



Supplementary Materials

Assessments of Alpha-amylase Inhibitory Potential of Tagetes Flavonoids through In-vitro, Molecular Docking, and Molecular Dynamic Simulation Studies

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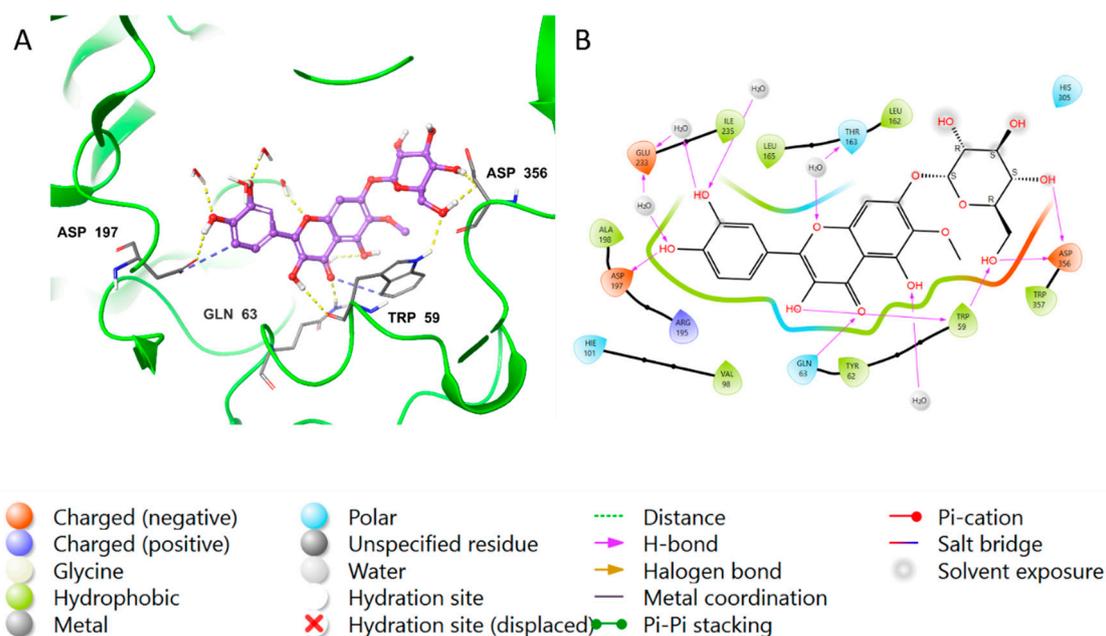


Figure S1. Proposed binding mode of patuletin-7-O- β -D-glucopyranoside (**5**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.

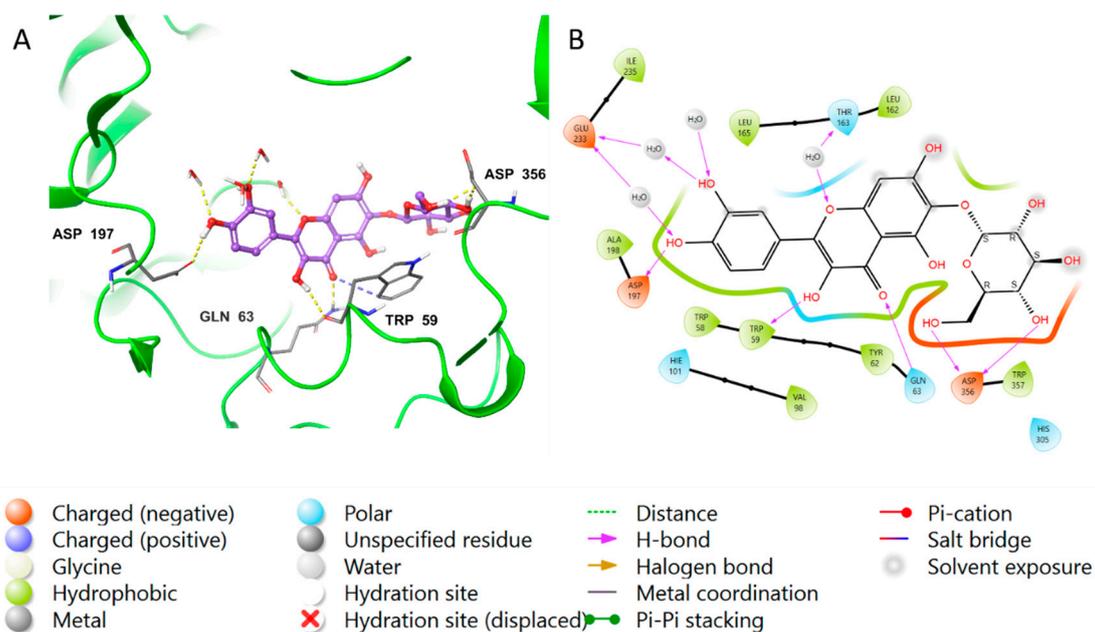


Figure S2. Proposed binding mode of quercetagenin-6-O- β -D-glucopyranoside (**3**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.

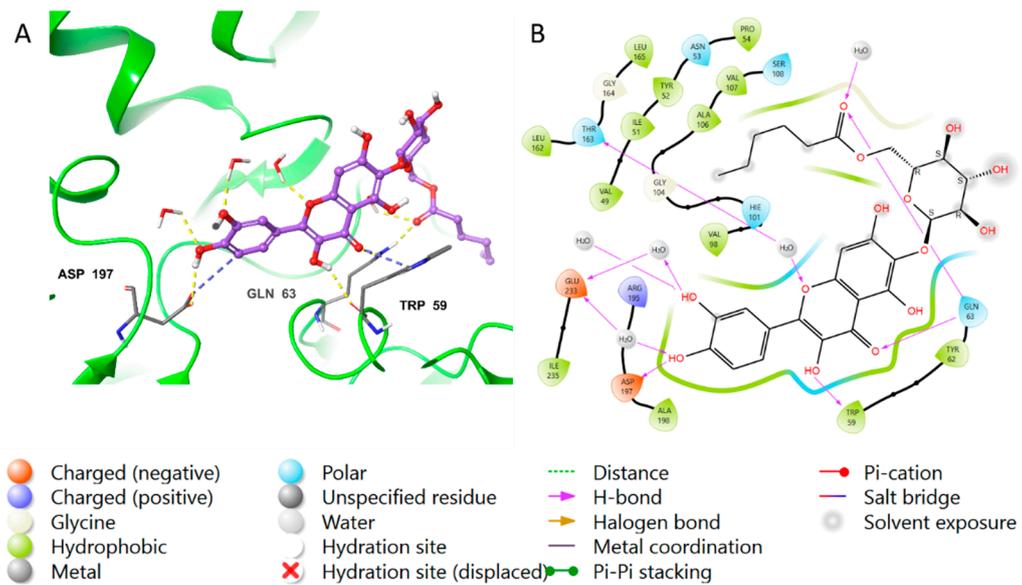


Figure S3. Proposed binding mode of minutaside A (**4**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.

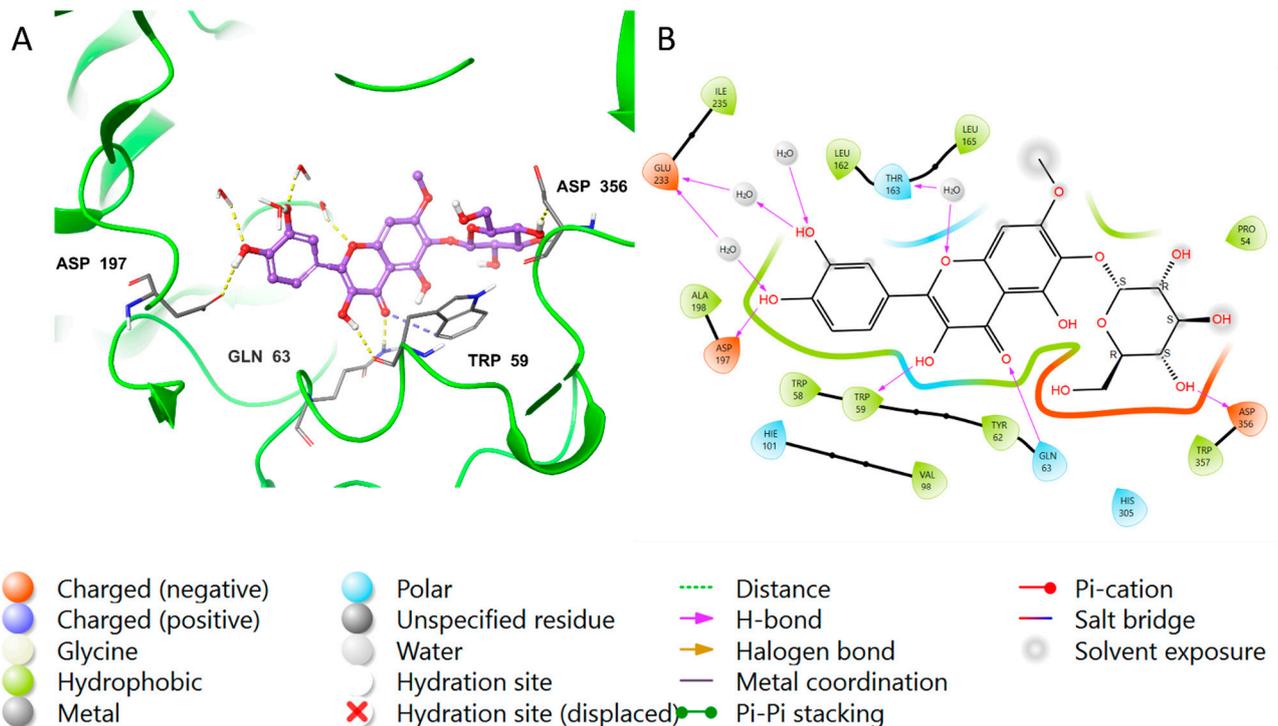


Figure S4. Proposed binding mode of quercetagenin-7-methoxy-6-O- β -D-glucopyranoside (**6**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.

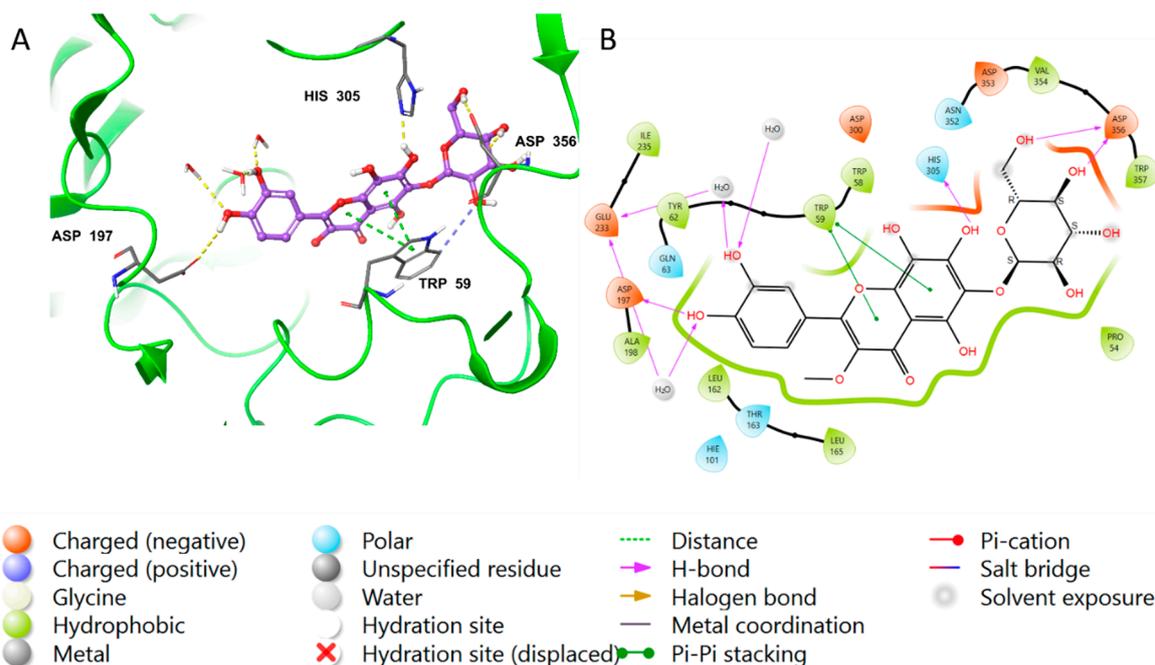


Figure S5. Proposed binding mode of tagenol B (**7**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.

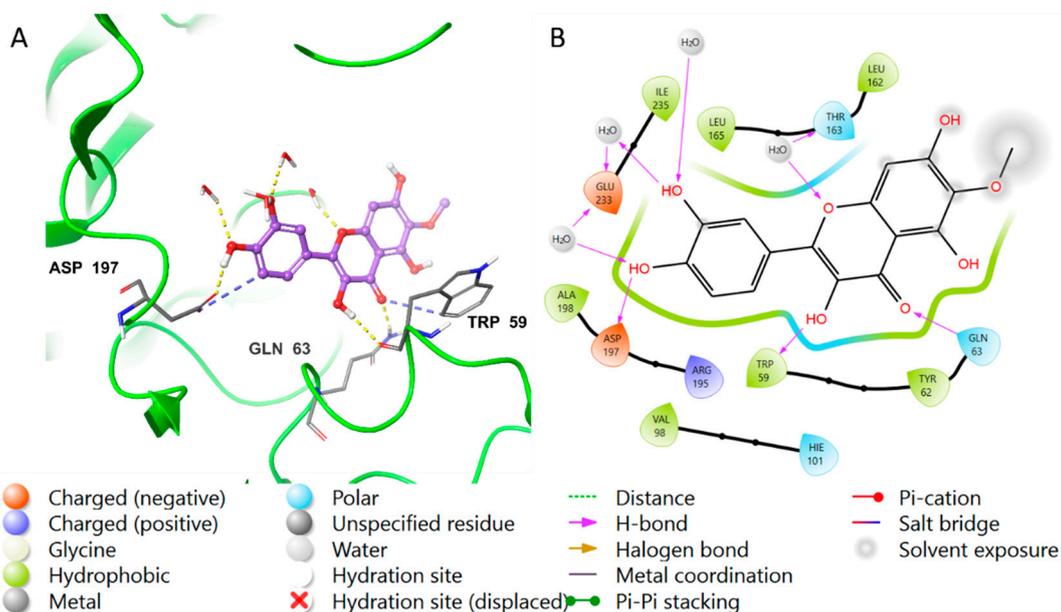


Figure S6. Proposed binding mode of patuletin (**8**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.

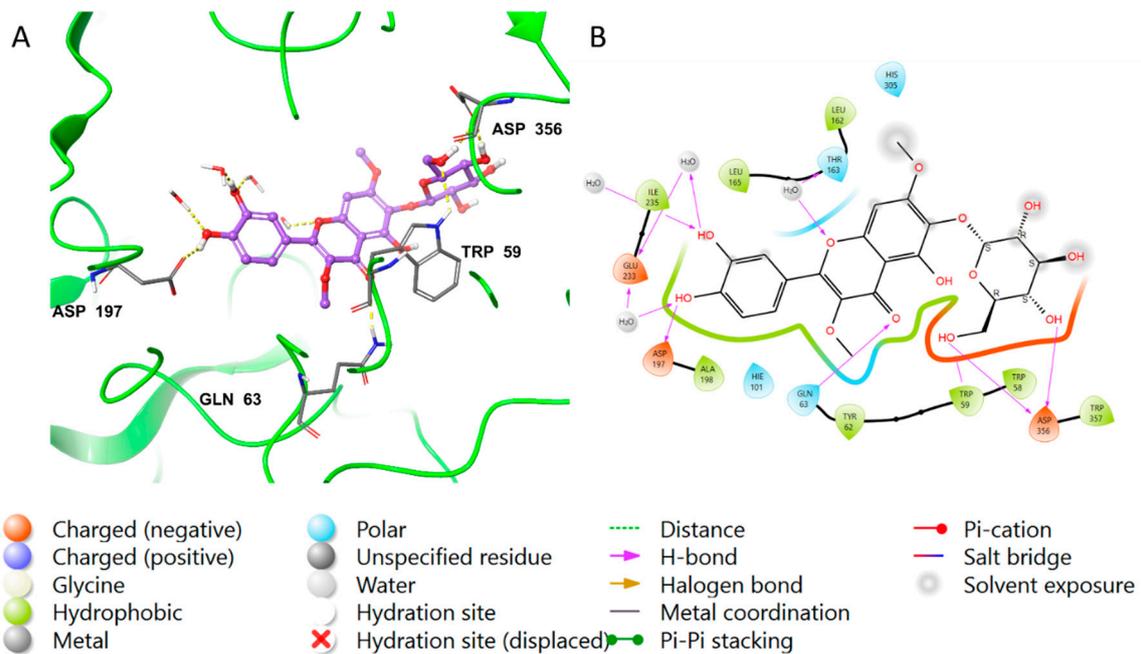


Figure S7. Proposed binding mode of quercetagenin-3,7-dimethoxy-6-O- β -D-glucopyranoside (**9**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (A) and 2D (B) views.

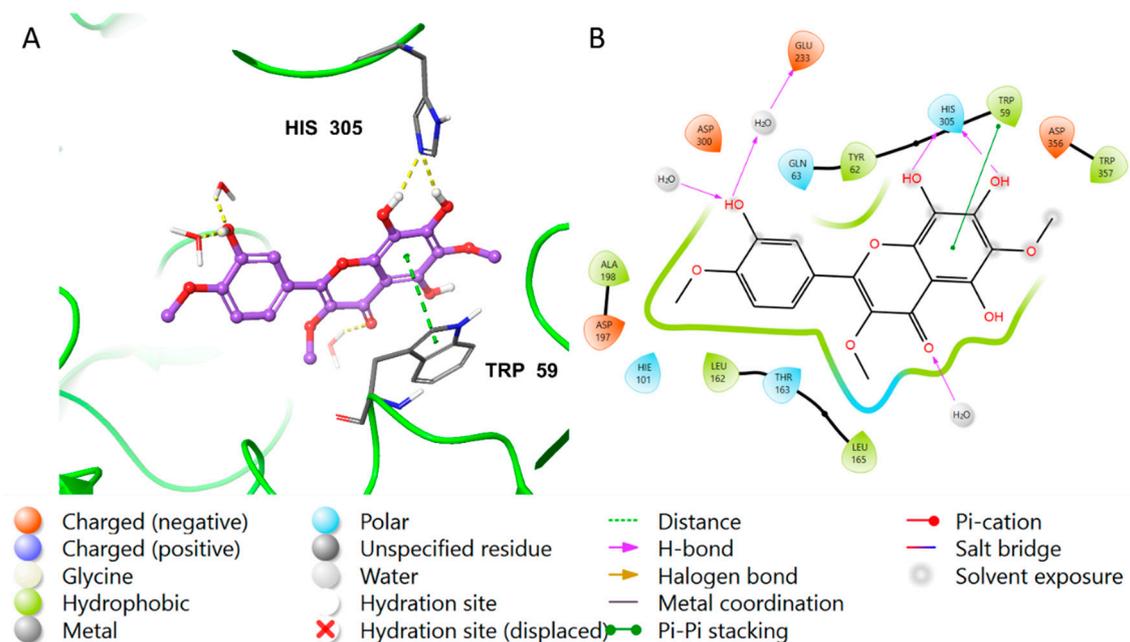


Figure S8. Proposed binding mode of tagenol A (**12**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (A) and 2D (B) views.

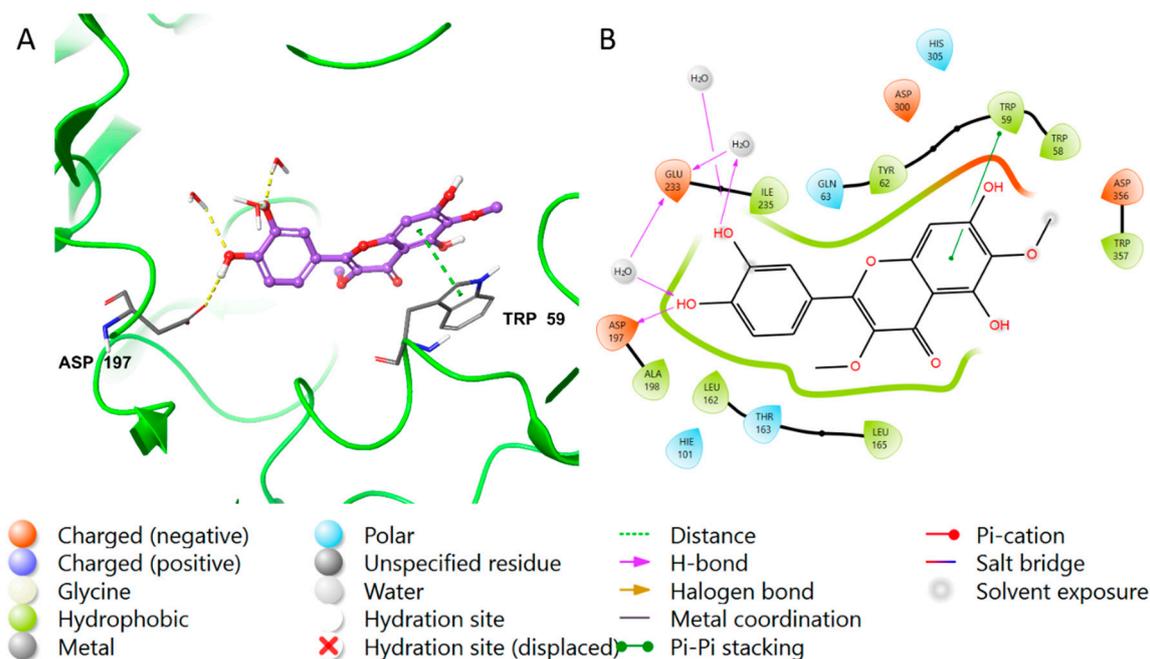


Figure S9. Proposed binding mode of quercetin-3,6-dimethyl ether (**11**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.

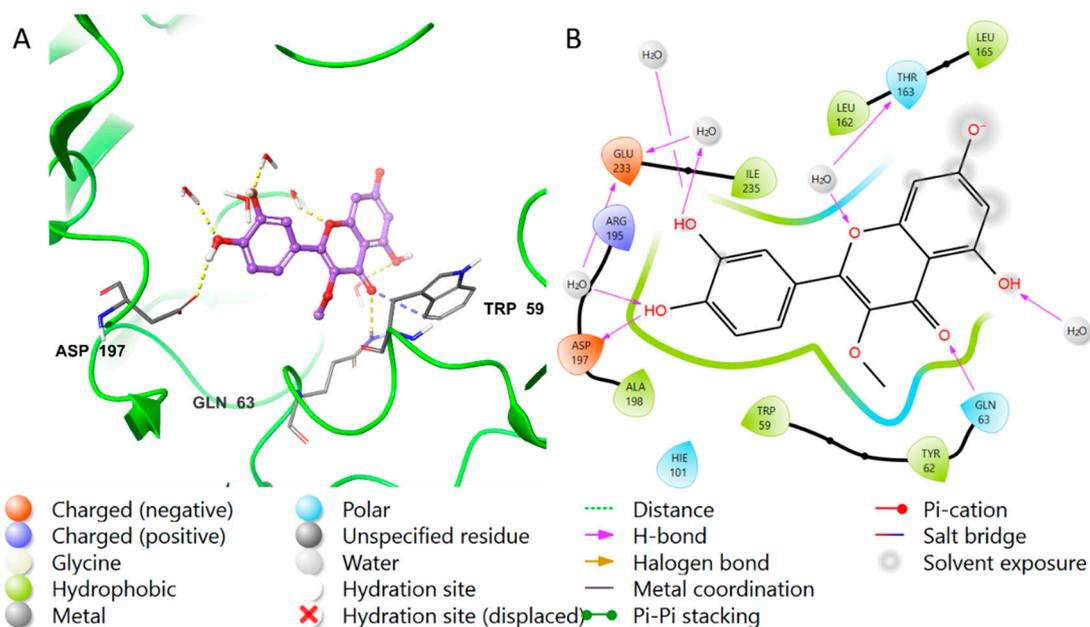


Figure S10. Proposed binding mode of quercetin-3-methyl ether (**10**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.

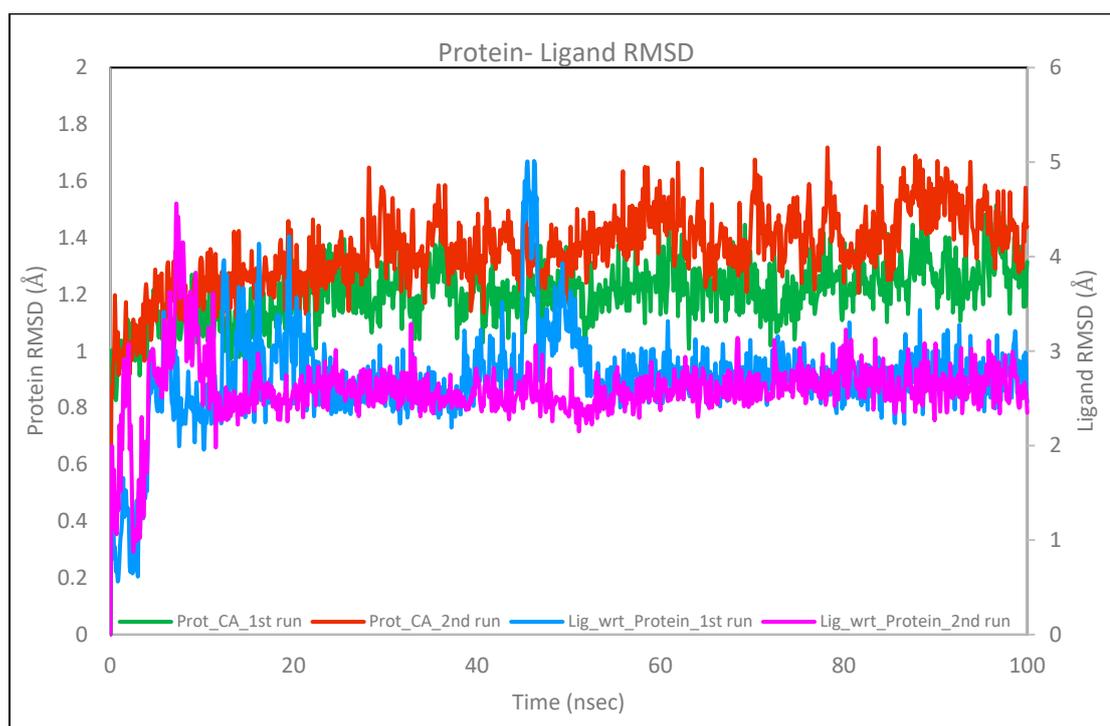


Figure S11. RMSD plot in duplicate for Quercetagenin-7-O-b-D-glucopyranoside (2) with pancreatic alpha-amylase (PDB-ID: 4GQR) during the MD simulation. Green and red represent the first and second run of protein, respectively. While blue and pink represent the first and second run of ligand

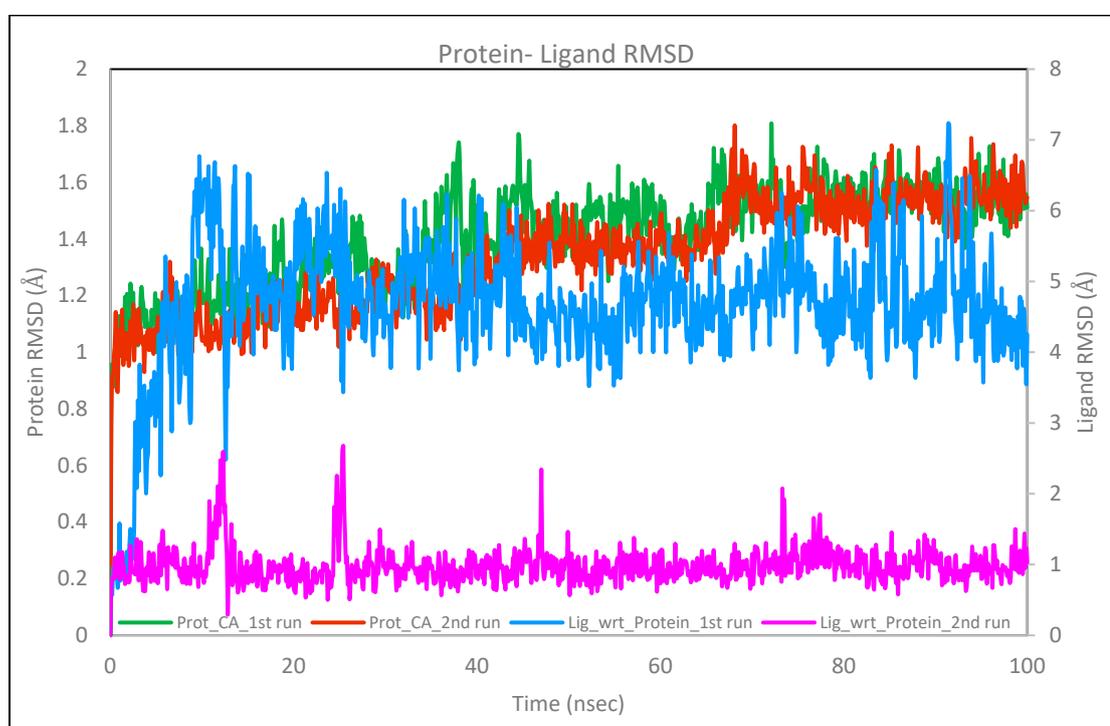


Figure S12. RMSD plot in duplicate for 3- Quercetagenin-6-O-b-D-glucopyranoside (3) with pancreatic alpha-amylase (PDB-ID: 4GQR) during the MD simulation. Green and red represent the first and second run of protein, respectively. While blue and pink represent the first and second run of ligand

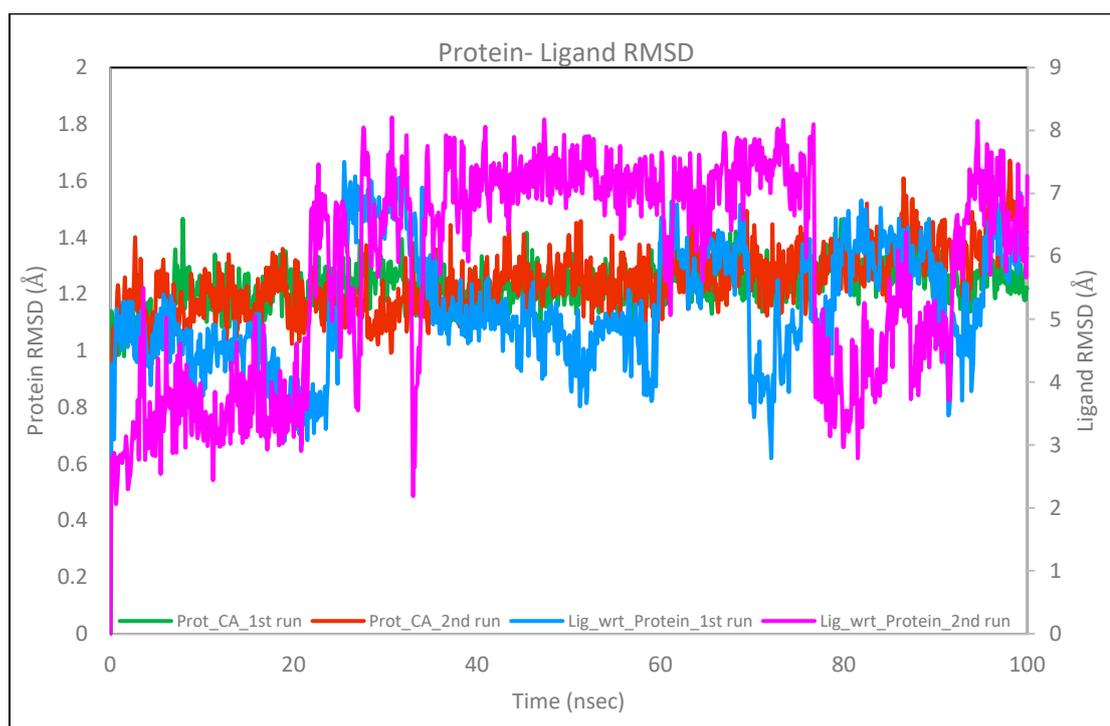


Figure S13. RMSD plot in duplicate for 4- MinuStructure574Minutaside A (4) with pancreatic alpha-amylase (PDB-ID: 4GQR) during the MD simulation Green and red represent the first and second run of protein, respectively. While blue and pink represent the first and second run of ligand

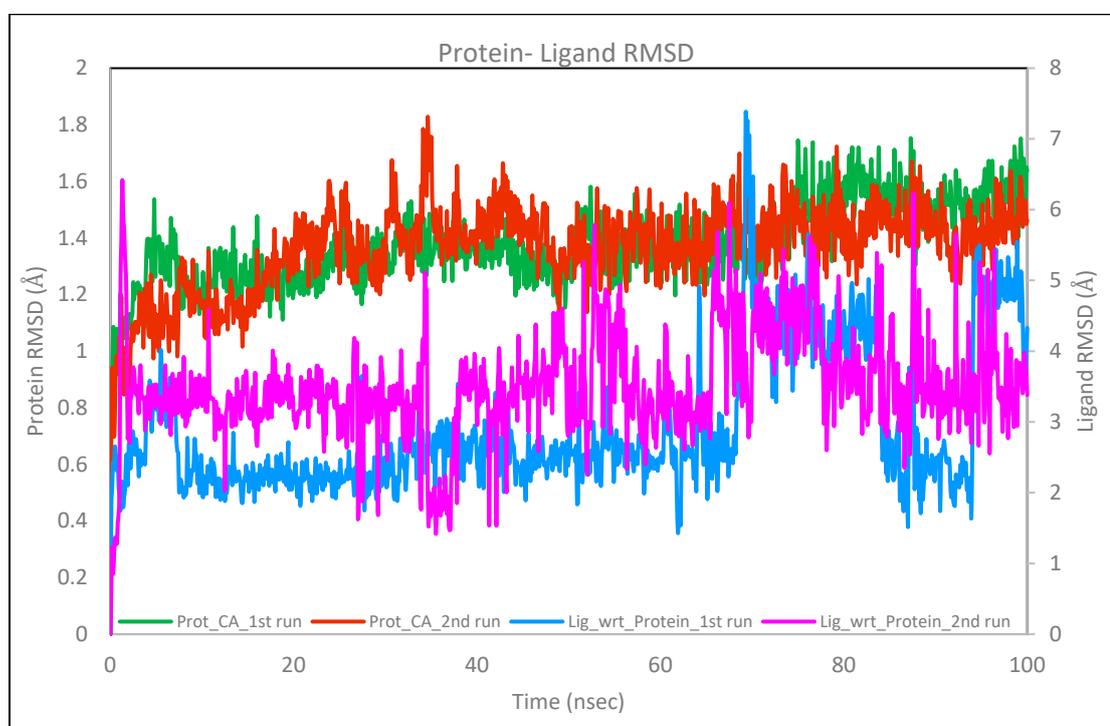


Figure S14. RMSD plot in duplicate for Patuletin-7-O-b-D-glucopyranoside (5) with pancreatic alpha-amylase (PDB-ID: 4GQR) during the MD simulation Green and red represent the first and second run of protein, respectively. While blue and pink represent the first and second run of ligand

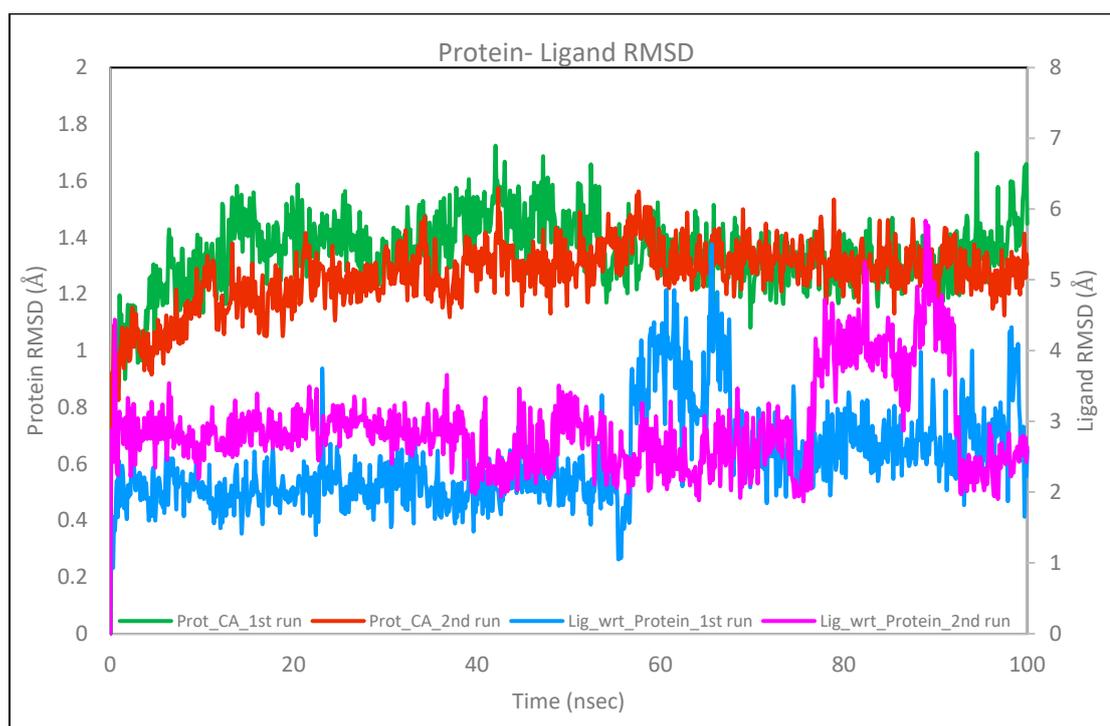


Figure S15. RMSD plot in duplicate for Quercetagenin-7-methoxy-6-O-b-D-glucopyranoside (6) with pancreatic alpha-amylase (PDB-ID: 4GQR) during the MD simulation Green and red represent the first and second run of protein, respectively. While blue and pink represent the first and second run of ligand

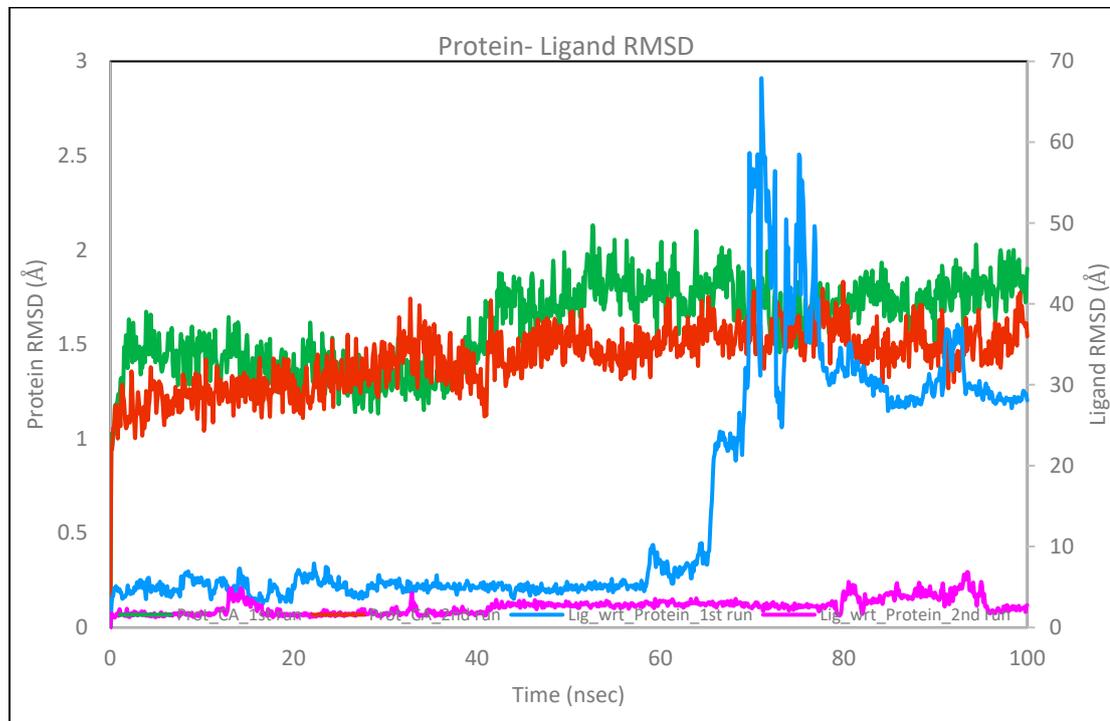


Figure S16. RMSD plot in duplicate for Acarbose with pancreatic alpha-amylase (PDB-ID: 4GQR) during the MD simulation Green and red represent the first and second run of protein, respectively. While blue and pink represent the first and second run of ligand

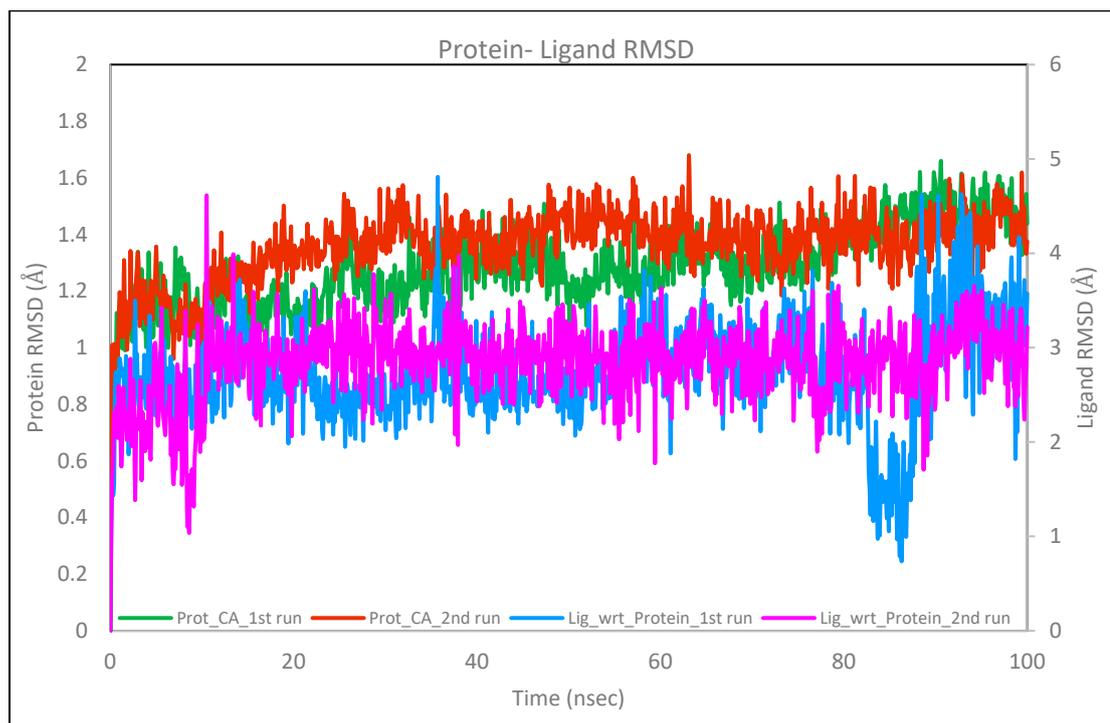


Figure S17. RMSD plot in duplicate for Myricetin with pancreatic alpha-amylase (PDB-ID: 4GQR) during the MD simulation. Green and red represent the first and second run of protein, respectively. While blue and pink represent the first and second run of ligand.