

Figure S1. Two-dimensional ligand-protein interaction diagram of (A) IBC-extracellular signal-regulated kinase 1 and (B) IBC-ribosomal S6 kinase 2 complex. IBC, isobavachalcone.

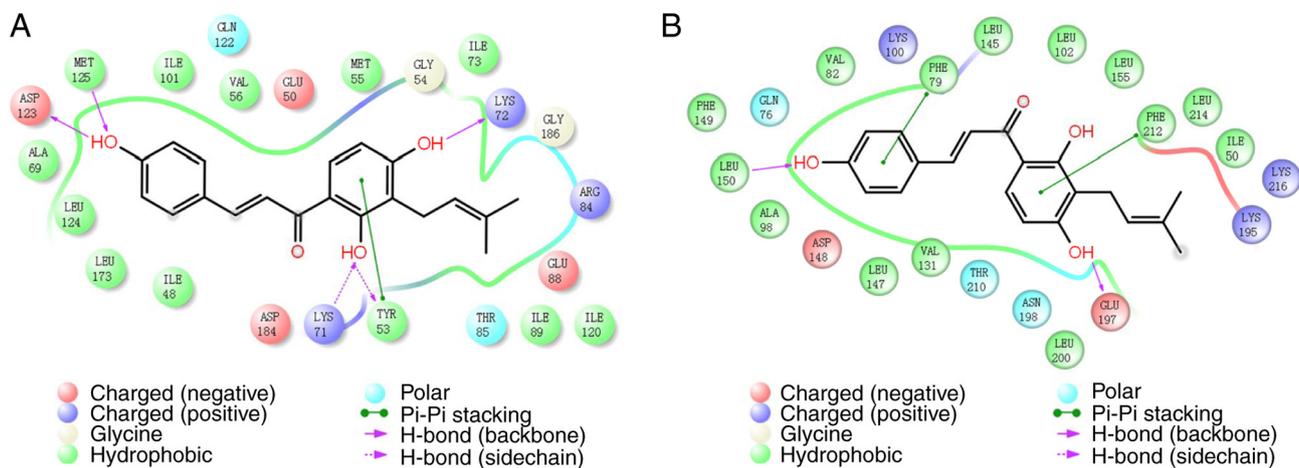


Figure S2. The effects of IBC on cell cycle distribution in liver cancer cells. HepG2 or Hep3B cells were treated with different concentrations of IBC for 48 h, and then cells were stained with propidium iodide and subjected to flow cytometry to assess cell cycle distribution. Data are presented as the mean \pm standard deviation ($n=3$). IBC, isobavachalcone.

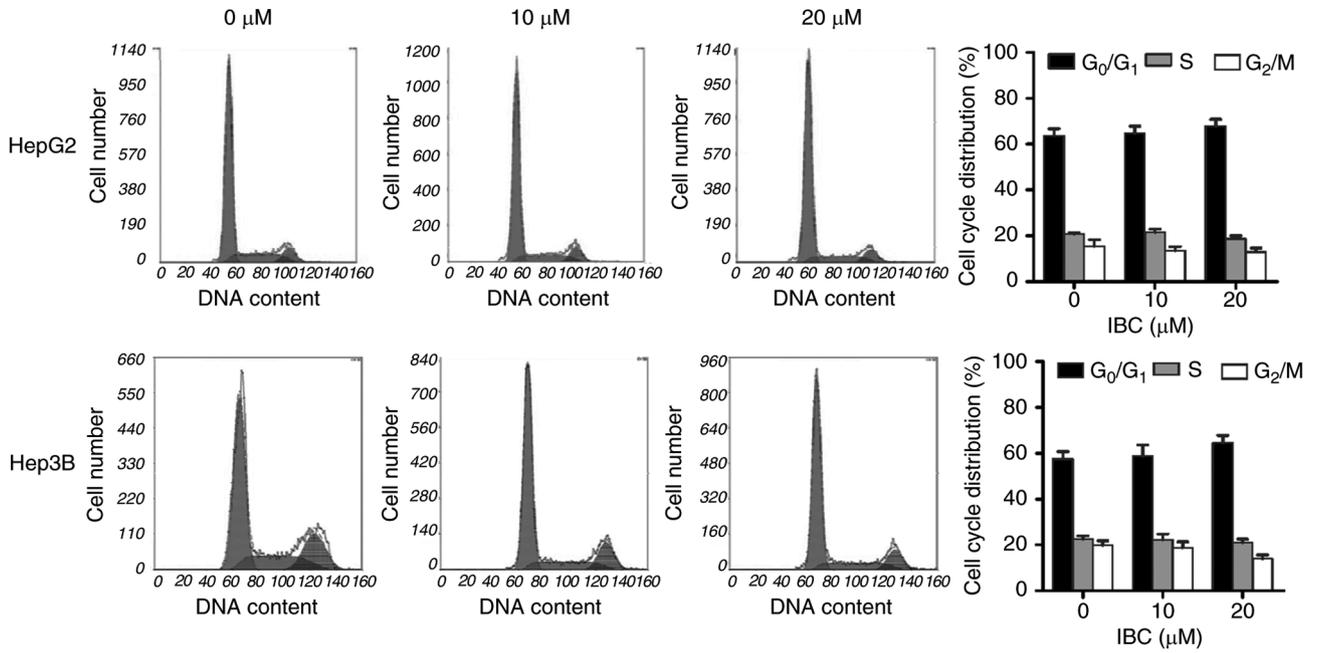


Figure S3. Enforced RSK2 expression promotes the proliferation of L02 cells. L02 cells were transfected with pCMV3-RSK2 or pCMV3 control vector. Following being transfected for 24 or 48 h, cell viability was assessed with a Cell Counting Kit-8 assay. Data are presented as the mean \pm standard deviation (n=3). *P<0.05 vs. cells transfected with control vector. RSK2, ribosomal S6 kinase 2; OD, optical density.

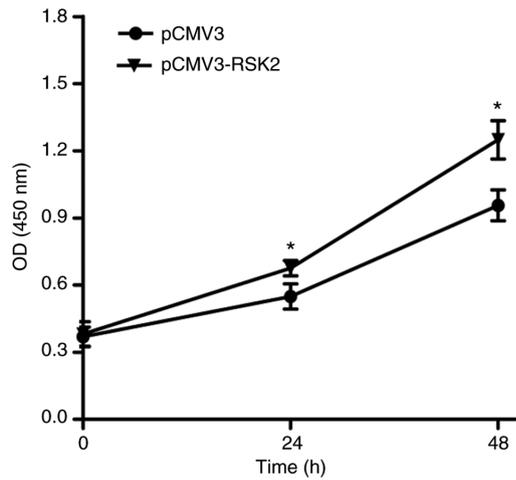


Table SI. The docking energies between isobavachalcone and RSK2^{NTKD} or RSK2^{CTKD} from both virtual screening and induced fit docking.

Docking methods	Binding domain docking energy (kcal/mol)	
	RSK2 ^{NTKD}	RSK2 ^{CTKD}
Virtual screening	-10.457	-8.567
Induced fit docking	-12.396	-10.621

RSK2, ribosomal S6 kinase 2; NTKD, N-terminal kinase domain; CTKD, C-terminal kinase domain.