

Supplementary Information

Synthesis, characterization, spectroscopic, DFT, antimicrobial and molecular docking analysis of butane-2,3-dione dioxime and its zinc (II) complex

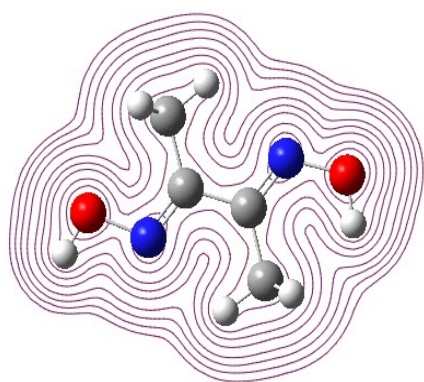
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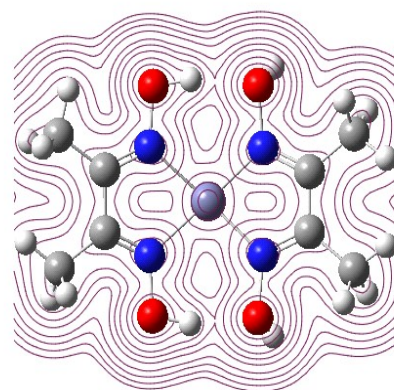
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Received 2 June 2025; accepted (revised) 25 September 2025



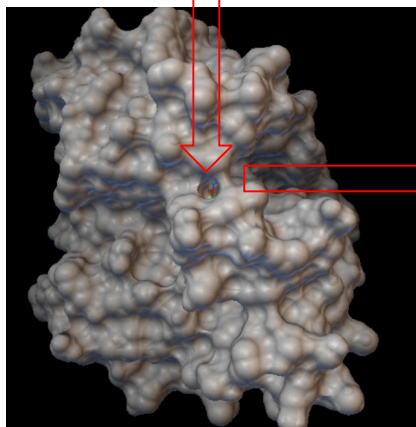
Ligand



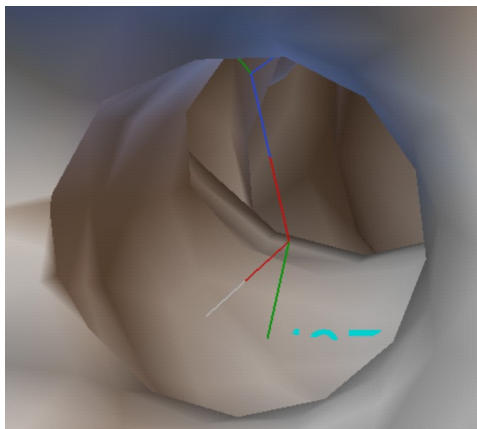
Zn metal complex

(Fig: S1) Total SCF Density of Ligand and its Zn metal Complex

Ligand binding in protein (1T46)

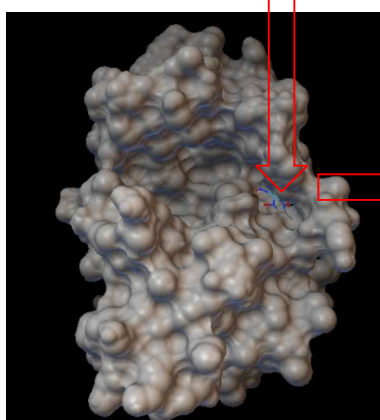


Ligand

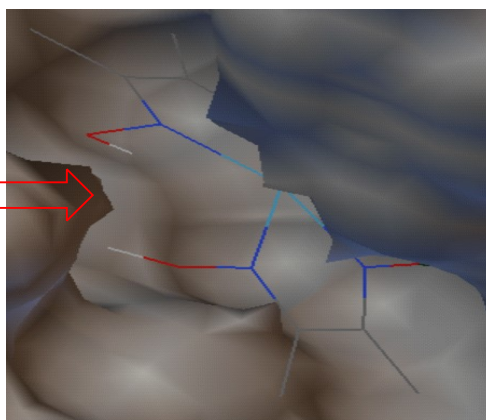


Zoom structure of protein and ligand interaction

Zn meta complex binding in protein(1T46)



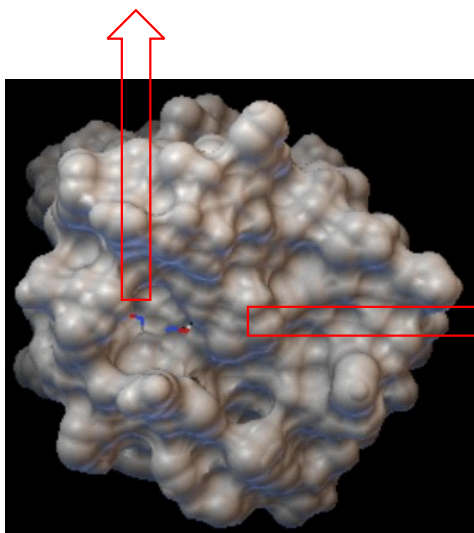
Zn Metal complex



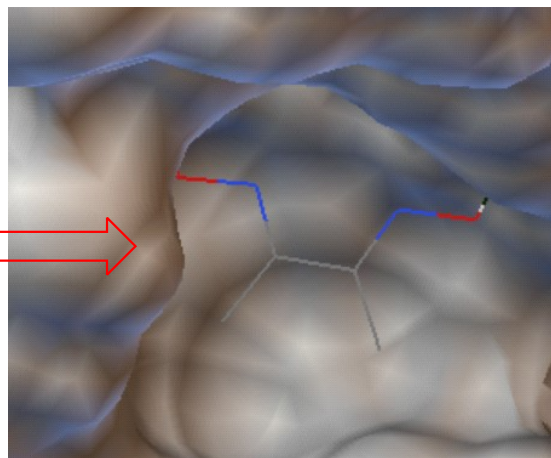
Zoom structure of protein and Zn metal complex interaction

(Fig:S2) Ligand and protein binding interaction (Bubble structures)

Ligand Binding in porotein(1HD2)

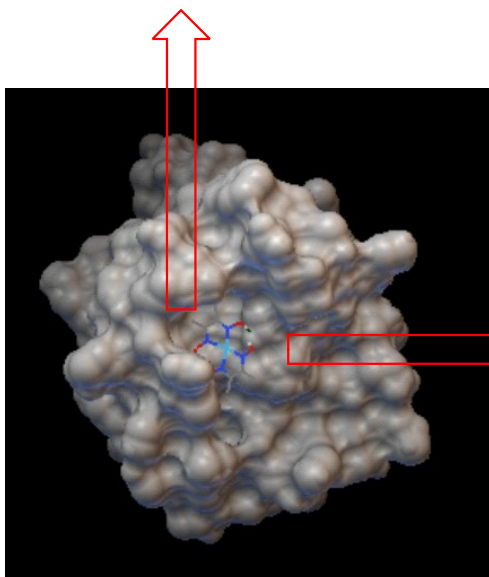


Ligand

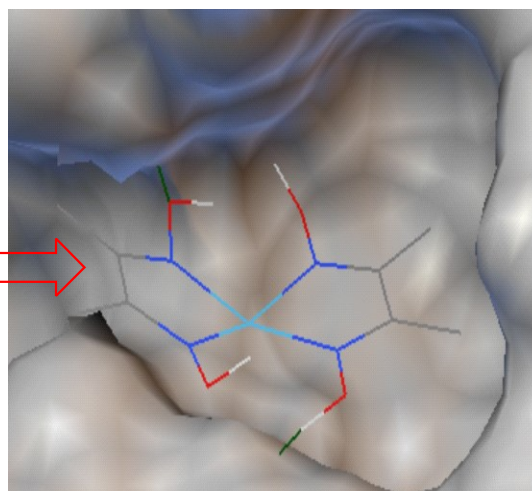


Zoom strucutre of ligand and protein interaction

Zn metal complex Binding in porotein (1HD2)



Zn metal complex



Zoom strucutre of Zn metal complex and protein interaction

(Fig: S3) Ligand and protein binding interaction (Bubble structures)