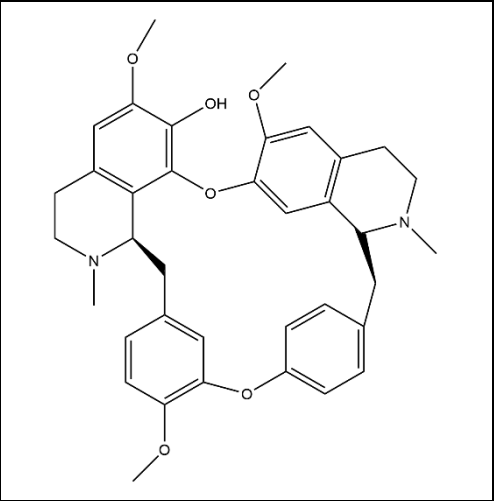
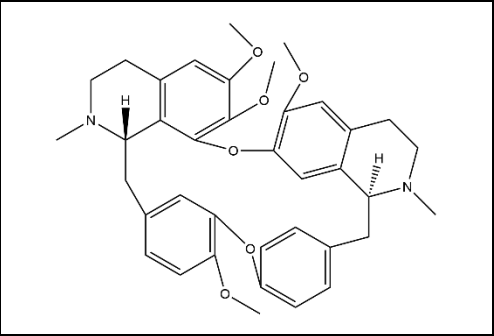
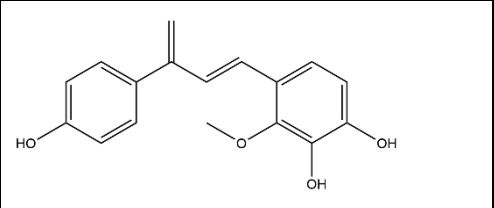
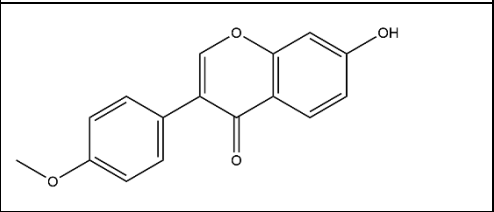
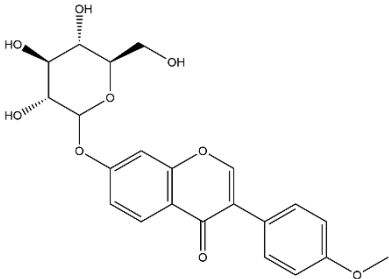
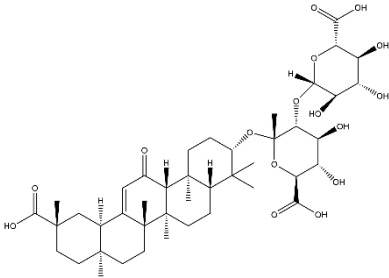
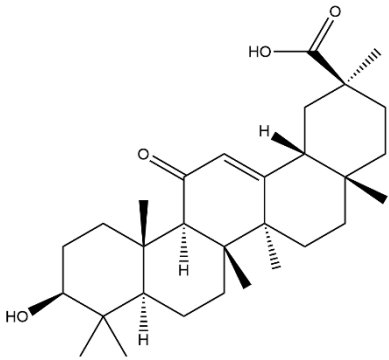
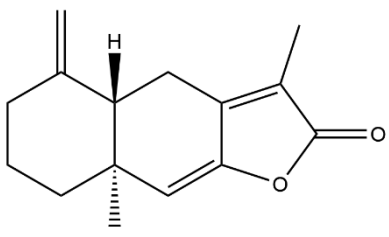


Number	tR/min	[M+H] ⁺ / (m/z)	Formula	Ppm	Chemical compound	Secondary mass spectrometry fragment	Chemical structure
1	2.37	314.13846	C ₁₈ H ₁₉ NO ₄	-0.7	Laurolictsine	58.0709,107.0514,151.0761,269.1169, 283.0833,299.1149,298.1072,314.1409	
2	3.18	595.16575	C ₂₇ H ₃₀ O ₁₅	-1.6	Nicotiflorin	134.0500,192.1060,271.1051,313.0671, 307.0617,321.0745,337.0689,355.0846, 379.0880,403.0765,421.0982,427.0971, 439.1092,457.1107,457.0887,481.0973, 475.0970,511.1251,541.1289,559.1499, 577.1477,595.2683	
3	4.77	193.04891	C ₁₀ H ₈ O ₄	-3.2	Scopoletin	56.9661,65.0432,75.0241,84.9566,92.8999, 103.0271,121.0286,133.9281,149.0820, 149.0208,150.0942,178.0855,178.0713, 193.0877,193.1057	
4	4.87	257.08084	C ₁₅ H ₁₂ O ₄	-0.2	Liquiritigenin	81.0359,91.0560,119.0491,137.0225, 147.0426,211.0732,257.0784	

5	5.83	609.29542	$C_{37}H_{40}N_2O_6$	-0.7	Fangchinoline	367.1631,578.2507,609.2913	
6	6.40	623.31112	$C_{38}H_{42}N_2O_6$	-0.7	Tetrandrine	623.308	
7	6.41	287.09128	$C_{16}H_{14}O_5$	-0.1	LicochalconeB	65.0400,84.9648,113.0586,123.0406, 138.0282,147.0397,153.0561,167.0344, 170.0962,181.0633,204.8821,204.9010, 287.0903,287.1192	
8	7.48	269.0808	$C_{16}H_{12}O_4$	-0.1	Formononetin	118.0416,170.0725,181.0641,197.0604, 213.0901,226.0617,237.0533,253.0508, 269.0809	

9	7.49	431.13366	<chem>C22H22O9</chem>	0.3	Ononin	269.079	
10	9.24	823.4104	<chem>C42H62O16</chem>	-0.8	Glycyrrhizic acid	454.3450,453.3339,471.3460,647.3761	
11	9.25	471.34659	<chem>C30H46O4</chem>	-0.6	18β-Glycyrrhetic Acid	135.1192,173.1333,189.1631,235.1735,317.2198,441.3193,453.3266	
12	9.98	231.13742	<chem>C15H18O2</chem>	-2.3	Atractylenolide I	77.0418,141.0012,157.1035,158.0265,214.0888,231.1376	

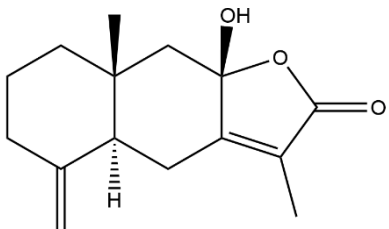
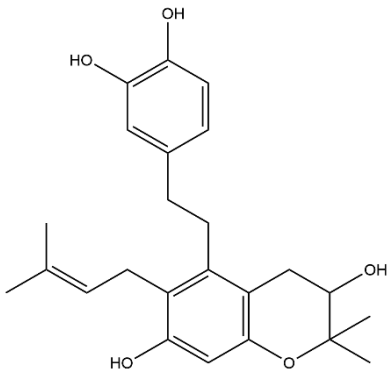
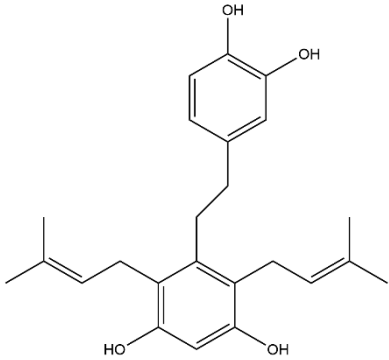
13	9.99	249.1481	C ₁₅ H ₂₀ O ₃	-1.6	Atractylenolide III	55.9382,67.0588,69.0740,77.0429,79.0581, 83.0887,91.0569,95.0876,105.0713,119.0857, 128.0615,135.0451,149.0588,157.1032,161.0588, 163.0751,175.0755,189.0886,195.1209,203.1454, 213.1257,231.1364,231.1655	
14	12.49	399.2166	C ₂₄ H ₃₀ O ₅	-3	Gancaonin T	84.9687,122.9770,127.9993,141.9836,143.9942, 155.9973,158.0100,170.0082,172.0253,184.0262, 186.0462,214.0817,228.0954,258.8092,270.1388, 270.7608,294.2094,295.2148,312.8080,314.2000, 340.2157,358.2033,357.2024,399.3479	
15	12.73	383.22169	C ₂₄ H ₃₀ O ₄	-0.4	Gancaonin R	101.9517,314.1836,318.2111,320.2264,337.2006, 337.2144,383.2204	

Figure S1. The main components' detailed information of Fangjihuangqi decoction