Supplementary Material

Combining eutectic solvents and pressurized liquid extraction coupled in-line with solid-phase extraction to recover, purify and stabilize anthocyanins from Brazilian berry wastes

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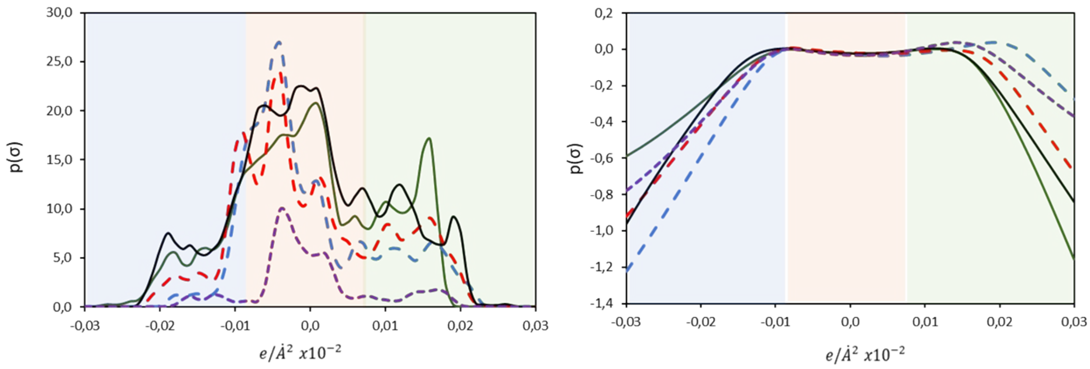

Fig. S1. The σ-profiles and σ-potential (μ(σ)) (COSMO-RS) of cyanidin-3-O-rutinoside (—), cyanidin-3-O-glucoside (—), ChCl:LA (---), Bet:LA (---) and ethanol (---).

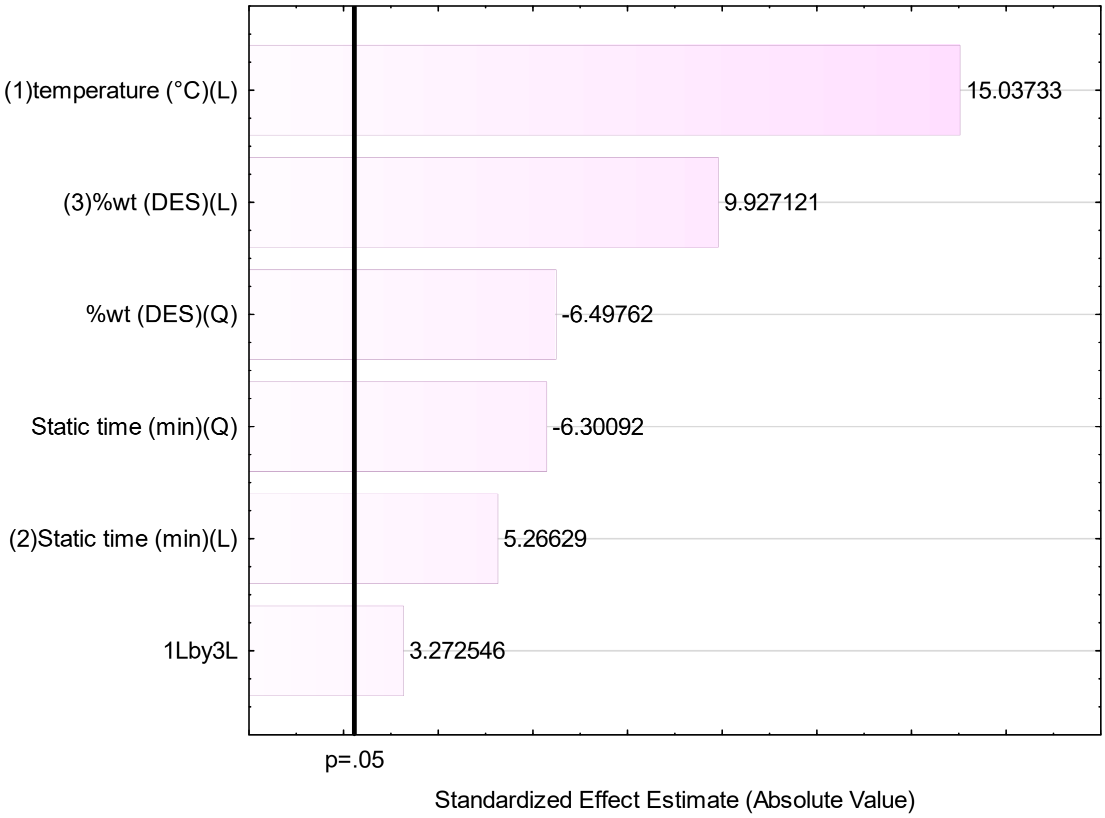

Fig S2. Pareto chart of the CCRD (2^3 + axial and central points) regarding the yield of extraction of anthocyanins from *Jabuticaba* wastes using ChCl:LA (35 wt%) as solvent.

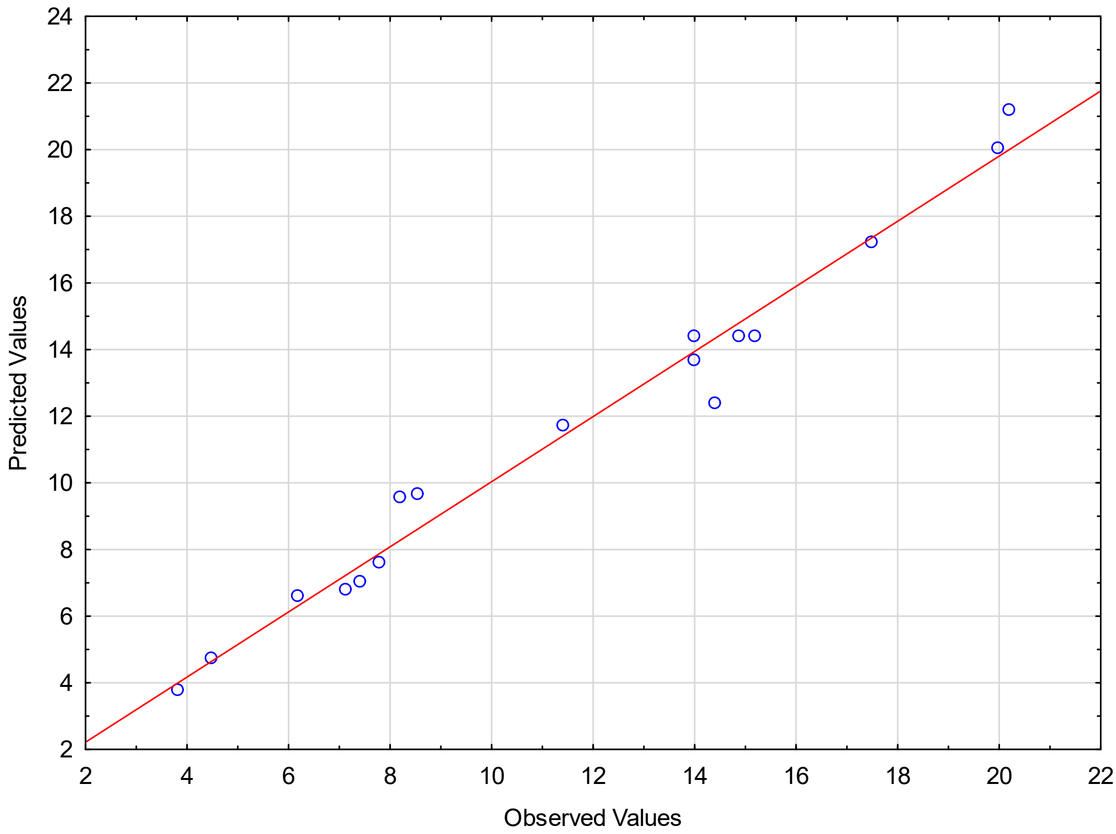

Fig. S3. Graphical representation of the predicted vs. experimental values obtained by the model when ChCl:LA (35wt%) was used as solvent in the extraction of anthocyanins from Jabuticaba wastes.

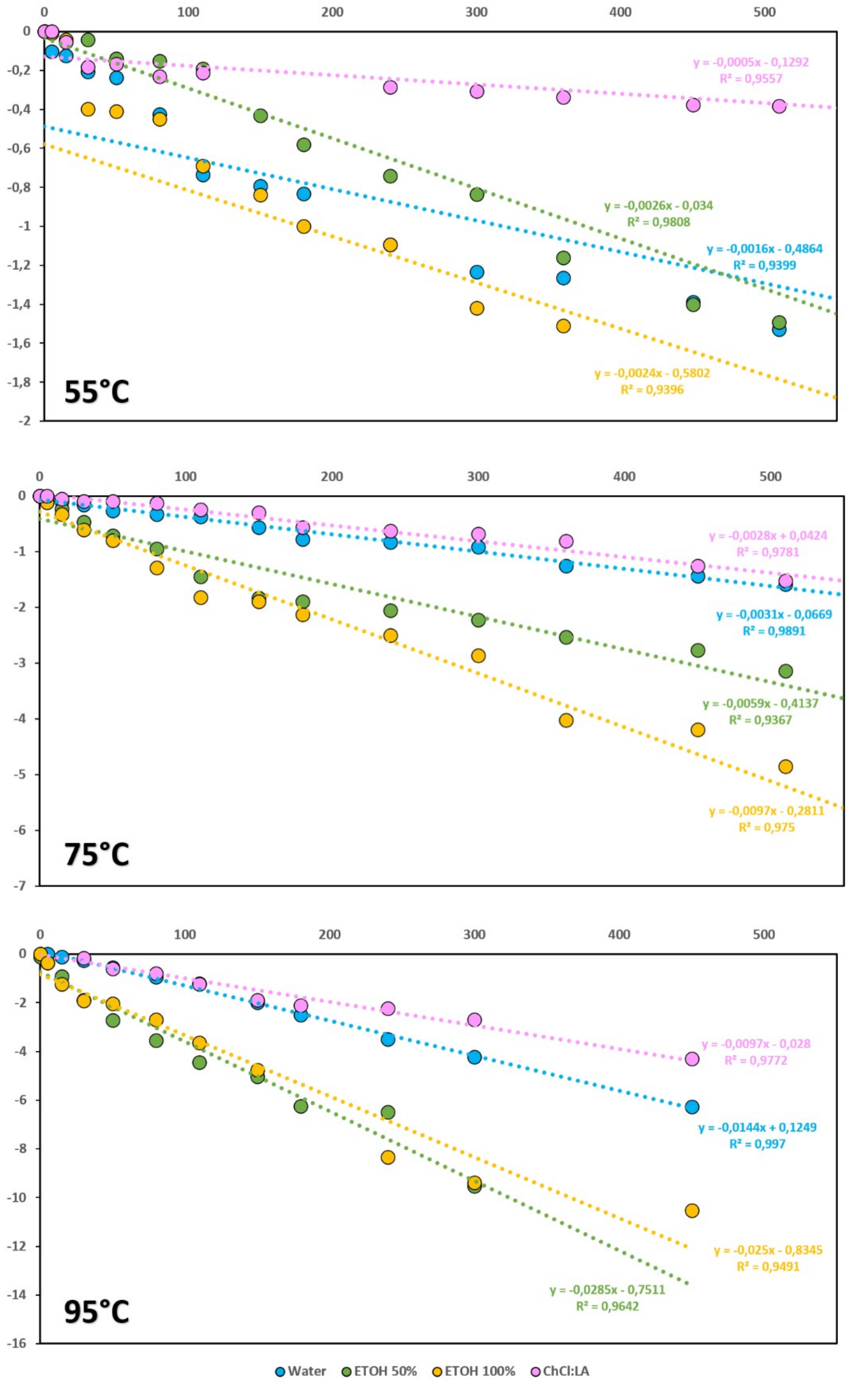

Fig. S4. Linear kinetic trends representing the anthocyanins' thermal stability for different solvents (water – blue dots, ethanol 50% v/v – green dots, ethanol 100% - yellow dots, and ChCl:LA, 35% $wt_{\%}$ - pink dots).

Tables

Table S1. List of HBAs and HBDs used in the COSMO-RS simulation screening assay.

Compound	HBA	Compound	HBA	Compound	HBA
1	Urea	11	Lactic acid	21	Ammonium acetate
2	Betaine	12	Malic acid	22	Ethylammonium chloride
3	Glycine	13	Citric acid	23	Acetylcholine chloride
4	Proline	14	Octanoic acid	24	Carnitine hydrochloride
5	Serine	15	Nonanoic acid	25	N,N-Diethylethanolammonium chloride
6	Alanine	16	Decanoic acid	26	Methyltriphenyl phosphonium bromide
7	Histidine	17	Dodecanoic acid	27	Menthol
8	Threonine	18	Glycerol	28	Thymol
9	Lysine	19	Cholinium chloride		
10	Arginine	20	Sodium acetate		

Compound	HBD	Compound	HBD	Compound	HBD
1	Urea	21	Arabinose	41	Malonic acid
2	Dimethylurea	22	Fructose	42	Propionic acid
3	Glycerol	23	Galactose	43	Succinic acid
4	Ethylene glycol	24	Glucose	44	Tartaric acid
5	1,2-Propanediol	25	Maltose	45	Octanoic acid
6	1,3-Butanediol	26	Mannose	46	Nonanoic acid
7	2,3-Butanediol	27	Raffinose	47	Decanoic acid
8	1,6-Hexanediol	28	Rhamnose	48	Dodecanoic acid
9	1,5-Pentanediol	29	Sorbose	49	Nicotinic acid
10	1,7-Heptanediol	30	Sucrose	50	Alanine
11	1,8-Octanediol	31	Trehalose	51	Arginine
12	1,9-Nonanediol	32	Xylose	52	Glycine
13	1,10-Decanediol	33	Acetic acid	53	Histidine
14	1,15-Pentadecanediol	34	Ascorbic acid	54	Lysine
15	1,4-Butanediol	35	Citric acid	55	Proline
16	Erythritol	36	Glycolic acid	56	Serine
17	Inositol	37	Lactic acid	57	Thereonine
18	Mannitol	38	Levulinic acid	58	Menthol
19	Sorbitol	39	Maleic acid	59	Thymol
20	Xylitol	40	Malic acid		

Table S2. Real and coded values (CCRD – 2^3 plus central and axial points) and experimental results for total anthocyanins extracted ($mg_{anthocyanins} \cdot g_{biomass}^{-1}$) from *Jabuticaba* wastes by PLE-SPE using ChC:LA (35 $wt_{\%}$).

Assay	Temperature (T, °C)	Static time (t_{sta}, min)	Water content ($wt_{\%}$)	Yield ($mg_{anthocyanins} \cdot g_{biomass}^{-1}$)
	V1	**V2**	**V3**	$Y_{(response)}$
1	50 (-1)	5 (-1)	25 (-1)	3.83
2	80 (1)	5 (-1)	25 (-1)	8.19
3	50 (-1)	20 (1)	25 (-1)	6.20
4	80 (1)	20 (1)	25 (-1)	14.42
5	50 (-1)	5 (-1)	35 (1)	7.12
6	80 (1)	5 (-1)	35 (1)	17.49

7	50 (-1)	20 (1)	35 (1)	8.56
8	80 (1)	20 (1)	35 (1)	19.98
9	39.8 (-1.68)	12.5 (0)	30 (0)	6.69
10	90.2 (1.68)	12.5 (0)	30 (0)	20.22
11	65 (0)	0 (-1.68)	30 (0)	7.43
12	65 (0)	25.1 (1.68)	30 (0)	11.41
13	65 (0)	12.5 (0)	21.6 (-1.68)	4.49
14	65 (0)	12.5 (0)	38.4 (1.68)	14.00
15	65 (0)	12.5 (0)	30 (0)	10.02
16	65 (0)	12.5 (0)	30 (0)	9.03
17	65 (0)	12.5 (0)	30 (0)	11.34