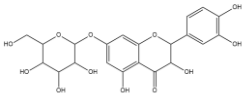
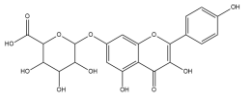
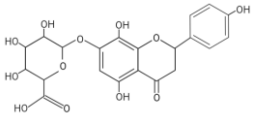
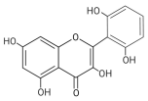
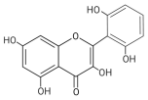
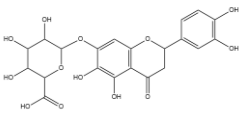
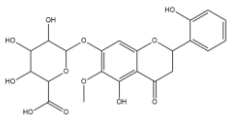
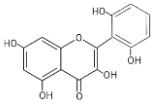
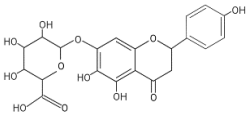
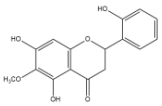
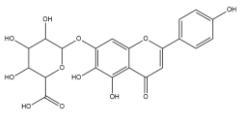
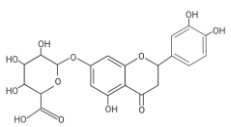
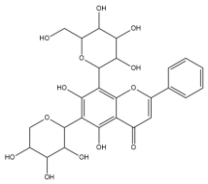
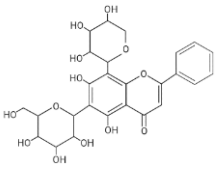
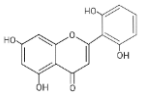
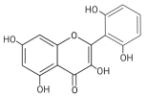
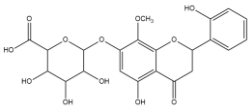
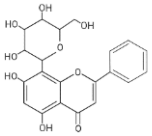
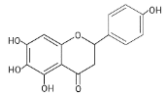
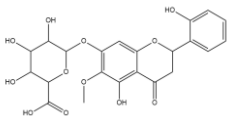
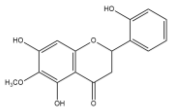
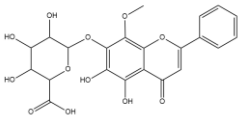
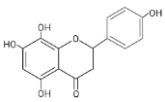
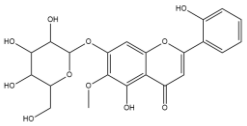
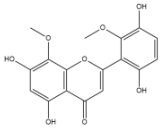
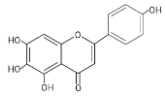
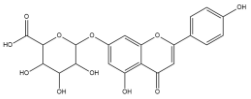
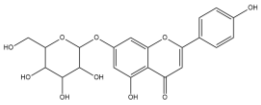
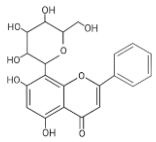
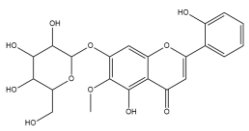
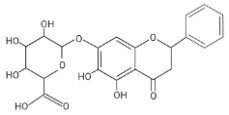
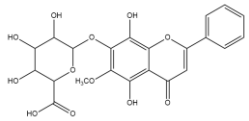
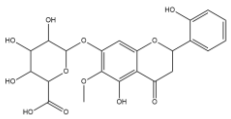
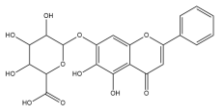
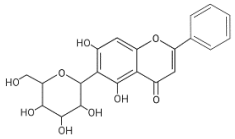
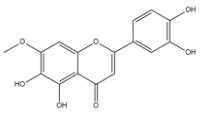
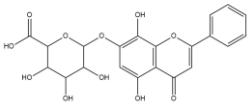
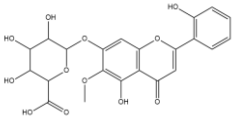
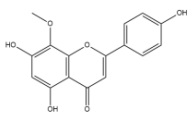
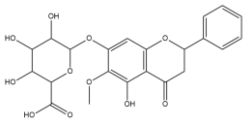
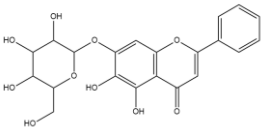
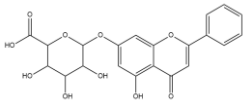
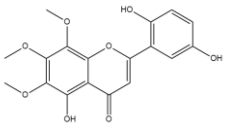
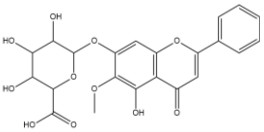
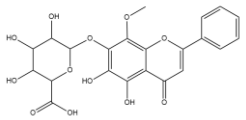
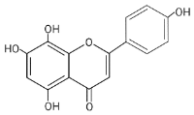
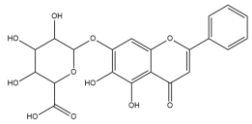
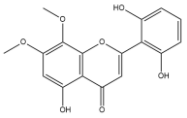
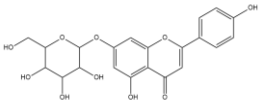
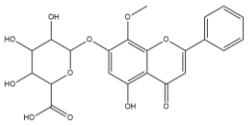
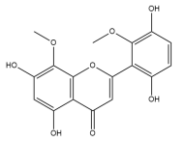
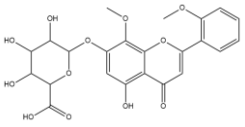
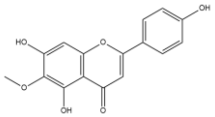
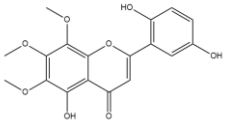
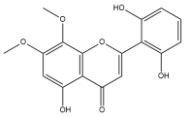
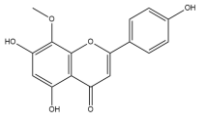
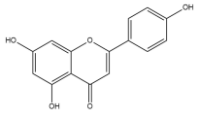
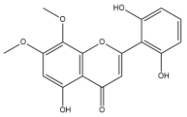
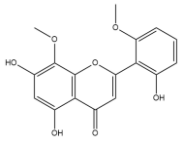
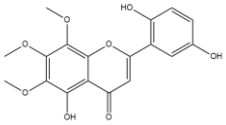
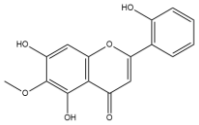
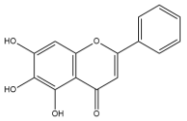
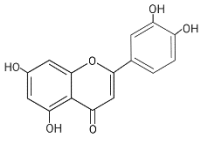
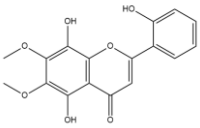
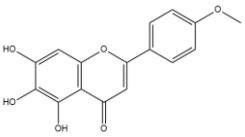
Table S1. Chemical structures and relative ion intensity of compounds identified in Huangqin (*Scutellaria baicalensis* Georgi. root).

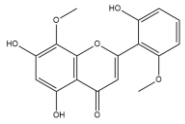
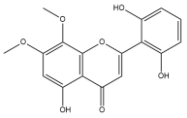
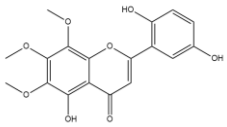
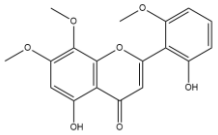
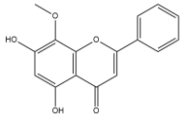
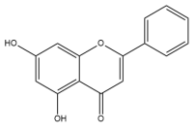
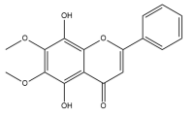
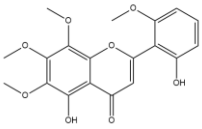
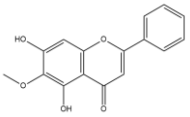
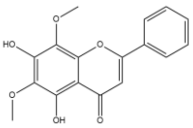
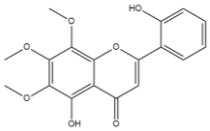
ID	Retention time		Formula	Name	Structure	Relative ion intensity (× 10^8)		Ref.
	ESI^+	ESI^-				WE (+/-)	EE (+/-)	
1.	12.81	13.16	$C_{21}H_{22}O_{12}$	Taxifolin 7-*O*-glucoside		0.190/0.470	nd/nd	[44]
2.	13.10	nd	$C_{21}H_{18}O_{12}$	Kaempferol 3-*O*-glucuronide		0.054/0.050	nd/nd	[44]
3.	16.00	15.75	$C_{21}H_{20}O_{12}$	Carthamidin 7-*O*-glucuronide		0.874/0.449	0.093/0.055	[45]
4.	16.43	16.23	$C_{15}H_{12}O_7$	Isomer of Pentahydroxyflavanone		7.574/9.298	1.150/2.182	[44]
5.	nd	18.13	$C_{15}H_{12}O_7$	Isomer of Pentahydroxyflavanone		nd/0.630	nd/0.173	
6.	19.59	19.35	$C_{21}H_{20}O_{13}$	5,6,7,3′,4′-Pentahydroxy Flavanon 7-*O*-glucuronide		0.094/0.130	nd/nd	[44]
7.	20.29	20.47	$C_{22}H_{22}O_{12}$	5,7,2′-Trihydroxy-6-methoxyflavanone 7-*O*-glucuronide		0.256/0.098	0.050/0.020	[44]
8.	20.34	20.46	$C_{15}H_{10}O_7$	Viscidulin I		4.954/3.297	0.628/0.445	[46]
9.	21.98	21.76	$C_{21}H_{20}O_{12}$	Isocarthamidin 7-*O*-glucuronide		2.498/2.835	0.040/0.045	[45]
10.	22.09	21.94	$C_{16}H_{14}O_6$	Isomer of trihydroxy-methoxyflavanone		3.364/0.808	0.346/0.176	[46]
11.	22.69	22.83	$C_{21}H_{18}O_{12}$	Scutellarin		8.815/3.250	0.089/0.044	[46]
12.	22.83	22.97	$C_{21}H_{20}O_{12}$	Eriodictyol 7-*O*-glucuronide		1.260/1.031	0.050/0.027	[45]

13.	22.89	23.06	$C_{26}H_{28}O_{13}$	Chrysin 6-*C*-arabinoside-8-*C*-glucoside		49.676/17.993	2.493/1.102	[44]
14.	23.97	23.74	$C_{26}H_{28}O_{13}$	Chrysin 6-*C*-glucoside-8-*C*-arabinoside		42.819/16.325	2.131/0.927	[44]
15.	24.20	24.05	$C_{15}H_{10}O_6$	5,7,2′,6′-Tetrahydroxyflavone		4.249/1.506	1.028/0.665	[44]
16.	24.29	24.12	$C_{15}H_{10}O_7$	Isomer of Pentahydroxyflavone		1.268/0.748	0.121/0.127	
17.	24.56	24.42	$C_{22}H_{22}O_{12}$	5,7,2′-Trihydroxy-8-methoxy Flavanone 7-*O*-glucuronide		0.312/0.526	0.009/nd	[44]
18.	24.90	25.04	$C_{21}H_{20}O_9$	Isomer of Chrysin 8-*C*-glucoside		3.737/1.846	0.509/0.321	[46]
19.	25.19	25.27	$C_{15}H_{12}O_6$	Carthamidin		0.765/0.713	0.186/0.271	[44]
20.	25.23	25.36	$C_{22}H_{22}O_{12}$	Isomer of trihydroxy-methoxyflavanone *O*-glucuronide		0.947/0.960	0.018/0.017	[44]
21.	25.47	25.49	$C_{16}H_{14}O_6$	Isomer of trihydroxy-methoxyflavanone		2.676/1.745	0.465/0.412	[46]
22.	25.95	25.76	$C_{22}H_{20}O_{12}$	5,6,7-Trihydroxy-8-methoxy-7-*O*-glucuronide		16.485/2.228	nd/nd	[44]
23.	26.02	25.87	$C_{15}H_{12}O_6$	Isocarthamidin		2.628/2.667	0.931/0.999	[44]
24.	26.10	25.92	$C_{22}H_{22}O_{11}$	5,7,2′-Trihydroxy-6-methoxyflavone 7-*O*-glucoside		0.723/0.221	0.038/0.016	[44]
25.	26.29	26.11	$C_{17}H_{14}O_8$	Viscidulin III		11.814/5.643	3.737/1.656	[46]
26.	26.48	26.37	$C_{15}H_{10}O_6$	Scutellarein		17.209/9.153	1.683/1.253	[44]

27.	26.88	26.97	$C_{21}H_{18}O_{11}$	Apigenin 7-*O*-glucuronide		197.928/16.837	8.856/2.021	[47]
28.	27.10	27.17	$C_{21}H_{20}O_{10}$	Apigenin 7-*O*-glucoside		12.855/1.895	0.743/0.318	[44]
29.	27.32	27.31	$C_{21}H_{20}O_{9}$	Isomer of Chrysin 8-*C*-glucoside		3.080/0.749	0.350/0.170	[46]
30.	27.59	27.41	$C_{22}H_{22}O_{11}$	Isomer of trihydroxy methoxyflavone *O*-glucoside		2.198/0.285	0.139/0.027	
31.	27.72	27.57	$C_{21}H_{20}O_{11}$	Dihydrobaicalin		19.663/8.404	0.335/0.321	[44]
32.	27.93	27.75	$C_{22}H_{20}O_{12}$	5,7,8-Trihydroxy-6-methoxy Flavone-7-*O*-glucuronide		3.704/1.051	nd/nd	[44]
33.	28.14	27.98	$C_{22}H_{22}O_{12}$	Isomer of trihydroxy-methoxyflavanone *O*-glucuronide		0.768/0.707	0.017/nd	
34.	28.22	28.09	$C_{21}H_{18}O_{11}$	Baicalin		42.845/13.435	0.879/0.454	[47]
35.	28.51	28.57	$C_{21}H_{20}O_{9}$	Chrysin 6-*C*-glucoside		0.815/0.385	0.015/0.018	[46]
36.	28.62	28.68	$C_{16}H_{12}O_{7}$	Pedalitin		5.078/2.554	0.272/0.254	[44]
37.	28.72	28.77	$C_{21}H_{18}O_{11}$	Norwogonin 7-*O*-glucuronide		13.347/4.952	0.404/0.215	[47]
38.	28.76	28.84	$C_{22}H_{20}O_{12}$	5,7,2′-Trihydroxy-6-methoxy Flavone 7-*O*-glucuronoide		25.725/6.427	0.226/0.114	[44]
39.	28.78	28.89	$C_{16}H_{12}O_{6}$	4′-Hydroxywogonin		12.063/1.048	0.359/0.148	[48]

40.	28.92	28.97	$C_{22}H_{22}O_{11}$	(2S)-5,7-Dihydroxy-6-methoxyflavanone 7-*O*-glucuronide		1.140/1.326	0.099/0.056	[46]
41.	28.95	28.99	$C_{21}H_{20}O_{10}$	Baicalein 7-*O*-glucoside		2.920/0.787	0.143/0.071	[46]
42.	29.21	29.13	$C_{21}H_{18}O_{10}$	Chrysin 7-*O*-glucuronide		25.746/6.500	0.687/0.325	[44]
43.	29.25	nd	$C_{18}H_{16}O_{8}$	Isomer of trihydroxy-trimethoxyflavone		0.343/nd	0.030/0.011	
44.	29.40	29.23	$C_{22}H_{20}O_{11}$	Oroxylin A-7-*O*-glucuronide		95.219/12.270	3.750/0.304	[44]
45.	29.62	29.48	$C_{22}H_{20}O_{12}$	Isomer of Trihydroxy methoxy Flavone *O*-glucuronoide		35.090/9.280	0.238/0.115	[44]
46.	29.76	29.61	$C_{15}H_{10}O_{6}$	Isoscutellarein		3.558/0.967	0.548/0.477	[44]
47.	29.81	29.69	$C_{21}H_{18}O_{11}$	Baicalein 6-*O*-glucuronide		19.076/6.575	0.057/0.032	[44]
48.	29.91	29.81	$C_{17}H_{14}O_{7}$	Isomer of trihydroxy dimethoxyflavone		1.538/0.737	0.432/0.288	[46]
49.	30.05	nd	$C_{21}H_{20}O_{10}$	Isomer of dihydroxyflavanone *O*-glucoside		3.871/nd	0.147/nd	
50.	30.08	30.08	$C_{22}H_{20}O_{11}$	Wogonoside		85.548/23.270	5.004/0.424	[44]
51.	30.40	30.44	$C_{17}H_{14}O_{8}$	Isomer of Tetrahydroxy-dimethoxyflavone		1.213/0.621	0.158/0.148	
52.	30.72	30.68	$C_{23}H_{22}O_{12}$	5,7-Dihydroxy-8,2′-dimethoxyflavone 7-*O*-glucuronide		20.360/6.678	0.339/0.130	[46]

53.	31.11	30.98	$C_{16}H_{12}O_6$	Hispidulin		6.154/3.165	0.840/0.605	[48]
54.	31.32	31.20	$C_{18}H_{16}O_8$	5,2',5'-Trihydroxy-6,7,8-trimethoxyflavone		1.658/0.823	0.393/0.238	[46]
55.	31.57	31.53	$C_{17}H_{14}O_7$	Isomer of trihydroxy dimethoxyflavone		1.022/0.469	0.089/0.055	[46]
56.	31.61	31.60	$C_{16}H_{12}O_6$	Isomer of trihydroxy-methoxyflavone		8.049/4.741	0.993/0.749	
57.	31.84	31.85	$C_{15}H_{10}O_5$	Apigenin		12.389/6.284	1.943/1.852	[44]
58.	31.93	31.96	$C_{17}H_{14}O_7$	Viscidulin II		0.587/0.224	0.085/0.031	[46]
59.	32.45	32.35	$C_{17}H_{14}O_7$	5,7,6'-Trihydroxy-8,2'-dimethoxyflavone		4.462/2.022	1.410/0.648	[46]
60.	32.66	32.55	$C_{18}H_{16}O_8$	Isomer of trihydroxy-trimethoxyflavone		2.084/0.675	0.169/0.034	[46]
61.	32.70	32.59	$C_{16}H_{12}O_6$	Tenaxin II		18.049/6.862	1.716/0.594	[46]
62.	32.83	32.73	$C_{15}H_{10}O_5$	Baicalein		151.087/44.968	35.019/9.471	[44]
63.	32.83	nd	$C_{15}H_{10}O_6$	Isomer of Tetrahydroxyflavone		2.057/nd	1.404/nd	[44]
64.	33.21	33.22	$C_{17}H_{14}O_7$	5,8,2′-Trihydroxy-6,7-dimethoxyflavone		3.612/1.756	0.414/0.219	[46]
65.	33.44	33.46	$C_{16}H_{12}O_6$	5,6,7-Trihydroxy-4′-methoxyflavone		5.534/2.928	1.398/0.791	[44, 46]

66.	33.82	33.76	$C_{17}H_{14}O_7$	5,7,2′-Trihydroxy-8,6'-dimethoxyflavone		1.027/0.512	0.205/0.089	[44]
67.	35.32	35.23	$C_{17}H_{14}O_7$	Isomer of trihydroxy dimethoxyflavone		0.787/0.645	0.182/0.163	[46]
68.	36.43	36.41	$C_{18}H_{16}O_8$	Isomer of trihydroxy-trimethoxyflavone		0.680/0.566	0.146/0.108	
69.	36.90	36.81	$C_{18}H_{16}O_7$	Skullcapflavone		5.657/1.753	2.193/0.285	[44]
70.	37.09	37.03	$C_{16}H_{12}O_5$	Wogonin		107.452/26.964	26.908/1.698	[44]
71.	37.18	37.12	$C_{15}H_{10}O_4$	Chrysin		9.151/6.996	2.767/1.531	[44]
72.	37.78	37.73	$C_{17}H_{14}O_6$	5,8-Dihydroxy-6,7-dimethoxyflavone		19.321/2.346	1.785/nd	[44]
73.	38.09	38.02	$C_{19}H_{18}O_8$	Skullcapflavone II		56.742/13.360	25.500/2.871	[44]
74.	38.14	38.10	$C_{16}H_{12}O_5$	Oroxylin A		47.933/6.529	13.894/0.181	[44]
75.	38.26	38.22	$C_{17}H_{14}O_6$	5,7-Dihydroxy-6,8-dimethoxyflavone		6.398/2.909	2.000/0.615	[44]
76.	39.26	39.21	$C_{18}H_{16}O_7$	Tenaxin I		5.772/2.654	1.649/0.578	[44]

ESI$^+$ represents in positive mode; ESI$^-$ represents in negative mode; WE: water extracts of Huangqin; EE: ethanol extracts of Huangqin; n/d represents not detectable.