

**Title** A preliminary approach to the prediction of 'Rocha' pear skin pigments by VIS/NIR reflectance spectroscopy

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**Citation** ISHS Acta Horticulturae 858:373-378. 2010.

**Keyword** carotenoids; chlorophyll; PLS; *Pyrus communis* L.

### Abstract

'Rocha' pear (*Pyrus communis* L.) is an exclusively Portuguese certified pear cultivar commercialized worldwide. Mature unripe 'Rocha' pears were obtained from COOPVAL (Cadaval, Portugal) after 8 months at  $-0.5^{\circ}\text{C}$ , 94-96% RH and CA (2%  $\text{O}_2$ +0.5%  $\text{CO}_2$ ). Then, they were maintained in a dark room at  $20\pm 2^{\circ}\text{C}$  and 70% RH to simulate shelf life. For three weeks these fruit were followed along using Vis/NIR reflectance spectroscopy in the wavelength range of 400 to 950 nm, and their colour and firmness were evaluated by standard techniques. 'Rocha' pear firmness decreased significantly during shelf life, paralleled by the yellowing of the fruit skin (increase in  $a^*$  and Hue angle). Pigments were extracted from fruit skin and assayed spectrophotometrically. Both Chla and Chlb contents decreased along ripening in shelf life, while contents of carotenoids remained constant. Vis/NIR reflectance spectra were correlated with the respective fruit skin pigments content by PLS. Prediction models were obtained for Chl ( $a$ ,  $b$ ,  $a+b$ ), but not for carotenoids. Models were reasonably significant in regression terms [ $r(\text{Chla})=0.898$ ;  $r(\text{Chlb})=0.897$ ;  $r(\text{Chla}+b)=0.918$ ], but the respective SDR (standard deviation ratio = standard deviation of the validation set /RMSEP)( $2.2^{\text{Chla}}$ ,  $2.3^{\text{Chlb}}$ ,  $2.2^{\text{Chla}+b}$ ) suggest that only a coarse quantitative prediction is possible for all models. Although Chla model required a higher number of latent variables [ $\text{Lv}(\text{Chla})=6$ ;  $\text{Lv}(\text{Chlb}$  or  $\text{Chla}+b)=3$ ], similarity between RMSEC and RMSEP was lower for the other parameters [ $\text{Chla}$ : 4.6 and 4.6  $\text{g m}^{-2}$   $\text{Chlb}$ : 3.9 and 2.3  $\text{g m}^{-2}$ ,  $\text{Chla}+b$ : 7.3 and 6.7  $\text{g m}^{-2}$ ]. A better performance for these models has been expected, because most of the differences found in the Vis/NIR spectra in shelf life were in the Chl absorption region. However, only a coarse prediction capability was found. Thus, the data obtained suggest that changes on the background around 670 nm decrease the prediction capability of the PLS model and should be further investigated.