



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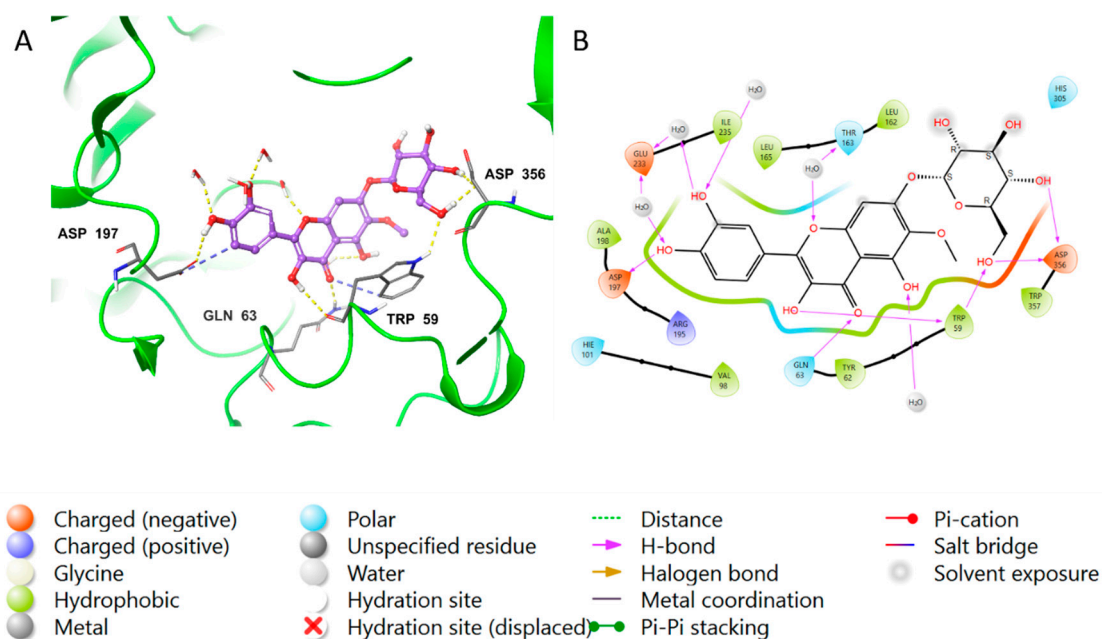
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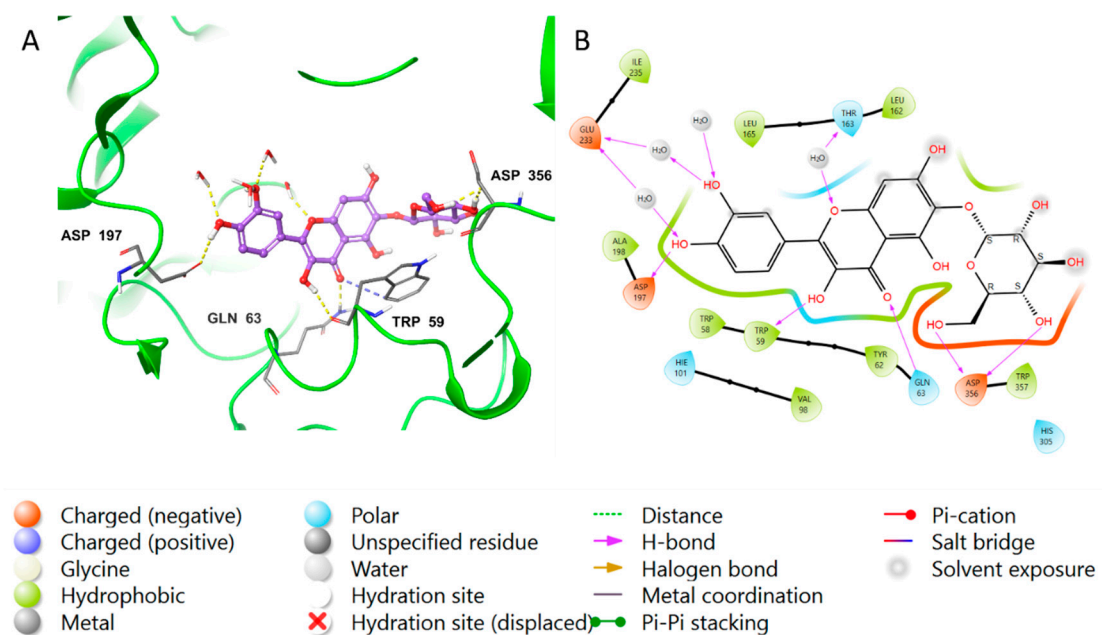
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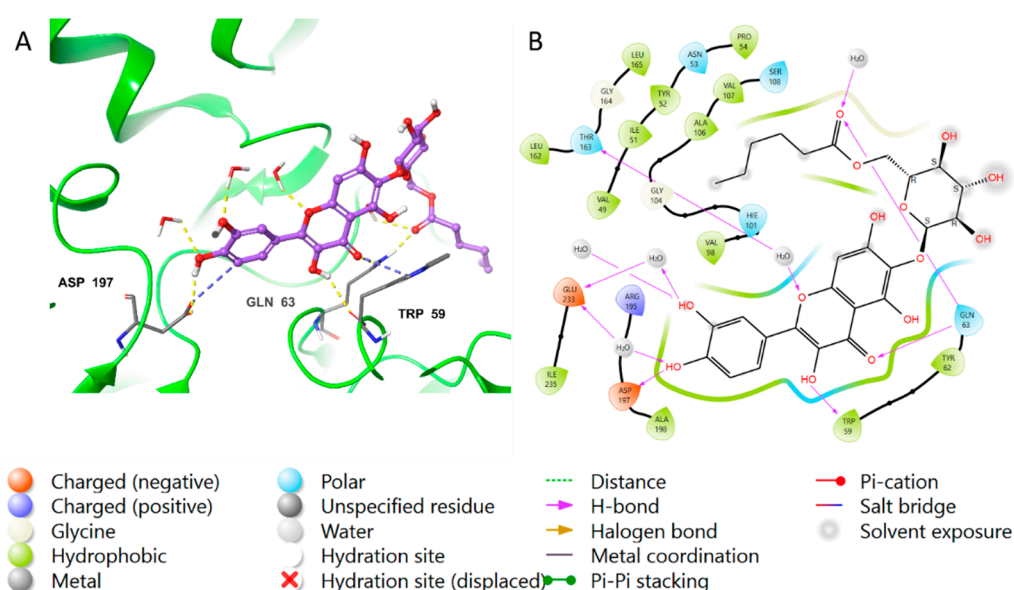
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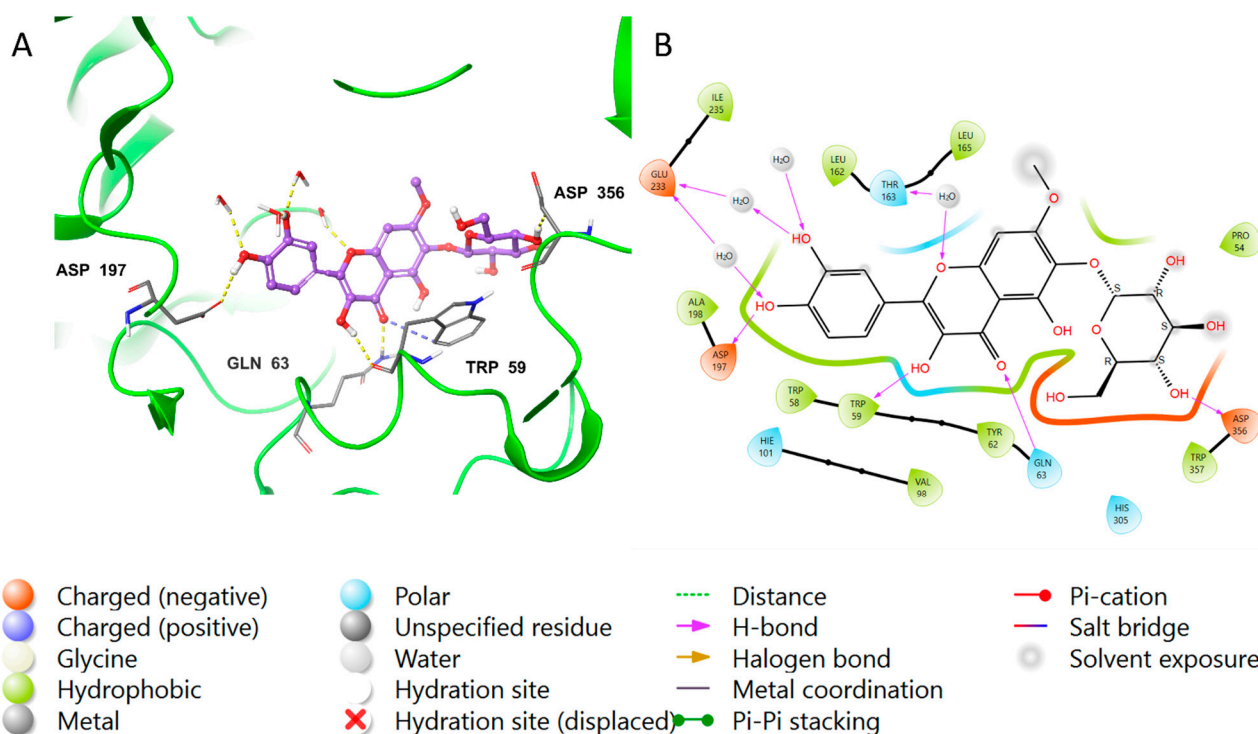
**Figure S1.** Proposed binding mode of patuletin-7-O-β-D-glucopyranoside (**5**) in the active site of the pancreatic α-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.



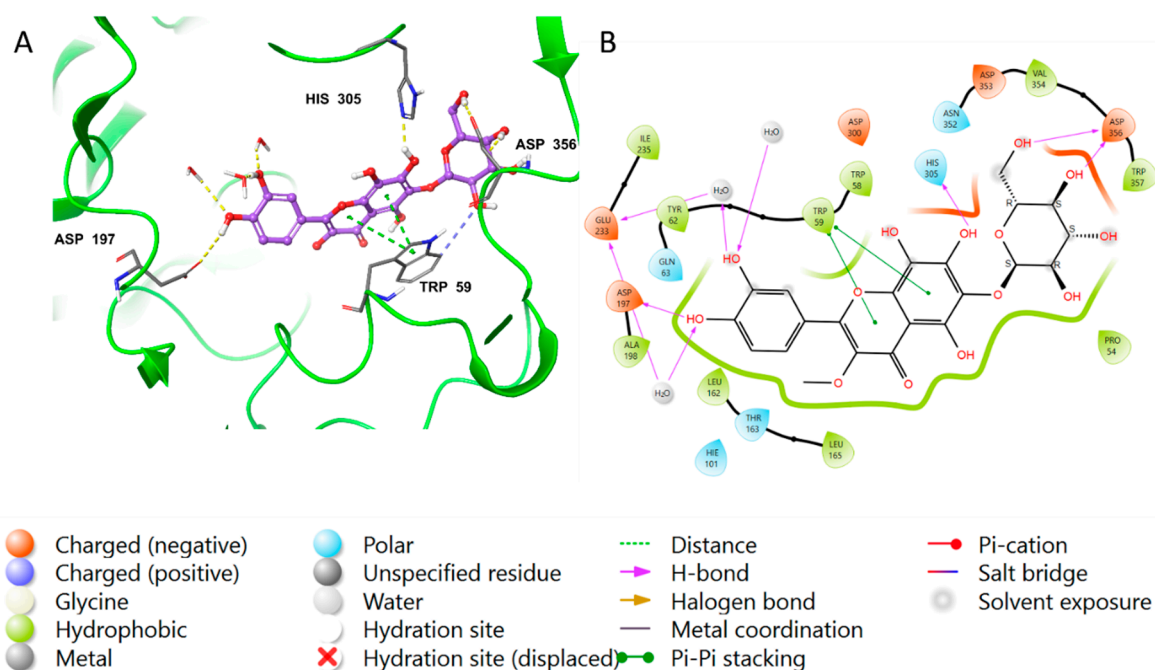
**Figure S2.** Proposed binding mode of quercetagenin-6-O-β-D-glucopyranoside (**3**) in the active site of the pancreatic α-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.



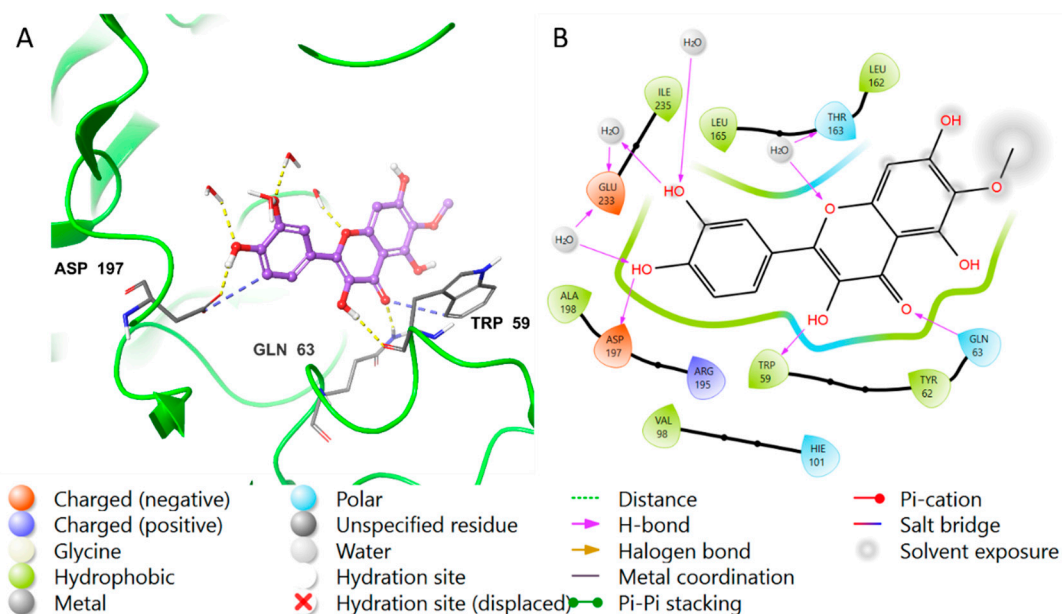
**Figure S3.** Proposed binding mode of minutaside A (**4**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (A) and 2D (B) views.



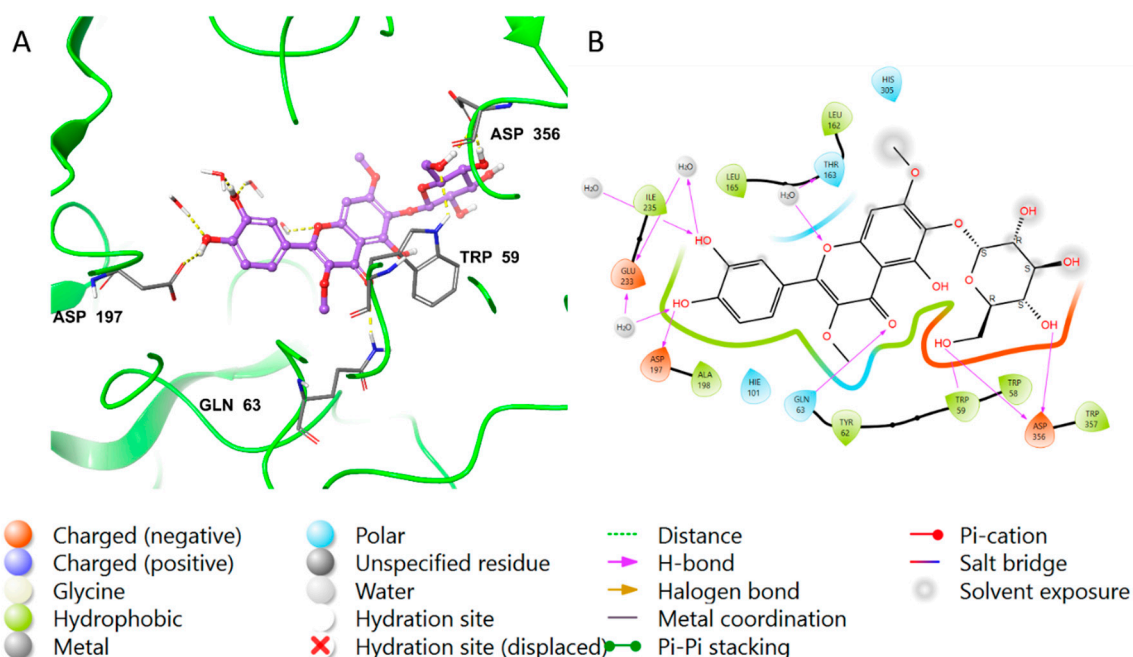
**Figure S4.** Proposed binding mode of quercetagetin-7-methoxy-6-O- $\beta$ -D-glucopyranoside (**6**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (A) and 2D (B) views.



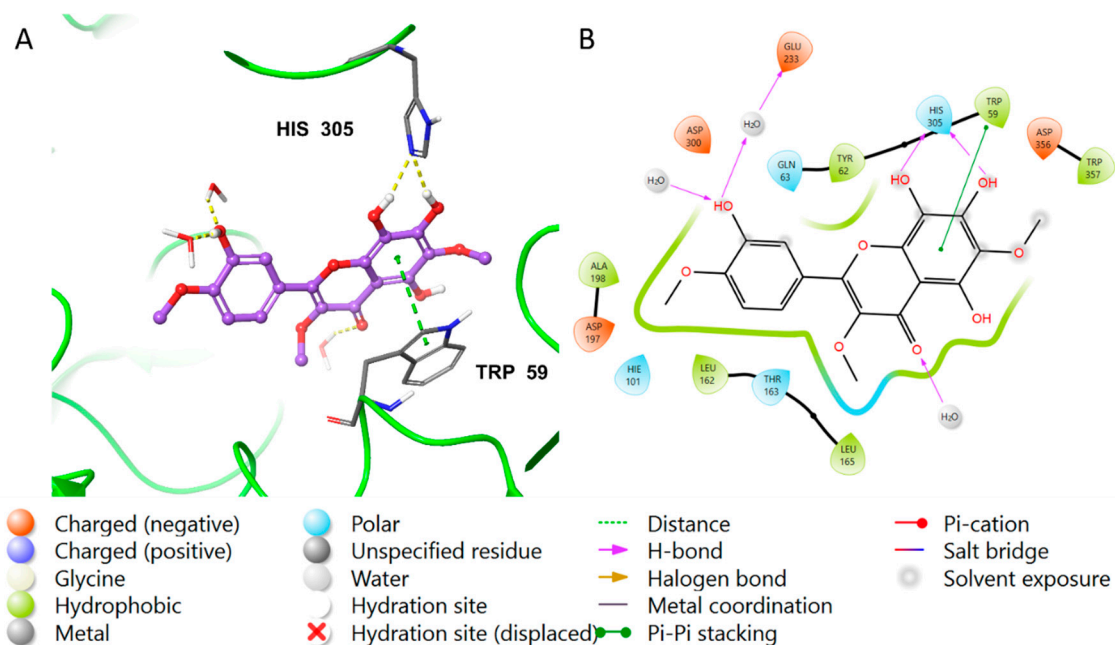
**Figure S5.** Proposed binding mode of tagenol B (**7**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.



**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.

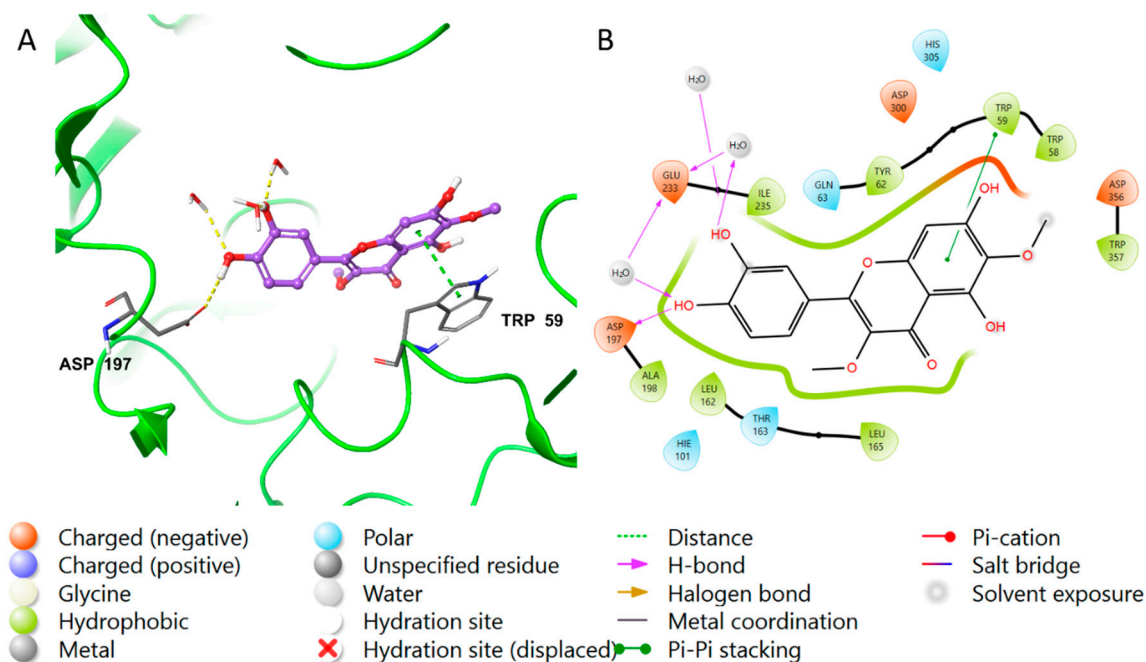


**Figure S7.** Proposed binding mode of quercetagenin-3,7-dimethoxy-6-O-β-D-glucopyranoside (**9**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (A) and 2D (B) views.

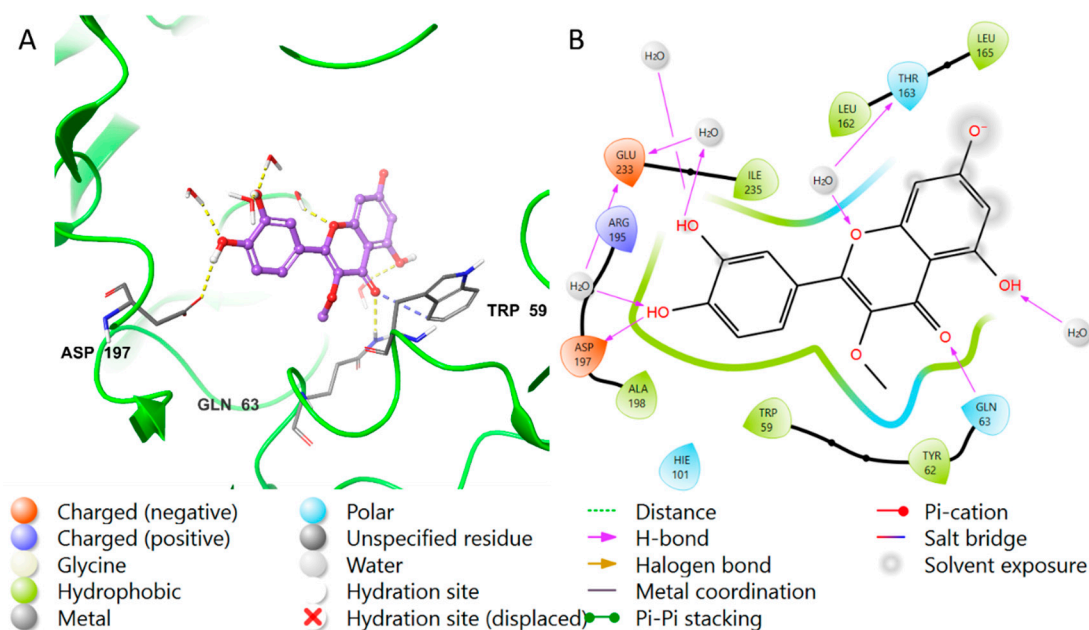


**Figure S8.** Proposed binding mode of tagenol A (**12**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (A) and 2D (B) views.

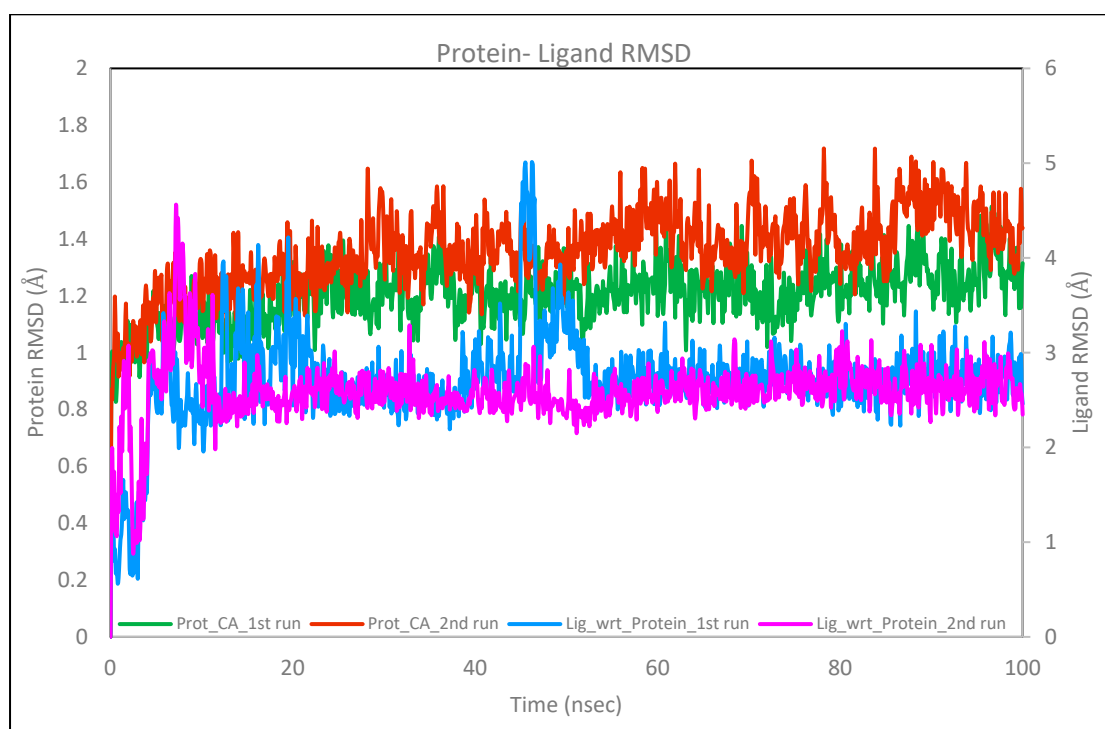




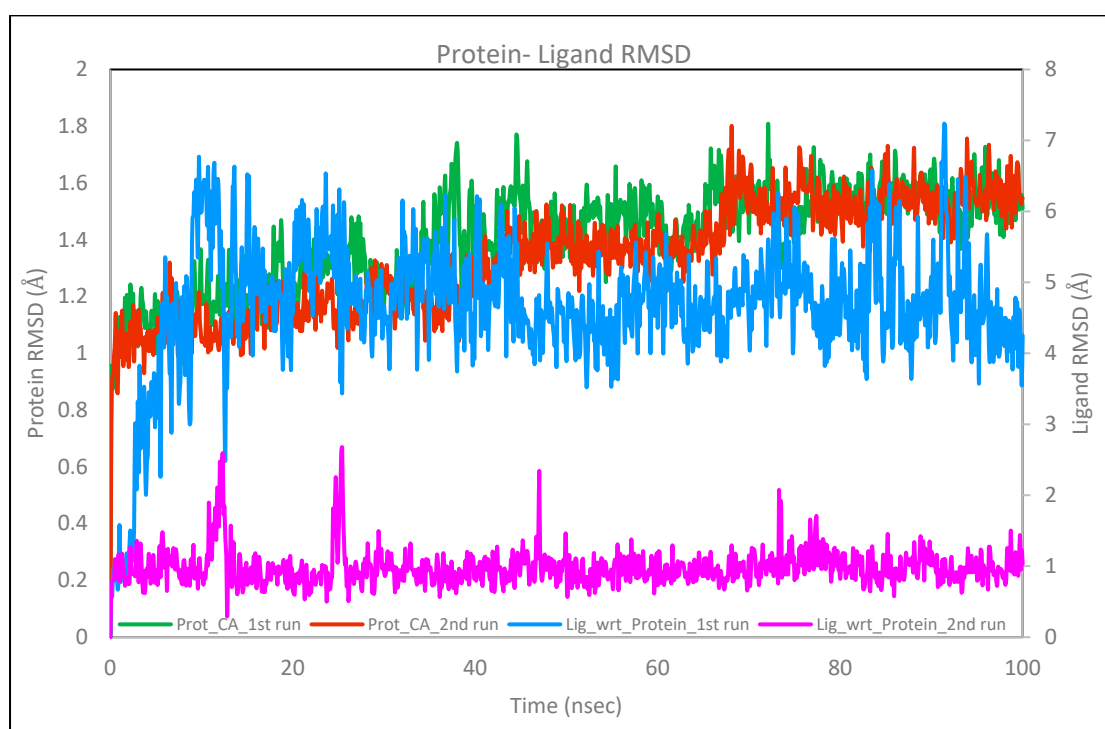
**Figure S9.** Proposed binding mode of quercetin-3,6-dimethyl ether (**11**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.



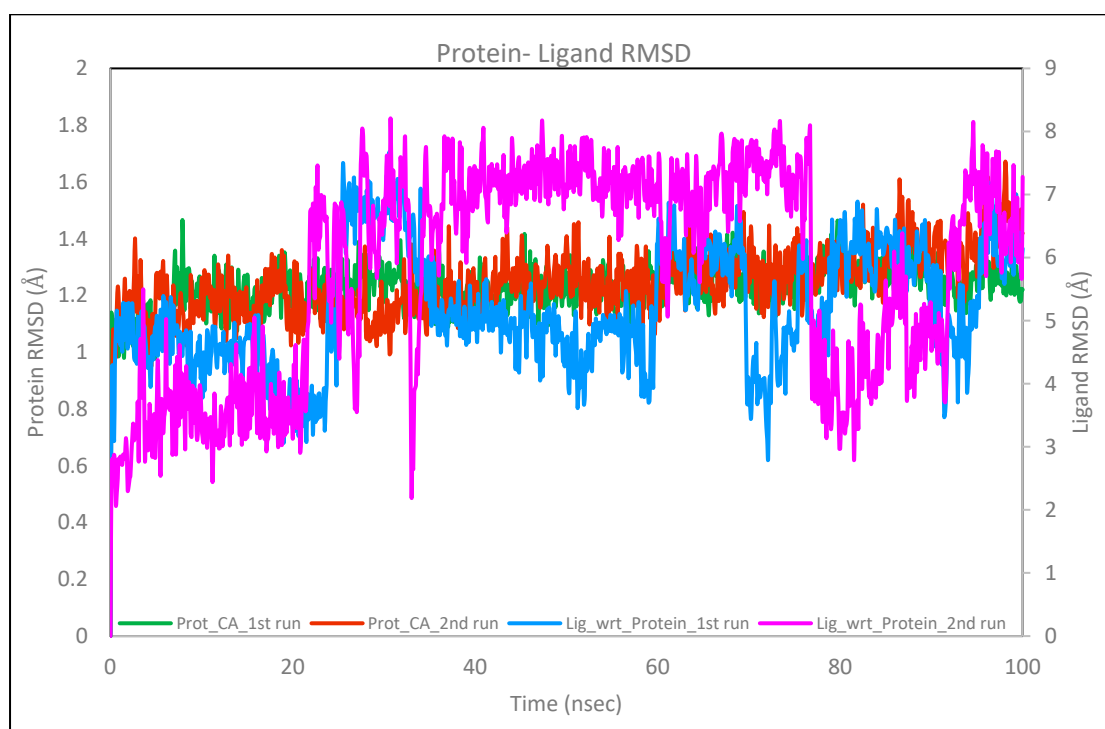
**Figure S10.** Proposed binding mode of quercetin-3-methyl ether (**10**) in the active site of the pancreatic alpha-amylase (PDB ID: 4GQR) in both 3D (**A**) and 2D (**B**) views.



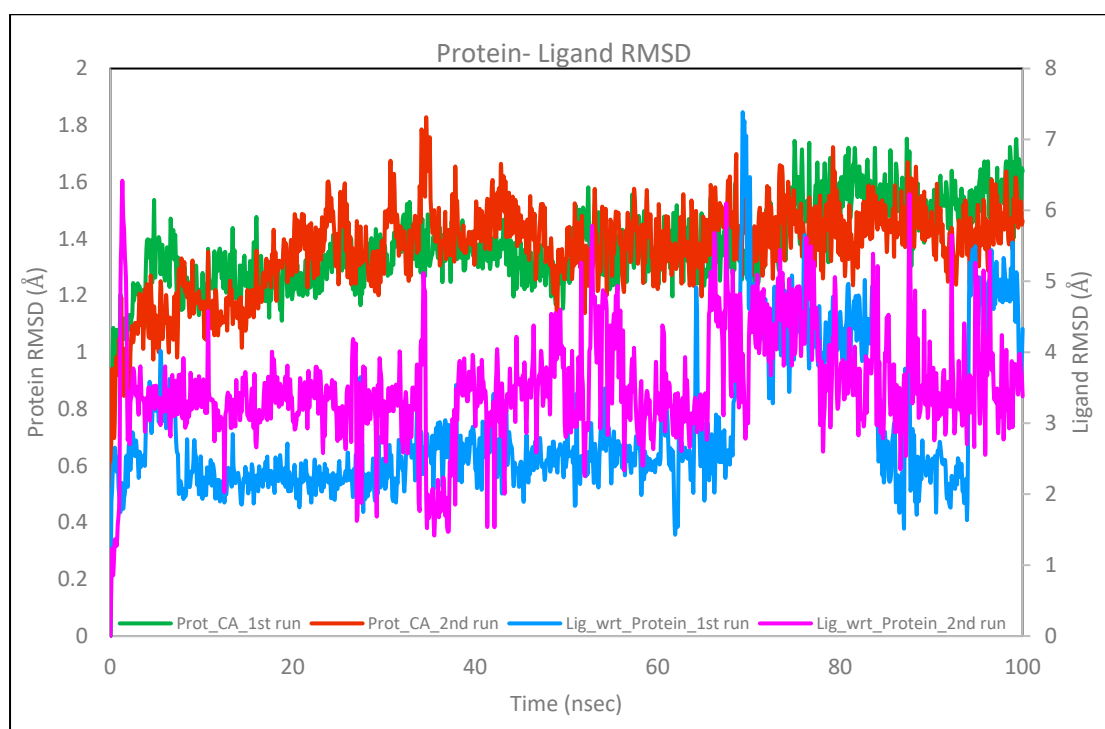
**Figure S11.** RMSD plot in duplicate for Quercetagenin-7-O-b-D-glucopyranoside (2) with pancreatic alpha-amylase (PDB-ID: 4GQR) during the MD simulation. Green and red represent the first and second run of protein, respectively. While blue and pink represent the first and second run of ligand



**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

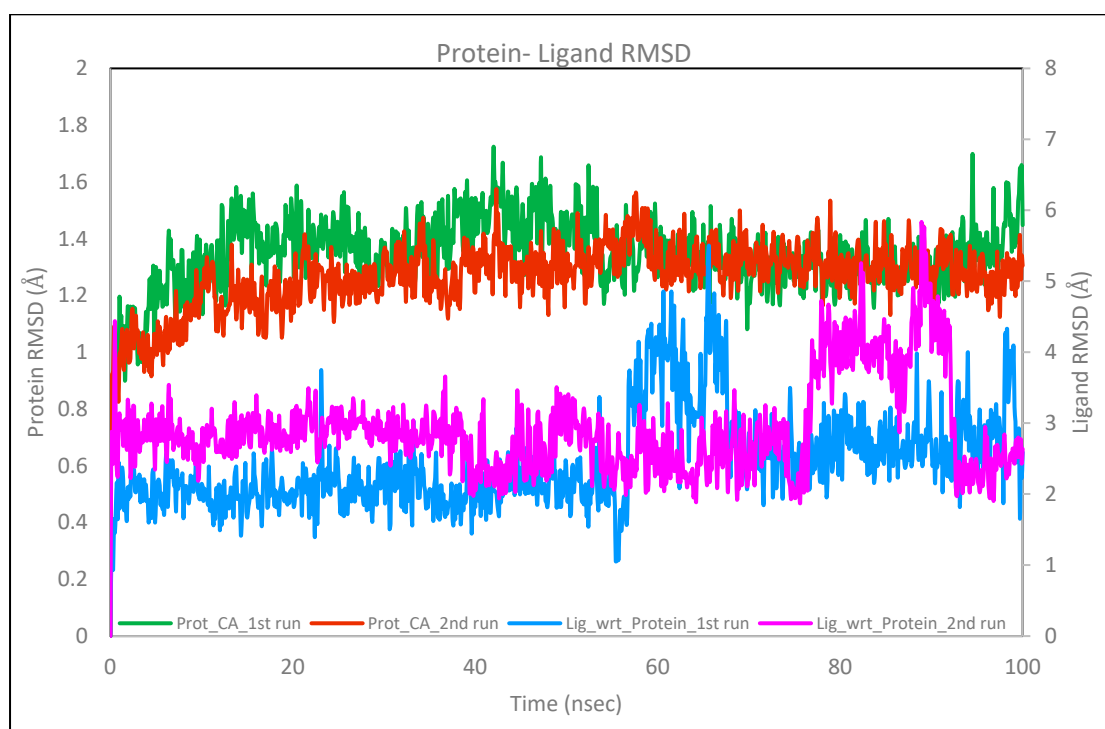


**Figure S13.** RMSD plot in duplicate for 4- MinuStructure574Minutaside A (4) with pancreatic alpha-amylase (PDB-ID: 4GQR) during the MD simulation Green and red represent the first and second run of protein, respectively. While blue and pink represent the first and second run of ligand

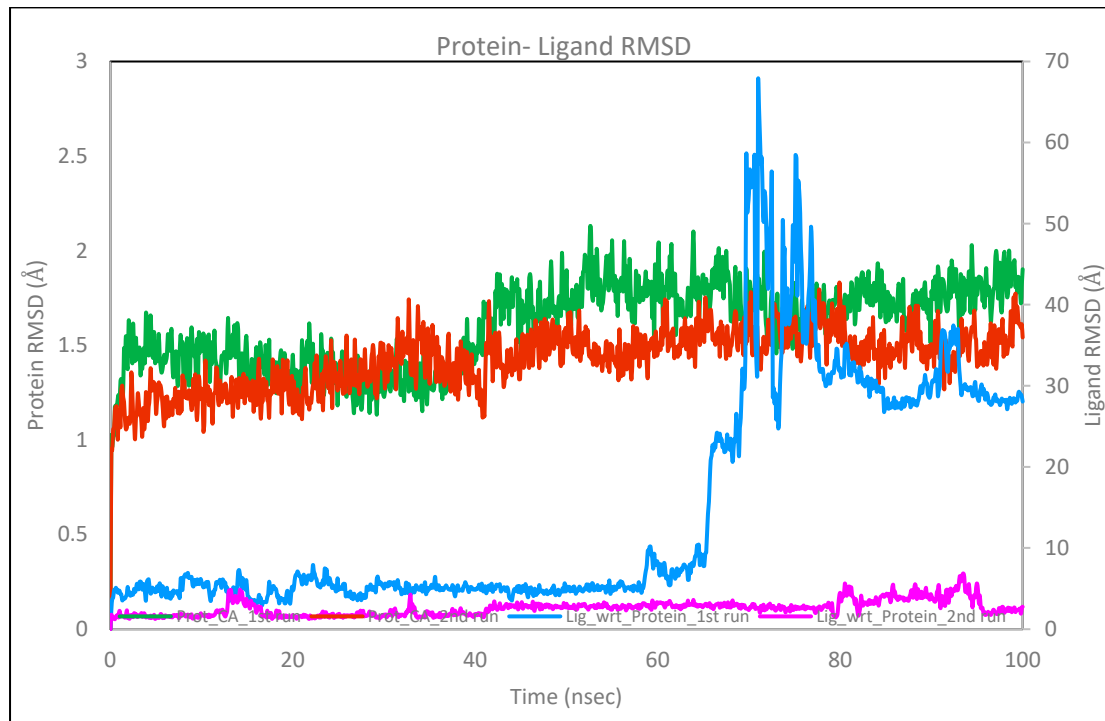


**Figure S14.** RMSD plot in duplicate for Patuletin-7-O-b-D-glucopyranoside (5) with pancreatic alpha-amylase (PDB-ID: 4GQR) during the MD simulation Green and red represent the first and second run of protein, respectively. While blue and pink represent the first and second run of ligand

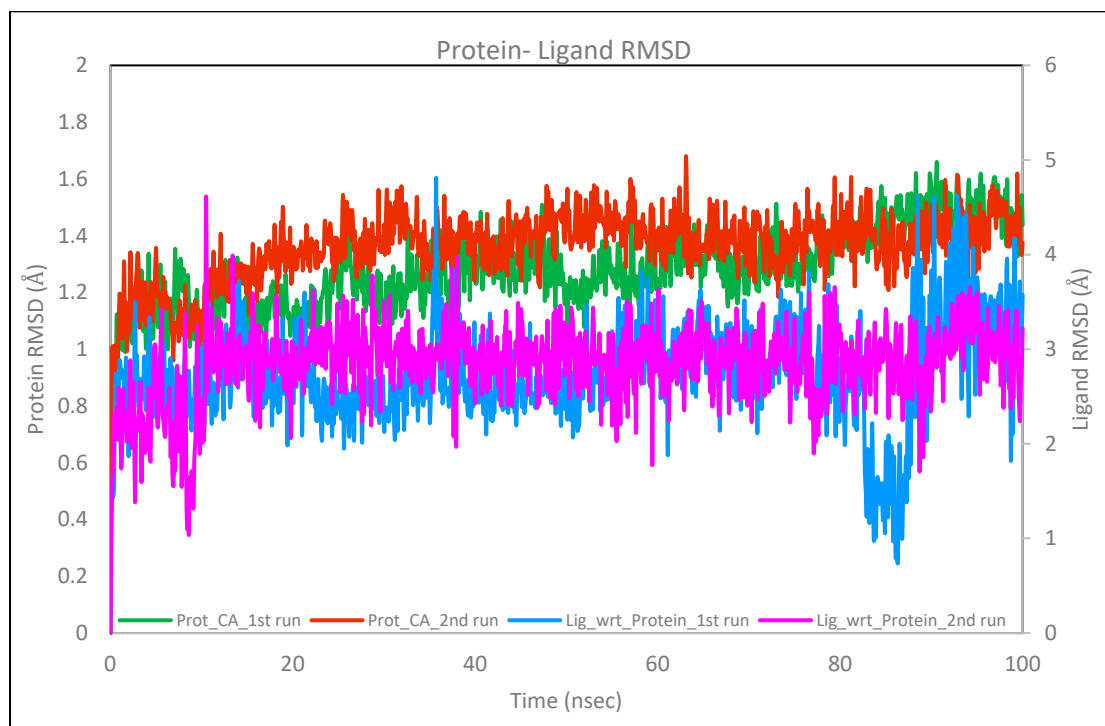




**Figure S15.** RMSD plot in duplicate for Quercetagenin-7-methoxy-6-O-b-D-glucopyranoside (6) with pancreatic alpha-amylase (PDB-ID: 4GQR) during the MD simulation. Green and red represent the first and second run of protein, respectively. While blue and pink represent the first and second run of ligand.



**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.