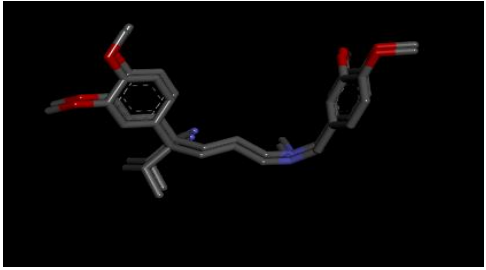
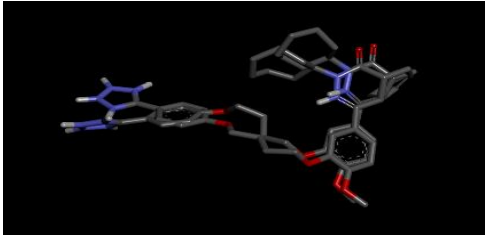

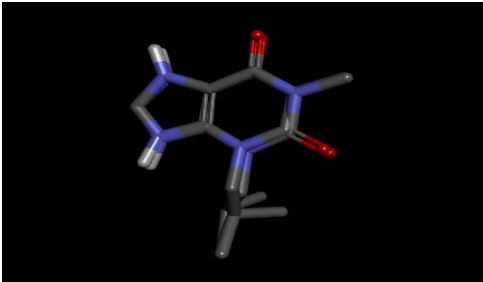


Table S1. Vina Grid Search Space and box size of the receptors

Receptors	Vina Grid Search Space
6JPA	center_x = 167.1143 center_y = 181.1604 center_z = 166.9501 size_x = 95.1036225891 size_y = 94.9972616577 size_z = 111.369475861
5LAQ	center_x = 2.13904252922 center_y = -40.8483539295 center_z = 3.81835521104 size_x = 39.6957028549 size_y = 33.1738787585 size_z = 31.192305625
4NPW	center_x = 22.0659489085 center_y = 27.8833197572 center_z = 47.3617937781 size_x = 27.6928237995 size_y = 23.6983115239 size_z = 24.1251809306
3ITU	center_x = 19.1413 center_y = 2.498 center_z = 38.682 size_x = 25 size_y = 25 size_z = 25
6EBM	center_x = 159.459569318 center_y = 162.184255506 center_z = 141.663830927 size_x = 44.0436834492 size_y = 28.7509110129 size_z = 47.7217175449
7VNP	center_x = 123.0037 center_y = 123.0189 center_z = 128.8314 size_x = 117.532685623 size_y = 115.65650032 size_z = 100.403661346

Table S2. Redocked structures overlayed on the co-crystallized ligands

Receptors	Co-crystallized ligand	Redocked co-crystallized ligand	RMSD
6JPA	Verapamil		0.8246
5LAq	NPD		1.6217
4npw_	0NY		0.5012
3ITU	IBMX		0.5801

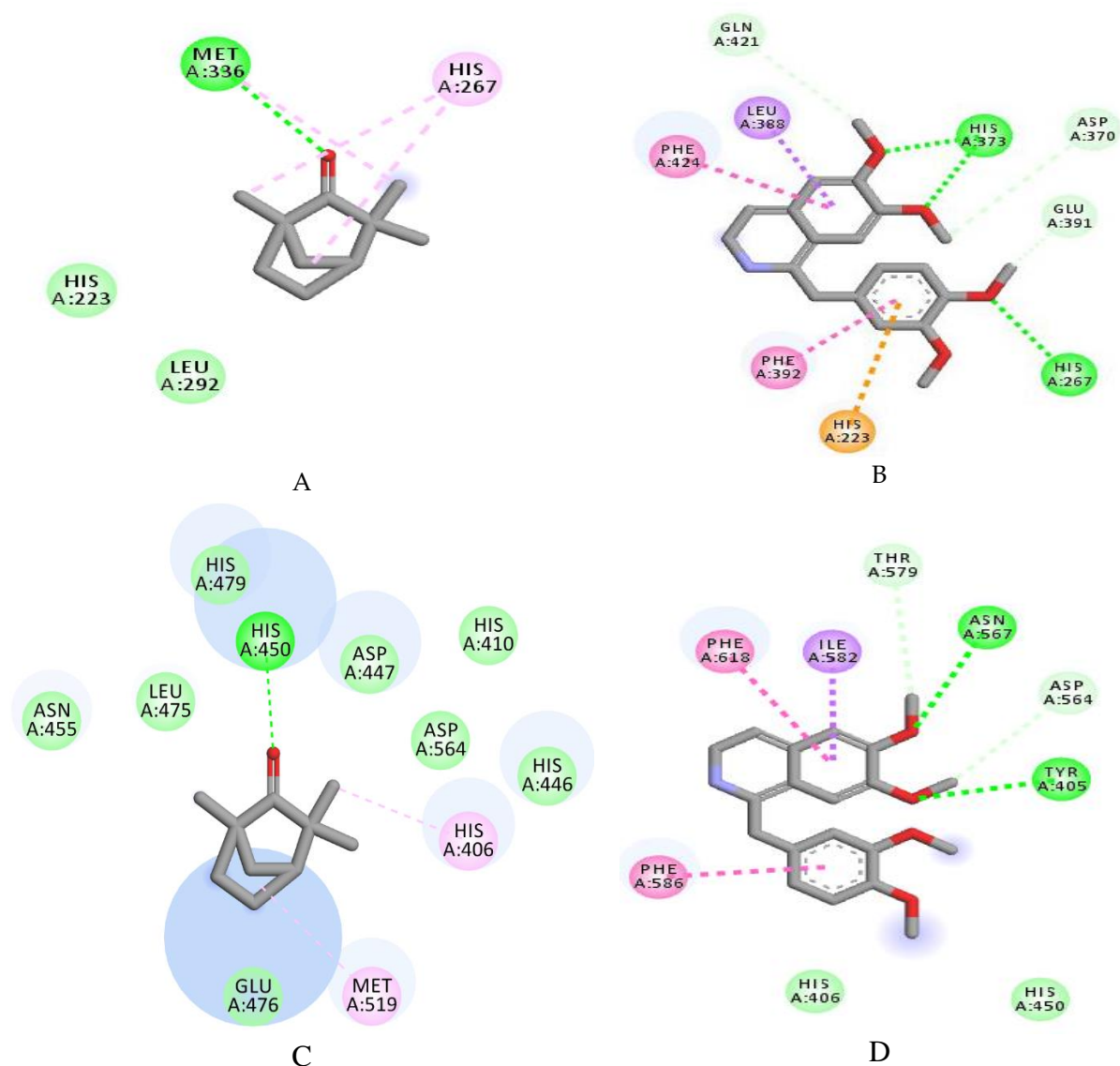


Figure S1. A to D show the ligand receptor interactions. Figure A-B and C-D show the binding mode of FNC and PPV with 4NPW and 5LAQ respectively. Dark green circles and lines show hydrogen bonds while the light green spheres are showing Vander Waal interaction between ligand and residues.