Supplementary material

Determination of Polyphenols in *Schinus terebinthifolius* Raddi bark extracts and chemometric analysis

Vitor Hugo Migues[a], Jorge Mauricio David*[a], Juceni Pereira David[a]*

[a] Instituto de Química, Universidade Federal da Bahia, 40170-290 - Salvador, BA, Brazil

* Corresponding author at: Instituto de Química, Universidade Federal da Bahia, 40170-290 - Salvador, BA, Brazil

E-mail address: jmdavid@ufba.br, juceni@ufba.br

Table 1S: Elution parameters of the polyphenolics employed in the chemical characterization of *S. terebinthifolius*

Standard	Rt	Wb	k	α	N	Rs
Gallic acid	9.97	0.345	1.00	3.23	13362,02	26.02
Catechin	21.12	0.512	3.25	1.54	27225.00	24.04
Chlorogenic acid	29.87	0.216	5.00	1.62	305972.87	64.04
*Epi*catechin	45.40	0.269	8.13	1.63	455750,47	89.58
Quercetin	71.02	0.303	13.28	1.01	879014.55	3.33
Rutin	71.89	0.219	13.45	1.02*	1724124.88	14.25*

* Where Rt=retention time of the peak; Wb=width of the peak base; k=retention factor; α=separation factor; N=number of theoretical plates and Rs=resolution.; * Values for the previous peak.

Table 2S. Summary of the ANOVA output for linear regression analysis by HPLC analyses.

Standard	$MS_{between}$	MS_{Within}	Fcalc	p-Value
EPI	1.14×10^3	7.91×10^2	1.45	0.248
GAL	2.44×10^9	1.51×10^9	1.61	0.205
QUE	9.87×10^{12}	3.42×10^{12}	2.88	0.06
RUT	3.69×10^2	1.38×10^2	2.67	0.06
CAT	1.38×10^4	7.30×10^3	1.89	0.150
CLO	1.43×10^3	9.27×10^2	1.54	0.224
MS = mean square; $F_{critic} = 2.90$				

Table 3S: Evaluation of method robustness by modifying the flow of the HPLC of *S. terebinthifolius* standards.

Compound	Flow(mLmin^{-1})	Conc. (%) (A1, A2, A3)	Average (%)	DP	DPR (%)
EPI	Proposed method	100.07	100.50	0.70	0.69
		101.30			
		100.12			
	1.2	100.06	100.11	0.22	0.22
		99.92			
		100.35			
	0.8	105.01	105.85	0.73	0.69
		106.32			
		106.22			
GAL	Proposed method	101.05	99.93	1.15	1.15
		98.76			
		99.99			
	1.2	108.05	104.21	4.02	3.85
		104.55			
		100.04			
	0.8	105.24	107.88	2.54	2.36
		100.31			
		100.09			
QUE	Proposed method	100.11	99.79	0.32	0.32
		99.48			
		99.77			
	1.2	105.21	104.83	0.53	0.51
		105.06			
		104.22			
	0.8	109.15	108.75	0.36	0.33

		108.45			
		108.66			
RUT	Proposed method	99.80	100.64	1.61	1.60
		99.63			
		102.49			
	1.2	105.14	105.49	1.07	1.01
		104.64			
		106.69			
	0.8	108.80	107.19	2.57	2.40
		108.56			
		104.23			
CAT	Proposed method	99.71	101.53	2.09	2.06
		101,06			
		103.81			
	1.2	104.89	106.10	1.48	1.39
		105.66			
		107.74			
	0.8	108.68	105.68	3.41	3.23
		106.39			
		101.97			
CLO	Proposed method	100.38	102.39	1.98	1.94
		102.44			
		104.35			
	1.2	105.28	106.73	1.47	1.38
		106.70			
		108.21			
	0.8	107.53	104.30	3.18	3.05
		104.18			
		101.18			

Table 4S: Values of "m", " b " e "R" obtained from linear regression of analytical curve.

Standard	m	b	R^2
EPI	0.0460	0.4478	0.9993
GAL	0.0681	0.1223	0.9939
QUE	0.0262	0.0999	0.9943
RUT	0.0519	0.4872	0.9951
CAT	0.1061	0.4934	0.9961
CLO	0.1825	1.6302	0.9979

Table 5S: Paired *t* Test for HPLC/DAD and UV applied for each analyte in *S. terebinthifolius.*

	GAL		CAT		CLO		EPI		CLO		RUT	
	HPLC	**UV**	**HPLC**	**UV**	**HPLC**	**UV**	**HPLC**	**UV**	**HPLC**	**UV**	**HPLC**	**UV**
Mean	3.727273	3.663636	5.681818	6.545455	6.572727	6.454545	3.890909	3.436364	6.527273	6.636364	3.227273	2.745455
Variance	0.132182	0.106545	0.791636	0.192727	0.114182	0.260727	0.654909	0.232545	0.370182	0.196545	0.772182	0.560727
Observations	11	11	11	11	11	11	11	11	11	11	11	11
Pearson correlations	0.119364		0.492182		0.187455		0.443727		0.283364		0.666455	
Hypothesized mean	0		0		0		0		0		0	
df	20		20		20		20		20		20	
T Stat	0.431967		-2.88702		0.640153		1.600297		-0.48062		1.384138	
P(T ≤ t) one-tail	0.335193		0.004557		0.26467		0.062605		0.318003		0.090784	
t Critic one-tail	1.724718		1.724718		1.724718		1.724718		1.724718		1.724718	
P(T ≤ t) two-tail	0.670387		0.009114		0.529339		0.125211		0.636005		0.181568	
t Critic two-tail	2.085963		2.085963		2.085963		2.085963		2.085963		2.085963	

Table 6S: Analyses of variance (ANOVA) from HPLC/DAD and UV determinations of the content of polyphenols in *S. terebinthifolius*.

Variation	gel	SQ	MQ	F	P - Valor	F significance meaning
Between groups	1	0.00216	0.028855	**0.010755***	0.04875	3.9139
Into the groups	130	348.7743	2.682879			
Total	139	348.8031				

* Significance $p < 0.05$
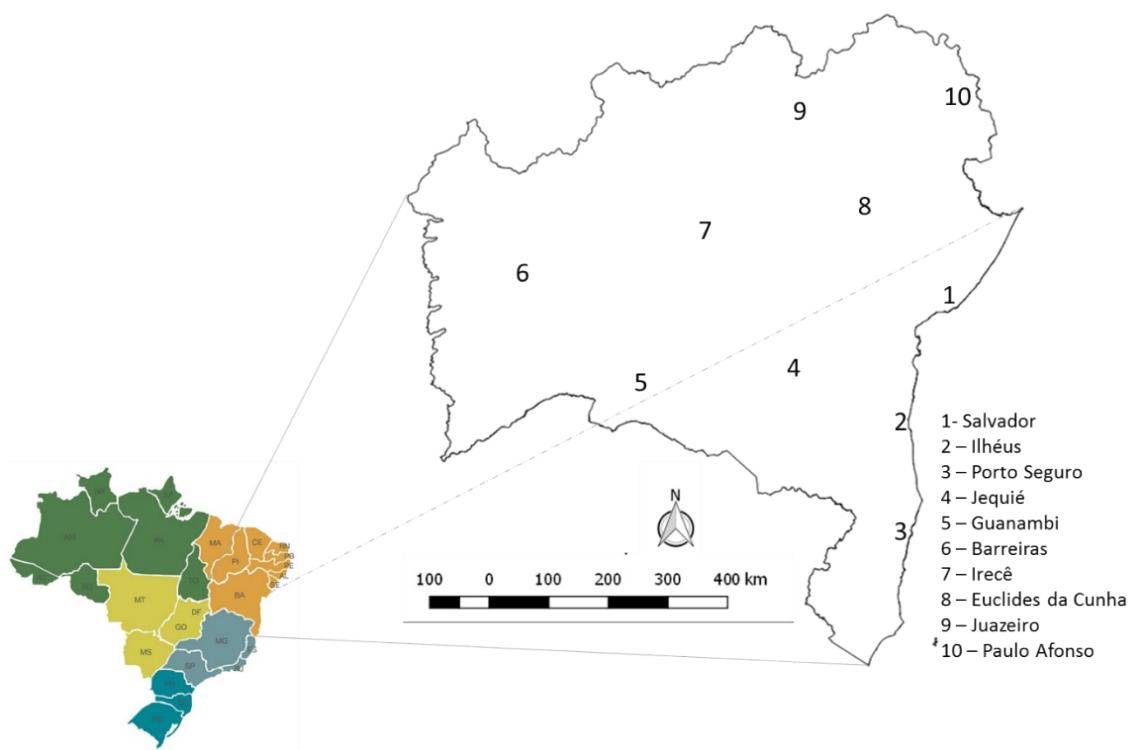
Figure 1S: Spots of *S. terebinthifolius* samples collect (Bahia State, Brazil)
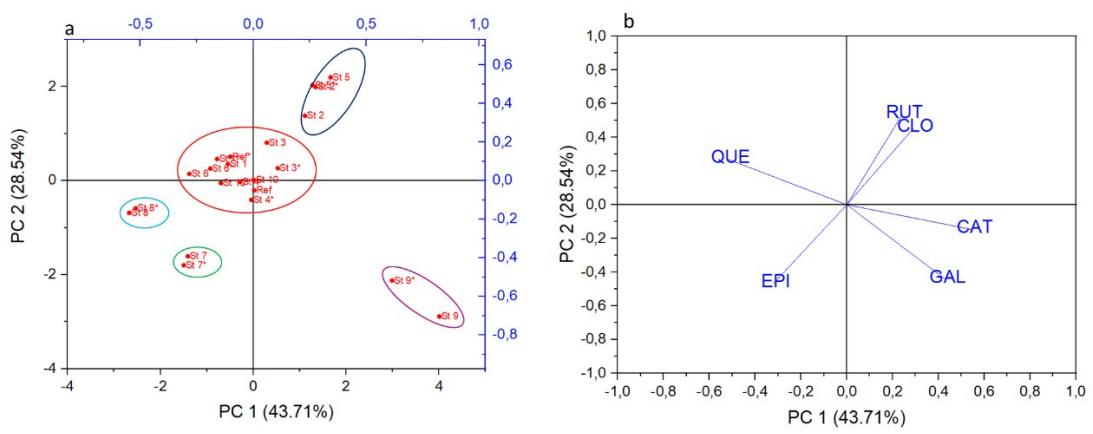
Figure 2S: Paired PCA of data obtained by UV and HPLC/DAD analysis in the samples of *S. terebinthifolius* by por PC1 e PC2. a) Dispersion diagram of samples in three groups (G1, G2, G3). b) Graphic loadings of the six analytes for PC1 and PC2.
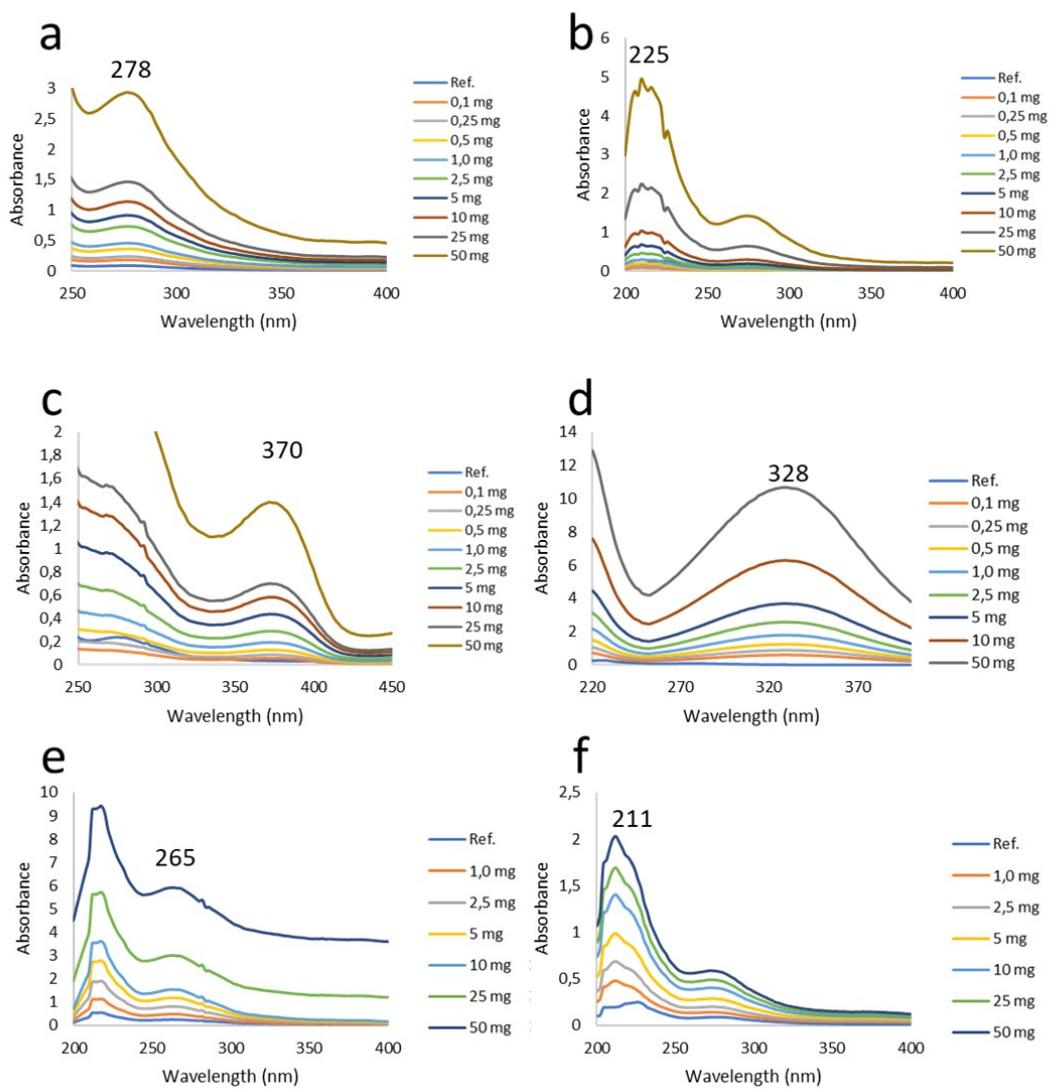
Figure 3S: UV spectra (200 a 400 nm) of samples of *S. terebinthifolius* with addition of different concentrations of standards. (a): *Epi*catechin, (b): gallic acid, (c): quercetin, (d): chlorogenic acid, (e): catechin and (f): rutin.