



Combinations of *Terminalia bellirica* (Gaertn.) Roxb. and *Terminalia chebula* Retz. extracts with selected antibiotics against antibiotic-resistant bacteria: Bioactivity and phytochemistry

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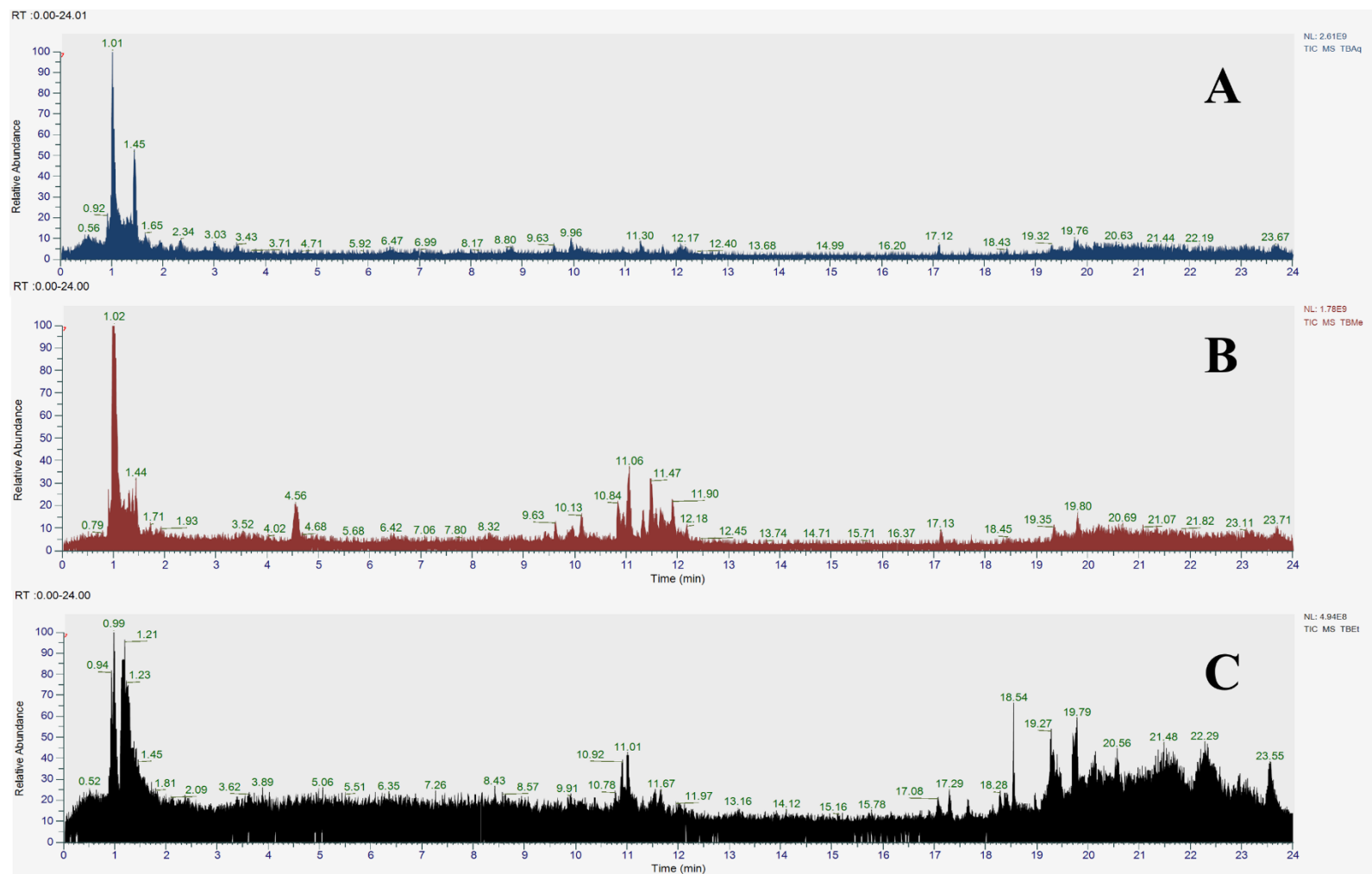


Figure S1: LC-MS total compound chromatograms of (A) TB-Aq (*Terminalia bellirica* aqueous), (B) TB-MeOH (*Terminalia bellirica* methanol), and (C) TB-EtOAc (*Terminalia bellirica* ethyl acetate).

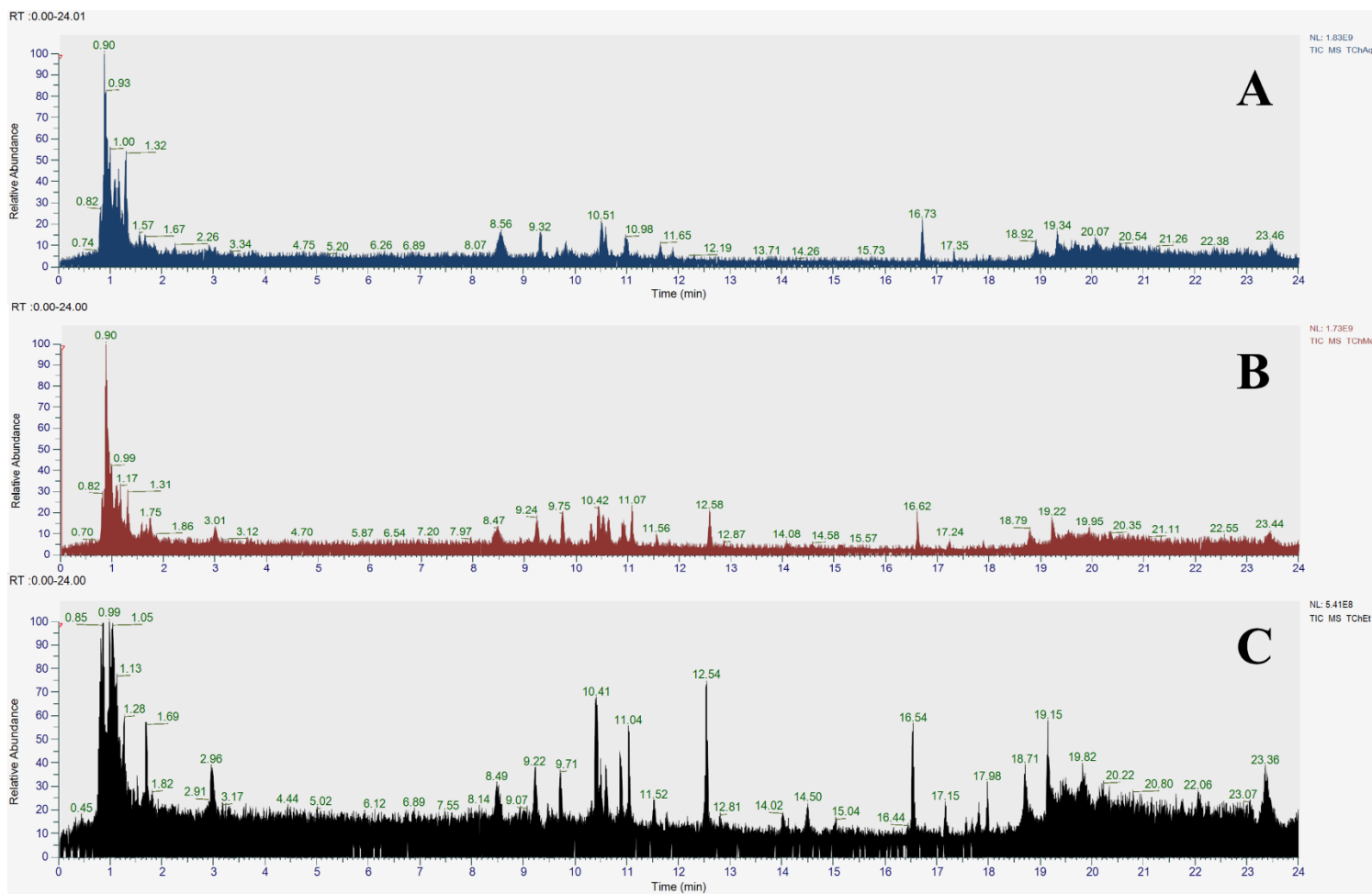


Figure S2: LC-MS total compound chromatograms of (A) TCh-Aq (*Terminalia chebula* aqueous), (B) TB-MeOH (*Terminalia chebula* methanol), and (C) TB-EtOAc (*Terminalia chebula* ethyl acetate).

Table S1: LC-MS putative identification and % relative abundance of phytochemicals identified in the fruit extracts of *Terminalia bellirica*. Compounds less than 0.01% of the total area were considered as trace amounts and denoted as T.

Retention time [min]	Molecular weight	Empirical Formula	Putative Compounds	Relative Abundance (% of Total Area)		
				AQ	MeOH	EtOAc
1.041	146.1054	C ₆ H ₁₄ N ₂ O ₂	L-Lysine	-	0.02%	-
1.05	132.0896	C ₅ H ₁₂ N ₂ O ₂	Ornithine	0.01%		
1.079	132.0533	C ₄ H ₈ N ₂ O ₃	Asparagine	0.20%		
1.086	174.1114	C ₆ H ₁₄ N ₄ O ₂	DL-Arginine	1.30%		
1.093	103.0995	C ₅ H ₁₃ N O	Choline	1.25%		
1.101	191.07876	C ₇ H ₁₃ N O ₅	Calystegine C1	0.03%	-	-
1.102	148.0481	C ₄ H ₈ N ₂ O ₄	Hydroxylated lecithin	0.82%	-	-
1.104	193.03725	C ₉ H ₇ N O ₄	5,6-Dihydroxyindole-2-carboxylic acid	-	0.27%	-
1.106	87.03176	C ₃ H ₅ N O ₂	2-Iminopropanoate	0.33%		
1.107	105.0423	C ₃ H ₇ N O ₃	L-Serine	0.22%		
1.108	203.0901	C ₇ H ₁₃ N ₃ O ₄	Alanyl asparagine	0.18%		
1.108	133.0372	C ₄ H ₇ N O ₄	L-Aspartic acid	0.24%		
1.108	133.03717	C ₄ H ₇ N O ₄	4-Hydroxybenzoic acid	0.24%	-	-
1.114	104.01073	C ₃ H ₄ O ₄	Malonic acid	0.03%	-	-
1.118	196.05797	C ₆ H ₁₂ O ₇	Gluconic acid	0.37%	0.54%	-
1.22	117.0789	C ₅ H ₁₁ N O ₂	L-Valine	-	0.20%	-
1.126	137.0475	C ₇ H ₇ N O ₂	Trigonelline	0.54%	0.69%	-
1.128	210.03725	C ₆ H ₁₀ O ₈	D-Saccharic acid	0.47%	-	-
1.132	210.03728	C ₆ H ₁₀ O ₈	Galactaric acid	0.01%	0.22%	-
1.132	186.0999	C ₈ H ₁₄ N ₂ O ₃	Alanyl proline	0.08%		
1.133	115.0631	C ₅ H ₉ N O ₂	Proline	17.00%		
1.14	162.05261	C ₆ H ₁₀ O ₅	3-Hydroxymethylglutaric acid	0.46%	1.94%	-
1.164	309.10538	C ₁₁ H ₁₉ N O ₉	N-Acetylneuraminic acid	-	0.90%	-
1.167	90.03157	C ₃ H ₆ O ₃	Glyceraldehyde	0.43%	0.74%	-
1.179	322.08954	C ₁₂ H ₁₈ O ₁₀	Lepidimoic acid	-	0.04%	-
1.198	174.05254	C ₇ H ₁₀ O ₅	Shikimic acid	-	0.41%	0.67%

1.201	116.01078	C ₄ H ₄ O ₄	Maleic acid	0.90%	-	0.71%
1.203	138.03151	C ₇ H ₆ O ₃	4-Hydroxybenzoic acid	0.07%	-	-
1.205	134.02136	C ₄ H ₆ O ₅	L- (-)-Malic acid	2.48%	-	-
1.209	116.01079	C ₄ H ₄ O ₄	Fumaric acid	0.01%	1.73%	-
1.223	129.07892	C ₆ H ₁₁ N O ₂	Pipecolic acid	0.04%	4.26%	-
1.229	516.13246	C ₁₈ H ₂₈ O ₁₇	β-D-Glucuronopyranosyl-(1->3)-α-D-galacturonopyranosyl-(1->2)-L-rhamnose	0.01%	-	-
1.232	85.01624	C ₃ H ₃ N O ₂	Cyanoacetic acid	0.23%		
1.236	174.0638	C ₆ H ₁₀ N ₂ O ₄	Formiminoglutamic acid	0.03%		
1.24	146.02125	C ₅ H ₆ O ₅	Oxoglutaric acid	0.01%	-	-
1.241	95.03688	C ₅ H ₅ N O	2-Hydroxypyridine	-	0.05%	-
1.245	130.0264	C ₅ H ₆ O ₄	Itaconic acid	0.60%	-	-
1.245	174.01587	C ₆ H ₆ O ₆	cis-Aconitic acid	-	0.07%	-
1.311	205.0379	C ₁₀ H ₇ N O ₄	Xanthurenic acid	-	-	0.05%
1.356	106.0264	C ₃ H ₆ O ₄	Glyceric acid	-	-	0.10%
1.36	206.04237	C ₇ H ₁₀ O ₇	2-Methylcitric acid	-	0.02%	0.11%
1.37	129.07886	C ₆ H ₁₁ N O ₂	Nipecotic acid	-	0.68%	-
1.372	122.0478	C ₆ H ₆ N ₂ O	Niacinamide	0.03%	-	-
1.377	156.0059	C ₆ H ₄ O ₅	2,5-Furandicarboxylic acid	0.04%		
1.38	130.02647	C ₅ H ₆ O ₄	Citraconic acid	0.74%	0.56%	-
1.394	115.0631	C ₅ H ₉ N O ₂	L-Proline	T		
1.395	198.0638	C ₈ H ₁₀ N ₂ O ₄	Mimosine	0.06%		
1.414	129.0425	C ₅ H ₇ N O ₃	L-Pyroglutamic acid	0.23%		
1.414	119.0584	C ₄ H ₉ N O ₃	L-Threonine	0.01%		
1.416	181.0737	C ₉ H ₁₁ N O ₃	L-Tyrosine		0.08%	
1.419	199.12056	C ₁₀ H ₁₇ N O ₃	Ecgonine methyl ester	0.09%	0.14%	-
1.427	176.03186	C ₆ H ₈ O ₆	Ascorbic acid	-	0.24%	0.06%
1.427	176.03184	C ₆ H ₈ O ₆	Glucuronic acid-3,6-lactone	0.11%	-	-
1.468	148.03695	C ₅ H ₈ O ₅	Citramalic acid	0.01%	-	-
1.472	344.07395	C ₁₄ H ₁₆ O ₁₀	Isovanillic acid glucuronide	0.75%	-	-
1.475	118.02646	C ₄ H ₆ O ₄	Succinic acid	0.04%	0.09%	0.12%
1.478	192.06314	C ₇ H ₁₂ O ₆	D- (-)-Quinic acid	3.13%	0.33%	0.19%
1.479	344.07397	C ₁₄ H ₁₆ O ₁₀	Theogallin	-	3.47%	-

1.521	261.12089	C ₁₁ H ₁₉ N O ₆	Lotaustralin	0.39%	-	-
1.541	192.02679	C ₆ H ₈ O ₇	Citric acid	0.18%	-	0.46%
1.545	112.01591	C ₅ H ₄ O ₃	2-Furoic acid	0.19%	-	-
1.56	142.0264	C ₆ H ₆ O ₄	trans,trans-Muconic acid		0.38%	
1.567	214.1314	C ₁₀ H ₁₈ N ₂ O ₃	Valylproline	0.09%		
1.568	131.0944	C ₆ H ₁₃ N O ₂	6-Aminocaproic acid	0.14%		
1.573	131.0945	C ₆ H ₁₃ N O ₂	L-Isoleucine		0.19%	
1.608	90.03159	C ₃ H ₆ O ₃	L-(+)-Lactic acid	-	-	0.26%
1.609	220.08452	C ₁₁ H ₁₂ N ₂ O ₃	5-Hydroxy-L-tryptophan	-	T	-
1.64	185.0687	C ₈ H ₁₁ N O ₄	2-Aminobicyclohexane-2,6-dicarboxylic acid	-	0.01%	-
1.658	240.0741	C ₁₀ H ₁₂ N ₂ O ₅	(±)-2-(1-Methylpropyl)-4,6-dinitrophenol	-	0.01%	-
1.668	161.0687	C ₆ H ₁₁ N O ₄	Aminoadipic acid	-	0.11%	-
1.668	294.0374	C ₁₃ H ₁₀ O ₈	Banksiamarin B	-	-	0.15%
1.679	85.08901	C ₅ H ₁₁ N	Piperidine	-	-	0.16%
1.701	92.02946	C ₃ H ₈ O S	Cibulins	-	-	0.58%
1.737	174.01629	C ₆ H ₆ O ₆	trans-Aconitic acid	0.24%	0.03%	-
1.737	136.03701	C ₄ H ₈ O ₅	<u>Erythronic acid</u>	T	-	-
1.739	130.02642	C ₅ H ₆ O ₄	Glutaconic acid	0.04%	-	-
1.747	98.03663	C ₅ H ₆ O ₂	2-Furanmethanol	-	-	0.09%
1.749	206.04246	C ₇ H ₁₀ O ₇	3-Hydroxy-3-(methoxycarbonyl) pentane dioic acid	-	0.05%	-
1.768	332.07417	C ₁₃ H ₁₆ O ₁₀	6-Galloylglucose	6.06%	3.97%	3.39%
1.778	312.04795	C ₁₃ H ₁₂ O ₉	Caftaric acid	0.02%	-	-
1.785	342.11611	C ₁₂ H ₂₂ O ₁₁	α, α-Trehalose	6.86%	12.27%	23.22%
1.793	244.0581	C ₁₀ H ₁₂ O ₇	1-O-Galloylglycerol	-	-	0.02%
1.813	88.0159	C ₃ H ₄ O ₃	Pyruvic acid	0.24%	-	-
1.824	147.05303	C ₅ H ₉ N O ₄	L-Glutamic acid	-	0.19%	-
1.858	144.04211	C ₆ H ₈ O ₄	5-hydroxy-4-methoxy-5,6-dihydro-2H-pyran-2-one	0.89%	0.17%	-
1.923	316.07932	C ₁₃ H ₁₆ O ₉	Ginnalin B	0.01%	-	-
1.976	88.05237	C ₄ H ₈ O ₂	Butyric acid	-	-	0.01%
2.027	134.02145	C ₄ H ₆ O ₅	DL-Malic acid	0.05%	0.07%	-
2.037	153.0788	C ₈ H ₁₁ N O ₂	3,5-Dimethoxyaniline	-	-	0.13%

2.193	288.08452	C ₁₂ H ₁₆ O ₈	Phlorin	-	0.02%	-
2.142	108.0211	C ₆ H ₄ O ₂	1,2-Benzoquinone	0.04%		
2.2	219.11062	C ₉ H ₁₇ N O ₅	Pantothenic acid	-	0.02%	-
2.214	134.0215	C ₄ H ₆ O ₅	Malic acid	-	-	0.05%
2.244	166.06293	C ₉ H ₁₀ O ₃	Apocynin	0.02%	0.04%	-
2.397	154.02654	C ₇ H ₆ O ₄	Gentisic acid	0.02%	0.05%	-
2.421	328.1157	C ₁₅ H ₂₀ O ₈	Ethylvanillin glucoside	-	-	0.01%
2.433	124.0272	C ₅ H ₄ N ₂ O ₂	Pyrazin-2-carboxylic acid	-	0.01%	-
2.645	356.03816	C ₁₄ H ₁₂ O ₁₁	(+)-Chebulic acid	0.54%	-	-
2.768	182.069	C ₈ H ₁₀ N ₂ O ₃	3-Hydroxy-5-(hydroxymethyl)-2-methylisonicotinaldehyde oxime	-	0.14%	-
2.844	212.0684	C ₁₀ H ₁₂ O ₅	Vanillactic acid	T		
2.911	302.06383	C ₁₂ H ₁₄ O ₉	Pyrogallol-2-O-glucuronide	-	0.21%	-
2.938	158.0579	C ₇ H ₁₀ O ₄	Succinylacetone		T	
3.059	204.08978	C ₁₁ H ₁₂ N ₂ O ₂	L-Tryptophan	-	0.03%	-
3.06	187.06318	C ₁₁ H ₉ N O ₂	trans-3-Indoleacrylic acid	0.11%	0.32%	-
3.061	145.05266	C ₉ H ₇ N O	4-Indolecarbaldehyde	-	0.04%	-
3.094	390.11625	C ₁₆ H ₂₂ O ₁₁	2,3,4,5,6-Penta-O-acetyl-D-glucose	0.01%	0.01%	-
3.11	484.08475	C ₂₀ H ₂₀ O ₁₄	Gallic acid 3-O-(6-galloylglucoside)	0.74%	-	-
3.145	228.1472	C ₁₁ H ₂₀ N ₂ O ₃	Prolylleucine	0.08%		
3.485	496.08487	C ₂₁ H ₂₀ O ₁₄	(1S,3R,4R,5R)-1,3-dihydroxy-4,5-bis(3,4,5-trihydroxybenzoyloxy) cyclohexane-1-carboxylic acid	-	0.28%	-
3.569	218.14169	C ₁₃ H ₁₈ N ₂ O	5-Methoxydimethyltryptamine	0.01%	-	-
3.652	112.05232	C ₆ H ₈ O ₂	(2E,4E)-2,4-Hexadienoic acid	0.08%	-	-
3.797	314.10014	C ₁₄ H ₁₈ O ₈	Vanilloside	-	0.01%	-
3.94	185.1049	C ₉ H ₁₅ N O ₃	Pseudoecgonine	-	-	0.02%
4.647	96.021	C ₅ H ₄ O ₂	2-Furancarboxaldehyde	-	0.02%	-
4.659	154.02638	C ₇ H ₆ O ₄	2,4-Dihydroxybenzoic acid	-	0.15%	-
4.667	122.03663	C ₇ H ₆ O ₂	4-Hydroxybenzaldehyde	-	0.49%	0.10%
4.756	342.0951	C ₁₅ H ₁₈ O ₉	Glucocaffeic acid	-	-	0.01%
4.921	292.02154	C ₁₃ H ₈ O ₈	Brevifolincarboxylic acid	0.09%	-	-
4.93	360.10563	C ₁₅ H ₂₀ O ₁₀	Glucosyringic acid	-	0.07%	-

5.164	176.06843	C ₇ H ₁₂ O ₅	2-Isopropylmalic acid	0.01%	0.02%	0.03%
5.757	216.08974	C ₁₂ H ₁₂ N ₂ O ₂	L-1,2,3,4-Tetrahydro-beta-carboline-3-carboxylic acid	-	0.01%	-
6.475	296.0529	C ₁₃ H ₁₂ O ₈	Caffeoylmalic acid	0.05%	-	-
6.812	187.06319	C ₁₁ H ₉ N O ₂	Indoleacrylic acid	T	-	-
6.827	230.10541	C ₁₃ H ₁₄ N ₂ O ₂	(1xi,3xi)-1,2,3,4-Tetrahydro-1-methyl-beta-carboline-3-carboxylic acid	-	0.02%	-
6.939	329.1988	C ₂₀ H ₂₇ N O ₃	Trilostane		0.03%	
8.333	636.09597	C ₂₇ H ₂₄ O ₁₈	1,3,6-Tri-O-galloyl-beta-D-glucose	-	0.25%	0.93%
8.44	484.08546	C ₂₀ H ₂₀ O ₁₄	1,6-Bis-O-(3,4,5-trihydroxybenzoyl) hexopyranose	5.13%	5.19%	2.52%
8.726	634.08076	C ₂₇ H ₂₂ O ₁₈	Sanguiin H4	0.84%	-	0.07%
8.941	512.15318	C ₂₃ H ₂₈ O ₁₃	3-(4-Hydroxy-3-methoxyphenyl)-1,2-propanediol 2-O-(galloyl-glucoside)	T	-	-
8.945	478.07477	C ₂₁ H ₁₈ O ₁₃	Miquelianin	0.04%	0.42%	-
8.948	308.0528	C ₁₄ H ₁₂ O ₈	Fulvic acid	0.02%		
8.985	478.07427	C ₂₁ H ₁₈ O ₁₃	Quercetin 3-O-glucuronide	-	0.08%	-
9.105	470.01185	C ₂₁ H ₁₀ O ₁₃	Sanguisorbic acid dilactone	0.56%	0.88%	-
9.21	126.03151	C ₆ H ₆ O ₃	Phloroglucinol	0.10%	1.93%	-
9.291	498.1009	C ₂₁ H ₂₂ O ₁₄	Methyl 4,6-di-O-galloyl-beta-D-glucopyranoside	T	-	-
9.532	338.09996	C ₁₆ H ₁₈ O ₈	3-O-p-Coumaroylquinic acid	T	-	-
9.538	314.06351	C ₁₃ H ₁₄ O ₉	Beta-D-Glucopyranuronic acid	2.37%	0.58%	0.33%
9.738	126.03149	C ₆ H ₆ O ₃	Maltol	0.02%	0.06%	-
9.74	236.06837	C ₁₂ H ₁₂ O ₅	Dillapional	0.01%	-	-
9.817	374.12117	C ₁₆ H ₂₂ O ₁₀	Geniposidic acid	-	0.02%	-
9.89	402.15262	C ₁₈ H ₂₆ O ₁₀	Benzyl beta-primeveroside	T	0.03%	-
10.064	636.09617	C ₂₇ H ₂₄ O ₁₈	1,2,6-Trigalloyl-β-D-glucopyranose	0.09%	5.44%	2.85%
10.235	96.02095	C ₅ H ₄ O ₂	2H-Pyran-2-one	0.05%	0.09%	1.02%
10.237	126.03161	C ₆ H ₆ O ₃	Pyrogallol	6.28%	5.28%	2.19%
10.357	524.15327	C ₂₄ H ₂₈ O ₁₃	Barbatoflavan	0.01%	-	-
10.382	160.05219	C ₁₀ H ₈ O ₂	6-Methylcoumarin	-	0.01%	-
10.406	126.0316	C ₆ H ₆ O ₃	1,2,3-Trihydroxybenzene	-	-	0.15%
10.448	432.12706	C ₁₈ H ₂₄ O ₁₂	Apiosylglucosyl 4-hydroxybenzoate	T	-	-

10.475	484.08519	C ₂₀ H ₂₀ O ₁₄	Hamamelitannin	2.10%	0.02%	0.62%
10.484	296.05287	C ₁₃ H ₁₂ O ₈	cis-Coutaric acid	0.33%	0.86%	0.19%
10.577	478.07496	C ₂₁ H ₁₈ O ₁₃	6-Hydroxyluteolin 6-glucuronide	0.01%	-	-
10.691	196.03709	C ₉ H ₈ O ₅	3-Methoxy-4,5-methylenedioxybenzoic acid	T	-	-
10.703	372.10552	C ₁₆ H ₂₀ O ₁₀	Veranisatin C	0.02%	0.04%	-
10.706	198.05269	C ₉ H ₁₀ O ₅	Syringic acid	0.16%	0.15%	-
10.796	448.10018	C ₂₁ H ₂₀ O ₁₁	(1ξ)-1,5-Anhydro-1-[2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4-oxo-4H-chromen-8-yl]-D-galactitol	-	0.03%	-
10.879	584.13777	C ₂₅ H ₂₈ O ₁₆	Neomangiferin	-	T	-
11.055	466.11077	C ₂₁ H ₂₂ O ₁₂	(2R,3R)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3- {[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl) oxan-2-yl] oxy} -3,4-dihydro-2H-1-benzopyran-4-one	0.01%	-	-
11.057	302.00606	C ₁₄ H ₆ O ₈	Ellagic acid	2.45%	10.74%	33.49%
11.159	236.03157	C ₁₁ H ₈ O ₆	6-Methoxy-8-hydroxyisocoumarin-3-carboxylic acid	-	0.58%	-
11.257	304.05785	C ₁₅ H ₁₂ O ₇	Nigrescin	T	0.02%	-
11.263	174.08907	C ₈ H ₁₄ O ₄	Suberic acid	T	-	0.06%
11.272	610.15272	C ₂₇ H ₃₀ O ₁₆	Quercetin 3-O-rhamnoside-7-O-glucoside	0.05%	-	-
11.295	610.15295	C ₂₇ H ₃₀ O ₁₆	Rutin	-	0.14%	0.10%
11.3	464.09518	C ₂₁ H ₂₀ O ₁₂	3,5,7-trihydroxy-2-(3-hydroxy-4- {[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl) oxan-2-yl]oxy}phenyl)-4H-chromen-4-one	-	0.02%	-
11.341	436.10043	C ₂₀ H ₂₀ O ₁₁	Taxifolin 3-apioside	T	-	-
11.348	184.07305	C ₉ H ₁₂ O ₄	Vanylglycol	0.01%	-	-
11.372	498.13718	C ₂₂ H ₂₆ O ₁₃	Verprosoid	0.03%	0.07%	-
11.473	464.09505	C ₂₁ H ₂₀ O ₁₂	Myricitrin	0.05%	0.13%	0.19%
11.487	168.126	C ₉ H ₁₆ N ₂ O	N-Methylloine	-	-	0.01%
11.507	554.16359	C ₂₅ H ₃₀ O ₁₄	Lippioside II	T	-	-
11.527	388.13676	C ₁₇ H ₂₄ O ₁₀	Geniposide	0.01%	0.01%	-
11.529	422.08464	C ₁₉ H ₁₈ O ₁₁	1,5,8-Trihydroxy-9-oxo-9H-xanthen-3-yl beta-D-glucopyranoside	0.02%	0.05%	-

11.533	400.1519	C ₂₂ H ₂₄ O ₇	Melafolone	T	-	-
11.546	522.21046	C ₂₆ H ₃₄ O ₁₁	Isolariciresinol 9-O-beta-D-glucoside	0.01%	-	-
11.55	184.10991	C ₁₀ H ₁₆ O ₃	(1'R)-Nepetalic acid	T	-	-
11.553	492.09059	C ₂₂ H ₂₀ O ₁₃	Carminic acid	0.04%	-	-
11.586	164.05849	C ₈ H ₈ N ₂ O ₂	Ricinine	0.01%	0.03%	0.12%
11.666	216.09953	C ₁₀ H ₁₆ O ₅	(4S,5S,8S,10R)-4,5,8-trihydroxy-10-methyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one	0.05%	-	-
11.674	478.11101	C ₂₂ H ₂₂ O ₁₂	6-Methoxyluteolin 7-glucoside	0.01%	-	-
11.692	132.04297	C ₆ H ₄ N ₄	Pteridine	-	0.01%	-
11.694	164.04717	C ₉ H ₈ O ₃	2-Hydroxycinnamic acid	0.02%	0.05%	-
11.788	260.0316	C ₁₃ H ₈ O ₆	Urolithin D	-	0.02%	-
11.953	448.10033	C ₂₁ H ₂₀ O ₁₁	Trifolin	0.01%	-	-
12.018	184.03695	C ₈ H ₈ O ₅	Methyl gallate	0.25%	11.39%	-
12.019	170.02144	C ₇ H ₆ O ₅	Gallic acid	26.23%	8.64%	2.60%
12.048	302.04238	C ₁₅ H ₁₀ O ₇	Quercetin	0.11%	0.33%	0.17%
12.053	448.1	C ₂₁ H ₂₀ O ₁₁	5-(5,7-Dihydroxy-3-methoxy-4-oxo-4H-chromen-2-yl)-2-hydroxyphenyl beta-D-xylopyranoside	-	0.05%	-
12.06	150.06809	C ₉ H ₁₀ O ₂	Hydrocinnamic acid	T	-	0.14%
12.138	396.15682	C ₂₃ H ₂₄ O ₆	Glabrachalcone	T	-	-
12.155	448.06386	C ₂₀ H ₁₆ O ₁₂	Ellagic acid 2-rhamnoside	0.11%	1.44%	0.69%
12.183	448.09955	C ₂₁ H ₂₀ O ₁₁	Maritimein	-	0.01%	0.02%
12.184	456.10534	C ₂₃ H ₂₀ O ₁₀	Epicatechin 3-O- (3-O-methylgallate)	-	0.02%	-
12.38	334.03252	C ₁₅ H ₁₀ O ₉	3,5,6,7,2',3',4'-Heptahydroxyflavone	-	0.20%	-
12.459	462.0795	C ₂₁ H ₁₈ O ₁₂	Aureusidin 6-glucuronide	-	-	2.52%
12.509	610.1894	C ₂₈ H ₃₄ O ₁₅	Neohesperidin	-	-	0.16%
12.539	292.1209	C ₁₈ H ₁₆ N ₂ O ₂	4-phenyl-2-[(3-pyridylamino) methylidene] cyclohexane-1,3-dione	-	0.02%	-
12.584	498.17406	C ₂₃ H ₃₀ O ₁₂	Eucaglobulin	-	0.02%	-
12.711	262.04766	C ₁₃ H ₁₀ O ₆	Maclurin	-	0.02%	-
12.82	188.1047	C ₉ H ₁₆ O ₄	Azelaic acid	-	-	0.33%
12.822	362.17305	C ₂₀ H ₂₆ O ₆	Secoisolariciresinol	-	T	-
12.843	580.21589	C ₂₈ H ₃₆ O ₁₃	(+)-7-epi-Syringaresinol 4'-glucoside	-	0.01%	-

12.844	518.1785	C ₂₆ H ₃₀ O ₁₁	Phellodensin E	-	-	0.05%
12.924	302.11519	C ₁₇ H ₁₈ O ₅	Lusianin	0.01%	-	-
13.088	241.1675	C ₁₃ H ₂₃ N O ₃	Dioscoretine	-	-	0.05%
13.307	556.15817	C ₂₈ H ₂₈ O ₁₂	Epicatechin 5-O-beta-D-glucopyranoside-3-benzoate	T	-	-
13.38	416.1681	C ₁₉ H ₂₈ O ₁₀	Phenylethyl primeveroside	T	-	-
13.41	170.02148	C ₇ H ₆ O ₅	Phloroglucinic acid	0.98%	1.80%	4.33%
13.428	442.1992	C ₂₅ H ₃₀ O ₇	Exiguaflavanone M	-	-	0.13%
13.455	462.11665	C ₂₂ H ₂₂ O ₁₁	Leptosin	-	0.01%	-
13.51	169.11009	C ₉ H ₁₅ N O ₂	Homoarecoline	T	-	-
13.527	191.0944	C ₁₁ H ₁₃ N O ₂	5-Methoxytryptophol	-	-	0.06%
13.593	502.1836	C ₂₆ H ₃₀ O ₁₀	Flavaprin	-	-	0.07%
13.611	358.14156	C ₂₀ H ₂₂ O ₆	Pedicellin	0.01%	-	-
13.701	308.07953	C ₁₇ H ₁₂ N ₂ O ₄	Flazine	-	0.01%	-
13.725	330.03743	C ₁₆ H ₁₀ O ₈	Blighinone	0.12%	-	-
13.822	227.09433	C ₁₄ H ₁₃ N O ₂	Koenoline	T	T	-
13.898	326.115	C ₁₉ H ₁₈ O ₅	4',7-Dimethoxy-6,8-dimethyl-5-hydroxyflavone	T	-	T
13.928	554.2148	C ₃₀ H ₃₄ O ₁₀	Lappaol C	-	T	-
13.958	520.1948	C ₂₆ H ₃₂ O ₁₁	Matairesinoside	-	-	0.01%
14.024	500.1674	C ₂₆ H ₂₈ O ₁₀	Ikarisioside A	-	-	0.03%
14.045	488.20476	C ₂₆ H ₃₂ O ₉	Terretonin	T	-	-
14.277	444.17847	C ₂₄ H ₂₈ O ₈	Astellolide F	-	0.02%	-
14.318	178.06285	C ₁₀ H ₁₀ O ₃	4-Methoxycinnamic acid	-	0.01%	-
14.364	312.13574	C ₁₉ H ₂₀ O ₄	Desmosdumotin C	T	-	0.02%
14.472	376.1882	C ₂₂ H ₂₄ N ₄ O ₂	N-{(3S,5S)-1-Methyl-5-[3-(4-methylphenyl)-1,2,4-oxadiazol-5-yl]-3-pyrrolidinyl}-2-phenylacetamide	-	0.05%	-
14.475	208.10971	C ₁₂ H ₁₆ O ₃	β-Asarone	-	0.04%	-
14.561	226.1203	C ₁₂ H ₁₈ O ₄	Allixin	-	-	0.03%
14.742	584.22534	C ₃₁ H ₃₆ O ₁₁	hemsleyanoside	-	0.02%	-
15.119	456.1776	C ₂₅ H ₂₈ O ₈	Lobaric acid	-	-	0.02%
15.874	328.2249	C ₁₈ H ₃₂ O ₅	Corchorifatty acid F	T	0.01%	0.29%
15.912	452.18324	C ₂₆ H ₂₈ O ₇	Derrichalcone	T	-	-

16.002	444.2512	C ₂₆ H ₃₆ O ₆	Pyrenulic acid C	-	-	0.19%
16.09	212.0947	C ₁₃ H ₁₂ N ₂ O	Harmine	-	-	0.08%
16.301	470.1941	C ₂₆ H ₃₀ O ₈	Limonin	-	-	0.14%
16.382	212.1407	C ₁₂ H ₂₀ O ₃	Cucurbic acid	-	-	0.01%
16.478	540.1663	C ₂₅ H ₃₂ O ₁₁ S	Sumalarin B	-	-	0.02%
16.51	256.07345	C ₁₅ H ₁₂ O ₄	Isoliquiritigenin	-	T	0.01%
16.532	316.1308	C ₁₈ H ₂₀ O ₅	Methylodoratol	-	-	0.02%
16.697	498.1884	C ₂₇ H ₃₀ O ₉	Solanoeclepin A	-	-	0.13%
16.787	472.2097	C ₂₆ H ₃₂ O ₈	Kushenol H	-	-	0.07%
16.844	344.0532	C ₁₇ H ₁₂ O ₈	3,4,3'-Tri-O-methylellagic acid	-	-	0.01%
16.889	300.1361	C ₁₈ H ₂₀ O ₄	Angoletin	-	-	T
16.968	286.08397	C ₁₆ H ₁₄ O ₅	Homobutein	-	T	0.01%
17.064	440.1828	C ₂₅ H ₂₈ O ₇	Lonchocarpol E	-	-	0.15%
17.209	544.2668	C ₃₀ H ₄₀ O ₉	Physagulin F	-	-	0.10%
17.217	149.0839	C ₉ H ₁₁ N O	Venoterpine	-	-	0.05%
17.219	184.0997	C ₁₂ H ₁₂ N ₂	Harmalan	-	-	0.11%
17.237	822.40293	C ₄₂ H ₆₂ O ₁₆	Glycyrrhizin	T	-	-
17.253	281.1408	C ₁₈ H ₁₉ N O ₂	Floribundine	-	-	0.01%
17.316	180.11485	C ₁₁ H ₁₆ O ₂	Jasmolone	-	0.61%	1.48%
17.341	310.12026	C ₁₉ H ₁₈ O ₄	Castillene B	T	-	-
17.368	282.12542	C ₁₈ H ₁₈ O ₃	Ohobanin	0.01%	T	0.09%
17.481	136.05228	C ₈ H ₈ O ₂	4-Methoxybenzaldehyde	-	0.04%	0.83%
17.615	188.0835	C ₁₂ H ₁₂ O ₂	Trigoforin	-	-	0.11%
17.633	286.2141	C ₁₆ H ₃₀ O ₄	Hexadecanedioic acid	-	-	0.04%
17.709	540.199	C ₂₉ H ₃₂ O ₁₀	Pilosanol A	-	-	0.03%
17.755	284.14097	C ₁₈ H ₂₀ O ₃	Minquartynoic acid	T	-	-
17.763	342.1465	C ₂₀ H ₂₂ O ₅	Brosimacutin C	-	-	0.03%
17.878	408.2296	C ₂₆ H ₃₂ O ₄	Methylinderatin	-	-	0.05%
17.902	424.1881	C ₂₅ H ₂₈ O ₆	Paratocarpin G	T	-	-
17.949	456.21436	C ₂₆ H ₃₂ O ₇	Antiarone J	-	0.54%	-
18.124	372.2509	C ₂₀ H ₃₆ O ₆	Sterebin Q4	-	-	0.01%
18.164	328.1309	C ₁₉ H ₂₀ O ₅	2',3',4',6'-Tetramethoxychalcone	-	-	0.05%

18.237	428.1831	C ₂₄ H ₂₈ O ₇	Heteroflavanone B	-	-	0.05%
18.392	292.2035	C ₁₈ H ₂₈ O ₃	9S,13R-12-Oxophytodienoic acid	-	-	0.15%
18.409	296.1411	C ₁₉ H ₂₀ O ₃	(1E)-1,7-bis(4-hydroxyphenyl) hept-1-en-3-one	-	0.60%	-
18.442	342.11601	C ₁₂ H ₂₂ O ₁₁	D-(+)-Maltose	-	0.51%	-
18.444	141.1152	C ₈ H ₁₅ N O	(R)-Pelletierine	-	-	0.03%
18.47	466.19888	C ₂₇ H ₃₀ O ₇	Eriotriochin	-	0.50%	-
18.513	288.2299	C ₁₆ H ₃₂ O ₄	(S)-10,16-Dihydroxyhexadecanoic acid	-	-	0.03%
18.542	296.141	C ₁₉ H ₂₀ O ₃	(1E)-1,7-bis(4-hydroxyphenyl) hept-1-en-3-one	-	-	0.56%
18.605	414.2037	C ₂₄ H ₃₀ O ₆	Bis(4-ethylbenzylidene) sorbitol	-	-	1.96%
18.712	268.1462	C ₁₈ H ₂₀ O ₂	Diethylstilbestrol	-	-	0.07%
18.72	268.13078	C ₁₄ H ₂₀ O ₅	Kamahine C	0.02%	0.01%	-
18.735	278.22429	C ₁₈ H ₃₀ O ₂	alpha-Linolenic acid	-	0.51%	0.22%
18.748	208.10964	C ₁₂ H ₁₆ O ₃	Isoelemicin	0.01%	-	0.19%
18.767	526.25646	C ₃₀ H ₃₈ O ₈	Kosamol A	-	0.52%	-
18.814	144.1147	C ₈ H ₁₆ O ₂	Caprylic acid	-	-	0.01%
18.824	300.0997	C ₁₇ H ₁₆ O ₅	2',4'-Dihydroxy-3,4-dimethoxychalcone	-	-	0.07%
18.863	134.073	C ₉ H ₁₀ O	2,4-Dimethylbenzaldehyde	-	-	0.63%
18.865	118.0782	C ₉ H ₁₀	beta-Methylstyrene	-	-	1.98%
18.899	554.28739	C ₃₂ H ₄₂ O ₈	11β-hydroxycolossolactone VIII	0.01%	-	-
18.987	372.1208	C ₂₀ H ₂₀ O ₇	Tangeretin	-	-	0.03%
19.444	132.0573	C ₉ H ₈ O	Cinnamaldehyde	-	-	0.09%
19.605	226.09933	C ₁₅ H ₁₄ O ₂	7-Hydroxyflavan	-	0.84%	-
19.657	304.1669	C ₁₈ H ₂₄ O ₄	2-Hydroxyestriol	-	-	1.12%
19.715	272.1406	C ₁₇ H ₂₀ O ₃	(S)-Verimol F	-	-	0.75%
21.005	592.2693	C ₃₅ H ₃₆ N ₄ O ₅	Pheophorbide a	-	-	0.15%
21.418	356.32872	C ₂₂ H ₄₄ O ₃	2(R)-hydroxydocosanoic acid	T	-	0.04%
22.345	472.3551	C ₃₀ H ₄₈ O ₄	Maslinic acid	-	-	0.64%
Grand Total				100%	100%	100%

Table S2: LC-MS putative identification and % relative abundance of phytochemicals identified in the fruit extracts of *Terminalia chebula*. Compounds less than 0.01% of the total area were considered as trace amounts and denoted as T.

Retention time [min]	Molecular weight	Empirical Formula	Putative Compounds	Relative Abundance (% of Total Area)		
				AQ	MeOH	EtOAc
1.205	114.04278	C ₄ H ₆ N ₂ O ₂	L-3-Cyanoalanine	-	0.04%	-
1.22	87.03192	C ₃ H ₅ N O ₂	2-Aminoacrylic acid	-	0.15%	-
1.221	189.09992	C ₈ H ₁₅ N O ₄	N-Methylcalystegine B2	-	0.18%	-
1.222	276.09543	C ₁₀ H ₁₆ N ₂ O ₇	gamma-Glutamylglutamic acid	-	1.08%	-
1.223	342.11587	C ₁₂ H ₂₂ O ₁₁	α,α -Trehalose	-	3.43%	-
1.224	105.0424	C ₃ H ₇ N O ₃	L-Serine	-	0.03%	-
1.225	215.0791	C ₉ H ₁₃ N O ₅	N-Methacryloyl-L-glutamic acid	-	0.61%	-
1.244	132.04206	C ₅ H ₈ O ₄	Methylsuccinic acid	-	11.54%	-
1.246	210.03738	C ₆ H ₁₀ O ₈	Galactaric acid	-	0.31%	-
1.279	356.13167	C ₁₃ H ₂₄ O ₁₁	4-O-Methylgalactinol	-	0.07%	-
1.296	144.04208	C ₆ H ₈ O ₄	Methylglutamic acid	-	0.29%	-
1.298	196.05798	C ₆ H ₁₂ O ₇	Galactonic acid	-	-	0.10%
1.3	145.08502	C ₅ H ₁₁ N ₃ O ₂	4-Guanidinobutyric acid	-	0.22%	-
1.376	342.11598	C ₁₂ H ₂₂ O ₁₁	Melibiose	-	0.05%	-
1.357	160.03685	C ₆ H ₈ O ₅	Oxoadipic acid	-	-	0.34%
1.383	134.02136	C ₄ H ₆ O ₅	L-(-)-Malic acid	-	-	1.09%
1.428	129.07882	C ₆ H ₁₁ N O ₂	Pipecolic acid	0.02%	0.01%	0.03%
1.444	174.11148	C ₆ H ₁₄ N ₄ O ₂	DL-Arginine	1.45%	-	-
1.479	132.05333	C ₄ H ₈ N ₂ O ₃	Asparagine	0.31%	0.23%	-
1.479	187.1207	C ₉ H ₁₇ N O ₃	(S)-(+)-N-Boc-3-pyrrolidinol	-	0.21%	-
1.481	103.09955	C ₅ H ₁₃ N O	Choline	2.23%	1.61%	-
1.484	182.07877	C ₆ H ₁₄ O ₆	L-Iditol	3.34%	7.32%	7.23%
1.486	90.03157	C ₃ H ₆ O ₃	Glyceraldehyde	5.35%	11.03%	26.76%
1.489	86.03662	C ₄ H ₆ O ₂	gamma-Butyrolactone	0.28%	0.11%	-
1.492	294.10599	C ₁₀ H ₁₈ N ₂ O ₈	Distichonic acid A	0.37%	-	-
1.492	133.03731	C ₄ H ₇ N O ₄	L-Aspartic acid	0.32%	0.16%	0.03%

1.495	147.05287	C ₅ H ₉ N O ₄	L-Glutamic acid	1.67%	1.15%	-
1.496	192.06305	C ₇ H ₁₂ O ₆	Quinic acid	0.39%	-	1.53%
1.501	196.05798	C ₆ H ₁₂ O ₇	Gluconic acid	0.39%	0.18%	-
1.501	117.07878	C ₅ H ₁₁ N O ₂	L-Valine	1.09%	0.90%	-
1.501	129.04249	C ₅ H ₇ N O ₃	L-Pyroglutamic acid	-	0.46%	-
1.505	137.04746	C ₇ H ₇ N O ₂	Trigonelline	0.24%	0.19%	-
1.506	210.03733	C ₆ H ₁₀ O ₈	D-Saccharic acid	1.03%	-	-
1.511	144.04206	C ₆ H ₈ O ₄	5-hydroxy-4-methoxy-5,6-dihydro-2H-pyran-2-one	0.59%	0.64%	-
1.526	104.01072	C ₃ H ₄ O ₄	Malonic acid	0.02%	-	-
1.548	180.06314	C ₆ H ₁₂ O ₆	D-(+)-Glucose	0.88%	-	-
1.554	148.03698	C ₅ H ₈ O ₅	D-Xylono-1,5-lactone	0.28%	-	-
1.562	118.02649	C ₄ H ₆ O ₄	Succinic acid	-	0.04%	0.08%
1.566	90.03152	C ₃ H ₆ O ₃	L-(+)-Lactic acid	-	-	0.34%
1.568	129.04239	C ₅ H ₇ N O ₃	4-Oxoproline	-	-	0.44%
1.572	138.03148	C ₇ H ₆ O ₃	4-Hydroxybenzoic acid	0.23%	0.25%	-
1.572	94.04171	C ₆ H ₆ O	Phenol	0.56%	-	-
1.573	344.07409	C ₁₄ H ₁₆ O ₁₀	Theogallin	-	0.03%	0.02%
1.58	116.01077	C ₄ H ₄ O ₄	Maleic acid	0.68%	-	0.39%
1.58	134.02133	C ₄ H ₆ O ₅	D-(+)-Malic acid	1.77%	1.65%	-
1.601	185.10486	C ₉ H ₁₅ N O ₃	Pseudoecgonine	0.07%	0.02%	0.01%
1.607	155.09432	C ₈ H ₁₃ N O ₂	Arecoline	0.05%	-	-
1.632	115.06327	C ₅ H ₉ N O ₂	L-Proline	-	0.26%	-
1.654	214.13153	C ₁₀ H ₁₈ N ₂ O ₃	Valylproline	-	0.15%	0.22%
1.702	109.05256	C ₆ H ₇ N O	Nicotinyl alcohol	0.31%	0.25%	-
1.745	192.0267	C ₆ H ₈ O ₇	Citric acid	0.97%	-	0.21%
1.748	112.01588	C ₅ H ₄ O ₃	2-Furoic acid	0.64%	0.52%	-
1.748	88.0159	C ₃ H ₄ O ₃	Pyruvic acid	0.15%	0.05%	0.01%
1.751	174.01619	C ₆ H ₆ O ₆	cis-Aconitic acid	0.33%	-	-
1.773	90.03153	C ₃ H ₆ O ₃	L-Lactic acid	0.09%	0.49%	-
1.775	181.07364	C ₉ H ₁₁ N O ₃	L-Tyrosine	0.54%	0.45%	-
1.778	96.02097	C ₅ H ₄ O ₂	2-Furancarboxaldehyde	0.18%	0.20%	0.02%
1.778	129.0424	C ₅ H ₇ N O ₃	D-(+)-Pyroglutamic Acid	0.47%	-	-

1.784	302.06328	C ₁₂ H ₁₄ O ₉	Pyrogallol-2-O-glucuronide	0.07%	-	-
1.785	199.12043	C ₁₀ H ₁₇ N O ₃	Ecgonine methyl ester	0.14%	0.17%	-
1.809	206.04257	C ₇ H ₁₀ O ₇	2-Methylcitric acid	-	0.03%	-
1.82	354.15268	C ₁₄ H ₂₆ O ₁₀	Isopropyl apiosylglucoside	-	0.07%	-
1.847	202.02667	C ₁₁ H ₆ O ₄	Bergaptol	0.02%	T	-
1.849	131.09458	C ₆ H ₁₃ N O ₂	L-Isoleucine	0.12%	0.09%	-
1.887	224.06841	C ₁₁ H ₁₂ O ₅	Elenolide	-	0.01%	-
1.905	236.0684	C ₁₂ H ₁₂ O ₅	Dillapional	-	T	0.01%
1.912	98.03661	C ₅ H ₆ O ₂	5-Hydroxy-4-pentenoic acid d-lactone	0.23%	-	-
1.93	85.08905	C ₅ H ₁₁ N	Piperidine	0.34%	-	0.10%
1.975	149.08397	C ₉ H ₁₁ N O	Venoterpine	0.04%	-	-
2.01	210.05269	C ₁₀ H ₁₀ O ₅	5-Hydroxyferulic acid	-	0.07%	-
2.022	254.07863	C ₆ H ₁₅ N ₄ O ₅ P	L-Phosphoarginine	-	0.01%	-
2.045	294.03749	C ₁₃ H ₁₀ O ₈	Banksiamarin B	0.17%	0.05%	0.13%
2.053	100.05235	C ₅ H ₈ O ₂	Senecioic acid	0.30%	-	-
2.058	174.05268	C ₇ H ₁₀ O ₅	Shikimic acid	2.64%	3.14%	4.80%
2.13	256.05811	C ₁₁ H ₁₂ O ₇	(2R,3S)-Piscidic acid	0.01%	-	-
2.169	115.06323	C ₅ H ₉ N O ₂	Proline	0.28%	-	-
2.175	222.05248	C ₁₁ H ₁₀ O ₅	Isofraxidin	0.02%	0.04%	-
2.176	178.06283	C ₁₀ H ₁₀ O ₃	4-Methoxycinnamic acid	0.01%	0.05%	0.01%
2.18	259.08409	C ₁₄ H ₁₃ N O ₄	Skimmianine	0.02%	-	-
2.184	236.03185	C ₁₁ H ₈ O ₆	Methylspinazarin	-	0.08%	-
2.237	154.02646	C ₇ H ₆ O ₄	Gentisic acid	0.01%	-	0.09%
2.277	165.07876	C ₉ H ₁₁ N O ₂	L-Phenylalanine	0.12%	0.11%	0.10%
2.284	190.02635	C ₁₀ H ₆ O ₄	8H-1,3-Dioxolo[4,5-h][1] benzopyran-8-one	0.26%	-	-
2.285	290.09975	C ₁₂ H ₁₈ O ₈	Osmundalin	0.04%	0.03%	-
2.296	448.15769	C ₁₉ H ₂₈ O ₁₂	8-O-Acetyl shanzhiside methyl ester	0.19%	0.18%	-
2.3	248.06824	C ₁₃ H ₁₂ O ₅	Coriandrone E	0.01%	0.01%	0.01%
2.356	332.07411	C ₁₃ H ₁₆ O ₁₀	6-Galloylglucose	3.74%	0.68%	-
2.38	134.02141	C ₄ H ₆ O ₅	Malic acid	0.08%	-	-
2.444	448.06386	C ₂₀ H ₁₆ O ₁₂	Ellagic acid 2-rhamnoside	0.01%	0.21%	0.33%
2.496	128.04739	C ₆ H ₈ O ₃	Osmundalactone	-	0.01%	-

2.51	292.02177	C ₁₃ H ₈ O ₈	Brevifolincarboxylic acid	0.11%	0.03%	0.61%
2.523	374.12161	C ₁₆ H ₂₂ O ₁₀	Geniposidic acid	T	-	-
2.527	279.11064	C ₁₄ H ₁₇ N O ₅	Niazirin	T	0.07%	-
2.56	288.0844	C ₁₂ H ₁₆ O ₈	Phlorin	0.03%	0.02%	-
2.618	234.01615	C ₁₂ H ₁₀ O S ₂	Arctinol A	T	-	-
2.718	110.03671	C ₆ H ₆ O ₂	Catechol	0.10%	0.11%	0.15%
2.72	154.02652	C ₇ H ₆ O ₄	Protocatechuic acid	0.07%	-	-
2.804	370.05335	C ₁₅ H ₁₄ O ₁₁	2-O-Caffeoylhydroxycitric acid	-	0.43%	-
2.849	314.06336	C ₁₃ H ₁₄ O ₉	Beta-D-Glucopyranuronic acid	0.18%	0.55%	0.49%
2.937	272.05311	C ₁₁ H ₁₂ O ₈	Fukiic acid	0.02%	0.94%	0.77%
3.158	212.06824	C ₁₀ H ₁₂ O ₅	Propyl gallate	0.30%	0.35%	0.12%
3.183	140.04729	C ₇ H ₈ O ₃	Ethyl maltol	T	-	-
3.432	228.14714	C ₁₁ H ₂₀ N ₂ O ₃	Prolylleucine	0.14%	0.16%	0.26%
3.578	112.05237	C ₆ H ₈ O ₂	Sorbic acid	-	0.24%	-
3.578	390.11607	C ₁₆ H ₂₂ O ₁₁	2,3,4,5,6-Penta-O-acetyl-D-glucose	-	-	0.02%
3.583	342.09523	C ₁₅ H ₁₈ O ₉	Glucocaffeic acid	-	0.01%	-
3.696	276.0269	C ₁₄ H ₁₂ O ₂ S ₂	5-(4-Acetoxy-1-butynyl)-2,2'-bithiophene	-	0.01%	-
3.862	162.03152	C ₉ H ₆ O ₃	3 Hydroxycoumarin	0.01%	-	-
4.102	366.14233	C ₁₇ H ₂₂ N ₂ O ₇	2-{2-[5-(Ethoxycarbonyl)-2-morpholinoanilino]-2-oxoethoxy} acetic acid	0.04%	-	-
4.138	312.04826	C ₁₃ H ₁₂ O ₉	Caftaric acid	T	0.08%	-
4.378	348.08452	C ₁₇ H ₁₆ O ₈	3,5,7,3',4',5'-Hexahydroxy-6,8-dimethylflavanone	0.03%	-	-
4.4	277.05821	C ₁₃ H ₁₁ N O ₆	Salfredin C1	0.14%	-	0.03%
4.78	262.13139	C ₁₄ H ₁₈ N ₂ O ₃	5-(tert-butyl)-2-methyl-N-(5-methyl-3-isoxazolyl)-3-furamide	0.06%	-	-
4.847	184.03703	C ₈ H ₈ O ₅	Methyl gallate	0.04%	1.05%	-
4.969	176.06842	C ₇ H ₁₂ O ₅	2-Isopropylmalic acid	-	0.01%	-
4.992	484.08533	C ₂₀ H ₂₀ O ₁₄	1,6-Bis-O-(3,4,5-trihydroxybenzoyl) hexopyranose	6.52%	2.16%	3.78%
5.167	360.10554	C ₁₅ H ₂₀ O ₁₀	Glucosyringic acid	0.08%	0.09%	-
5.539	216.08974	C ₁₂ H ₁₂ N ₂ O ₂	L-1,2,3,4-Tetrahydro-beta-carboline-3-carboxylic acid	-	0.02%	-
5.638	444.19969	C ₂₁ H ₃₂ O ₁₀	Cynaroside A	0.02%	0.02%	-
5.779	478.07474	C ₂₁ H ₁₈ O ₁₃	6-Hydroxyluteolin 6-glucuronide	0.04%	0.03%	-

5.919	432.16322	C ₁₉ H ₂₈ O ₁₁	Zizybeoside I	-	0.01%	-
6.16	168.04204	C ₈ H ₈ O ₄	Isovanillic acid	0.08%	0.08%	-
6.538	187.0632	C ₁₁ H ₉ N O ₂	Indoleacrylic acid	-	0.02%	-
6.726	136.05239	C ₈ H ₈ O ₂	4-Methoxybenzaldehyde	0.12%	0.11%	-
6.909	404.13157	C ₁₇ H ₂₄ O ₁₁	Oleoside 11-methyl ester	T	0.03%	-
6.911	230.10533	C ₁₃ H ₁₄ N ₂ O ₂	(1xi,3xi)-1,2,3,4-Tetrahydro-1-methyl-beta-carboline-3-carboxylic acid	0.04%	-	-
7.074	272.10472	C ₁₆ H ₁₆ O ₄	4'-O-Methyldavidigenin	0.03%	T	-
7.513	196.0733	C ₁₀ H ₁₂ O ₄	Cantharidin	0.10%	0.11%	-
8.848	636.09627	C ₂₇ H ₂₄ O ₁₈	1,3,4-Trigalloyl-β-D-glucopyranose	-	0.07%	0.25%
8.961	478.07436	C ₂₁ H ₁₈ O ₁₃	Quercetin 7-glucuronide	-	-	0.49%
8.973	326.10005	C ₁₅ H ₁₈ O ₈	Melilotoside	0.08%	0.03%	-
8.981	206.05798	C ₁₁ H ₁₀ O ₄	Eugenitol	0.10%	0.03%	0.03%
9.029	338.06378	C ₁₅ H ₁₄ O ₉	Umbelliferone glucuronide	-	0.11%	-
9.206	107.03707	C ₆ H ₅ N O	2-Pyridinecarboxaldehyde	-	0.03%	-
9.316	470.01176	C ₂₁ H ₁₀ O ₁₃	Sanguisorbic acid dilactone	0.56%	0.61%	0.19%
9.343	184.09991	C ₁₂ H ₁₂ N ₂	Harmalan	T	-	-
9.501	196.14612	C ₁₂ H ₂₀ O ₂	Dihydro-5-(2-octenyl)-2(3H)-furanone	-	-	0.01%
9.567	634.08082	C ₂₇ H ₂₂ O ₁₈	Sanguiin H4	-	5.63%	0.54%
9.81	308.05281	C ₁₄ H ₁₂ O ₈	Fulvic acid	0.03%	0.06%	-
9.811	478.07452	C ₂₁ H ₁₈ O ₁₃	Miquelianin	0.37%	0.60%	0.39%
9.818	98.03669	C ₅ H ₆ O ₂	2-Furanmethanol	-	0.21%	-
9.876	246.01651	C ₁₃ H ₁₀ O S ₂	Arctinone	-	0.01%	-
9.902	152.04703	C ₈ H ₈ O ₃	Vanillin	0.16%	0.17%	0.17%
9.92	260.03188	C ₁₃ H ₈ O ₆	Urolithin D	-	0.02%	-
9.921	126.03146	C ₆ H ₆ O ₃	Phloroglucinol	0.07%	0.24%	0.27%
10.043	636.09614	C ₂₇ H ₂₄ O ₁₈	1,2,6-Trigalloyl-beta-D-glucopyranose	0.11%	1.42%	2.22%
10.158	634.08037	C ₂₇ H ₂₂ O ₁₈	Corilagin	-	0.15%	-
10.191	242.07893	C ₁₁ H ₁₄ O ₆	Genipinic acid	0.03%	-	-
10.256	296.05303	C ₁₃ H ₁₂ O ₈	Caffeoylmalic acid	0.22%	0.02%	0.06%
10.256	224.03176	C ₁₀ H ₈ O ₆	Dehydrochorismic acid	0.02%	-	-
10.29	233.06862	C ₁₂ H ₁₁ N O ₄	Casimiroin	T	-	-
10.419	96.02088	C ₅ H ₄ O ₂	2H-Pyran-2-one	0.05%	-	-

10.419	484.08522	C ₂₀ H ₂₀ O ₁₄	Hamamelitannin	0.02%	0.11%	-
10.421	126.0316	C ₆ H ₆ O ₃	Pyrogallol	6.29%	3.82%	4.87%
10.422	296.05248	C ₁₃ H ₁₂ O ₈	cis-Coutaric acid	0.31%	0.93%	1.05%
10.445	262.01122	C ₁₃ H ₁₀ O ₂ S ₂	Arctinone A	-	0.03%	-
10.476	636.09612	C ₂₇ H ₂₄ O ₁₈	1,4,6-Trigalloyl-beta-D-glucopyranose	-	-	0.63%
10.55	601.99658	C ₂₈ H ₁₀ O ₁₆	Diellagilactone	1.13%	0.60%	-
10.68	211.11067	C ₁₃ H ₁₃ N ₃	N,N'-Diphenylguanidine	0.03%	-	-
10.668	448.10005	C ₂₁ H ₂₀ O ₁₁	(1ξ)-1,5-Anhydro-1-[2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4-oxo-4H-chromen-8-yl]-D-galactitol	-	-	0.06%
10.754	636.09608	C ₂₇ H ₂₄ O ₁₈	1,3,6-Tri-O-galloyl-beta-D-glucose	0.64%	-	-
10.785	198.05265	C ₉ H ₁₀ O ₅	Syringic acid	0.35%	0.44%	0.48%
10.885	306.03729	C ₁₄ H ₁₀ O ₈	2-(3,4-Dihydroxybenzoyloxy)-4,6-dihydroxybenzoate	-	0.45%	-
10.967	236.03182	C ₁₁ H ₈ O ₆	6-Methoxy-8-hydroxyisocoumarin-3-carboxylic acid	-	0.07%	0.11%
11.305	170.02138	C ₇ H ₆ O ₅	Phloroglucinic acid	0.98%	0.83%	1.24%
11.091	610.1535	C ₂₇ H ₃₀ O ₁₆	Rutin	-	0.03%	0.08%
11.176	432.10539	C ₂₁ H ₂₀ O ₁₀	Vitexin	-	0.05%	-
11.323	162.05261	C ₆ H ₁₀ O ₅	2-Hydroxyadipic acid	T	0.85%	-
11.361	116.01079	C ₄ H ₄ O ₄	Fumaric acid	0.01%	0.63%	-
11.41	194.05781	C ₁₀ H ₁₀ O ₄	Ferulic acid	0.04%	0.02%	-
11.444	236.06825	C ₁₂ H ₁₂ O ₅	1-{4-hydroxy-2-oxo-6-[(1E)-prop-1-en-1-yl]-2H-pyran-3-yl} butane-1,2-dione	0.03%	0.03%	-
11.448	302.04213	C ₁₅ H ₁₀ O ₇	Quercetin	0.02%	-	-
11.485	164.04731	C ₉ H ₈ O ₃	2-Hydroxycinnamic acid	-	0.03%	-
11.556	478.11088	C ₂₂ H ₂₂ O ₁₂	6-O-[(2E)-3-(4-Hydroxyphenyl)-2-propenoyl]-1-O-(3,4,5-trihydroxybenzoyl)hexopyranose	-	-	0.14%
11.558	676.23652	C ₃₃ H ₄₀ O ₁₅	Icariin	-	0.01%	-
11.589	170.02147	C ₇ H ₆ O ₅	Gallic acid	23.90%	1.90%	1.56%
11.675	264.08989	C ₁₆ H ₁₂ N ₂ O ₂	Perlolyrine	-	0.01%	-
11.699	540.22102	C ₂₆ H ₃₆ O ₁₂	Sambacin	-	-	0.01%
11.702	630.12227	C ₂₉ H ₂₆ O ₁₆	Isorhamnetin 3- (6"-galloylglucoside)	-	T	0.01%
11.738	146.05786	C ₆ H ₁₀ O ₄	2-Methylglutaric acid	-	0.01%	-

11.756	216.0994	C ₁₀ H ₁₆ O ₅	(4S,5S,8S,10R)-4,5,8-trihydroxy-10-methyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one	0.06%	-	1.23%
11.822	462.07961	C ₂₁ H ₁₈ O ₁₂	Aureusidin 6-glucuronide	-	-	0.04%
11.905	286.04729	C ₁₅ H ₁₀ O ₆	Maritimetin	T	0.01%	0.01%
11.906	594.15829	C ₂₇ H ₃₀ O ₁₅	Palasitrin	0.01%	-	0.03%
11.921	316.02205	C ₁₅ H ₈ O ₈	2-hydroxyemodic acid	-	0.01%	-
11.938	176.04708	C ₁₀ H ₈ O ₃	4-Methylumbelliferone hydrate	0.03%	0.03%	-
11.949	280.05779	C ₁₃ H ₁₂ O ₇	D-Malic acid p-coumarate	-	-	0.09%
11.953	310.10477	C ₁₅ H ₁₈ O ₇	(E)-1-O-Cinnamoyl-beta-D-glucose	-	-	1.67%
11.955	102.0315	C ₄ H ₆ O ₃	2-Ketobutyric acid	-	-	0.05%
12.024	201.13638	C ₁₀ H ₁₉ N O ₃	Capryloylglycine	-	-	0.04%
12.05	275.11535	C ₁₅ H ₁₇ N O ₄	(±)-Ribaline	0.01%	-	-
12.054	450.16789	C ₂₆ H ₂₆ O ₇	Artonin T	-	T	-
12.095	270.08895	C ₁₆ H ₁₄ O ₄	Isoliquiritigenin 4-methyl ether	T	-	T
12.141	584.1169	C ₂₈ H ₂₄ O ₁₄	2"-O-Galloylisovitexin	-	-	0.01%
12.147	538.20527	C ₂₆ H ₃₄ O ₁₂	Diosbulbinoside F	T	-	-
12.147	256.07309	C ₁₅ H ₁₂ O ₄	Isoliquiritigenin	T	-	-
12.155	436.10094	C ₂₀ H ₂₀ O ₁₁	Taxifolin 3-apioside	-	0.01%	-
12.184	280.09477	C ₁₄ H ₁₆ O ₆	Gravolenic acid	-	T	-
12.185	302.00627	C ₁₄ H ₆ O ₈	Ellagic acid	8.39%	10.46%	11.96%
12.201	220.07336	C ₁₂ H ₁₂ O ₄	Eugenitin	-	-	0.04%
12.233	262.0476	C ₁₃ H ₁₀ O ₆	Maclurin	0.04%	-	-
12.252	126.03158	C ₆ H ₆ O ₃	1,2,3-Trihydroxybenzene	0.10%	0.15%	-
12.254	148.05223	C ₉ H ₈ O ₂	trans-Cinnamic acid	0.76%	0.96%	0.87%
12.255	160.05226	C ₁₀ H ₈ O ₂	6-Methylcoumarin	0.02%	0.01%	-
12.282	374.1364	C ₂₀ H ₂₂ O ₇	8-Hydroxypinoresinol	-	0.26%	-
12.29	318.11033	C ₁₇ H ₁₈ O ₆	Protofarrerol	T	-	0.03%
12.331	174.08908	C ₈ H ₁₄ O ₄	Suberic acid	0.01%	-	0.10%
12.396	262.14158	C ₁₂ H ₂₂ O ₆	Phaseolic acid	0.01%	-	-
12.411	146.03665	C ₉ H ₆ O ₂	Coumarin	0.12%	0.06%	-
12.436	126.10434	C ₈ H ₁₄ O	(E)-2-octenal	-	-	0.06%
12.48	402.15266	C ₁₈ H ₂₆ O ₁₀	Benzyl beta-primeveroside	0.01%	-	-
12.487	226.06259	C ₁₄ H ₁₀ O ₃	2-Methoxyxanthone	0.01%	-	-

12.492	244.07339	C ₁₄ H ₁₂ O ₄	3,3',4'5-Tetrahydroxystilbene	0.01%	0.01%	-
12.502	114.03157	C ₅ H ₆ O ₃	Norfuraneol	0.06%	0.55%	0.08%
12.503	132.0574	C ₉ H ₈ O	Cinnamaldehyde	0.01%	-	0.01%
12.503	192.07847	C ₁₁ H ₁₂ O ₃	(R)-Shinanolone	0.04%	0.03%	0.05%
12.504	310.10483	C ₁₅ H ₁₈ O ₇	(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl) oxan-2-yl (2E)-3-phenylprop-2-enoate	2.25%	-	-
12.547	288.06332	C ₁₅ H ₁₂ O ₆	2,4,6-Trihydroxy-2-(4-hydroxybenzyl)-1-benzofuran-3(2H)-one	0.03%	-	-
12.55	344.1256	C ₁₉ H ₂₀ O ₆	Okanin 3,4,3',4'-tetramethyl ether	0.02%	-	-
12.552	374.13624	C ₂₀ H ₂₂ O ₇	3-hydroxy-3,4-bis[(4-hydroxy-3-methoxyphenyl)methyl] oxolan-2-one	0.14%	-	-
12.558	362.17308	C ₂₀ H ₂₆ O ₆	Secoisolariciresinol	-	0.01%	-
12.573	388.11562	C ₂₀ H ₂₀ O ₈	Sigmoidin G	-	T	-
12.593	436.13688	C ₂₁ H ₂₄ O ₁₀	Nothofagin	-	-	0.12%
12.642	150.06799	C ₉ H ₁₀ O ₂	Hydrocinnamic acid	0.01%	0.03%	0.01%
12.666	646.37157	C ₃₆ H ₅₄ O ₁₀	Gypsogenin 3-O-b-D-glucuronide	-	T	-
12.721	680.37692	C ₃₆ H ₅₆ O ₁₂	Tenuifolin	-	0.11%	0.37%
12.739	550.16884	C ₂₆ H ₃₀ O ₁₃	Licuroside	0.01%	-	-
12.739	442.34453	C ₂₉ H ₄₆ O ₃	4alpha-Methylzymosterol-4-carboxylate	-	T	-
12.745	188.10473	C ₉ H ₁₆ O ₄	Azelaic acid	0.07%	-	0.35%
12.799	218.05765	C ₁₂ H ₁₀ O ₄	Liqcoumarin	T	0.01%	T
12.8	486.33397	C ₃₀ H ₄₆ O ₅	Bassic acid	-	-	0.05%
12.889	346.1052	C ₁₈ H ₁₈ O ₇	Hamilcone	0.02%	-	0.01%
12.914	190.13544	C ₁₃ H ₁₈ O	beta-Damascenone	-	0.02%	0.06%
12.915	666.39739	C ₃₆ H ₅₈ O ₁₁	Chebuloide II	-	3.85%	-
12.915	326.15138	C ₂₀ H ₂₂ O ₄	2-[1-(2H-1,3-benzodioxol-5-yl) propan-2-yl]-6-methoxy-4-(prop-2-en-1-yl) phenol	0.03%	0.03%	-
12.929	356.03763	C ₁₄ H ₁₂ O ₁₁	(+)-Chebulic acid	3.98%	1.40%	2.88%
12.967	330.14651	C ₁₉ H ₂₂ O ₅	Hericenone A	-	0.03%	-
12.969	440.32894	C ₂₉ H ₄₄ O ₃	13'-Hydroxy-alpha-tocotrienol	-	-	0.05%
12.969	504.34417	C ₃₀ H ₄₈ O ₆	Madecassic acid	-	-	1.42%
12.971	202.13522	C ₁₄ H ₁₈ O	(±)-Anisoxide	-	-	0.05%
12.973	244.14583	C ₁₆ H ₂₀ O ₂	Lahorenoic acid C	-	-	0.02%

12.975	674.36638	C ₃₇ H ₅₄ O ₁₁	Cimicifugoside	T	-	-
13.01	358.14147	C ₂₀ H ₂₂ O ₆	Pedicellin	-	0.01%	-
13.081	462.11632	C ₂₂ H ₂₂ O ₁₁	Azalein	-	0.03%	-
13.084	191.09447	C ₁₁ H ₁₃ N O ₂	5-Methoxytryptophol	-	-	0.02%
13.208	288.06318	C ₁₅ H ₁₂ O ₆	Eriodictyol	-	-	0.27%
13.238	148.05233	C ₉ H ₈ O ₂	Cinnamic acid	0.07%	-	0.50%
13.245	360.15695	C ₂₀ H ₂₄ O ₆	Brosimacutin H	0.01%	-	-
13.279	310.12035	C ₁₉ H ₁₈ O ₄	Castillene B	0.01%	-	-
13.354	314.1154	C ₁₈ H ₁₈ O ₅	Crotaoprostrin	-	-	0.01%
13.431	298.08379	C ₁₇ H ₁₄ O ₅	Isonobavachalcone	T	-	-
13.443	460.13716	C ₂₃ H ₂₄ O ₁₀	7-Hydroxy-5,6-dimethoxyflavone 7-glucoside	-	0.01%	-
13.451	274.08371	C ₁₅ H ₁₄ O ₅	Phloretin	0.01%	0.02%	0.01%
13.536	462.11641	C ₂₂ H ₂₂ O ₁₁	Leptosin	0.01%	0.06%	-
13.562	302.07902	C ₁₆ H ₁₄ O ₆	2,6,3'-Trihydroxy-4'-methoxy-2-benzylcoumaranone	-	0.01%	-
13.59	302.04255	C ₁₅ H ₁₀ O ₇	Bracteatin	0.01%	0.01%	-
13.592	450.07961	C ₂₀ H ₁₈ O ₁₂	Quercetin 4'-galactoside	0.01%	-	-
13.642	514.18403	C ₂₇ H ₃₀ O ₁₀	Baohuoside 1	T	0.01%	-
13.678	568.12178	C ₂₈ H ₂₄ O ₁₃	Isoorientin 2"-p-hydroxybenzoate	-	-	0.04%
13.703	280.13067	C ₁₅ H ₂₀ O ₅	Artabsinolide A	-	-	0.02%
13.805	444.10499	C ₂₂ H ₂₀ O ₁₀	3'-O-Methyldehamnosylmaysin	0.04%	0.12%	0.08%
13.805	292.09447	C ₁₅ H ₁₆ O ₆	(S)-Angelicaic	0.05%	-	-
13.806	462.11629	C ₂₂ H ₂₂ O ₁₁	6-O-[(2E)-3-Phenyl-2-propenoyl]-1-O-(3,4,5-trihydroxybenzoyl)-β-D-glucopyranose	0.08%	1.02%	0.18%
13.855	227.09438	C ₁₄ H ₁₃ N O ₂	Koenoline	T	0.02%	-
13.936	614.12731	C ₂₉ H ₂₆ O ₁₅	6-Cinnamoyl-1,2-digalloylglucose	-	0.07%	-
13.971	586.24153	C ₃₁ H ₃₈ O ₁₁	Baccatin III	T	-	0.01%
14.036	664.38246	C ₃₆ H ₅₆ O ₁₁	Medicagenic acid 3-O-beta-D-glucoside	T	-	-
14.066	434.12116	C ₂₁ H ₂₂ O ₁₀	Monospermoside	T	-	-
14.078	534.28285	C ₂₉ H ₄₂ O ₉	Corchoroside A	-	-	0.02%
14.122	578.16359	C ₂₇ H ₃₀ O ₁₄	(1S)-1,5-Anhydro-2-O-(6-deoxy-α-L-mannopyranosyl)-1-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-6-yl]-D-glucitol	0.03%	-	-

14.277	340.13047	C ₂₀ H ₂₀ O ₅	Bakuchalcone	0.01%	-	0.01%
14.358	272.06832	C ₁₅ H ₁₂ O ₅	Naringenin	-	-	0.18%
14.367	470.33907	C ₃₀ H ₄₆ O ₄	Glycyrrhetic acid	-	0.08%	0.01%
14.413	188.15618	C ₁₄ H ₂₀	Congressane		0.01%	0.06%
14.49	614.12725	C ₂₉ H ₂₆ O ₁₅	2-Cinnamoyl-1,6-digalloyl-beta-D-glucopyranose	-	-	0.07%
14.495	148.05227	C ₉ H ₈ O ₂	p-Coumaraldehyde	0.84%	0.15%	0.96%
14.57	614.2364	C ₃₂ H ₃₈ O ₁₂	chrysoeriol 7-O-neohesperidoside	-	T	-
14.618	322.08357	C ₁₉ H ₁₄ O ₅	Ovalitenin C	T	-	-
14.783	234.16167	C ₁₅ H ₂₂ O ₂	Valerenic acid	-	-	0.13%
14.895	518.324	C ₃₀ H ₄₆ O ₇	Perulactone	0.12%	T	0.06%
14.928	202.17175	C ₁₅ H ₂₂	Rulepidadiene B	-	-	0.08%
14.93	222.16153	C ₁₄ H ₂₂ O ₂	Rishitin	-	-	0.04%
14.933	330.24009	C ₁₈ H ₃₄ O ₅	9,12,13-TriHOME	-	-	0.05%
15.046	426.09477	C ₂₂ H ₁₈ O ₉	Epiatzelechin 3-O-gallate	-	-	0.01%
15.126	342.11024	C ₁₉ H ₁₈ O ₆	Rengasin trimethyl ether	-	T	-
15.398	470.30287	C ₂₉ H ₄₂ O ₅	17,23-Epoxy-29-hydroxy-27-norlanost-8-ene-3,15,24-trione	T	-	-
15.448	424.33398	C ₂₉ H ₄₄ O ₂	alpha-Tocotrienol	-	0.02%	0.07%
15.454	650.4026	C ₃₆ H ₅₈ O ₁₀	Pedunculoside	-	1.18%	2.61%
15.624	296.10439	C ₁₈ H ₁₆ O ₄	5,7-Dimethoxy-6-C-methylflavone	-	-	0.01%
15.704	316.13099	C ₁₈ H ₂₀ O ₅	O-Methylodoratol	-	T	-
16.257	738.41926	C ₃₉ H ₆₂ O ₁₃	Isonuatigenin 3-[rhamnosyl-(1->2)-glucoside]	-	0.04%	0.12%
16.585	330.24071	C ₁₈ H ₃₄ O ₅	(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid	-	0.03%	0.33%
15.825	346.14158	C ₂₀ H ₁₈ N ₄ O ₂	Lepidine B	-	-	0.01%
16.852	260.17732	C ₁₇ H ₂₄ O ₂	Falcarindiol	-	-	0.01%
16.854	270.21926	C ₁₆ H ₃₀ O ₃	3-Oxohexadecanoic acid	-	0.01%	-
16.876	252.20856	C ₁₆ H ₂₈ O ₂	Isoambrettolide	-	-	0.32%
16.942	406.28628	C ₂₈ H ₃₈ O ₂	Gymnasterone D	-	0.01%	-
17.155	246.08918	C ₁₄ H ₁₄ O ₄	Marmesin	-	T	-
17.244	288.22977	C ₁₆ H ₃₂ O ₄	(S)-10,16-Dihydroxyhexadecanoic acid	0.03%	-	0.73%
17.275	342.14638	C ₂₀ H ₂₂ O ₅	Brosimacutin C	-	T	-
17.276	180.11471	C ₁₁ H ₁₆ O ₂	Jasmolone	0.05%	-	-
17.30	248.14064	C ₁₅ H ₂₀ O ₃	(S)-Pterosin A	0.02%	-	-

17.31	504.34409	C ₃₀ H ₄₈ O ₆	Protobassic acid	1.26%	0.02%	0.01%
17.33	468.32326	C ₃₀ H ₄₄ O ₄	Glabrolide	0.87%	-	3.19%
17.33	502.32964	C ₃₀ H ₄₆ O ₆	Medicagenic acid	-	T	0.07%
17.331	200.15605	C ₁₅ H ₂₀	(S)-gamma-Calacorene	0.02%	-	0.29%
17.363	696.40877	C ₃₇ H ₆₀ O ₁₂	Momordicoside E	-	0.01%	0.04%
17.411	822.40306	C ₄₂ H ₆₂ O ₁₆	Glycyrrhizin	0.01%	-	-
17.489	212.09457	C ₁₃ H ₁₂ N ₂ O	Harmine	T	-	0.02%
17.491	284.14093	C ₁₈ H ₂₀ O ₃	(S)-17-Hydroxy-9,11,13,15-octadecatetraynoic acid	-	-	0.13%
17.496	368.16222	C ₂₂ H ₂₄ O ₅	4'-O-Methylxanthohumol	-	T	-
17.595	254.15153	C ₁₄ H ₂₂ O ₄	(2R,5R,6R)-3-[(1E,3E)-hepta-1,3-dien-1-yl]-5,6-dihydroxy-2-(hydroxymethyl) cyclohexan-1-one	-	-	0.46%
17.621	326.11524	C ₁₉ H ₁₈ O ₅	Eucalyptin	-	T	-
17.626	286.08357	C ₁₆ H ₁₄ O ₅	Homobutein	-	-	0.01%
17.635	282.12541	C ₁₈ H ₁₈ O ₃	Ohobanin	T	-	0.06%
17.671	652.27302	C ₃₂ H ₄₄ O ₁₄	Dicrocin	-	-	0.03%
17.847	326.11506	C ₁₉ H ₁₈ O ₅	7-{[(2E)-3-methyl-4-(4-methyl-5-oxo-2,5-dihydrofuran-2-yl) but-2-en-1-yl]oxy}-2H-chromen-2-one	0.02%	-	-
17.946	476.35021	C ₂₉ H ₄₈ O ₅	Homodolichosterone	-	-	T
17.949	224.18904	C ₁₃ H ₂₄ N ₂ O	Cuscohygrine	-	0.28%	-
17.956	141.11525	C ₈ H ₁₅ N O	(R)-Pelletierine	-	-	0.02%
18.237	312.13615	C ₁₉ H ₂₀ O ₄	Desmosdumotin C	T	-	0.02%
18.269	268.14619	C ₁₈ H ₂₀ O ₂	Diethylstilbestrol	-	-	0.02%
18.292	546.35535	C ₃₂ H ₅₀ O ₇	Hovenidulcigenin B	0.04%	-	-
18.339	236.1776	C ₁₅ H ₂₄ O ₂	Capsidiol	-	-	0.02%
18.346	268.13069	C ₁₄ H ₂₀ O ₅	Kamahine C	-	0.01%	0.15%
18.363	336.0994	C ₂₀ H ₁₆ O ₅	Ciliatin A	-	0.01%	-
18.455	328.2249	C ₁₈ H ₃₂ O ₅	Corchorifatty acid F	0.05%	0.01%	0.24%
18.498	340.09447	C ₁₉ H ₁₆ O ₆	Ambanol	-	0.01%	-
18.501	314.2455	C ₁₈ H ₃₄ O ₄	(+/-)9,10-dihydroxy-12Z-octadecenoic acid	-	-	0.30%
18.507	484.31803	C ₃₀ H ₄₄ O ₅	Liquoric acid	T	0.01%	0.04%
18.623	488.35017	C ₃₀ H ₄₈ O ₅	Pitheduloside I	T	0.06%	0.11%
18.792	278.22417	C ₁₈ H ₃₀ O ₂	α -Eleostearic acid	0.02%	0.03%	0.35%

19.621	272.14089	C ₁₇ H ₂₀ O ₃	(S)-Verimol F	0.01%	-	-
19.641	226.09903	C ₁₅ H ₁₄ O ₂	7-Hydroxyflavan	0.03%	-	0.05%
23.2	410.31819	C ₂₈ H ₄₂ O ₂	gamma-Tocotrienol	-	-	0.06%
Grand Total				100%	100%	100%