

Table S1 The identification results of *Cimicifugae Rhizoma* extract

Label	Component	Formula	mass (Da)	<i>m/z</i> (precursor ion)	Mass error (ppm)	Observed RT (min)	Adducts	MS/MS Fragment (product ion)	Reference
1	Norcimifugin	C ₁₅ H ₁₆ O ₆	292.0947	291.0863	-3.8	20.45	-H	253.0358/191.0351	
2	12β-O- acetyl-Cimiacerin A	C ₃₇ H ₅₆ O ₁₁	676.3823	677.3877	-2.7	27.93	+H	449.3067/195.1211	[1]
3	12β-O-acetyl-Cimiacerin B	C ₃₇ H ₅₈ O ₁₁	678.3979	677.3903	-0.5	36.79	-H	617.3696/59.0132	[1]
4	12β-hydroxycimigenol arabinopyranoside	C ₃₅ H ₅₆ O ₁₀	636.3874	635.3801	0.0	32.93	-H	577.3382	[2]
5	12β- hydroxycimigenol glucoside	C ₃₅ H ₅₆ O ₁₀	636.3874	635.3802	0.2	31.10	-H	577.3383	[1]
6	15α-Hydroxyl cimicifugoside H ₂	C ₃₅ H ₅₄ O ₁₁	650.3666	649.3599	0.8	25.15	-H	633.3650	[3]
7	2'-O- Acetyl- cimicifugoside H ₁	C ₃₇ H ₅₄ O ₁₀	658.3717	659.375	-6.1	31.09	+H	433.3119/184.0773	
8	23-Epi-26-Dehydroxyacortin	C ₃₇ H ₅₆ O ₁₀	660.3874	659.3804	0.4	38.50	-H	599.3594/559.3292	[2]
9	24-O-acetyl-7,8-Didehydrocimigenol xyloside	C ₃₇ H ₅₈ O ₁₁	678.3979	677.3906	-0.1	33.62	-H	617.3700/59.0133	[2]
10	24-O-acetyl-Cimifugin-xyloside	C ₃₇ H ₆₀ O ₁₁	680.4136	679.4049	-2.0	37.19	-H	619.3837	[2]
11	25-O-acetyl-7,8-Didehydrocimigenol xyloside	C ₃₇ H ₅₆ O ₁₀	660.3874	659.3804	0.5	39.25	-H	599.3590/559.3289	[1]
12	25-O-acetyl-cimifugin-3-O-β-D-xylopyranoside (23R, 24S)	C ₃₇ H ₅₈ O ₁₀	662.4030	663.4069	-5.1	33.88	+H	585.3773/435.3268	[3]
13	Acetylcimigenol 3-O-alpha-L-arabinopyranside	C ₃₇ H ₅₈ O ₁₀	662.4030	663.4072	-4.6	37.18	+H	585.3769/435.3266	[3]

14	25-Anhydrocimigenol-xyloside	C ₃₅ H ₅₄ O ₈	602.3819	603.3881	-1.8	33.73	+H	397.277/184.0772	[3]
15	3'-O-acetyl-Cimicifugoside H1	C ₃₇ H ₅₄ O ₁₀	658.3717	657.3618	-4.0	34.51	-H	303.2335/255.2332/134.0409	
16	7,8-didehydrocimigenol xyloside	C ₃₅ H ₅₄ O ₉	618.3768	619.3829	-1.8	31.10	+H	583.3627/451.3222/433.3119	[2]
17	7β-Hydroxycimigenol xyloside	C ₃₅ H ₅₆ O ₁₀	636.3874	635.3804	0.5	33.62	-H	617.3700/577.3388	[2]
18	Actein	C ₃₇ H ₅₆ O ₁₁	676.3823	677.3884	-1.6	26.75	+H	583.3632/433.3121/451.3223	
19	Cimigenol xyloside	C ₃₅ H ₅₆ O ₉	620.3924	643.3826	1.5	28.00	+Na, +H	435.3249	
20	Cimiside A	C ₃₅ H ₅₆ O ₁₀	636.3874	635.3806	0.8	28.19	-H	577.3391	[1]
21	Cimiside C	C ₄₃ H ₇₀ O ₁₆	842.4664	841.4591	0.0	31.48	-H	637.3950/447.3115	
22	Cimiside D	C ₄₃ H ₇₀ O ₁₆	842.4664	841.4594	0.4	34.22	-H	677.3913	
23	Cimiside F	C ₃₆ H ₅₈ O ₁₀	650.4030	673.3917	-0.8	32.47	+Na	435.3277	
24	Cimicifugoside H1	C ₃₅ H ₅₂ O ₉	616.3611	615.3527	-1.8	36.34	-H	369.2440	[1]
25	Cimicifugoside H2	C ₃₅ H ₅₄ O ₁₀	634.3717	633.3644	0.0	27.78	-H	501.2871/369.2438	[1]
26	Cimicifugine	C ₃₅ H ₅₁ NO ₈	613.3615	614.3685	-0.4	22.45	+H	596.3591/446.3082	[4]
27	Cimicifugic acid B	C ₂₁ H ₂₀ O ₁₁	448.1006	447.0944	2.4	23.53	-H	149.0465/89.0243	[3]
28	Neocimiside	C ₃₂ H ₄₈ O ₉	576.3298	575.323	0.7	27.78	-H		
29	Cimaroside V	C ₄₇ H ₇₆ O ₁₉	944.4981	943.4941	3.5	30.82	-H	781.4358	[3]
30	Cimaroside VI	C ₃₈ H ₆₀ O ₁₁	692.4136	693.4202	-0.9	35.22	+H	469.3326/451.3223/433.3121	
31	Cimaroside VII	C ₄₃ H ₇₀ O ₁₆	842.4664	841.4601	1.2	33.7	-H	577.3389	
32	Cimaroside IV	C ₄₃ H ₆₈ O ₁₅	824.4558	825.46	-3.7	31.49	+H		
33	Cimaroside I	C ₃₆ H ₅₈ O ₁₁	666.3979	665.3909	0.4	33.74	-H	619.3822	[2]
34	Cimiacerin A	C ₃₅ H ₅₄ O ₉	618.3768	619.3828	-2.0	35.81	+H, +Na	451.3219/433.3117	[3]
35	Cimiacerin B	C ₃₅ H ₅₆ O ₉	620.3924	643.3829	1.9	29.17	+Na, +H	453.3370	[1]
36	Cimidahuside C	C ₃₇ H ₅₈ O ₁₂	694.3928	693.3854	-0.2	27.93	-H	633.3647	[1]
37	Cimidahuside D	C ₃₇ H ₅₆ O ₁₂	692.3772	693.3847	0.3	27.77	+H	657.3600	
38	Cimidahuside E	C ₃₅ H ₅₂ O ₈	600.3662	601.3725	-1.7	35.81	+H	451.3220	[1]
39	Cimidahuside F	C ₃₅ H ₅₂ O ₉	616.3611	617.3677	-1.1	27.87	+H	467.3153	[3]

40	Cimidahuside G	C ₃₅ H ₅₆ O ₉	620.3924	621.3971	-4.3	31.55	+H	585.3776	
41	Cimidahuside H	C ₃₅ H ₅₄ O ₉	618.3768	641.3651	-1.4	35.32	+Na		[3]
42	Cimidahuside J	C ₃₇ H ₅₆ O ₁₁	676.3823	677.388	-2.2	33.47	+H, +Na	635.3802	[3]
43	12β-hydroxycimigenol	C ₃₀ H ₄₈ O ₆	504.3451	503.338	0.5	36.64	-H	445.2962	[1]
44	Dahurinol	C ₃₀ H ₄₈ O ₅	488.3502	487.3418	-2.2	44.27	-H		
45	Cimigenol	C ₃₀ H ₄₈ O ₅	488.3502	489.3561	-2.7	36.04	+H	453.3359	
46	Cimicidanol	C ₃₀ H ₄₄ O ₅	484.3189	485.3239	-4.6	27.83	+H	467.3153/449.3067	[3]
47	Isodahurinol	C ₃₀ H ₄₈ O ₅	488.3502	489.3562	-2.6	31.55	+H	381.2811	[3]
48	3,4-dimethoxycinnamylic alcohol	C ₁₁ H ₁₂ O ₄	208.0736	207.0679	7.6	14.79	-H	151.0400	
49	3-O-Acetyl-caffeic acid	C ₁₁ H ₁₀ O ₅	222.0528	221.0455	-0.4	26.04	-H	193.0508/149.0589	
50	Caffeic acid	C ₉ H ₈ O ₄	180.0423	179.0352	1.1	12.54	-H		standards data
51	Citric acid	C ₆ H ₈ O ₇	192.0270	191.02	1.2	2.15	-H	111.0088	
52	Ferulic acid	C ₁₀ H ₁₀ O ₄	194.0579	193.0509	1.4	19.48	-H		standards data
53	Cimidahurinine	C ₁₄ H ₂₀ O ₈	316.1158	315.1067	-5.7	9.07	-H	153.0558	
54	Paeonol	C ₉ H ₁₀ O ₃	166.0630	165.0556	-0.6	25.08	-H		standards data
55	4-Hydroxyphenylacetic acid	C ₈ H ₈ O ₃	152.0473	151.04	-0.5	11.73	-H		standards data
56	Sinapic acid	C ₁₁ H ₁₂ O ₅	224.0685	223.0616	1.6	16.48	-H		standards data
57	Methyl caffeate	C ₁₀ H ₁₀ O ₄	194.0579	193.0509	1.4	16.17	-H		standards data
58	Ethyl caffeate	C ₁₁ H ₁₂ O ₄	208.0736	207.0666	1.5	22.82	-H		standards data
59	Cimicifugic acid	C ₂₀ H ₂₀ O ₇	372.1209	371.1138	0.5	27.82	-H	193.0508/134.0378	
60	Cimicifugic acid A	C ₂₁ H ₂₀ O ₁₁	448.1006	447.0937	0.9	20.40	-H	253.0358/181.0507	[3]
61	Cimicifugic acid C	C ₂₀ H ₁₈ O ₁₀	418.0900	417.0833	1.4	18.99	-H	179.0353	[3]

62	Cimicifugic acid D	C ₂₀ H ₁₈ O ₁₀	418.0900	417.0836	2.1	22.17	-H		
63	Cimicifugic acid E	C ₂₁ H ₂₀ O ₁₀	432.1057	431.0984	0.0	21.94	-H	237.0406/193.0506/165.0556	[3]
64	Isoferulic acid	C ₁₀ H ₁₀ O ₄	194.0579	193.0509	1.6	16.86	-H		std
65	Isocimicifugamide	C ₂₅ H ₃₁ NO ₁₀	505.1948	504.1876	0.1	21.78	-H	343.0839	[3]
66	Cimicifugaside A	C ₃₂ H ₃₈ O ₁₇	694.3923	693.3894	-3.5	28.09	-H	555.0280	[1]
67	Cimicifugaside B	C ₃₃ H ₄₀ O ₁₈	724.3952	723.3962	-3.7	33.6	-H	723.3962	[5]
68	Cimicifugaside C/D	C ₂₇ H ₃₄ O ₁₃	566.4257	589.4105	-2.2	17.7	+H, +Na	567.4341	[5]
69	Shomaside B	C ₂₇ H ₃₀ O ₁₅	594.1533	593.1528	-6.1	16.82	-H	193.0500	[1]
70	Shomaside C	C ₂₇ H ₃₀ O ₁₅	594.3709	617.3677	-2.5	27.86	+H, +Na	177.0562	[1]
71	3-Methoxyisoferulic acid	C ₁₁ H ₁₂ O ₅	224.0602	223.0609	-6.7	12.26	-H		[3]
72	Meth-ferulic acid	C ₁₁ H ₁₂ O ₄	208.0679	207.0673	-6.8	23	-H	165.0547	
73	Shomaside A	C ₂₇ H ₃₀ O ₁₆	610.1463	609.1432	-6.1	15.63	-H	193.0499	[3]
74	Carboxymethyl isoferulic acid	C ₁₂ H ₁₂ O ₆	252.0597	251.055	-6.4	19.55	-H		
75	Pyroglutamic acid	C ₅ H ₇ NO ₃	129.0426	128.0354	0.4	2.35	-H	128.0354	massbank
76	D-(+)-Sorbose	C ₆ H ₁₂ O ₆	180.0634	181.0705	-1.1	1.15	+H	383.0332	
77	Khelloside	C ₁₉ H ₂₀ O ₁₀	408.1057	409.1117	-2.9	12.33	+H	351.1695/177.05912	massbank
78	6,7-Dihydroxycoumarin	C ₉ H ₆ O ₄	178.0266	177.0193	-0.2	20.46	-H		massbank
79	Cimicifugamide	C ₂₅ H ₃₁ NO ₁₀	505.1948	504.1877	0.4	17.72	-H	344.1395	[3]
80	Methyl ferulate	C ₁₁ H ₁₂ O ₄	208.0736	207.0666	1.6	23.44	-H		standards data
81	Succinic acid	C ₄ H ₆ O ₄	118.0266	117.0193	-0.5	2.81	-H	89.0244	
82	Cimifugin	C ₁₆ H ₁₈ O ₆	306.2455	305.2455	-2.1	56.33	-H	235.9991	[1]

Note: Ref. i.e. relevant research literature, standards data, database (massbank) referenced on behalf of the constituents, so as to screen and analyse the drug constituents of *Cimicifugae Rhizoma* extract.

Reference:

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