Determination of characteristic absorption bands for carbohydrates and organic acids in mango purée

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Introduction

Mango (*Mangifera indica* L.) is a tropical fruit with large export markets in Asia, Europe and North America. Mangoes contain simple and complex carbohydrates, organic acids, proteins, fats and vitamins,[1] all of which contribute to fruit quality. Many of these molecules contain O-H, C-H and N-H bonds that absorb energy at NIR frequency,[2] meaning that mango quality can be non-destructively determined using NIRS.[3,4] NIR absorption peaks are broad and overlap, making it almost impossible to assign chemical identity to the absorption at any wavelength, or to develop quantitative calibration equations for specific compounds based on single peak heights. The accuracy and precision of calibrations depends on the quality of both the spectral and the reference measurements, and the choice of samples used to construct the calibration and validation databases. It is often found that model performance can be improved by restricting the number of wavelengths initially entered in the model. This can be done by unsupervised selection methods, such as genetic algorithms, or by choosing wavelengths known to correspond to the compound of interest. The purpose of this research was to identify wavelengths corresponding to compounds that contribute to mango quality, in the expectation that the relevant wavelengths could be identified from PLSR coefficients.

Material and methods

Six different compounds found in mango fruits, were studied: glucose and sucrose (simple sugars), starch and cellulose (complex polysaccharides), and citric acid and malic acid (organic acids). Mango purée (cv. Keitt) and the pure substances were mixed at various concentrations (glucose, sucrose, citric and malic acids at 0, 5, 10, 15 and 20 % w/w; starch and cellulose at 0, 2.5, 5, 7.5 and 10 % w/w). A NIRSystems Model 6500 (Foss) was used to obtain spectra between 400 nm to 1100 nm. Partial least squares regression (PLSR) was used to develop calibration

equations for each component. Wavelengths related to each compound were identified from plots of the regression coefficients.

Results and discussion

The spectra of the six pure substances are shown in Figure 1 and the main absorption peaks identified in Table 1.

Glucose and sucrose shared peaks at 920/926 nm, a peak also shared with starch, and at 1030/1040 nm. Two additional peaks were present in the sucrose spectrum, at 760 nm, also shared with starch, and at 984 nm. A peak at 996 nm was present in the spectra of both starch and cellulose. Citric acid and malic acid shared three peaks at 782/790 nm, at 902 nm and at 1010/1016 nm. There was an additional peak at 1074 nm in the spectrum of citric acid. The spectra of mango purée and of the purée mixtures showed only two clear absorption peaks, one at 456 nm corresponding to carotenoids.[5]and one at 978 nm corresponding to water.[4] the major component of the purée by mass.

The spectral data of purée mixtures were pre-treated with multiplicative scatter correction (MSC), standard normal variate (SNV) and second derivative to reduce the effects of overlapping peaks.[2] The wavelength range of interest was initially determined by examining PLSR model performance after varying the starting and ending wavelengths of the part of the spectrum used. Calibration equations were then developed to identify wavelengths that might be related to each component. PLSR calibration model statistics for glucose, sucrose, citric acid, malic acid, starch and cellulose are shown in Table 2.

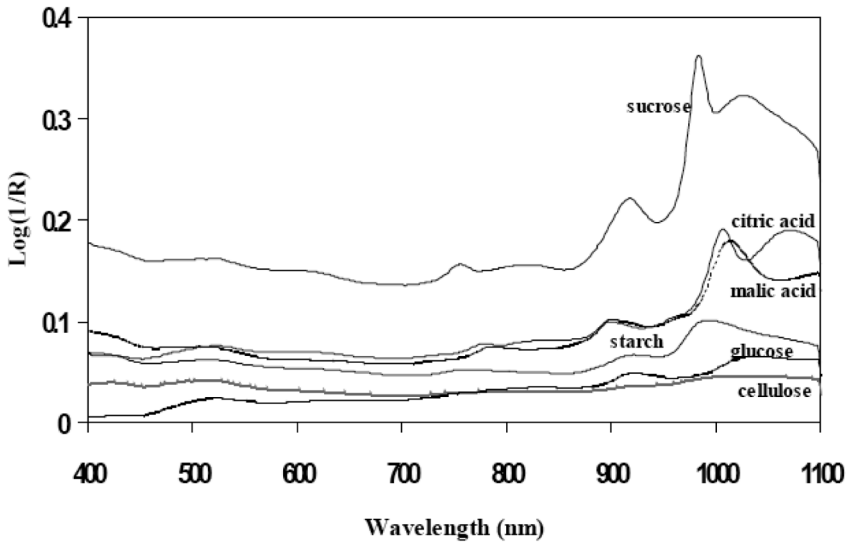

Figure 1. Spectra of six pure substances following multiplicative scatter correction.

Table 1. Identified absorption peaks of six pure substances.

Substance	Wavelength (nm)								
Glucose				926				1040	
Sucrose	760			920	984			1030	
Starch	760			924		996			
Cellulose						996			
Citric acid		782	902				1010		1074
Malic acid		790	902				1016		

The coefficient of determination (R^2) of all models was 0.99 with values of *SEC* and *SEP* less than 0.5 % (w/w).

As up to 20 % by weight of each substance was added to the purée, the calibrations might be expected to rely heavily on the water content of the mixture, and indeed wavelengths between 974 nm and 984 nm were identified as contributing to the PLSR calibration models for glucose, cellulose, citric acid and malic acid (Table 3).

The model for starch shared wavelengths with the model for glucose (1084/ 1086 nm) and that for sucrose (954/966 nm; 1068 nm). The model for starch also identified the wavelength 996 nm, which was present in the spectrum of the pure substance. The model for cellulose shared the wavelength 1084/1086 nm with both the glucose and starch models, but 996 nm, also present in the pure substance spectrum for cellulose, was not identified by the PLSR model in the mango purée. Whilst the spectra for pure citric acid and malic acid shared three common absorption peaks, no shared wavelengths were identified by the PLSR models for these substances in the purée.

Table 2. PLSR calibration statistics for mango purée mixed with six substances at various concentrations between 0 and 20 % (w/w).

Substance	Pre-treatment	Wavelength (nm)	R^2	*SEC*	*SEP*	Bias
Glucose	log(1/R)	900–1100	0.99	0.49	0.42	−0.02
Sucrose	MSC	860–1100	0.99	0.37	0.37	−0.02
Starch	SNV + 2nd	900–1100	0.99	0.23	0.23	−0.05
Cellulose	SNV + 2nd	550–1100	0.99	0.19	0.19	0.01
Citric acid	SNV + MSC	950–1100	0.99	0.34	0.34	−0.01
Malic acid	MSC + 2nd	950–1100	0.99	0.26	0.26	0.01

MSC: Multiplicative scatter correction; SNV: Standard normal variate; 2^{nd}: second derivative; *F*: number of factors used in the calibration equation; R^2: coefficient of determination; *SEC*: standard error of calibration; *SEP*: standard error of prediction; Bias: average of difference between actual value and NIR predicted value.

Table 3. Wavelengths identified from PLSR coefficient plots for calibration equations of mango purée mixed with six substances at various concentrations between 0 and 20% (w/w).

Substance	Pre-treatment	Wavelength (nm)									
Glucose	log(1/R)			914			974				1086
Sucrose	MSC					966				1068	
Starch	SNV + 2nd					954		996		1068	1084
Cellulose	SNV + 2nd	602	664		940		984				1084
Citric acid	SNV + MSC						974				1080
Malic acid	MSC + 2nd					956	980		1024	1070	

Conclusions and future work

We conclude that the wavelengths identified by the PLSR models were those at which the absorbance is most affected by the addition of each substance to mango purée and are therefore characteristic of that compound. We will next examine whether models for prediction of these compounds for whole fruits can be improved by using these wavelengths (or wavelength regions) compared to models that use complete spectra or unsupervised wavelength selection methods. We will also repeat the work with other mango varieties to examine whether these wavelengths can be considered independent of variety.

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