Supplementary Materials

Evaluation of 3,5-diphenyl-2-pyrazolines for antimitotic activity by inhibition of tubulin polymerization

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Supplementary Figures

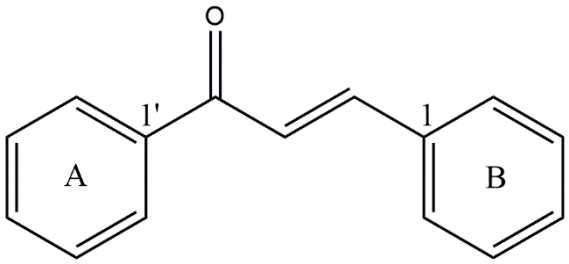


Fig. S1. The chemical structure and numbering of chalcone.

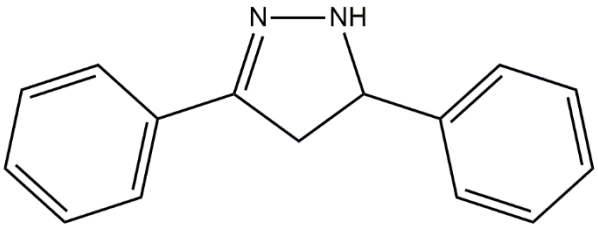


Fig. S2. The chemical structure of 3,5-diphenyl-2-pyrazoline.

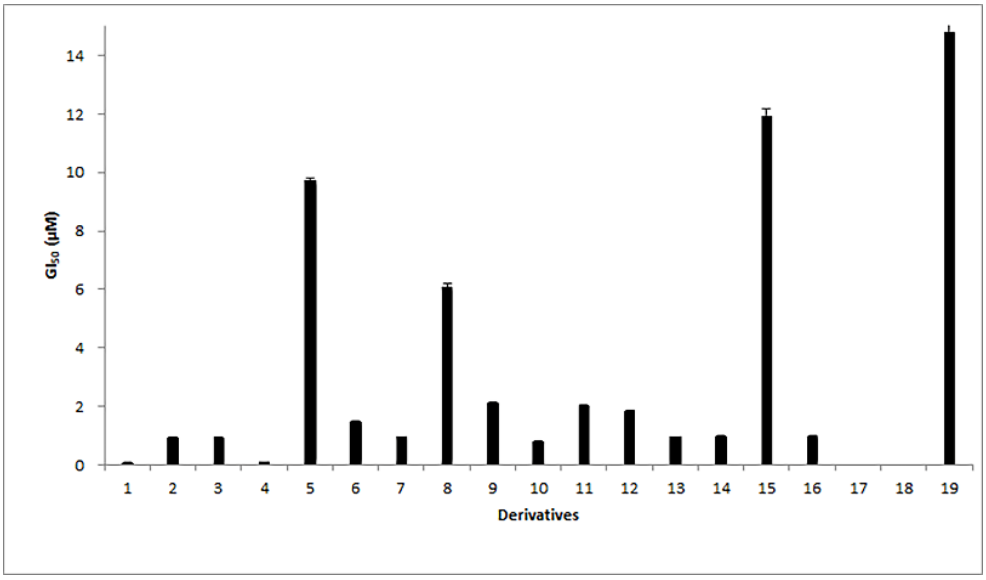


Fig. S3. Graph of the half-maximal cell growth inhibitory concentrations (GI_{50}) of 3,5-diphenyl-2-pyrazoline derivatives (with error bars).

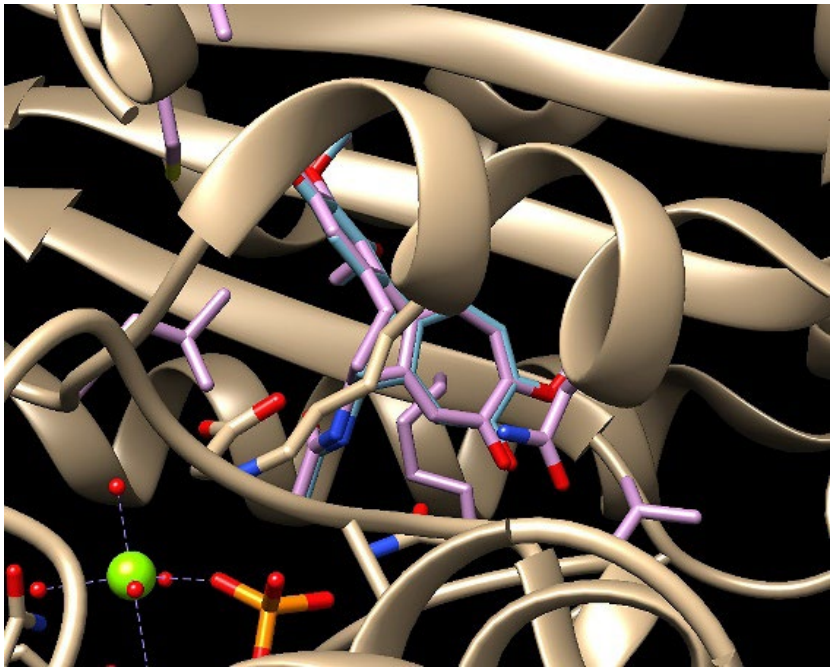
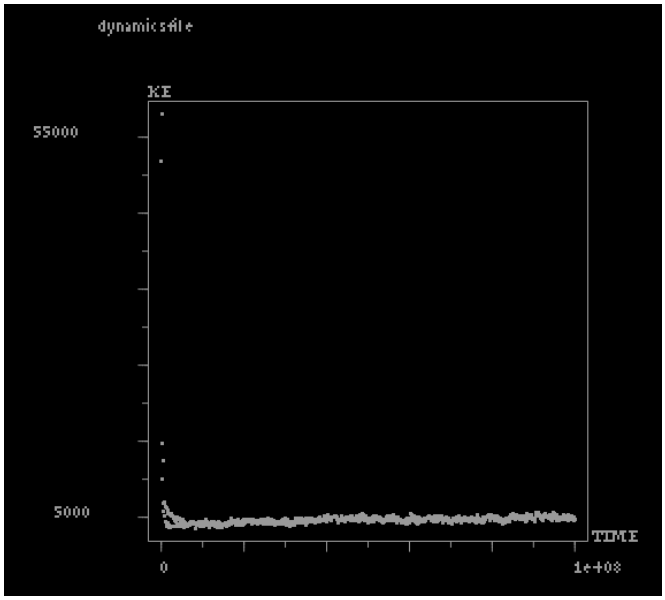


Fig. S4. 3D images of colchicine obtained from the current docking (pink) and colchicine contained in the crystallographic structure of tubulin 6xer.pdb as its ligand (cyan) in the binding pocket of the 6xer.pdb generated using PyMol.

(A)



(B)

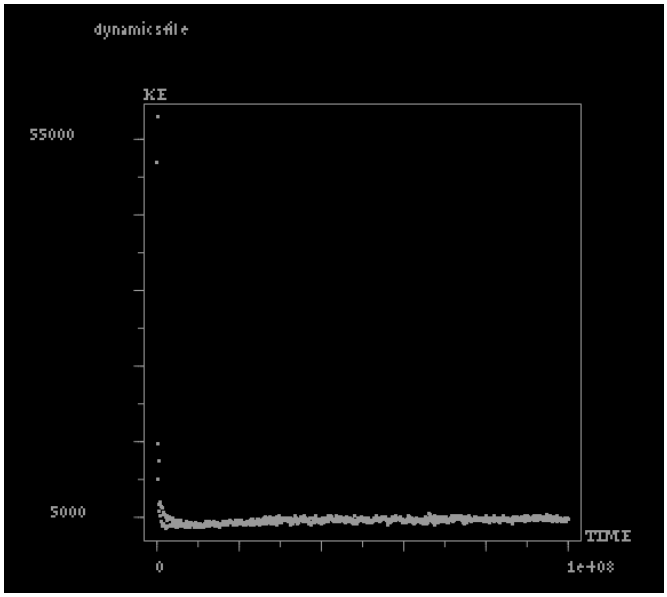


Fig. S5. Plots of kinetic energy of colchicine-tubulin complex (A) and derivative **4** (B) against the simulation time 100 nsec.

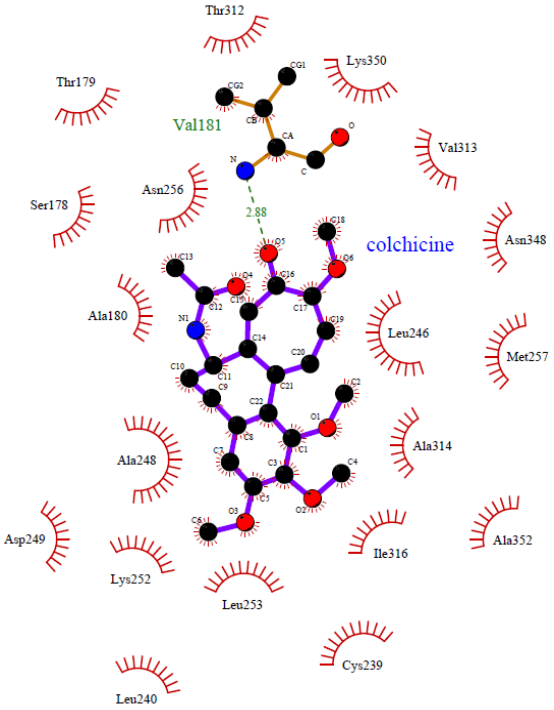


Fig. S6. Interactions between colchicine and residues of the holo-protein of 6xer.pdb analyzed using LigPlot. Residues in the red half-circles denote hydrophobic interactions, and Val181 of the A chain forms a hydrogen bond with colchicine.

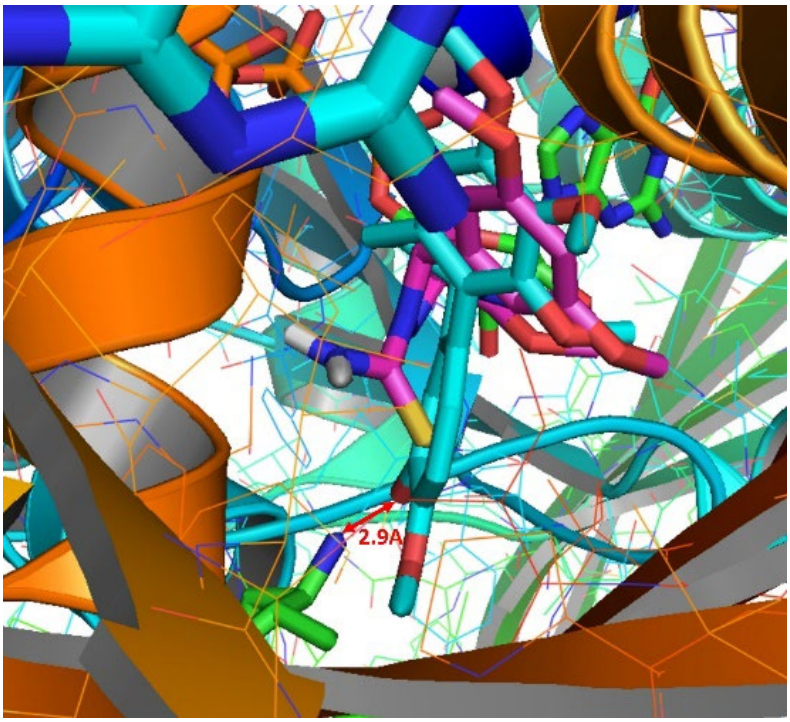


Fig. S7. 3D images of colchicine (cyan) and derivative **4** (magenta) contained in the binding pocket of 6xer.pdb generated using PyMol. The hydroxyl group of colchicine forms a hydrogen bond with the nitrogen of Val181 of the A chain (2.9 Å).