

ORIGINAL RESEARCH ARTICLE

*In silico* assessment of cannabinoids and related compounds as multi-target modulators of IL-2, TNF- $\alpha$ , HSP70/HSP90, EGF signaling, and MMP-2/MMP-9 in ovarian cancer

Supplementary Files

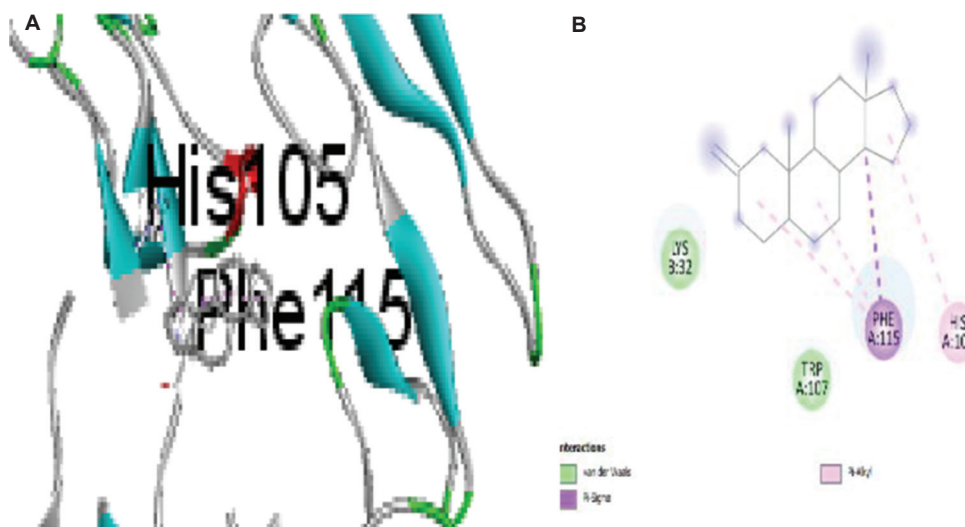


Figure S1. Binding interaction of 2-methylenecholestan-3-ol with TNF- $\alpha$ . (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.

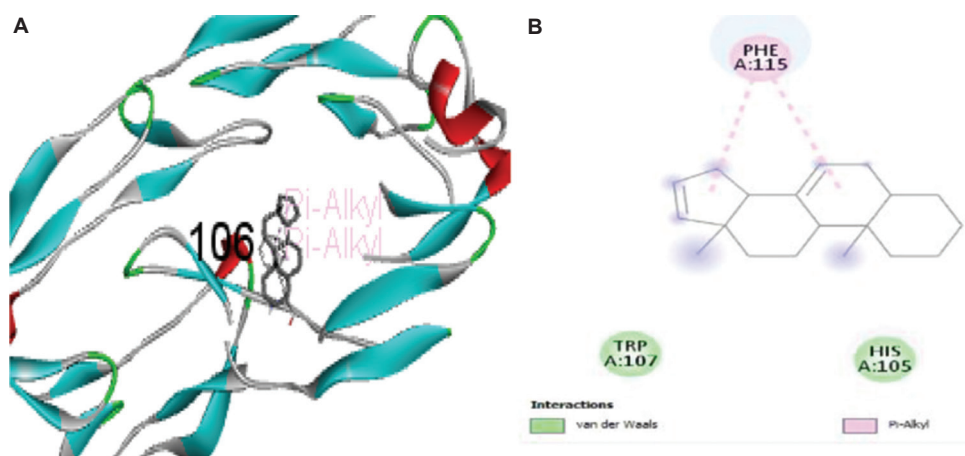
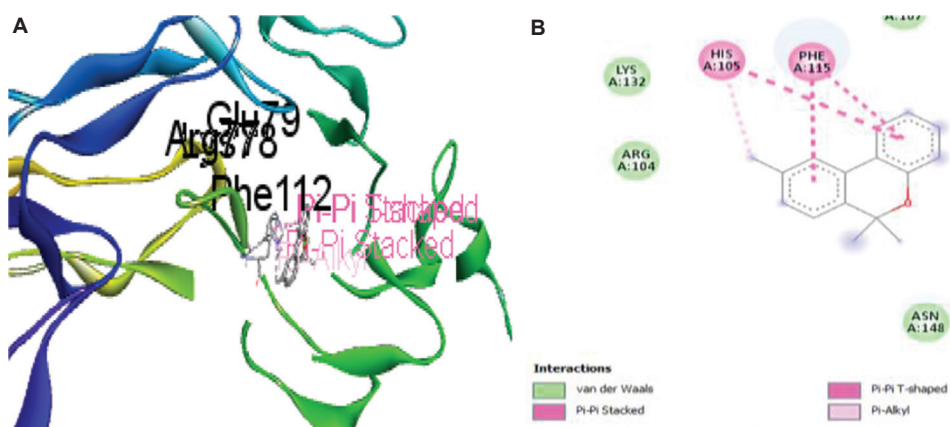
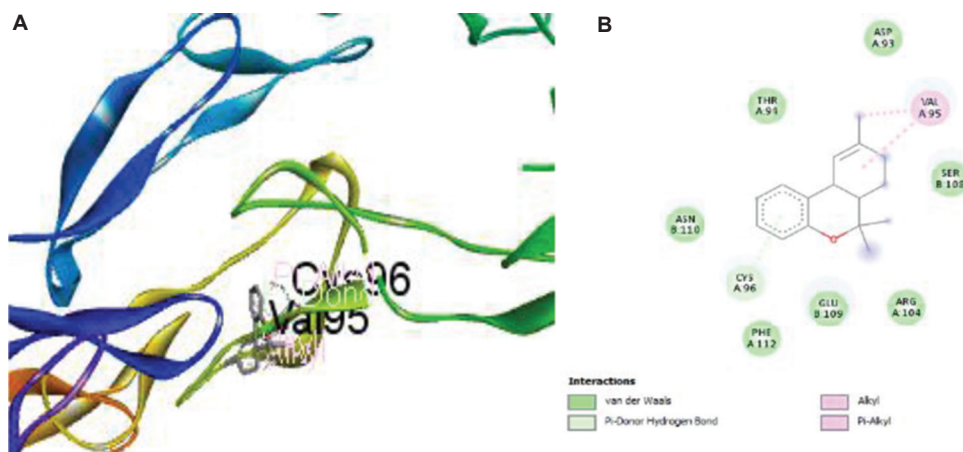


Figure S2. Binding interaction of elasterol with TNF- $\alpha$ . (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.

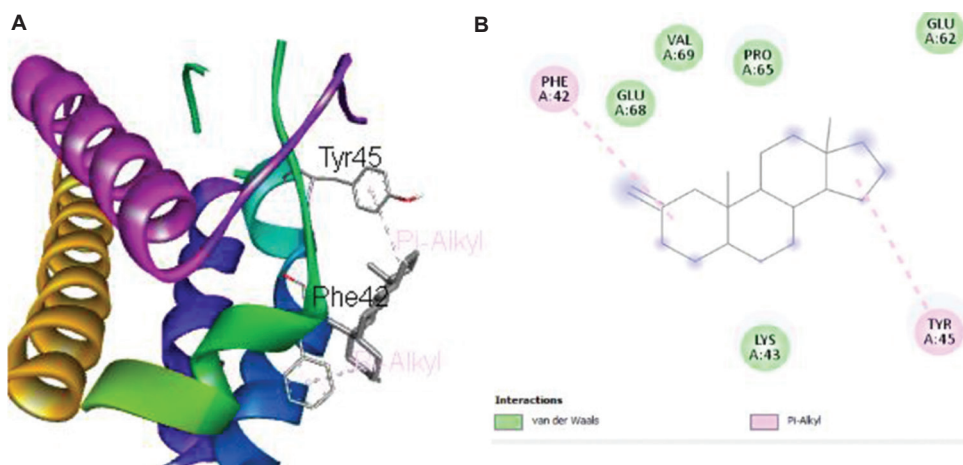


**Figure S3.** Binding interaction of cannabiniol with TNF- $\alpha$ . (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.

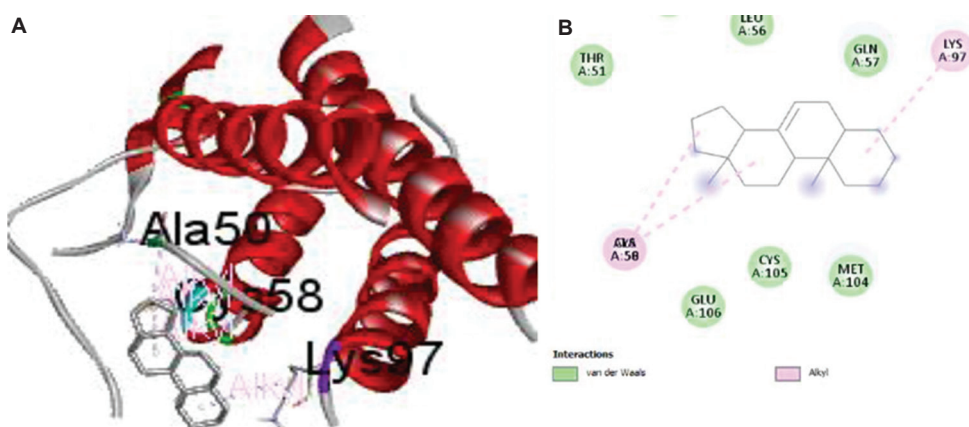


**Figure S4.** Binding interaction of tetrahydrocannabivarin with TNF- $\alpha$ . (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.

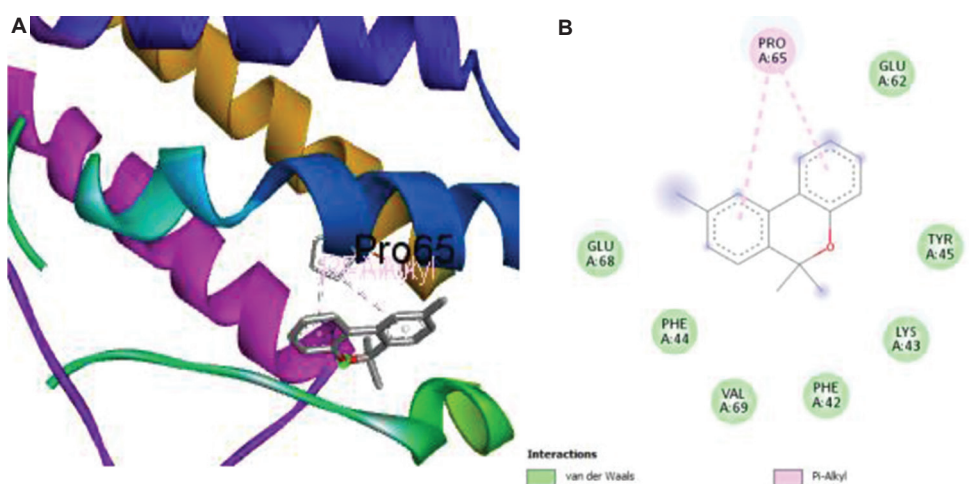
**Interleukin-2**



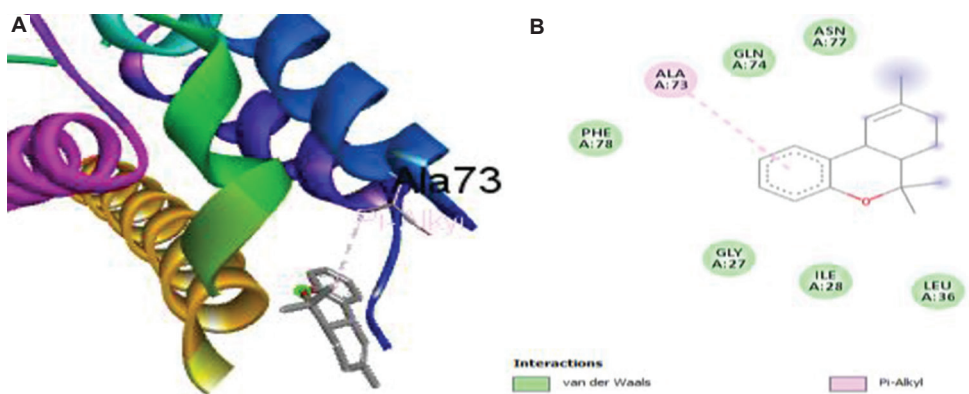
**Figure S5.** Binding interaction of 2-methylenecholestan-3-ol with IL-2. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



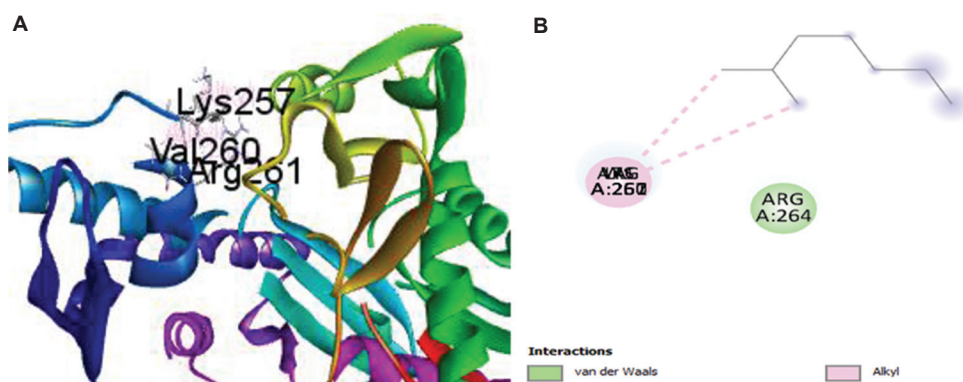
**Figure S6.** Binding interaction of elasterol with IL-2. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



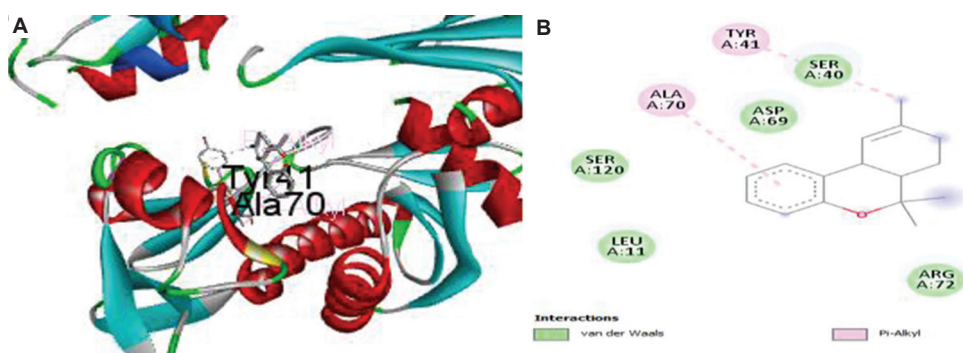
**Figure S7.** Binding interaction of cannabinal with IL-2. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



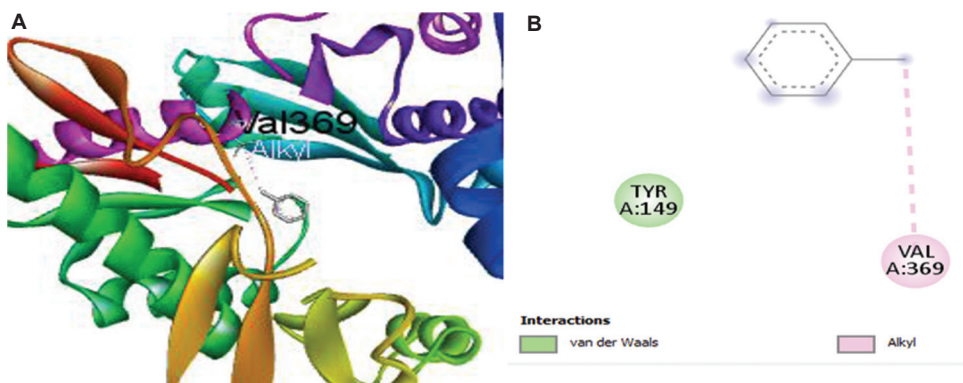
**Figure S8.** Binding interaction of tetrahydrocannabivarin with IL-2. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



**Figure S9.** Binding interaction of 2-methylenecholestan-3-ol with HSP70. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



**Figure S10.** Binding interaction of tetrahydrocannabinol with HSP70. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



**Figure S11.** Binding interaction of 4,6-dimethoxy-o-toluate with HSP70. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.

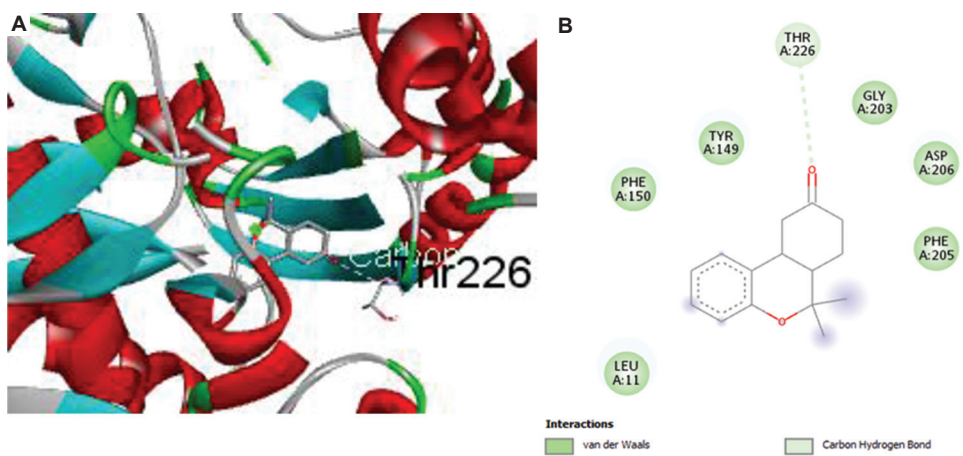


Figure S12. Binding interaction of nabilone with HSP70. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.

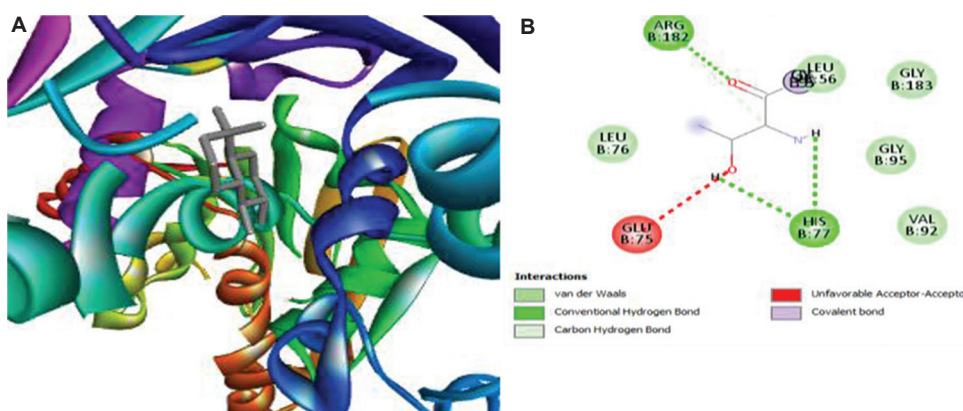


Figure S13. Binding interaction of 2-methylenecholestan-3-ol with HSP-90. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.

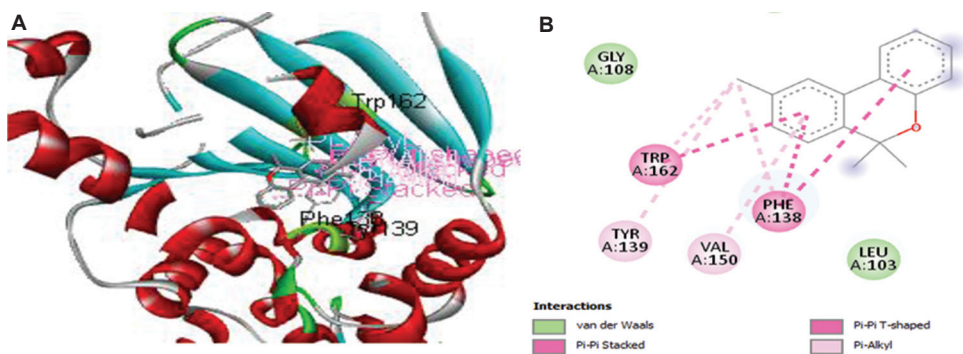
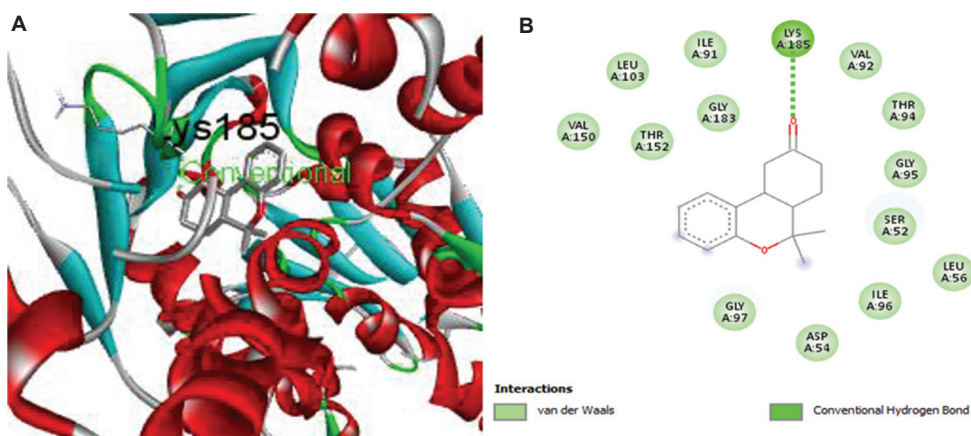
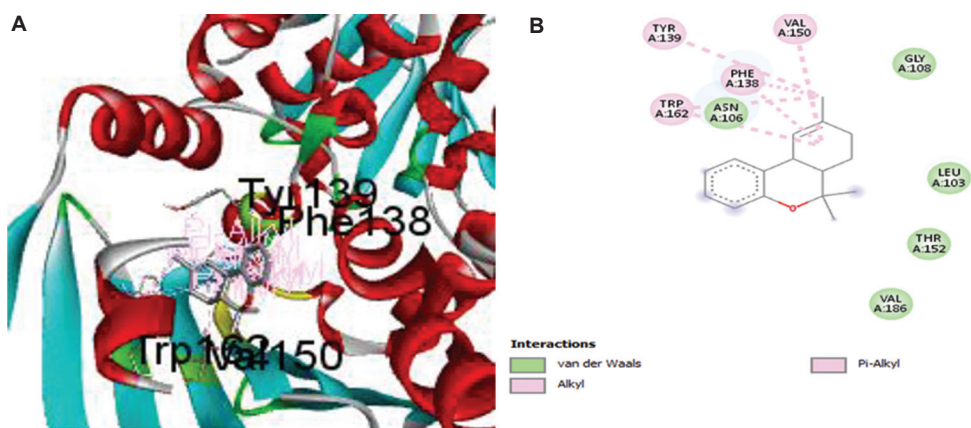


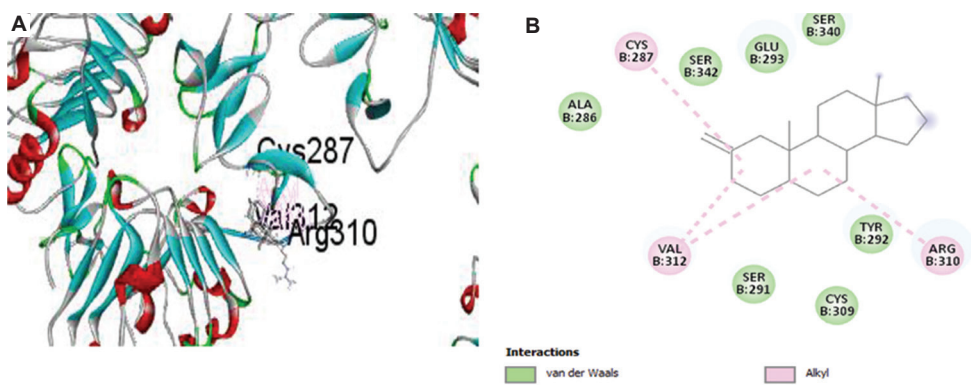
Figure S14. Binding interaction of cannabinal with HSP-90. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



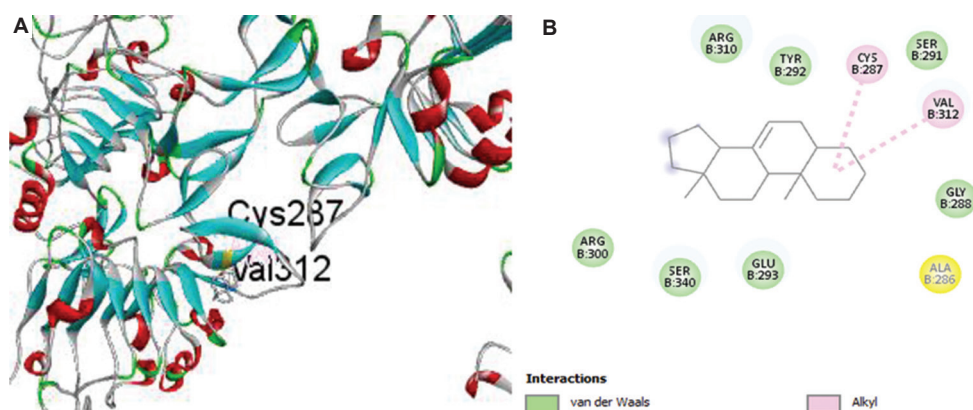
**Figure S15.** Binding interaction of nabilone with HSP-90. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



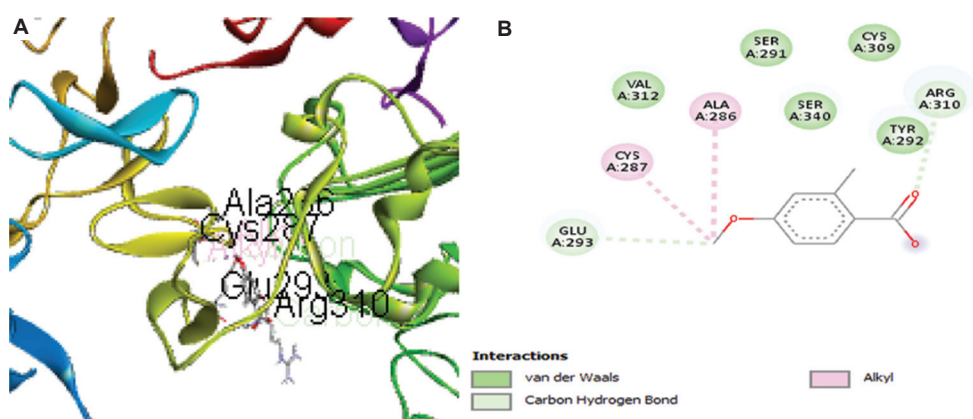
**Figure S16.** Binding interaction of tetrahydrocannabivarin with HSP-90. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



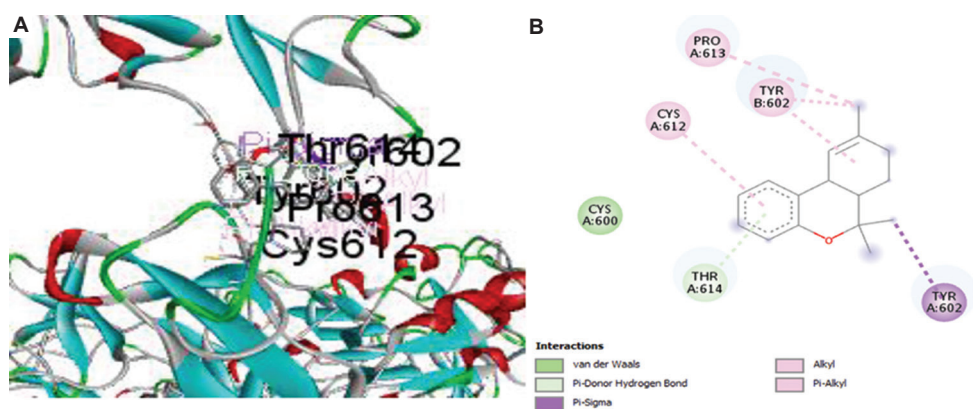
**Figure S17.** Binding interaction of 2-methylenecholestan-3-ol with EGF. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



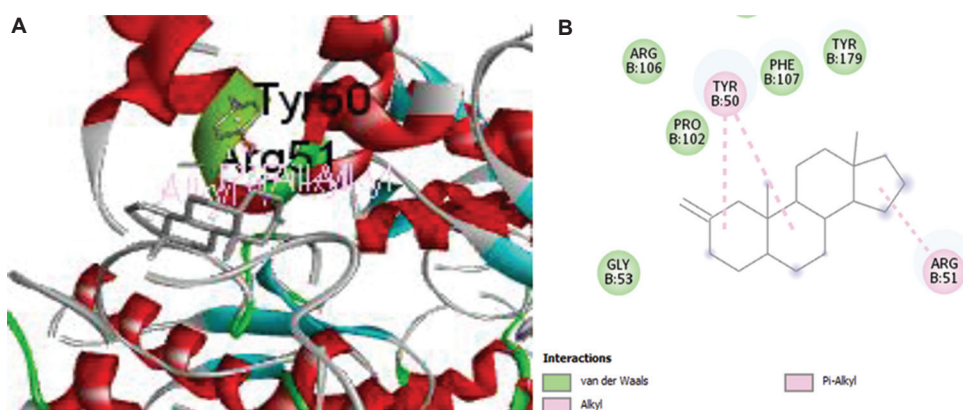
**Figure S18.** Binding interaction of elasterol with EGF. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



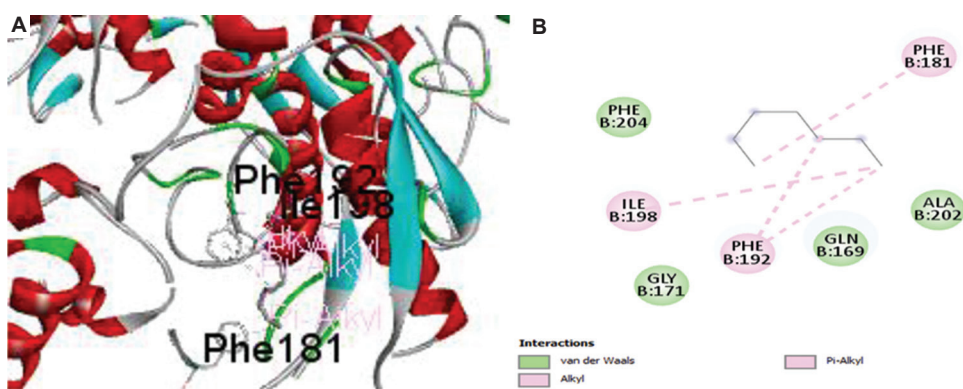
**Figure S19.** Binding interaction of 4,6-dimethoxy-o-toluate with EGF. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



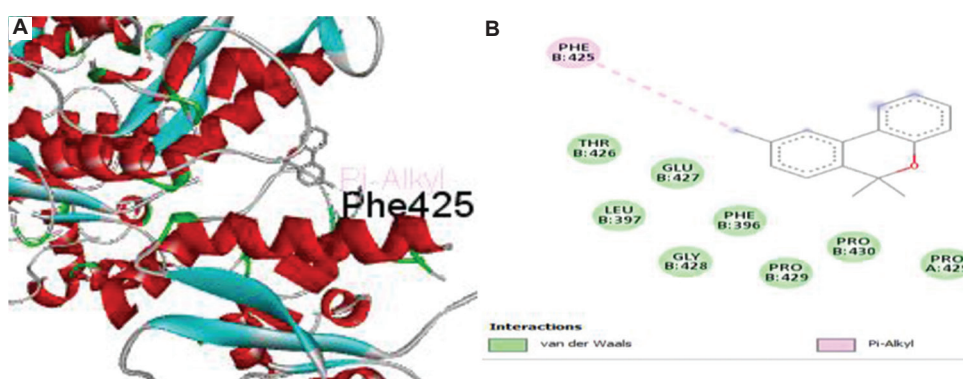
**Figure S20.** Binding interaction of tetrahydrocannabivarin with EGF. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



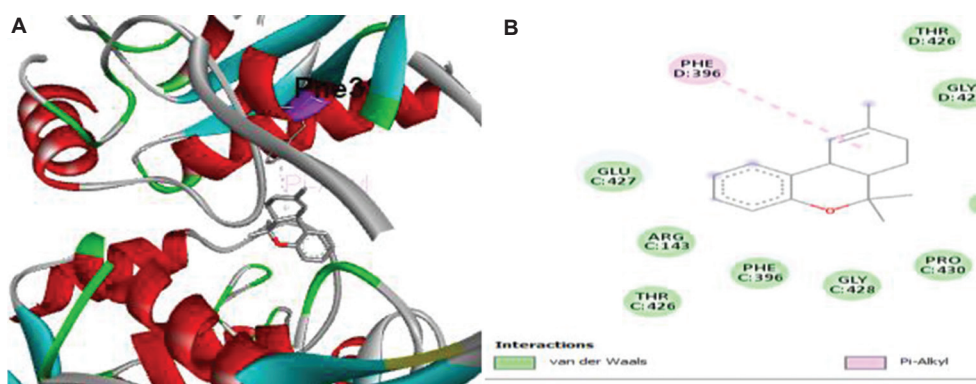
**Figure S21.** Binding interaction of 2-methylenecholestan-3-ol with MMP-9. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



**Figure S22.** Binding interaction of elasterol with MMP-9. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



**Figure S23.** Binding interaction of cannabinal with MMP-9. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.



**Figure S24.** Binding interaction of tetrahydrocannabivarin with MMP-9. (A) 3D binding pose highlighting key interacting residues; (B) corresponding 2D interaction map.