Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Interactions analyses

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Figure S101. Trajectory snapshots from the complexes formed between the proteins FabZ and FabI and their respective five best ligands. The frames shown were chosen based on the mode (i.e. most repetitive value) of the RMSD value for each frame. Yellow spheres represent hydrophobic interactions (H), green vectors represent hydrogen bond donors (HBD), red vectors represent hydrogen bond acceptors (HBA), and purple rings represent aromatic ring interactions (AR). **A)** Ligand 6'-Hydroxyangolensin bound to the active site of FabZ; **B)** Ligand Angolensin bound to the active site of FabZ; **C)** Ligand Butein bound to the active site of FabZ; **D)** Ligand 6-Hydroxy-*O*-Desmethylangolensin bound to the active site of FabZ; **E)** Ligand 4-*O*-Methylequol bound to the active site of FabZ; **F)** Ligand *O*-Desmethylangolensin bound to the active site of FabI; **G)** Dihydrodaizein 7-*O*-Glucuronide bound to the active site of FabI; **H)** Ligand Cyanidin bound to the active site of FabI; **I)** Ligand 3'-4'-5-7-Tetrahydroxyisoflavanone bound to the active site of FabI; **J)** Ligand Equol 4'-*O*-Glucuronide bound to the active site of FabI

