

Rapid quantification of the adulteration of fresh coconut water by dilution and sugars using Raman spectroscopy and chemometrics

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Table S1: Sample contents for each sugar solution

Coconut water (μL)	Sugar solution (μL)	Deionised water (μL)	Total (μL)
250	0	250	500
250	25	225	500
250	50	200	500
...
250	250	0	500

Table S2: Sample contents for each of the three adulterants (deionised water, individual sugar solution, mixed sugar solution)

Coconut water (μL)	Adulterant (μL)	Adulteration (%)
1000	0	0
950	50	5
900	100	10
...
0	1000	100

Table S3: Table of main Raman spectral peaks present in coconut water. The presence of these peaks in relation to specific sugars along with their tentative vibrational assignments is reported

Peak (cm ⁻¹)	Present in:	Assignment ^{1,2}
423.3	Guc, Fuc	(CCC) Bend
519.7	Guc, Fuc (521), Suc (524)	(CCO) Bend
627	Fuc	(CCO) Bend
706	Fuc	(CCO) Bend
821	Fuc	(C-C) Stretch
835 (shoulder)	Suc	(C-C) Stretch
869	Fuc, Suc (shoulder)	(C-C) Stretch
918	Guc, Fuc	(CCH) Bend
1063	Guc (1061), Suc (1065), Fuc (1065)	(C-O) Stretch
1123	Guc, Suc (1132)	(COH) Bend
1265	Fuc, Suc, Suc	(CHH) Twist
1367	Guc, Suc, Fuc	(CHH) Wag
1457	Fuc, Suc, Suc	(CH ₂) Stretch
Bold: standard addition reference peak for each sugar		

1: Mathoulthi , M. Luu, D. V. Carbohydrate Research, 78 (1980) 225-233

2: Mathoulthi , M. Luu, D. V. Carbohydrate Research, 81 (1980) 203-212

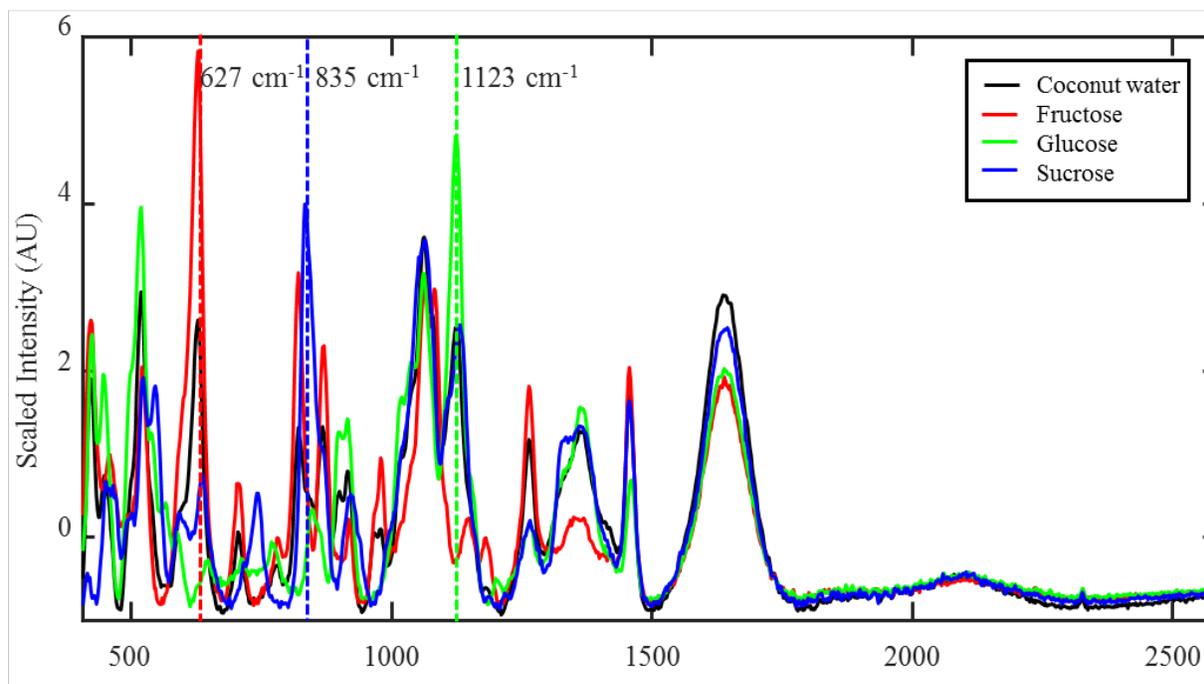


Figure S1: Overlaid spectra for pure coconut water (black) and 63 mg mL⁻¹ solutions of fructose (red), glucose (green) and sucrose (blue). Spectra are averages of four machine replicates after least squares baseline correction and autoscaling. Reference peaks for each sugar have been highlighted.

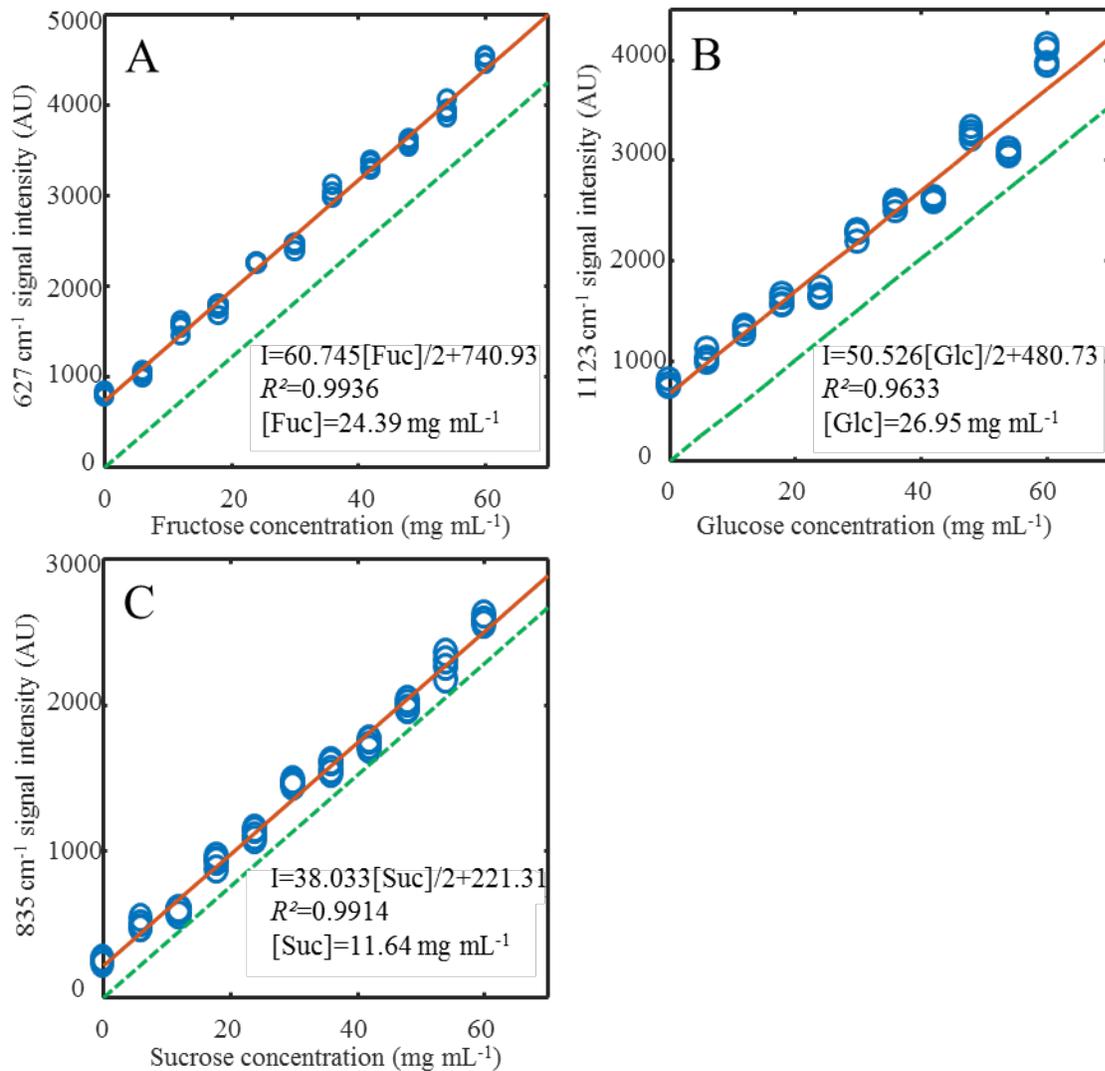


Figure S2: Standard addition calibration results for fructose (A), glucose (B) and sucrose (C). The orange line represents the linear $I = mx + b$ regression results where I is the signal intensity at each peak and x is the concentration of the sugar being examined, and the green dashed line represents the “real” expected relationship ($y = x$) between concentration and signal intensity excluding the effect of coconut water. The equation of best fit, R^2 and calculated concentration is also reported.

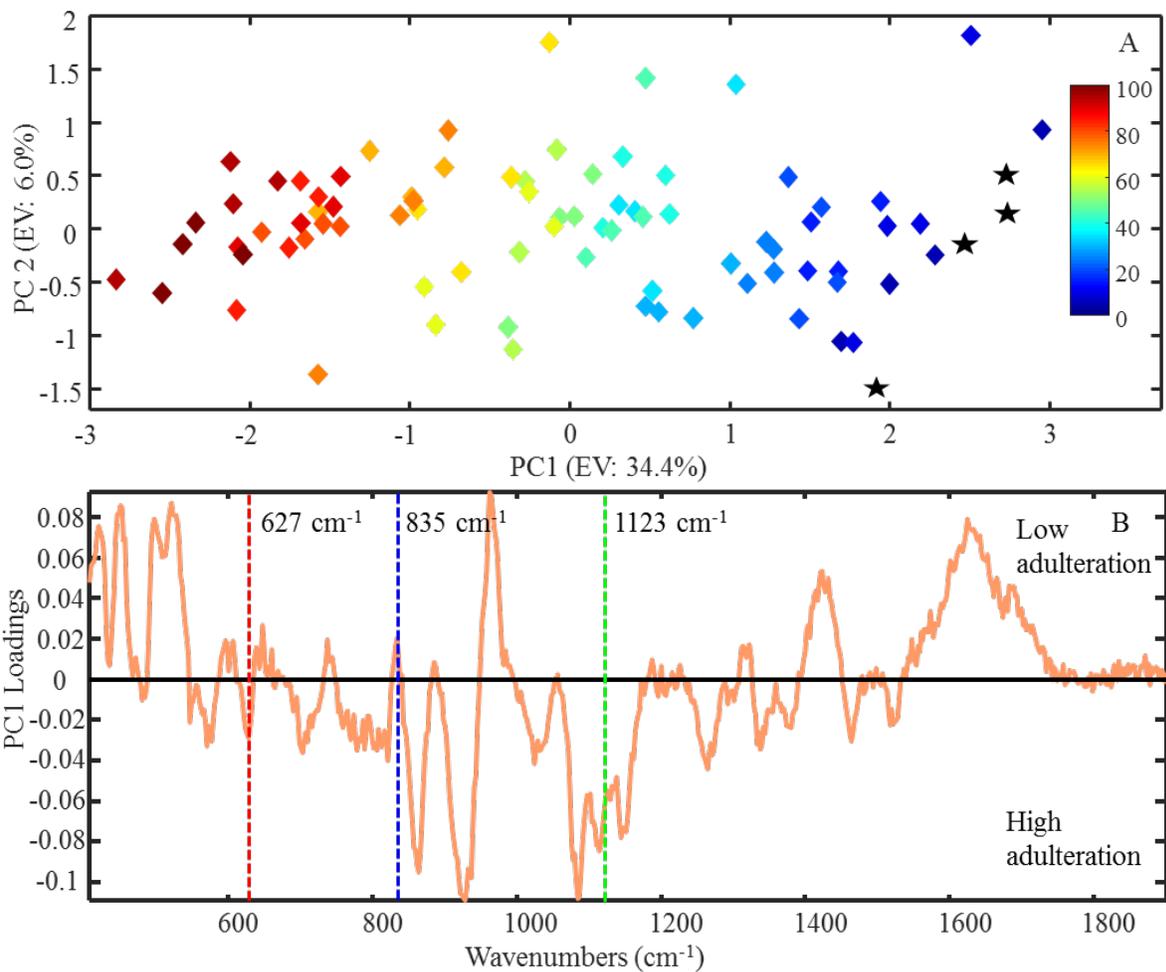


Figure S3 PCA scores plot (A) of the adulteration of coconut water (yellow stars) with HFCS (downwards-facing triangles) ranging from 0-100% (black to beige). The analysis was performed using two PCs and achieved 40.5% TEV. PCA loadings plot (B) describing the variance in PC 1 for the PCA analysis of the adulteration of coconut water with HFCS. Positive loadings indicate a higher intensity at low adulteration, while negative loadings indicate a higher intensity at high adulteration. Red, blue and green lines indicate the variance present in the main fructose, sucrose and glucose peaks respectively.

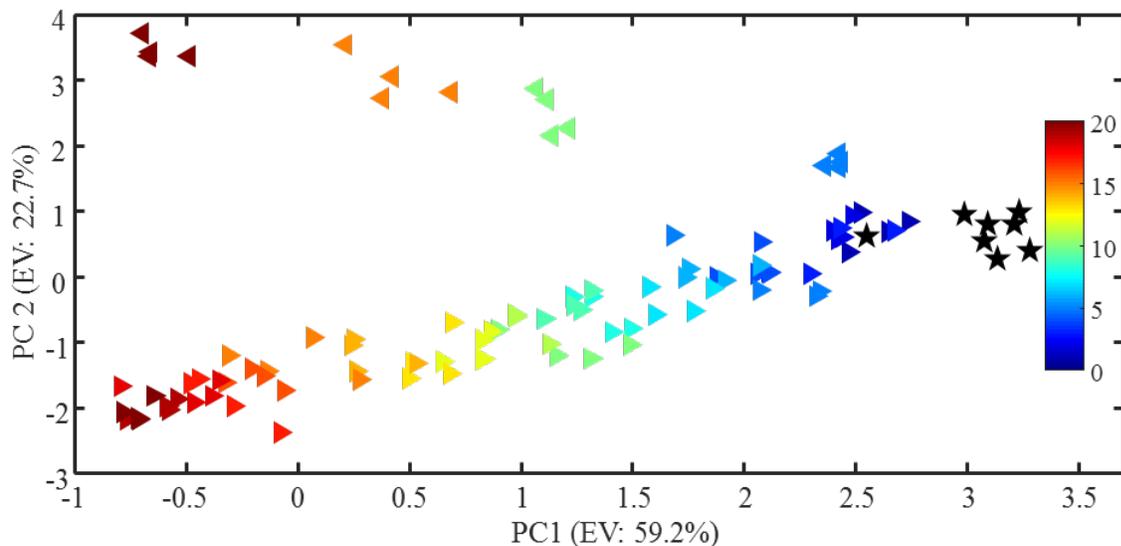


Figure S4: PCA scores plot outlining the adulteration of coconut water (black stars) with a 63 mg mL^{-1} laboratory grade glucose powder solution (left-facing triangles) and a $6.4 \text{ }^\circ\text{Bx}$ commercial corn (glucose) syrup (Daesang America, inc.) (right-facing triangles). Adulteration ranges from 0-20% in 5% and 1% increments for glucose powder and syrup respectively. The analysis was performed using 2 PCs and achieved 81.9% TEV.

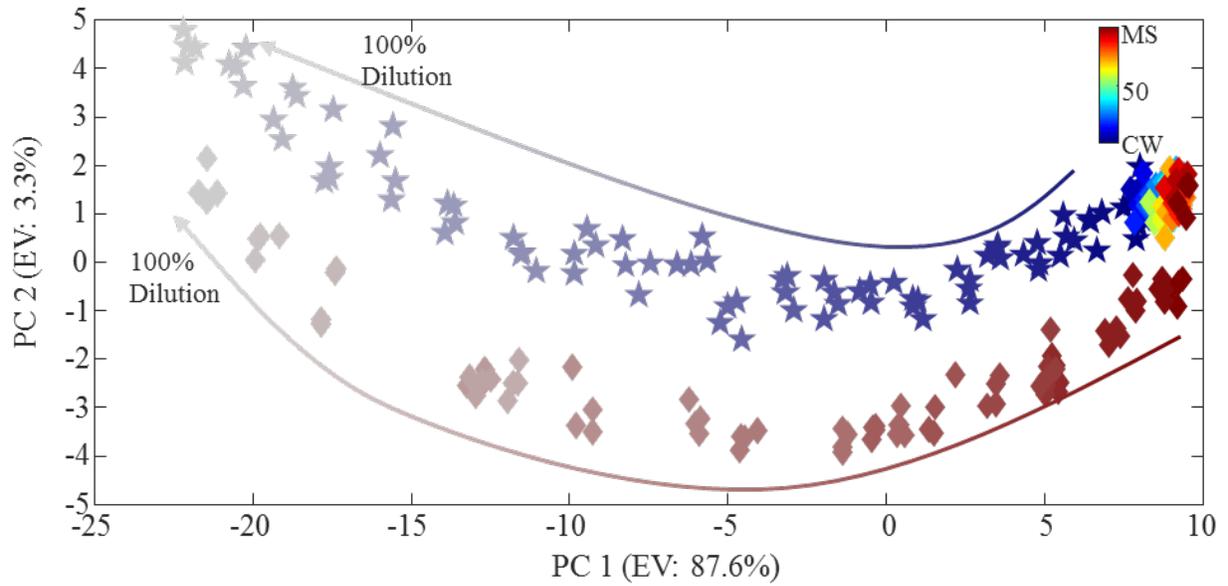


Figure S5: PCA scores plot of the adulteration of coconut water (blue stars) with water (blue to grey stars), mixed sugar solution (red diamonds) with water (red to grey diamonds) and coconut water with sugar solution (blue to red diamonds). The analysis was performed using 2 PCs and achieved 90.8% TEV.