

Table S1 Information for molecular docking

Number	Hub gene	PDB ID	Mol ID	Compound	Docking affinity (kcal/mol)
1	PIK3CA	6OAC	MOL008411	11-Hydroxyrankinidine	-5.4
			MOL000239	Jaranol	-5.2
			MOL003896	7-Methoxy-2-methyl isoflavone	-5.6
			MOL000380	(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	-4.9
			MOL000354	isorhamnetin	-3.9
2	PIK3R1	5UBT	MOL008411	11-Hydroxyrankinidine	-5.9
			MOL000239	Jaranol	-7.8
			MOL003896	7-Methoxy-2-methyl isoflavone	-7.8
			MOL000380	(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	-7.8
			MOL000354	isorhamnetin	-8
3	SRC	1KSW	MOL008411	11-Hydroxyrankinidine	-9.1
			MOL000239	Jaranol	-8.7
			MOL003896	7-Methoxy-2-methyl isoflavone	-8.8
			MOL000380	(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	-8.4
			MOL000354	isorhamnetin	-8.7
4	HRAS	2C5L	MOL008411	11-Hydroxyrankinidine	-6.7
			MOL000239	Jaranol	-6.1
			MOL003896	7-Methoxy-2-methyl isoflavone	-6.5
			MOL000380	(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	-6
			MOL000354	isorhamnetin	-7.2
5	MAPK1	6G9J	MOL008411	11-Hydroxyrankinidine	-8.6
			MOL000239	Jaranol	-7.2
			MOL003896	7-Methoxy-2-methyl isoflavone	-7.7
			MOL000380	(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	-8.3
			MOL000354	isorhamnetin	-8.2
6	AKT1	2C5L	MOL008411	11-Hydroxyrankinidine	-10
			MOL000239	Jaranol	-7.9
			MOL003896	7-Methoxy-2-methyl isoflavone	-8.3
			MOL000380	(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	-8.3
			MOL000354	isorhamnetin	-8.2

average docking
affinity: -7.37333

Table S2 Information of top 10 Gene Ontology (GO) analysis

Number	Catogary	Term ID	Description	-Log ₁₀ (P)	Count
1	Biological processes(BP)	GO:0033674	positive regulation of kinase activity	-42.9	50
2	BP	GO:1901699	cellular response to nitrogen compound	-31.15	42
3	BP	GO:0009611	response to wounding	-27.77	40
4	BP	GO:0008015	blood circulation	-27.15	36
5	BP	GO:0010035	response to inorganic substance	-26.61	36
6	BP	GO:0043491	protein kinase B signaling	-26.13	28
7	BP	GO:0043269	regulation of ion transport	-25.52	38
8	BP	GO:0050804	modulation of chemical synaptic transmission	-23.79	31
9	BP	GO:0010817	regulation of hormone levels	-23.57	33
10	BP	GO:0031667	response to nutrient levels	-23.31	32
1	Cell component(CC)	GO:0045121	membrane raft	-22.72	27
2	CC	GO:0043235	receptor complex	-18.75	28
3	CC	GO:0030424	axon	-14.36	26
4	CC	GO:0000323	lytic vacuole	-14.22	27
5	CC	GO:0048471	perinuclear region of cytoplasm	-13.12	26
6	CC	GO:0005769	early endosome	-11.08	18
7	CC	GO:0045177	apical part of cell	-10.19	18
8	CC	GO:0098793	presynapse	-8.88	18
9	CC	GO:0098552	side of membrane	-7.71	18
10	CC	GO:0098978	glutamatergic synapse	-7.67	14
1	Molecular function(MF)	GO:0004672	protein kinase activity	-26.37	36
2	MF	GO:0019902	phosphatase binding	-14.9	17
3	MF	GO:0019904	protein domain specific binding	-13.32	26
4	MF	GO:0019900	kinase binding	-12.77	26
5	MF	GO:0042803	protein homodimerization activity	-12.23	24
6	MF	GO:0043560	insulin receptor substrate binding	-11.2	6
7	MF	GO:0042562	hormone binding	-10.89	11
8	MF	GO:0008289	lipid binding	-10.67	24
9	MF	GO:0020037	heme binding	-10.61	12
10	MF	GO:0051219	phosphoprotein binding	-10.24	10