Use of near infrared spectroscopy to predict oil content components and fatty acid composition in intact olive fruit

L. León-Moreno,[a] A. Garrido-Varo[b] and L. Rallo-Romero[a]

[a]*Plant Production Department, School of Agriculture and Forestry Engineering, University of Cordoba, Avda Menéndez Pidal s/n, PO Box 3048, E-14080 Córdoba, Spain.*
E-mail: ag2lemol@uco.es

[b]*Animal Production Department, School of Agriculture and Forestry Engineering, University of Cordoba, Avda Menéndez Pidal s/n, PO Box 3048, E-14080 Córdoba, Spain*

Introduction

Since 1991 the University of Córdoba has been conducting a breeding programme to obtain new olive cultivars from intraspecific crosses. The objective of this programme is to obtain new early bearing and high-quality cultivars.[1] In the framework of this breeding programme hundreds of samples should be tested every year to increase the chance of getting desirable genotypes. Therefore, fast, inexpensive and accurate methods of analysis are necessary. Conventional laboratory techniques are expensive and time-consuming. Near infrared (NIR) spectroscopy can satisfy the characteristics requested by plant breeders as it offers many advantages such as the simultaneous analysis of many traits and low cost. NIR analysis has enabled plant breeders to quickly select superior genotypes in breeding programmes and this has been one of the most important applications of NIR in agriculture.[2]

The objective of this work was to assess the performance of NIR to estimate oil fruit components (fruit weight, flesh moisture, flesh/stone ratio and oil flesh content in dry weight basis) and fatty acid composition in intact olive fruit.

Material and methods

Genotypes from reciprocal crosses between 'Arbequina', 'Frantoio' and 'Picual' cultivars have been used in this study. A total of 287 samples, each from a single plant, were scanned using a DA-7000 Diode Array vis/NIR Spectrophotometer (Perten Instruments DA 7000 Flexi-Mode), which covers the visible and NIR range from 400–1700 nm.

Intact frozen olive fruit samples were scanned in the "Down-View" mode. The sample is placed in a circular dish and is illuminated from above by light shining directly on the surface of the sample.[3]

All samples were analysed for fatty acid composition by means of gas chromatography (GC) analyses of fatty acid methyl esters. They were prepared following the procedure developed by Garces and Mancha[4] and analysed on a Hewlett Packard gas chromatograph equipped with a flame-ionisation detector. 220 of the 287 samples were analysed for oil fruit components. The oil content was measured by means of nuclear magnetic resonance (NMR).

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Calibration development and validation was carried out by Nircal Version 3.0 Software.[5] Partial least squares (PLS) was used to obtain regression equations for all the reference data. The wavelength region used was 900–1500 nm.

Nircal does not use cross-validation so the sample file was randomly split into two files, one containing 70% of the samples (calibration set) and the other containing the remaining 30% of the samples (validation set).

Table 1. Mean, standard deviation and range of variability of oil fruit components (150 samples) and fatty acid composition (201 samples) in the calibration set.

	Mean	Minimum	Maximum	*SD*
Oil fruit components				
Fruit weight (g)	3.8	1.6	7.0	0.9
Flesh/stone ratio	8.0	4.6	12.0	1.5
Flesh moisture (%)	75.8	64.2	86.2	4.2
Oil flesh content (%)	62.1	40.3	74.3	5.7
Fatty acid composition (%)				
Palmitic (C16 : 0)	15.0	9.1	21.5	2.4
Palmitoleic (C16 : 1)	2.8	0.7	7.9	1.2
Stearic (C18 : 0)	1.8	1.1	7.9	0.7
Oleic (C18 : 1)	65.8	43.3	84.7	9.0
Linoleic (C18 : 2)	11.5	1.9	29.7	6.6

Table 2. Mean, standard deviation and range of variability of oil fruit components (74 samples) and fatty acid composition (86 samples) in the validation set.

	Mean	Minimum	Maximum	*SD*
Oil fruit components				
Fruit weight (g)	3.7	2.1	6.4	1.0
Flesh/stone ratio	7.8	4.7	11.7	1.3
Flesh moisture (%)	75.2	63.4	83.9	3.9
Oil flesh content (%)	62.8	51.6	73.2	5.1
Fatty acid composition (%)				
Palmitic (C16 : 0)	15.1	9.0	21.1	2.7
Palmitoleic (C16 : 1)	2.7	0.8	5.7	1.1
Stearic (C18 : 0)	1.8	1.0	4.9	0.6
Oleic (C18 : 1)	65.6	46.0	84.5	9.3
Linoleic (C18 : 2)	12.0	1.7	26.3	6.4

Different data pretreatments (derivative and MSC) were used to improve calibration results. The equation models obtained for each reference data were evaluated following the statistics and rules provided by Nircal, as the standard error of calibration (*SEC*), prediction (*SEP*), coefficient of determination for calibration (R^2) and prediction (r^2).

Results and discussion

Tables 1 and 2 show the oil content components and fatty acid composition of the calibration and validation sets. The breeding programme produces genotypes with a high variability of the characteristics evaluated. Therefore, these samples are very suitable for producing robust NIR analysis. The largest variability was found in flesh moisture, oil flesh content and oleic and linoleic acid content. The available range of variability for the other traits was more limited.

The preliminary results show that calibration for oleic and linoleic acids were highly accurate with coefficients of determination of 0.91 and 0.95 for calibration and of 0.88 and 0.91 for validation (Table 3). Similar results were obtained analysing the fatty acid composition of edible vegetables oils,[6] intact oil seeds such as rapeseed,[7] mustard[8] and other Brassicaceae species.[9] Calibration for palmitoleic and

Table 3. Calibration and prediction statistics in NIRS equations for fatty acid composition.

Fatty acid	Calibration		Prediction	
	R^2	*SEC*	r^2	*SEP*
Palmitic (C16 : 0)	0.85	1.28	0.76	1.75
Palmitoleic (C16 : 1)	0.72	0.83	0.44	1.04
Stearic (C18 : 0)	0.41	0.68	0.14	0.68
Oleic (C18 : 1)	0.94	3.04	0.88	4.40
Linoleic (C18 : 2)	0.95	1.96	0.90	2.73

R^2 = Coefficient of determination for calibration
r^2 = Coefficient of determination for prediction
SEC = Standard error of calibration
SEP = Standard error of prediction

Table 4.- Calibration and prediction statistics in NIRS equations for oil fruit components.

Oil Fruit Components	Calibration		Prediction	
	R^2	*SEC*	r^2	*SEP*
Fruit weight (G)	0.73	0.62	0.72	0.71
Flesh/stone ratio	0.80	0.91	0.68	0.96
Flesh moisture (%)	0.97	0.96	0.94	1.33
Oil flesh content (%)	0.96	1.67	0.91	2.20

R^2 = Coefficient of determination for calibration
r^2 = Coefficient of determination for prediction
SEC = Standard error of calibration
SEP = Standard error of prediction

estearic acids were less accurate, probably because of the narrow range of variability available for these fatty acids.

For the oil fruit components (Table 4), calibration was highly accurate for flesh moisture and oil flesh content in dry weight basis (R^2 and r^2 higher than 0.90) and less accurate for the other characteristics evaluated. These results agree with the ones obtained analysing the oil content in Brassicaceae germplasm,[9] sunflower[10] and the oil and moisture contents in soybean seeds.[11]

Conclusion

The first results obtained indicate that NIR analysis could be an ideal technique to reduce the cost, time and chemical waste necessary to evaluate a large number of olive genotypes. NIR is accurate enough to preselect genotypes for oil content and oleic acid content, two of the most important objectives in our olive tree breeding programme.

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