

*In silico characterization of a potential Zn²⁺ ABC transporter*Suraj Kumar Mandal¹, Shankar Prasad Kanaujia¹¹Department Of Biosciences And Bioengineering, Indian Institute Of Technology Guw, Guwahati, India

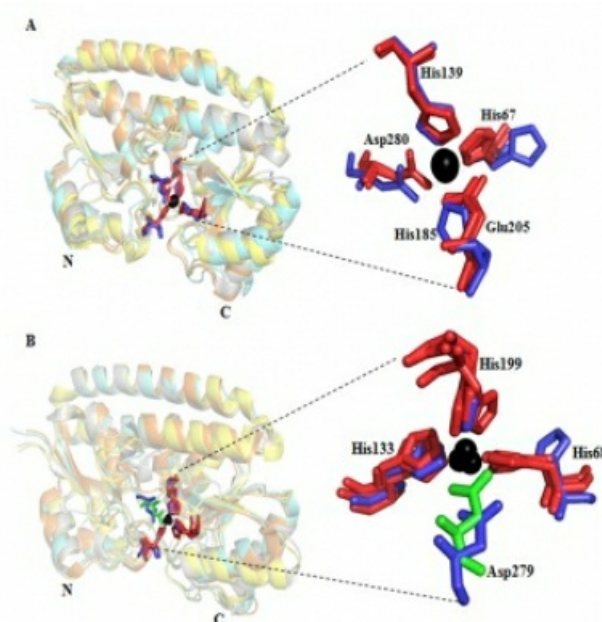
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Metalloproteins, the most diverse classes of proteins, require metal ions (Mn²⁺, Zn²⁺, Ni²⁺, Fe^{2+/3+}, etc.) for their regulatory, catalytic and/or structural activities making them inevitable for survival of an organism. One of the most efficient systems of acquiring metal ions inside a bacterial cell is the ATP-binding cassette (ABC) transporters, which are further classified into importers and exporters. Structurally, ABC importers comprises of a transmembrane domain, a nucleotide binding domain and a substrate binding protein (SBP) for substrate acquisition. Being specific to prokaryotes and often accountable for their pathogenicity, SBPs are recognized as potential drug targets. In this study, TTHA0596, a SBP from *Thermus thermophilus* HB8 is characterized using *in silico* approaches. Homology search and phylogenetic tree analysis exhibit that TTHA0596 is similar to a group of Zn²⁺/Mn²⁺ binding SBPs. Furthermore, TTHA0596 protein attains an unusual structural prototype similar to that of cluster A-I SBPs. Akin to Zn²⁺ binding SBPs, binding pocket of TTHA0596 is constituted of three histidine residues (His52, His123 and His185). However, the presence of an aspartate (Asp259) and absence of the histidine-rich loop, an attribute of Zn²⁺ binding SBPs, indicates its possible affinity towards Mn²⁺ ion. This further led us to identify a subdivision within the Zn²⁺ binding SBPs, group I display affinity for both Zn²⁺ and Mn²⁺ ions, while group II are highly specific towards Zn²⁺ ion. Our analysis concludes that TTHA0596 protein belongs to group I Zn²⁺ binding SBPs and thus bear a tendency to bind both Zn²⁺ and Mn²⁺ ions.

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