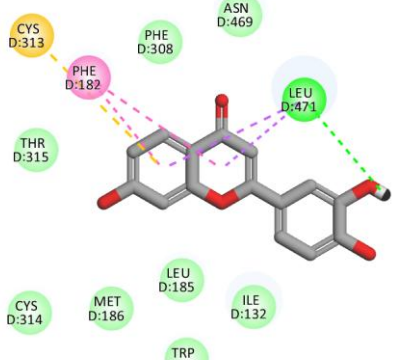
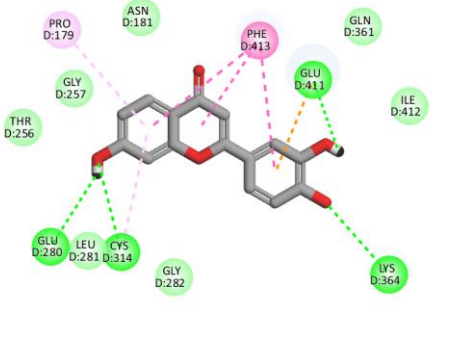
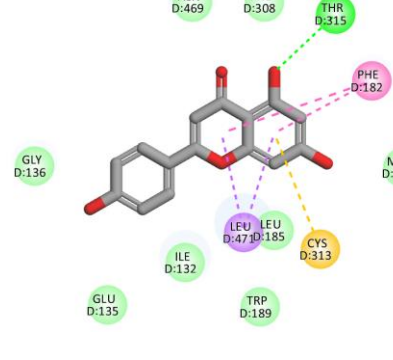
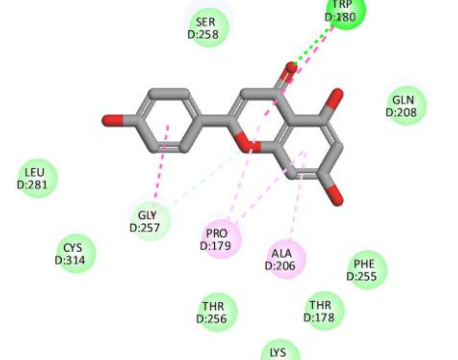
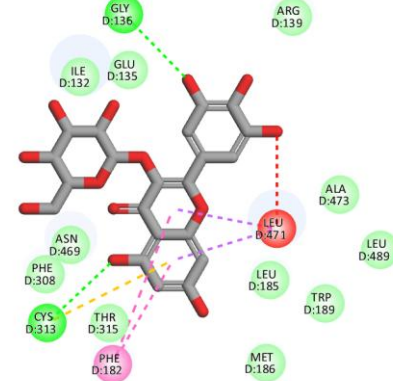
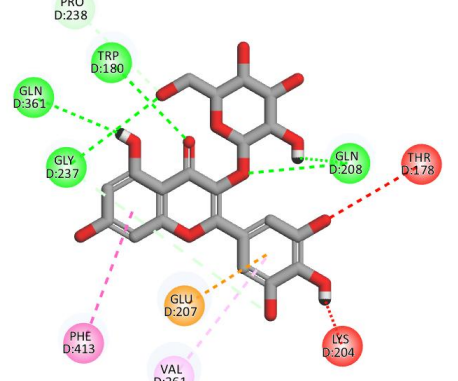
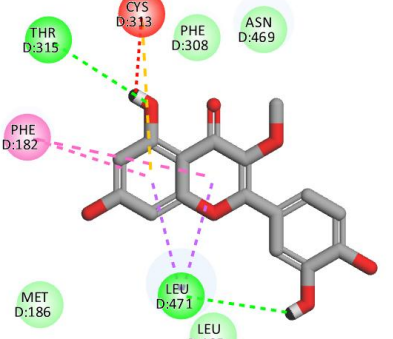
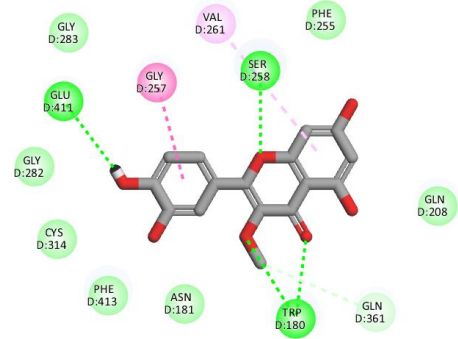
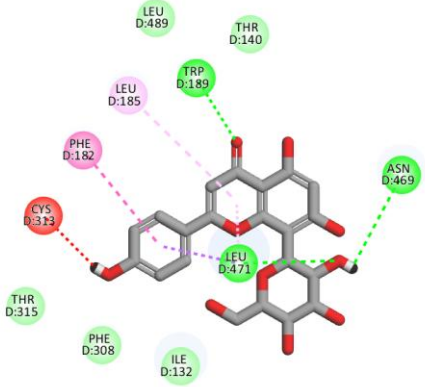
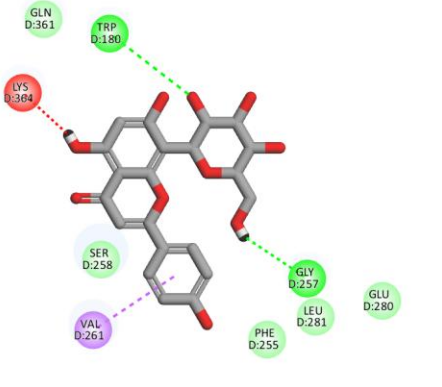
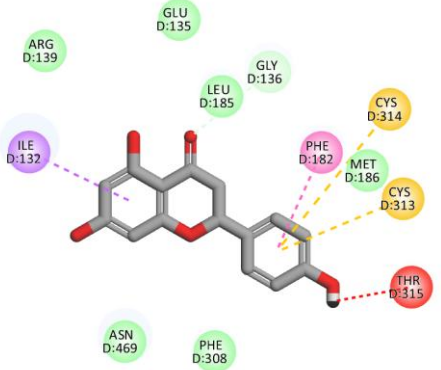
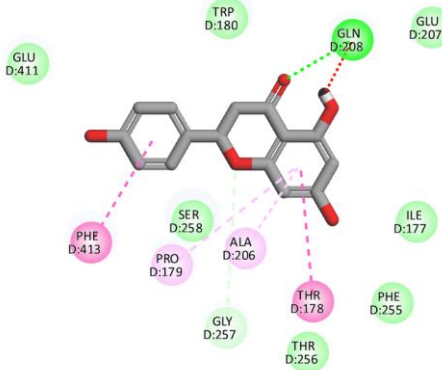
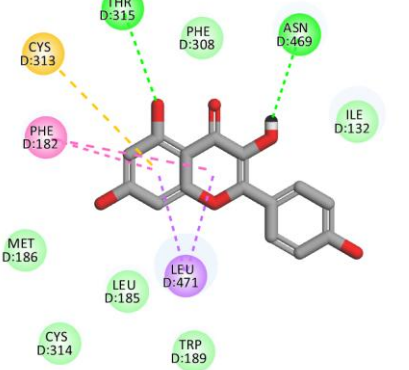
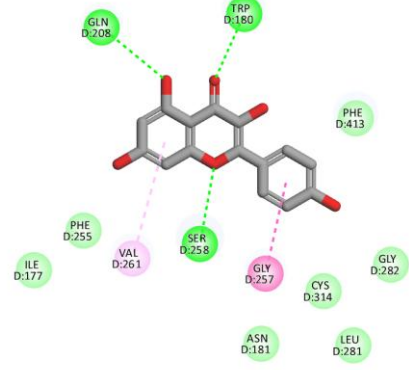
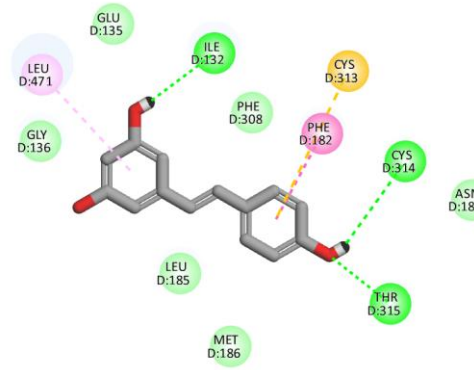
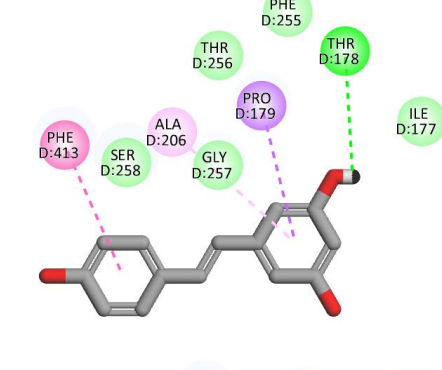


Ligand		Predicted position within the substrate-binding site	Predicted position within the cofactor-binding site
Luteolin 7-O-glucoside			
Luteolin glucoside	3'		
Myricetin			
Isovitexin			

Rutin		
Luteolin		
Quercetin 3-O-galactoside		
Chlorogenic Acid		

5-deoxy luteolin		
Apigenin		
Myricetin 3-O-glucoside		
Quercetin 3-methyl ether		

Vitexin		
Naringenin		
Kaempferol		
Resveratrol		

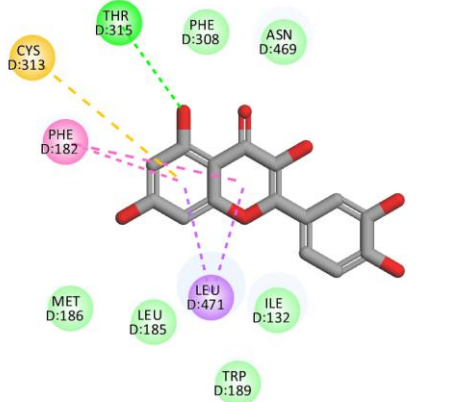
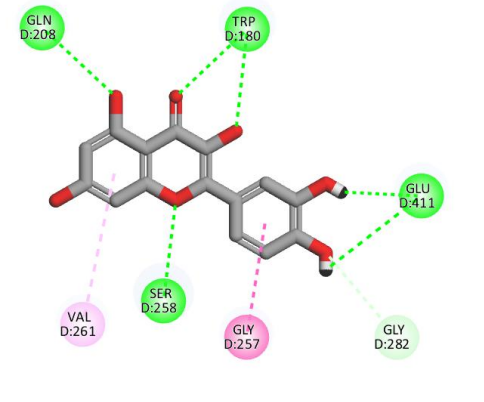
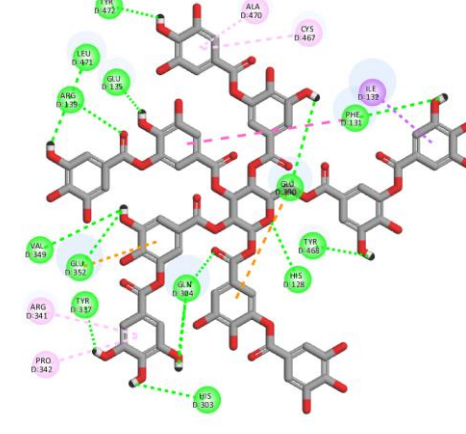
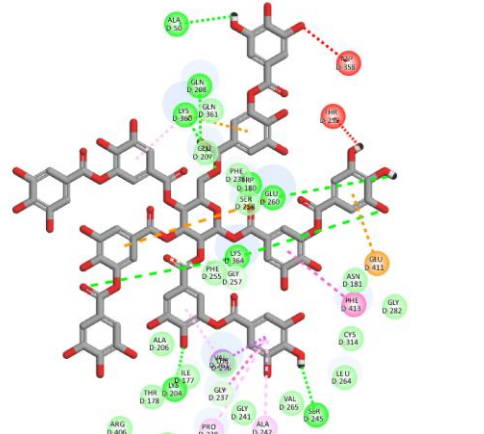
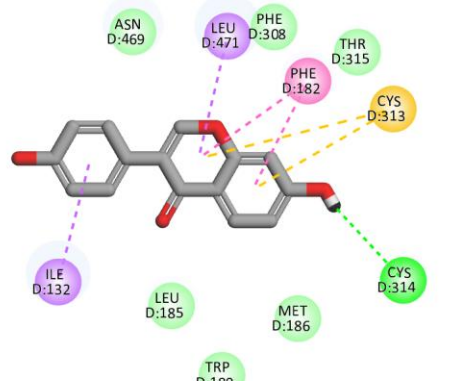
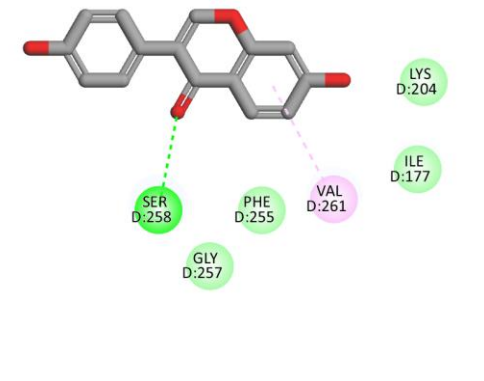
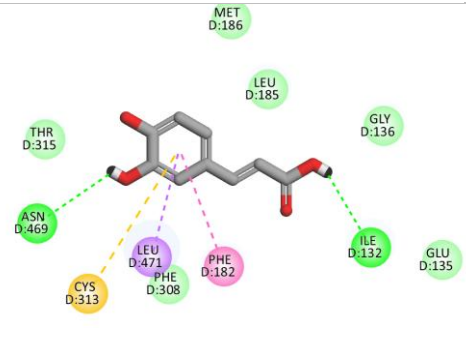
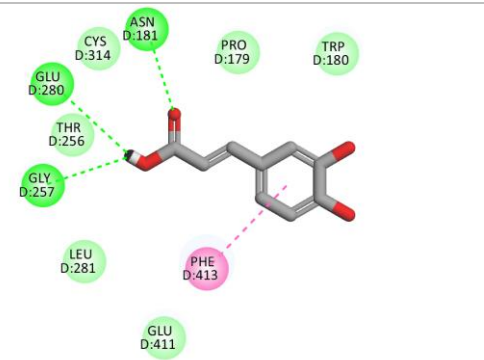
Quercetin	 Quercetin molecule showing interactions with protein residues: CYS D:313, THR D:315, PHE D:308, ASN D:469, MET D:186, LEU D:185, LEU D:471, ILE D:132, TRP D:189, and PHE D:182.	 Quercetin molecule showing interactions with protein residues: GLN D:208, TRP D:180, VAL D:261, SER D:258, GLY D:257, GLY D:282, and GLU D:411.
Tannic acid	 Tannic acid molecule showing interactions with protein residues: THR D:315, LEU D:471, PHE D:308, ASN D:469, MET D:186, LEU D:185, LEU D:471, ILE D:132, TRP D:189, PHE D:182, and CYS D:313.	 Tannic acid molecule showing interactions with protein residues: GLN D:208, TRP D:180, VAL D:261, SER D:258, GLY D:257, GLY D:282, GLU D:411, and CYS D:313.
Diadzein	 Diadzein molecule showing interactions with protein residues: ASN D:469, LEU D:471, PHE D:308, THR D:315, CYS D:313, ILE D:132, LEU D:185, MET D:186, TRP D:189, and CYS D:314.	 Diadzein molecule showing interactions with protein residues: LYS D:204, ILE D:177, VAL D:261, PHE D:255, SER D:258, and GLY D:257.
Caffeic acid	 Caffeic acid molecule showing interactions with protein residues: THR D:315, ASN D:469, LEU D:185, GLY D:136, ILE D:132, GLU D:135, CYS D:313, LEU D:471, PHE D:308, and PHE D:182.	 Caffeic acid molecule showing interactions with protein residues: ASN D:181, PRO D:179, TRP D:180, GLU D:280, THR D:256, GLY D:257, LEU D:281, PHE D:413, and GLU D:411.

Figure S1. Predicted docking poses of the evaluated phytochemicals within the substrate-binding and cofactor-binding sites of ALDH1A3.

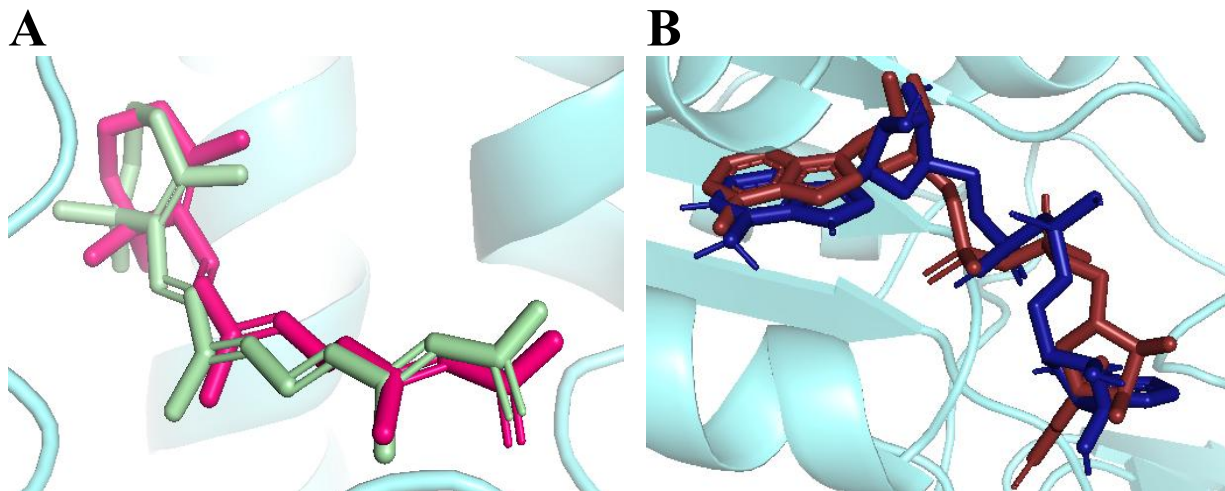


Figure S2. Superimposition of the re-docked and crystallographic ligand poses in ALDH1A3. (A) Re-docked retinoic acid–ALDH1A3 complex (pink) superimposed on the corresponding crystallographic pose (pale green) within the substrate-binding site (RMSD = 0.85 Å). (B) Re-docked NAD–ALDH1A3 complex (navy blue) superimposed on the corresponding crystallographic pose (ruby) within the cofactor-binding site (RMSD = 1.99 Å).

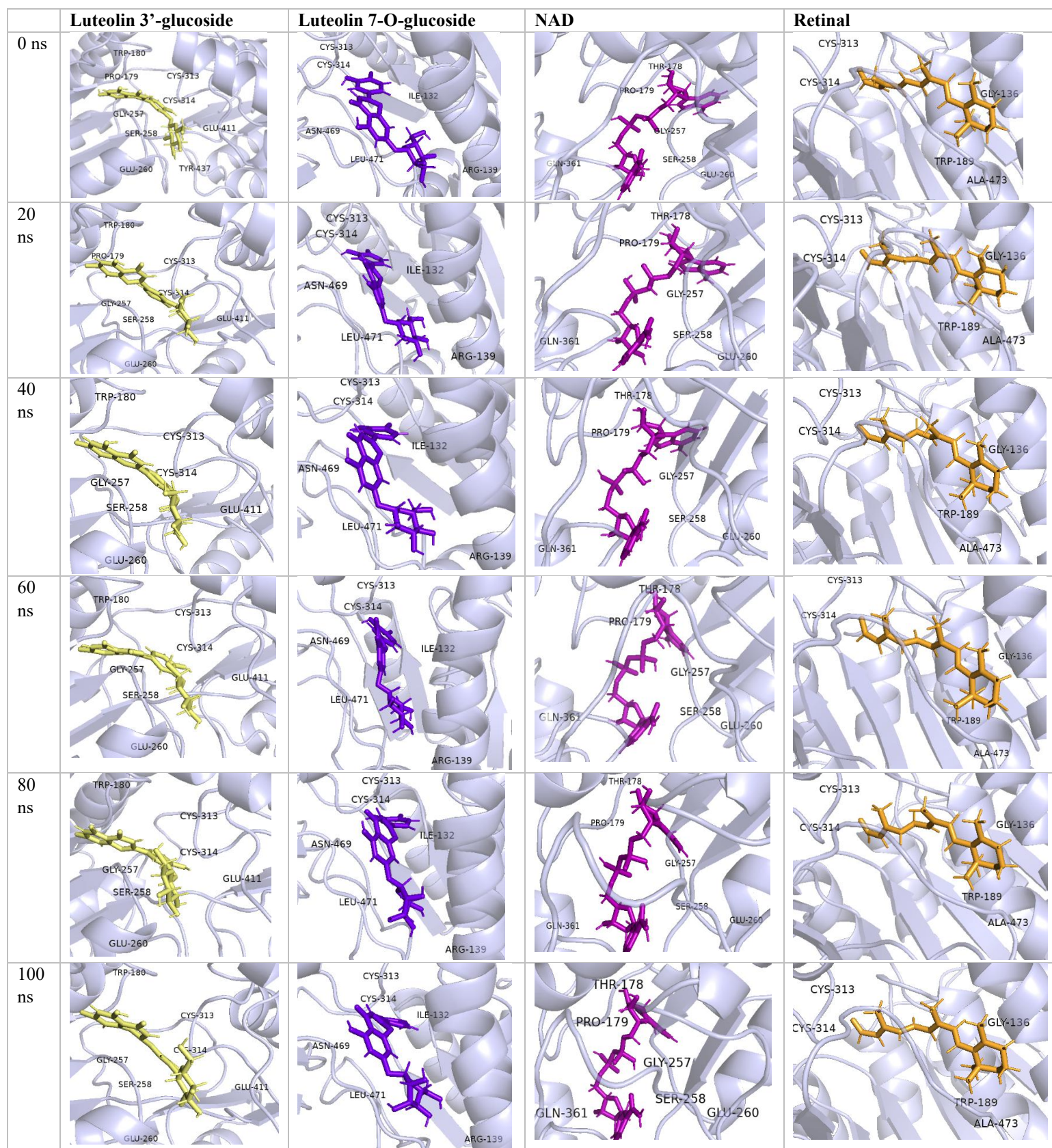


Figure S3. Frames of protein–ligand binding modes every 20 ns for each ligand during simulation.