

Structural and spectroscopic characterisation of a heme peroxidase from sorghum

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Figure S1. Sequence alignment of sorghum peroxidase, BP1, HRP and PNP. The sorghum peroxidase has the highest sequence identity to BP1 (69 %) then to PNP (45 %) and HRP (44 %). The figure was generated by ESPript (1).

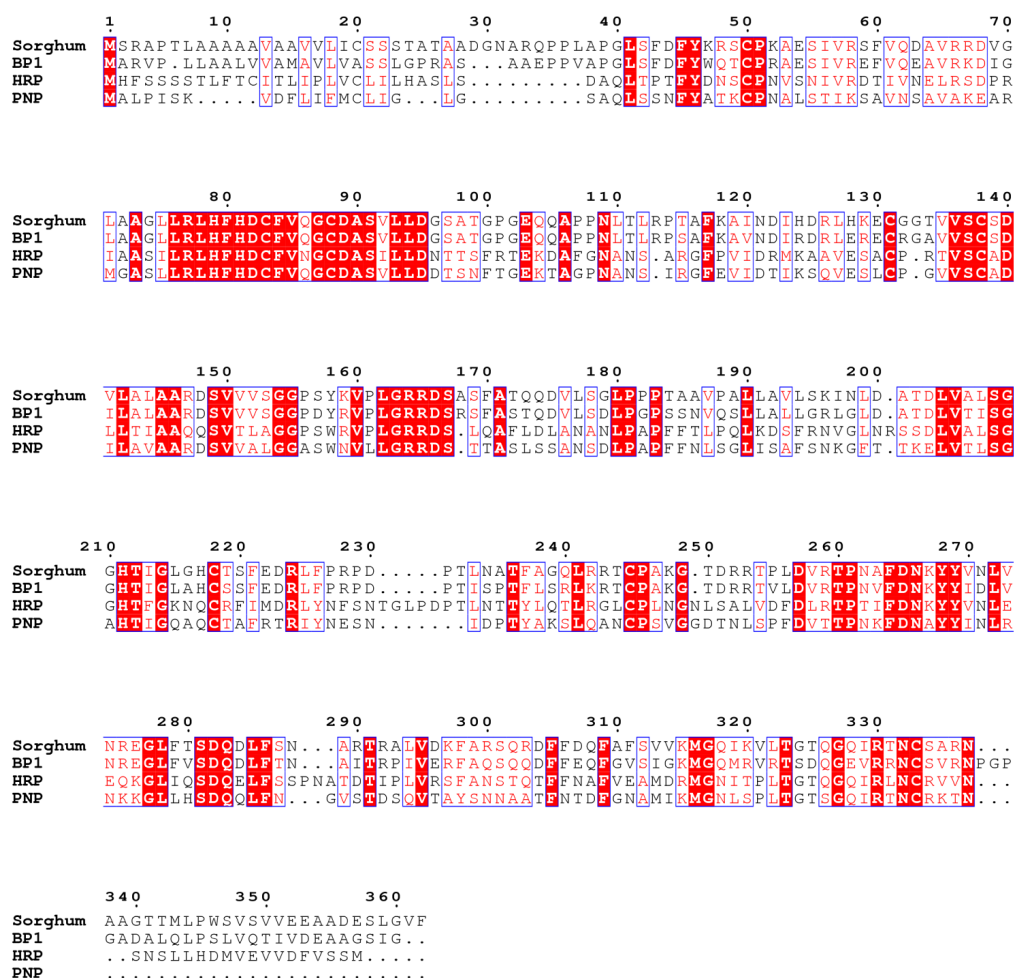
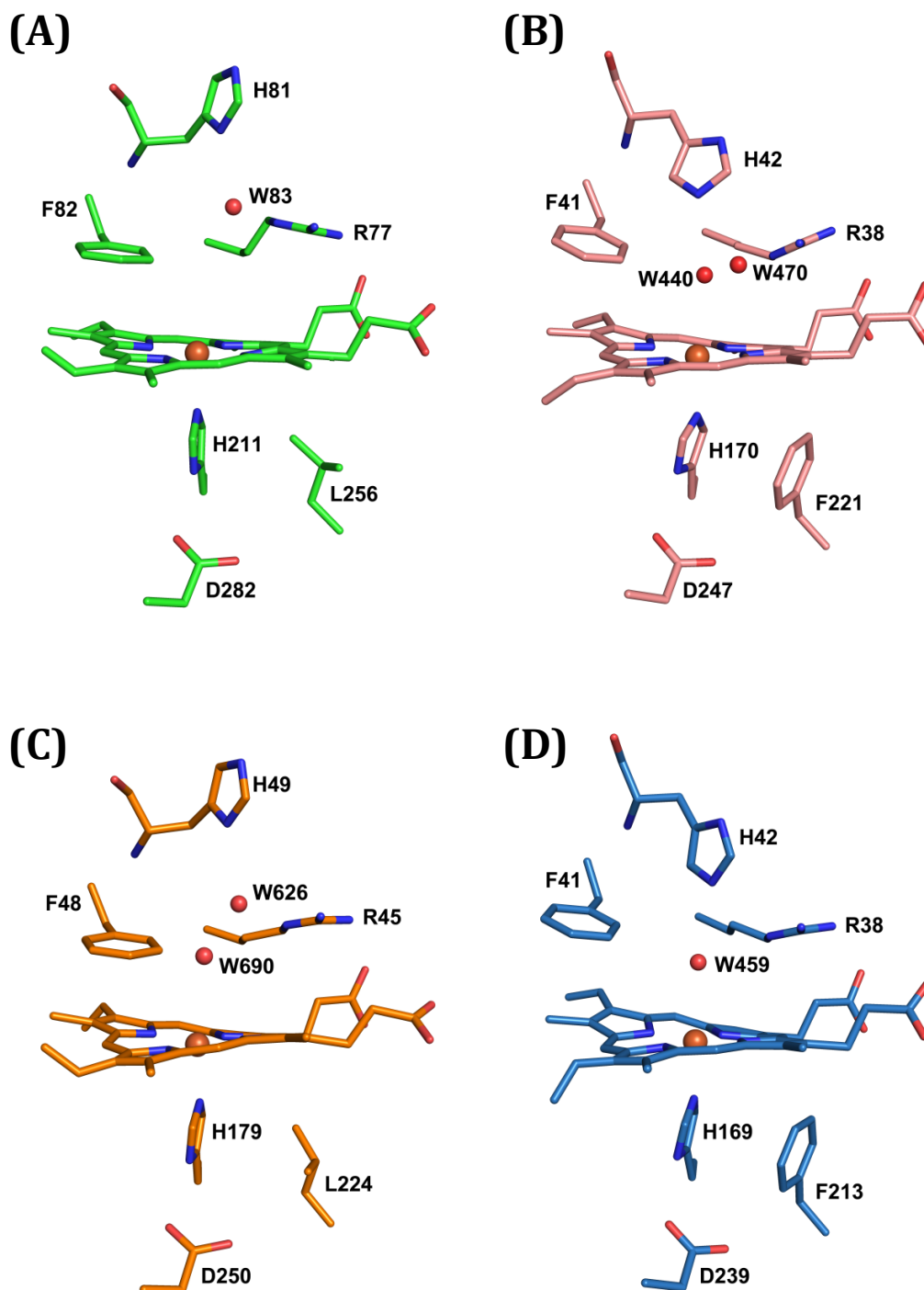


Figure S2. Comparison of the active sites of (A) sorghum peroxidase, (B) HRP, (C) BP1 and (D) PNP. The sorghum peroxidase is the only structure with 5-coordinated heme. The sorghum and BP1 enzymes shares some structural characteristics such as re-orientation of the distal histidine, presence of structural water molecules (W83 in sorghum and W626 in BP1) and the presence of a leucine residue in the proximal heme pocket (instead of phenylalanine residues found in HRP and PNP). Water molecules are shown as red spheres.



1. Gouet P, Robert X, & Courcelle E (2003) ESPript/ENDscript: Extracting and rendering sequence and 3D information from atomic structures of proteins. *Nucleic acids research* 31(13):3320-3323.