

Extraction of *T. cordifolia* (Thunb.) by multiple solvents to investigate phytochemical recovery by LC-MS and greenness evaluation by AGREEprep and AGREE

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Supplementary Tables

Table S1 — Secondary metabolites detected by LC-MS/MS in chloroform extract of *T. cordifolia* stem

S. No.	Retention time (R _t)	Ionisation mode	Secondary metabolites	Mol. Wt.	precursor <i>m/z</i> values
1	0.88	(-) ve	Tinosporine, C ₂₀ H ₂₂ O ₆	406.16	407.18 [M-H] ⁺
2	1.62	(+) ve	Magnoflorine, C ₂₀ H ₂₄ NO ₄	342.45	343.17 [M-H] ⁺
3	2.97	(+) ve	Tinosporaside, C ₂₅ H ₃₂ O ₁₀	492.52	491.42 [M-H] ⁻
4	7.82	(-) ve	Berberine, C ₂₀ H ₁₈ NO ₄	336.41	337.12 [M-H] ⁺
5	7.83	(+) ve	Berberine, C ₂₀ H ₁₈ NO ₄	336.41	337.12 [M-H] ⁺
6	8.70	(+) ve	Tembetarine, C ₂₀ H ₂₆ NO ₄	344.43	345.23 [M-H] ⁺
7	9.17	(-) ve	Sinapic acid, C ₁₁ H ₁₂ O ₅	224.21	225.32 [M-H] ⁺
8	9.94	(+) ve	Tinosporaside, C ₂₅ H ₃₂ O ₁₀	492.51	493.25 [M-H] ⁺
9	10.89	(-) ve	Beta-sitosterol, C ₂₉ H ₅₀ O	414.71	415.36 [M-H] ⁺
10	10.94	(+) ve	Tinosporide, C ₂₀ H ₂₂ O ₇	374.43	375.65 [M-H] ⁺
11	11.33	(+) ve	Ecdyson, C ₂₇ H ₄₄ O ₆	464.63	464.35 [M-H] ⁺
12	11.88	(-) ve	Berberine, C ₂₀ H ₁₈ NO ₄	336.41	335.41 [M-H] ⁻
13	13.07	(-) ve	Choline, C ₅ H ₁₄ NO ₄	104.17	103.21 [M-H] ⁻
14	13.88	(-) ve	Choline, C ₅ H ₁₄ NO ₄	104.17	103.21 [M-H] ⁻
15	15.32	(-) ve	Beta-sitosterol, C ₂₉ H ₅₀ O	414.73	415.62 [M-H] ⁺
16	15.44	(+) ve	Jatrorrhizine, C ₂₀ H ₂₀ NO ₄	338.42	339.51 [M-H] ⁺
17	22.36	(-) ve	Tinocordifolin, C ₁₅ H ₂₂ O ₃	250.33	249.34 [M-H] ⁻
18	22.81	(+) ve	Jatrorrhizine, C ₂₀ H ₂₀ NO ₄	338.41	339.45 [M-H] ⁺
19	23.00	(+) ve	Tinocordifolin, C ₁₅ H ₂₂ O ₃	250.33	251.34 [M-H] ⁺
20	23.41	(-) ve	Tembetarine, C ₂₀ H ₂₆ NO ₄	344.29	343.25 [M-H] ⁻
21	29.10	(-) ve	Tinocordifolioside, C ₂₁ H ₃₂ O ₈	412.53	413.25 [M-H] ⁺

Table S2 — Secondary metabolites detected by LC-MS/MS in ethyl acetate extract of *T. cordifolia* stem

S. No.	Retention time (R _t)	Ionisation mode	Secondary metabolites	Mol. Wt.	precursor <i>m/z</i> values
1	1.22	(+) ve	Magnoflorine, C ₂₀ H ₂₄ NO ₄	342.45	343.17 [M-H] ⁺
2	1.30	(-) ve	Tinosporaside, C ₂₅ H ₃₂ O ₁₀	492.52	493.25 [M-H] ⁺
3	2.60	(-) ve	Tembetarine, C ₂₀ H ₂₆ NO ₄	344.41	343.21 [M-H] ⁻
4	2.70	(+) ve	Octacosanol, C ₂₈ H ₅₈ O ₁	410.81	411.78 [M-H] ⁺
5	7.88	(+) ve	Berberine, C ₂₀ H ₁₈ NO ₄	336.42	335.41 [M-H] ⁻
6	7.89	(-) ve	Berberine, C ₂₀ H ₁₈ NO ₄	336.43	337.41 [M-H] ⁺
7	11.46	(+) ve	Choline, C ₅ H ₁₄ NO ₄	104.17	105.21 [M-H] ⁺
8	11.47	(-) ve	Ecdyson, C ₂₇ H ₄₄ O ₆	464.63	465.32 [M-H] ⁺
9	12.20	(+) ve	Kaempferol, C ₁₅ H ₁₀ O ₆	286.23	285.32 [M-H] ⁻
10	13.20	(-) ve	Cordioside, C ₂₆ H ₃₄ O ₁₂	538.55	539.24 [M-H] ⁺
11	18.33	(-) ve	Palmatoside, C ₂₅ H ₃₂ O ₁₀	492.12	491.13 [M-H] ⁻
12	19.46	(+) ve	Palmatine, C ₂₁ H ₂₂ NO ₄	352.14	353.26 [M-H] ⁺
13	21.75	(-) ve	Clerodane, C ₂₀ H ₃₈	278.51	279.35 [M-H] ⁺
14	22.96	(+) ve	Ecdysterone, C ₂₇ H ₄₄ O ₇	480.54	479.36 [M-H] ⁻
15	23.30	(-) ve	Tinosponone, C ₁₉ H ₂₂ O ₅	330.43	331.71 [M-H] ⁻
16	23.39	(+) ve	Tinosporine, C ₂₀ H ₂₂ O ₆	388.76	387.36 [M-H] ⁻
17	23.80	(-) ve	Clerodane, C ₂₀ H ₃₈	278.51	279.36 [M-H] ⁺
18	28.63	(-) ve	Cordioside, C ₂₆ H ₃₄ O ₁₂	538.55	539.37 [M-H] ⁺
19	29.13	(-) ve	Tinosporide, C ₂₀ H ₂₂ O ₇	374.38	373.23 [M-H] ⁻
20	29.24	(+) ve	Beta-sitosterol, C ₂₉ H ₅₀ O	414.71	413.32 [M-H] ⁻
21	30.40	(-) ve	Sinapic acid, C ₁₁ H ₁₂ O ₅	224.21	223.32[M-H] ⁻
22	30.87	(-) ve	Sinapic acid, C ₁₁ H ₁₂ O ₅	224.21	225.32 [M-H] ⁺

Table S3 — Secondary metabolites detected by LC-MS/MS in methanolic extract of *T. cordifolia* stem

S. No.	Retention time (R _t)	Ionisation mode	Secondary metabolites	Mol. Wt.	Precursor <i>m/z</i> values
1	0.87	(+) ve	Tinosporine, C ₂₀ H ₂₂ O ₆	388.76	387.36 [M-H] ⁺
2	0.95	(-) ve	Tinosporine, C ₂₀ H ₂₂ O ₆	388.76	387.36 [M-H] ⁺
3	1.27	(-) ve	Magnoflorine, C ₂₀ H ₂₄ NO ₄	342.43	343.17 [M-H] ⁺
4	1.28	(+) ve	Tinosporaside, C ₂₅ H ₃₂ O ₁₀	492.51	493.25 [M-H] ⁺
5	2.38	(+) ve	Tinosporide, C ₂₀ H ₂₂ O ₇	374.38	373.23 [M-H] ⁻
6	3.19	(-) ve	Jatrorrhizine, C ₂₀ H ₂₀ NO ₄	338.44	339.41 [M-H] ⁺
7	4.26	(+) ve	Octacosanol, C ₂₈ H ₅₈ O ₁	410.84	411.78 [M-H] ⁺
8	5.40	(-) ve	Stigmastertol, C ₂₉ H ₄₈ O	412.69	411.43 [M-H] ⁻
9	6.45	(+) ve	Cordioside, C ₂₆ H ₃₄ O ₁₂	538.55	537.36 [M-H] ⁻
10	7.82	(+) ve	Berberine, C ₂₀ H ₁₈ NO ₄	336.43	335.41 [M-H] ⁻
11	7.88	(-) ve	Ecdyson, C ₂₇ H ₄₄ O ₆	464.63	465.36 [M-H] ⁺
12	8.73	(+) ve	Berberine, C ₂₀ H ₁₈ NO ₄	336.45	335.41 [M-H] ⁻
13	10.29	(-) ve	Beta-sitosterol, C ₂₉ H ₅₀ O	414.71	413.32 [M-H] ⁻
14	10.34	(+) ve	Kaempferol, C ₁₅ H ₁₀ O ₆	286.23	287.24 [M-H] ⁺
15	10.95	(+) ve	Tinosporide, C ₂₀ H ₂₂ O ₇	374.38	373.23 [M-H] ⁻
16	12.85	(+) ve	Cordifolioside A, C ₂₂ H ₃₂ O ₁₃	504.52	505.23 [M-H] ⁺
17	12.86	(-) ve	Cordifolioside B, C ₂₂ H ₃₂ O ₁₃	504.52	505.32 [M-H] ⁺
18	13.73	(-) ve	Cordifolioside A, C ₂₂ H ₃₂ O ₁₃	504.52	503.32 [M-H] ⁻
19	14.86	(-) ve	Heptacosanol, C ₂₇ H ₅₆ O	396.71	397.35 [M-H] ⁺
20	22.41	(-) ve	Tinocordifolin, C ₁₅ H ₂₂ O ₃	250.33	251.48 [M-H] ⁺
21	22.44	(+) ve	Tinosponone, C ₁₉ H ₂₂ O ₅	330.42	331.54 [M-H] ⁺
22	23.57	(-) ve	Ecdysterone, C ₂₇ H ₄₄ O ₇	480.61	481.36 [M-H] ⁺
23	23.91	(-) ve	Clerodane, C ₂₀ H ₃₈	278.52	279.65 [M-H] ⁺
24	28.64	(-) ve	Cordioside, C ₂₆ H ₃₄ O ₁₂	538.55	539.37 [M-H] ⁺
25	29.11	(-) ve	Tinocordifolioside, C ₂₁ H ₃₂ O ₈	412.51	413.65 [M-H] ⁺
26	30.51	(-) ve	Tinocordioside, C ₂₁ H ₃₂ O ₇	396.52	397.54 [M-H] ⁺

Table S4 — Secondary metabolites detected by LC-MS/MS in water extract of *T. cordifolia* stem

S. No.	Retention time (R _t)	Ionisation mode	Secondary metabolites	Mol. Wt.	precursor <i>m/z</i> values
1	1.01	(-) ve	Magnoflorine, C ₂₀ H ₂₄ NO ₄	342.41	343.25 [M-H] ⁺
2	1.37	(+) ve	Magnoflorine, C ₂₀ H ₂₄ NO ₄	342.41	341.26 [M-H] ⁻
3	1.71	(+) ve	Tinosporine, C ₂₀ H ₂₂ O ₆	388.76	387.36 [M-H] ⁻
4	2.13	(+) ve	Beta-sitosterol, C ₂₉ H ₅₀ O	414.73	415.36 [M-H] ⁺
5	3.53	(-) ve	Berberine, C ₂₀ H ₁₈ NO ₄	336.45	335.63 [M-H] ⁻
6	3.59	(+) ve	Jatrorrhizine, C ₂₀ H ₂₀ NO ₄	338.42	337.61 [M-H] ⁻
7	4.32	(+) ve	Cordifolioside E, C ₂₂ H ₃₂ O ₁₃	504.52	505.36 [M-H] ⁺
8	7.88	(+) ve	Cordioside, C ₂₆ H ₃₄ O ₁₂	538.55	537.68 [M-H] ⁻
9	8.15	(-) ve	Stigmastertol, C ₂₉ H ₄₈ O	412.69	411.36 [M-H] ⁻
10	8.77	(+) ve	Beta-sitosterol, C ₂₉ H ₅₀ O	414.47	413.36 [M-H] ⁻
11	10.29	(-) ve	Cordifolioside A, C ₂₂ H ₃₂ O ₁₃	504.52	505.34 [M-H] ⁺
12	11.30	(+) ve	Cordifolioside C, C ₂₂ H ₃₂ O ₁₃	504.52	503.32 [M-H] ⁻
13	12.86	(+) ve	Sinapic acid, C ₁₁ H ₁₂ O ₅	224.21	225.36 [M-H] ⁺
14	12.87	(-) ve	Stigmastertol, C ₂₉ H ₄₈ O	412.69	413.23 [M-H] ⁺
15	14.52	(-) ve	Clerodane, C ₂₀ H ₃₈	278.51	277.65 [M-H] ⁻
16	15.19	(+) ve	Cordifolioside B, C ₂₂ H ₃₂ O ₁₃	504.53	505.36 [M-H] ⁺
17	19.64	(-) ve	Makisterone, C ₂₈ H ₄₆ O ₇	494.47	495.36 [M-H] ⁺
18	23.20	(-) ve	Cordifolioside D, C ₂₂ H ₃₂ O ₁₃	504.52	505.36 [M-H] ⁺
19	23.52	(-) ve	Palmatine, C ₂₁ H ₂₂ NO ₄	352.14	351.37 [M-H] ⁻
20	23.76	(-) ve	Tinocordioside, C ₂₁ H ₃₂ O ₇	396.5	397.36 [M-H] ⁺
21	24.26	(+) ve	Clerodane, C ₂₀ H ₃₈	278.52	277.46 [M-H] ⁻
22	28.40	(+) ve	Tinosporide, C ₂₀ H ₂₂ O ₇	374.38	375.36 [M-H] ⁺
23	28.63	(-) ve	Giloin, C ₂₅ H ₃₂ O ₁₀	492.58	493.65 [M-H] ⁺
24	29.12	(-) ve	Tinocordifolioside, C ₂₁ H ₃₂ O ₈	412.51	413.26 [M-H] ⁺
25	29.19	(+) ve	Ecdyson, C ₂₇ H ₄₄ O ₆	464.63	463.32 [M-H] ⁻
26	31.12	(-) ve	Palmatoside, C ₂₆ H ₃₂ O ₁₂	536.52	537.63 [M-H] ⁺