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An *in silico* study on molecular level interactions of host Siderocalin with siderophores from *Mycobacterium tuberculosis* and other bacterial species

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Background

Tuberculosis (TB) drug research and development has witnessed resurgence in recent times primarily due to the high mortality rates despite the availability of front line drugs and a prominent BCG vaccine. Synergy of TB with HIV is another factor which has warranted a search for newer therapeutic interventions. Treatment of latent TB infection is also the need of the hour. Iron acquisition is an important virulence mechanism of *Mycobacterium tuberculosis* (MTB). To scavenge iron, bacterial species have developed high affinity, low molecular weight iron chelators termed as siderophores. To counteract the detrimental effect of microbial iron acquisition systems, the host secretes a 21kDa lipocalin protein (Siderocalin) that binds with these iron laden siderophores in an attempt to restrict the growth of MTB within host macrophages.

Methods

In the current study, using molecular docking tools, we assessed the interactions of host Siderocalin with Mycobactin, Parabactin and Cepabactin structurally non similar siderophores from three different bacterial species-MTB, Paracoccus and *Burkholderia cepacia*. A comparison of molecular level interactions of Siderocalin with these siderophores was performed.

Results

Siderocalin forms energetically favourable and stable complexes with parabactin and cepabactin. However the unfavourable positive binding energies for mycobactin- a salicylate derived MTB siderophore indicated that siderocalin does not dock well with mycobactin.

Conclusion

Siderocalin probably fails to disrupt the role of mycobactin in acquiring iron for mycobacteria thereby helping the pathogen to survive leading to progression of disease.

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