SUPPLEMENTAL MATERIAL

Table S1. PATHWAYs predicted coupling values (using HARLEM software) (17-19) and optimal electron-transfer paths for various Tyr and Trp candidates in *Mtb* KatG (PDB Code 2CCA)[a]:

Donor/Acceptor	Optimal pathway	Pathway distance (Å)	Predicted coupling
Y229/Heme Fe Y353/Heme Fe W107/Heme Fe W91/Heme Fe	Y229⇒W107⇒Heme Y353⇒MET377→LEU378⇒Heme W107⇒Heme W91⇒HOH47⇒HOH487⇒Heme	5.009 11.180 3.350 6.882	1.8896×10^{-3} 3.7048×10^{-5} 2.1812×10^{-2} 2.0077×10^{-4}
Y337(predicted doublet)/Heme	Y337→LEU336⇒PHE332⇒HIS270→ Heme	14.768	1.1826×10^{-6}
Y413(predicted doublet)/Heme	Y413→TRP412⇒Heme	8.815	4.3806×10^{-4}
Y197(predicted doublet)/Heme	Y197⇒ARG114→TYR113⇒MET255⇒ TYR229⇒TRP107⇒Heme	19.421	2.4165×10^{-8}
Y28(predicted doublet)/Heme	Y28→LYS27⇒PRO40→TRP39⇒ SER134→TRP135→PRO136→ASP137⇒ HOH89⇒Heme	36.249	2.7150×10^{-14}
Y210(predicted singlet)/Heme	Y210⇒ASP247→ILE248⇒Heme	12.343	1.1444×10^{-6}
Y339(predicted singlet)/Heme	Y339⇒PRO375→THR376→MET377→ LEU378⇒Heme	18.553	1.6502×10^{-7}
Y353/Y229	Y353→GLN352→TRP351⇒HOH247⇒ PRO232→ASN231→VAL230→Y229	16.613	1.7736×10^{-6}
W91/Y229	W91⇒SER140→ALA139→ASN138→ ASP137→ILE228→Y229	19.549	1.8413×10^{-7}

[a] A through-bond coupling is indicated by →; through-space jumps and hydrogen bonds are indicated by ⇒.