

Table 1 Different chemical composition of the raw and HPWS *C. officinalis* products.

		Formula	Mass (Da)	Adduct	Extraction Mass (Da)	Error (ppm)	RT (min)	t-value	p-value	changedirection
1	5-Hydroxymethylfurfural	C ₆ H ₆ O ₃	126.0317	[M+H] ⁺	127.03897	1.5	1.9	3.548359	0.00528	+
2	Dimethyl malate	C ₆ H ₁₀ O ₅	162.0528	[M-H] ⁻	161.04555	5.2	2.32	-4.381084	0.00138	-
3	3,4,6-tri-O-Galloyl-b-D-glucose	C ₂₇ H ₂₄ O ₁₈	636.0963	[M-H] ⁻	635.08899	4.5	3.87	-2.576338	0.02759	-
4	1,2,3-tri-O-Galloyl-b-D-glucose	C ₂₇ H ₂₄ O ₁₈	636.0963	[M-H] ⁻	635.08899	5.7	3.9	3.263964	0.00852	+
5	Tellimagrandin I	C ₃₄ H ₂₆ O ₂₂	786.0916	[M-H] ⁻	785.0843	5.8	4.54	2.879021	0.01641	+
6	7-O-Methyl-morroniside	C ₁₈ H ₂₈ O ₁₁	420.1632	[M-H] ⁻	419.15589	2.6	4.97	4.730597	0.0008	+
7	Caffeoyltartaric acid dimethyl ester	C ₁₅ H ₁₆ O ₉	340.0794	[M+H] ⁺	341.08671	0.1	5.01	5.844058	0.00016	+
8	Naringenin	C ₁₅ H ₁₂ O ₅	272.0685	[M+H] ⁺	273.07575	0.9	6.73	4.134988	0.00203	+
9	Kaempferol-3-O-β-D-rutinoside	C ₂₇ H ₃₀ O ₁₅	594.1585	[M+H] ⁺	595.16575	0.7	7.29	3.041758	0.01243	+
10	Oenothien C	C ₃₄ H ₂₄ O ₂₂	784.0759	[M+H] ⁺	785.0832	0.1	7.32	5.861379	0.00016	+
11	Quercetin	C ₁₅ H ₁₀ O ₇	302.0427	[M-H] ⁻	301.03538	6.9	10.42	-3.405739	0.00671	-
12	Apigenin	C ₁₅ H ₁₀ O ₅	270.0528	[M-H] ⁻	269.04555	7.1	11.59	4.657361	0.0009	+
13	ArjunglucosideII	C ₃₆ H ₅₈ O ₁₀	650.403	[M-H] ⁻	649.39572	2.5	11.72	3.264763	0.00851	+
14	Ethyl 2-hydroxytetradecanoate	C ₁₆ H ₃₂ O ₃	272.2352	[M-H] ⁻	271.22787	6.5	14	6.580312	6.23E-05	+
15	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	C ₁₅ H ₂₂ O ₂	234.162	[M-H] ⁻	233.1547	6.9	14.12	2.370131	0.03927	+

16	Maslinic acid	C ₃₀ H ₄₈ O ₄	472.3553	[M-H] ⁻	471.34798	5.6	14.16	9.815299	1.89E-06	+
17	Diisobutyl phthalate	C ₁₆ H ₂₂ O ₄	278.1518	[M+H] ⁺	279.15909	0.8	14.62	-8.161049	9.88E-06	-
18	9,12,15-Octadecatrienoic acid	C ₁₈ H ₃₀ O ₂	278.2246	[M+H] ⁺	279.23186	0.8	15.77	3.118799	0.0109	+
19	Ethyl (9E,12E,15E)-octadeca-9,12,15-trienoate	C ₂₀ H ₃₄ O ₂	306.2559	[M+H] ⁺	307.26316	-0.9	15.82	4.285773	0.0016	+
20	Ursolic acid	C ₃₀ H ₄₈ O ₃	456.3604	[M-H] ⁻	455.35307	6.1	16.06	-2.962918	0.01422	-
21	Betulic acid	C ₃₀ H ₄₈ O ₃	456.3604	[M-H] ⁻	455.35307	6.1	16.06	-2.962918	0.01422	-
22	Oleanolic acid	C ₃₀ H ₄₈ O ₃	456.3604	[M-H] ⁻	455.35307	5.6	16.07	-2.962918	0.01422	-
23	Cistanoside H	C ₁₆ H ₃₀ O ₂	254.2246	[M-H] ⁻	253.2173	5.7	16.27	4.714915	0.00082	+
24	Palmitoleic acid	C ₁₆ H ₃₀ O ₂	254.2246	[M-H] ⁻	253.2173	3.9	16.27	4.714915	0.00082	+
25	Linoleic acid	C ₁₈ H ₃₂ O ₂	280.2402	[M-H] ⁻	279.23295	7	16.54	10.40155	1.11E-06	+
26	Z,Z-10,12-Hexadecadien-1-ol acetate	C ₁₈ H ₃₂ O ₂	280.2402	[M-H] ⁻	279.23295	7	16.54	10.40155	1.11E-06	+
27	Linoelaidic acid	C ₁₈ H ₃₂ O ₂	280.2402	[M-H] ⁻	279.23295	4.6	16.55	10.40155	1.11E-06	+
