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

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

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

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