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Quality evaluation of intact açaí and juçara fruit by means of near infrared spectroscopy

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ABSTRACT

The objective of this study was to report the robustness of partial least squares regression (PLSR) models developed using FT-NIR reflectance spectra obtained from intact açaí and juçara fruit. Mature fruit were collected over two years (6 populations of açaí and juçara, totalling 505 samples). Diffuse reflectance spectra were acquired (64 scans and spectral resolution of 8 cm^{-1}) using ~25 fruits per batch on a 90 mm diameter glass dish in a single layer. Spectra were subject to several pre-processing procedures and two variable selection methods to develop the PLSR models. For total anthocyanin content (TAC) in açaí, a PLSR model developed using the wavelength range of 1606–1793 nm, standard normal variate (SNV) and second derivative of Savitzky–Golay (SNV + d^2A) achieved a bias corrected root mean square error (SEP) of 3.6 g kg^{-1} and a R^2_p of 0.7 in predicting an external independent set, which was better than PLSR models for juçara (SEP of 3.7 g kg^{-1},R^2_p of 0.5), and for both species combined (SEP of 5.7 g kg^{-1}, R^2_p of 0.5). For soluble solids content (SSC) in açaí the models developed using SNV + d^2A spectra over the window of 1640–1738 nm achieved a bias-corrected SEP of 2.9% and R^2_p of 0.8, similar to juçara (SEP of 1.1%, R^2_p of 0.9) and for both species combined (SEP of 2.3%, R^2_p of 0.8). The developed models can be used to sort açaí and juçara based on SSC and TAC into two grades (low and high contents).

1. Introduction

Among the Brazilian palm species açaí (*Euterpe oleracea* Mart.) and juçara (*Euterpe edulis* Mart.) are mentioned as "super foods" (Smith, 2013). Açaí is endemic in the Amazonian floodplains (Santos and Jardim, 2006) and juçara in the Atlantic Forest (Inácio et al., 2013). The fruit of both species mature within approximately 180 d after flowering, with a single bunch containing fruit with a wide range of maturity (Calvi and Pina-Rodrigues, 2005; Pessoa and Teixeira, 2012). A typical fruit of both species weighs around 2 g of which 15% is the exocarp and mesocarp (pulp) surrounding a single seed (Borges et al., 2011; Schauss et al., 2006a; Schauss et al., 2006b). Fruit is purple when ripe as a result of anthocyanin accumulation in the exocarp and mesocarp tissues during fruit maturation (Gordon et al., 2012).

These fruits have been promoted for their functional properties, linked to an exceptionally high antioxidant activity (Poulose et al., 2012), which in turn is associated with a high anthocyanin content (Inácio et al., 2013), with values typically an order of magnitude greater than that is reported in red wine grape (Ferrer-Gallego et al., 2011; Schauss et al., 2006a). Açaí and juçara pulp extracts have demonstrated effectiveness to combat some of the inflammatory and oxidative mediators involved in ageing (Poulose et al., 2012). There is also potential to use the fruit as a source of coloring agent (anthocyanin) for the food industry (Vieira et al., 2013), as demand for natural colorants has increased by almost 35% from 2005 to 2009 (Foods, 2011). The main anthocyanins detected in the juçara and açaí fruits were identified as cyanidin3-glucoside and cyanidin3-rutinoside (Brito et al., 2007; Pessoa and Teixeira, 2012; Schauss et al., 2006b). The major current source of natural anthocyanin pigment used in the food industry is known as

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colorant E163 or enocyanin and is extracted from grape skins (Melo et al., 2009 Vieira et al., 2013).

The açaí and juçara postharvest fruit handling was presented by Pessoa and Teixeira (2012). On arrival at the processing plant, fruits are visually assessed based on defects (diseases, bruises, insect damage) and skin color (deep purple, as an index of fruit maturity). Fruits are then softened in water (~40 °C), and processed in a juicer (Pessoa and Teixeira, 2012; Rogez et al., 2012). The pulp is standardized based on total solids content into three grades: A, >14%; B, 11–14%; and C, 8–11%, as defined by the Brazilian Ministry of Agriculture and Husbandry (BRASIL, 2000).

With the fruit valued for its anthocyanin content, it is logical to grade fruit based on this compound concentration, as exists a wide variation in anthocyanin content among fruits on a single bunch and between harvest times, trees, origin, etc. For example, Malcher and Carvalho (2011) reported that anthocyanin content of açaí fruit harvested in December was 10 times higher on a per weight basis than fruit harvested in September. A wide variation in fruit external color exists between fruit of a bunch at any time of bunch harvest, from green or purple to deep purple–black (Inácio et al., 2013; Pessoa and Teixeira, 2012). While this color is an index of maturity, and linked to anthocyanin accumulation, it is not well correlated to absolute anthocyanin level. For example, fruit of same color (completely purple) from two localities was assessed to possess between 1.5–82.0 g kg^{-1} total anthocyanin content (TAC), on a pulp fresh weight basis (Inácio et al., 2013). Also, Rogez et al. (2011) noted the maximum TAC in açaí was achieved some time after development of 100% purple–black skin color, and the amount of waxy on the cuticle was suggested as an alternative maturity index, the relationship to TAC level was not demonstrated, though.

Near infrared (NIR) spectroscopy is a candidate analytical technology for fruit grading, conditional to the ability to create a robust calibration for this indirect analysis technique. Given the presence of a hard seed within a thin (1–3 mm thick) pericarp that contains the attributes of interest, reflectance spectroscopy is recommended over partial or full transmission geometry. Ferrer-Gallego et al. (2011) used reflectance spectra (wavelength range of 1100–2000 nm) and partial least squares regression (PLSR) to estimate TAC of intact grape berries, reporting a root mean squared error of prediction (RMSEP) of 810–1100 mg kg^{-1} fresh weight. Cozzolino et al. (2004) acquired absorbance spectra over the wavelength range of 400–1100 nm of intact grape berries and berry homogenates. A root mean square error of cross calibration ($RMSE_{CV}$) of 60 and 140 mg kg^{-1} fresh weight, and a ratio of the standard deviation (S.D.) (110 mg kg^{-1}) to the standard error of calibration (RPD) of 4.2 and 1.8, was achieved for of TAC of whole and homogenised grape, respectively.

Various procedures can be undertaken to ensure that a model is not over-fitted to a data set, causing inflated calibration statistics, e.g. careful selection of cross validation sets, and interpretation of model coefficients. However, variation in fruit properties between populations (in chemical composition, in cell density, etc.) exists, and in practical demonstration of the robustness of a model in predicting an attribute of interest in fruit grown under a range of conditions is required (Nicolaï et al., 2007; Subedi and Walsh, 2009). For example, diffuse reflectance spectra are sensitive to changes in sample surface layers (Lammertyn et al., 2000; Nicolaï et al., 2007). Different fruit batches vary in the amount of cuticle of wax over the exocarp, and also in the depth of edible tissue (exocarp and mesocarp, 1–3 mm to hard seed) (Pessoa and Teixeira,

Table 1
Populations of açaí (*Euterpe oleracea*Mart.) and juçara (*Euterpe Edulis*Mart.) fruits and respective population statistics for total anthocyanin (TAC, g cyanidin-3-glucoside per kilogram of fresh weight) and soluble solids content (SSC, %).

Species	Locality	Year	Population	TAC		SSC		*N*	Season	TAC		SSC	
				Mean	[a]S.D.	Mean	S.D.			Mean	S.D.	Mean	S.D.
Açaí (A)	Amer (i)	2012	Pop 1	11.16	3.93	17.27	2.05	40	June	13.56	3.70	16.40	2.43
								39	August	8.68	2.39	18.16	1.03
		2013	Pop 2	2.78	1.91	11.52	1.14	15	May	2.91	2.49	11.34	1.44
								10	June	2.59	0.67	11.78	0.49
	Jab1 (ii)	2012	Pop 3	15.08	2.17	23.23	1.34	14	July	14.63	2.49	23.23	1.39
		2013	Pop 4	8.27	2.94	17.63	1.33	17	May	8.27	3.03	17.62	1.37
	Jab2 (iii)	2012	Pop 5	27.81	4.25	26.81	3.78	40	July	27.81	4.30	26.81	3.83
		2013	Pop 6	27.81	6.66	26.51	6.07	40	June	29.95	6.73	29.60	5.40
								60	July	24.51	5.28	22.02	3.90
	i	12–13	Pop 1–2	9.14	5.07	15.89	3.11	104					
	i + ii	12–13	Pop 1–3	9.85	5.16	16.76	3.79	118					
	i + ii	12–13	Pop 1–4	9.64	4.96	16.87	3.59	135					
	i + ii + iii	12–13	Pop 1–5	13.80	9.03	19.14	5.54	175					
Juçara (J)	Amer (i)	2012	Pop 7	32.82	4.25	22.82	2.59	20	June	32.82	4.36	22.85	2.66
		2013	Pop 8	20.68	3.85	21.27	1.42	20	April	20.68	3.95	21.27	1.46
	Jab1(ii)	2012	Pop 9	20.37	5.72	16.80	3.39	10	March	17.97	3.94	15.78	3.36
								30	April	27.58	4.27	19.84	1.46
		2013	Pop 10	13.53	7.44	14.71	5.04	41	April	9.04	2.35	11.62	1.92
								19	June	23.23	5.19	21.39	2.76
	Rib(iv)	2012	Pop 11	18.53	7.53	17.94	5.07	30	March	13.37	4.14	14.29	2.67
								10	April	30.41	2.08	25.02	1.26
								30	June	19.74	6.37	19.22	4.66
		2013	Pop 12	4.77	4.98	9.55	2.73	10	February	9.38	2.80	12.21	0.62
								10	April	0.16	0.05	6.89	0.74
	i	12–13	Pop 7–8	26.75	7.39	22.05	2.25	40					
	i + ii	12–13	Pop7–9	23.56	7.34	19.42	3.91	80					
	i + ii	12–13	Pop 7–10	19.26	8.90	17.40	5.01	140					
	i + ii + iv	12–13	Pop 7–11	19.02	8.47	17.58	5.04	210					
J+A	i	12–13	Pop 1–2;7–8	12.96	10.00	17.60	3.99	144					
	ii	12–13	Pop 3–4;9–10	15.10	7.26	16.64	4.71	131					
	iii + iv	12–13	Pop 5–6 + 11–12	23.00	9.53	22.50	7.62	230					
	i + iii + iv	12–13	Pop 1–2 + 5–8 + 11–12	19.56	10.56	20.62	6.90	374					

[a] S.D.: standard deviation.