Supporting Information

A subtle structural change in the distal haem pocket has a remarkable effect on tuning hydrogen peroxide reactivity in dye decolourising peroxidases from *Streptomyces lividans*

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RESULTS

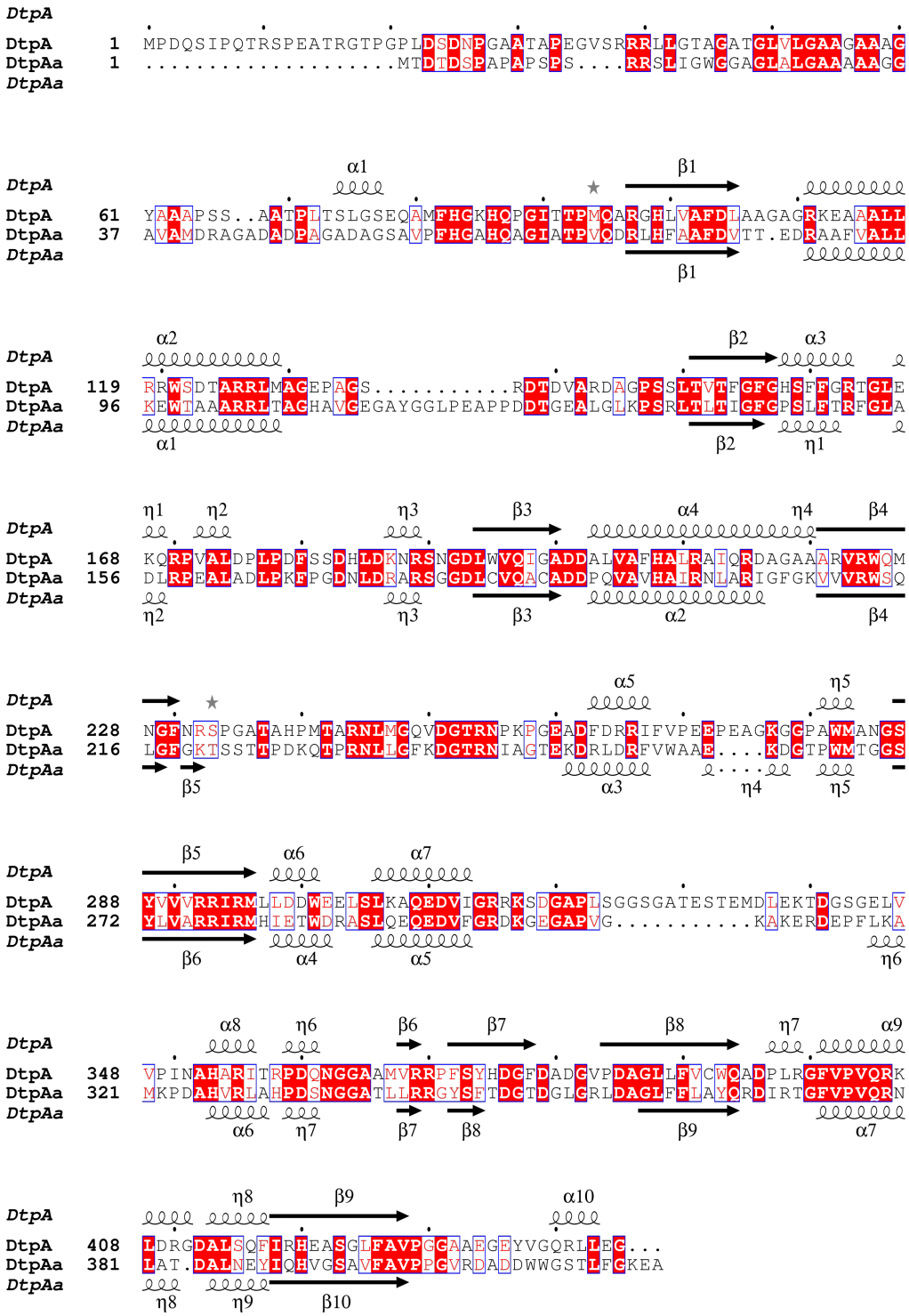
DtpA
DtpAa
DtpAa
MPDQSIPQTRSPEATRGTPGPLDSDNPGAATAPEGVSRRRLLGTAGATGLVLGAAGAAAG
MTDTDSPAPAPSPS....RRSLIGWGGAGLALGAAAAAGG
α1
β1
β1
YAAAPSS..AATPLTSLGSEQAMFHGKHQPGITTPMQARGHLVAFDLAAGAGRKEAAALL
AVAMDRAGADADPAGADAGSAVPFHGAHQAGIATPVQDRLHFAAFDVTT.EDRAAFVALL
α2
β2
α3
α1
β2
η1
RRWSDTARRLMAGEPAGS..........RDTDVARDAGPSSLTVTFGFGHSFFGRTGLE
KEWTAAARRLTAGHAVGEGAYGGLPEAPPDDTGEALGLKPSRLTLTIGFGPSLFTRFGLA
η1
η2
η3
β3
α4
η4
β4
η2
η3
β3
α2
β4
KQRPVALDPLPDFSSDHLDKNRSNGDIWVQIGADDALVAFHALRAIQRDAGAAARVRWQM
DLRPEALADLPKFPGDNLDRARSGGDICVQACADDPQVAVHAIRNLARIGFGKVVVRWSQ
α5
η5
β5
α3
η4
η5
NGFNRSPGATAHPMTARNLMGQVDGTRNPKPGEADFDRRIFVPEEPEAGKGGPAWMANGS
LGFGKTSSTTPDKQTPRNLLGFKDGTRNIAGTEKDRLDRFVWAAE....KDGTPWMTGGS
β5
α6
α7
β6
α4
α5
η6
YVVVRRIRMLLDDWEELSLKAQEDVIGRRKSDGAPLSGGSGATESTEMDLEKTDGSGELV
YLVARRIRMHIETWDRASLQEQEDVFGRDKGEGAPVG..........KAKERDEPFLKA
α8
η6
β6
β7
β8
η7
α9
α6
η7
β7
β8
β9
α7
VPINAHARITRPDQNGGAAMVRRPFSYHDGFDADGVPDAGLLFVCWQADPLRGFVPVQRK
MKPDAHVRLAHPDSNGGATLIRRGYSFTDGTDGLGRLDAGLFFLAYQRDIRTGFVPVQRN
η8
β9
α10
η8
η9
β10
LDRGDALSQFIRHEASGLFAVPGGAAEGEYVGQRLLEG...
LAT.DALNEYIQHVGSAVFAVPPGVRDADDWWGSTLFGKEA

Figure S1: Amino acid sequence alignment of DtpA and DtpAa from *Streptomyces lividans.* ESPript 3.0[1] was used to generate the alignment and calculate a sequence identity of 43.09 % as indicated by residues in a red box. Secondary structure elements as determined from the respective X-ray structures of DtpA and DtpAa are also depicted.

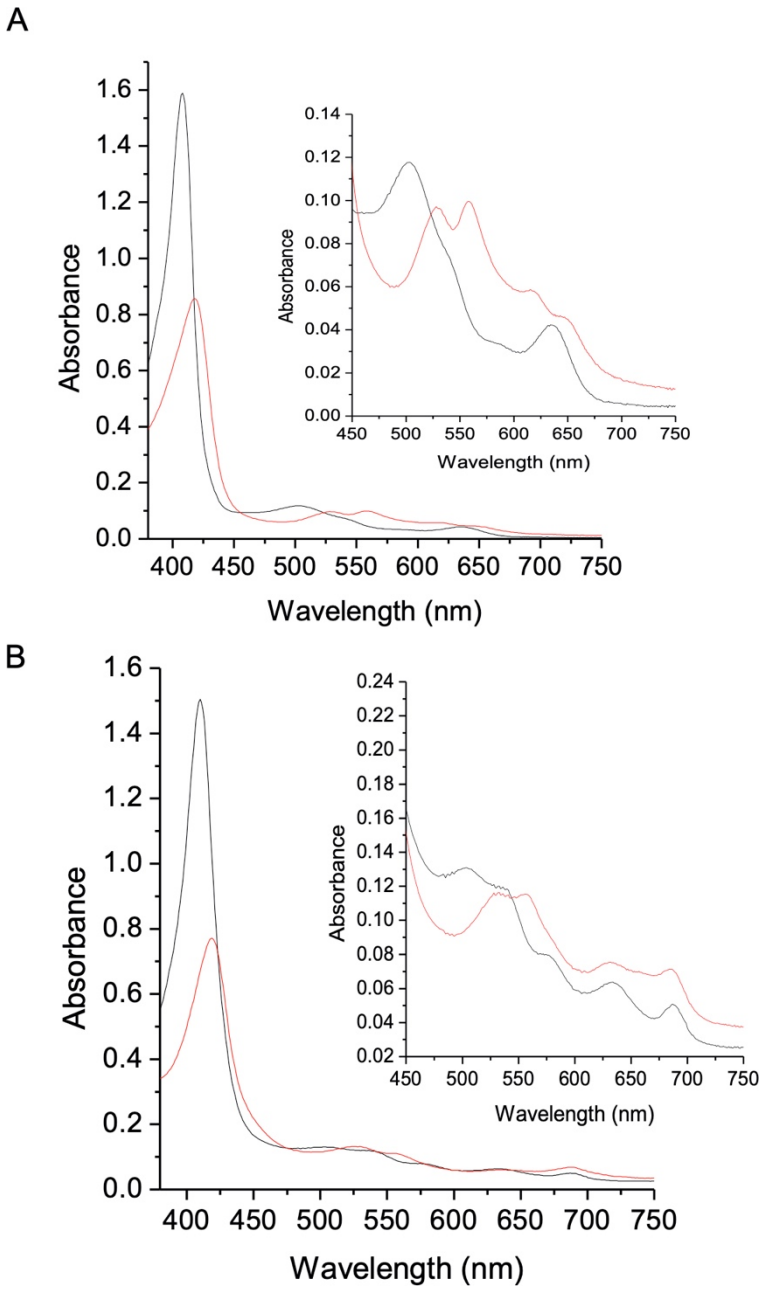

Figure S2: Absorbance spectra of the Asp variants at pH 7.0. A) The D251A DtpA variant and B) the D239A DtpAa variant. The black spectra indicates the ferric form and the red spectra following addition of one molar equivalent of H_2O_2. Insets show a close-up of the Q-bands.

REFERENCES

1. X. Robert and P. Gouet, *Nucleic acids research*, 2014, **42**, W320-324.