

Supplementary Information

Optimizing the Extraction of Anthocyanins from the Skin and Phenolic Compounds from the Seed of Jaboticaba Fruits (*Myrciaria jaboticaba* (Vell.) O. Berg) with Ternary Mixture Experimental Designs

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Table S1. Solvent optimization experiments: simplex lattice design and observed responses

| Run number | Independent variable ^a | | | | | | Response | |
|------------|-----------------------------------|----------------|----------------------------|----------------|-------------------------|----------------|---|--|
| | Ethanol (X ₁) | | Methanol (X ₂) | | Water (X ₃) | | Total phenolic compounds (seed) / (mg of gallic acid equivalent g ⁻¹ of freeze-dried sample) | Total monomeric anthocyanins (skin) / (mg of cyanidin-3-glycoside equivalent 100 g ⁻¹ of freeze-dried sample) |
| | Coded value | Real value / % | Coded value | Real value / % | Coded value | Real value / % | | |
| 1 | 1 | 100 | 0 | 0 | 0 | 0 | 73.34 | 509.31 |
| 10 | 0 | 0 | 1 | 100 | 0 | 0 | 91.22 | 1111.86 |
| 11 | 0 | 0 | 0 | 0 | 1 | 100 | 61.89 | 301.97 |
| 9 | 1/2 | 50 | 1/2 | 50 | 0 | 0 | 62.07 | 920.17 |
| 12 | 1/2 | 50 | 0 | 0 | 1/2 | 50 | 110.13 | 1020.02 |
| 5 | 0 | 0 | 1/2 | 50 | 1/2 | 50 | 106.02 | 1149.44 |
| 4 | 1/3 | 33.3 | 1/3 | 33.3 | 1/3 | 33.3 | 120.81 | 1213.45 |
| 2 | 1/3 | 33.3 | 1/3 | 33.3 | 1/3 | 33.3 | 115.1 | 1141.09 |
| 7 | 1/3 | 33.3 | 1/3 | 33.3 | 1/3 | 33.3 | 122.86 | 1185.62 |
| 6 | 2/3 | 66.6 | 1/6 | 16.6 | 1/6 | 16.6 | 109.77 | 1156.39 |
| 8 | 1/6 | 16.6 | 2/3 | 66.6 | 1/6 | 16.6 | 112.07 | 1235.71 |
| 3 | 1/6 | 16.6 | 1/6 | 16.6 | 2/3 | 66.6 | 84.67 | 947.66 |

^aAcetic acid (0.5%) was added to each experiment of the experimental design for total monomeric anthocyanins extraction from the skin.

