Development of robust calibrations to predict oil content and fatty acid composition in olive breeding programmes

L. León,[a] A. Garrido-Varo[a] and G. Downey[b]

[a]*Faculty of Agriculture and Forestry Engineering, ETSIAM, University of Córdoba, Apdo 3048, 14080 Córdoba, Spain. ag2lemol@uco.es*

[b]*TEAGASC, The National Food Centre, Ashtown, Dublin 15, Ireland*

Introduction

Near infrared (NIR) spectroscopy can satisfy the characteristics requested by plant breeders and offers many advantages such as the rapid and simultaneous analysis of many traits and low cost. For this reason, NIR has been previously evaluated to estimate the oil content and fatty acid composition in intact olive fruits, two of the most important objectives in olive breeding programmes.[1]

NIR Prediction statistics obtained from calibration and prediction sets from the same population showed high accuracy although there is a lack of information regarding the robustness of calibration models for the prediction of independent populations. NIR calibrations have shown to be sensitive to year, cultivar, species or crop location in other fruit species.[2–6]

The objective of the present is to asses the performance of calibrations across different populations of olive fruit samples (seedlings from different olive crosses, years and crop number within year) to estimate the oil and oleic acid contents in intact olive fruits.

Materials and methods

Genotypes from crosses between 'Arbequina', 'Frantoio' and 'Picual' females have been used in this study. Samples, each for a single plant, were collected in two consecutive years and analysed for oil content and fatty acids composition by the reference methods as described by Del Río and Romero[7] and Garcés and Mancha,[8] respectively.

Intact olive fruit samples were scanned using a NIR diode-array spectrophotometer (Perten DA-7000 Flexi-Mode), working in reflectance mode in the spectral range between 400 to 1700 nm (at 5 nm intervals). Spectral data were recorded with the software Simplicity.

The log 1/*R* values were corrected with the data pre-treatment previously reported as the best one for each contituent to calibrate.[1] Calibration models were performed by using partial least squares regression (PLS) with Nircal software.

A data file was made for each year, for each crop number separately within the second year data and for each female genitor in the whole data. Samples in each group were randomly assigned for the calibration (2/3) and validation sets (1/3), except samples coming from 'Frantoio' female which were only used for validating results of the other female groups. For each variable (year, crop and female genitor) calibration models were developed for each group and validated against the other groups.

Results and discussion

Oil content and oleic acid percentage of olive fruits in each group is shown in Table 1. The breeding program produces genotypes with variable values of the characteristics evaluated in all

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groups. Oil content and oleic acid percentage of fruits tested in the whole population varied from 5.9 to 28.8% and from 43.5 to 84.7%, respectively.

Table 1. Number of samples, mean and range for oil content and oleic acid percentage by groups.

	Oil content (%)			Oleic acid (%)		
Group	n	Mean	Range	n	Mean	Range
First year	96	18.33	7.7–28.8	147	71.37	50.9–82.7
Second year	224	14.28	5.9–22.9	287	65.70	43.5–84.7
First crop	79	14.45	6.1–22.9	111	65.90	43.5–84.7
Second crop	145	14.18	5.9–22.5	176	65.57	45.8–84.6
Combined	320	15.49	5.9–28.8	434	67.62	43.5–84.7
Female A	164	14.94	6.1–24.8	223	66.45	43.5–84.6
Female F	35	15.65	9.7–25.3	58	69.06	50.1–82.5
Female P	121	16.19	5.9–28.8	153	68.76	46.5–84.7

Global and specific calibrations showed high accuracy with correlation coefficient (*r*) values from 0.93 to 0.98 for oil content and 0.88 to 0.93 for oleic acid percentage, and standard error of calibration (*SEC*) from 0.68 to 1.56 and 3.13 to 4.29 respectively (Table 2).

Table 2. Coefficient of correlation (*r*) and standard error of calibration (*SEC*) for oil content and oleic acid percentage by groups.

	Oil content (%)		Oleic acid content (%)	
Group	*r*	*SEC*	*r*	*SEC*
First year	0.93	1.52	0.89	3.20
Second year	0.98	0.69	0.93	3.13
First crop	0.98	0.68	0.90	3.92
Second crop	0.97	0.74	0.90	3.89
Combined	0.94	1.32	0.88	4.12
Female A	0.93	1.56	0.89	4.30
Female P	0.96	0.93	0.92	3.44

Within the second year, samples of the second crop were better predicted than first crop independently of the calibration model used (Table 3) and no differences were observed between the models developed from the different female genitors (Table 4). The opposite results have been reported in other fruit species in which the calibrations derived for specific cultivars validated poorly against other cultivar populations.[2,4,5]

Table 3. Standard error of prediction (*SEP*) of individual crop calibrations for oil content and oleic acid percentage.

Validation Group	Calibration group	
	First crop	Second crop
Oil content (%)		
First crop	1.38	1.32
Second crop	0.74	0.72
Oleic acid content (%)		
First crop	5.47	5.41
Second crop	4.66	4.14

Table 4. Standard error of prediction (*SEP*) of individual female calibrations for oil content and oleic acid percentage.

Validation Group	Calibration group	
	Female A	Female P
Oil content (%)		
Female A	1.26	1.44
Female F	1.26	1.36
Female P	1.11	1.30
Oleic acid content (%)		
Female A	4.52	4.96
Female F	4.99	4.28
Female P	4.72	4.88

Table 5. Standard error of prediction (*SEP*) of individual year calibrations for oil content and oleic acid percentage.

Validation Group	Calibration group	
	First year	Second year
Oil content (%)		
First year	1.72	2.11
Second year	2.64	0.95
Oleic acid content (%)		
First year	3.87	6.07
Second year	6.67	4.43

For the year variable, however, each calibration group (first year and second year) predicted its own validation sample set successfully but the errors increase when they were applied to another group (Table 5), although a combined calibration model (first + second years) was sufficiently

robust to predict both years (r = 0.93, *SEP* = 1.32 and r = 0.90, *SEP* = 4.13 for oil content and oleic acid percentage respectively). The dramatic decrease in performance of a calibration when applied to another year has been previously reported in other fruit species such as peach,[4] apple,[6] mandarin[3] and pineapple.[2]

Conclusions

The performance of calibrations across new populations of olive samples from different olive crosses and crop number within a year was accurate enough to estimate the oil content and oleic acid percentage in intact olive fruits. However, calibration models for each year were not transferable to the other year, although a robust calibration equation was obtained from the combined data. Further research is required to determine whether the combined calibration can be used to predict oil content and oleic acid percentage for subsequent years and to determine the best strategy for improving calibration performance over the years.

References

1. L. León, A. Garrido and L. Rallo, in *Near Infrared Spectroscopy: Proceedings of the 10th International Conference*, Ed by A.M.C. Davies and R.K. Cho. NIR Publications, Chichester, UK, p. 221 (2002).
2. J.A. Guthrie, B. Wedding and K. Walsh, *J. Near Infrared Spectrosc.* **6,** 259 (1998).
3. J.A. Guthrie and K.B. Walsh, in *Near Infrared Spectroscopy: Proceedings of the 10th International Conference*, Ed by A.M.C. Davies and R.K. Cho. NIR Publications, Chichester, UK, p. 151 (2002).
4. K.H.S. Peiris, G.G. Dull, R.G. Leffler and S.J. Kays, *J. Am. Soc. Hort. Sci.* **123(5),** 898 (1998).
5. M.B. Esler, M. Gishen, I.L. Francis, R.G. Dambergs, A. Kambouris, W.U. Cynkar and D.R. Boehm, in *Near Infrared Spectroscopy: Proceedings of the 10th International Conference*, Ed by A.M.C. Davies and R.K. Cho. NIR Publications, Chichester, UK, p. 249 (2002).
6. M.-R. Sohn, Y.-K. Kwon and R.-K. Cho, in *Near Infrared Spectroscopy: Proceedings of the 10th International Conference*, Ed by A.M.C. Davies and R.K. Cho. NIR Publications, Chichester, UK, p. 319 (2002).
7. C. Del Río and A.M. Romero, *Hortech.* **9,** 675 (1999).
8. R. Garcés and M. Mancha, *Anal. Biochem.* **211,** 139 (1993).