

The Malarial Drug Target *Plasmodium falciparum* 1-Deoxy-D-Xylulose-5-Phosphate Reductoisomerase (PfDXR): Development of a 3-D Model for Identification of Novel, Structural and Functional Features and for Inhibitor Screening

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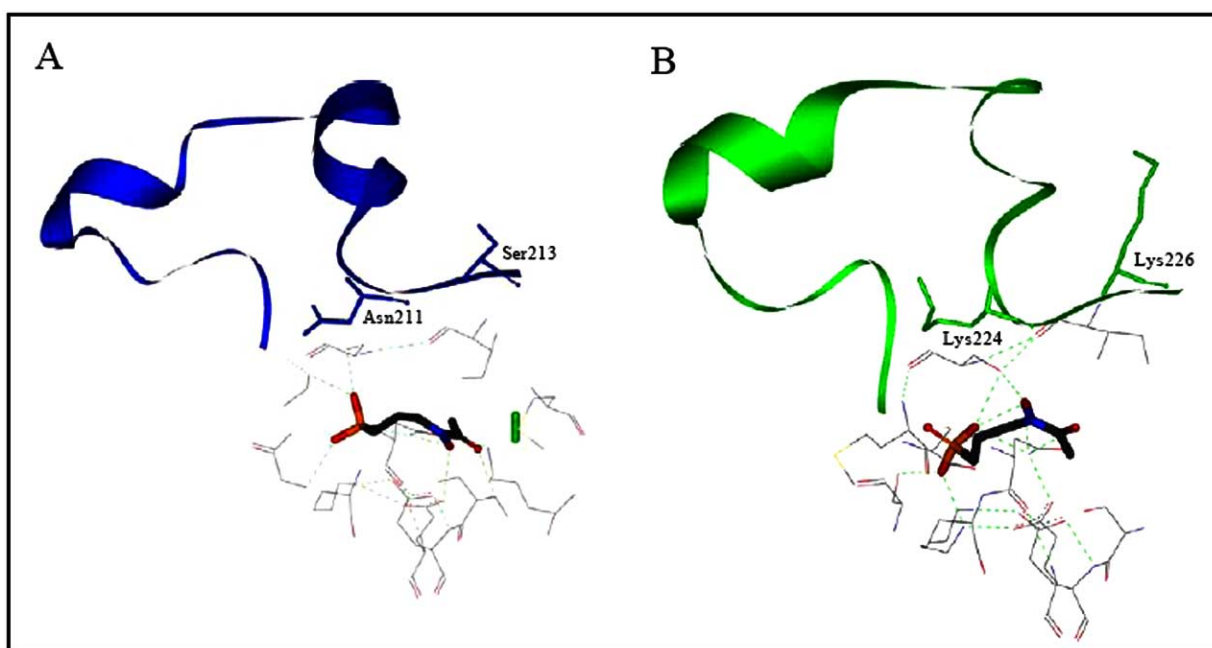


Figure S1. (A) FR900098 docked into *EcDXR*, showing residues within 4 Angstroms of the inhibitor, as well as the hatch in ribbon representation (coloured *blue*), with the side chains of Asn211 and Ser213 shown. Hydrogen bonding is shown in green. (B) FR900098 docked into *PfDXR*, showing residues within 4 Angstroms of the inhibitor, as well as the hatch in ribbon representation (coloured *green*), with the side chains of Lys224 and Lys226 shown. Hydrogen bonding is shown in green.

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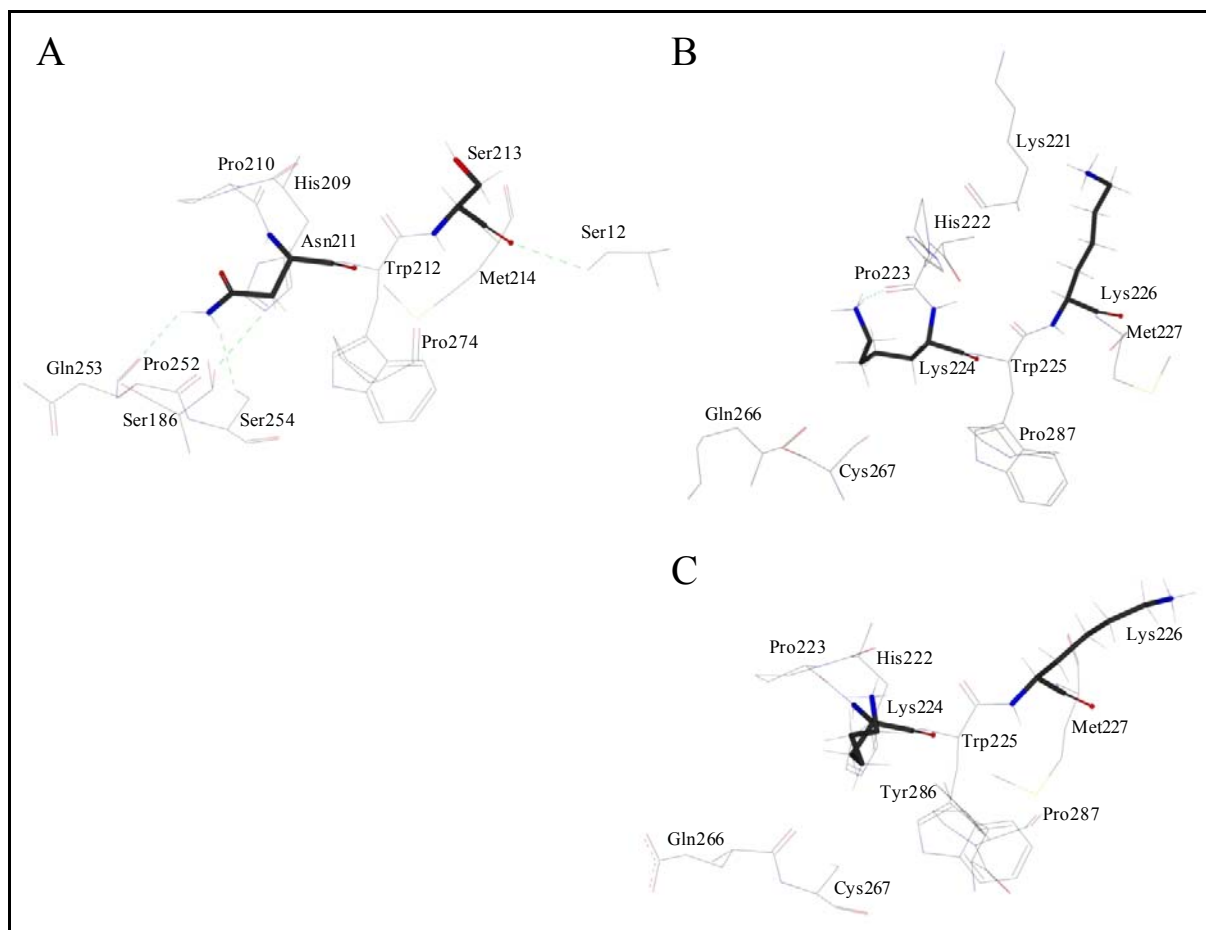
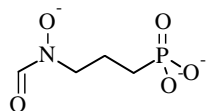
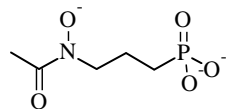


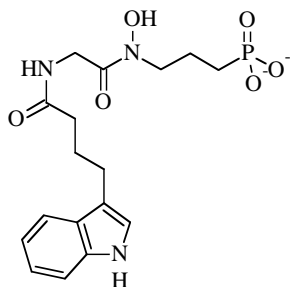
Figure S2. (A) FR900098 docked into *EcDXR*, showing only the residues within 4 Angstroms of Asn211 and Ser213. Hydrogen bonding is shown in green. (B) FR900098 docked into *PfDXR* showing only the residues within 4 Angstroms of Lys224 and Lys226. Hydrogen bonding is shown in green. (C) Three-dimensional *PfDXR* model with only NADPH with no ligand and no cofactor docked, showing only the residues within 4 Angstroms of Lys224 and Lys226. Hydrogen bonding is shown in green.



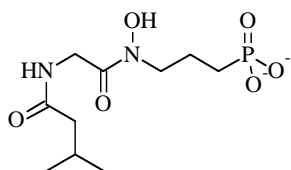
Fosmidomycin



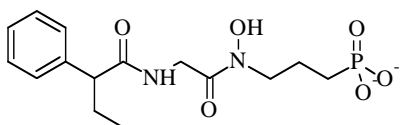
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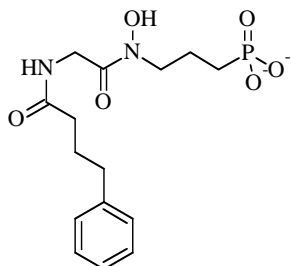
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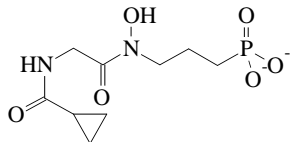
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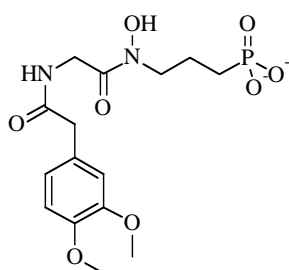
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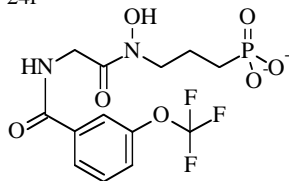
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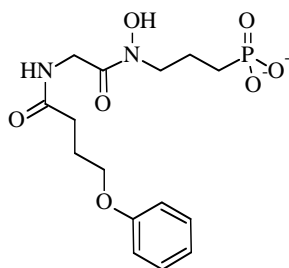
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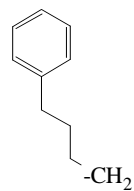
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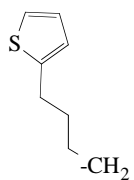
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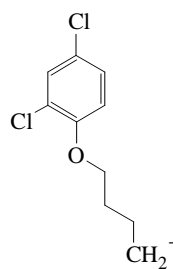
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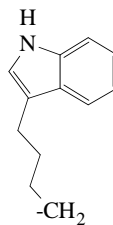
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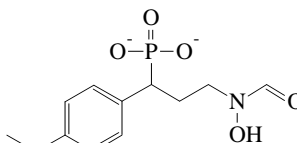
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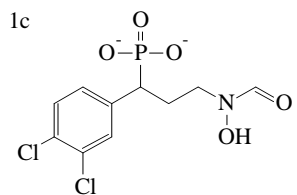
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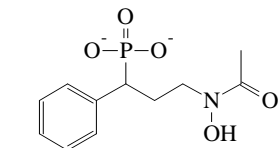
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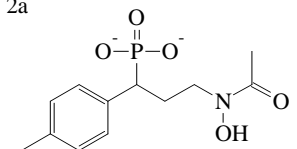
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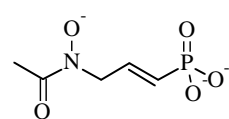
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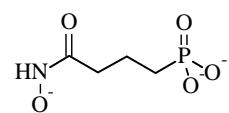
2a



2b



KD562



LD_1_1

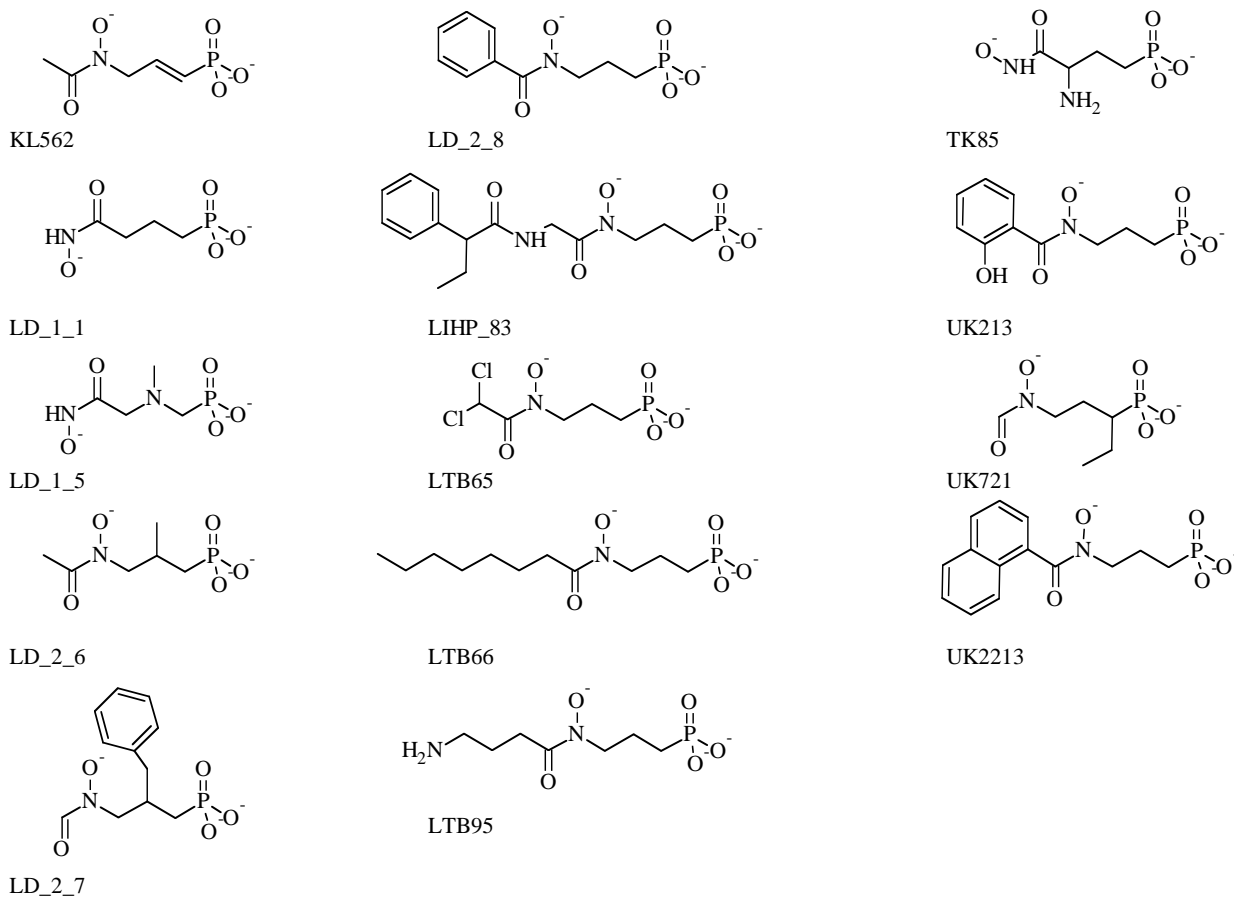


Figure S3. The chemical structures of inhibitors used for docking studies, namely fosmidomycin, FR900098, Gießmann *et al.* (2008) ligands (24a – h) [23], Herforth *et al.* (2004) ligands (9a – d) [20], Haemers *et al.* (2006) ligands (fosmidomycin analogues 1c, 1e, 2a, 2b) [22] and Silber *et al.* (2005) ligands KD562, LD_1_1, LD_1_5, LD_2_6, LD_2_7, LD_2_8, LIHP_83, LTB65, LTB66, LTB95, TK85, UK213, UK2213, UK721 [21].