Ultrasonic-Assisted Extraction (UAE) and NADES Combination: A green strategy to Improve the Recovery of Phenolic Compounds from *Lavandula pedunculata* subsp. *lusitanica* (Chaytor) Franco

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Supplementary information

Table S1. HPLC-HRMS data of identified phenolic compounds from *Lavandula pedunculata* subsp. *lusitanica* extracts.

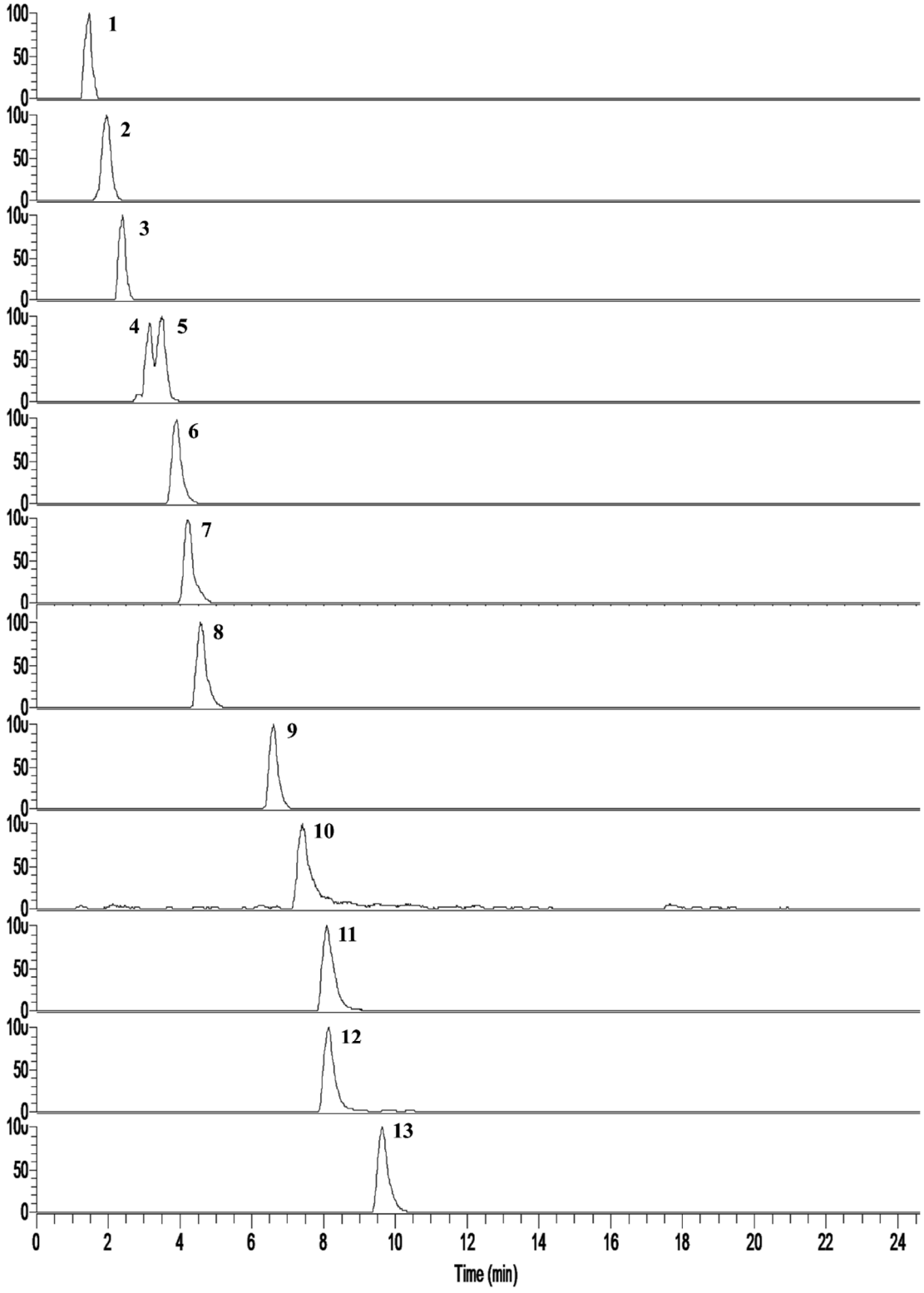
Peak	Compound identity	Chemical formula	Theoretical exact mass [M-H]$^-$ (*m/z*)	Delta ppm (error)	RT (min)	MSI MI level*
1	O-Caffeoylquinic acid[a]	$C_{16}H_{18}O_9$	353.0867	2.103	1.48	2
2	Gallic acid[b]	$C_7H_6O_5$	169.0131	-0.638	1.92	1
3	Vanillic acid[b]	$C_8H_8O_4$	167.0350	-2.606	2.37	2
4	Caffeic acid hexoside[a]	$C_{15}H_{18}O_9$	341.0867	-0.007	2.9	2
5	Caffeic acid hexoside[a]	$C_{15}H_{18}O_9$	341.0867	0.143	3.5	2
6	Chlorogenic acid (5-O-caffeoylquinic acid) [a]	$C_{16}H_{18}O_9$	353.0867	0.543	3.82	1
7	Fertaric acid[a]	$C_{14}H_{14}O_9$	325.0557	0.774	4.23	2
8	Caffeic acid[a]	$C_9H_8O_4$	179.0338	-0.604	4.59	1
9	Feruloyl hexose[a]	$C_{16}H_{20}O_9$	355.1028	1.187	6.60	2
10	Ferulic acid[a]	$C_{10}H_{10}O_4$	193.0495	-0.374	7.59	1
11	Luteolin-7-O-glucuronide[d]	$C_{21}H_{18}O_{12}$	461.0714	0.569	8.11	2
12	Luteolin-7-O-glucoside[d]	$C_{21}H_{20}O_{11}$	447.0929	1.660	8.12	2
13	Rosmarinic acid[a]	$C_{18}H_{16}O_8$	359.0761	0.488	9.57	1
14	Apigenin-7-O-glucoside[d]	$C_{21}H_{20}O_{10}$	431.0977	0.9594	9.72	2
15	Salvianolic acid A isomer I[a]	$C_{26}H_{22}O_{10}$	493.1129	0.508	10.11	2
16	Salvianolic acid A isomer II[a]	$C_{26}H_{22}O_{10}$	493.1129	0.358	10.97	2
17	Salvianolic acid I[a]	$C_{27}H_{22}O_{12}$	537.1027	1.499	11.13	2
18	Salvianolic acid B[a]	$C_{36}H_{30}O_{16}$	717.1450	-0.049	11.23	2
19	Apigenin-7-O-acetylglucoside[d]	$C_{23}H_{22}O_{11}$	473.1082	0.808	11.55	2
20	Herniarin[c]	$C_{10}H_8O_3$	175.0389	-0.429	12.14	2
21	Salvianolic acid A isomer III[a]	$C_{26}H_{22}O_{10}$	493.1129	-0.132	12.8	2
22	Luteolin[d]	$C_{15}H_{10}O_6$	285.0393	0.277	13.5	1
23	Naringenin[e]	$C_{15}H_{12}O_5$	271.0600	0.172	14.01	1
24	Apigenin[d]	$C_{15}H_{10}O_5$	269.0444	0.172	14.8	1

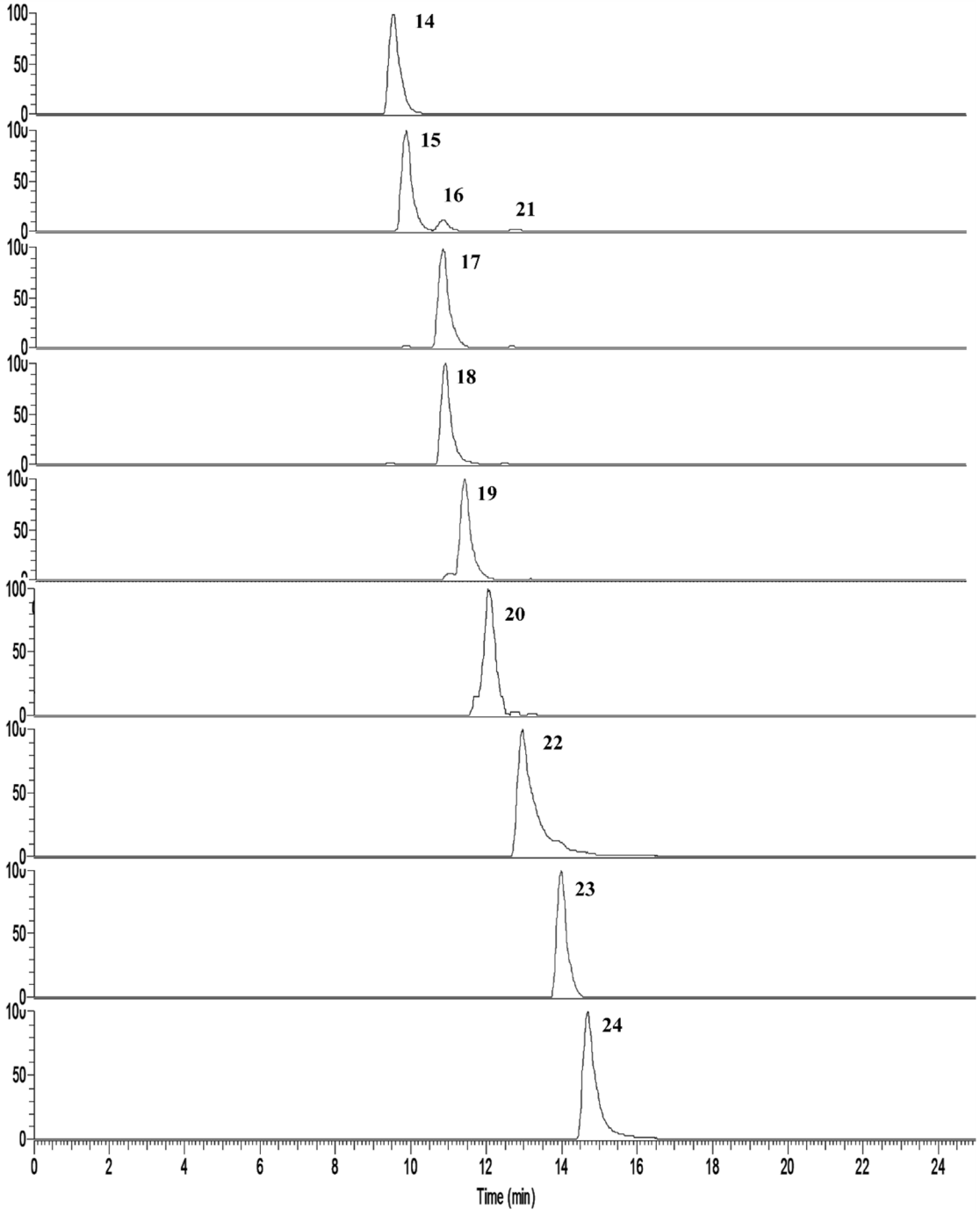
*Metabolite standards initiative metabolite identification (MSI MI) levels. Reference standards were available for all compounds identified at MSI MI level 1. Class of compounds: phenolic acids ([a]hydroxycinnamic acids and [b]hydroxybenzoic acids); [c]Coumarin derivative; flavonoids ([d]flavones and [e]flavanones).

Table S2. Summary of HPLC-HRMS parameters for quantification of phenolic compounds in *Lavandula pedunculata* subsp. *lusitanica* extracts.

Compound	Linear range (mg/L)	Intercept	Slope	R^2	LOD (mg/mL)	LOQ (mg/mL)
Rosmarinic acid	0.1-100	-103410	1598747	0.9992	0.06	0.19
Caffeic acid	0.1-10	1436398	3950274	0.9990	0.50	1.68
Ferulic acid	0.2-60	2487	9717	0.9995	0.37	1.25
Gallic acid	0.2-15	-330994	2547719	0.9998	0.00	0.01
Chlorogenic acid	0.2-15	-243627	1363025	0.9993	0.00	0.01
Luteolin	0.2-15	1464030	5454860	0.9990	0.29	0.96
Apigenin	0.2-15	185082	6649959	0.9995	0.00	0.01
Naringenin	0.2-15	-314843	2143048	0.9996	0.37	1.23
p-Coumaric acid	0.2-15	-2024	73034	0.9999	0.22	0.72

Figure S1. HPLC-HRMS extracted-ion chromatogram of phenolic compounds in *Lavandula pedunculata* subsp. *lusitanica* extracts obtained by ultrasound-assisted extraction for 60 min in combination with different NADES and conventional solvents. The compound name corresponding to each number of peaks can be consulted in Supplementary Table 1.

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