Electronic Supplementary Material (ESI) for RSC Advances.

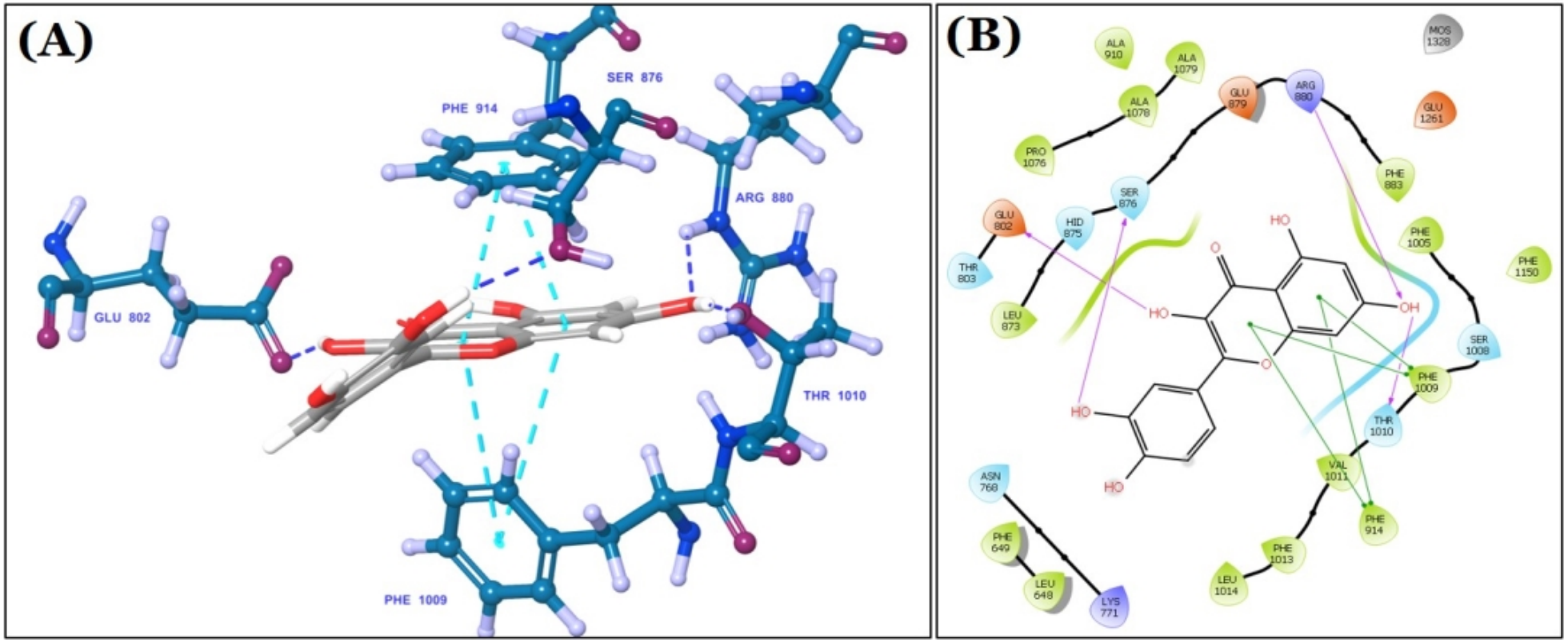

Figure S1: 3D **(A)** and 2D **(B)** diagrams of docked pose of quercetin (co-crystallized ligand) interacting with XO active site's amino acid residues (PDB ID: 3NVY), as generated using the Schrödinger software. Blue dotted lines indicate the hydrogen bonds while light blue dotted lines show Pi-Pi stacking interactions in 3D view. Magenta solid arrows indicate hydrogen bonds (backbone) while green solid lines represent Pi-Pi stacking interactions in 2D view.

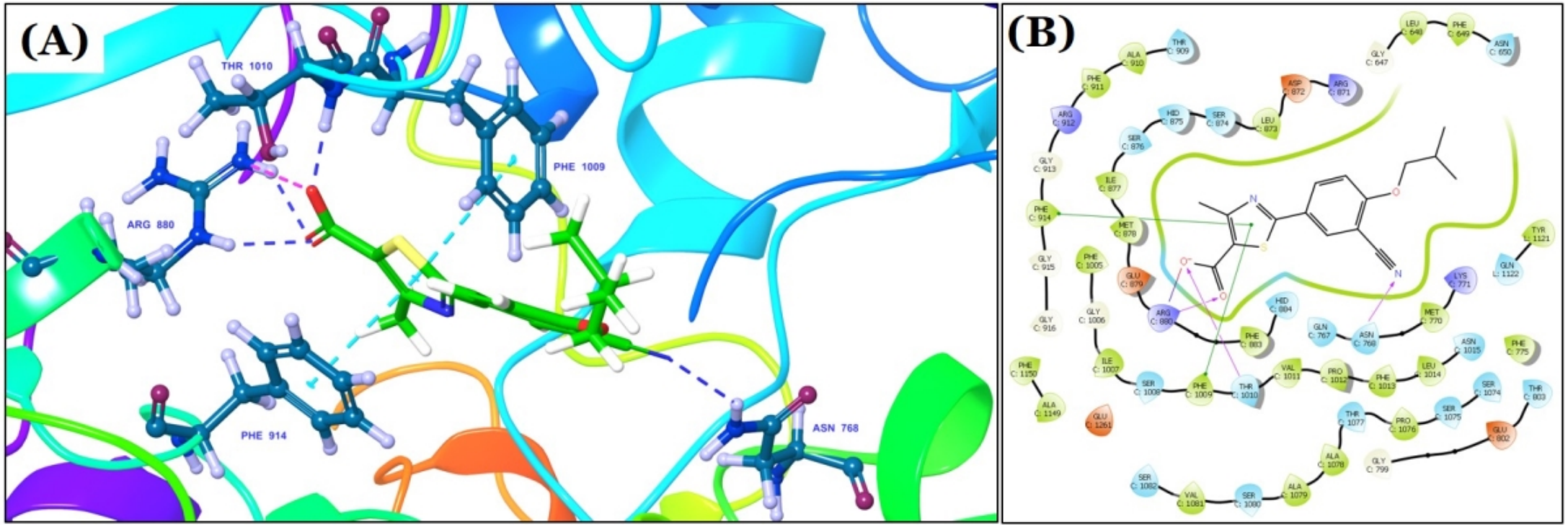

Figure S2: 3D **(A)** and 2D **(B)** diagrams of docked pose of febuxostat interacting with XO active site's amino acid residues (PDB ID: 3NVY), the protein is shown in three-dimensional cartoon presentation as generated using the Schrödinger software. Blue & light blue dotted lines indicate hydrogen bonds and Pi-Pi stacking interactions, respectively, while magenta dotted lines denote salt bridges in 3D view. Magenta solid arrows indicate hydrogen bonds (backbone) while green & purplish red solid lines represent Pi-Pi stacking interactions and salt bridges, respectively, in 2D view.

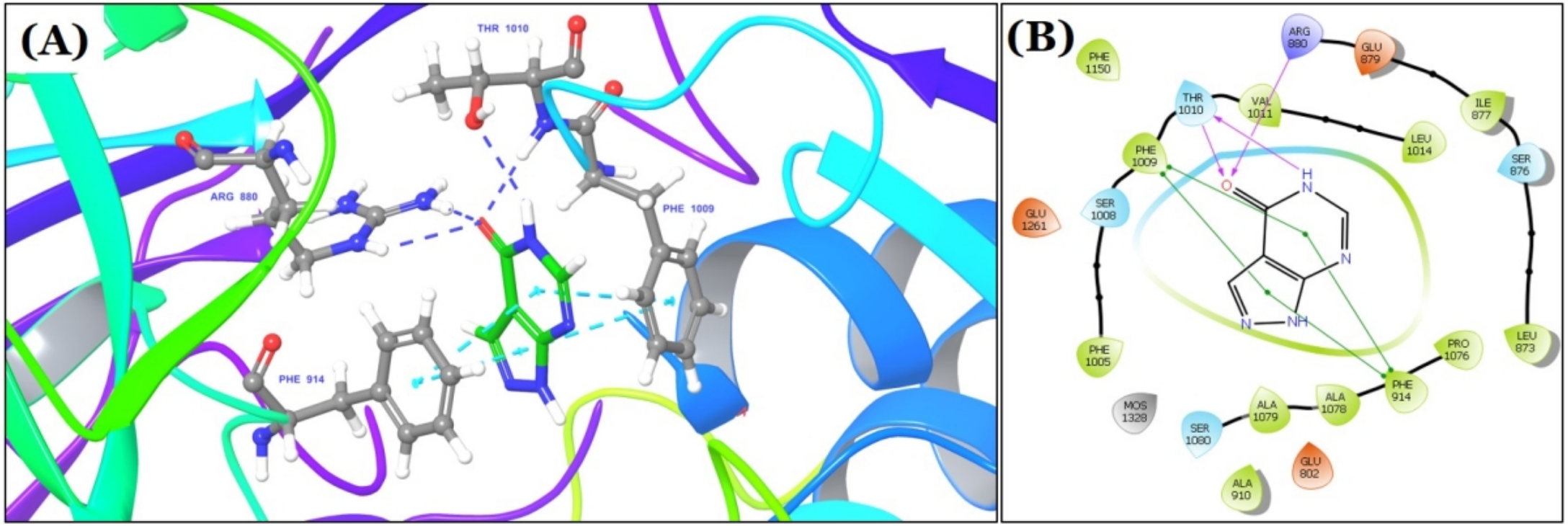

Figure S3: 3D **(A)** and 2D **(B)** diagrams of docked pose of allopurinol interacting with XO active site's amino acid residues (PDB ID: 3NVY), the protein is shown in three-dimensional cartoon presentation as generated using the Schrödinger software. Blue dotted lines indicate the hydrogen bonds while light blue dotted lines show Pi-Pi stacking interactions in 3D view. Magenta solid arrows indicate hydrogen bonds (backbone) while green solid lines represent Pi-Pi stacking interactions in 2D view.

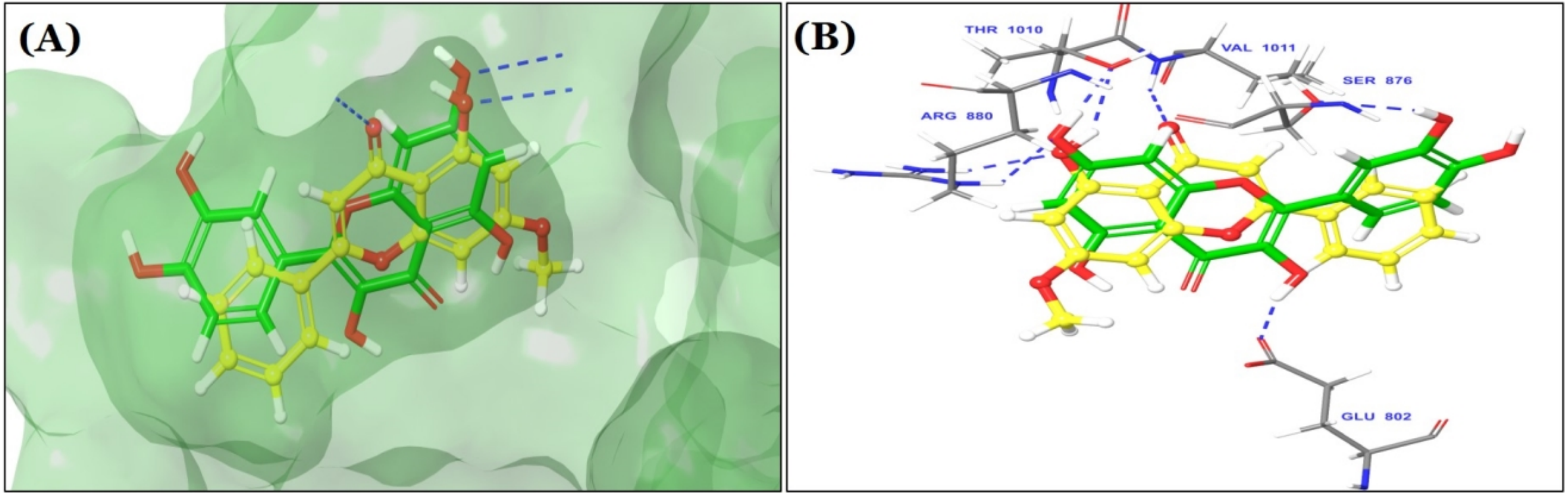

Figure S4: (A) Structure overlay for techtochrysin shown in yellow ball and stick representation with the original ligand quercetin conformations shown in green tube, as obtained from the crystal structure of XO (PDB ID: 3NVY) via docking simulations. The protein surface is shown in aquamarine transparent surface representation. **(B)** Overlaid docked poses of techtochrysin, shown in yellow ball and stick representation, and quercetin, shown in green tube, interacting with XO active site's amino acid residues (PDB ID: 3NVY), as generated using the Schrödinger software. Blue dotted lines indicate hydrogen bonds.

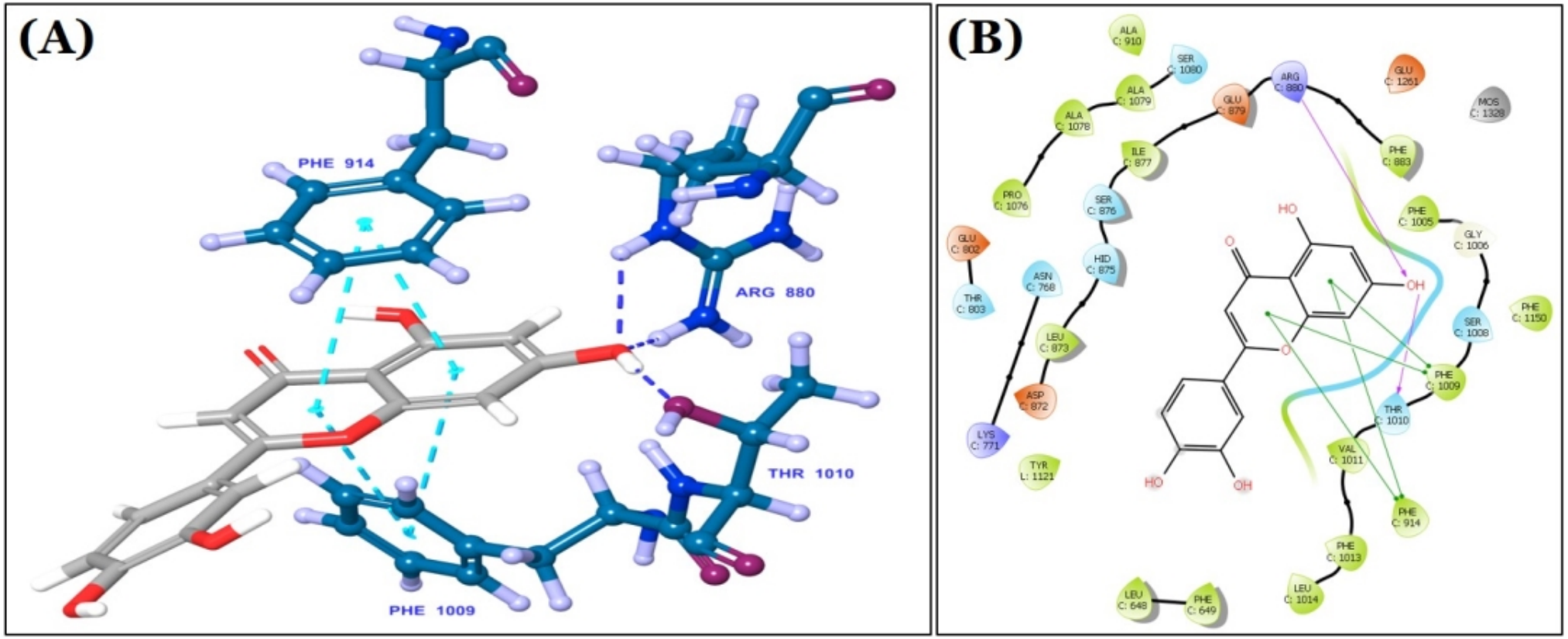

Figure S5: 3D **(A)** and 2D **(B)** diagrams of docked pose of luteolin interacting with XO active site's amino acid residues (PDB ID: 3NVY), as generated using the Schrödinger software. Blue dotted lines indicate the hydrogen bonds while light blue dotted lines show Pi-Pi stacking interactions in 3D view. Magenta solid arrows indicate hydrogen bonds (backbone) while green solid lines represent Pi-Pi stacking interactions in 2D view.

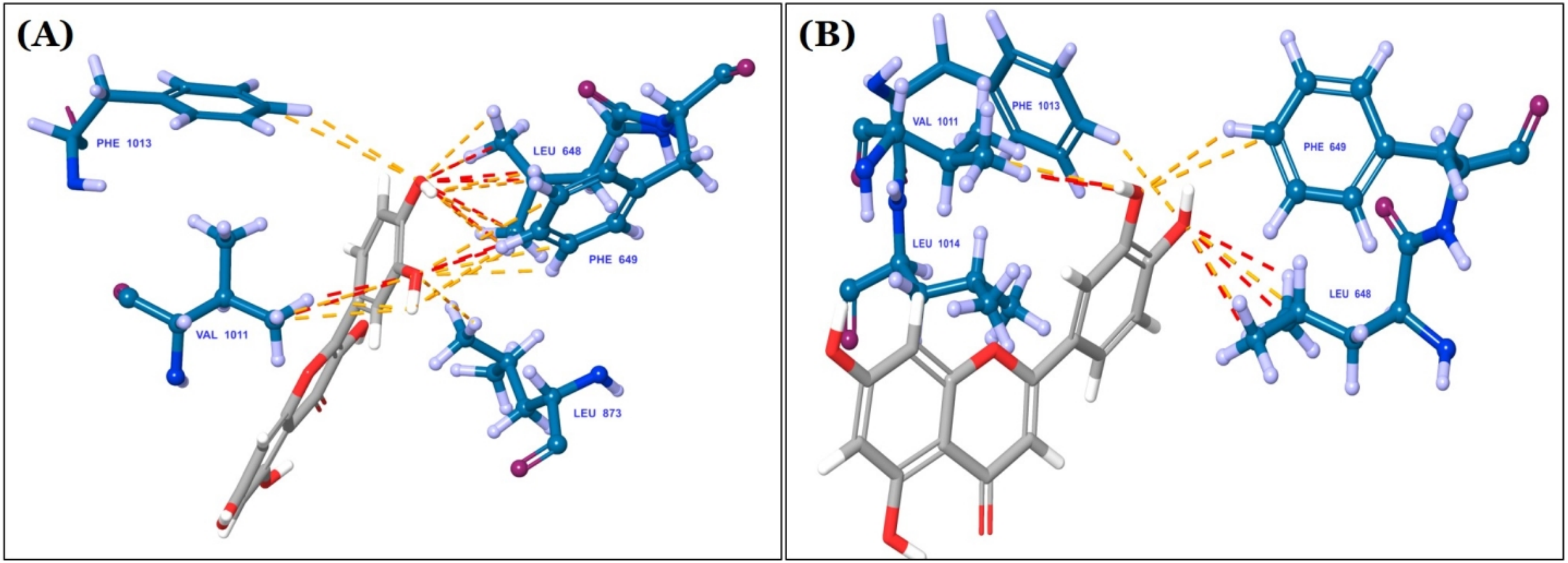

Figure S6: 3D docked poses of **(A)** quercetin and **(B)** luteolin interacting with XO active site's amino acid residues (PDB ID: 3NVY), as generated using the Schrödinger software. Red and orange dotted lines indicate ugly and bad clashes, respectively (unfavorable ligand-receptor interactions).

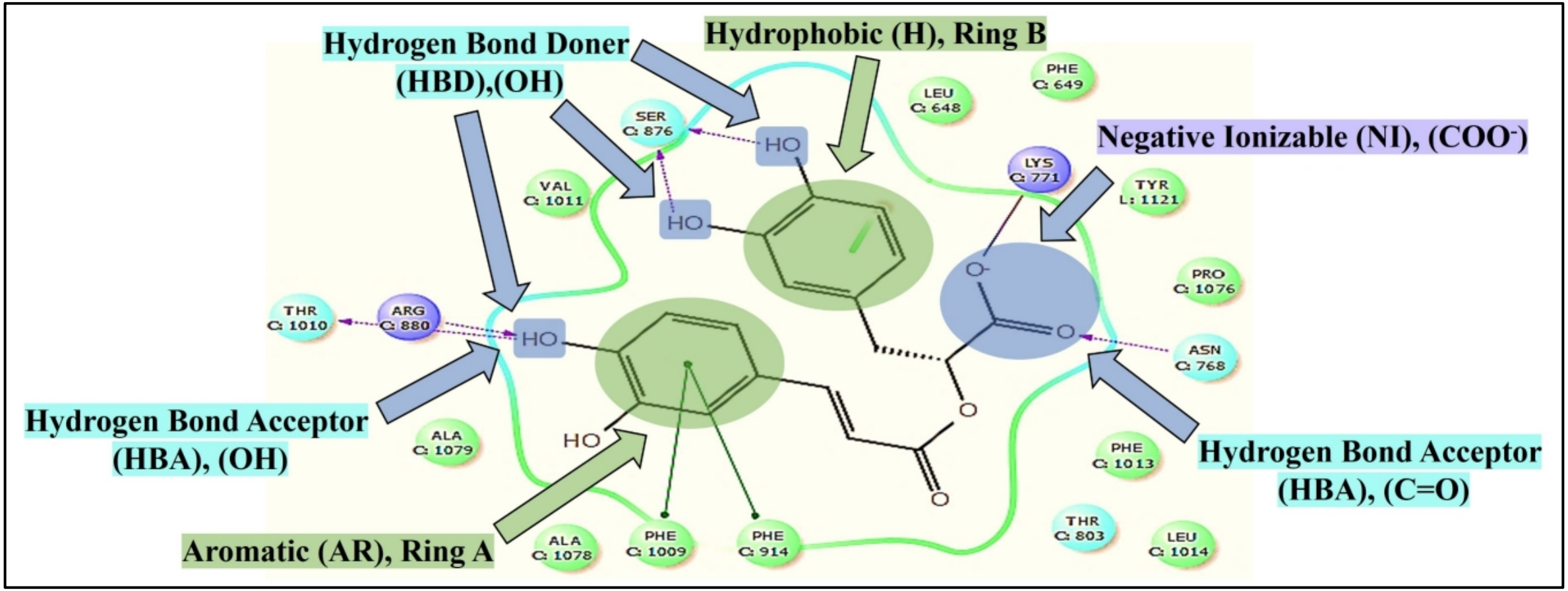

Figure S7: 2D Rosmarinic acid/XO active site's amino acid residues interactions diagram summarizing the observed structure-activity relationship studies (SARs) of rosmarinic acid (i.e. phenolic acids/esters class) for effective XO inhibition.

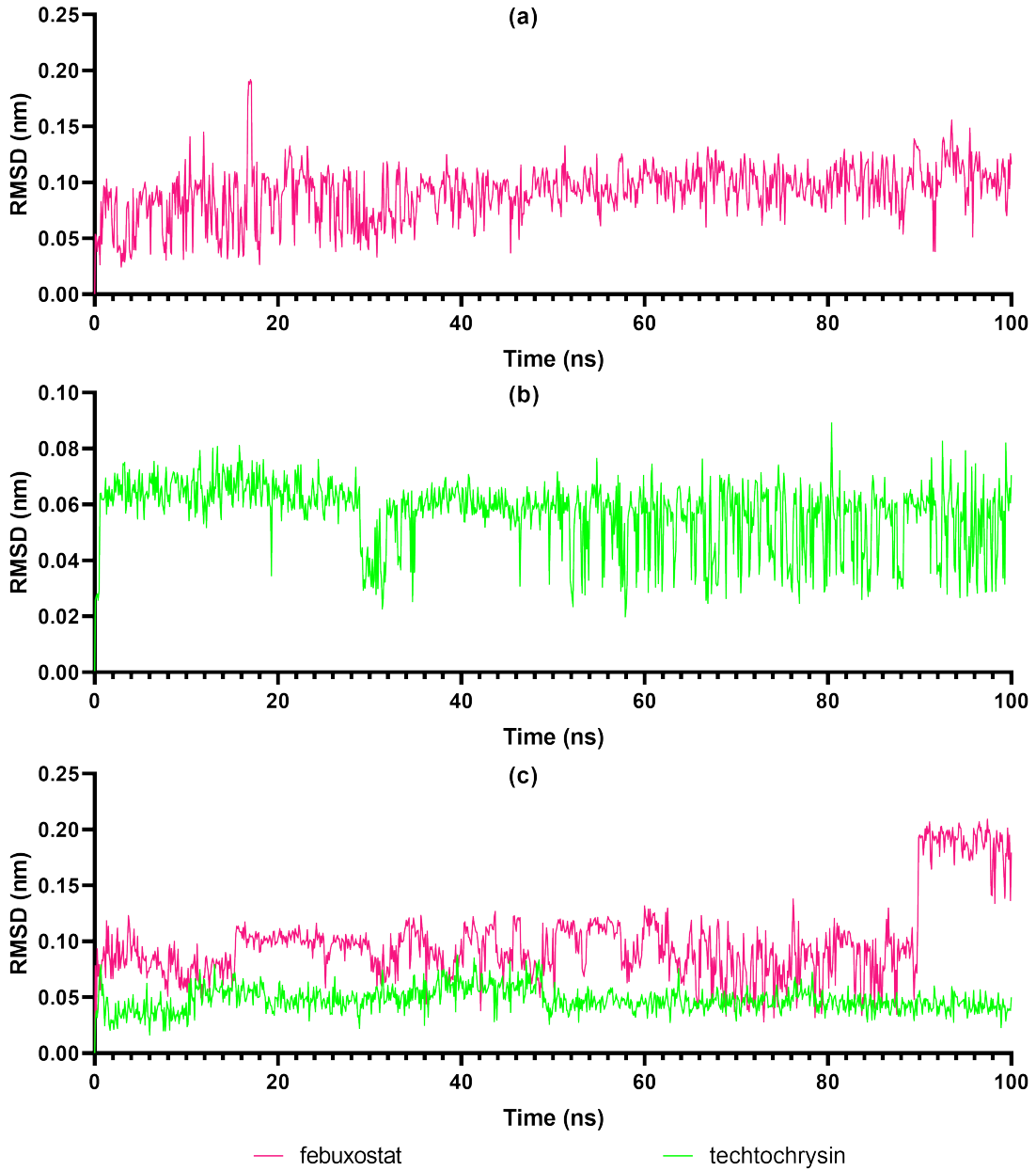

Figure S8: Plots of RMSD measurements of ligands over 100 ns MD simulations for (a) febuxostat in XO-febuxostat complex, mean RMSD value 0.91 Å, (b) techtochrysin in XO-techtochrysin complex, mean RMSD value of 0.56 Å, and (c) combined