Supporting Information

Heterocyclic Diamines with Leishmanicidal Activity

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Figure S2. Detail of the interaction of a methylated (8) and a non-methylated system (10) with the active centre of Fe-SOD. The increase in the number of hydrogen bonds that can be established and the reduction of the steric hindrances generated by the non-methylated system increases the effectiveness of the interaction of the ligand with the residue Gln71, leading to a higher distortion of the active centre.

Figure S3. Detail of the interaction of a quinoline (**10**) and a pyridine system (**1**) with the active centre of Fe-SOD. The increase of the surface area of the aromatic moiety favours the interaction with residue Tyr75 though π -stacking, thus increasing the affinity between both systems.

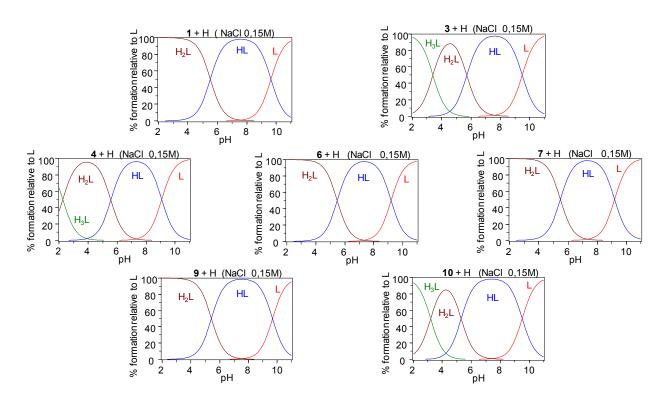


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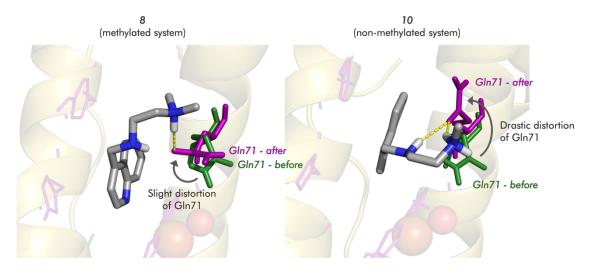


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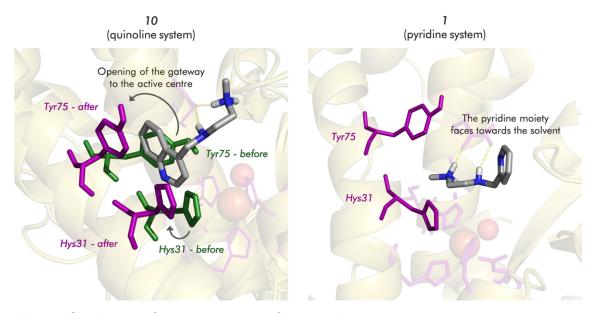


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