

Response of *Thymus lotocephalus* in vitro cultures to drought stress and role of green extracts in cosmetics

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Supplementary information

Table S1. HPLC-HRMS data of identified phenolics in *Thymus lotocephalus* López and Morales extracts.

Peak	Compound identity	Chemical formula	Theoretical exact mass [M-H] ⁻ (<i>m/z</i>)	Delta ppm (error)	RT (min)	MSI MI level*
1	Methyl 6-O-galloyl-β-D-glucopyranoside ^{a, 1}	C ₁₄ H ₁₈ O ₁₀	345.0793	-5.81	2.64	2
2	Protocatechuic aldehyde ^{d, 2}	C ₇ H ₆ O ₃	137.0239	0.07	3.96	2
3	Caffeic acid ^a	C ₉ H ₈ O ₄	179.0338	-0.14	4.81	1
4	Epigallocatechin gallate ^b	C ₂₂ H ₁₈ O ₁₁	457.0765	0.27	5.34	1
5	Salvianolic acid C ^{a, 3}	C ₁₈ H ₁₇ O ₉	377.0873	-0.74	5.37	2
6	Dihydromorelloflavone ^{b, 4}	C ₃₀ H ₂₂ O ₁₁	557.1083	0.13	5.37	2
7	Salviaflaside ^{a, 3}	C ₂₄ H ₂₆ O ₁₃	521.1288	0.12	8.1	2
8	Luteolin-7-O-glucuronide ^{b, 5}	C ₂₁ H ₁₈ O ₁₂	461.0714	-0.03	8.67	2
9	Salvianolic acid B /Salvianolic acid L isomer I ^{a, 3}	C ₃₆ H ₃₀ O ₁₆	717.1456	-2.62	9.22	2
10	Rosmarinic acid ^a	C ₁₈ H ₁₆ O ₈	359.0761	0.77	10	1
11	Theaflavic acid ^{b, 6}	C ₂₁ H ₁₆ O ₁₀	427.0636	-5.28	10.04	2
12	Sagerinic acid ^{a, 3}	C ₃₆ H ₃₂ O ₁₆	719.1612	-1.21	10.07	2
13	Salvianolic acid A isomer I ^{a, 3}	C ₂₆ H ₂₂ O ₁₀	493.1129	-0.76	10.6	2
14	Salvianolic acid A isomer II ^{a, 3}	C ₂₆ H ₂₂ O ₁₀	493.1129	0.36	11.47	2
15	Melitric acid A / Salvianolic acid I ^{a, 3}	C ₂₇ H ₂₂ O ₁₂	537.1034	-0.73	11.55	2
16	Salvianolic acid B /Salvianolic acid L isomer II ^{a, 3}	C ₃₆ H ₃₀ O ₁₆	717.1456	-0.58	11.63	2
17	Herniarin ^{c, 7}	C ₁₀ H ₈ O ₃	175.0389	-1.83	12.51	2
18	Methylrosmarinic acid isomer I ^{a, 3}	C ₁₉ H ₁₈ O ₈	373.0921	1.14	12.56	2
19	Salvianolic acid A isomer IV ^{a, 3}	C ₂₆ H ₂₂ O ₁₀	493.1129	-0.82	13.1	2
20	Salvianolic acid B /Salvianolic acid L isomer III ^{a, 3}	C ₃₆ H ₃₀ O ₁₆	717.1456	-0.59	13.16	2
21	Luteolin ^b	C ₁₅ H ₁₀ O ₆	285.0393	0.55	13.97	1
22	Methylrosmarinic acid isomer III ^{a, 3}	C ₁₉ H ₁₈ O ₈	373.0921	0.98	13.97	2
23	Melitric acid B ^{a, 3}	C ₂₇ H ₂₀ O ₁₁	519.0922	-0.63	14.3	2
24	Salvianolic acid B / Salvianolic acid L isomer IV ^{a, 3}	C ₃₆ H ₃₀ O ₁₆	717.1456	-0.50	14.34	2
25	Salvianolic acid F isomer I ^{a, 3}	C ₁₇ H ₁₃ O ₆	313.0712	1.61	14.6	2
26	Salvianolic acid F isomer II ^{a, 3}	C ₁₇ H ₁₃ O ₆	313.0712	0.15	15.26	2

*Metabolite standards initiative metabolite identification (MSI MI) levels. Reference standards were available for all compounds identified at MSI MI level 1. Class of compounds: ^aPhenolic acids; ^bFlavonoids; ^cCoumarin derivative; ^dHydroxybenzaldehydes. Results expressed as equivalents of gallic acid (1), protocatechuic acid (2), rosmarinic acid (3), quercetin (4), luteolin (5), catechin (6), *p* -coumaric acid (7).

Table S2. Summary of HPLC-HRMS criterion for quantification of phenolics in *Thymus lotocephalus* López and Morales extracts.

Compound	Linear range (mg/L)	Intercept	Slope	R ²	LOD (µg/L)	LOQ (µg/L)
Epigallocatechin gallate	3.12-50	-69150	21667	0.9976	228.13	760.46
Caffeic acid	0.05-8	209431	5791726	0.9999	0.95	3.16
Protocatechuic acid	0.05-10	150321	2058784	0.9995	3.92	13.06
Gallic acid	0.1-50	124985	3119019	0.9993	1.38	4.60
<i>p</i> -Coumaric acid	0.5-6	2090	84084	0.9979	43.91	146.38
Luteolin	0.03-91	7840120	-158687	0.9997	0.60	2.00
Quercetin	0.1-3.12	-1347970	9918400	0.9975	0.10	0.33
Catechin	0.8-25	-632768	2024864	0.9994	3.25	10.82
Rosmarinic acid	0.10-80	-2568152	1567304	0.9917	30.11	100.38

Table S3. $EE(\lambda) \times I(\lambda)$ constants used in the determination of SPF for each wavelength (Sayre et al., 1979)

Wavelength λ (nm)	$EE(\lambda) \times I(\lambda)$
290	0.0150
295	0.0817
300	0.2874
305	0.3278
310	0.1864
315	0.0837
320	0.0180

$EE(\lambda)$: erythral effect spectrum; $I(\lambda)$: solar intensity spectrum.