

Supplementary Data

Figure S1: Example PAC traces for dissociation of CO from CO-FHP (black) and 4SP reference compound (grey) at 20 °C in 10 mM sodium phosphate and 10 mM potassium chloride buffer, pH 7.5.

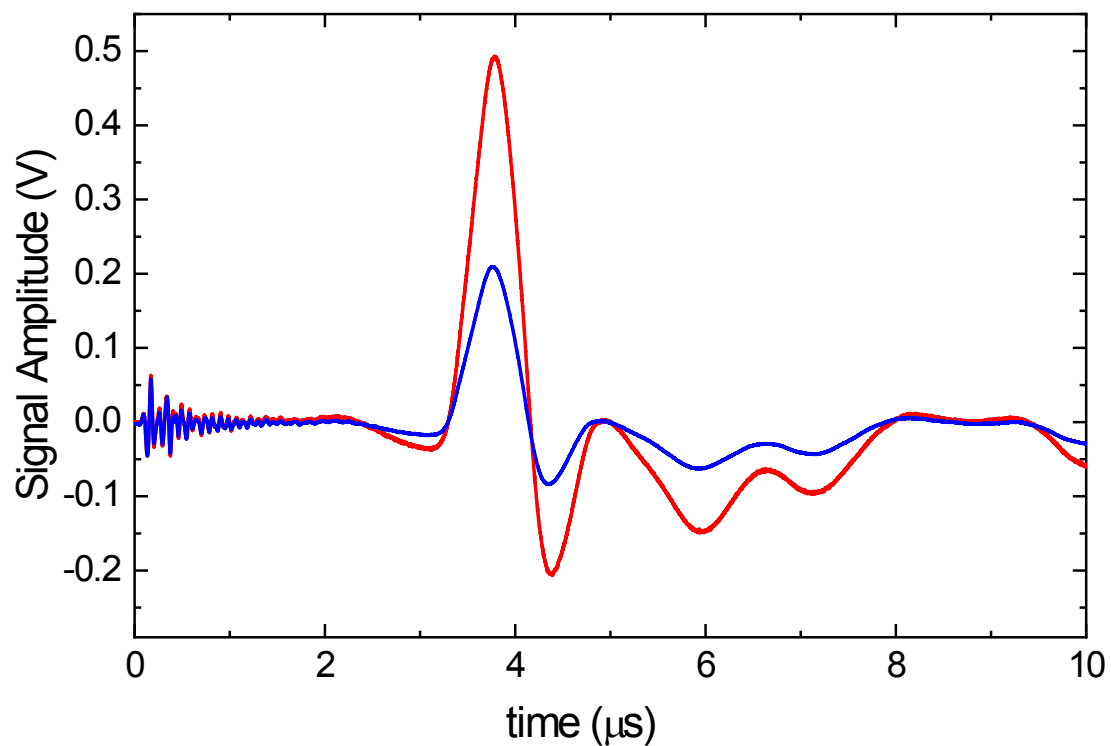


Figure S2: Example TA traces for bimolecular rebinding of CO to deoxy-FHP in the absence ofazole drugs at 20 °C.

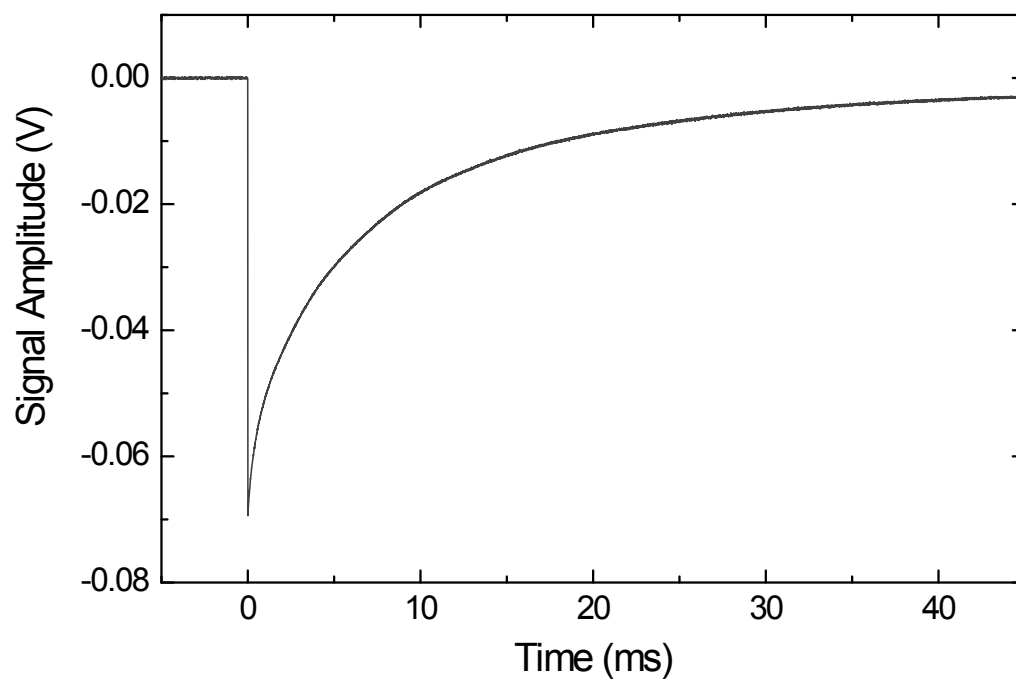


Figure S3: Binding location of ketoconazole to CO-FHP predicted by Autodock Vina. Heme, CO, Tyr29 and His85 are shown as licorice and the five ketoconazole conformations with highest binding affinity are shown as in green. FAD is shown in yellow. The globin domain is shown in cyan, the reductase domain is shown in blue, and heme is shown in orange.

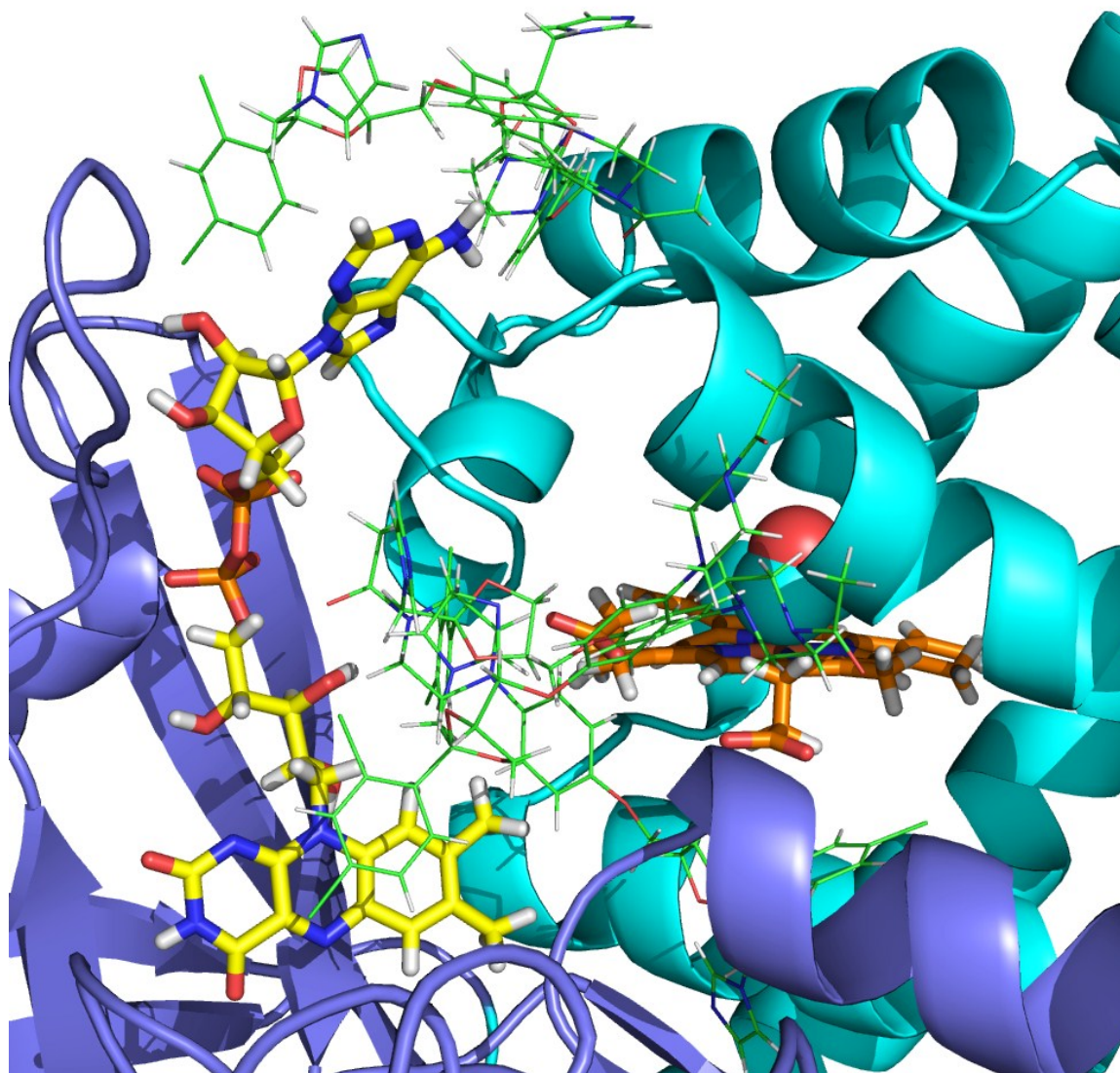


Figure S4: Binding locations of miconazole to CO-FHP as predicted by Autodock Vina. The CO molecule is shown in VdW representation. Heme B, Tyr29 and His85 are shown as licorice and the five miconazole binding locations with highest binding affinity are shown in magenta. The globin domain is shown in cyan, the reductase domain is shown in blue, and heme is shown in orange.

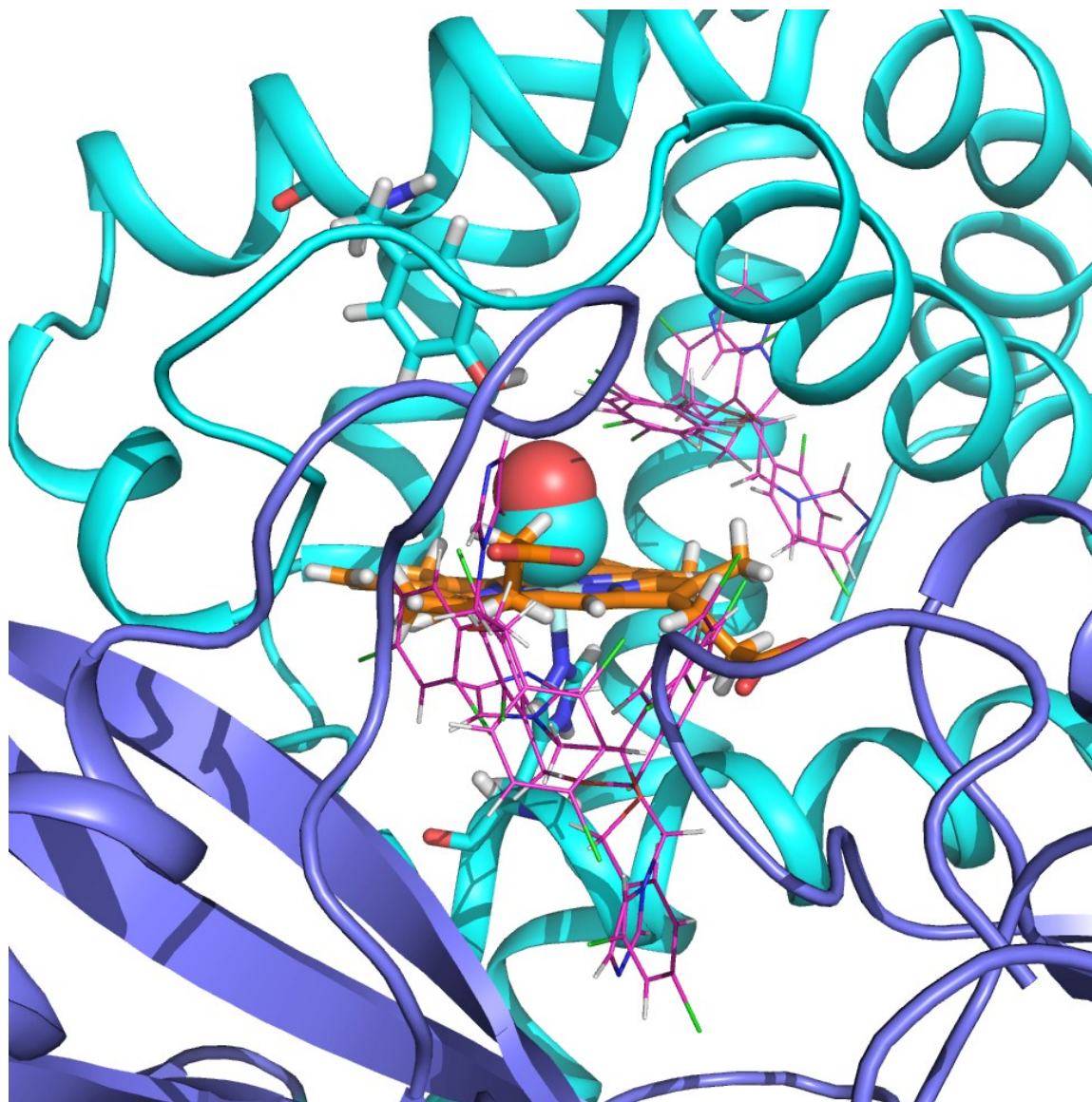


Figure S5: An alternate view of the heme binding pocket of CO-FHP with miconazole bound after 20 ns of MD simulation. Hydrophobic interactions are shown as gray lines.

