

Integrated network pharmacology, molecular docking and experimental validation to investigate the mechanism of tannic acid in nasopharyngeal cancer

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Table S1. The hub genes screened from PPI network by CytoHubba.

Gene symbol	MCC	MNC	Degree	EPC	BottleNeck	EcCentricity	Closeness	Radiality	Betweenness	Stress
AKT1	527445136	32	32	17.469	2	0.5	36	2.9	206.36108	768
HSP90AA1	520090970	29	29	16.814	3	0.5	34.5	2.825	156.88547	658
ALB	527414665	26	27	16.559	4	0.5	33.5	2.775	102.18943	472
MMP9	520154286	25	25	16.382	5	0.33333	32.33333	2.7	55.62476	332
CCND1	520075807	24	25	16.253	3	0.5	32.5	2.725	89.73204	432
SRC	523011960	24	24	16.105	1	0.33333	31.83333	2.675	39.70186	260
MAPK3	489990486	24	24	16.175	2	0.33333	31.83333	2.675	72.07398	386
PTGS2	267180510	23	23	15.949	1	0.5	31.5	2.675	53.01202	302
HRAS	263874504	22	22	15.829	2	0.5	31	2.65	32.7465	230
IGF1	263462880	22	22	15.622	3	0.33333	30.83333	2.625	36.4503	224

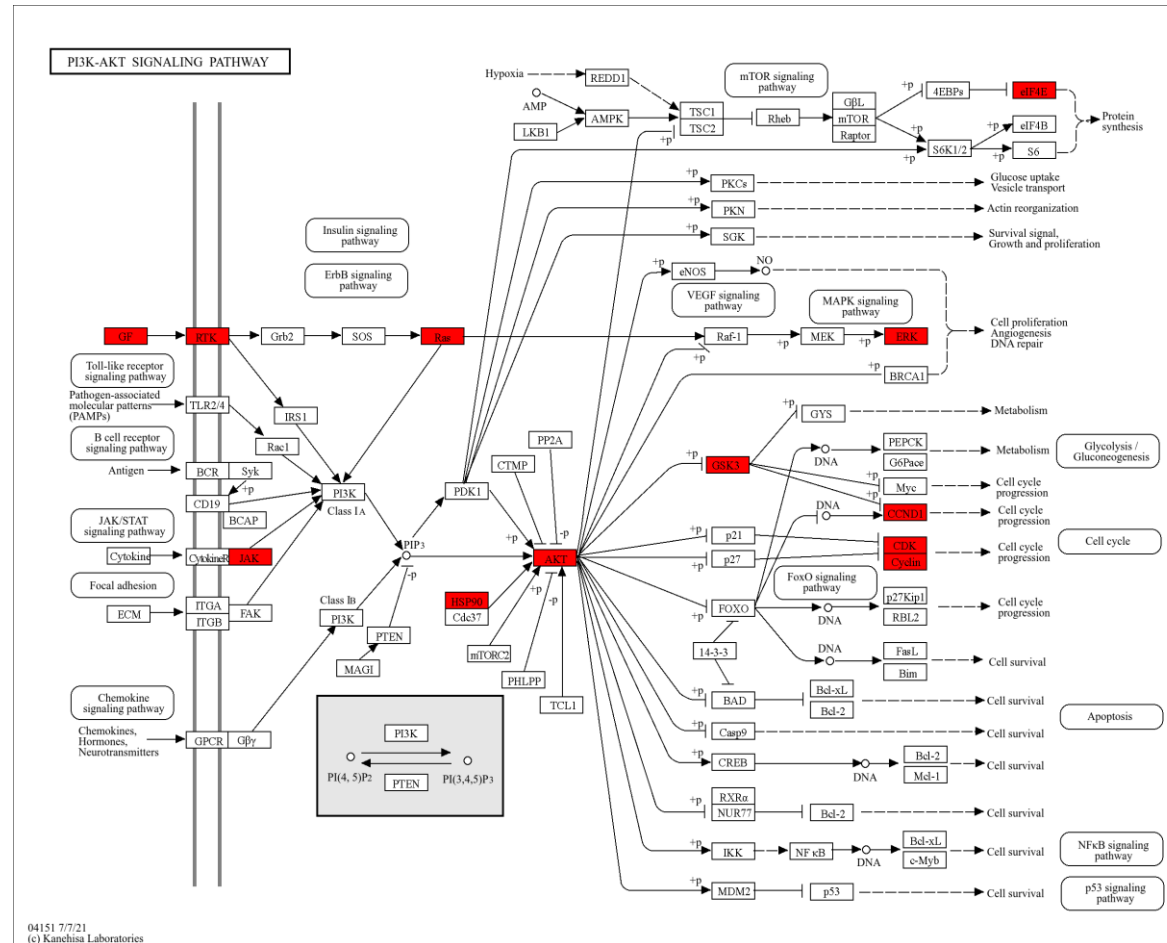


Figure S1 The effect of PI3K/AKT signaling pathway in the treatment of NPC by TA. Red block diagrams represent genes that are enriched in the pathway.

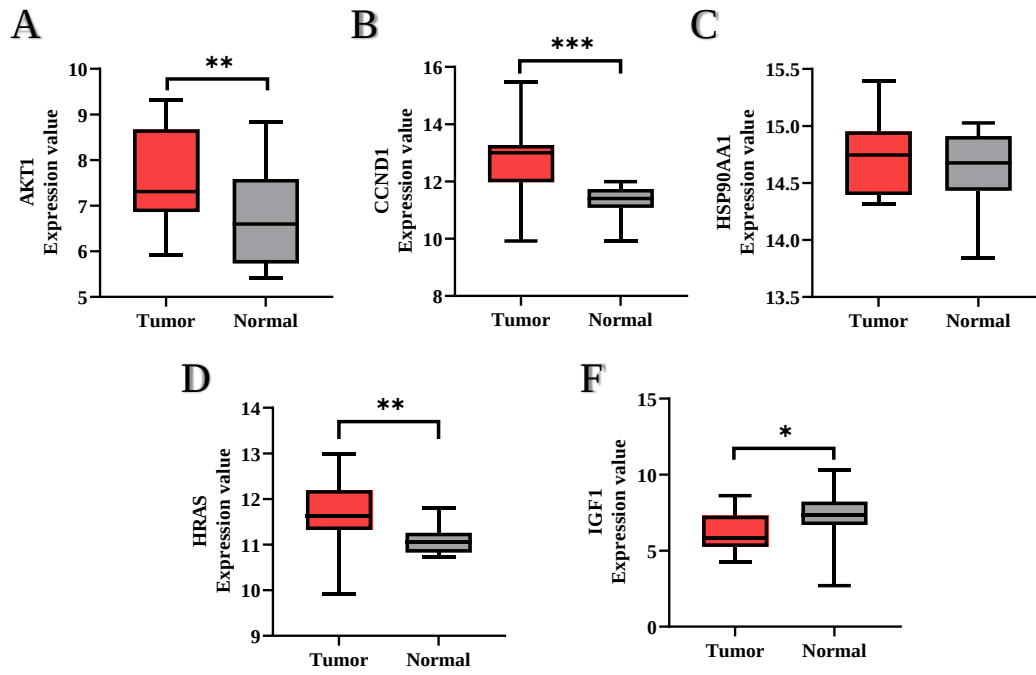


Figure S2 Boxplot of hub gene mRNA expression levels in the GSE53819 dataset. (A) AKT1, (B) CCND1, (C) HSP90AA1, (D) HRAS, (F) IGF1. * $P < 0.05$, ** $P < 0.01$, *** $P < 0.001$.

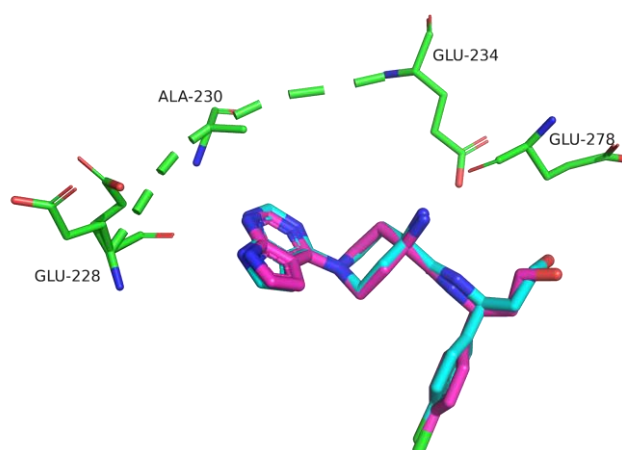


Figure S3 The comparison of experimental and predicted conformations of the bound ligand in AKT1 (PDB: 4GV1); Green represents amino acid residues, blue represents experimental ligand conformation, and purple represents calculated ligand conformation.

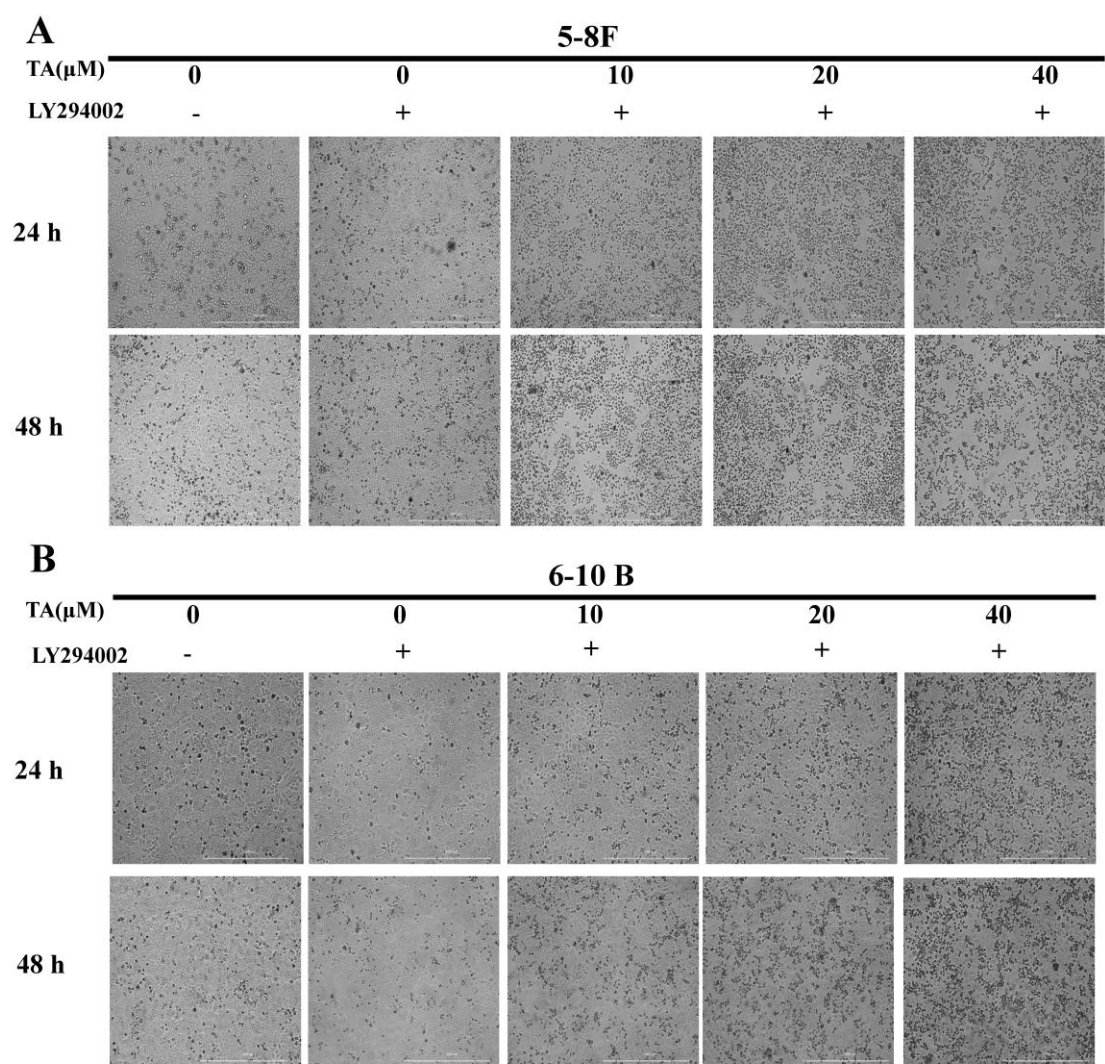


Figure S4 The representative images of cell morphology in PI3K inhibitors in nasopharyngeal carcinoma cells, scale bar = 1000 μ m.