

ORIGINAL RESEARCH ARTICLE

Antibacterial potential, phytochemical constituents, and toxicity assessment of *Azadirachta indica* leaf extracts in combination with antibiotics

Supplementary File

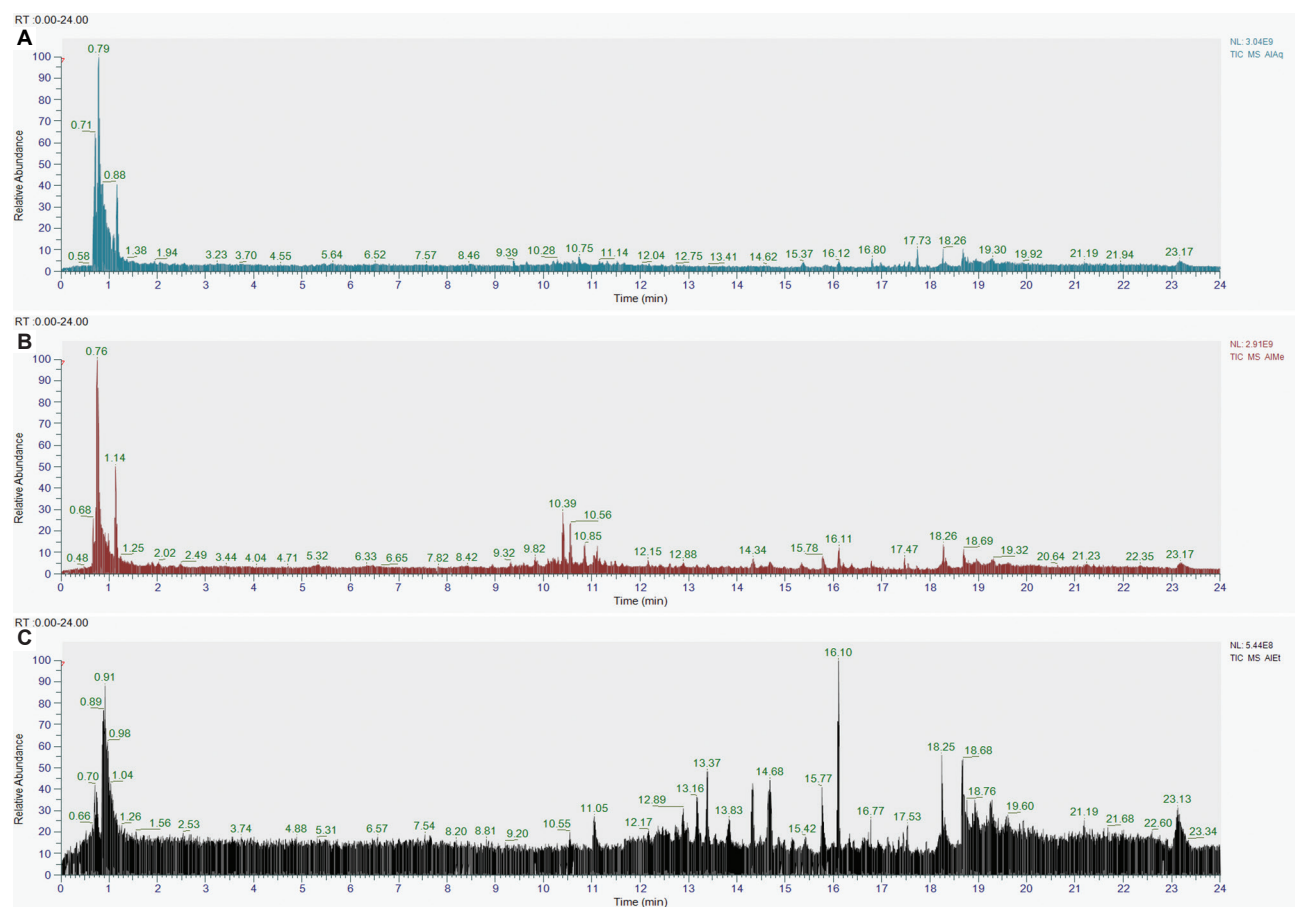


Figure S1. Liquid chromatography–mass spectrometry total compound chromatograms of (A) AzI-Aq (*Azadirachta indica* aqueous), (B) AzI-MeOH (*A. indica* methanol), and (C) AzI-EtOAc (*A. indica* ethyl acetate) extracts

Table S1. Liquid chromatography–mass spectrometry putative identification and % relative abundance of phytochemicals identified in the aqueous (AQ), methanol (MeOH) and ethyl acetate (EtOAc) leaf extracts of *Azadirachta indica*

Retention time (minutes)	Molecular weight	Empirical formula	Putative compounds	Relative abundance (% of total area)		
				AQ (%)	MeOH (%)	EtOAc (%)
1.622	192.06319	C ₇ H ₁₂ O ₆	D-(-)-Quinic acid	0.12	0.17	-
1.633	129.04252	C ₅ H ₇ N O ₃	4-Oxoproline	0.04	0.26	0.98
1.648	356.0376	C ₁₄ H ₁₂ O ₁₁	(+)-Chebulic acid	0.24	-	-
1.671	134.02139	C ₄ H ₆ O ₅	D-(+)-Malic acid	-	5.76	-
1.772	118.02651	C ₄ H ₆ O ₄	Succinic acid	6.35	0.33	-
1.81	393.16326	C ₁₆ H ₂₇ N O ₁₀	6'-Apiosyllotaustralin	-	0.10	-
1.838	272.05304	C ₁₁ H ₁₂ O ₈	Fukiic acid	-	1.03	-
1.855	128.04717	C ₆ H ₈ O ₃	Osmundalactone	0.07	-	-
1.871	376.13673	C ₁₆ H ₂₄ O ₁₀	Mussaenosidic acid	-	0.02	-
1.881	322.03203	C ₁₄ H ₁₀ O ₉	Digallic acid	0.06	-	-
1.893	332.07405	C ₁₃ H ₁₆ O ₁₀	6-Galloylglucose	0.11	0.08	-
1.911	131.09457	C ₆ H ₁₃ N O ₂	L-Isoleucine	-	0.24	1.03
1.973	126.03156	C ₆ H ₆ O ₃	Pyrogallol	-	0.52	-
2.092	244.06936	C ₉ H ₁₂ N ₂ O ₆	Uridine	-	-	0.76
2.114	112.05231	C ₆ H ₈ O ₂	Sorbic acid	0.02	0.03	-
2.215	244.05813	C ₁₀ H ₁₂ O ₇	1-O-Galloyllycerol	-	0.11	-
2.857	210.0374	C ₆ H ₁₀ O ₈	D-Saccharic acid	8.28	-	-
2.859	372.06918	C ₁₅ H ₁₆ O ₁₁	2-O-caffeoylglucaric acid	0.40	-	-
2.928	484.08511	C ₂₀ H ₂₀ O ₁₄	Hamamelitannin	-	0.01	-
3.215	340.07946	C ₁₅ H ₁₆ O ₉	Aesculin	-	S	-
3.238	324.1782	C ₁₄ H ₂₈ O ₈	Caryophyllan	0.04	-	-
3.25	228.14716	C ₁₁ H ₂₀ N ₂ O ₃	Leucylproline	0.04	-	-
3.504	306.07383	C ₁₅ H ₁₄ O ₇	(+)-Gallocatechin	-	0.02	-
3.385	212.06823	C ₁₀ H ₁₂ O ₅	Propyl gallate	-	-	0.87
3.953	189.04237	C ₁₀ H ₇ N O ₃	Kynurenic acid	0.56	0.61	-
3.962	154.0264	C ₇ H ₆ O ₄	Gentisic acid	0.07	0.08	-
4.292	484.08512	C ₂₀ H ₂₀ O ₁₄	1,6-Bis-O-(3,4,5-trihydroxybenzoyl) hexopyranose	-	0.14	-
4.679	388.13699	C ₁₇ H ₂₄ O ₁₀	Geniposide	0.02	0.04	-
5.428	178.02645	C ₉ H ₆ O ₄	Aesculetin	-	0.03	-
5.5	168.0421	C ₈ H ₈ O ₄	4-Methoxysalicylic acid	-	0.17	-
5.618	258.14656	C ₁₃ H ₂₂ O ₅	Trans-7,9-dihydroxy-3-methyl-8-oxo-dodecan-4-olide	0.15	-	-
6.89	192.02685	C ₆ H ₈ O ₇	Citric acid	0.24	0.15	-
7.114	196.07336	C ₁₀ H ₁₂ O ₄	Cantharidin	0.08	0.08	-
8.728	288.08412	C ₁₂ H ₁₆ O ₈	Phlorin	0.02	-	-
9.117	294.09484	C ₁₁ H ₁₈ O ₉	Tuliposide B	S	-	-
9.18	264.12079	C ₁₁ H ₂₀ O ₇	2-Hydroxy-2-methyl-3-buten-1-yl β-D-glucopyranoside	0.13	0.13	-
9.125	478.07395	C ₂₁ H ₁₈ O ₁₃	6-Hydroxyluteolin 6-glucuronide	-	S	-
9.559	596.17414	C ₂₇ H ₃₂ O ₁₅	Hovetrichoside D	0.03	-	-
9.677	478.07486	C ₂₁ H ₁₈ O ₁₃	8-Hydroxyluteolin 8-glucuronide	-	0.03	-

(Cont'd...)

Table S1. (Continued)

Retention time (minutes)	Molecular weight	Empirical formula	Putative compounds	Relative abundance (% of total area)		
				AQ (%)	MeOH (%)	EtOAc (%)
9.72	208.03693	C ₁₀ H ₈ O ₅	6,8-Dihydroxy-3-hydroxymethylisocoumarin	-	0.02	
9.758	342.13117	C ₁₆ H ₂₂ O ₈	Coniferin	-	S	
9.853	206.04251	C ₇ H ₁₀ O ₇	2-Methylcitric acid	0.04	-	
9.871	164.04731	C ₉ H ₈ O ₃	2-Hydroxycinnamic acid	0.58	0.09	
9.996	610.15321	C ₂₇ H ₃₀ O ₁₆	Rutin	0.01	10.23	1.27
10.069	259.99811	C ₉ H ₈ O ₇ S	Caffeic acid 3-O-sulfate	S	-	
10.211	224.06838	C ₁₁ H ₁₂ O ₅	Sinapinic acid	0.06	0.06	
10.216	304.05805	C ₁₅ H ₁₂ O ₇	Nigrescin	S	0.10	
9.758	342.13117	C ₁₆ H ₂₂ O ₈	Coniferin	-	S	
10.252	636.0961	C ₂₇ H ₂₄ O ₁₈	1,2,6-Trigalloyl-β-D-glucopyranose	-	0.58	
10.253	126.03153	C ₆ H ₆ O ₃	Maltol	-	0.04	
10.331	280.09338	C ₁₄ H ₁₆ O ₆	Gravolenic acid	0.03	-	
10.384	522.20996	C ₂₆ H ₃₄ O ₁₁	Isolariciresinol 9-O-β-D-glucoside	S	-	
10.438	402.15291	C ₁₈ H ₂₆ O ₁₀	Benzyl β-primeveroside	0.03	-	
10.468	490.205	C ₂₂ H ₃₄ O ₁₂	Cymorcin diglucoside	0.02	-	
10.494	450.11711	C ₂₁ H ₂₂ O ₁₁	Hovetrichoside C	0.02	-	
10.58	610.15312	C ₂₇ H ₃₀ O ₁₆	Quercetin 3-O-rhamnoside-7-O-glucoside	0.02	-	
10.645	242.0788	C ₁₁ H ₁₄ O ₆	Genipinic acid	0.03	-	
10.66	434.04844	C ₁₉ H ₁₄ O ₁₂	Ellagic acid arabinoside	S	-	
10.672	290.09988	C ₁₂ H ₁₈ O ₈	Osmundalin	S	-	
10.679	222.0526	C ₁₁ H ₁₀ O ₅	Isofraxidin	S	-	
10.706	480.09005	C ₂₁ H ₂₀ O ₁₃	myricetin 3-O-β-D-galactopyranoside	-	0.95	
10.731	284.10442	C ₁₇ H ₁₆ O ₄	Isoliquiritigenin 4,4'-dimethyl ether	S	-	
10.75	610.15306	C ₂₇ H ₃₀ O ₁₆	Aureusidin 4,6-diglucoside	S	-	
10.784	338.09999	C ₁₆ H ₁₈ O ₈	3-O-p-Coumaroylquinic acid	-	S	
10.869	192.04216	C ₁₀ H ₈ O ₄	7-Hydroxy-6-methoxy-2H-chromen-2-one	1.32	0.55	9.26
10.885	302.00606	C ₁₄ H ₆ O ₈	Ellagic acid	1.93	4.17	
10.89	312.12068	C ₁₅ H ₂₀ O ₇	p-Coumaryl alcohol 4-glucoside	0.03	-	
10.893	318.00087	C ₁₄ H ₆ O ₉	flavellagic acid	0.02	-	
10.931	254.07899	C ₁₂ H ₁₄ O ₆	Balticol C	0.02	-	
10.955	568.21535	C ₂₇ H ₃₆ O ₁₃	Citrusin B	0.04	-	
10.965	192.04212	C ₁₀ H ₈ O ₄	Scopoletin	-	1.06	
10.971	190.13559	C ₁₃ H ₁₈ O	Heptanophenone	0.07	-	1.67
10.974	388.20955	C ₁₉ H ₃₂ O ₈	Dihydroseoside	0.61	0.82	
10.987	286.04744	C ₁₅ H ₁₀ O ₆	Maritimetin	0.02	-	
11.06	550.20385	C ₂₇ H ₃₄ O ₁₂	Tracheloside	-	0.02	
11.018	174.08911	C ₈ H ₁₄ O ₄	Suberic acid	0.03	0.03	
11.025	580.21571	C ₂₈ H ₃₆ O ₁₃	(+)-7-epi-Syringaresinol 4'-glucoside	S	-	
11.026	418.16258	C ₂₂ H ₂₆ O ₈	Lirioresinol A	S	-	
11.026	176.04729	C ₁₀ H ₈ O ₃	4-Methylumbelliferone hydrate	0.28	-	

(Cont'd...)

Table S1. (Continued)

Retention time (minutes)	Molecular weight	Empirical formula	Putative compounds	Relative abundance (% of total area)		
				AQ (%)	MeOH (%)	EtOAc (%)
11.066	262.04771	C ₁₃ H ₁₀ O ₆	Maclurin	S	S	
11.103	524.22562	C ₂₆ H ₃₆ O ₁₁	Mascaroside	0.09	-	
11.135	304.05816	C ₁₅ H ₁₂ O ₇	(2R,3R)-Taxifolin	0.03	-	
11.233	464.09493	C ₂₁ H ₂₀ O ₁₂	Hyperoside	-	1.41	
11.287	196.10975	C ₁₁ H ₁₆ O ₃	Angupyron E	0.15	-	
11.287	464.09536	C ₂₁ H ₂₀ O ₁₂	Myricitrin	0.61	6.71	
11.348	312.12097	C ₁₅ H ₂₀ O ₇	Nivalenol	-	S	
11.42	126.03156	C ₆ H ₆ O ₃	Phloroglucinol	0.16	0.16	
11.445	522.2101	C ₂₆ H ₃₄ O ₁₁	Lariciresinol 4-O-glucoside	0.05	0.13	
11.459	194.05782	C ₁₀ H ₁₀ O ₄	Ferulic acid	0.14	0.08	
11.485	304.058	C ₁₅ H ₁₂ O ₇	Taxifolin	0.03	0.08	
11.487	302.04207	C ₁₅ H ₁₀ O ₇	Bracteatin	S	-	
11.487	450.11609	C ₂₁ H ₂₂ O ₁₁	Astilbin	0.06	0.25	0.40
11.493	594.15831	C ₂₇ H ₃₀ O ₁₅	Nictoflorin	-	0.36	
11.502	598.18966	C ₂₇ H ₃₄ O ₁₅	Phloretin 3',5'-Di-C-glucoside	-	0.16	
11.549	506.10615	C ₂₃ H ₂₂ O ₁₃	Quercetin 3- (6 ^o -acetylgalactoside)	0.03	-	
11.669	378.16759	C ₂₀ H ₂₆ O ₇	Carinol	S	-	
11.684	594.158	C ₂₇ H ₃₀ O ₁₅	5,7-Dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-3-yl 6-O-(6-deoxyhexopyranosyl) hexopyranoside	-	3.85	3.61
11.685	362.13776	C ₁₉ H ₂₂ O ₇	Machaerol B	S	-	
11.721	139.02678	C ₆ H ₅ N O ₃	4-Nitrophenol	-	0.04	1.62
11.759	448.10062	C ₂₁ H ₂₀ O ₁₁	Trifolin	0.13	0.50	1.92
11.83	302.04253	C ₁₅ H ₁₀ O ₇	Quercetin	1.08	6.59	1.43
11.845	436.13653	C ₂₁ H ₂₄ O ₁₀	Phloridzin	-	0.02	
11.899	374.15775	C ₁₇ H ₂₆ O ₉	Deoxyloganin	0.02	-	
11.999	264.09963	C ₁₄ H ₁₆ O ₅	1'-Acetoxyeugenol acetate	0.04	-	
12.002	316.05803	C ₁₆ H ₁₂ O ₇	Isorhamnetin	-	0.13	
12.015	262.14157	C ₁₂ H ₂₂ O ₆	Phaseolic acid	0.11	-	
12.018	680.37682	C ₃₆ H ₅₆ O ₁₂	Tenuifolin	-	S	
12.076	404.11076	C ₂₀ H ₂₀ O ₉	Chalconaringenin 2'-xyloside	S	-	
12.079	464.09535	C ₂₁ H ₂₀ O ₁₂	Quercetin-3β-D-glucoside	-	0.06	0.36
12.175	374.23036	C ₁₉ H ₃₄ O ₇	Tsangane L 3-glucoside	S	-	
12.183	286.04753	C ₁₅ H ₁₀ O ₆	Fisetin	-	0.05	0.69
12.192	534.1007	C ₂₄ H ₂₂ O ₁₄	Kaempferol 3-O-(6-malonyl-glucoside)	-	0.10	
12.194	338.09994	C ₁₆ H ₁₈ O ₈	4-Methylumbelliferyl-α-D-glucopyranoside	0.04	0.09	
12.195	340.14987	C ₁₂ H ₂₄ N ₂ O ₉	βD-glucosaminyl-(1->4)-β-D-glucosamine	S	-	
12.214	462.17169	C ₂₀ H ₃₀ O ₁₂	Bioside	0.04	-	
12.215	310.10514	C ₁₅ H ₁₈ O ₇	(E)-1-O-Cinnamoyl-β-D-glucose	-	S	
12.228	386.19415	C ₁₉ H ₃₀ O ₈	Corchoionol C 9-glucoside	0.02	-	
12.258	288.06315	C ₁₅ H ₁₂ O ₆	Maesopsin	-	0.07	

(Cont'd...)

Table S1. (Continued)

Retention time (minutes)	Molecular weight	Empirical formula	Putative compounds	Relative abundance (% of total area)		
				AQ (%)	MeOH (%)	EtOAc (%)
12.331	188.10475	C ₉ H ₁₆ O ₄	Azelaic acid	0.24	0.25	3.23
12.356	126.03159	C ₆ H ₆ O ₃	1,3,5-Trihydroxybenzene	0.03	-	
12.356	170.02143	C ₇ H ₆ O ₅	Gallic acid	3.32	0.15	
12.359	286.04733	C ₁₅ H ₁₀ O ₆	Kaempferol	0.04	0.16	0.37
12.371	582.2314	C ₂₈ H ₃₈ O ₁₃	(7'R)-(+)-Lyoniresinol 9'-glucoside	0.04	-	
12.433	348.142	C ₁₅ H ₂₄ O ₉	Ajugol	0.02	0.03	
12.469	170.02138	C ₇ H ₆ O ₅	2,4,6-Trihydroxybenzoic acid	-	0.03	
12.477	432.1056	C ₂₁ H ₂₀ O ₁₀	Afzelin	-	0.27	
12.49	346.10525	C ₁₈ H ₁₈ O ₇	Hamilcone	0.01	-	
12.532	544.19419	C ₂₈ H ₃₂ O ₁₁	Physalin E	S	-	
12.539	320.05324	C ₁₅ H ₁₂ O ₈	Amaranol A	0.01	-	
12.547	292.02196	C ₁₃ H ₈ O ₈	Brevifolincarboxylic acid	0.01	-	
12.564	244.13085	C ₁₂ H ₂₀ O ₅	4-oxododecanedioic acid	-	0.02	
12.588	372.21482	C ₁₉ H ₃₂ O ₇	Blumenol C glucoside	S	-	
12.61	384.12093	C ₂₁ H ₂₀ O ₇	Oxyisocyclointegrin	-	S	
12.702	192.04213	C ₁₀ H ₈ O ₄	5,7-Dihydroxy-4-methylcoumarin	0.08	0.04	0.64
12.727	88.05234	C ₄ H ₈ O ₂	Butyric acid	0.03	-	
12.727	98.0731	C ₆ H ₁₀ O	2-Hexenal	0.03	-	
12.79	250.08394	C ₁₃ H ₁₄ O ₅	Samini	S	-	
12.88	194.05781	C ₁₀ H ₁₀ O ₄	Isoferulic acid	0.22	0.04	0.65
12.912	230.05771	C ₁₃ H ₁₀ O ₄	Coriandrin	S	-	
12.966	281.14153	C ₁₈ H ₁₉ N O ₂	Floribundine	S	-	
13.039	274.08413	C ₁₅ H ₁₄ O ₅	Phloretin	0.07	-	
13.1	200.1411	C ₁₁ H ₂₀ O ₃	(S)-9-Hydroxy-10-undecenoic acid	S	-	
13.129	342.11005	C ₁₉ H ₁₈ O ₆	2-(2,6-dimethoxyphenyl)-5,6-dimethoxy-4H-chromen-4-one	0.03	0.05	
13.144	666.19453	C ₃₄ H ₃₄ O ₁₄	Deacetylphomoxanthone B	S	-	
13.15	386.12123	C ₁₇ H ₂₂ O ₁₀	1-O-Sinapoylglucose	0.09	0.21	
13.269	138.03165	C ₇ H ₆ O ₃	Salicylic acid	-	0.03	
13.291	400.15229	C ₂₂ H ₂₄ O ₇	Melafolone	S	-	
13.343	246.12534	C ₁₅ H ₁₈ O ₃	2-[(4,5-dimethyl-2-furyl) methylidene]-5,5-dimethylcyclohexane-1,3-dione	0.02	-	
13.437	296.17731	C ₂₀ H ₂₄ O ₂	Eicosatetraenoic acid		0.05	
13.499	232.10982	C ₁₄ H ₁₆ O ₃	Dihydrokawain	0.02	-	
13.527	202.17201	C ₁₅ H ₂₂	α-Curcumene	0.03	-	-
13.697	314.18749	C ₂₀ H ₂₆ O ₃	Kahweol	-	-	0.50
13.736	456.1783	C ₂₅ H ₂₈ O ₈	7-Hydroxy-2,6,9,12,17,17-hexamethyl-22-methylidene-5,16,19,21-tetraoxaheptacyclo-docos-13-ene-4,8,15-trione	-	0.09	
13.777	428.18319	C ₂₄ H ₂₈ O ₇	Heteroflavanone B	S	-	
13.809	148.05234	C ₉ H ₈ O ₂	p-Coumaraldehyde	0.07	0.03	
13.811	534.28193	C ₂₉ H ₄₂ O ₉	Corchoroside A	S	-	
13.849	162.10438	C ₁₁ H ₁₄ O	Valerophenone	0.02	-	

(Cont'd...)

Table S1. (Continued)

Retention time (minutes)	Molecular weight	Empirical formula	Putative compounds	Relative abundance (% of total area)		
				AQ (%)	MeOH (%)	EtOAc (%)
13.851	226.12029	C ₁₂ H ₁₈ O ₄	Allixin	0.06	-	
13.874	446.23048	C ₂₅ H ₃₄ O ₇	7-Formyl-4,6'-dihydroxy-6-(hydroxymethyl)-2',5',5',8a'-tetramethyl-3',4',4a',5',6',7',8',8a'-octahydro-2'H,3H-spiro[1-benzofuran-2,1'-naphthalen]-7'-yl acetate			0.72
13.888	472.20995	C ₂₆ H ₃₂ O ₈	Kushenol H	0.02	-	
13.891	484.17313	C ₂₆ H ₂₈ O ₉	(2R,7S,13R,14R,16S,19R,20S)-19-(furan-3-yl)-11-hydroxy-9,9,13,20-tetramethyl-4,8,15,18-tetraoxahexacyclodocos-10-ene-5,12,17-trione	0.08	-	17.93
13.92	148.05238	C ₉ H ₈ O ₂	(E)-3-(2-Hydroxyphenyl)-2-propenal	0.03	-	
13.949	208.11007	C ₁₂ H ₁₆ O ₃	β-Asarone	0.02	0.02	
13.953	532.1949	C ₂₇ H ₃₂ O ₁₁	Icaritin 3-rhamnoside	S	-	
13.97	804.37825	C ₃₈ H ₆₀ O ₁₈	Stevioside	-	S	
14.035	248.10456	C ₁₄ H ₁₆ O ₄	(+)-cis-5,6-Dihydro-5-hydroxy-4-methoxy-6-(2-phenylethyl)-2H-pyran-2-one	0.01	-	
14.078	257.1046	C ₁₅ H ₁₅ N ₃ O ₃	Haplamine	-	-	0.46
14.08	256.12062	C ₁₅ H ₁₆ N ₂ O ₂	Ancymidol	-	-	0.64
14.094	376.28227	C ₂₀ H ₄₀ O ₆	Tetradecyl β-D-glucopyranoside	S	-	
14.102	722.31464	C ₃₆ H ₅₀ O ₁₅	Physagulin G	0.11	-	
14.137	272.0684	C ₁₅ H ₁₂ O ₅	Naringenin	0.03	0.02	
14.379	548.22578	C ₂₈ H ₃₆ O ₁₁	3,7-Dihydroxy-4,5-dimethoxy-8-prenylflavan 7-O-β-D-glucopyranoside	0.01	-	
14.499	470.19435	C ₂₆ H ₃₀ O ₈	Zapoterin	-	0.07	
14.552	406.12623	C ₂₀ H ₂₂ O ₉	Anadanthoside	S	-	
14.559	558.28306	C ₃₁ H ₄₂ O ₉	Glycinoeclepin B	0.02	-	
14.769	470.33943	C ₃₀ H ₄₆ O ₄	Glycyrrhetic acid	-	S	
15.056	486.1892	C ₂₆ H ₃₀ O ₉	2',4',4'-Trihydroxy-3'-prenylchalcone 4'-O-glucoside	-	S	
15.341	534.2827	C ₂₉ H ₄₂ O ₉	(3β,9×i)-3-(β-D-Glucopyranosyloxy)-14-hydroxycarda-5,20 (22)-dienolide	0.06	0.07	
15.424	641.31987	C ₃₅ H ₄₇ N ₁₀ O ₁₀	Taxine	0.06	0.19	
15.488	346.21419	C ₂₂ H ₂₆ N ₄	(+)-Calycanthine	S	-	
15.564	166.13556	C ₁₁ H ₁₈ O	(-)-Nopol	S	-	
15.587	530.21479	C ₂₈ H ₃₄ O ₁₀	7-Acetoxy-6-hydroxylimonin	-	0.39	
15.825	440.18354	C ₂₆ H ₂₄ N ₄ O ₃	1,4:3,6-Dianhydro-5-O-benzyl-2-[5-(4-biphenyl)-1H-tetrazol-1-yl]-2-deoxy-D-glucitol		0.38	5.51
16.063	324.20863	C ₂₂ H ₂₈ O ₂	Cannabinol monomethyl ether	0.04	-	
16.241	504.34515	C ₃₀ H ₄₈ O ₆	Protobassic acid	S	-	
16.317	440.18338	C ₂₆ H ₂₄ N ₄ O ₃	Holyrine A	S	-	
16.337	328.22487	C ₁₈ H ₃₂ O ₅	Corchorifatty acid F	0.09	0.48	3.05
16.382	312.20833	C ₂₁ H ₂₈ O ₂	Tetrahydrogestrinone	-	-	1.27
16.386	348.22944	C ₂₁ H ₃₂ O ₄	(4aS,5R,6S,8aS)-5-[(3E)-5-methoxy-3-methyl-5-oxopent-3-en-1-yl]-5,6,8a-trimethyl-3,4,4a, 5,6,7,8,8a-octahydronaphthalene-1-carboxylic acid	-	-	4.66
16.687	216.18777	C ₁₆ H ₂₄	Cyperotundone	S	-	
16.69	288.23031	C ₁₆ H ₃₂ O ₄	(S)-10,16-Dihydroxyhexadecanoic acid	0.12	-	
16.72	408.23001	C ₂₆ H ₃₂ O ₄	Methylinderatin	S	-	
16.786	504.34497	C ₃₀ H ₄₈ O ₆	Arjungenin	0.53	0.08	
16.848	583.31466	C ₃₃ H ₄₅ N ₃ O ₈	Taxine B	-	S	
16.977	822.40365	C ₄₂ H ₆₂ O ₁₆	Glycyrrhizin	0.04	-	

(Cont'd...)

Table S1. (Continued)

Retention time (minutes)	Molecular weight	Empirical formula	Putative compounds	Relative abundance (% of total area)		
				AQ (%)	MeOH (%)	EtOAc (%)
17.015	560.33477	C ₃₂ H ₄₈ O ₈	Cucurbitacin C	S	-	
17.081	468.2149	C ₂₇ H ₃₂ O ₇	Exiguaflavanone E	-	0.02	
17.127	646.37157	C ₃₆ H ₅₄ O ₁₀	Gypsogenin 3-O-b-D-glucuronide	-	S	
17.201	574.3505	C ₃₃ H ₅₀ O ₈	Favolon B	S	-	
17.366	676.23644	C ₃₃ H ₄₀ O ₁₅	Icariin	0.03	-	
17.478	620.28401	C ₃₂ H ₄₄ O ₁₂	Scilliroside	0.92	-	
17.552	256.07338	C ₁₅ H ₁₂ O ₄	Isoliquiritigenin	0.02	-	
17.56	254.11522	C ₁₃ H ₁₈ O ₅	Aplojaveediin C	0.02	-	
17.574	452.18324	C ₂₆ H ₂₈ O ₇	Derrichalcone	S	-	
17.578	252.17231	C ₁₅ H ₂₄ O ₃	1-Hydroxyepiacorone	0.06	-	
17.673	650.32998	C ₃₄ H ₅₀ O ₁₂	Thapsigargin	-	0.11	
17.728	294.1828	C ₁₇ H ₂₆ O ₄	(+/-)-Gingerol	-	0.05	
17.968	406.17781	C ₂₅ H ₂₆ O ₅	Flemiwallichin D	S	-	
17.982	482.23027	C ₂₈ H ₃₄ O ₇	Gedunin	0.02	-	
18.457	466.19849	C ₂₇ H ₃₀ O ₇	Nimbolide	-	0.07	
19.166	354.14656	C ₂₁ H ₂₂ O ₅	Xanthohumol	-	-	3.13
21.143	412.37023	C ₂₉ H ₄₈ O	β-Sitostenone	0.13	-	
21.302	426.37018	C ₂₆ H ₅₀ O ₄	Bis (2-ethylhexyl) sebacate	-	-	1.85
21.881	390.27653	C ₂₄ H ₃₈ O ₄	Bis (2-ethylhexyl) terephthalate	0.49	0.52	
22.055	472.39152	C ₃₁ H ₅₂ O ₃	α-Tocopherol acetate	T	-	
22.132	412.37029	C ₂₉ H ₄₈ O	Stigmasterol	-	S	
22.533	410.31813	C ₂₈ H ₄₂ O ₂	γ-Tocotrienol	0.02	-	

Notes: Relative percentage abundance (%) indicates the proportion of each compound detected in the extract, based on its peak area in chromatographic analysis. It reflects how much of each compound is present relative to the total composition. Compounds detected in very small amounts ≤0.01% are considered minor and marked with 'S'. Phytochemicals that are not present in either of the extracts are denoted by dash (-).