

Supporting Information for

Identification of proximal and distal axial ligands in *Leishmania major*
pseudoperoxidase.

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Supporting Information Table S1. Oligonucleotides list for mutations. Mutagenic codons designate as an underlined letter.

Mutation	Primer name	Oligonucleotides
C71A	Sense	5'-GACGTGGTAGCATCGGCGG <u>CCA</u> AAGCAGTTCGAG-3'
	Antisense	5'-CTCGAACTGCTTGGCCGCCGATGCTACCACGTC-3'
E105L	Sense	5'-GCCGAGACGGTTGAC <u>CTG</u> TCGTGTGCAGTG-3'
	Antisense	5'-CACTGCACACGACAGGTCAACCGTCTCGGC-3'
C107A	Sense	5'-GTTGACGAGTCGG <u>CCG</u> CAGTGGTGCGGGG-3'
	Antisense	5'-CCCCCGCACCCTGCGGCCGACTCGTCAAC-3'
M120A	Sense	5'-CGTGGCGGGCATC <u>GCG</u> AACTATCTCTCCAGC-3'
	Antisense	5'-GCTGGAGAGATAGTTCGCGATGCCCGCCACG-3'
C199A	Sense	5'-CTAACCGAGGCAGAG <u>GCC</u> GTGGCGCTGCTC-3'
	Antisense	5'-GAGCAGCGCCACGGCCTCTGCCTCGGTTAG-3'
C205A	Sense	5'-GGCGCTGCTCGCC <u>GCG</u> CACAGCGTCGGCG-3'
	Antisense	5'-CGCCGACGCTGTGCGGGCGAGCAGCGCC-3'
H206A	Sense	5'-CGCTGCTCGCCTG <u>GCG</u> AGCGTCGGCGAGTTCC-3'
	Antisense	5'-GGAACTCGCCGACGCTCGCGCAGGCGAGCAGCG-3'
C268A	Sense	5'-CCGCAAACGTTGCGGG <u>CCG</u> TCTACGTGAAGGAG-3'
	Antisense	5'-CTCCTTCACGTAGACGGCCCGCAACGTTTGCGG-3'
C284A	Sense	5'-GCGAAGAAGCGGCAG <u>GCC</u> GTCGTGAACGCG-3'
	Antisense	5'-CGCGTTCACGACGGCCTGCCGCTTCTTCGC-3'
M324A	Sense	5'-TCGGCCTTCACAAAG <u>GCG</u> ATCGAGAGCAAC-3'
	Antisense	5'-GTTGCTCTCGATCGCCTTTGTGAAGGCCGA-3'

C205A/H206A	Sense	5'-GGCGCTGCTCGCC <u>GCGGCC</u> GAGCGTCGGCG-3'
	Antisense	5'-CGCCGACGCTCGCCGCGGCCGAGCAGCGCC-3'

Supporting Information Table S2. Comparison of Soret and visible absorption maxima (nm) for CO bound ferrous wild type LmPP, mutants LmPP and other heme proteins in presence of 50 mM Tris-HCl buffer pH 8.8. nr indicates not reported. The value of (milli)molar absorptivity ($\text{mM}^{-1} \text{cm}^{-1}$) is presented within Parentheses.

CO bound enzyme	Soret	β	α	Ref.
Wild LmPP	420 (97)	540 (10)	568 (8.6)	This work
C71A LmPP	420 (101)	540 (9.9)	568 (8.7)	This work
M120A LmPP	420 (110)	540 (10.2)	568 (8.8)	This work
C199A LmPP	420 (105)	540 (10.4)	568 (8.6)	This work
C205A LmPP	420 (116)	540 (7.8)	568 (7.0)	This work
C268A LmPP	420 (103)	540 (9.2)	568 (7.7)	This work
C284A LmPP	420 (104)	540 (9.7)	568 (7.8)	This work
M324A LmPP	420 (107)	540 (8.7)	568 (7.7)	This work
E105L LmPP	420 (80)	540 (5.0)	567 (3.9)	This work
<i>RrCooA</i>	422 (nr)	540 (nr)	569 (nr)	1
<i>BxRcoM-2</i>	423 (nr)	540 (nr)	570 (nr)	2
hCBS	422 (nr)	nr	nr	3
H206A LmPP	420 (170)	540 (14.2)	568 (13.2)	This work
C205A/H206A LmPP	420 (165)	540 (13.9)	568 (13.0)	This work
P420	420 (190)	539 (16)	569 (15)	4
C107A LmPP	420 (155)	540 (14.4)	567 (12.7)	This work
LmP	424 (nr)	543 (nr)	571 (nr)	5

References

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