 4, somewhat lower than would be needed if the method were to be suitable for quality control. This issue is under further study.

Fatty acid composition. Fatty acid composition studies were only carried out with the NIRSystems 6500 instrument. Major fatty acids were studied (Table 4), including palmitic (C16:0), stearic (C18:0), oleic (C18:1), linoleic (C18:2), linolenic (C18:3) and total saturated fatty acids (C14:0 + C16:0 + C18:0 + C20:0 + C22:0 + C24:0). Erucic acid was also included, although values for this parameter were usually less than 1% of the total fatty acids.

Earlier studies (31,32) identified wavelengths near 1700 and 2100 nm as being important to fatty acid determination by NIR. Spectra of triacylglycerols from various oils showed differences in these regions and enabled differentiation of oils from different sources (33). Quantitative analysis of fatty acids in rapeseed has been reported by Reinhardt and co-workers (34,35). These workers were able to obtain acceptable calibrations when working with a set of samples selected to cover wide ranges of fatty acid composition.

In our study, calibrations based on fatty acids expressed as percentages of total fatty acids gave low correlations ($r \leq 0.3$). When individual fatty acids were expressed as mg/g seed, rather than as percentage of total fatty acids, the NIR instrument was able to calibrate on the actual concentration of each fatty acid as it was presented to the instrument. Errors induced by variable oil content were removed, and acceptable calibration and correlations were obtained for the major fatty acids (Table 5). Except for C18:1, MLR results were slightly better than PLS results. These "up and down" differences between MLR and the (favored) PLS method are quite common, with MLR calibrations often being slightly better.

Prediction results expressed as mg fatty acid per g of seed (Table 5) gave RPD values greater than 2 for all major

TABLE 4

Analytical Data for Fatty Acid Composition

Fatty acid	As % of total fatty acids					mg/g Seed (dry basis)				
	Mean	Standard deviation	Minimum	Maximum	Range	Mean	Standard deviation	Minimum	Maximum	Range
All samples										
C16:0	3.8	0.3	3.1	4.3	1.2	17.1	1.3	13.5	20.0	6.5
C18:0	1.8	0.2	1.4	2.3	0.9	8.4	0.7	6.5	10.0	3.5
C18:1	61.4	2.1	55.6	65.6	9.9	279.7	13.7	230.8	313.0	82.1
C18:2	19.5	0.9	17.5	22.6	5.1	89.0	6.1	74.7	100.2	25.5
C18:3	9.4	1.5	6.9	12.9	6.0	43.0	7.9	28.9	60.7	31.8
C22:1	0.6	0.8	0.1	6.7	6.5	2.7	4.0	0.6	31.7	31.2
Sats. ^a	5.6	0.6	1.6	6.6	5.0	25.3	2.4	7.8	29.2	21.5
Calibration										
C16:0	3.7	0.3	3.1	4.3	1.2	17.1	1.3	13.5	20.0	6.5
C18:0	1.8	0.2	1.4	2.3	0.9	8.4	0.7	6.5	10.0	3.5
C18:1	61.4	2.2	55.7	65.6	9.8	281.0	14.0	230.8	313.0	82.1
C18:2	19.5	0.9	17.5	22.6	5.1	89.5	6.0	75.2	99.8	24.6
C18:3	9.5	1.5	6.9	12.9	6.0	43.5	7.9	28.9	60.7	31.8
C22:1	0.6	0.8	0.1	6.7	6.5	2.8	4.0	0.6	31.7	31.1
Sats.	5.5	0.6	1.6	6.6	5.0	25.3	2.7	7.8	29.2	21.5
Prediction										
C16:0	3.8	0.3	3.1	4.2	1.1	16.9	1.1	14.0	19.2	5.3
C18:0	1.9	0.2	1.4	2.2	0.8	8.3	0.6	6.7	9.3	2.6
C18:1	61.5	2.1	55.6	64.9	9.2	275.8	12.2	249.6	302.1	52.5
C18:2	19.5	0.8	18.3	21.8	3.5	87.7	6.2	74.7	100.2	25.5
C18:3	9.2	1.5	7.1	12.8	5.7	41.7	8.0	29.9	60.6	30.7
C22:1	0.6	0.8	0.1	5.8	5.6	2.7	3.9	0.6	28.1	27.5
Sats.	5.6	0.4	4.5	6.3	1.8	25.2	1.6	20.6	28.1	7.5

^aSum of saturated fatty acids (C14:0 + C16:0 + C18:0 + C20:0 + C22:0 + C24:0).

COMPARISON OF THREE WHOLE SEED NEAR-INFRARED ANALYZERS

TABLE 5

Summary of Calibration and Prediction Results for Fatty Acid Compositions in Canola from the NIRSystems 6500^a

Fatty acid	Calibration			Prediction			
	Factors	R	SEE	R	SEP	RPD	R/SEP
Partial least squares							
C16:0	9	0.927	0.47	0.916	0.41	2.66	12.9
C18:0	13	0.887	0.30	0.884	0.26	2.31	10.0
C18:1	13	0.964	3.0	0.903	4.8	2.54	10.9
C18:2	10	0.964	1.5	0.965	1.5	4.15	17.1
C18:3	12	0.986	1.2	0.986	1.3	6.21	24.0
C22:1	13	0.481	2.1	0.208	3.5	1.11	7.8
Total saturated	9	0.923	0.68	0.906	0.61	2.56	12.3
Multiple step-wise regression							
C16:0		0.903	0.38	0.937	0.35	3.12	15.1
C18:0		0.772	0.29	0.857	0.28	2.11	9.1
C18:1		0.867	4.6	0.909	4.7	2.62	11.2
C18:2		0.940	1.3	0.971	1.4	4.58	18.9
C18:3		0.977	1.1	0.986	1.2	6.52	25.2
C22:1		0.208	3.3	0.367	3.4	1.17	8.2
Total saturated		0.898	0.55	0.919	0.56	2.77	13.3

^aFrom NIR Systems, Inc. (Silver Spring, MD). Definitions and abbreviations as in Table 2.

TABLE 6

Prediction of Fatty Acid Composition (% total fatty acids) from a Combination of Near-Infrared Oil Content and Fatty Acid Composition^a

Fatty acid	R	SEP	RPD	R/SEP
Partial least squares				
C16:0	0.846	0.14	2.1	7.9
C18:0	0.853	0.09	2.2	8.9
C18:1	0.532	1.96	1.1	4.7
C18:2	0.541	1.14	0.7	3.1
C18:3	0.857	0.86	1.7	6.6
C22:1	0.003	0.66	1.2	8.5
Total saturated	0.816	0.25	1.6	7.2
Multiple step-wise regression				
C16:0	0.840	0.14	2.1	7.9
C18:0	0.886	0.08	2.5	10.0
C18:1	0.496	2.12	1.0	4.3
C18:2	0.814	0.68	1.2	5.1
C18:3	0.951	0.50	3.0	11.4
C22:1	0.330	0.38	2.1	14.7
Total saturated	0.863	0.20	2.0	9.0

^aAbbreviations and definitions as in Table 2.

fatty acids in canola. Results for erucic acid were not good, but this fatty acid was found in small quantities (less than 1% relative) in most of the samples. It was also possible to predict the relative concentration of the major fatty acids from the NIR calculated oil content (Table 6). Although the results were not acceptable for routine use, significant regression coefficients were obtained, except for oleic and erucic acid. Accuracy of prediction of these two fatty acids was sufficient to warrant further study in this area. Wavelengths selected for fatty acid composition included wavelengths that have been associated with fatty acids composition by other workers (Table 7) (31,32).

One of the main objectives of the above study was to determine which of the three NIR instruments would be most suitable for use in analysis of oilseeds at terminal elevators, for survey work and in breeding programs. The results showed that for certain components (oil and pro-

TABLE 7

Principle Wavelengths Used for Calibration of Fatty Acid Compositions from the NIRSystems 6500 Instrument^a

C16:0	C18:0	Total sats. ^b	C18:1	C18:2	C18:3	C22:1
400	460	400	550	820	730	670
610	730	610	760	940	1030	700
850	1060	820	970	1150	1150	1210
880	1150	1000	1270	1570	1510	1240
1000	1480	1420	1300	1660 ^c	1630	1540
1420	1780 ^c	1570	1360	1810 ^c	1690 ^c	1570
1810 ^c	1930 ^c	1810 ^c	1690 ^c	2020	1750 ^c	2020
1990 ^c	2050	1990	1750 ^c	2260	1810 ^c	2140 ^c
2410	2380	2410	1960 ^c	2380	2050	2230

^aFrom NIR Systems, Inc. (Silver Spring, MD).^bSum of saturated fatty acids (C14:0 + C16:0 + C18:0 + C20:0 + C22:0 + C24:0).^cWavelengths associated with fatty acid absorbers (Refs. 27 and 28).

tein), all three instruments would serve. The second objective was to examine the extent to which the minor but important constituents, chlorophyll and glucosinolates, could be determined by an NIR instrument. The NIR-Systems Model 6500 gave the best results for glucosinolates and chlorophyll, as well as for oil and Kjeldahl protein. The SEPs for chlorophyll and glucosinolates indicated that the Model 6500 could be a valuable tool in screening for low glucosinolates in breeding programs.

ACKNOWLEDGMENTS

We thank the PerCon Company for lending us the Inframatic 8144 instrument so that we could carry out this and other studies. H.K. Howard, B.A.S. Misener, B. Ng and P.B. Mazur provided assistance with analyses. Paper number 719 of the Grain Research Laboratory.

REFERENCES

- Williams, P.C., and Karl H. Norris (eds.), *Near-Infrared Technology in the Agricultural and Food Industries*, American Association of Cereal Chemists Inc., St. Paul, 1987.

2. McGregor, D.I., in *Canola and Rapeseed Production, Chemistry, and Processing Technology*, edited by F. Shahidi, Van Nostrand Reinhold, New York, 1990, pp. 221-231.
3. Tkachuk, R., V.J. Mellish, J.K. Daun and L.J. Macri, *J. Am. Oil Chem. Soc.* 65:381 (1988).
4. Biston, R., P. Dardenne, M. Cwikowski, M. Marlier, M. Severin and J.-P. Wathelet, *Ibid.* 65:1599 (1988).
5. Salgó, A., Z. Weinbrenner-Varga, Z. Fábán and E. Ungár, in *Making Light Work: Advances in Near Infrared Spectroscopy*, edited by I. Murray, and I.A. Cowe, VCH, Weinheim, 1992, pp. 328-332.
6. Williams, P.C., and D.C. Sobering, *J. Near Infrared Spectrosc.* 1:25 (1993).
7. *Official Methods and Recommended Practices of the American Oil Chemists' Society*, edited by D.R. Firestone, 4th edn., American Oil Chemists' Society, Champaign, 1989.
8. Hurburgh, C.R., Jr., L.N. Panynter and S.G. Schmitt, *Appl. Eng. Agric.* 3:159 (1987).
9. Starr, C., A.G. Morgan and D.B. Smith, *J. Agric. Sci., Camb.* 97:107 (1981).
10. Starr, C., J. Suttle, A.G. Morgan and D.B. Smith, *Ibid.* 104:317 (1985).
11. Bengtsson, L., *Fette Seifen Anstrichm.* 87:262 (1985).
12. Hartwig, R.A., and C.R. Hurburgh, Jr., *J. Am. Oil Chem. Soc.* 67:435 (1990).
13. Panford, J.A., P.C. Williams and J.M. deMan, *J. Am. Oil Chem. Soc.* 65:1627 (1988).
14. Ribaillier, D., and M.-F. Maviel, *Rev. Franc. Corps Gras* 31:181 (1984).
15. Tkachuk, R., *J. Am. Oil Chem. Soc.* 58:819 (1981).
16. Salgó, A., Z. Fábán, E. Ungár and Z. Weinbrenner-Varga, in *Making Light Work: Advances in Near Infrared Spectroscopy*, edited by I. Murray, and I.A. Cowe, VCH, Weinheim, 1992, pp. 336-341.
17. DeClercq, D.R., J.K. Daun and K.H. Tipples, *Quality of Western Canadian Canola 1989*, Crop Bulletin 175, Canadian Grain Commission Grain Research Laboratory, Winnipeg, 1989.
18. *FOSFA International the Manual Part 2. Standard Contractual Methods*, Federation of Oil Seeds and Fats Association International, London, 1989, pp. 65-67.
19. Williams, P.C., *J. Sci. Food Agric.* 24:343 (1973).
20. *Official Methods of Analysis*, 15th edn., 1st Supplement, Association of Official Analytical Chemistry International, Arlington, 1990, Sec. 990.03.
21. *Official Methods and Recommended Practices of the American Oil Chemists' Society*, edited by D.R. Firestone, American Oil Chemists' Society, Champaign, 1989, Method Ak 2-92.
22. Heaney, R.K., and G.R. Fenwick, *J. Sci. Food Agric.* 31:593 (1980).
23. *Official Methods and Recommended Practices of the American Oil Chemists' Society*, edited by D.R. Firestone, American Oil Chemists' Society, Champaign, 1989, Method Ak 1-92.
24. ISO Method 5508:1990 (E) Animal and vegetable fats and oils—Analysis by gas chromatography of methyl esters of fatty acids, International Organization for Standardization, Geneva.
25. *Ibid.*, Method 665.
26. Williams, P.C., and K.H. Norris, in *Near-Infrared Technology in the Agricultural and Food Industries*, edited by P.C. Williams, and K.H. Norris, American Association of Cereal Chemists Inc., St. Paul, 1987, pp. 241-246.
27. Evans, E.J., P. Bilborrow, A. Gran, C.A. Kwiatkowska, E.A. Spinks, R.K. Heaney and G.R. Fenwick, *J. Sci. Food Agric.* 49:297 (1989).
28. Michalski, K., and J. Krzymański, in *Third International Conference on Near Infrared Spectroscopy Proceedings*, Vol. 2., Agricultural Research Center, Gembloux, 1991, pp. 582-586.
29. Lila, M., and V. Furstoss, *Agronomie* 6:703 (1986).
30. Tkachuk, R., V.J. Mellish, J.K. Daun and L.J. Macri, *J. Am. Oil Chem. Soc.* 65:381 (1988).
31. Holman, R.T., and P.R. Edmondson, *Anal. Chem.* 28:1533 (1956).
32. Murray, I., in *Near Infrared Diffuse Reflectance/Transmittance Spectroscopy*, edited by J. Hollo, K.J. Kaffka and J.L. Gonczy, Akademiai Kiado, Budapest, 1987, pp. 13-28.
33. Sato, T., S. Kawano and M. Iwamoto, *J. Am. Oil Chem. Soc.* 68:827 (1991).
34. Reinhardt, T.-C., and G. Robellin, in *Proceedings of the GCIRC Eighth International Rapeseed Congress* edited by D.I. McGregor, GCIRC, Paris and Canola Council of Canada, Winnipeg, 1991, pp. 1380-1384.
35. Reinhardt, T.-C., C. Paul and G. Robellin, in *Making Light Work: Advances in Near Infrared Spectroscopy*, edited by I. Murray, and I.A. Cowe, VCH, Weinheim, 1992, pp. 323-327.

[Received February 28, 1994; accepted July 8, 1994]