Pharmacological characterization, structural studies, and *in vivo* Activity of Anti-Chagas Disease Lead Compounds Derived from Tipifarnib

Supplementary Material

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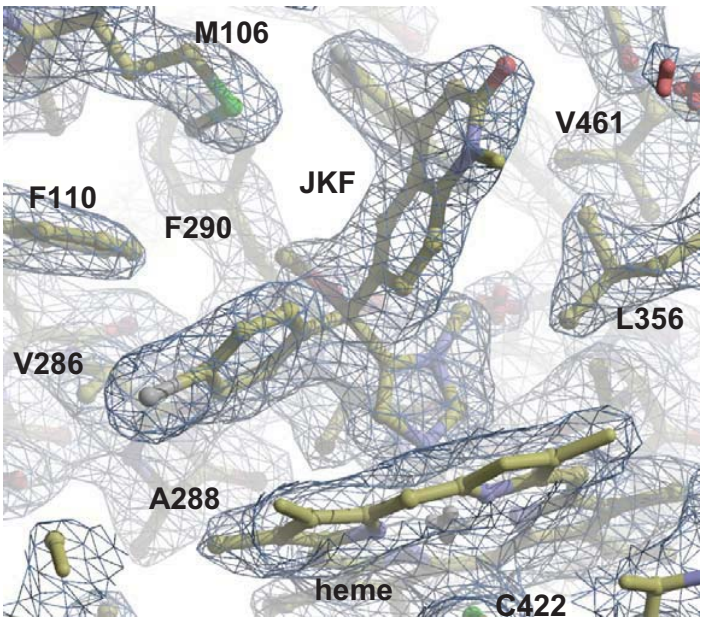
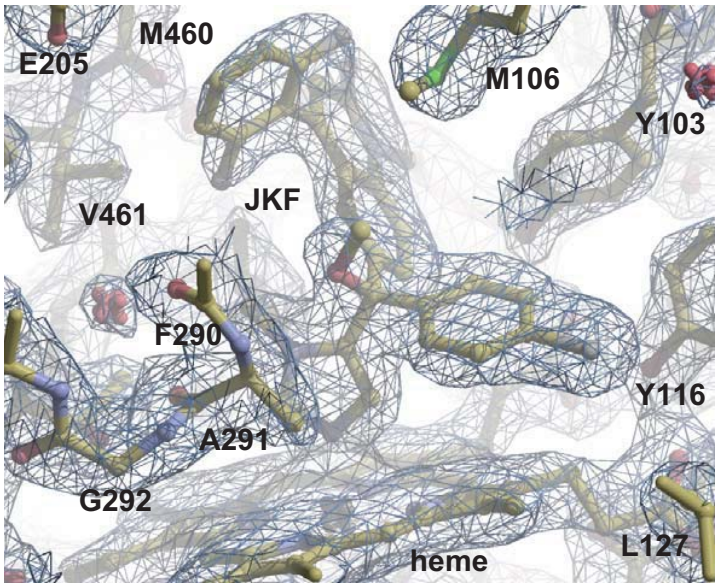
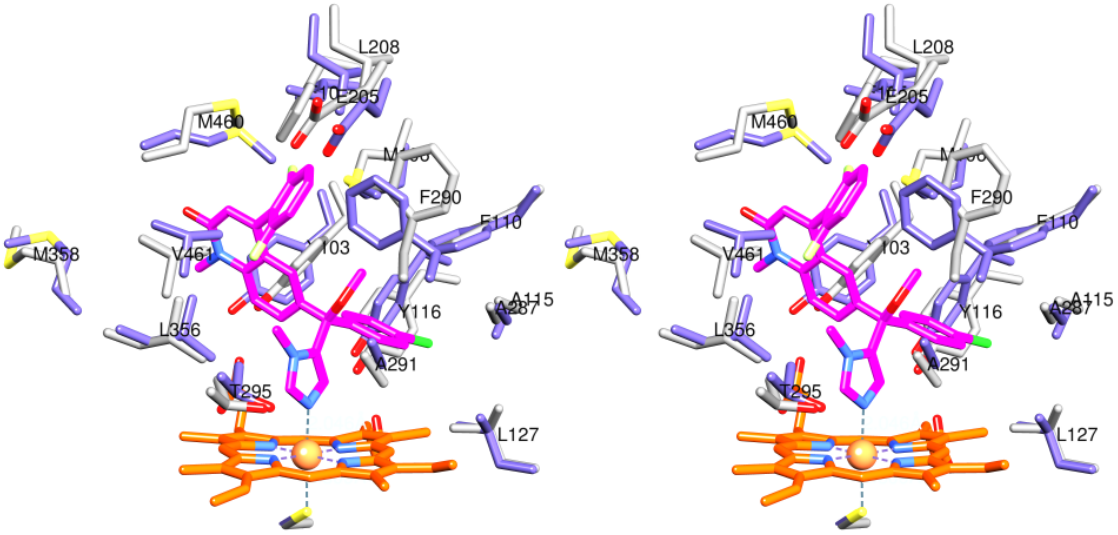
Supplemental Table 1. Data collection and refinement statistics

T. brucei CYP51-JKF complex (PDB code 3TIK)	
Data collection	
Wavelength, Å	0.979
Space group	P1
Cell dimensions	
a, b, c, Å	59.7, 79.7, 117.5
α, β, γ, °	74.5, 81.6, 68.1
Molecules per asymmetric unit	4
Solvent content, %	48
Resolution (last shell), Å	30.0 2.05(2.09-2.05)
R_{merge} (last shell)	0.049(0.595)
I/σ (last shell)	43.6 (2.8)
Completeness (last shell), %	99.7 (99.6)
Redundancy (last shell)	6.0 (5.9)
Refinement	
Resolution, Å	50.0-2.05
R-factor	0.186
R-free	0.243
Reflections used	115222
Test set size, %	5.0
Rms deviations from ideal geometry	
Bond lengths, Å	0.009
Bond angles, °	1.13
Ramachandran plot	
Residues in favorable regions	99.7%
Residues in allowed regions	100%
Outliers	0%
Model	
Total number of atoms	14916
Residues per chain (average B-factor, $Å^2$)	
protein	450 / 450 / 450 / 450 (49.7)
heme	1 / 1 / 1 / 1 (34.0)
JKF (inhibitor)	1 / 1 / 1 / 1 (45.3)
Water	295 (57.6)





Supplemental Figure 1. 2Fo-Fc electron density map for JKF in the active site of T. brucei CYP51 contoured at 1.5 σ. **a** and **b** represent opposite views obtained at ~180º rotation of JKF centered on its chiral C-atom around axis Y.



Supplemental Fig. 2. Stereoview of the CYP51 active site . Stick model representation. Orientation is approximately the same as in **Fig. 5**. Carbon atoms in the enzymes from *T. cruzi* and *T. brucei* are purple and grey, respectively.