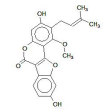
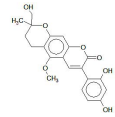
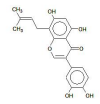
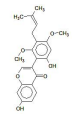
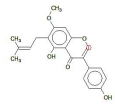
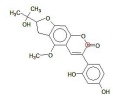
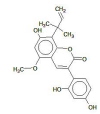
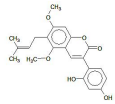
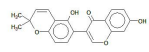
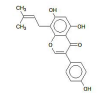
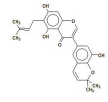
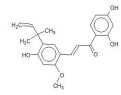
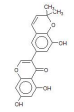
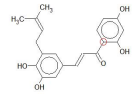
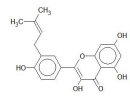
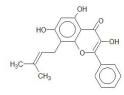
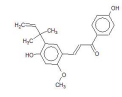
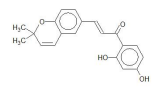
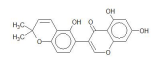
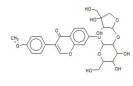
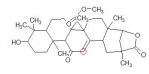
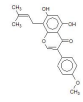
Supplementary Table 3. Active compounds

Mol ID	Molecule Name	OB (%)	DL	Classification	Structure
MOL002311	GLL	90.78	0.67	Coumarin	
MOL004904	Llicopyranocoumarin	80.36	0.65	Coumarin	
MOL004863	3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-8-(3-methylbut-2-enyl) Chromone	66.37	0.41	Isoflavones	
MOL004855	Licoricone	63.58	0.47	Isoflavones	
MOL005000	Gancaonin G	60.44	0.39	Isoflavones	
MOL004824	(2S)-6-(2,4-dihydroxyphenyl)-2-(2-hydroxypropan-2-yl)-4-methoxy-2,3-dihydrofuro[3,2-g]chromen-7-one	60.25	0.63	Coumarin	
MOL004849	3-(2,4-dihydroxyphenyl)-8-(1,1-dimethylprop-2-enyl)-7-hydroxy-5-methoxy-coumarin	59.62	0.43	Coumarin	
MOL004879	Glycyrin	52.61	0.47	Coumarin	
MOL004912	Glabrone	52.51	0.5	Isoflavones	
MOL003656	Lupiwighteone	51.64	0.37	Isoflavones	
MOL004856	Gancaonin A	51.08	0.4	Isoflavones	
MOL005001	Gancaonin H	50.1	0.78	Isoflavones	

MOL004848	Licochalcone G	49.25	0.32	Chalcones	
MOL004857	Gancaonin B	48.79	0.45	Isoflavones	
MOL004827	Semilicoisoflavone B	48.78	0.55	Isoflavones	
MOL004898	(E)-3-[3,4-dihydroxy-5-(3-methylbut-2-enyl)phenyl]-1-(2,4-dihydroxyphenyl)prop-2-en-1-one	46.27	0.31	Chalcones	
MOL004949	ILF	45.17	0.42	Flavonoids	
MOL004828	Glepidotin A	44.72	0.35	Flavonoids	
MOL004948	Isoglycyrol	44.7	0.84	Coumarin	
MOL004866	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-(3-methylbut-2-enyl) chromone	44.15	0.41	Flavonoids	
MOL004915	Eurycarpin A	43.28	0.37	Isoflavones	
MOL004883	LIA	41.61	0.42	Isoflavones	
MOL000497	LCA	40.79	0.29	Chalcones	
MOL004815	Kanzonol B	39.62	0.35	Chalcones	
MOL004884	Licoisoflavone B	38.93	0.55	Isoflavones	
MOL004917	Glycyroside	37.25	0.79	Isoflavones	

MOL004905	3,22-Dihydroxy-11-oxo-delta(12)-oleanene-27-alpha-methoxycarbonyl-29-oic acid	34.32	0.55	Triterpenes	
MOL004864	5,7-dihydroxy-3-(4-methoxyphenyl)-8-(3-methylbut-2-enyl)chromone	30.49	0.41	Isoflavones	

The ingredients of OB≥30% and DL≥0.1 in licorice.Bioavailability play a key role in the drug development period for both new drug products and their generic equivalents. High OB is usually a key indicator of bioactive molecules in juding. (chen et al, 2001). DL is widely used to assess the possibility of compounds becoming drugs. Screening high DL can eliminate the interference of non-pharmaceutical compounds and save the cost and time of drug research and development. (Walters and murcko, 2002). So we rank the OB and DL values from high to low, and the choice of compounds with high oral bioavailability and drug-like properties are very helpful to our drug development and research.