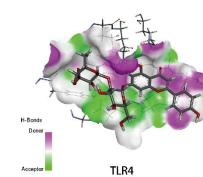


**Supplementary Figure 1**. Isolation of ROF from *Citrus grandis* 'Tomentosa': The flow chart of extraction and isolation of ROF (A), the chemical structure of ROF (B), and the Chromatograms of a standard ROF, sample ROF and *Citrus grandis* 'Tomentosa' that contains target compound (254 nm)

В

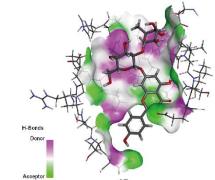


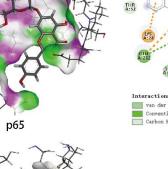


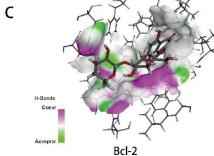


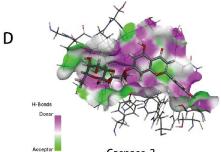
ASP A:53

SER A:51

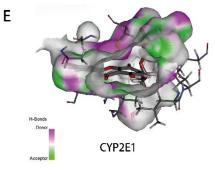


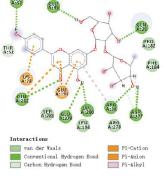






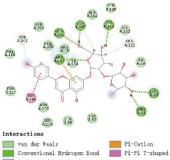




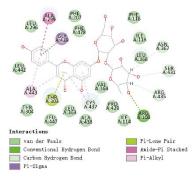




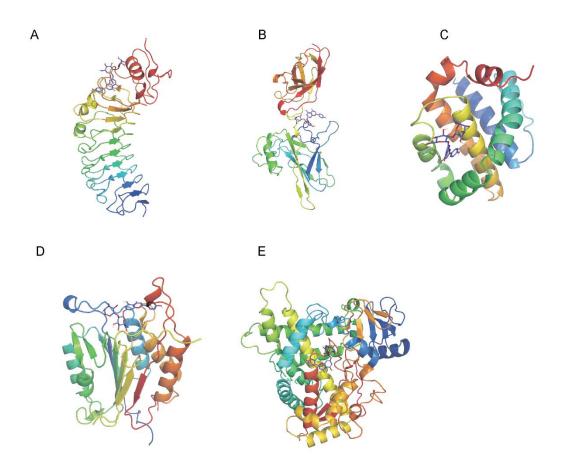




van der Vaals Conventional Hydrogen Bond Carbon Hydrogen Bond

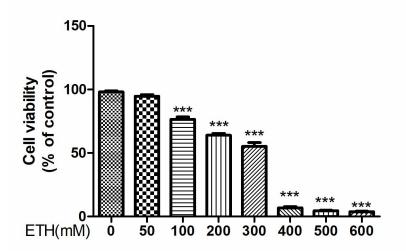


Supplementary Figure 2. Bioactive compound-protein docking combination: (A)TLR4, (B)p65, (C)Bcl-2, (D)Caspase-3, (E) CYP2E1.



Supplementary Figure 3. Bioactive compound-protein docking combination (3D binding structure):

(A)TLR4, (B)p65, (C)Bcl-2, (D)Caspase-3, (E) CYP2E1.



Supplementary Figure 4. Effects of ethanol on cell apoptosis and viability. Mean  $\pm$  SEM (n=6). \*\*\*P<0.001 vs. the CON group.