Table S1. Grid box coordinates and size parameters used for molecular docking.

	ADGRG3
Dimension (Å)	
x	91.513
y	113.233
z	100.418
Centre (Å)	
x	46
y	62
z	80

Table S2. Active site prediction for ADGRG3 using DoGSiteScorer.

Protein	Site	Volume Å^3	Surface Å^2	Drug Score	Simple Score
ADGRG3	S1	2190.02	2063.71	0.81	0.72
	S2	170.75	284.28	0.26	0.08
	S3	155.84	298.64	0.23	0.0

Table S3. Parameters evaluated for drug-likeness of ginsenosides and the control drugs.

Compound	MCE-18	SAscore	Fsp^3	PAINS	NPScore	Pfizer
Ginsenoside Rg3	132.92	5.84	0.95	0	2.66	Accepted
Ginsenoside Rk3	108.59	5.48	0.88	0	3.21	Accepted
Ginsenoside F5	132.5	5.96	0.95	0	2.70	Accepted
Ginsenoside Rg7	135.58	6.03	0.95	0	2.43	Accepted
Ginsenoside F1	113.02	5.57	0.94	0	3.01	Accepted
Dexamethasone	81.57	4.63	0.72	0	2.20	Accepted
HCY	76.63	4.35	0.81	0	2.40	Accepted

Table S4. Parameters evaluated for absorption of ginsenosides and the control drugs.

Compound	Caco-2 permeability	MDCK permeability	Pgp-inhibitor	Pgp-substrate	HIA	F (20%)	F (30%)
Ginsenoside Rg3	- 5.292	9.3e-05	0.98	0.008	0.974	0.731	0.973
Ginsenoside Rk3	- 5.008	3.1e-05	0.791	0.009	0.88	0.137	0.065
Ginsenoside F5	- 5.362	7.7e-05	0.987	0.022	0.988	0.856	0.985
Ginsenoside Rg7	- 5.512	0.000114	0.859	0.006	0.945	0.911	0.974
Ginsenoside F1	- 4.994	5e-05	0.917	0.018	0.927	0.306	0.725
Dexamethasone	-4.82	2e-05	0.12	0.008	0.04	0.004	0.003
HCY	- 4.832	2.5e-05	0.562	0.01	0.235	0.008	0.01

Table S5. Parameters evaluated for distribution of ginsenosides and the control drugs.

Compound	PPB (%)	VD (L/kg)	BBB (log BB)	Fu (%)
Ginsenoside Rg3	84.94	0.527	0.081	6.466
Ginsenoside Rk3	91.37	1.611	0.085	5.933
Ginsenoside F5	78.03	0.444	0.09	9.110
Ginsenoside Rg7	63.99	0.274	0.274	15.23
Ginsenoside F1	88.14	0.845	0.079	6.905
Dexamethasone	79.46	0.99	0.99	12.83
HCY	85.17	0.513	0.957	16.20

Table S6. Parameters evaluated for metabolism of ginsenosides and the control drugs.

Compound	CYP1A2 inhibitor	CYP1A2 substrate	CYP2C19 inhibitor	CYP2C19 substrate	CYP2C9 inhibitor	CYP2C9 substrate	CYP2D6 inhibitor	CYP2D6 substrate	CYP3A4 inhibitor	CYP3A4 substrate
Ginsenoside Rg3	0.0	0.085	0.0	0.522	0.0	0.086	0.0	0.09	0.011	0.042
Ginsenoside Rk3	0.001	0.108	0.003	0.738	0.004	0.259	0.0	0.189	0.042	0.107
Ginsenoside F5	0.0	0.09	0.0	0.409	0.0	0.105	0.0	0.106	0.01	0.034
Ginsenoside Rg7	0.0	0.075	0.0	0.355	0.0	0.101	0.0	0.131	0.005	0.041
Ginsenoside F1	0.001	0.114	0.001	0.807	0.003	0.236	0.0	0.113	0.032	0.073
Dexamethasone	0.012	0.608	0.025	0.802	0.024	0.129	0.01	0.072	0.425	0.914
HCY	0.008	0.775	0.026	0.845	0.031	0.262	0.002	0.161	0.098	0.917

Table S7. Parameters evaluated for excretion of ginsenosides and the control drugs.

Compound	CL	$T_{1/2}$
Ginsenoside Rg3	0.628	0.037
Ginsenoside Rk3	3.868	0.024
Ginsenoside F5	0.751	0.034
Ginsenoside Rg7	0.613	0.123
Ginsenoside F1	3.983	0.033
Dexamethasone	3.363	0.765
HCY	3.748	0.865

Table S8. Parameters evaluated for toxicity of ginsenosides and the control drugs.

Compound	hERG Blockers	H-HT	DILI	AMES Toxicity	ROA	Skin Sensitization	Carcinogenicity	Eye Corrosion	Respiratory Toxicity
Ginsenoside Rg3	0.032	0.227	0.006	0.069	0.204	0.012	0.005	0.003	0.352
Ginsenoside Rk3	0.017	0.245	0.01	0.05	0.568	0.024	0.01	0.003	0.811
Ginsenoside F5	0.042	0.21	0.006	0.072	0.347	0.019	0.007	0.003	0.556
Ginsenoside Rg7	0.065	0.232	0.007	0.059	0.127	0.019	0.003	0.003	0.399
Ginsenoside F1	0.038	0.274	0.008	0.042	0.316	0.036	0.007	0.003	0.863
Dexamethasone	0.033	0.543	0.018	0.04	0.398	0.041	0.774	0.003	0.95
HCY	0.044	0.49	0.039	0.056	0.091	0.032	0.18	0.003	0.387