

Supplementary Material

Gallic Acid Alkyl Esters: Trypanocidal and Leishmanicidal Activity, and Target Identification via Modeling Studies

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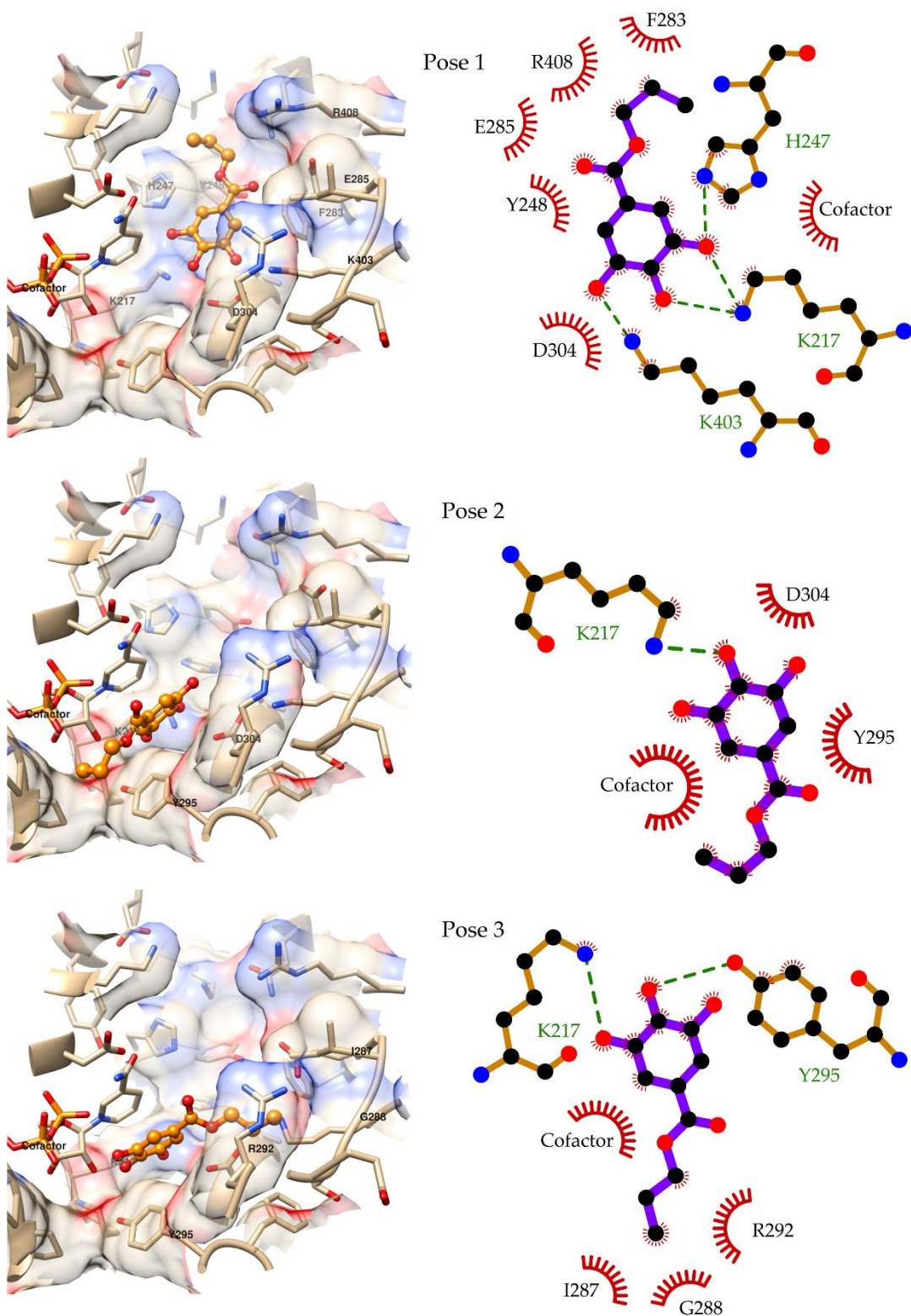
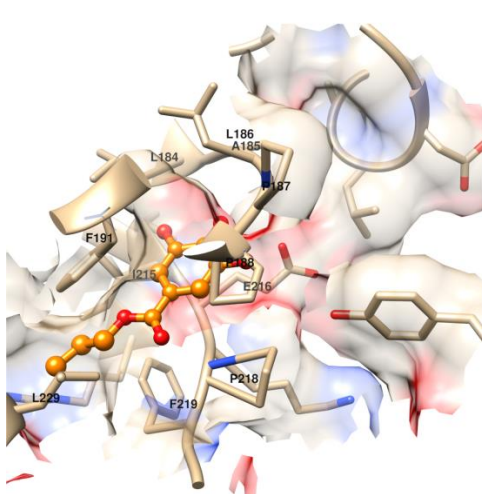
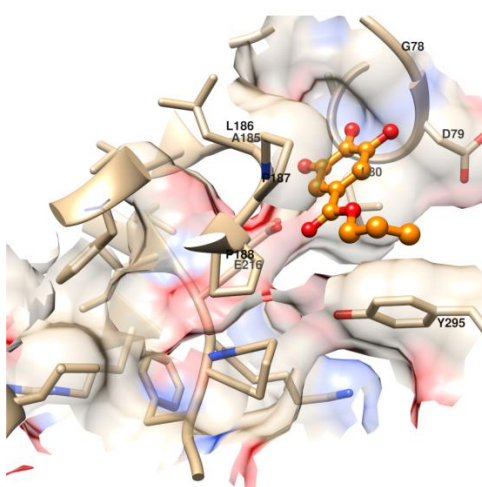
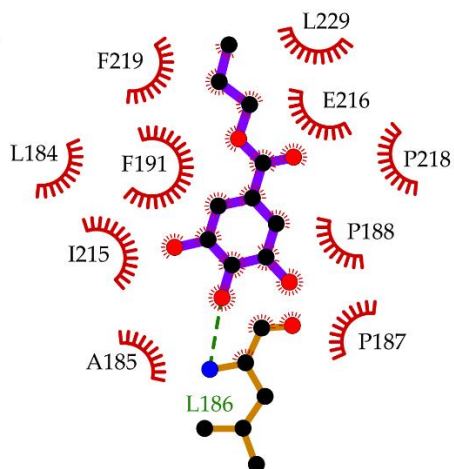


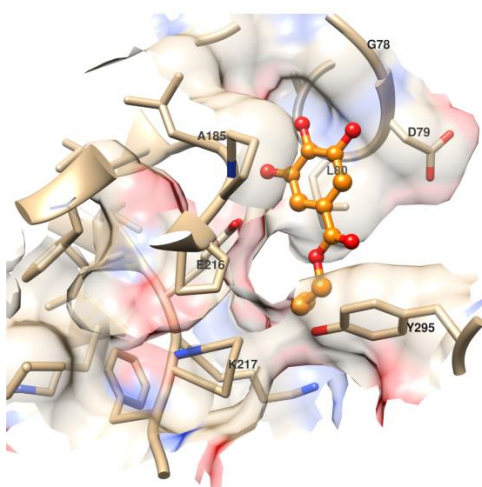
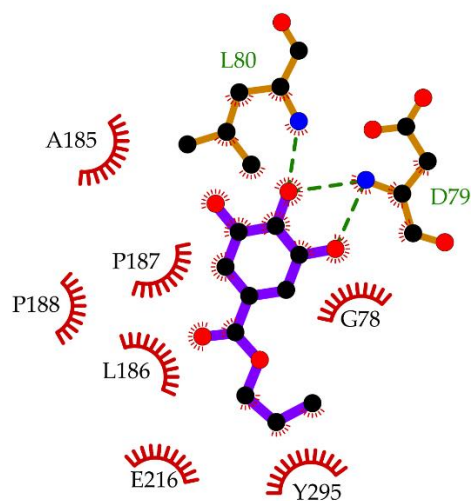
Figure S1. Predicted binding modes and networks of intermolecular interactions obtained from the molecular docking of compound **4** to the substrate binding site of G6PD. Compound **4** is colored orange and represented as balls and sticks.



Pose 1



Pose 2



Pose 3

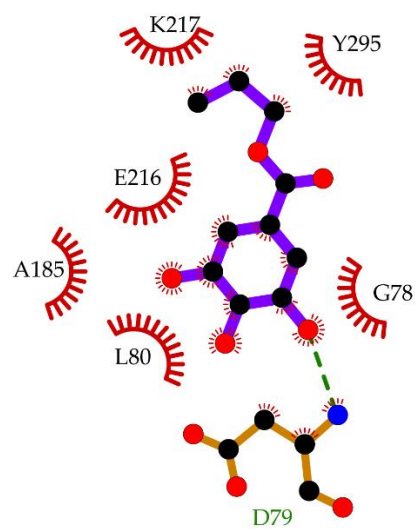


Figure S2. Predicted binding modes and networks of intermolecular interactions obtained from the molecular docking of compound **4** to the cofactor binding site of G6PD. Compound **4** is colored orange and represented as balls and sticks.

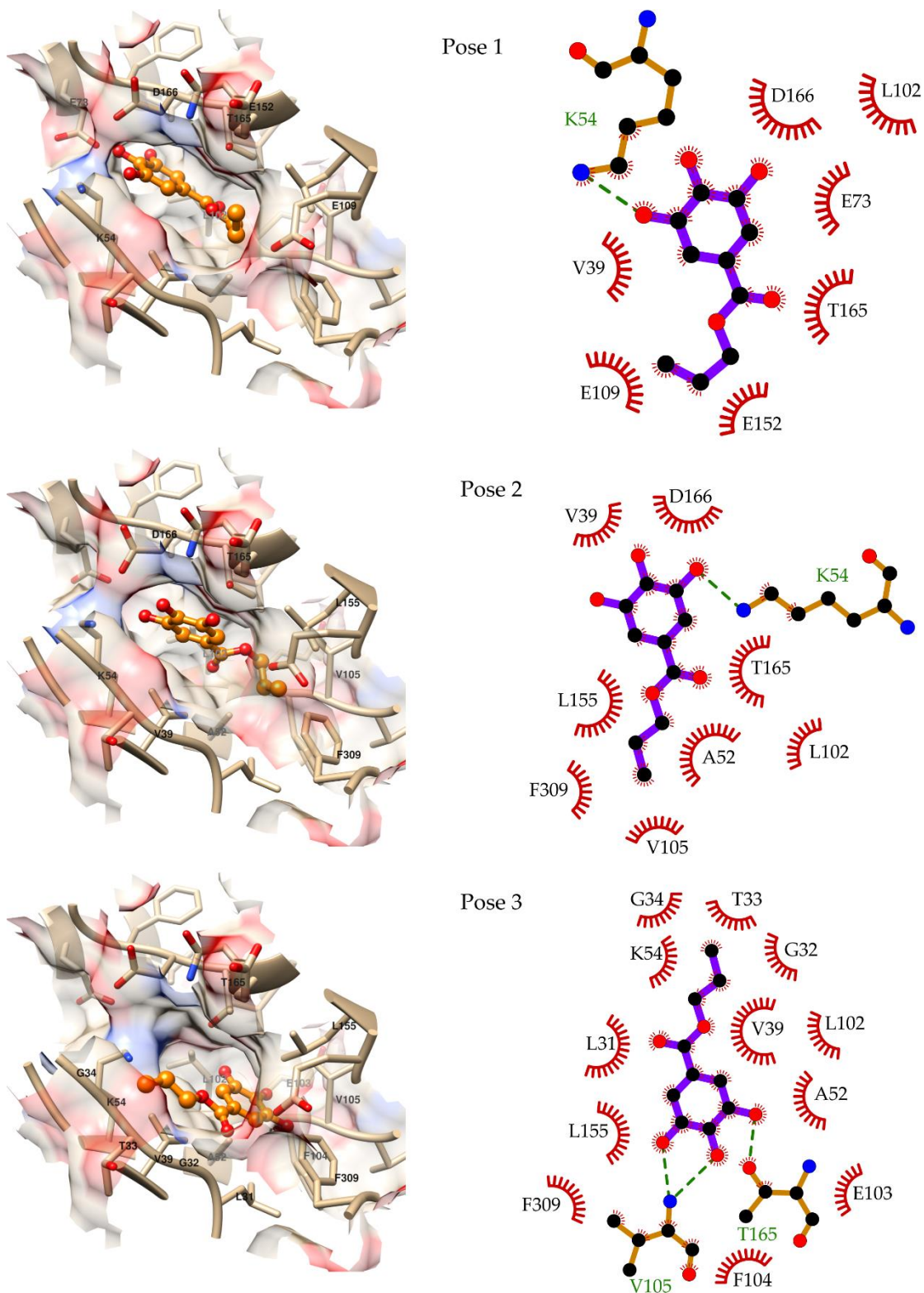
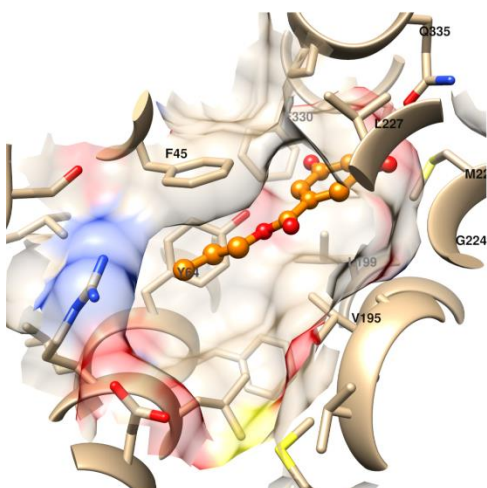
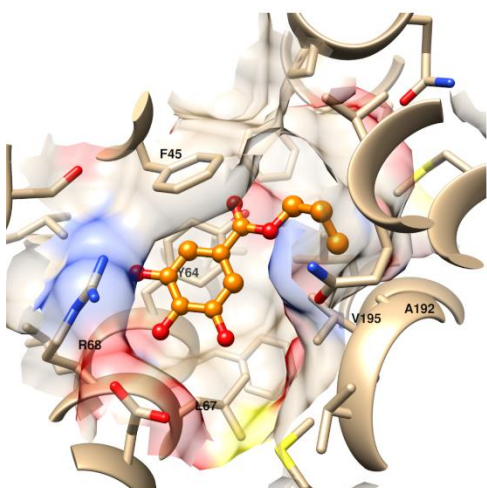
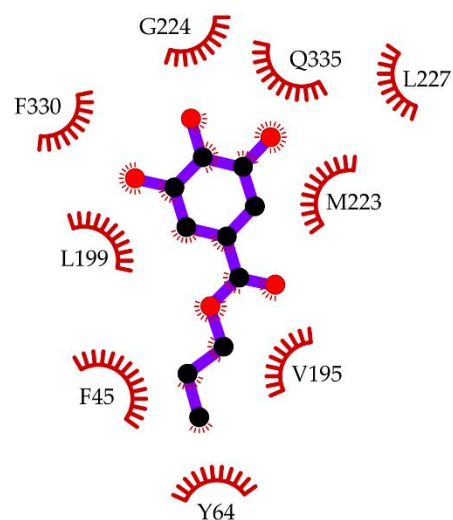


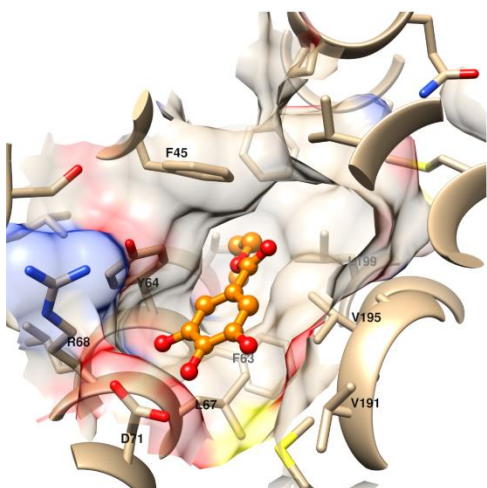
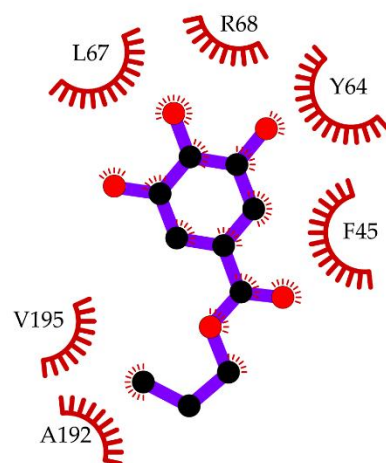
Figure S3. Predicted binding modes and networks of intermolecular interactions obtained from the molecular docking of compound **4** to PKA1. Compound **4** is colored orange and represented as balls and sticks.



Pose 1



Pose 2



Pose 3

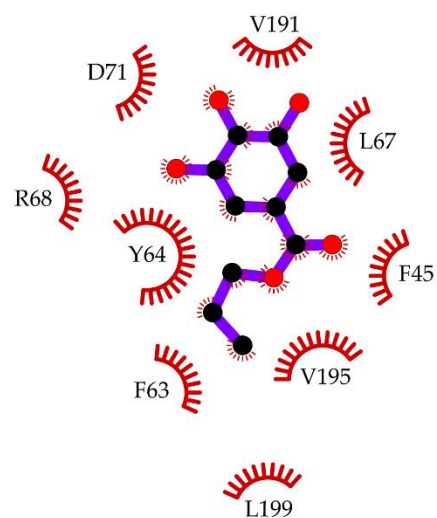
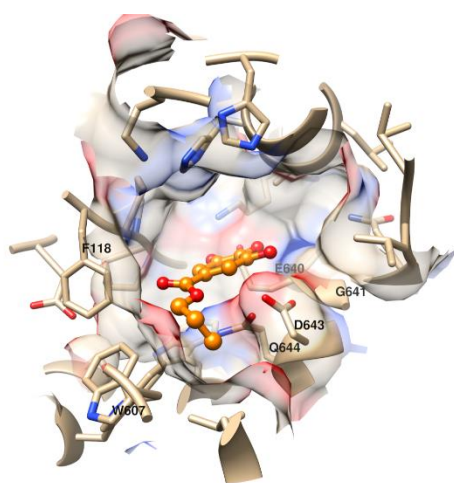
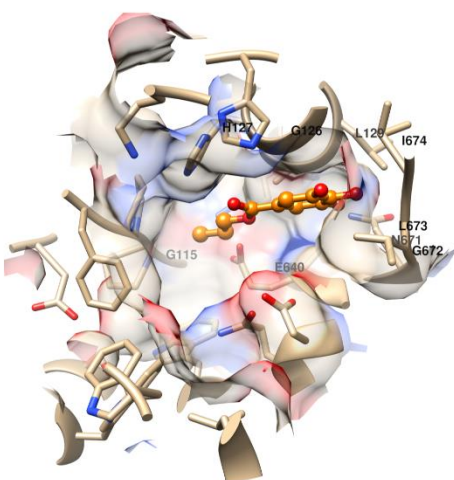
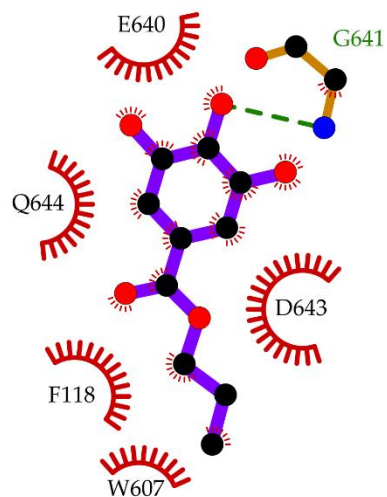


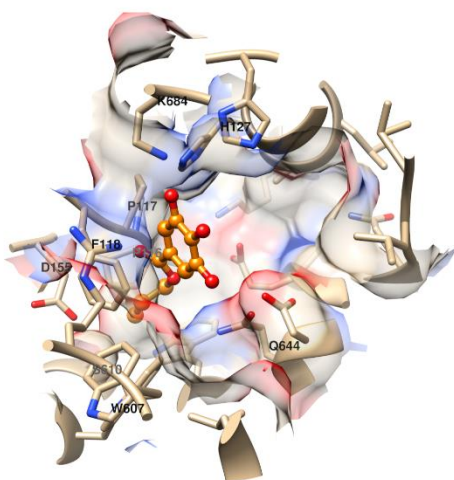
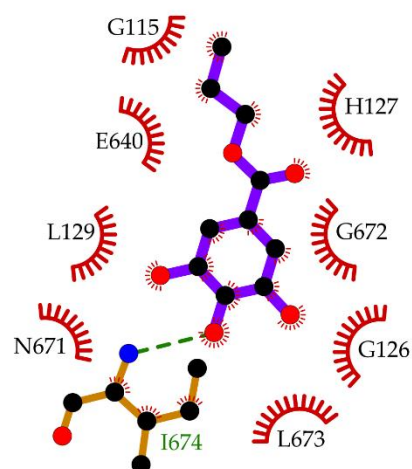
Figure S4. Predicted binding modes and networks of intermolecular interactions obtained from the molecular docking of compound **4** to FT. Compound **4** is colored orange and represented as balls and sticks.



Pose 1



Pose 2



Pose 3

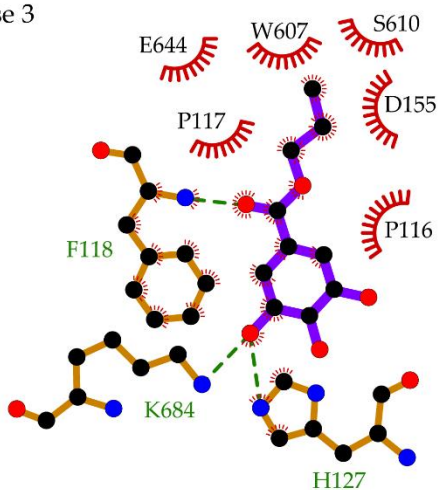


Figure S5. Predicted binding modes and networks of intermolecular interactions obtained from the molecular docking of compound 4 to IleRL. Compound 4 is colored orange and represented as balls and sticks.

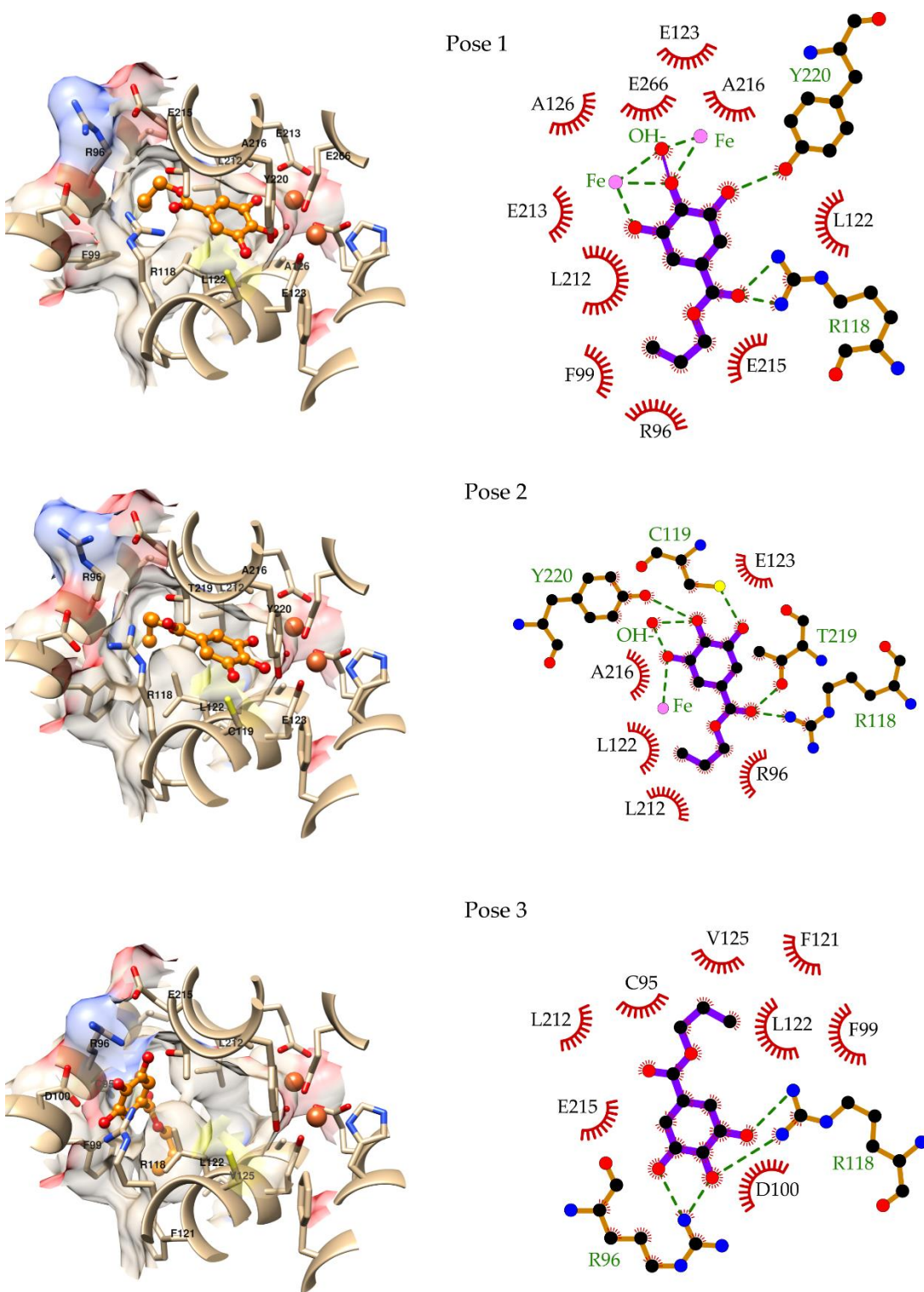
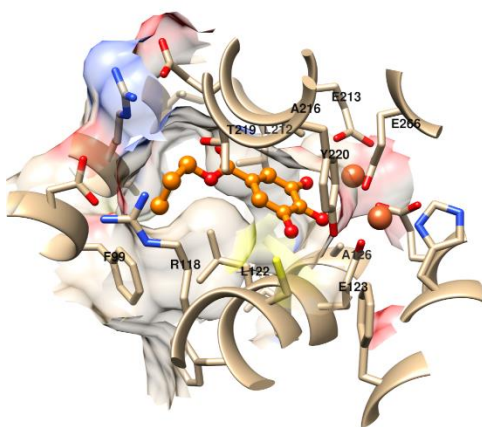
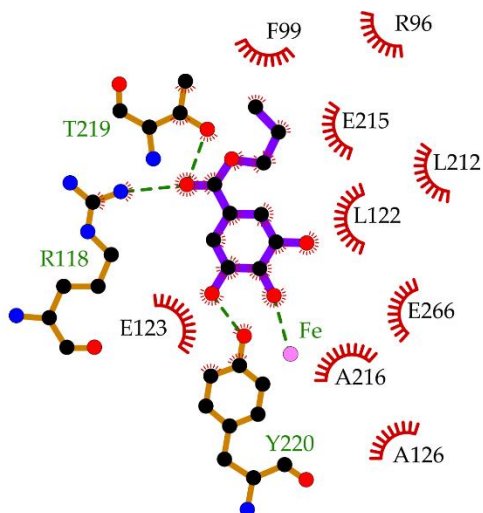
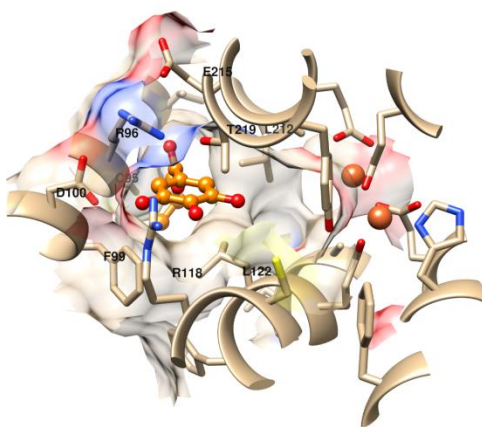
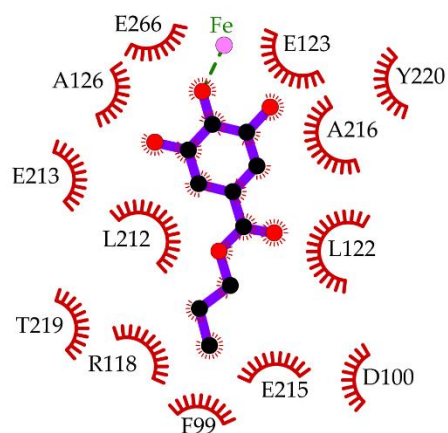


Figure S6. Predicted binding modes and networks of intermolecular interactions obtained from the molecular docking of compound 4-to TAO in presence of the hydroxide anion. Compound 4 is colored orange and represented as balls and sticks.

Pose 1



Pose 2



Pose 3

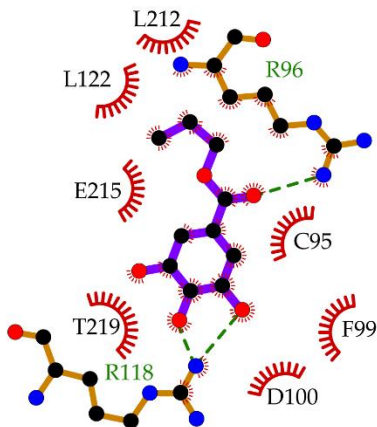


Figure S7. Predicted binding modes and networks of intermolecular interactions obtained from the molecular docking of compound **4** to TAO without the hydroxide anion. Compound **4** is colored orange and represented as balls and sticks.