

Supplementary Information

Bioprospecting Ultrasound-Assisted Phenolic Extracts from *Psidium guineense*: Antioxidant, Antimicrobial and UV Protection Potential

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Optimization of the UAE

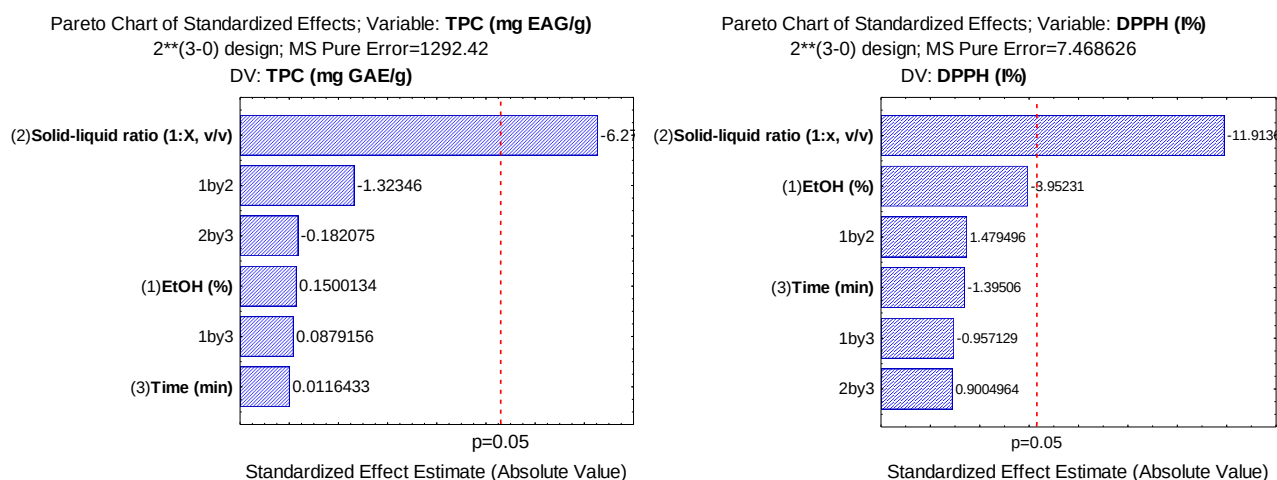


Figure S1. Pareto charts for the main effects (EtOH concentration, solid-liquid ratio and time) of input factors and interaction effects (1by2, 1by3 and 2by3) for total phenolic compounds (TPC) and antioxidant capacity against DPPH radicals.

Table S1. Pearson correlation matrix for the ultrasound-assisted extraction of phenolic compounds in the central composite design experiments

		EtOH / %	SLR	time	TPC	DPPH (I) / %
EtOH / %	R de Pearson	—				
	<i>p</i> -value	—				
SLR	R de Pearson	0.000	—			
	<i>p</i> -value	1.000	—			
time	R de Pearson	0.000	0.000	—		
	<i>p</i> -value	1.000	1.000	—		
TPC	R de Pearson	0.022	−0.937 ^a	0.002	—	
	<i>p</i> -value	0.948	< 0.001	0.996	—	
DPPH (I) / %	R de Pearson	−0.294	−0.888 ^a	−0.104	0.847 ^a	—
	<i>p</i> -value	0.379	< 0.001	0.761	< 0.001	—

^a*p*-value < 0.05 factor with significant influence. SLR: solid/liquid ratio; TPC: total phenolics content; DPPH: 2,2-diphenyl-1-picrylhydrazyl radical.

Table S2. ANOVA (95% significance) for the adequacy of the linear response surface models to determine the contents of total phenolic compounds (TPC), and antioxidant capacity against DPPH radicals (DPPH) of *Psidium guineense* fruits during the ultrasound-assisted extraction procedure optimization

Variation source	Sum of squares	Degrees of freedom	Mean square	F_{value}^a	R^2	Adjusted R^2
$\text{TPC / (mg GAE g}^{-1}\text{)} = 193.89 + 1.91X_1 - 79.77X_2 + 0.15X_3 - 16.82X_1X_2 + 1.12X_1X_3 - 2.31X_2X_3$						
Regression	53247.95	6	8874.66	7.43	0.9176	0.7940
Residue	4779.77	4	1194.94			
Lack of fit ($p > 0.05$)	2194.93	2	648.67	0.50		
Pure error	2584.84	2	1292.42			
Total	58027.72	10				
$\text{DPPH (I\%)} = 53.47 - 3.82X_1 - 11.51X_2 - 1.35X_3 + 1.43X_1X_2 - 0.92X_1X_3 + 0.87X_2X_3$						
Regression	1220.49	6	203.42	6.50	0.9070	0.7634
Residue	125.21	4	31.30			
Lack of fit ($p > 0.05$)	110.272	2	55.136	7.38		
Pure error	14.937	2	7.469			
Total	1345.700	10				

^a $F_{0.05; 6; 4} = 6.16$; $F_{0.05; 2; 2} = 19$ (F = Tabulated value from Fisher test). The mathematical models were considered significant ($p \leq 0.05$) when the regression F_{values} were higher than $F_{\text{tabulated}}$ and as predicted when the lack of fit F_{values} were lower than the $F_{\text{tabulated}}$ value. GAE: gallic acid equivalent. TPC: total phenolics content; DPPH: 2,2-diphenyl-1-picrylhydrazyl radical; GAE: gallic acid equivalent.

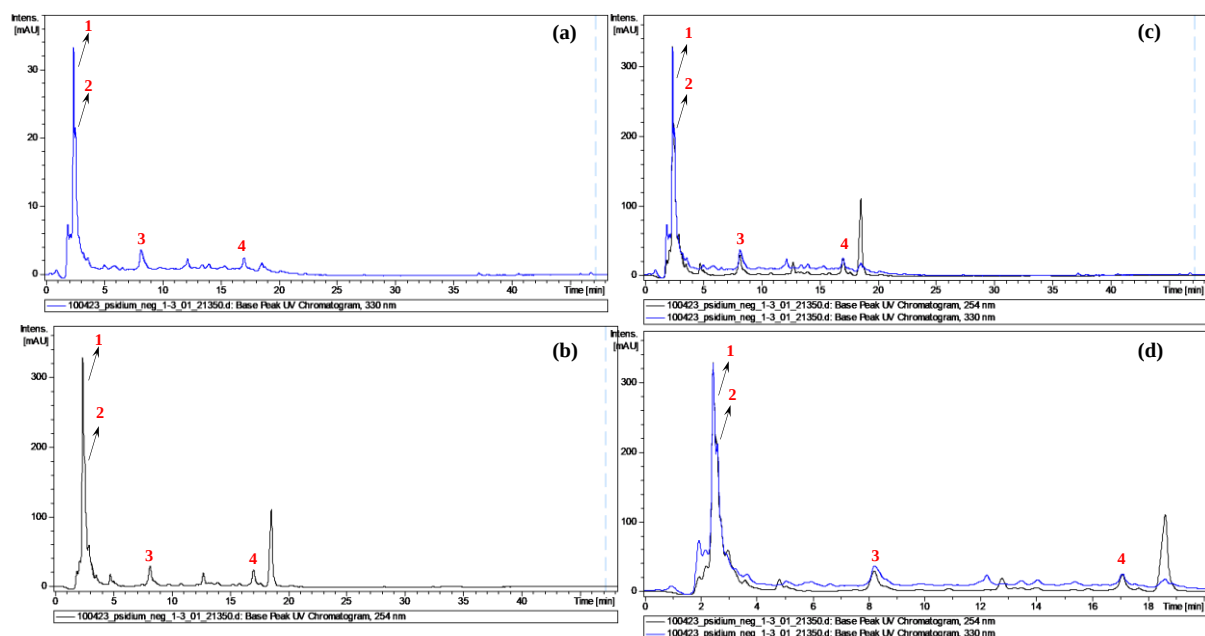


Figure S2. Chromatogram of the optimized extract of *Psidium guineense* fruits (a) = UV-Vis chromatogram at 330 nm; (b) = UV-Vis chromatogram at 254 nm; (c) = UV-Vis chromatogram superimposed at wavelengths of 254 nm (in black) and 330 nm (in blue); (d) = UV-Vis chromatogram expanded at times 0-20 min.

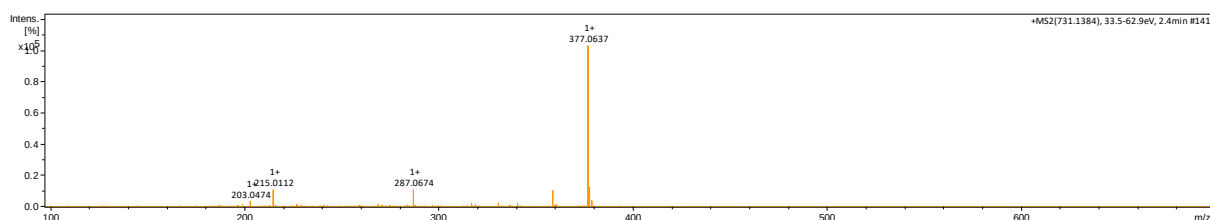


Figure S3. Mass spectrum of compound 1, caffeoylquinic acid.

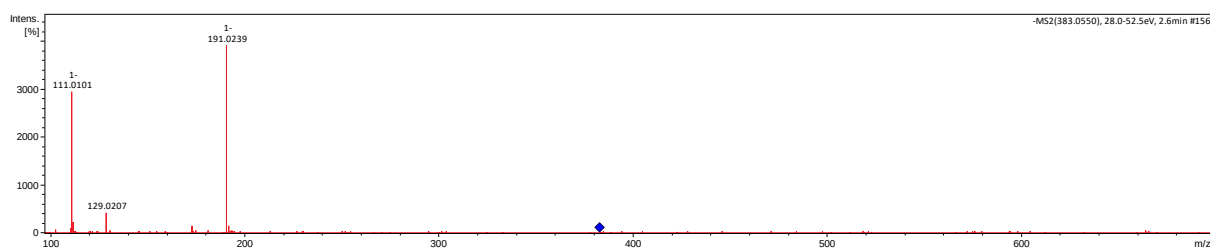


Figure S4. Mass spectrum of compound 2, quinic acid.

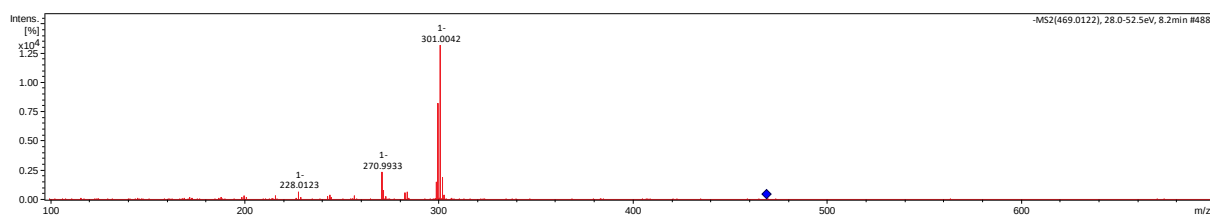


Figure S5. Mass spectrum of compound 3, dilactone valonic acid.

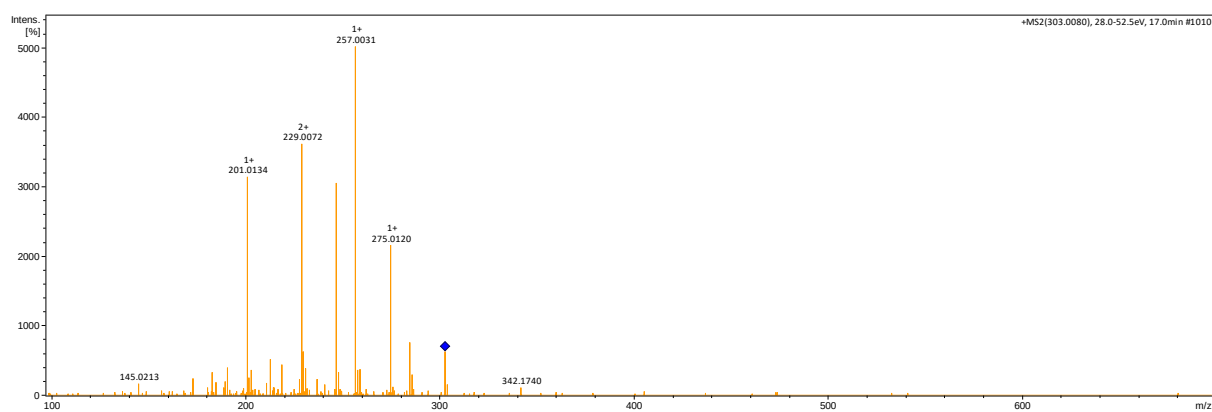


Figure S6. Mass spectrum of compound **4**, ellagic acid.