Figure legends for the article titled as: "*In silico* investigation of phenolic derivatives from *Silybum marianum* against SARS-CoV-2 proteins as a pharmacological drug repurposing strategies to mitigate the pandemic"

Graphical Abstract of the manuscript:

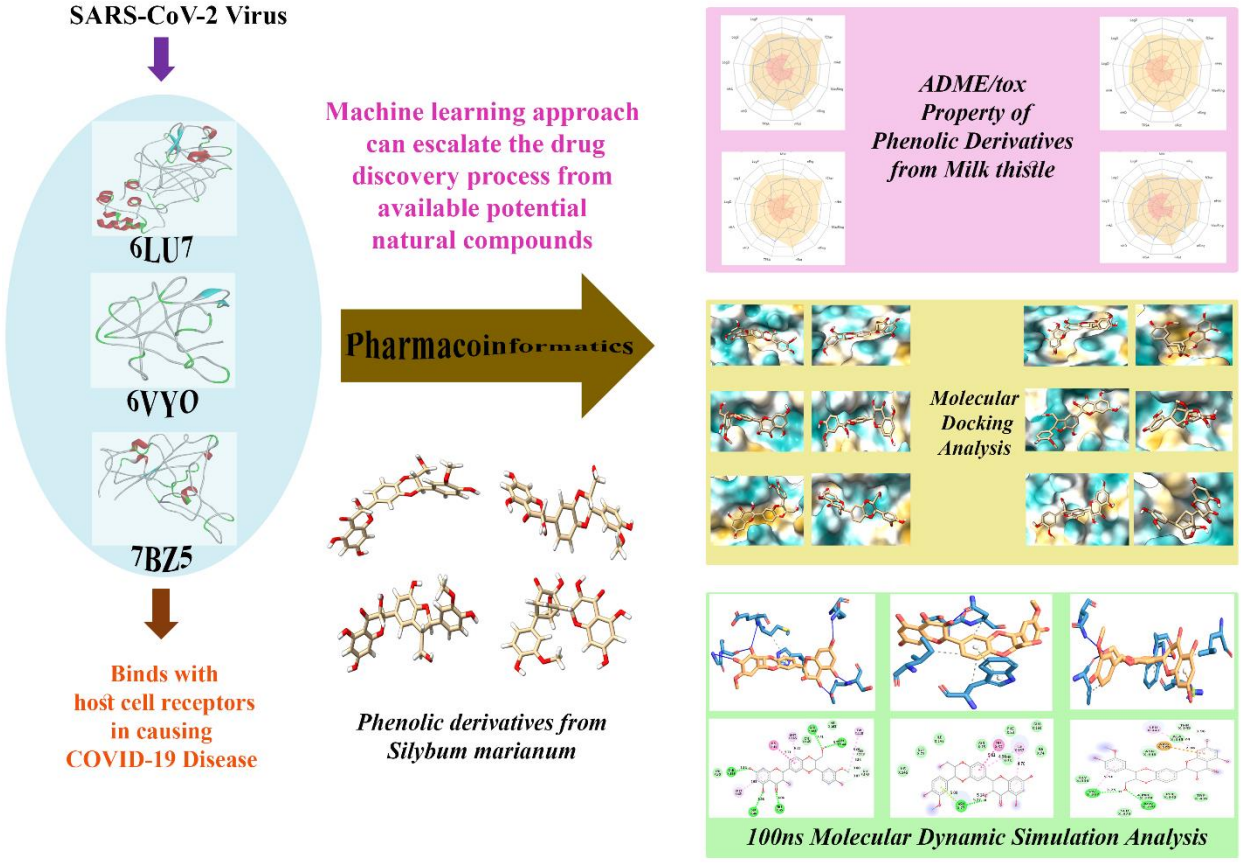

Figure 1: The genome organization of SARS-CoV-2 and its translational regions

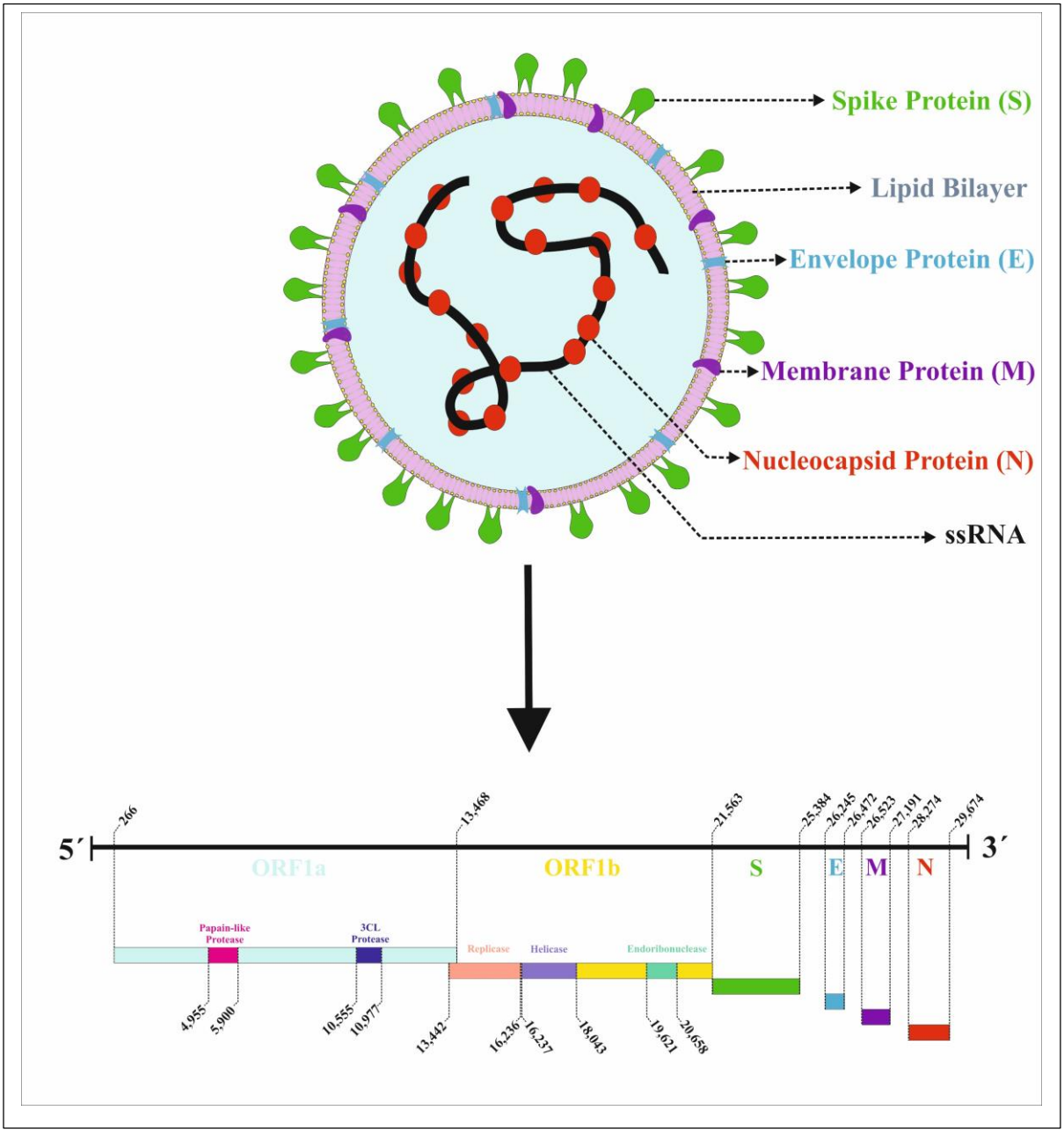

Figure 2: The image represents the bioavailability radar for the ligand molecules Silibinin(a), Isosilybin(b), Silychristin(c) and Silidianin(d)

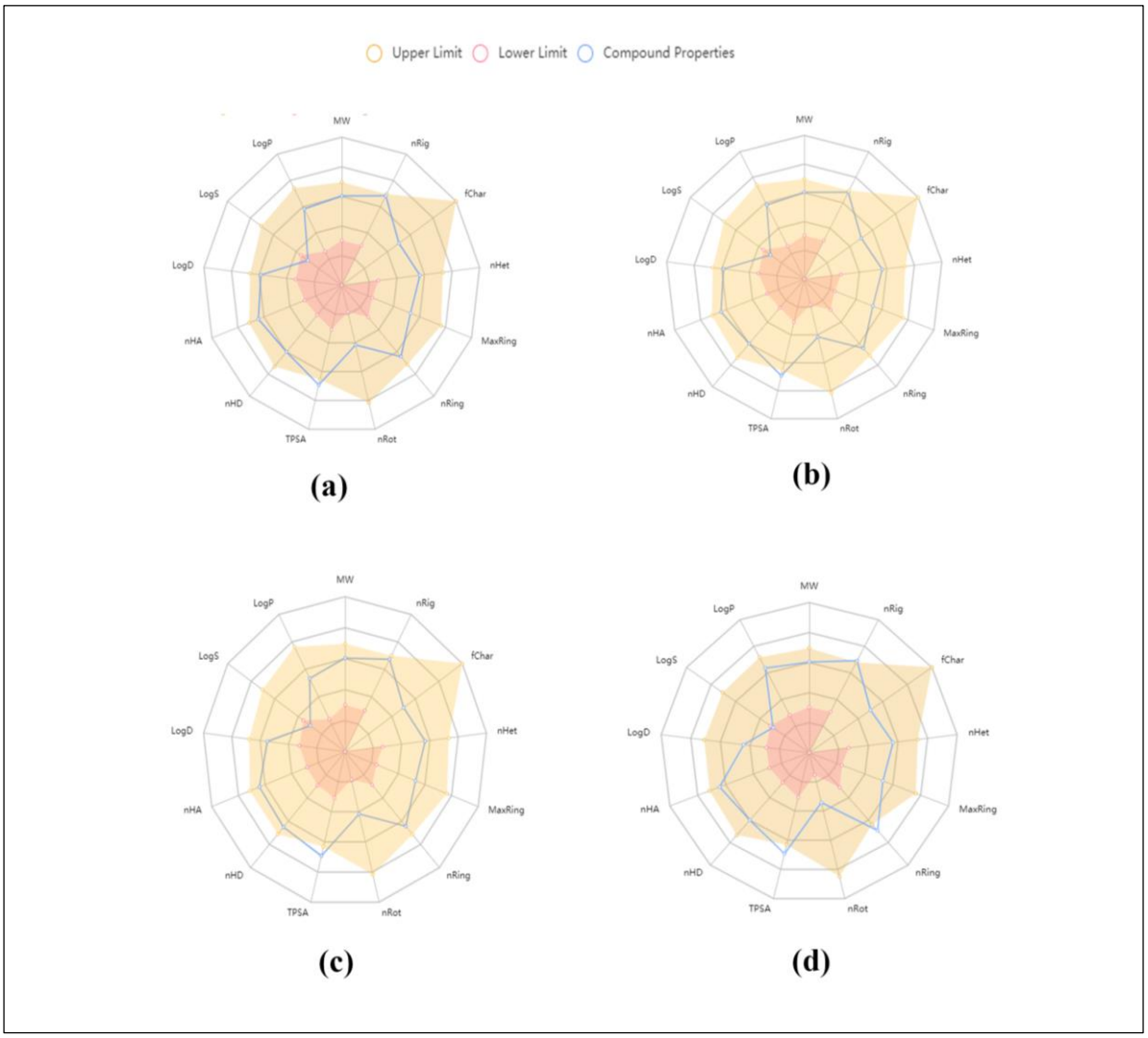

Figure 3: Interaction of main protease(6LU7) with different ligand molecules(Silibinin, Isosilybin, Silychristin & Silidianin) in 3D diagrammatic view(a) and 2D schematic view(b)

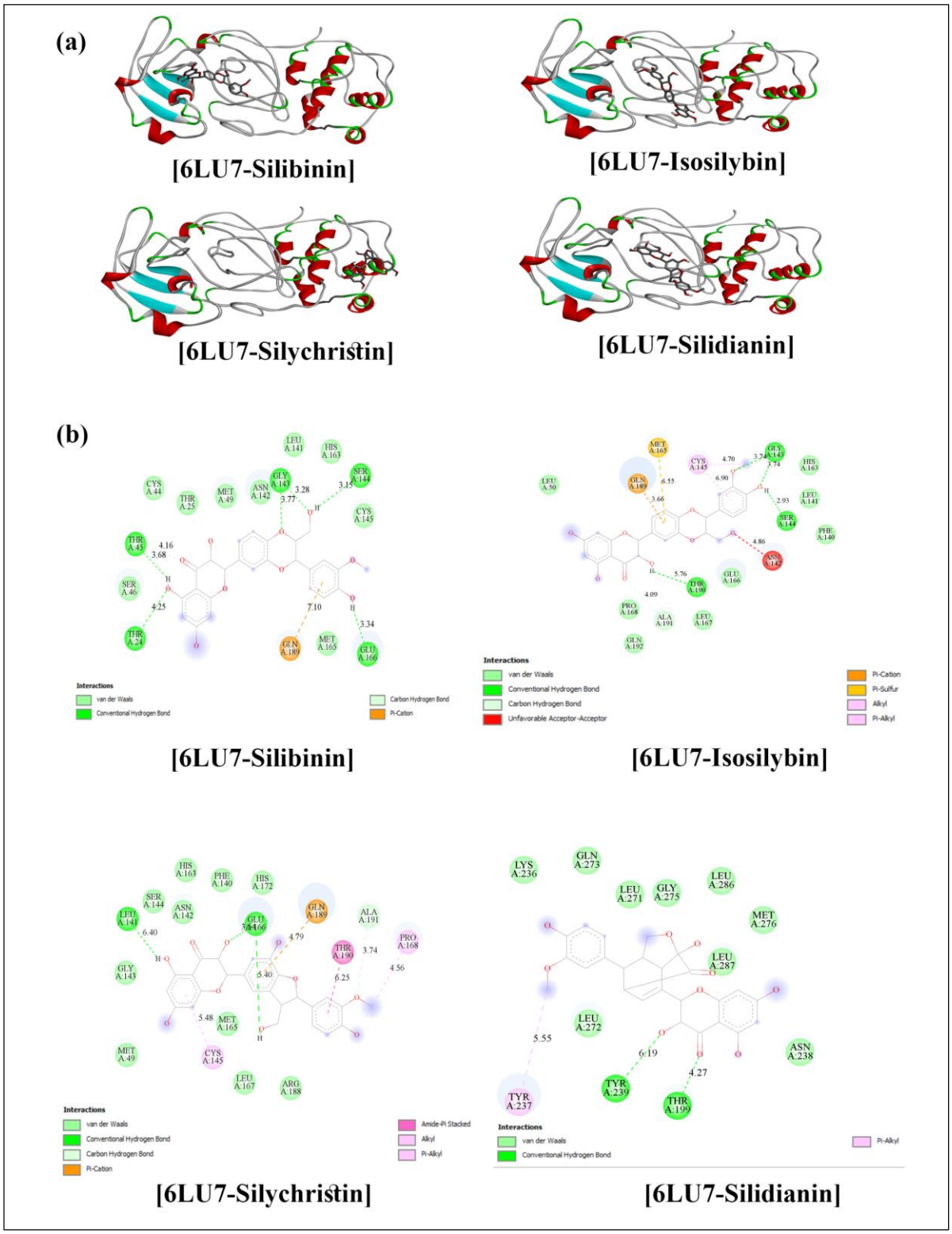

Figure 4: Interaction of RNA binding domain of nucleocapsid phosphoprotein(6VYO) with different ligand molecules(Silibinin, Isosilybin, Silychristin & Silidianin) in 3D diagrammatic view(a) and 2D schematic view(b)

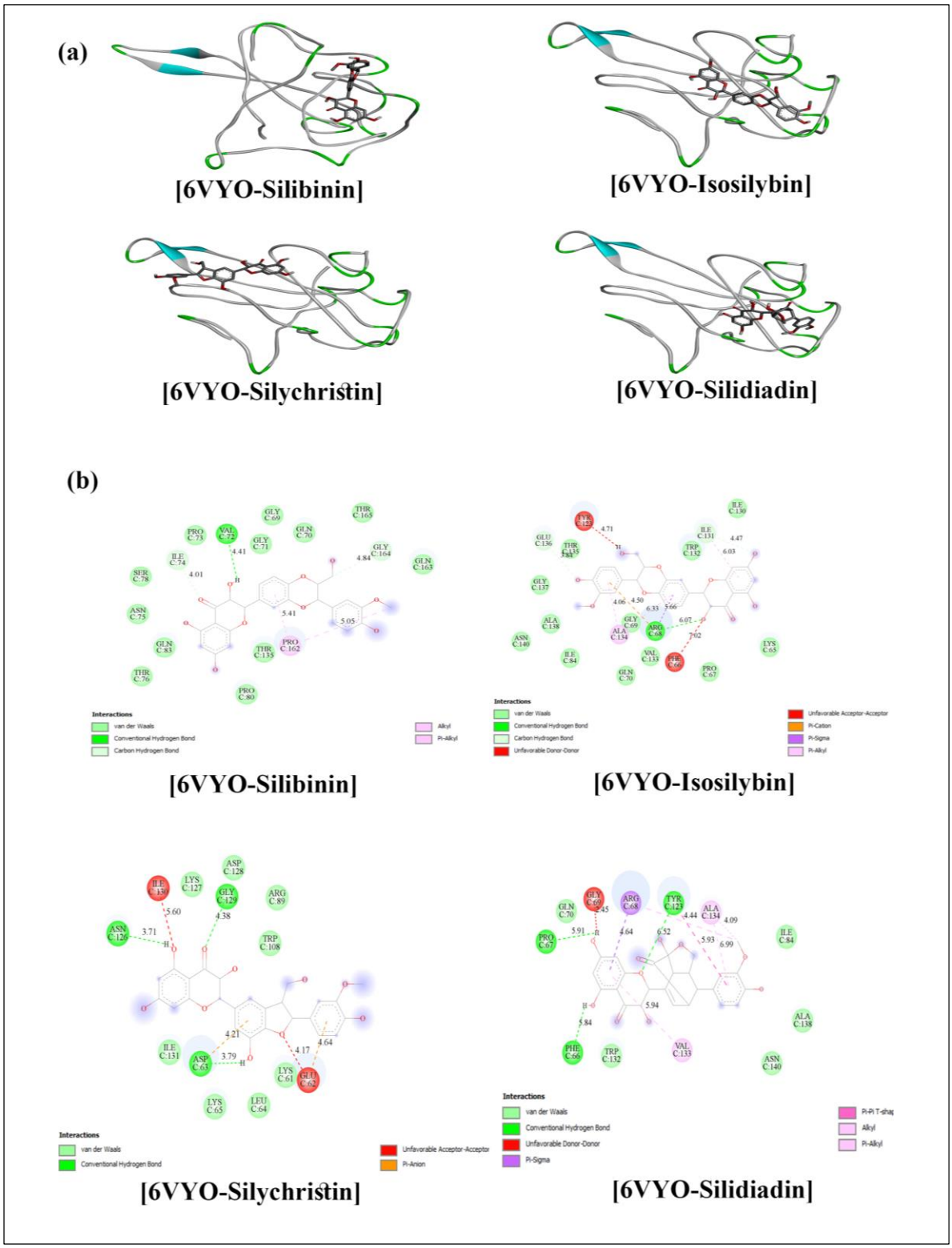

Figure 5: Interaction of spike receptor binding domain(7BZ5) with different ligand molecules(Silibinin, Isosilybin, Silychristin & Silidianin) in 3D diagrammatic view(a) and 2D schematic view(b)

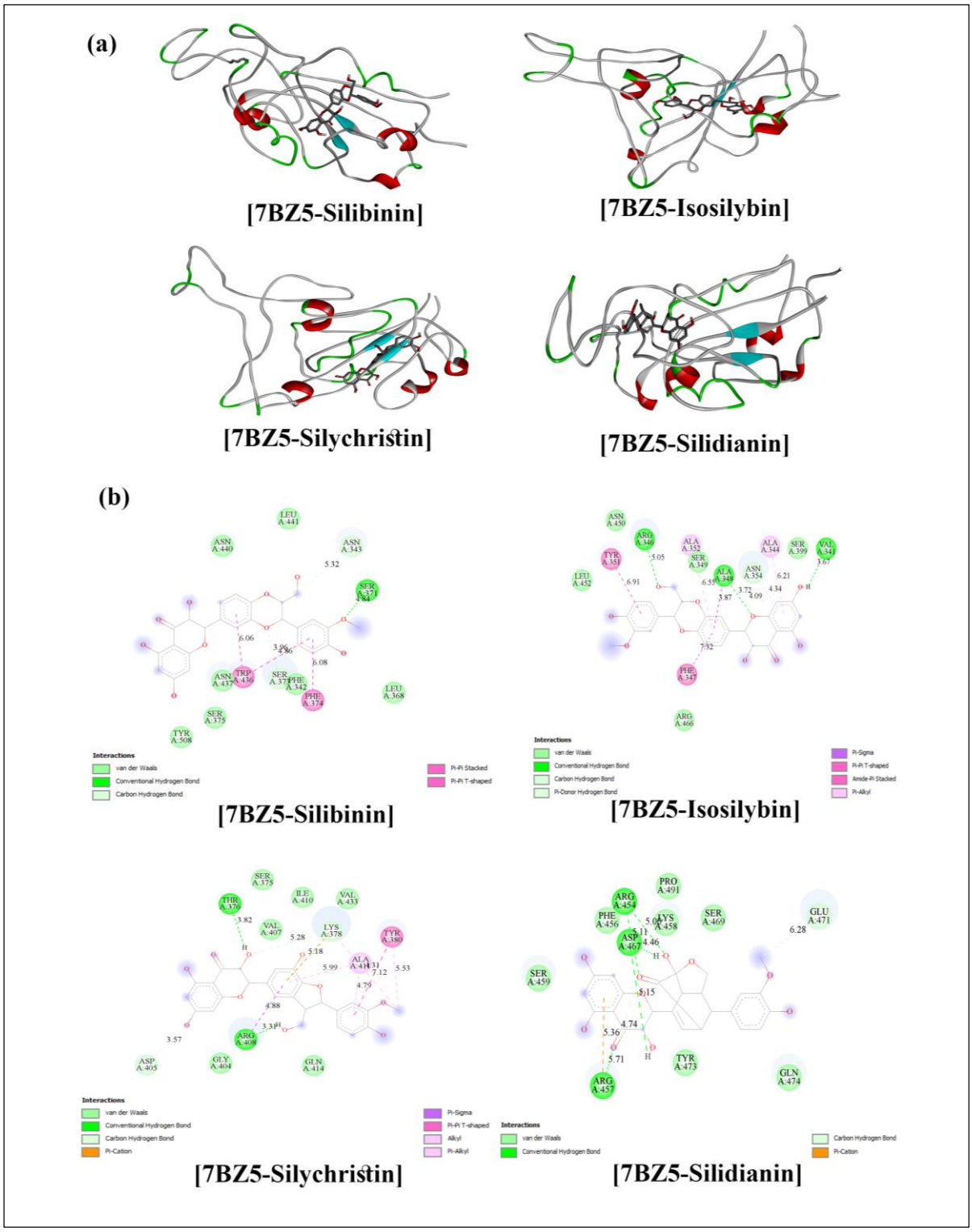

Figure 6: (a)Root mean square deviation(RMSD) trajectories of macromolecules(6LU7, 6VYO & 7BZ5)(BLACK) with silibinin molecule(RED) and (b)Root mean square fluctuation(RMSF) trajectories of macromolecules(6LU7, 6VYO & 7BZ5) during 100ns molecular dynamics simulation

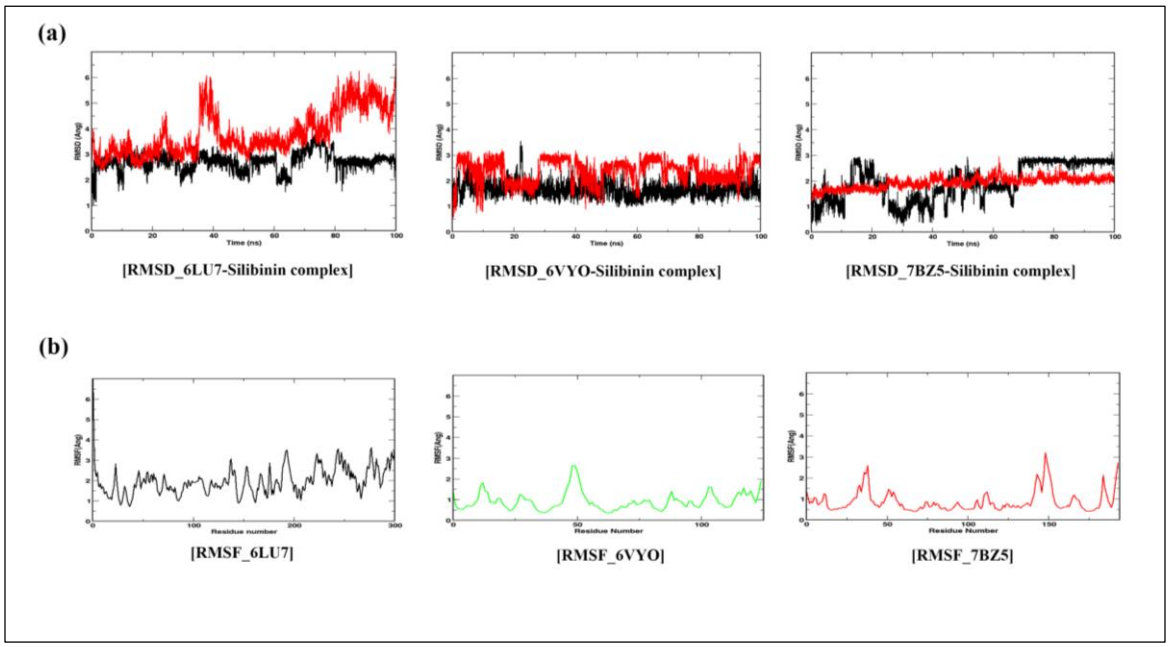

Figure 7: PCA of different macromolecules(6LU7, 6VYO & 7BZ5) and eigen values of the covariance matrix during 100ns simulation process

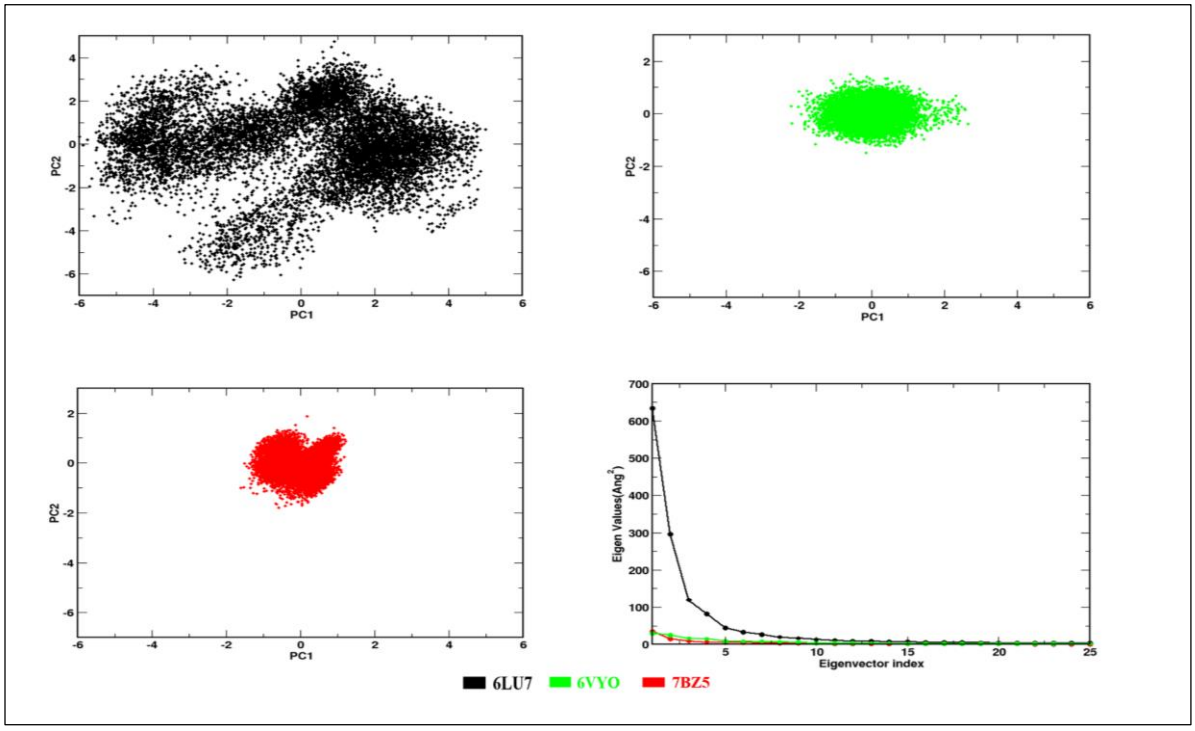

Figure 8: Secondary structure of macromolecules(6LU7, 6VYO & 7BZ5) during 100ns MD simulation process

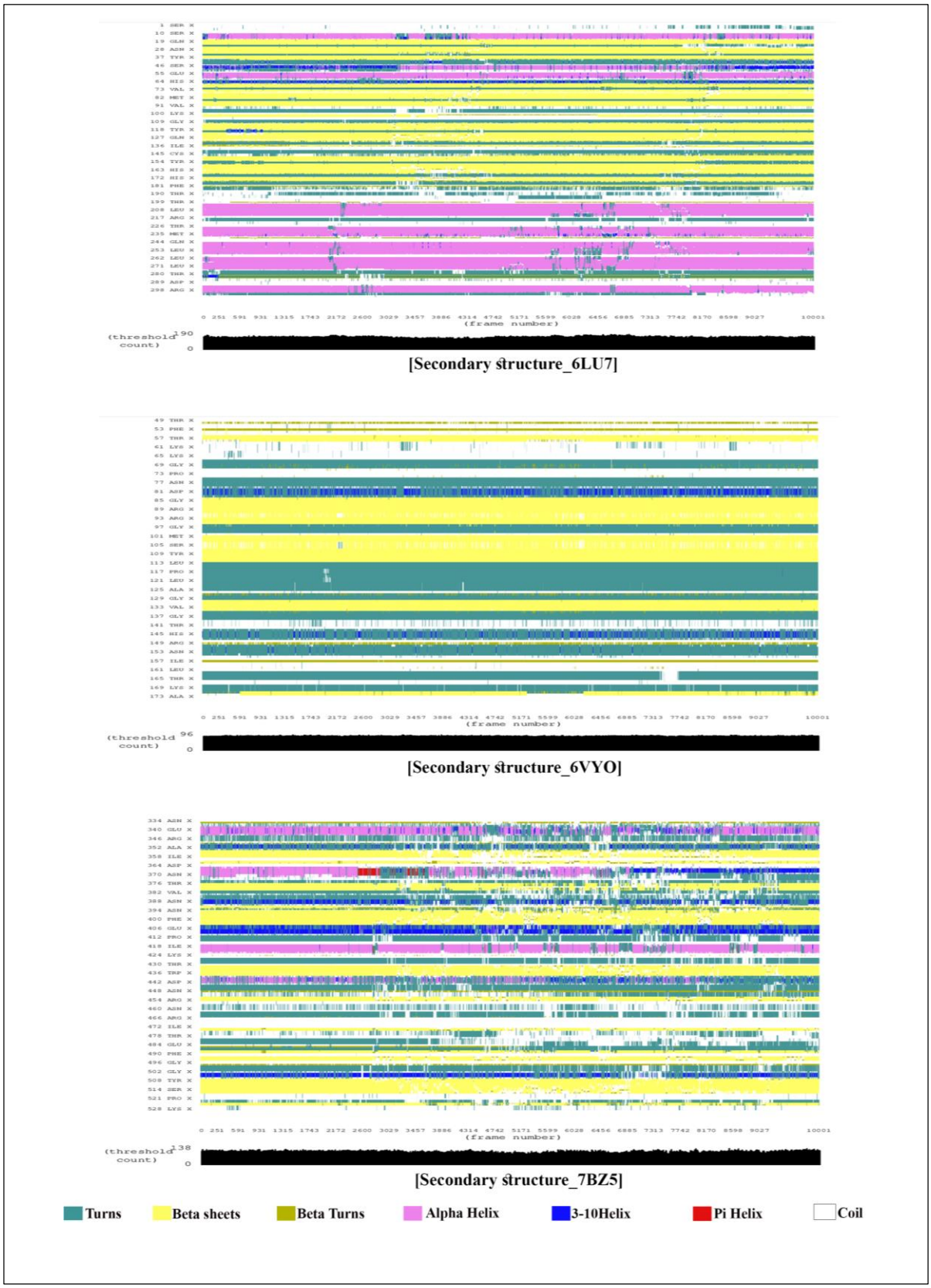

Figure 9: RMSF of silibinin ligand with different macromolecules(6LU7, 6VYO & 7BZ5) during 100ns MD simulation

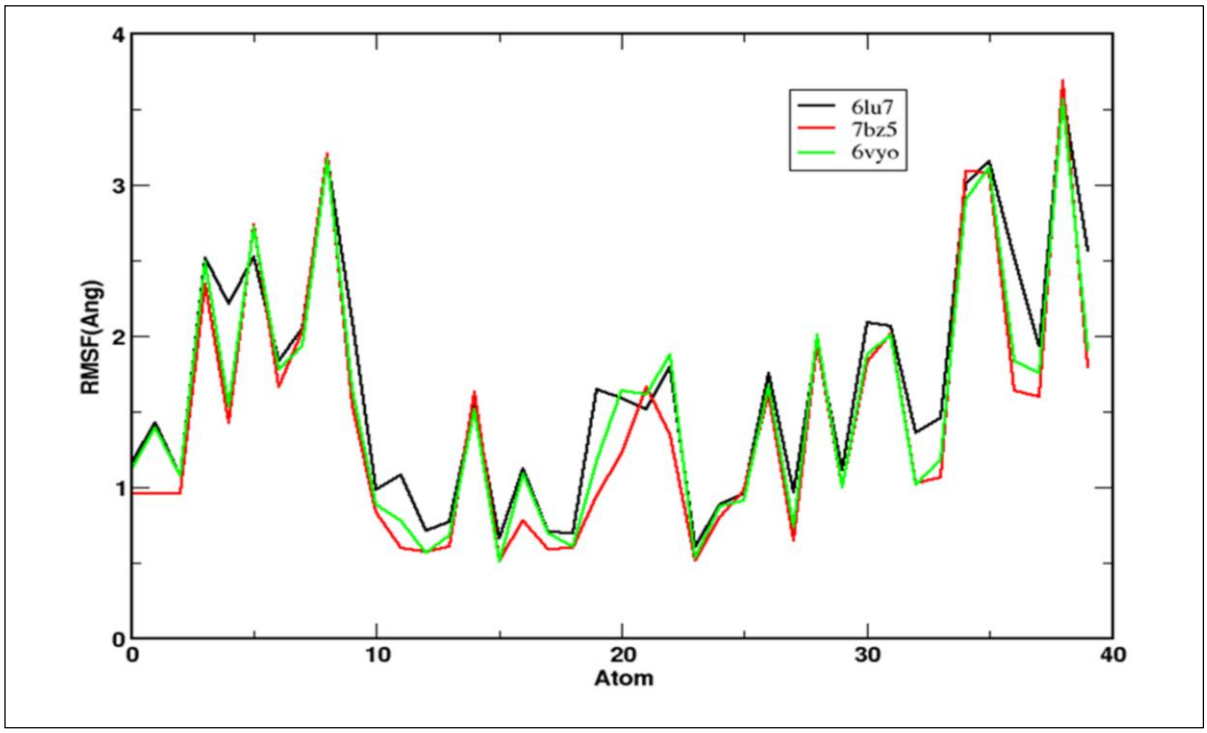

Figure 10: Radius of Gyration(a) and solvent accessible surface area(b) of different macromolecules(6LU7, 6VYO & 7BZ5) during 100ns MD simulation process

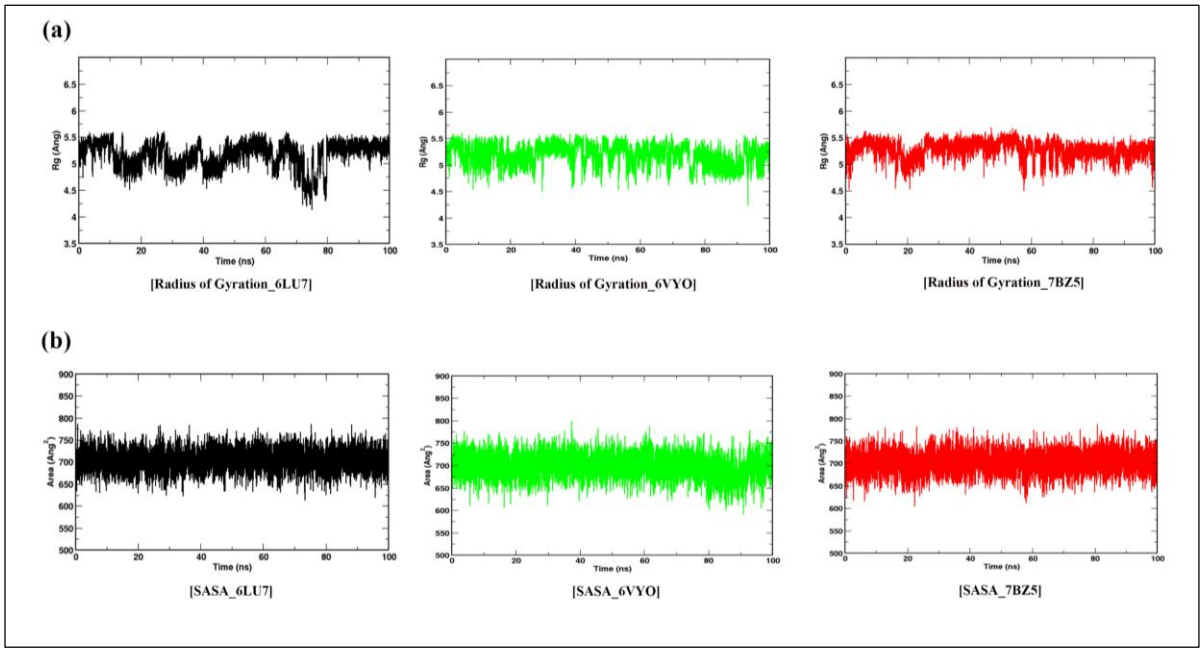

Figure 11: Protein-ligand interaction profile(PLIP) of Silibinin with different macromolecules(6LU7, 6VYO & 7BZ5) in 3D(a) & 2D(b) schematic view representing different bonds and bond length after 100ns MD simulation last frame