

Using Pharmacokinetic–Pharmacodynamic Modeling to Study the Main Active Substances of the Anticancer Effect in Mice from *Panax ginseng*–*Ophiopogon japonicus*

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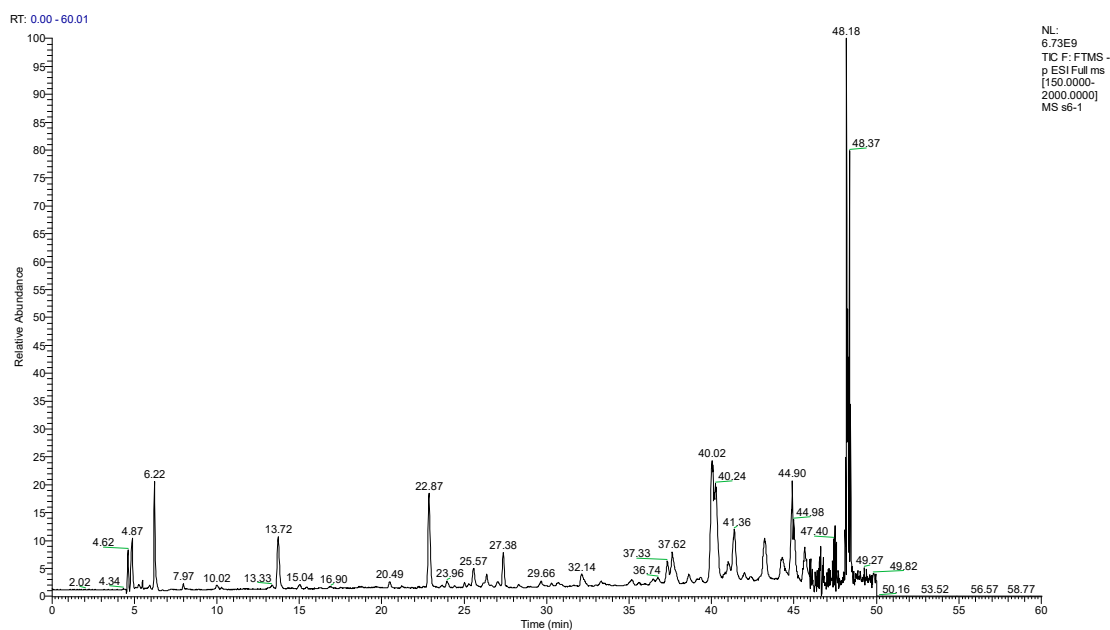


Figure S1. Total ion chromatogram of lung tissue samples in negative ion mode.

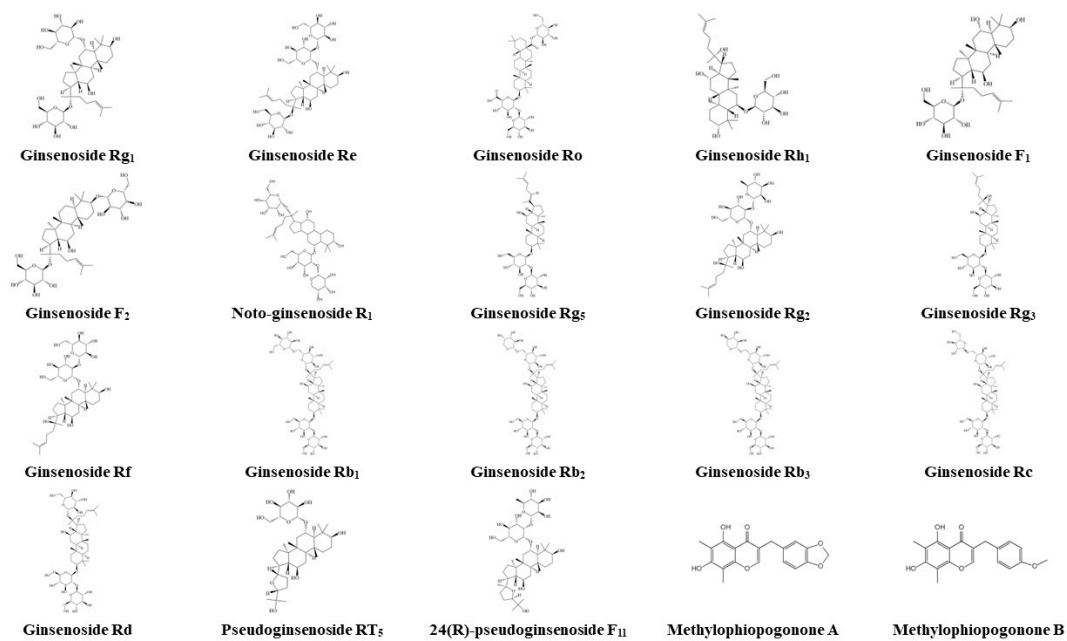


Figure S2. Chemical structures of the 20 compounds.

Table S1. The comprehensive weighted scoring of drug efficacy indicators.

Time (h)	IFN- γ	TNF- α	TGF- β 1	Combined Weighted Score (S)
0.083	0.9418	0.9379	0.2634	0.1389
0.167	0.1200	1.3515	0.6516	0.1924
0.25	0.3715	0.4455	0.4645	0.0651
0.5	0.3134	0.3145	1.3691	0.0810
0.75	0.7140	0.2269	1.5642	0.0958
1	0.6402	0.0542	0.7059	0.0491
2	0.8941	0.1797	1.5414	0.0874
3	1.2556	0.9594	2.2131	0.2158
4	0.3165	0.1596	0.7663	0.0458
6	0.2799	0.0593	0.7245	0.0194
8	0.0361	0.0351	0.4682	0.0095
12	0.0378	0.0369	0.4742	0.0154
24	0.0385	0.04055	0.5016	0.0308

Table S2-1. Detection results of drug-containing lung tissue content at different time points (mean \pm SD, n =6).

Time (h)	Ginsenoside Rg ₁ (ng/g)	Ginsenoside Re (ng/g)	Ginsenoside Ro (ng/g)	Ginsenoside Rh ₁ (ng/g)	Ginsenoside F1 (ng/g)	Ginsenoside F2 (ng/g)	Notoginsenoside R1 (ng/g)	Ginsenoside Rg ₅ (ng/g)	Ginsenoside Rg ₂ (ng/g)	Ginsenoside Rg ₃ (ng/g)
0.083	41.21 \pm 9.63	132.49 \pm 32.88	11.83 \pm 0.79	8.29 \pm 0.69	0.42 \pm 0.07	14.7 \pm 0.96	5.86 \pm 1.30	4135.21 \pm 269.18	61.52 \pm 2.18	4.61 \pm 0.20
0.167	2.8 \pm 0.1	5.33 \pm 0.56	1.69 \pm 0.13	0.05 \pm 0.04	0.05 \pm 0.03	1.84 \pm 0.3	5.16 \pm 2.87	386.08 \pm 26.98	8.29 \pm 0.36	3.45 \pm 0.09

0.25	50.24±6.67	64.38±5.85	11.32±1.58	8.53±0.99	0.57±0.08	4.89±1.3	3.51±2.35	2348.06±325.95	67.24±10.16	3.91±0.16
0.5	9.25±1.73	55±21.54	3.65±0.5	1.4±0.66	0.15±0.06	6.12±3.57	3.46±1.15	658.61±156.18	17.29±1.44	3.85±0.25
0.75	4.95±0.04	5.83±0.04	1.4±0.05	2.79±0.05	0.46±0.04	17.18±0.13	0.03±0.04	4804.2±37.85	31.91±0.04	3.86±0.04
1	3.53±0.20	3.09±0.66	3.09±0.16	3.7±0.11	2.38±0.21	135.65±2.66	0.04±0.01	5679.31±158.09	52.13±1.23	4.34±0.19
2	0.82±0.06	1.54±0.11	1.39±0.05	0.31±0.02	0.11±0.02	3.7±1.03	5.17±0.37	136.75±14.00	7.15±0.24	3.98±0.73
3	3.19±0.35	12.42±0.27	2.03±0.43	1.6±0.25	1.46±0.18	45.74±2.56	6.4±1.28	2337.69±334.68	24.2±1.49	4.46±0.03
4	8.63±0.51	3.72±0.09	2.34±0.16	7.49±0.55	4.12±0.45	128.46±8.7	5.47±0.38	7967.81±441.77	69.08±2.87	4.41±0.29
6	0.58±0.02	1.7±0.15	1.35±0.13	0.42±0.01	0.27±0.01	2.55±0.73	2.22±0.12	81.51±18.10	6.00±0.09	3.4±0.08
8	0.4±0.02	0.77±0.04	1.33±0.01	0.47±0.02	0.25±0.01	1.55±0.09	0.58±0.05	138.3±22.36	6.04±0.03	3.39±0.05
12	0±0	0±0	0±0	0±0	0±0	0±0	0±0	0±0	0±0	0±0
24	0±0	0±0	0±0	0±0	0±0	0±0	0±0	0±0	0±0	0±0

Table S2-2. Detection results of drug-containing lung tissue content at different time points (mean ± SD, n =6).

Time (h)	Ginsenoside Rf (ng/g)	Ginsenoside Rb ₁ (ng/g)	Ginsenoside Rb ₂ (ng/g)	Ginsenoside Rb ₃ (ng/g)	Ginsenoside Rc (ng/g)	Ginsenoside Rd (ng/g)	Pseudoginsenoside RT ₅ (ng/g)	24(R)-pseudoginsenoside F11	Methyloph iopogon flavanone A	Methyloph iopogon flavanone B
0.083	36.13±1.77	84.51±3.17	2.22±0.15	2.54±0.16	17.39±0.64	43.37±1.94	2.62±0.23	35.98±1.93	6.21±5.23	6.44±3.18
0.167	2.22±0.12	10.62±2.98	0.67±0.05	1.63±0.05	10.91±0.29	2.86±0.40	1.77±0.36	1.98±0.11	4.2±0.11	4.54±0.80
0.25	47.9±6.96	91.22±17.84	1.9±0.29	2.62±0.12	16.7±1.45	34.48±2.62	5.11±0.88	47.49±6.94	2.04±0.29	3.45±0.17

0.5	9.09±1.97	34.9±13.81	1.01±0.10	1.84±0.01	13.87±0.58	71.57±12.27	3.38±0.76	9.23±1.73	2.33±0.27	4.37±0.60
0.75	8.08±0.04	4.52±0.04	0.72±0.04	1.53±0.04	1.31±0.04	2.93±0.04	1.79±0.04	7.8±0.04	2.95±0.04	4.9±0.04
1	8.87±0.20	26.77±1.71	0.92±0.08	1.74±0.04	0.92±0.15	23.56±0.34	1.46±0.07	10.44±0.94	2.76±0.16	1.58±0.53
2	1.25±0.20	5.33±0.56	1.09±0.17	1.54±0.06	3.89±0.13	2.57±0.10	1.31±0.09	3.83±0.21	2.06±0.11	2.12±0.17
3	5.27±0.26	128.72±5.25	1.17±0.26	1.68±0.10	1.75±0.90	9.88±0.30	1.71±0.10	7.58±0.28	5.41±0.92	20.61±2.38
4	18.78±0.77	25.54±1.63	0.79±0.02	1.54±0.02	2.32±0.20	17.81±1.40	2.28±0.12	21.21±0.93	2.92±0.10	3.51±0.66
6	0.37±0.02	14.85±0.45	0.69±0.01	1.44±0.02	4.05±0.04	2.86±0.18	1.64±0.06	2.82±0.01	2.04±0.07	2.09±0.89
8	0.12±0.01	8.75±0.16	0.69±0.01	1.44±0.03	4.16±0.01	1.74±0.02	1.46±0.08	2.62±0.05	2.32±0.38	1.54±0.20
12	0±0	440.68±15.67	7.2±0.96	5.92±0.45	42.95±2.11	82.95±2.11	0±0	0±0	0±0	0±0
24	0±0	5.51±0.36	0.78±0.06	1.79±0.08	2.35±0.89	3.16±0.54	0±0	0±0	0±0	0±0

Table S3. Reference substance concentration gradient and QC sample concentration.

Components	Nominal Concentration (mg/g)	Concentrations of QC Samples (ng/g)		
		Low	Medium	High
Ginsenoside Rg ₁	1.07	5	50	500
Ginsenoside Re	0.98	5	50	500
Ginsenoside Ro	1.06	5	50	500
Ginsenoside Rh ₁	1.01	5	50	500
Ginsenoside F ₁	1.11	5	50	500
Ginsenoside F ₂	0.97	5	50	500
Notoginsenoside R ₁	1.07	5	50	500
Ginsenoside Rg ₅	1.00	5	50	500
Ginsenoside Rg ₂	1.18	5	50	500

Ginsenoside Rg ₃	1.12	5	50	500
Ginsenoside Rf	1.06	5	50	500
Ginsenoside Rb ₁	1.03	5	50	500
Ginsenoside Rb ₂	0.93	5	50	500
Ginsenoside Rb ₃	1.01	5	50	500
Ginsenoside Rc	1.05	5	50	500
Ginsenoside Rd	1.04	5	50	500
Pseudoginsenoside RT ₅	1.11	5	50	500
24(R)-pseudoginsenoside F ₁₁	1.03	5	50	500
Methylophiopogon flavanone A	0.95	5	50	500
Methy ophiopogon flavanone B	0.97	5	50	500
