

## Supplementary Material

# Molecular Modeling and Structural Stability of Wild-Type and Mutant CYP51 from *Leishmania Major*: In Vitro and In Silico Analysis of a Laboratory Strain

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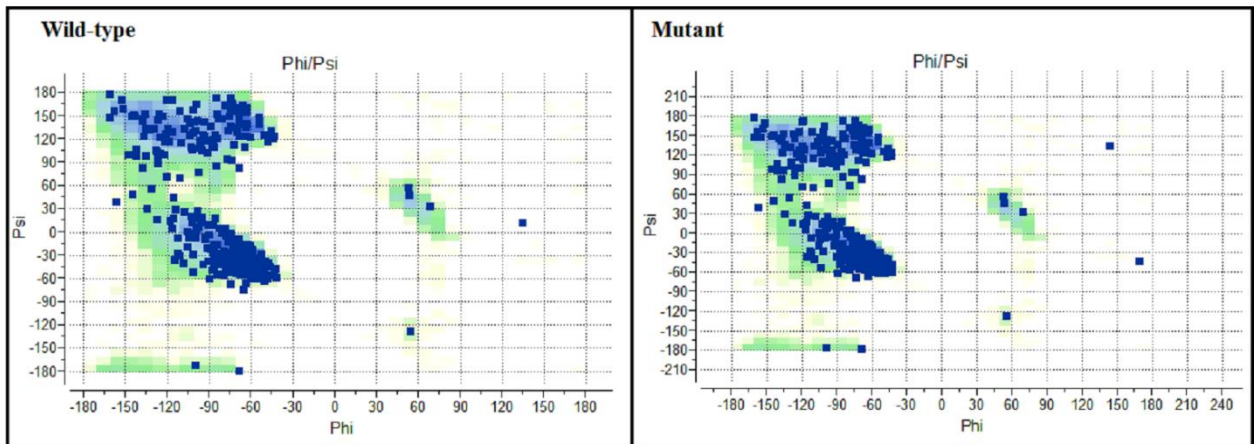
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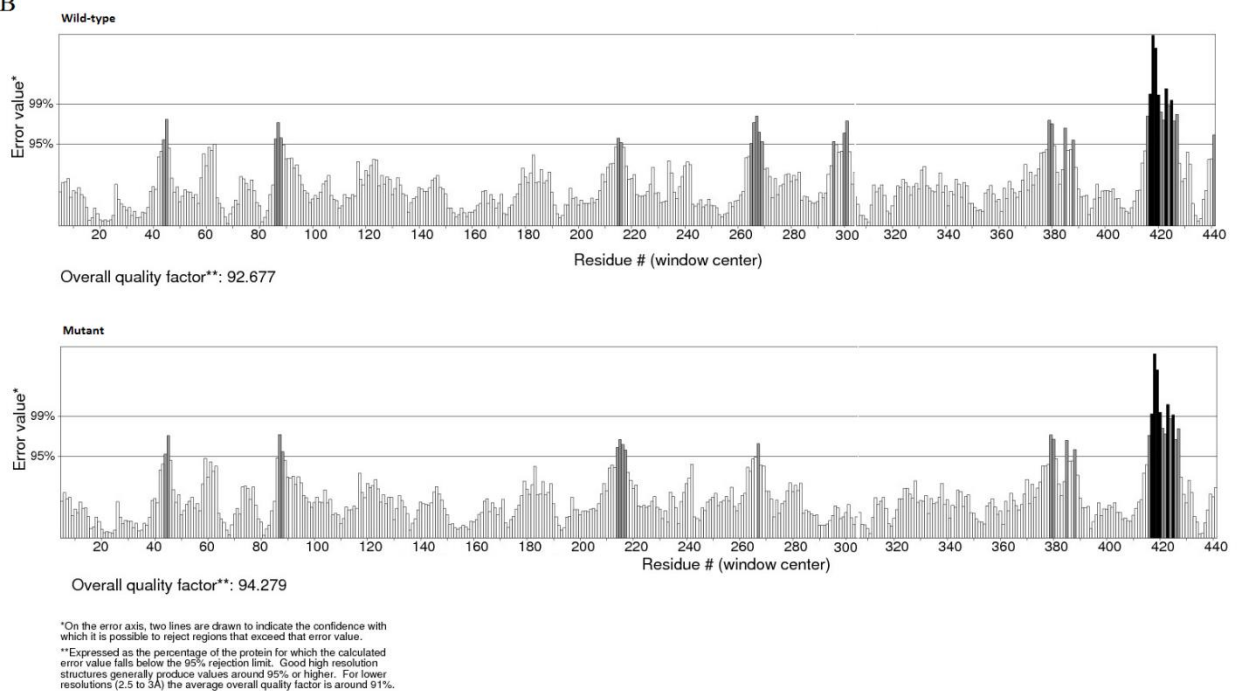
**Supplementary Table S1:** List of putative CYP51 sequences identified in different *Leishmania* species.

Species	Accession number	Genomic region	CDs size (bp)
<i>L. infantum</i>	NC_009395	453693 to 455135	1443
<i>L. donovani</i>	NC_018238	456337 to 457779	1443
<i>L. major</i> strain Friedlin	NC_007252	464294 to 465733	1440
<i>L. mexicana</i>	NC_018315	442773 to 444209	1440
<i>L. braziliensis</i>	NC_009303	413210 to 414649	1440
<i>L. panamensis</i>	NC_025856	467143 to 468582	1440
<i>L. enrietti</i>	ATAF01000270	152371 to 153807	1440
<i>L. tropica</i>	ATAT01001267	68292 to 69731	1440
<i>L. arabica</i>	ATBH01000314	17025 to 18464	1440
<i>L. gerbilli</i>	ATBK01000445	95610 to 97049	1440
<i>L. turanica</i>	ATBU01000855	1011 to 2450	1440
<i>L. amazonensis</i>	APNT01003038	2608 to 4047	1440
<i>L. aethiopica</i>	AUMB01000834	3589 to 5028	1440
<i>L. major</i> strain (MRHO/IR/75/ER)	KU843873	15 to 1454	1440
<i>L. major</i> (wild-type Tork-245)	KU843874	15 to 1454	1440

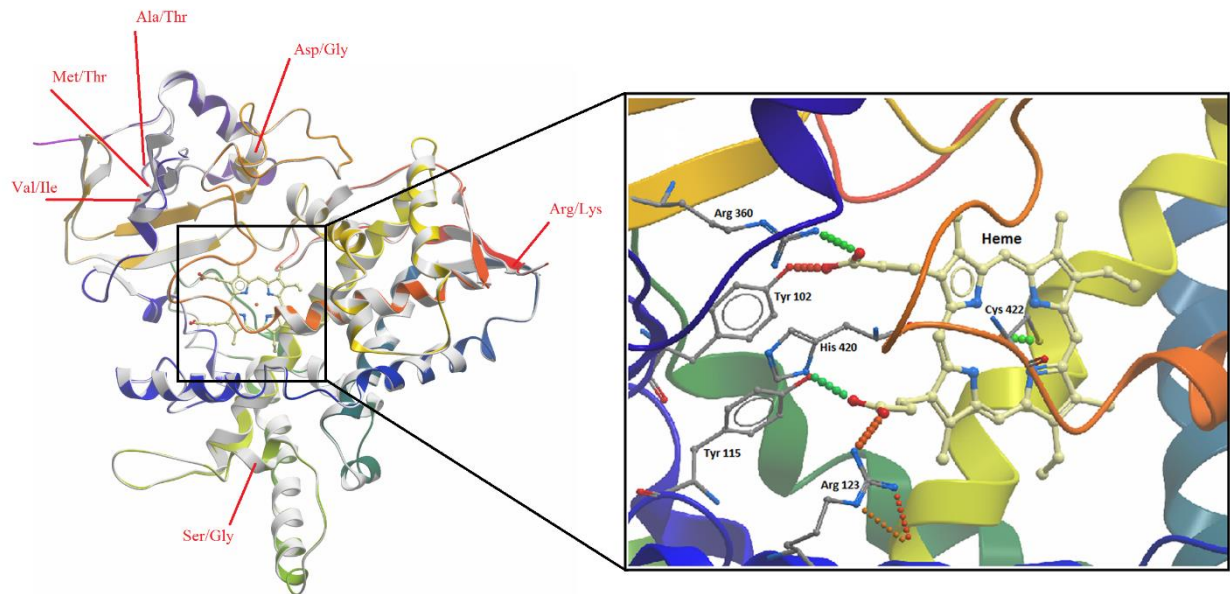
A



B



**Supplementary Figure S1:** Ramachandran plots for conformational model of CYP51 in wild-type and laboratory strain of *L. major*. The dark green regions contain the most favorable combinations of phi and psi while the light green regions indicate the allowed regions. The amino acids are shown with blue squares. B) ERRAT analysis (32) of wild-type and mutant structure showed that the overall quality factor for wild-type and mutant models were 92.677% and 94.279%, respectively.



**Supplementary Figure S2:** Structural model of superimposed CYP51 from *L. infantum* (PDB code: 3L4D), wild-type and strain MRHO/IR/75/ER of *L. major*. (A) The three structures were superimposed. The position of non-synonymous mutations have been mapped on the structure with red lines. Different colors were used for better visualization of the secondary structures in the model (B) The porphyrin ring of heme structure was coordinated by hydrogen bonds with Tyr102, Tyr115, Arg123, Arg360 and His420 and the iron atom in the heme is linked to Cys422. The green and brown spheres indicates hydrogen bonds. The figure was generated by ICM-pro software.