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Assessment of Apple Juice by Aquaphotomics in a Temperature Dependent Environment

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Introduction

The near infrared (NIR) spectrum of water is sensitive to temperature variations¹. Since apple juice consists of more than 85% water, its spectral signature is also affected by temperature perturbations, often resulting in bias when applying a predictive model developed at one temperature to another². We are studying a new field called "Aquaphotomics" to help to develop improved models which are robust against temperature perturbations. In this study, we examine predictions of soluble solids content (SSC; measured as °Brix) in apple juice made at various temperatures using a Fourier transform (FT)-NIR spectrometer operating around the major water absorbance peak at ~1450 nm.

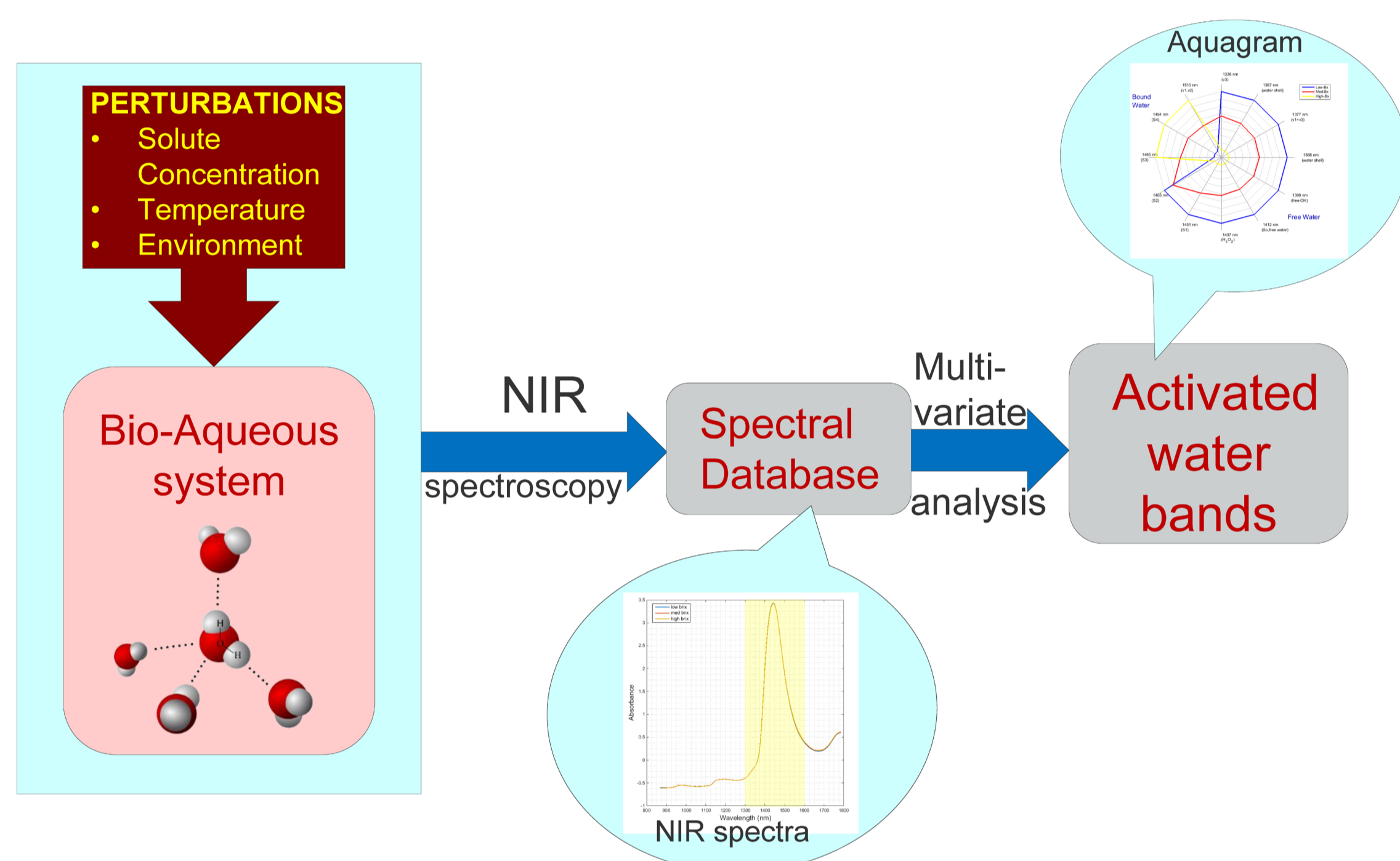


Figure 1: Aquaphotomics: analysing samples using NIR spectroscopy in the first overtone region (1300-1600 nm) of water³.

Material and Methods

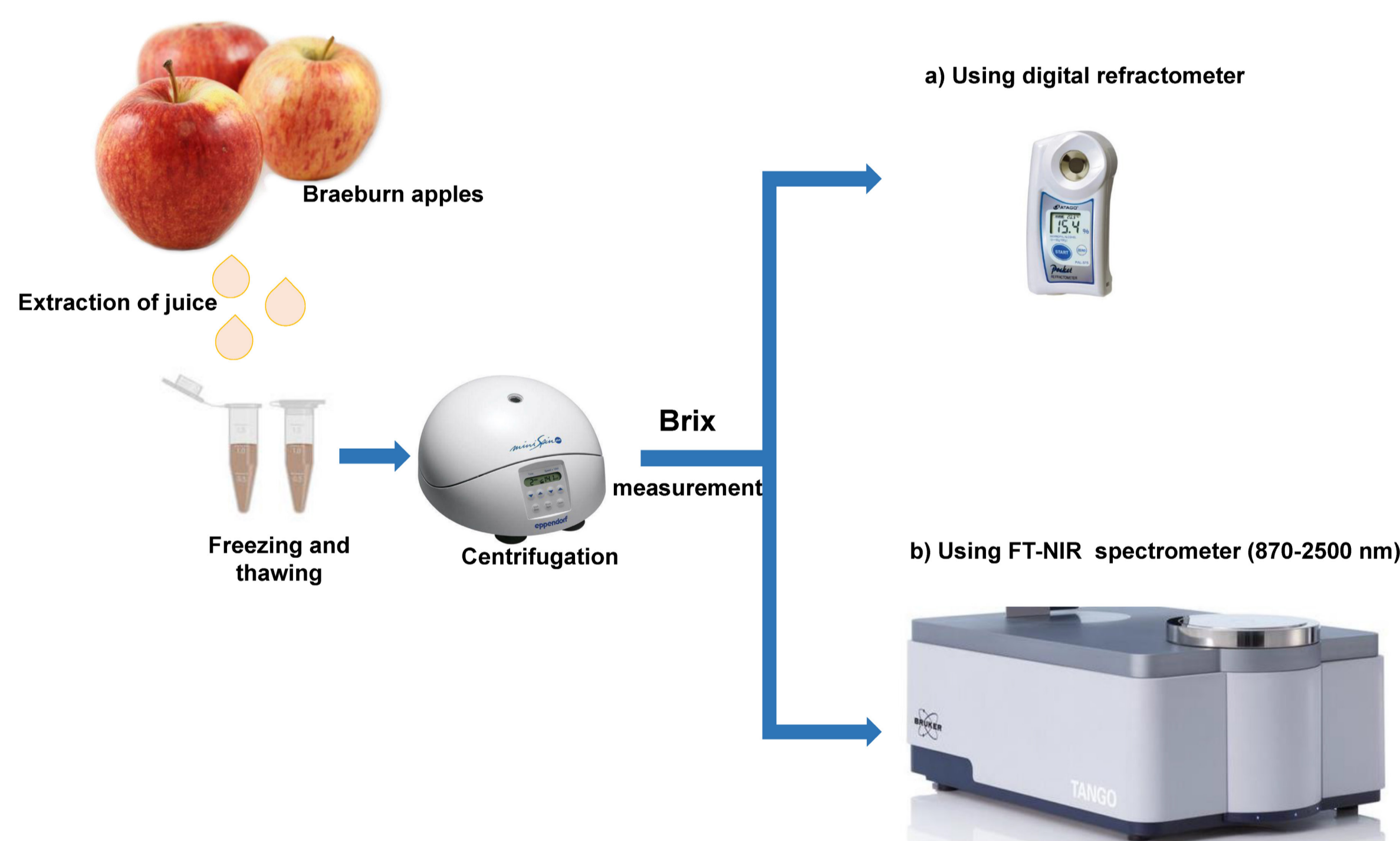


Figure 2: Experimental setup for soluble solids content (°Brix) measurement in apple juice samples using (a) digital refractometer (b) FT-NIR spectrometer at three temperatures 20, 25, and 30°C.

The SSC of 111 apple juice samples was measured by a digital refractometer (Atago Co. Ltd, Japan). Transmittance spectra of the juice samples in 1300-1600 nm range were measured at 20, 25, and 30°C (±1°C) with a FT-NIR spectrometer (Tango, Bruker Corporation, Germany) having a temperature-controlled quartz cuvette (1 mm optical path length). A spectrum of Milli-Q water was measured after every 11th sample reading as an interferent spectrum. Predictive models were developed using Partial Least Squares (PLS; MATLAB and PLS toolbox) with four-fold venetian blind cross validation. Aquaphotomics encouraged investigation of the extended multiplicative scatter correction (EMSC) spectral pre-treatment method:

$$X = b_0 + b_1\bar{X} + b_2I + e \quad (1)$$

where X is the observed spectra, \bar{X} is the reference spectrum (the mean of spectra of calibration data), I is an interferent spectrum (PC1 loading of water samples in our case), b_0 , b_1 , and b_2 are fitting constants, and e is the residual. The EMSC approach was compared with standard methods involving the combination of standard normal variate and second derivative spectral (SNV+2D) pre-treatments.

Results

The aquagram in Figure 3 illustrates that free water increases with temperature because of breaking of H-bonds. As the SSC increases, the number of strongly H-bonded water molecules increases, resulting in highly organised water structures.

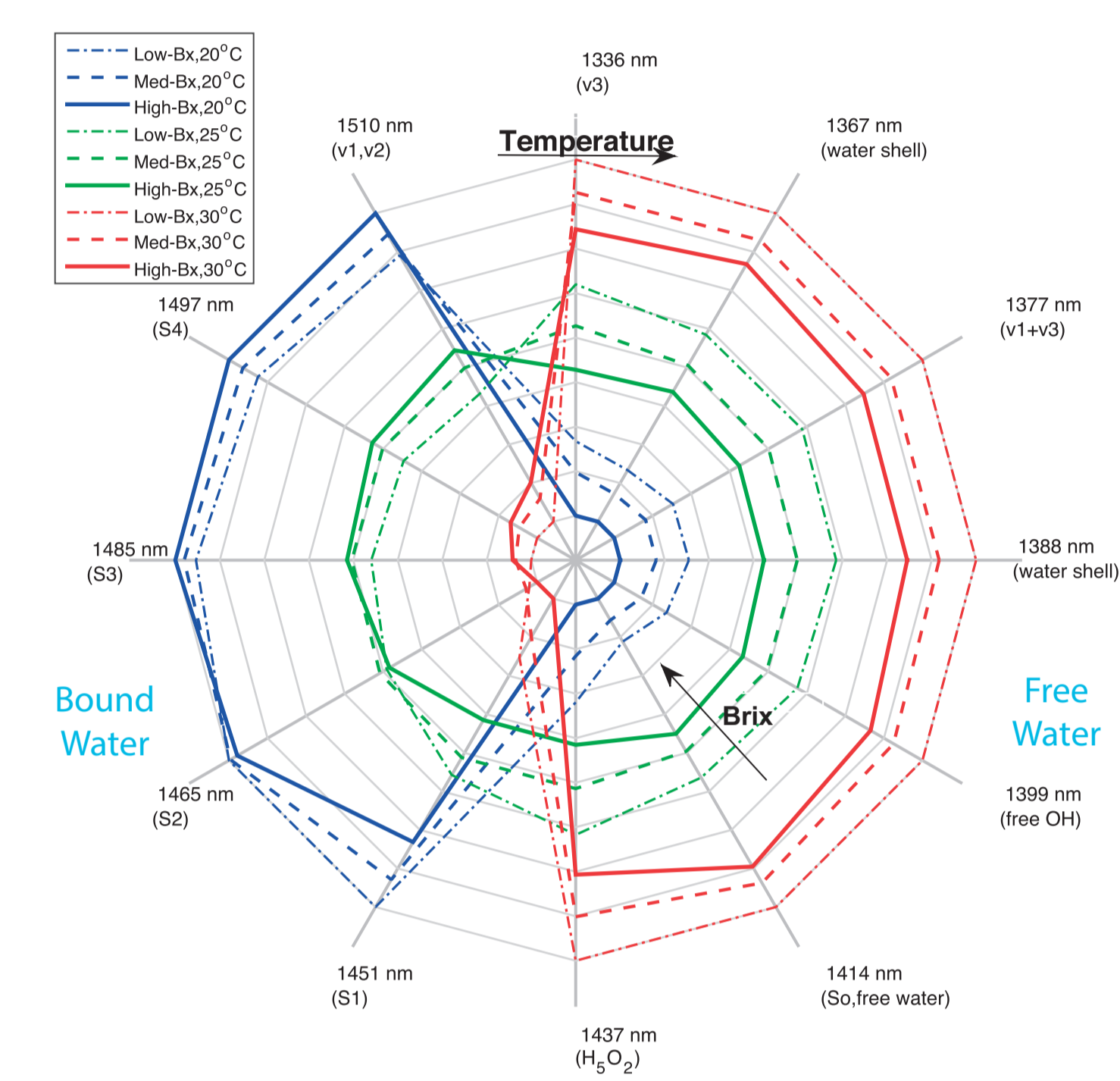


Figure 3: Aquagram at three temperatures for low, medium and high soluble solids content (°Brix; Bx) apple juice samples, based on water matrix coordinates³.

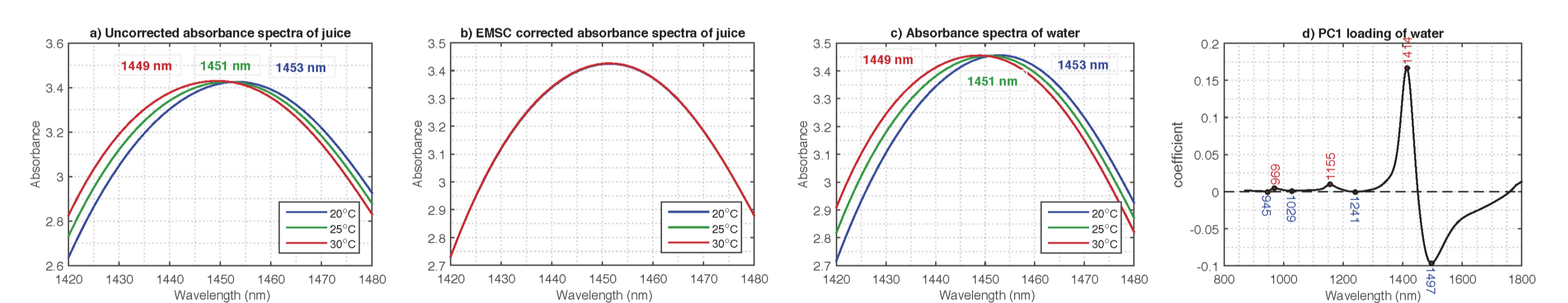


Figure 4: Uncorrected (a) and extended multiplicative scatter correction (EMSC)-corrected (b) apple juice spectra generated by removing PC1 loading component of water samples from apple juice spectra. (c) Absorbance spectra of water at three temperatures (d) PC1 loading of water. Labels indicate the wavelengths of the peaks.

Table 1: Comparison of SNV+2D and EMSC pre-processing methods.

Cal = 20°C		(N _{cal} =83 and N _{val} =28)						
Val =	Pre-processing	R ² _{cv}	RMSECV	LV	R ² _p	RMSEP	Bias	SEP
20°C	SNV+2D	0.82	0.50(± 0.03)	2	0.81	0.52(± 0.11)	0.07	0.51
	EMSC	0.83	0.49(± 0.03)	1	0.83	0.49(± 0.09)	0.07	0.48
25°C	SNV+2D	0.82	0.50(± 0.03)	2	0.81	0.62(± 0.10)	0.29	0.51
	EMSC	0.83	0.49(± 0.03)	1	0.83	0.49(± 0.10)	0.06	0.48
30°C	SNV+2D	0.82	0.50(± 0.03)	2	0.77	1.01(± 0.25)	0.77	0.58
	EMSC	0.83	0.49(± 0.03)	1	0.79	0.54(± 0.11)	0.05	0.53

N_{cal}/N_{val}: the number of samples in calibration/validation set; R²_{cv}/R²_p: the coefficient of determination for calibration/prediction; RMSECV/RMSEP: root mean square error of calibration/prediction; SEP: standard error of prediction (bias corrected RMSEP); LV: latent variable.

Conclusions

- The aquagram pattern showed the trend of increasing free water with temperature and bound water with SSC.
- EMSC pre-processing reduced bias by 79% and 93.5% compared with standard pre-processing (SNV+2D) when predicting SSC at 25 and 30°C using a model developed at 20°C.
- Model precision (SEP) was also improved by 6-8%.

Acknowledgements

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