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Supplementary Information

Evaluation of Chemical Changes during *Myrciaria cauliflora* (Jabuticaba Fruit) Fermentation by ^{1}H NMR Spectroscopy and Chemometric Analyses

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Table S1. Calculation of compound concentration quantified by ^{1}H NMR spectroscopy

Compound/integral/chemical shift	Protons	Relative moles	MW / (g mol^{-1})	Mass / g	Concentration / (g kg^{-1})
Sucrose (a) 5.24 ppm	1	a/1	342.3	(a/1) × 342.3	((a/1) × 342.3)/total × 1000
Water (b) 4.68 ppm	2	b-f/2	18.02	(b-f/2) × 18.02	((b-f/2) × 18.02)/total × 1000
Fructose (c) 3.92-4.08 ppm	2	c-a/2	180.2	(c-a/2) × 180.2	((c-a/2) × 180.2)/total × 1000
Glycerol (d) 3.37-3.42 ppm	4	d/4	92.09	(d/4) × 92.09	((d/4) × 92.09)/total × 1000
Methanol (e) 3.20 ppm	3	e/3	32.0	(e/3) × 32.0	((e/3) × 32.0)/total × 1000
β-Glucose (f) 3.08 ppm	0.64	f/0.64	180.2	(f/0.64) × 180.2	((f/0.64) × 180.2)/total × 1000
Citric acid (g) 2.60-2.83 ppm	4	g/4	192.13	(g/4) × 192.13	((g/4) × 192.13)/total × 1000
Succinic acid (h) 2.49 ppm	4	h/4	118.09	(h/4) × 118.09	((h/4) × 118.09)/total × 1000
Acetic acid (i) 1.92 ppm	3	i/3	60.05	(i/3) × 60.05	((i/3) × 60.05)/total × 1000
Ethanol (j) 1.02 ppm	3	j/3	46.07	(j/3) × 46.07	((j/3) × 46.07)/total × 1000
Total				Total / g	1000

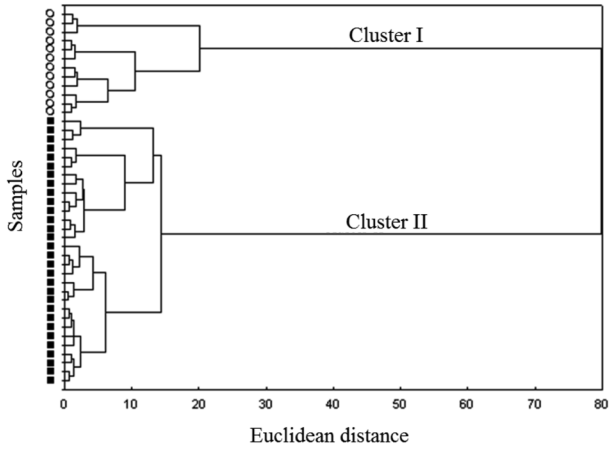

Figure S1. Dendrogram obtained by cluster analysis of must samples using Ward's linkage method.

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