Supporting information

Phytochemicals of *Swertia chirayita* Roxb. *ex* Fleming Against Malarial Dihydroorotate Dehydrogenase: An *in silico* Study

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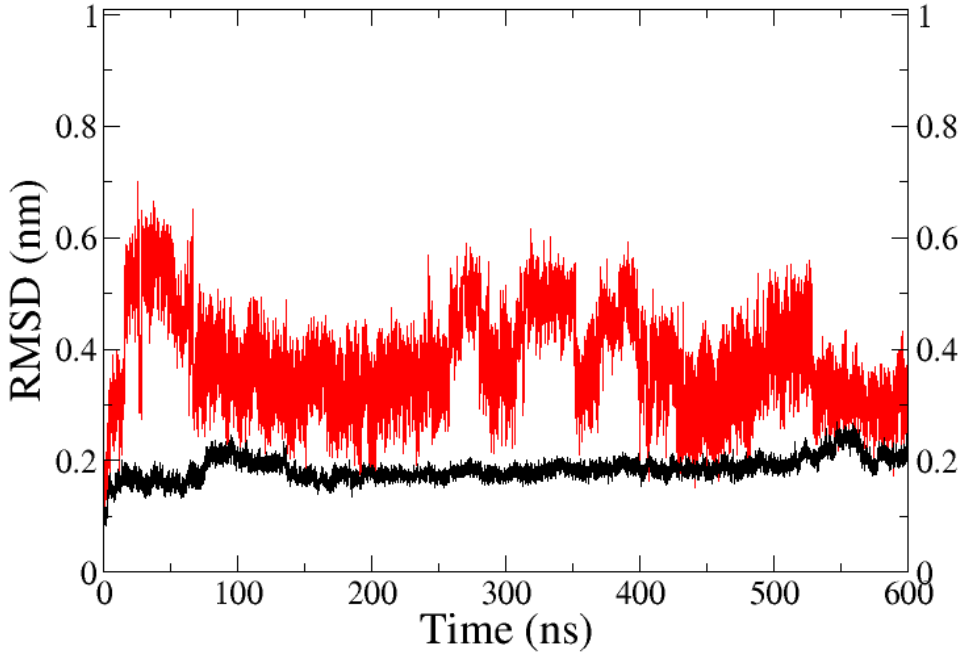

Figure S1. RMSD of ligand, decussatin (red) and protein backbone (dark) both relative to protein backbone in a separate 600 ns simulation run of Complex01

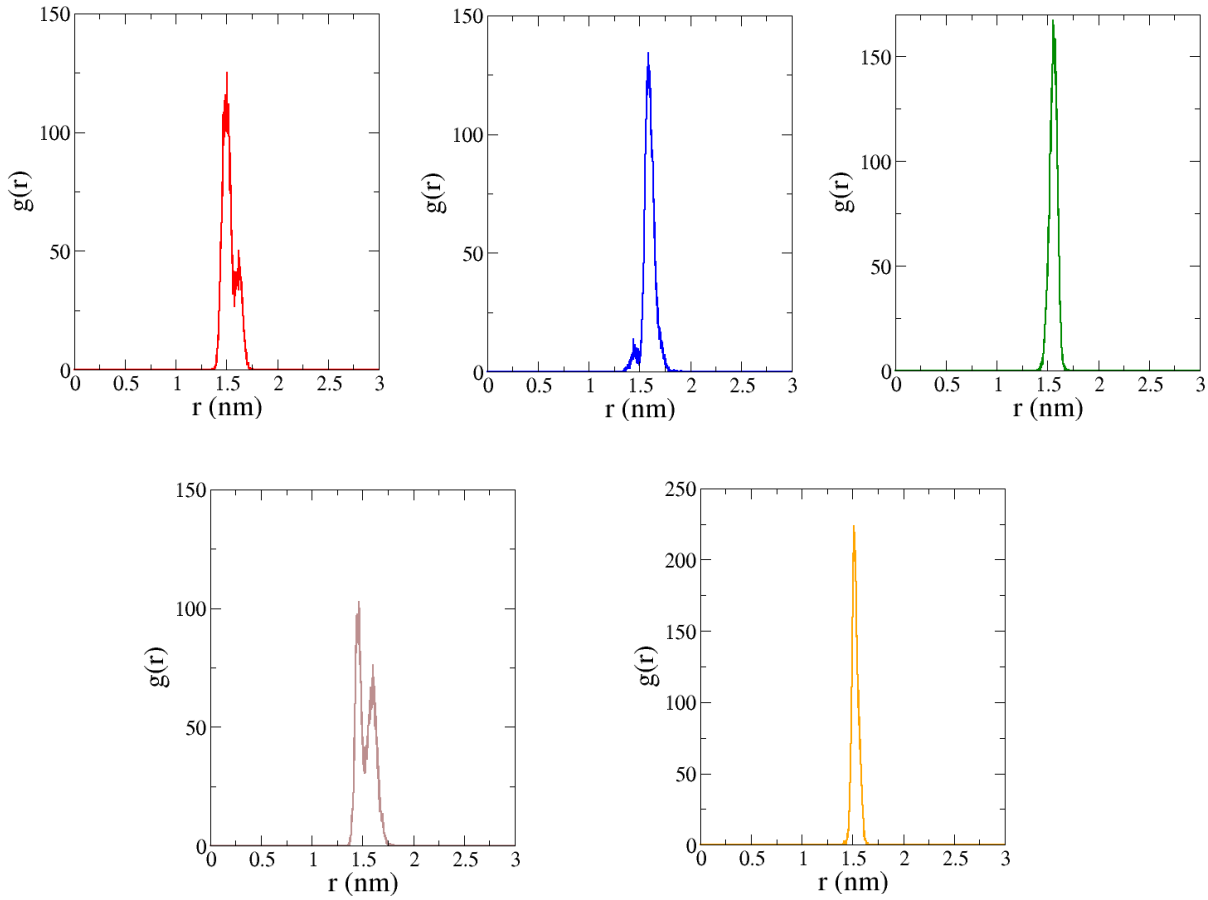

Figure S2. Radial pair distribution function (RPDF, g(r)) of the ligands' center of mass with reference to that of the protein's in five different adducts (Complex01=red, Complex02= blue, Complex03= green, Complex04=brown, and Complex05=gold) from 200 ns MDS

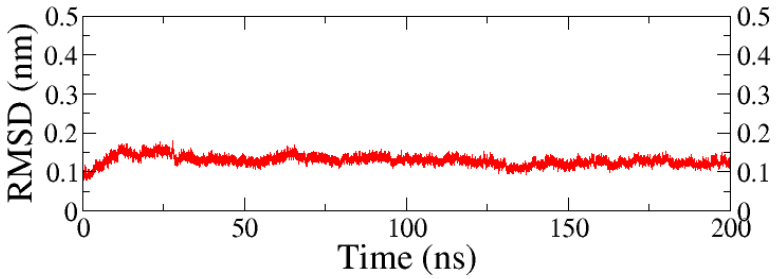

Figure S3. RMSD of protein backbone relative to protein backbone in the apo form of the receptor from a separate MDS (smooth trajectory with RMSD less than 1.5 Å)

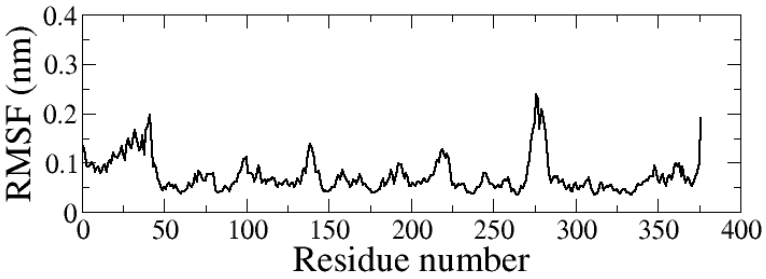

Figure S4. RMSF of alpha carbon atoms of protein backbone in the apo form

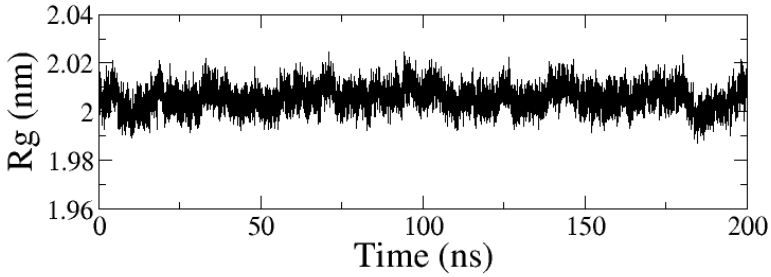

Figure S5. Variation of radius of gyration of protein in the apo form with time

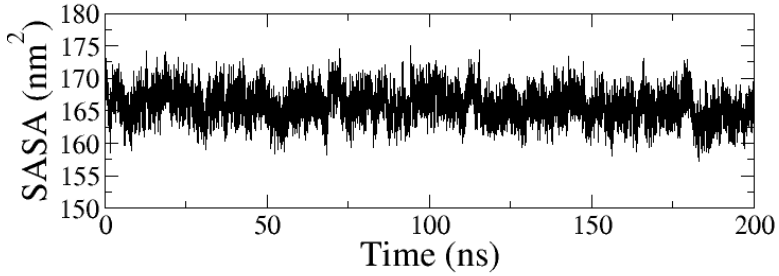

Figure S6. Variation of SASA of protein in the apo form with time

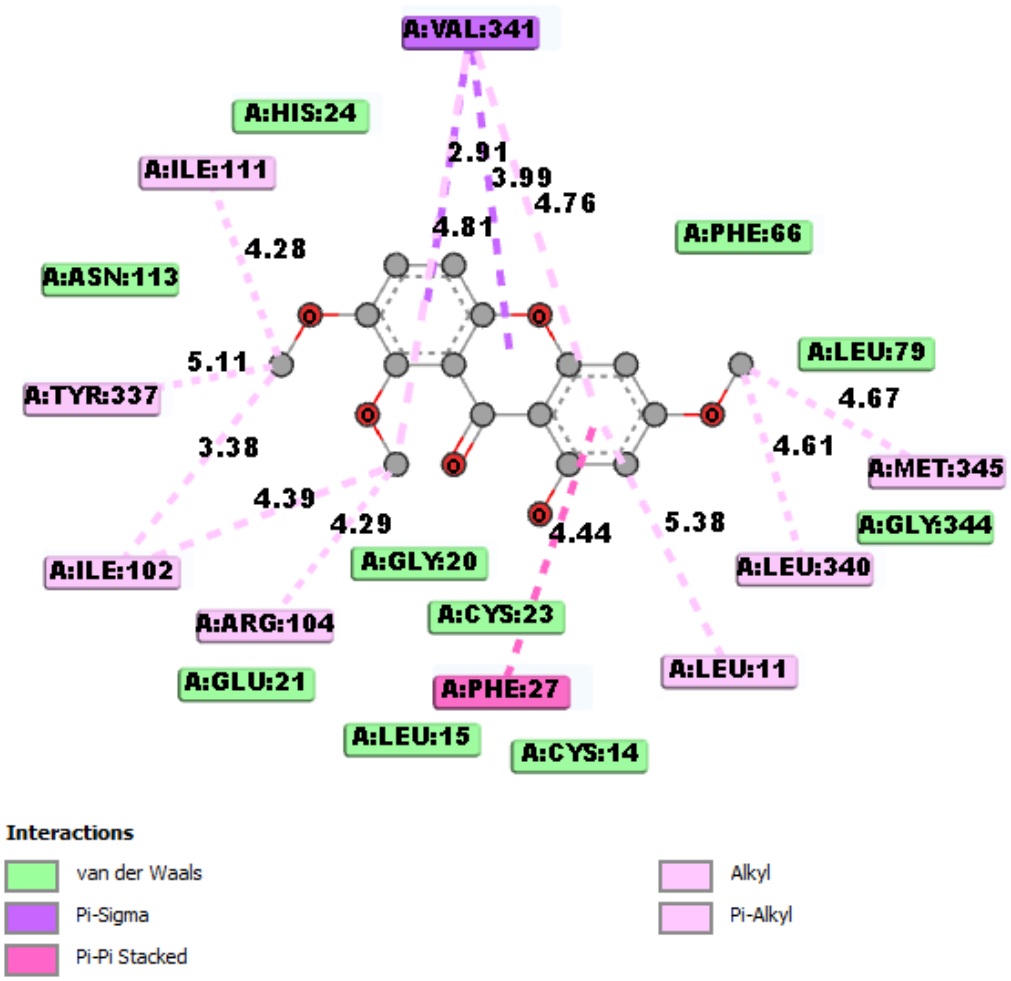

Figure S7. 2D projection of the interactions between the ligand and amino acid residues of the receptor protein in Complex01 along with the distances (Å)

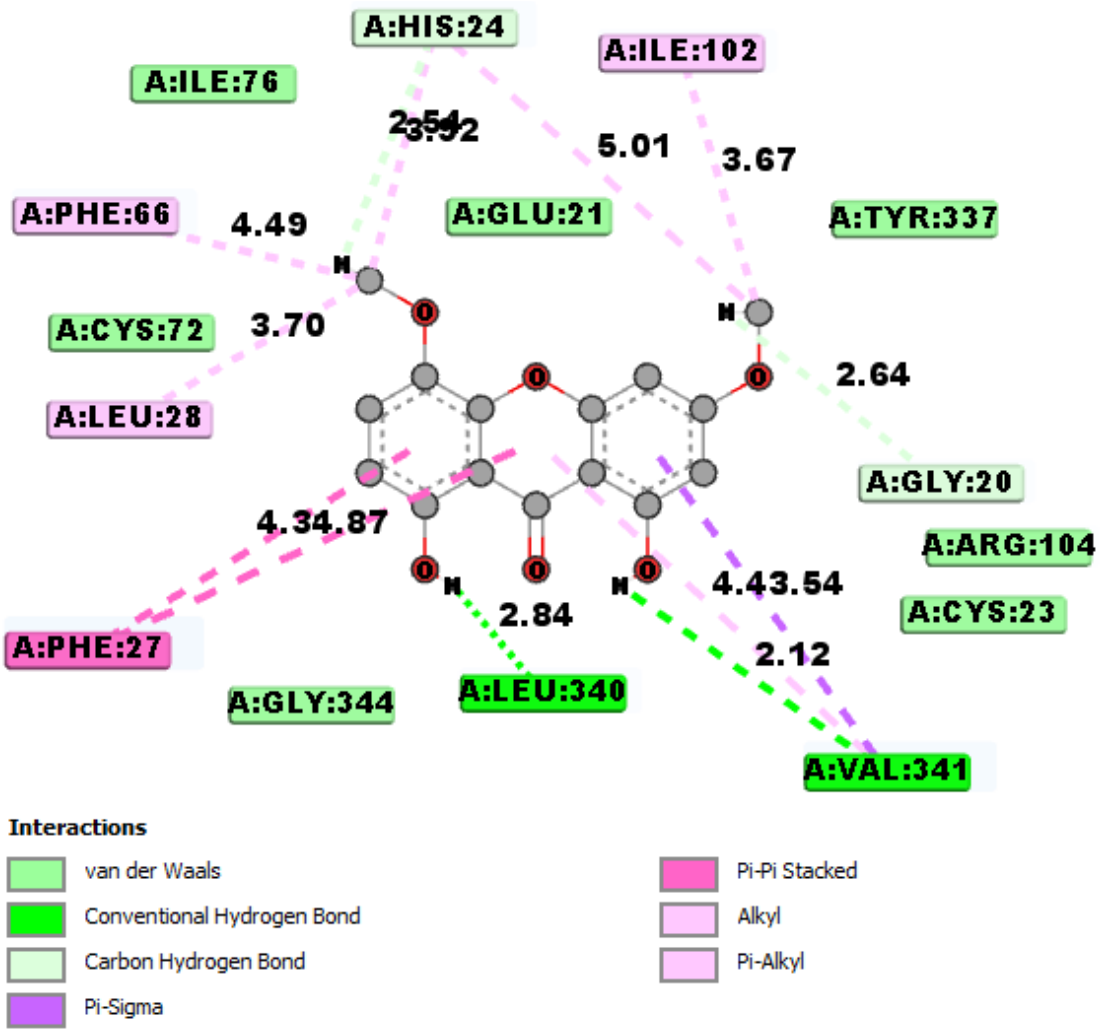

Figure S8. 2D projection of the interactions between the ligand and amino acid residues of the receptor protein in Complex02 along with the distances (Å)

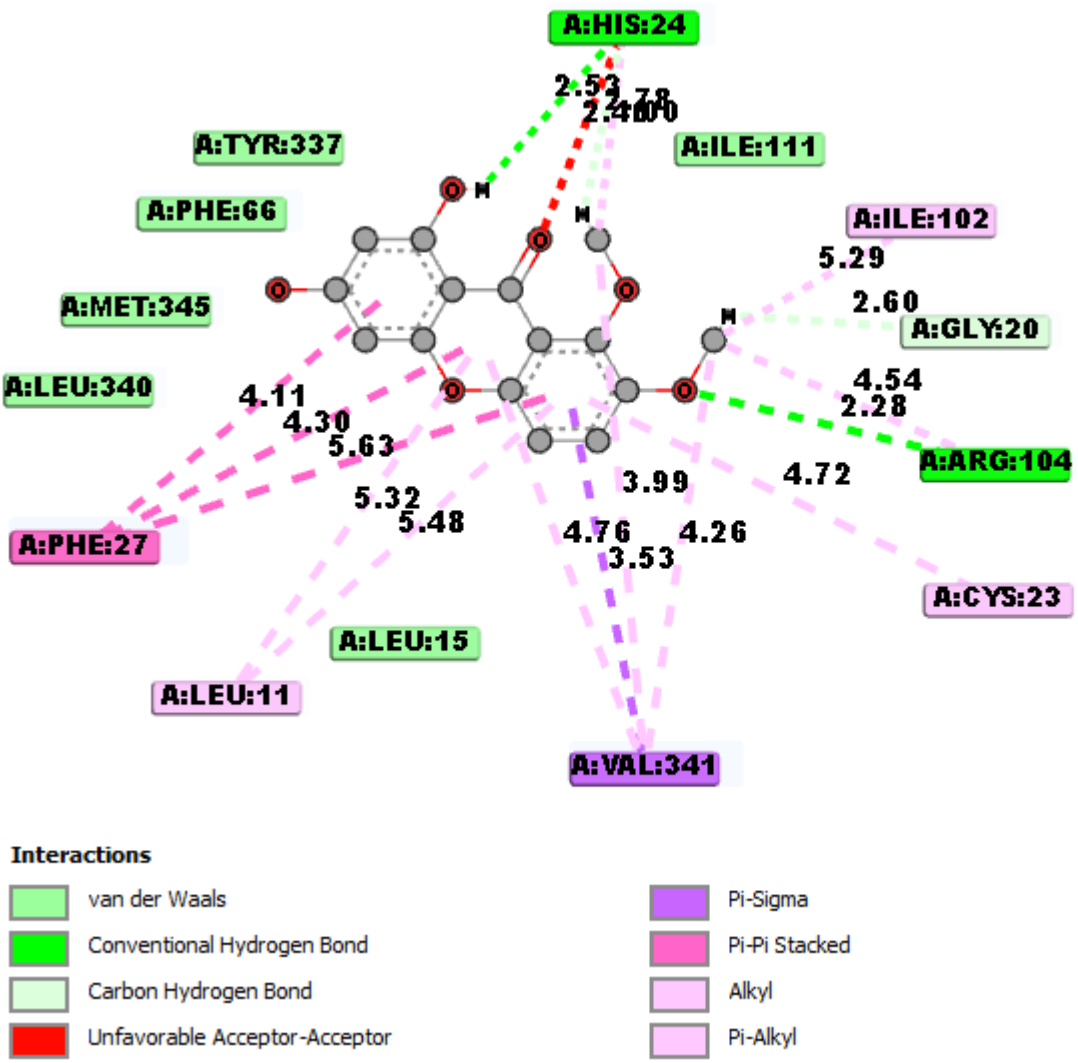

Figure S9. 2D projection of the interactions between the ligand and amino acid residues of the receptor protein in Complex03 along with the distances (Å)

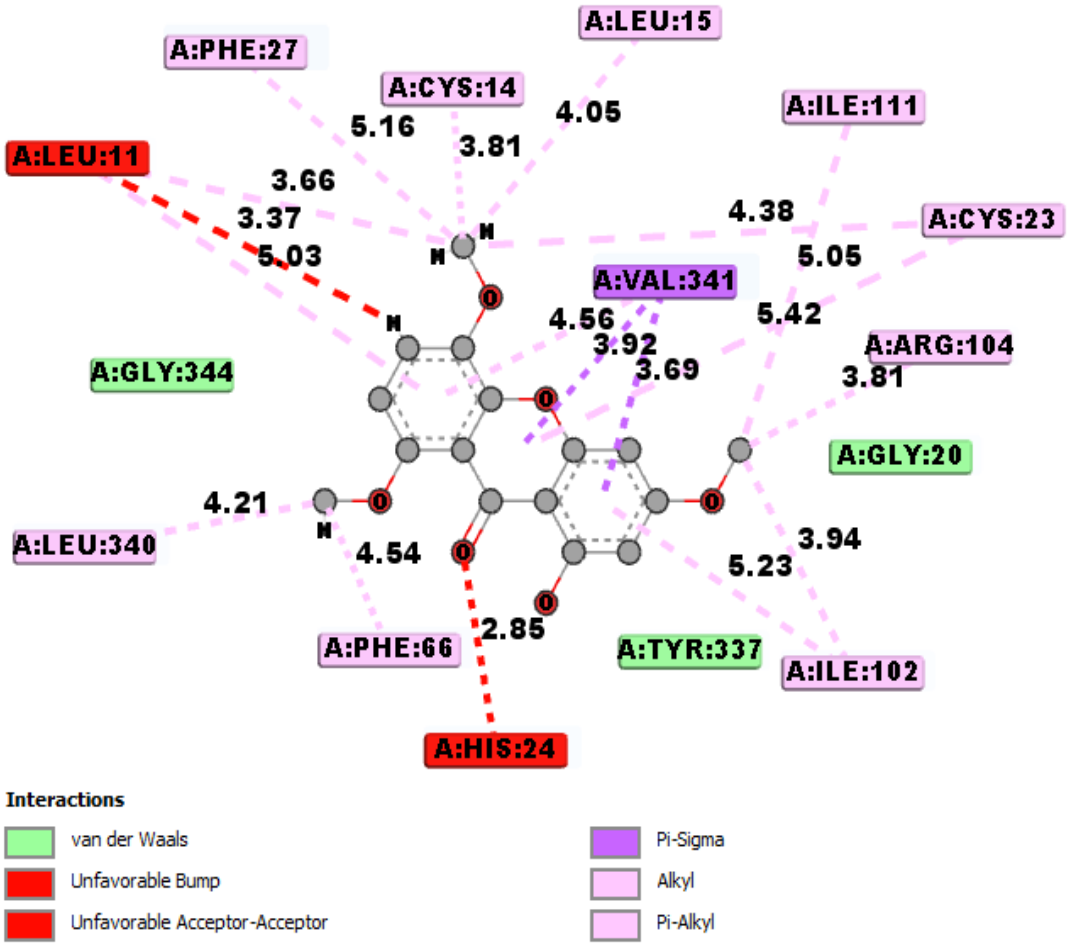

Figure S10. 2D projection of the interactions between the ligand and amino acid residues of the receptor protein in Complex04 along with the distances (Å)

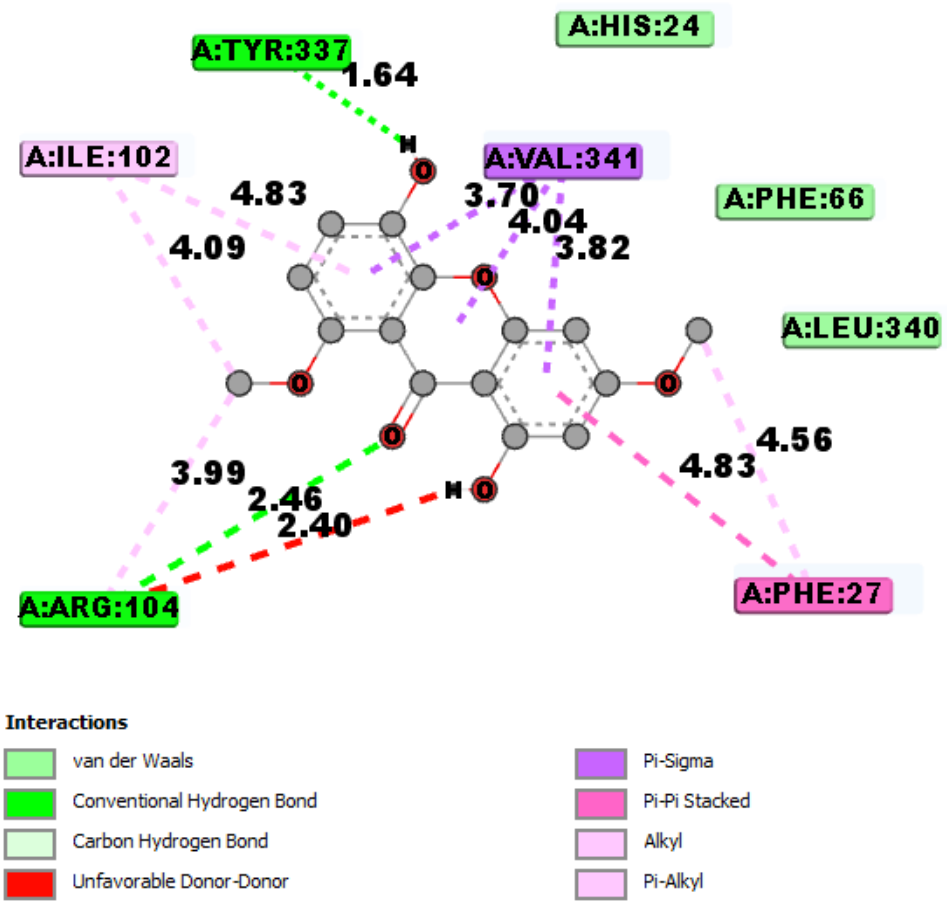

Figure S11. 2D projection of the interactions between the ligand and amino acid residues of the receptor protein in Complex05 along with the distances (Å)