Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - MD trajectories

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Figure S91. Ligand 6'-Hydroxyangolensin trajectory inside FabZ's (3AZA) binding pocket. Red colour indicate initial frames and blue colour indicate last frames. The ligand's positions are shown in every 100 frames for the whole trajectory.

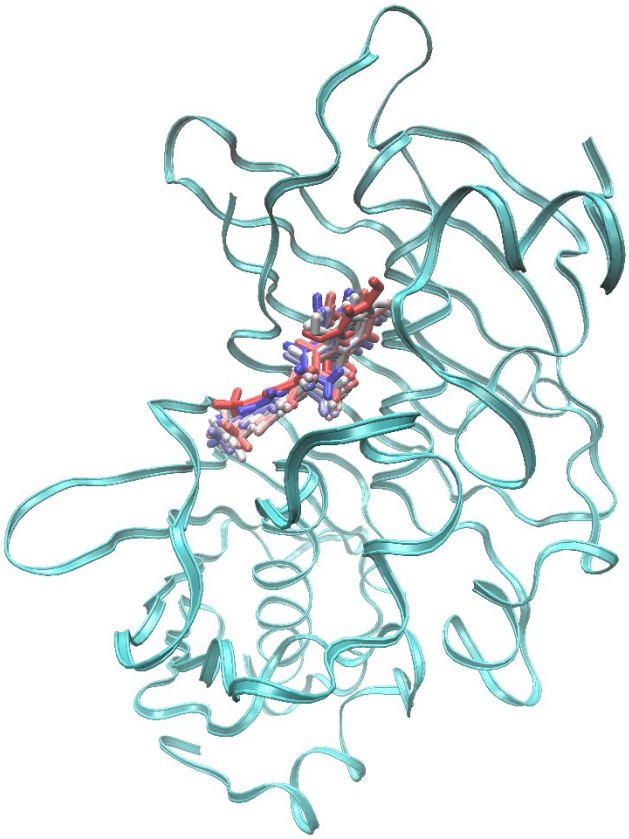

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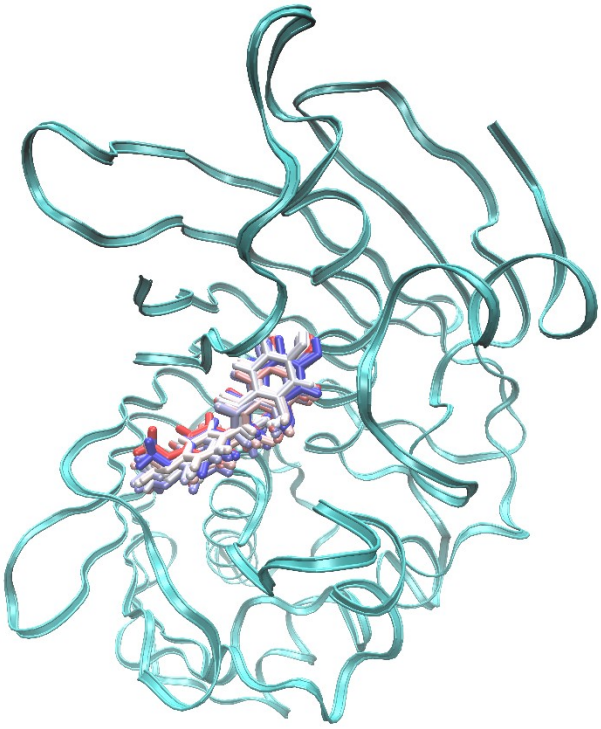
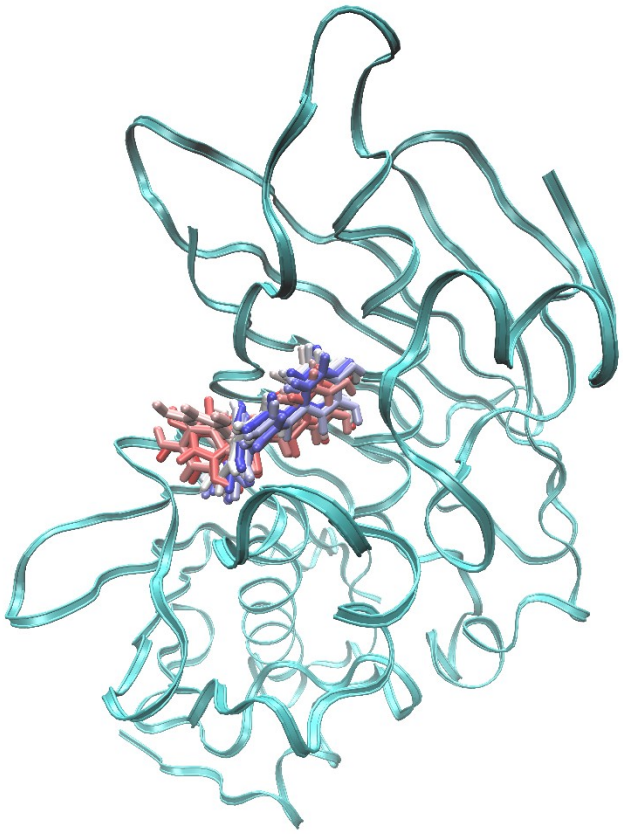
Figure S92. Ligand Angolensin trajectory inside FabZ's (3AZA) binding pocket. Red colour indicate initial frames and blue colour indicate last frames. The ligand's positions are shown in every 100 frames for the whole trajectory.



Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - MD trajectories

Figure S93. Ligand Butein trajectory inside FabZ's (3AZA) binding pocket. Red colour indicate initial frames and blue colour indicate last frames. The ligand's positions are shown in every 100 frames for the whole trajectory.



Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - MD trajectories

Figure S94. Ligand 6-Hydroxy-*O*-Desmethylangolensin trajectory inside FabZ's (3AZA) binding pocket. Red colour indicate initial frames and blue colour indicate last frames. The ligand's positions are shown in every 100 frames for the whole trajectory.

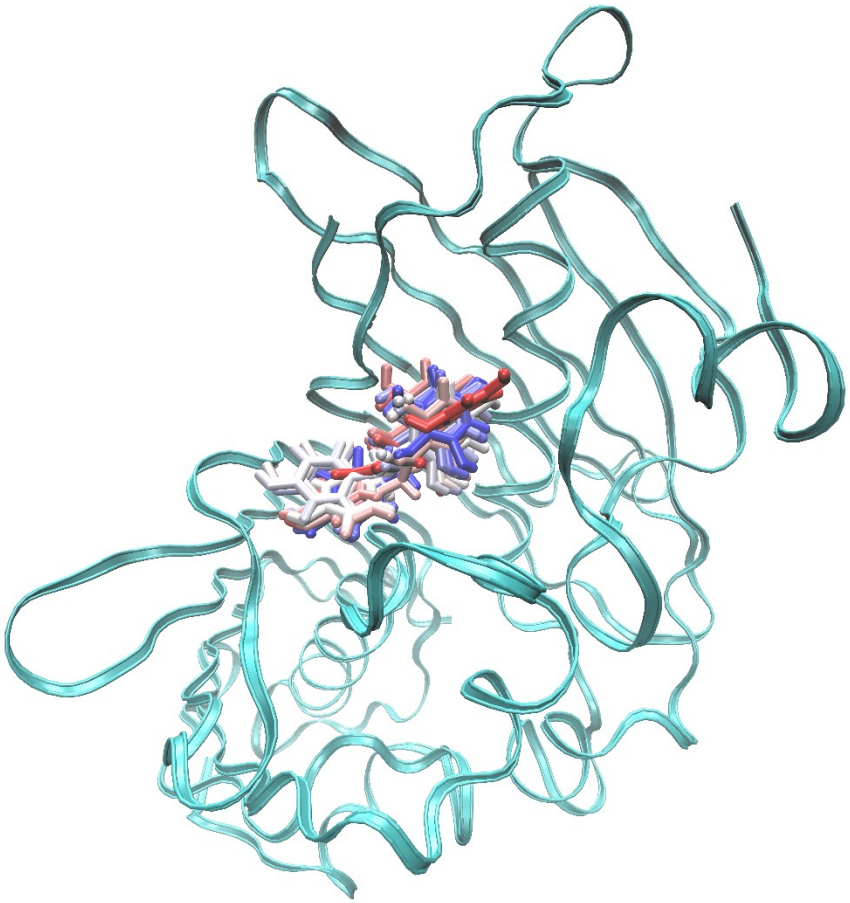


Figure S95. Ligand 4-*O*-Methylequol trajectory inside FabZ's (3AZA) binding pocket. Red colour indicate initial frames and blue colour indicate last frames. The ligand's positions are shown in every 100 frames for the whole trajectory.

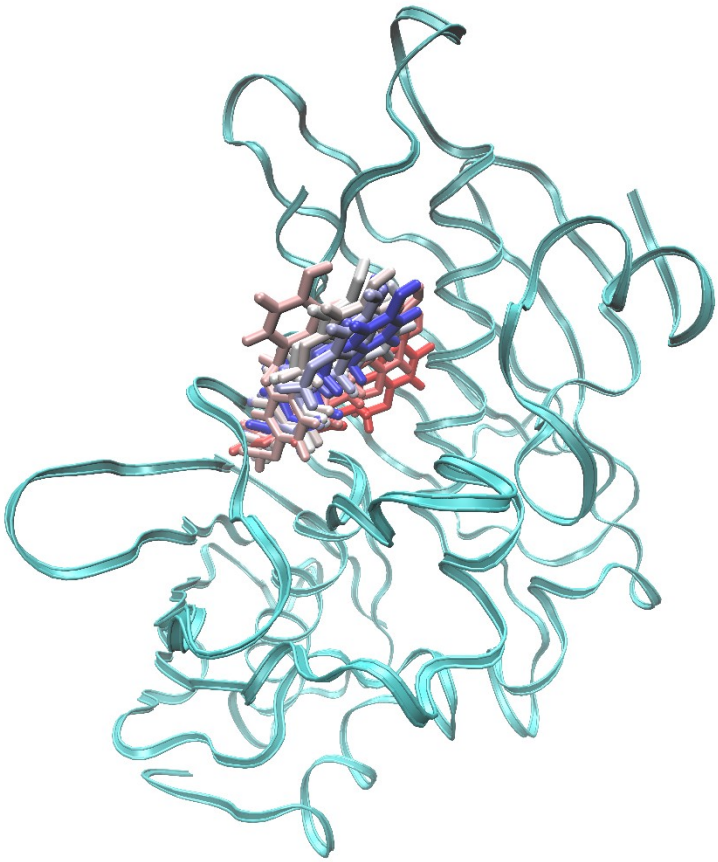


Figure S96. Ligand *O*-Desmethylangolensin trajectory inside FabI's (3LT4) binding pocket. Red colour indicate initial frames and blue colour indicate last frames. The ligand's positions are shown in every 100 frames for the whole trajectory.

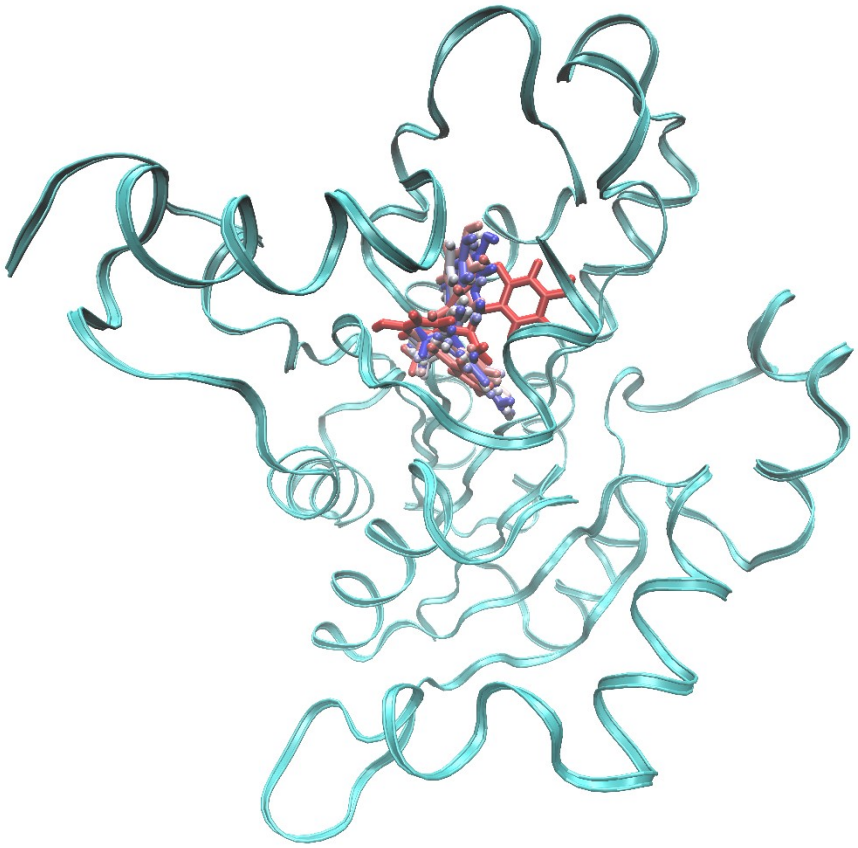


Figure S97. Ligand Dihydrodaidzein 7-*O*-Glucuronide trajectory inside FabI's (3LT4) binding pocket. Red colour indicate initial frames and blue colour indicate last frames. The ligand's positions are shown in every 100 frames for the whole trajectory.

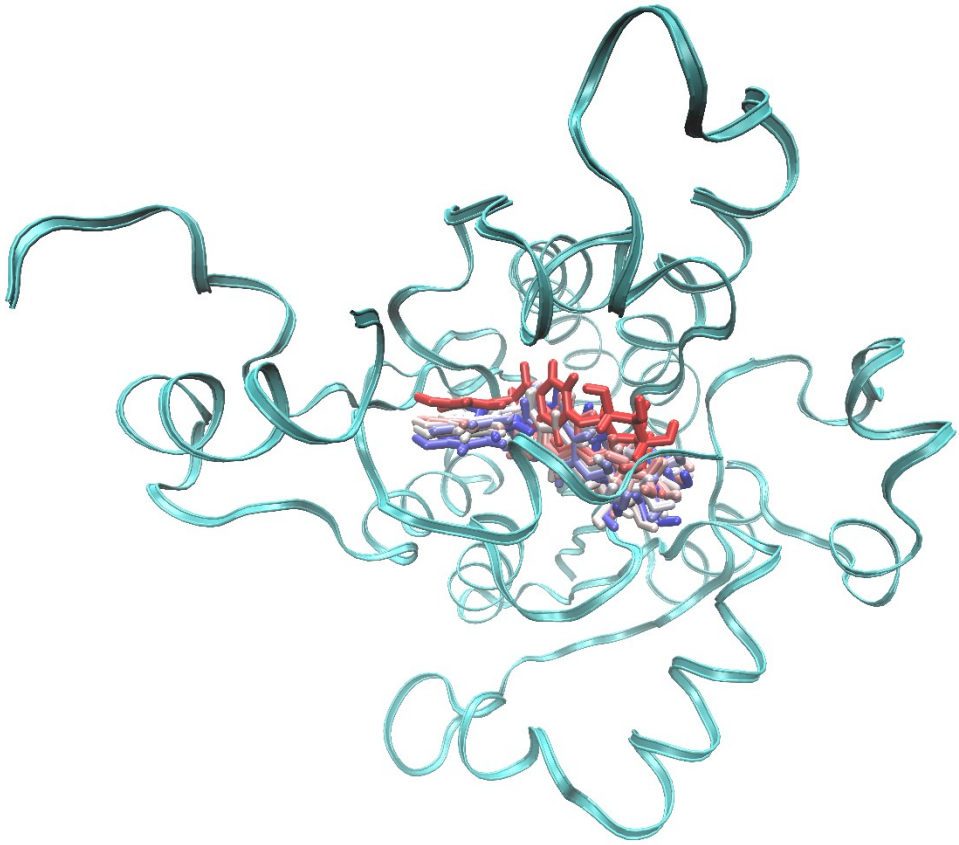


Figure S98. Ligand Cyanidin trajectory inside FabI's (3LT4) binding pocket. Red colour indicate initial frames and blue colour indicate last frames. The ligand's positions are shown in every 100 frames for the whole trajectory.

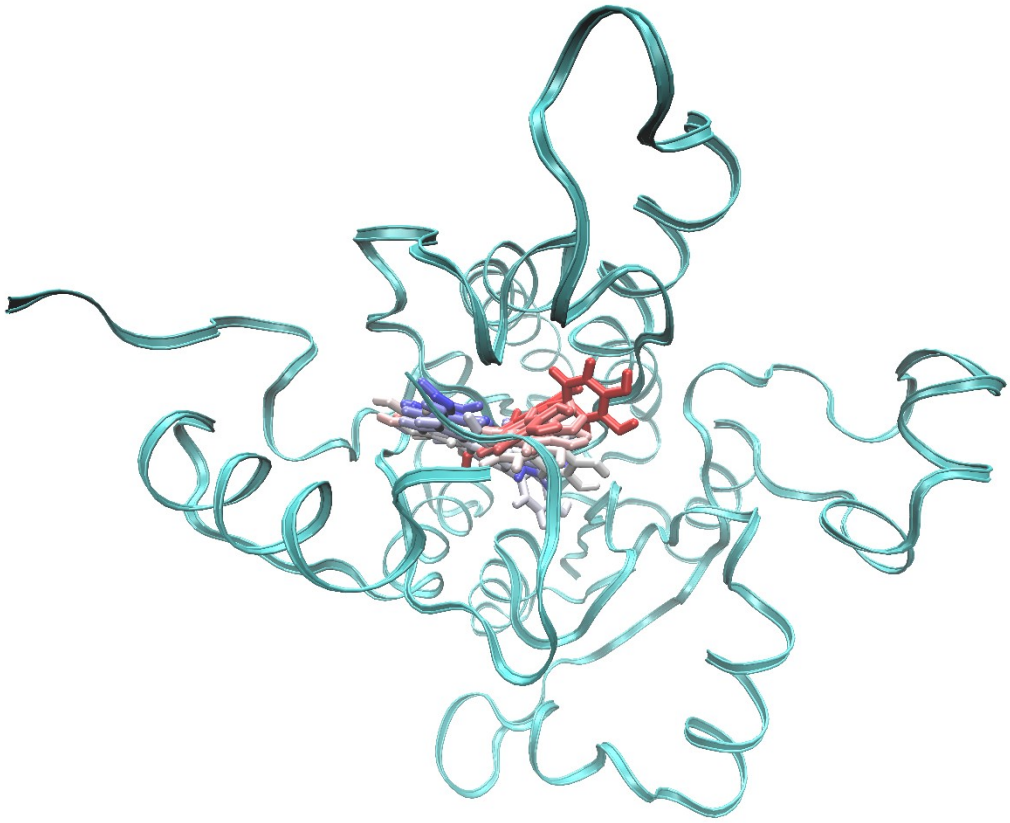


Figure S99. Ligand 3′, 4′, 5, 7-Tetrahydroxyisoflavanone trajectory inside FabI's (3LT4) binding pocket. Red colour indicate initial frames and blue colour indicate last frames. The ligand's positions are shown in every 100 frames for the whole trajectory.

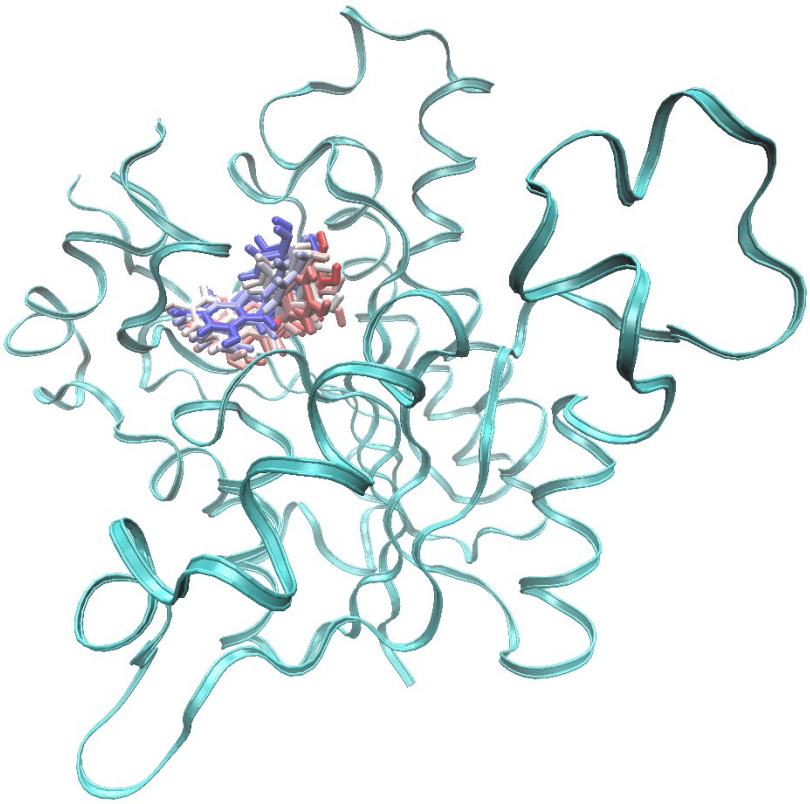


Figure S100. Ligand Equol 4′-*O*-Glucuronide trajectory inside FabI's (3LT4) binding pocket. Red colour indicate initial frames and blue colour indicate last frames. The ligand's positions are shown in every 100 frames for the whole trajectory.

