

利用网络药理学方法研究热毒宁注射液抗流感病毒的分子作用机制

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Study on Mechanism of the Reduning Injection on the Influenza Virus Using Network Pharmacology Method

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Table S1 78 molecules contained in Reduning injection

index	CAS_NO.	UNPD_ID^[a]	Chemical_Name
1	99-50-3	UNPD60430	Protocatechuic acid
2	92-61-5	UNPD123796	scopoletine
3	91-64-5	UNPD21132	coumarin
4	906-33-2	UNPD129293	neochlorogenic acid
5	17608-52-5	UNPD84139	Kryptochlorogensaeure
6	6049-17-8	UNPD69393	Cryptochlorogensaeure
7	82638-23-1	UNPD62662	4-O-trans-caffeoylquininc acid
8	82638-22-0	UNPD164733	3alpha,5alpha-dihydroxy-4alpha-O-caffeoyl quinic acid
9	905-99-7	UNPD49725	4-O-caffeoylquinic acid
10	78-70-6	UNPD106513	(3R)-()-Linalool
11	126-90-9	UNPD139439	(3S)-()-Linalool
12	77-92-9	UNPD145647	citric acid
13	76-22-2	UNPD59933	Camphor
14	69-72-7	UNPD59192	salicylic acid
15	6902-77-8	UNPD70448	Genipin
16	63968-64-9	UNPD189689	Artemisin
17	62218-53-5	UNPD24300	Picrocrocinic acid
18	62218-53-5	UNPD125855	O-beta-D-Glucopyranoside-4-Hydroxy-2,6, 6-trimethyl-1-cyclohexenecarboxylic acid
19	60077-47-6	UNPD86130	7-epi-vogeloside
20	118627-52-4	UNPD181272	7alpha-methoxysweroside
21	60077-47-6	UNPD136955	Vogeloside
22	58822-47-2	UNPD26834	Secoxyloganin
23	546-49-6	UNPD102035	Artemisia ketone
24	5373-11-5	UNPD51223	Cynaroside
25	491-70-3	UNPD149880	Luteolin
26	482-36-0	UNPD127168	Hyperoside
27	480-19-3	UNPD60650	Isorhamnetin
28	479-91-4	UNPD186353	Casticine
29	470-82-6	UNPD63596	Cineole
30	331-39-5	UNPD133665	Caffeic acid
31	327-97-9	UNPD106185	chlorogenic acid
32	301-16-6	UNPD130563	Scoparin
33	29307-60-6	UNPD31542	Genipin-1beta-D-gentiobiosid
34	29307-60-6	UNPD158162	genipin-1-beta-gentiobioside
35	27856-66-2	UNPD197203	secologanin tetraacetate
36	27856-66-2	UNPD197202	O',O',O',O'-tetraacetylsecologanin
37	27741-01-1	UNPD162860	geniposidic acid
38	27741-01-1	UNPD155880	geniposidic acid
39	27741-01-1	UNPD106583	Geniposidinsaeure
40	25694-72-8	UNPD29278	Veronicastrósíde
41	25694-72-8	UNPD12881	luteolin 7-O-beta-D-neohesperidoside
42	24512-63-8	UNPD120048	Geniposide
43	16758-05-7	UNPD18949	3,5-di-O-trans-caffeoylquininc acid

44	89919-61-9	UNPD101522	isochlorogenic acid A
45	2450-53-5	UNPD138107	3,5-dicaffeoyl quinic acid
46	22864-93-3	UNPD138269	Secologansaeure
47	21149-19-9	UNPD49553	Santolina alcohol
48	19587-65-6	UNPD135322	Eupatin
49	1632-73-1	UNPD26605	(-)-beta-fenchol
50	470-08-6	UNPD22238	(+)-beta-Fenchol
51	4695-62-9	UNPD30210	(-)-alpha-fenchol
52	2217-02-9	UNPD7069	(+)-alpha-Fenchol
53	153-18-4	UNPD150726	Rutin
54	14965-20-9	UNPD186030	Chrysosplenol-D
55	14534-61-3	UNPD192822	3,4-dicaffeoyl-quinic acid
56	17912-89-9	UNPD13564	4,5-di-O-caffeoylquinic acid
57	14259-55-3	UNPD93830	10-Deacetylasperulosidinsaeure
58	18842-99-4	UNPD24222	Scandoside
59	18842-99-4	UNPD163595	desacetyl asperulosidic acid
60	14259-55-3	UNPD147471	Decetylasperulosidic acid
61	117-39-5	UNPD49205	Quercetine
62	114653-46-2	UNPD125055	6''-p-coumaroyl genipin gentiobioside
63	1014-83-1	UNPD142498	(Z)-ferulic acid
64	537-98-4	UNPD12047	(E)-ferulic acid
65	1135-24-6	UNPD168255	3-O-methyl caffeic acid
66	106-24-1	UNPD171634	Geraniol
67	118627-52-4	UNPD123	7-epi-vogeloside
68	123372-74-7	UNPD128	Methyl 4-O-caffeoylquininate
69	29708-87-0	UNPD1210	Methyl 5-O-caffeoylquininate
70	2450-53-5	UNPD1212	Isochlorogenic acid C
71	879293-21-7	UNPD1213	Methyl 3,5-di-O-caffeoylquininate
72	114637-83-1	UNPD1214	4,5-di-O-caffeoylquininate
73	471271-55-3	UNPD1218	(E)-aldosecologanin
74	1174662-63-5	UNPD1219	6''-O-trans-sinapoylgenipin gentiobioside
75	82474-97-3	UNPD1224	(Z)-aldosecologanin
76	1782-55-4	UNPD1225	3-(3,4-dihydroxy-5-methoxyphenyl)-Cinnamic acid
77	1340540-40-4	UNPD1229	Methyl 3,4-di-O-caffeoylquininate
78	123150-12-9	UNPD1230	5H,8H-Pyrano[4,3-d]thiazolo[3,2-a]pyridine-3-carboxylic acid

[a] UNPD: universal natural product database, which is constructed by Xiao-Jie Xu professor et al.

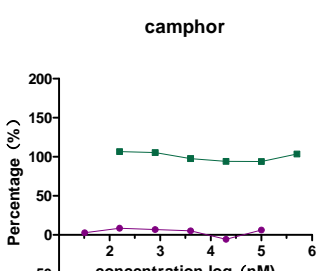
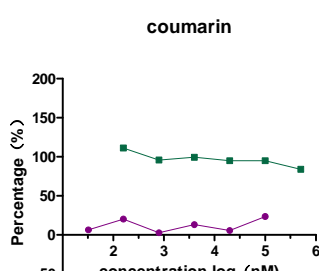
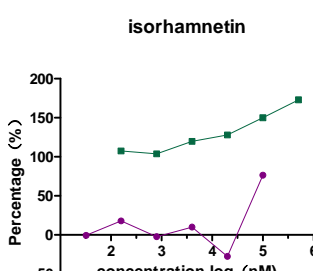
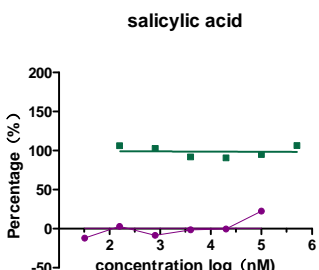
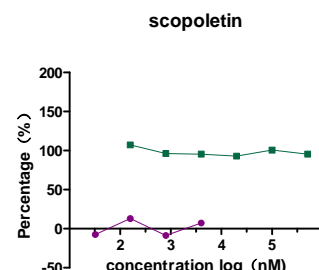
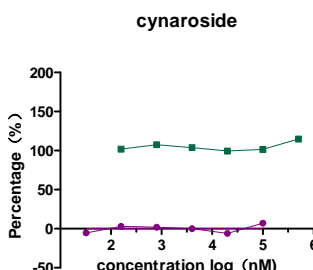
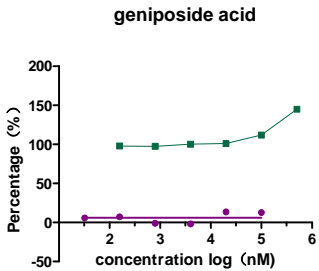
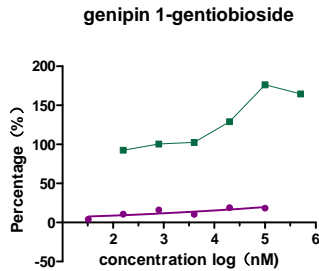
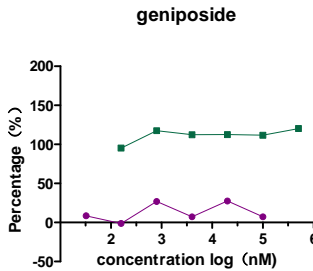
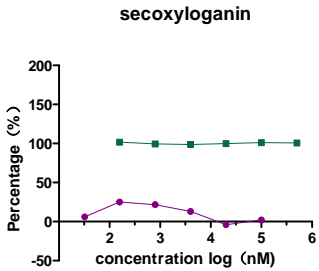
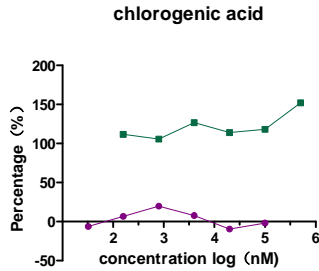
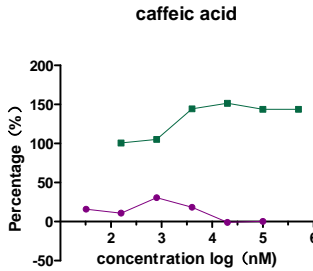
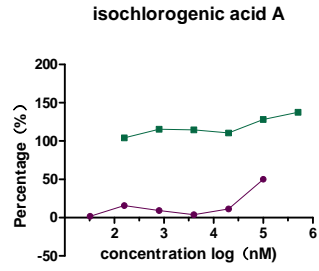
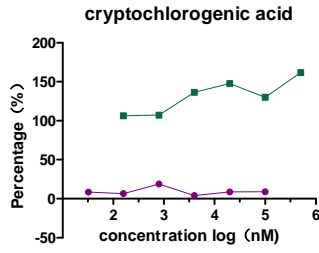
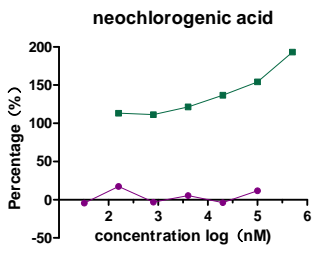
Table S2 The predicted CC50, EC50, SI of the compounds in Reduning injection

compound	CC ₅₀	EC ₅₀	SI	compound	CC ₅₀	EC ₅₀	SI
luteolin	701.219	28.44	24.66	cryptochlorogenic acid	-	ND	ND
quercetin	-	91.284	>5.48	hyperoside	-	ND	ND
genipin	-	104.355	>4.79	cynaroside	-	ND	ND
Isochlorogenic acid B	-	113.143	>4.42	caffeic acid	-	ND	ND
scopoletin	-	ND	ND	Neochlorogenic acid	-	ND	ND
geniposide	-	ND	ND	chlorogenic acid	-	ND	ND
isorhamnetin	-	ND	ND	rutin	-	ND	ND
Isochlorogenic acid A	-	ND	ND	citric acid	-	ND	ND
coumarin	-	ND	ND	artemisinin	-	ND	ND
camphor	-	ND	ND	linalol	-	ND	ND
geniposide acid	-	ND	ND	artensia ketone	-	ND	ND
protocatechuic acid	-	ND	ND	secoxyloganin	-	ND	ND
Salicylic acid	-	ND	ND	Genipin	-	ND	ND
ferulic acid	-	ND	ND	1-gentiobioside	-	ND	ND

“-”-no significant cytotoxicity(CC₅₀>>100μmol.L⁻¹).

“ND”-not determined antiviral activity.

◆ Inhibition
■ Cell viability



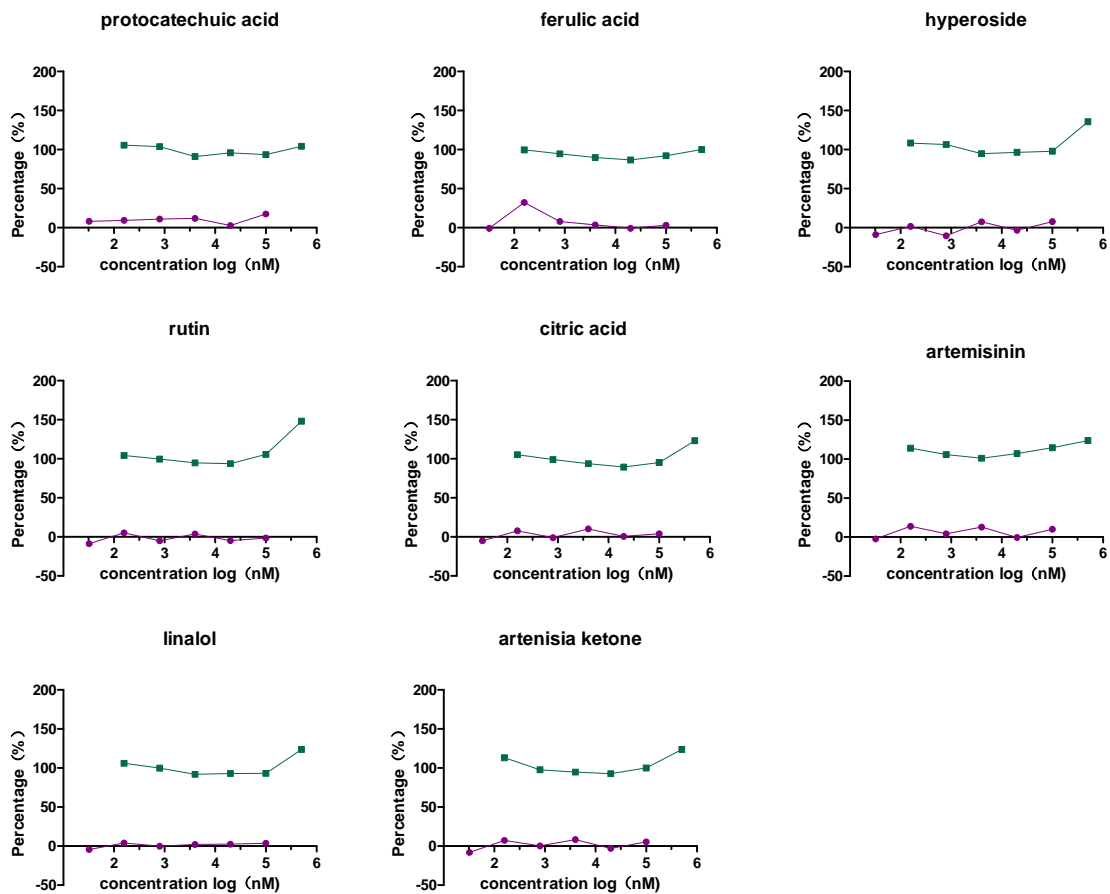


Fig.S1 The dose-response curve of compounds in Reduning injection