RESEARCH ARTICLE



Development of non-destructive models to predict oil content and fatty acid composition of Gomenzer (Ethiopian mustard) using near-infrared reflectance spectroscopy

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Abstract

Background: "Gomenzer" or Ethiopian mustard is the potential oilseed crop that is economically important. Ethiopian mustard and rapeseed quality breeding has focused on altering the fatty acid contents of seed oil to create novel genotypes with different oil characteristics. The goal of this research was to establish calibration equations' using a method called near-infrared reflectance spectroscopy with modified partial least squares (MPLS) regression.

Result: The spectra of 180 mustard samples were collected and their oil and fatty acid compositions were determined by n-hexane extraction and GC-MS methods respectively. With 130 samples, calibration equations were developed for oil and fatty acid compositions. All developed equation had an acceptable value of R 2c, RPDc, and also had suitable 1-VR values. Prediction of an external validation with 50 datasets revealed a blameless correlation between reference values and NIRS values based on the R 2v in prediction, SEP, and the ratio of SD to SEP (RPDv) for oil, oleic, linoleic, linolenic, and erucic acids. These had suitable values of RPDv and R 2v, with the range of 2.0 to 8.8 and 0.79 to 0.99 respectively.

Conclusion: The developed models gave meaningful quantitative data, however, the equations generated for palmitic, stearic, and eicosenoic acids were insufficient for data analysis. Hence, the developed NIRS model, which was satisfactory, could be used to assess and evaluate the oil and fatty acid content for the unknown mustard samples on a regular basis in the oilseed breeding quality program.

KEYWORDS

calibrations, fatty acid, mustard, near infrared spectroscopy, nondestructive technique, spectra

INTRODUCTION

"Gomenzer" or Ethiopian mustard (Brassica carinata) is the potential oilseed crop, which is mostly grown in the Ethiopia highlands.¹ Mustard is a worldwide significant oilseed crop; therefore, studying the genetic diversity of different germplasm collections is crucial for its genetic improvement.² It is an important edible oil crop, broadly includes rapeseed and mustards which are used as a food, especially in the arid and semi-arid areas.^{3,4} In addition, rapeseed is used to

substitute for fossil diesel fuel. Selection of mustard variety and genotype quality is based on fatty acid compositions and protein content. It is carried out according to the end-use of the oil such as for humans, meal for animal nutrition, and industrial application like biodiesel.⁵ Ethiopian mustard oil covered about 40% of its seed weight. It is mainly composed of fatty acids such as palmitic (16:0), stearic (18:0), oleic (18:1), linoleic (18:2), linolenic (18:3), Eicosenoic (20:1), and erucic (22:1) acids. The major components in rapeseed oil are unsaturated fatty acids (mainly oleic, erucic, and linoleic acid).^{2,5} The

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majority of the mustard and rapeseed cultivars grown in Ethiopia contain high levels of erucic acid.⁶ Because of this, Ethiopian mustard and rapeseed quality breeding has focused on altering the fatty acid contents of seed oil to create novel genotypes with different oil characteristics.

Fatty acid compositions of the oils of breeding lines were determined by gas chromatography. This analytical technique is the most commonly used approach for fatty acid compositions. 7,8 Although the obtained result by using this technique is accurate, it must be pointed out that there were limitations to the method. However, it is incongruous for a large number of samples as it is not cost-effective, is time-consuming, requires expensive chemicals, needs professionals with technical qualifications, is destructive, and generates wastes. 9,10 Interestingly, near-infrared spectroscopy (NIRS) is a powerful tool for the quantitative and qualitative analysis of chemicals and physical variables. Since the early 1960s, this method has been used to determine the moisture content of seeds. 11 NIRS could be applied to samples of various types, such as from the pharmaceutical, petrochemical, food, and agricultural industries. 12,13 Mainly, this technique is aimed to facilitate the screening for genotypes and varieties of cereal crops, oilseed crops, and forages. Furthermore, the NIRS technique offers numerous advantages over wet chemistry analytical techniques, such as a lowcost, quick, non-destructive, high-precision, high-throughput, and environmentally friendly approach. NIRS could predict contents of organic constituents by combining laboratory data and spectral information.14

NIRS is widely utilized for the evaluation of forage quality, according to the content of nitrogen, moisture, fiber, structural carbohydrates, amino acids, and minerals. 10,15 In addition, NIRS is used to evaluate the oilseed crop quality according to the value of oils and fatty acids. Oil content and main fatty acids of rapeseed oil had been accurately quantified by the NIRS technique. Besides, NIRS had been also successfully used to quantify the content of sterol composition in sesame¹⁶ and it was used in the screening of earlygeneration material in cereal breeding programs. Furthermore, NIRS is an efficient analytical technique for the rapid determination of chemical compositions for screening different oil crops, cereal crops, and forage grasses. 9 Besides, it is a green approach that does not require the use of organic solvents or reagents, avoids environmental pollution, and is regarded as an eco-friendly method, which is in accordance with the principles of sustainable chemistry. 17 The literature survey indicated that there is no study on the development of NIRS calibration models for predicting the content of oil and fatty acids compositions of mustard and rapeseed grown in different parts of Ethiopia.

Hence, the goal of this work was to create a model to examine the oil and fatty acid contents of mustard and rapeseed varieties and genotypes in breeding programs using the NIRS technique. Because the oil and fatty acid content of mustard and rapeseed are the important oil crops. The developed NIRS models were to quantitatively measured the oil and fatty acid content in low-cost and high-throughput ways to speed up the breeding process and to improve the quality of Ethiopian mustard.

MATERIALS AND METHODS

Sample collection and preparation

A total of 180 Ethiopian mustard samples were collected from four different main growing locations. 100 from the Holeta Agricultural Research Center; they were cultivated at Holeta, Debremarkos, Ambo, Fiche, and Debrebirhan districts. In addition, 60 samples were obtained from the Kulmsa Agricultural Research Center; they were cultivated at Kulmsa, beqoji, Shashmene, and 20 samples were collected from local markets. All samples were harvested from the 2020 and 2021 crop seasons. 130 were used for calibration development, and 50 were used for external validation of Ethiopian mustard oil and fatty acids

Oil content

Oil content of mustard was determined by n-hexane extraction with soxtec method according to Tsegay et al. 18 protocol with some modifications. Two grams of the ground sample was weighed into the extraction thimble and cotton was used as a plug to avoid loss of the sample. This was placed in the adapter part of the instrument and a 150 ml aluminum cup with 75 ml of n-hexane was put on the 60° C adjusted heat mantle sequentially. The crude oil was recovered after solvent evaporation and the residual solvent was dried in an oven. Later it was cooled in desiccators and weighed.

$$Fat\% = \frac{oil(g)}{weight of sample} * 100$$

Determination of fatty acid composition

According to the Yisak et al. 19 protocol, oil was extracted using Foss SoxtecTM 8000 extraction equipment from 5 g of Gomenzer (Ethiopian Mustard) pulverized with n-hexane. The fatty acids were investigated using gas chromatography (GC) with an MS detector, as described by Tsegay et al. 18 after methylation of the sample with methanolic potassium hydroxide solution for saponification. Its solution was prepared with a concentration of 0.5 µg/ml of the derivatized sample (dissolve 1 µg FAME in 2 ml of hexane). These were analyzed using GC-MS Agilent Technology 7820A GC and 5977 E MSD systems equipped using an auto sampler. Chromatographic separations were carried out using a stabilwax column (RESTEK 10623, USA) with 30 m length, 0.25 mm internal diameter, and 0.2 µm column phase thickness. Injection mode was performed with a 1:40 split ratio, helium gas was used as a carrier gas, and 1 µl volume of the sample was injected into the inlet heated to 250°C. The oven temperature was set to 180°C for the initial hold and increased to 230°C after 2 min. The program was divided into two parts: a rate of 5°C/min until 200°C with a 5-min hold time and a rate of 10°C/min until 230°C with a 2-min hold time. The conditions used for the mass

spectrometer were a source temperature of 230° C, a scan range of 40–650 m/z, and operated in positive electron impact mode with ionization energy of 70 eV. The data were processed by using the instrument's built in software (MS ChemStation; Agilent Technologies) and the percentage of each component in the total fatty acid was calculated by area normalization.

Sample scanning through near-infrared reflectance spectrophotometry (NIRS)

A near-infrared reflectance spectrometer was used to collect the spectral data of all mustard samples. For each sample, 2–4 g of mustard grain samples was placed in the ring cup. Each sample was scanned in duplicate by NIRS monochromator model FOSS 6500 (FOSS NIRS Systems, Inc., Silver Spring, Denmark) equipped with small ring cups (internal diameter of 35 mm and depth of 8 mm). The spectra were taken between 400 and 2500 nm, with a 2 nm interval and 32 scans per sample. For the production of NIRS spectra, the average reflectance value (R) was calculated and transformed to log (1/R).

Model calibration and validation for near-infrared spectroscopy

To construct the near-infrared spectra models, all the average spectral data of each sample were uploaded onto WinISI II software (Windows version 1.60, Foss and Infrasoft International LLC) for chemometric modeling and correlate with the GC-MS result. After correlating the reference analytical data, several potential calibration models were created using a number of spectral pre-treatment combinations, which were evaluated to investigate the optimum prediction model configurations for oil and fatty acid analysis. From those, the best calibration model was selected. In this study, calibration models were built using modified partial least squares regression (MPLS) techniques.

The statistical methods applied in this study included the correlation coefficient of calibration (R²c), cross-validation coefficient (1-VR), standard error of calibration (SEC), correlation coefficient of validation (R²v), standard error of prediction (SEP), which were used to test the accuracy of the calibration models. R²c obtained from the calibration process can be modeled linearly. SEC and SEP were used to evaluate the predictive ability of the calibration and validation model.²⁰ The correlations between the SD of the wet chemical analyzed data and the prediction data by NIRS model (SECV or SEP) 10 were used to estimate the prediction ability of the model and calibrations, as well as the accuracy of the equations.⁵ Equations with the highest R², RPD, and 1-VR and the lowest SECV and SEP were considered the best models.^{21–23} Samples with NIRS spectra that were significantly different from other samples were considered abnormal and removed from the dataset when the Mahalanobis distance global-H (GH) value or the neighboring-H (NH) value was greater than 3.0 or less than 0.6.24,25

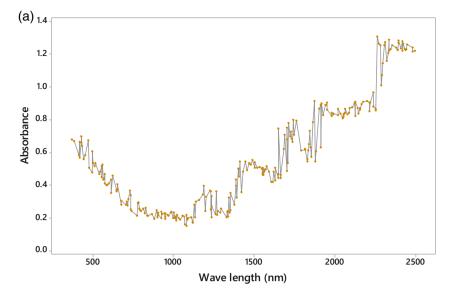
RESULT AND DISCUSSIONS

Spectral analysis

As a consequence of the investigation, absorbance spectra of Ethiopian mustard were obtained in the wavelength range of 400 to 2500 nm with a 2 nm interval. The mean raw spectral data (without pretreatment), treatment with invers MSC, and second-derivative of Ethiopian mustard samples were shown in Figure 1. The second derivative was calculated from the log (1/R) spectra at gaps of four data points and smoothing over segments of four data points 2,4,4,1 with scatter correction of invers MSC. Absorption peaks and vallevs were observed in those spectra based on the chemical component characteristics of mustard samples, with main strong bands observed at 1206, 1474, 1722, and 1946 nm. At the transition between visible and near-infrared (around 930 nm) was observed a band related to third overtones of the C—H stretching in various groups. The strong band observed at 1206 nm was related to the C-H stretching of the second overtone in various groups (-CH2). A band related to CO stretching of the third overtone (-CO) and O-H stretching of the first overtone (water) occured around 1474 nm, and the second overtone of N-H stretching in amides and aromatic amines occurred occured around 1506 nm. In addition, another strong band was observed at 1722 nm related to C-O of oil and C-H stretching of the first overtone -CH₂ as reported by Xu et al. 26 At 1760 nm, we found a stretching related to the C-H of oil and C-H of the first overtone of -CH2 was found. Another strong peak was observed nearly at 1950 nm, it was possibly related to the O-H bending of the second overtone (water), and the peak around 2304 nm is the combination absorbance of C-H stretching and the deformation of CH₂, which is related to oil. The overlapping of combination absorbance of C=O-stretching and the deformation of -CO-NH- and the combination absorbance of N-H stretching and the deformation of —CO—NH— can be attributed to the range of 2000-2250 nm; these are possibly related to oil and hydrocarbons. In general, the spectrum shows a strong absorption band related to oil and water. The spectrums of mustard were almost parallel to the spectrum of sesame, Camellia, and Perilla, 5,20 but, the spectrum of this study was different from the safflower spectrum reported by Elfadl et al.²⁷ According the review, most of oilseed crops has comparable NIR spectra.

Data analysis and statistical descriptions

In Ethiopian mustard oil samples, more than 15 fatty acids were detected and identified by GC-MS. From the detected 15 fatty acids, only seven fatty acids were proposed for NIRS model development. As the NIRS method cannot be used to predict components at lower percentage values, ²⁸ the study focused on the major fatty acid components present in Ethiopian mustard. The statistical values, including mean, standard deviation (SD), minimum, and maximum, of the individual selected fatty acids and oils of Ethiopian mustard used in the calibration and validation sets are shown in



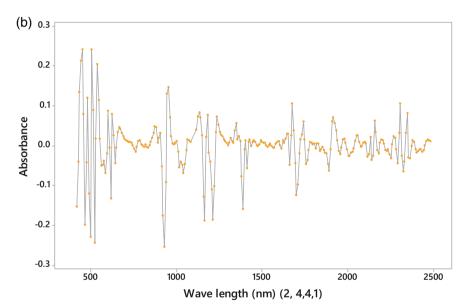


FIGURE 1 (a) Near infrared mean spectra, without pretreatment and (b) mean spectra with second derivative (2, 4, 4, 1 + invers MSC of Ethiopian mustard samples

TABLE 1 Statistical value of oil (%) and percent fatty acid content of mustard analyzed by GC-MS used for the calibration and validation

Constituent	Calibration ((n = 130)		Validation (n = 50)			
	SD	Mean	Range	SD	Mean	Range	
Oil	3.4	43.9	34.9-49.9	4.7	42.6	30.3-56.0	
Palmitic acid	0.4	2.9	2.2-4.1	0.2	3.0	2.7-3.3	
Stearic acid	0.3	1.3	1.0-2.3	0.3	1.3	1.1-2.2	
Oleic acid	11.5	10.5	4.9-52.6	27.2	25.4	2.7-65	
Linoleic acid	2.1	17.4	12.8-21.9	3.1	17.0	8.7-29.7	
Linolenic acid	2.2	10.1	5.9-15.4	1.7	9.7	7.7-17.9	
Eicosenoic acid	1.7	9.7	6.4-16	1.9	10.6	9.0-18	
Erucic acid	10.5	42.1	6.9-50.9	19.6	27.5	6.5-45.0	

Table 1. The mean values of oil and selected fatty acid content were 43.9% oil, 2.9% palmitic acid, 1.3% stearic acid, 10.5% oleic acid, 17.4% linoleic acid, 10.1% linolenic acid, 9.7% eicosenoic acid, and 42.1% erucic acid in the calibration set. The values present in the validation set were almost identical to the calibration sample datasets.

Calibration and cross-validation of NIRS model

The best calibration equations for oil, fatty acid compositions using mathematical treatment 2.4.4.1 with invers MSC scatter were selected with the value of R2c, RPDc (SD/SECV), SEC, and SECV as shown in Table 2. The NIRS models created for stearic, oleic, and erucic acids were excellent with R²c value of 0.90, 0.99, and 0.99 respectively. These results were almost similar to the study by Sato et al.²⁹ with his finding (0.860, 0.998, and 0.995 respectively). In addition, the equation developed for oil and linoleic acid content of mustard grains exhibited reliable R²c values, 0.84, 0.80, respectively, which is almost similar to the study by Kim et al. 5 (R² = 0.795-0.983) and Liu et al.8 (R² > 0.8). On the other hand, the model developed for palmitic, linolenic, and eicosenoic acids were moderately suitable with R² value of 0.68, 0.77, and 0.74 respectively. These were in agreement to NIRS models developed for tryptophan in maize³⁰ and fibers in feeds²³ that reported by Escuredo et al.³¹ The RPD_C values of calibration equations developed for oil, palmitic, stearic, oleic, linoleic, and erucic acids are more than two as shown in Table 2, which were acceptable result in the good range as studied by Aldo et al.32 Furthermore, the RPD_C values for palmitic, linolenic, and eicosenoic acid were 1.6, 1.8, and 1.7, respectively, which were lower than the other equations but still adequate for screening, according to Khamchum et al.³³ RER values of all equation of this study varied from 10.0 to 23.0 which agreed with the recommended values for screening purposes as reported by Yang et al. 10 except models developed for palmitic, linolenic, and eicosenoic acid.

1-VR as a statistic parameter for cross-validation on the calibration development was an important factor in addition to R^2c and RPDc. Even models with greater R^2c values could not show a decent correlation between reference values and NIRS estimated values unless they had a high 1-VR value close to R^2c . As shown in Table 2 the equation developed for palmitic, linolenic and eicosenoic acid had an acceptable R^2c value, but it has low 1-VR value observed in the cross-validation, which indicated that it was not a strong model. In general, all the models developed for oil and fatty acid compositions were evaluated by external validation.

External validation of the developed NIRS model

The robustness of the calibration models developed was tested through external validation with 50 samples, which were not included

TABLE 3 External validation statistics values were obtained from regression equations of chemical determination values of oils and fatty acids contents of Ethiopian mustard seeds and NIRS predicted values for the validation set.

	Validation						
Constituent	Mean	SD	SEP	R ² v	RPD		
Oil	42.6	4.20	1.90	0.79	2.2		
Palmitic acid	3.0	0.20	0.25	0.07	0.8		
Stearic acid	1.3	0.30	0.26	0.04	1.2		
Oleic acid	25.4	27.2	3.10	0.98	8.8		
Linoleic acid	17.0	3.10	0.50	0.84	6.2		
Linolenic acid	9.7	1.70	0.50	0.70	3.4		
Eicosenoic acid	10.6	1.90	1.80	0.3	1.1		
Erucic acid	27.5	17.6	2.10	0.92	8.4		

Note: SD, standard deviation; R^2v , coefficient of determination of prediction models; SEP, standard error of prediction; RPDv, the ratio of SD of reference data to SEP (SD/SEP).

TABLE 2 Model development statistics for the NIRS model of Ethiopian mustard oil and fatty acid contents using MPLS regression and scatter correction.

	Mean	SD	Calibration		Cross-validation			
Constituent			SEC	R ² c	SECV	1-VR	RPDc	RER
Oil	44.1	3.4	0.96	0.84	1.10	0.70	3.1	13.6
Palmitic acid (C16:0)	2.9	0.4	0.21	0.67	0.25	0.54	1.6	7.6
Stearic acid (C18:0)	1.3	0.3	0.09	0.90	0.11	0.80	2.7	11.8
Oleic acid (C18:1)	21.5	11.5	1.6	0.99	2.20	0.98	5.2	21.7
Linoleic acid (C18:2)	17.5	2.1	0.74	0.84	0.89	0.77	2.4	11.0
Linolenic acid (C18:3)	9.9	2.2	1.0	0.74	1.20	0.67	1.8	7.9
Eicosenoic acid (C20:1)	9.7	1.7	0.89	0.74	1.06	0.63	1.7	9.1
Erucic acid (C22:1)	33.9	10.3	1.80	0.99	2.61	0.98	4.0	16.9

Abbreviations: MPLS, modified partial least-squares; R²c, coefficient of determination of calibration; 1-VR, one minus the ratio of unexplained variance divided by variance; RER, relative range of error ((max-min)/SECV); RPDc, the ratio of SD (standard deviation of reference data) to SECV in the calibration set; SEC, standard error of calibration; SECV, standard error of cross-validation.

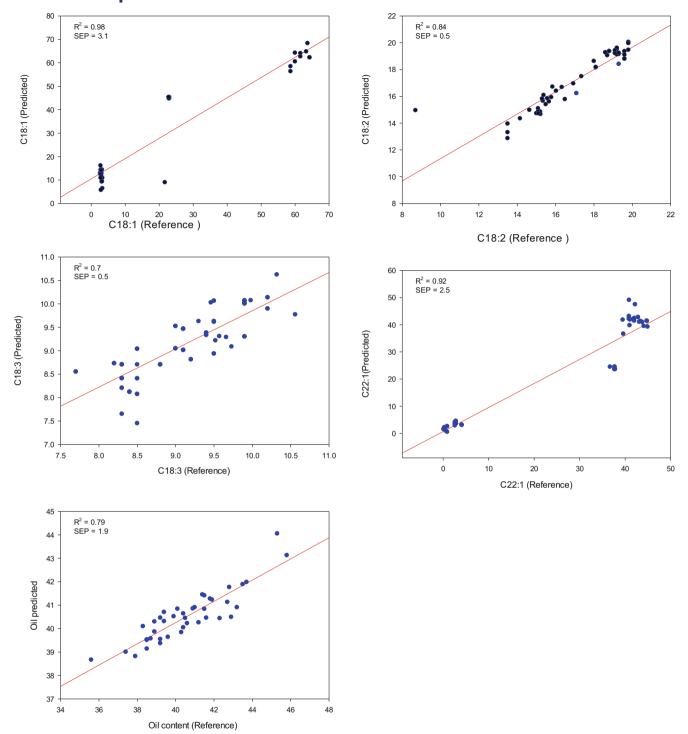


FIGURE 2 Relationship between the values predicted by the NIR method applying the developed calibration equations and the result obtained by the chemical reference method for oil, oleic acid (C18:1), linoleic acid (C18:2), linolenic acid (C18:3), and erucic acid (C22:1) contents of Ethiopian mustard.

in the calibration process and which were nearly similar in distribution with the dataset used in calibration. The statistical parameters (R^2v , SEP, RPDv,) used to evaluate the reliability of the calibration model of external validation for oil and fatty acids compositions of Ethiopian mustard samples are shown in Table 3. An accurate prediction can be monitored with the reliability of the established calibration models

with the lower value of SEP and higher R^2 and RPD_V. The predictions for oil content, oleic, linoleic, and erucic acid were confirmed with the R^2 v value of 0.79, 0.98, 0.84, 0.70, and 0.92 respectively. In addition, the RPDV values of these adequate external validation models were in the range of 2.2–8.8 as shown in Table 3, which were in agreement with the study of Kim et al.³⁴ These models were indicating a good

correlation between reference values and NIRS predicted values in the application of the calibration equations. However, palmitic, stearic, and eicosenoic acid had a coefficient of determination of prediction models (R²v) of 0.02, 0.0.04, and 0.3, respectively, which indicated that the reference and NIRS value were not correlated and they were the bad equations. Furthermore, according to Murphy et al. 35 and Zahera,²³ the RPDv values of these models were less than the required value of 1.5. In addition, models developed for palmitic, stearic acid, and eicosenoic acid had narrow distribution datasets and showed a poor correlation between reference values and NIRS predicted values. As a result, the palmitic, stearic, and eicosenoic acid models were unsuitable for screening data since the prediction model's R2v was very poor. In general, except for palmitic, stearic, and ecosonoic acids, all validations were found to be robust and accurately reflect the equations developed. Hence, the satisfactorily developed NIRS model could be used to assess and evaluate the oil and fatty acid content of Ethiopian mustard seeds on a regular basis in the oilseed breeding quality program.

The linear relationships between laboratory reference values (validation dataset) and NIRS predicted values of mustard oil and individual fatty acid contents using calibration equations for respective parameters were outlined in Figure 2. These results validated the prediction abilities of the calibration models for the oil, oleic acid, linoleic acid, linolenic acid, and erucic acid contents using the non-destructive NIRS technique in mustard cultivated in Ethiopia. one of the factores that allowed these models to produce reliable forecasts was the variety of their constituents.

The NIRS model developed for oil and fatty acid content was shown to be accurate, practical, and applicable. These well-developed calibration equations are utilized for routine analysis in the mustard breeding program, Ethiopian standard agency, and Ethiopia Commodity Exchange analyses. However, the reliability of the calibration model for determining palmitic, stearic, and eicosanoic acids was considerably lower and could not be considered adequate for use in routine analysis. The lack of precision and accuracy in palmitic, stearic, and eicosanoic acids could be addressed in the future by expanding the number and diversity of reference samples.

CONCLUSION

Using a non-destructive NIRS technique, the oil and fatty acid contents of Ethiopian mustard could be successfully predicted with high accuracy. NIRS is a feasible and useful tool for screening purposes and has the potential to predict oil and major fatty acids. Six suitable calibration NIRS models were built in the present study to predict the oil and fatty acid contents of Ethiopian mustard. These models have good coefficients of determination and were validated using a completely different set of samples. The coefficients of determination (R²v) for all constituents were laid out in the range of 0.79–0.98, and the ratio of prediction to deviation (RPD) was laid out in the range of 2.2–8.8. It is possible to conclude that the results found via the NIRS model developed could be used for routine analysis of the oil and fatty acid content of Ethiopian mustard for screening germplasm in

the agricultural breeding program. Besides, this is the first reported study of a NIRS calibration model developed for the prediction of oil and fatty acid content in Ethiopian mustard. Although NIRS is a practical method, the developed equations should be updated, expanded, and improved with future samples from different environments and germplasms, which can cover a wider range of oil and fatty acid values in the samples used for the calibration models.

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CONFLICT OF INTEREST

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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