Table 1. Screening results of the main active ingredients of *A. paniculata*

No.	Mol ID	Molecule Name	MW	OB (%)	DL	Caco-2
1	MOL000173	wogonin	284.28	30.68	0.23	0.79
2	MOL002928	oroxylin a	284.28	41.37	0.23	0.76
3	MOL002932	Panicolin	314.31	76.26	0.29	0.84
4	MOL008203	14-deoxy-11-oxo-andrographolide	348.48	57.06	0.34	-0.09
5	MOL008204	Mono-O-methylwightin	358.37	103.11	0.40	0.94
6	MOL008206	Moslosooflavone	298.31	44.09	0.25	1.01
7	MOL008209	Deoxycamptothecine	332.38	50.01	0.77	0.68
8	MOL008210	Deoxyelephantopin	344.39	105.32	0.4	0.26
9	MOL008213	14-deoxy-12-methoxyandrographolide	364.53	70.29	0.36	-0.03
10	MOL008215	Paniculide B	280.35	52.27	0.21	0.03
11	MOL008216	Paniculide C	278.33	79.73	0.21	0.02
12	MOL008217	Paniculogenin	448.71	47.66	0.75	-0.2
13	MOL008218	1-Monoolein	356.61	34.13	0.3	0.23
14	MOL008219	3-[2-[(1R,4aS,5R,8aS)-5,8a-dimethyl-2-methylene-5-methylol-decalin-1-yl]ethyl]-5H-furan-2-one	318.50	51.78	0.28	0.69
15	MOL008222	andrographidine B_qt	330.31	72.72	0.33	0.6
16	MOL008223	andrographidine C	460.47	56.85	0.77	-0.6
17	MOL008226	14-deoxyandrographolide	334.50	56.3	0.31	0.17
18	MOL008228	Andrographin	328.34	37.57	0.33	0.73
19	MOL008229	Andrographin F	536.53	33.34	0.85	-0.84
20	MOL008230	andrographidine F_qt	374.37	77.13	0.45	0.91
21	MOL008232	Andrographolide	350.50	46.96	0.36	-0.25
22	MOL008234	andrographolide-19-β-D-glucoside_qt	350.50	53.44	0.35	-0.30
23	MOL008238	3-[2-[(1S,4aR,5S,8aR)-5,8a-dimethyl-2-methylene-5-methylol-decalin-1-yl] ethyl]-5H-furan-2-one	318.50	63.54	0.28	0.68
24	MOL008239	Quercetin tetramethyl (3',4',5,7) ether	358.37	31.57	0.41	0.90

Sybyl 1.3		AutoDock Vina	
Symbol/Ligand	Total Score	Symbol/Ligand	Binding energy (kcal mol-1)
NOS2/MOL008218	10.076	NOS2/MOL008209	-11.0
PPARG/MOL008218	9.718	F10/MOL008223	-9.8
EGFR/MOL008218	9.3271	NOS2/MOL000173	-9.7
PIK3CG/MOL008218	9.3038	NOS2/MOL002932	-9.7
ACE2/MOL008218	9.1932	NOS2/MOL002928	-9.6
F10/MOL008218	8.8676	NOS2/MOL008206	-9.6
PTGS1/MOL008218	8.7675	NOS2/MOL008228	-9.6
PTGS2/MOL008218	8.1999	NOS2/MOL008223	-9.4
DPP4/MOL008218	7.7884	PPARG/MOL008209	-9.4
MAPK14/MOL008239	7.3153	PIK3CG/MOL008209	-9.3
PARP1/MOL008229	5.5767	ACE2/MOL008217	-9.8

Table 2. The best ingredients to interface with key proteins predicted by Sybyl 1.3 and AutoDock Vina