

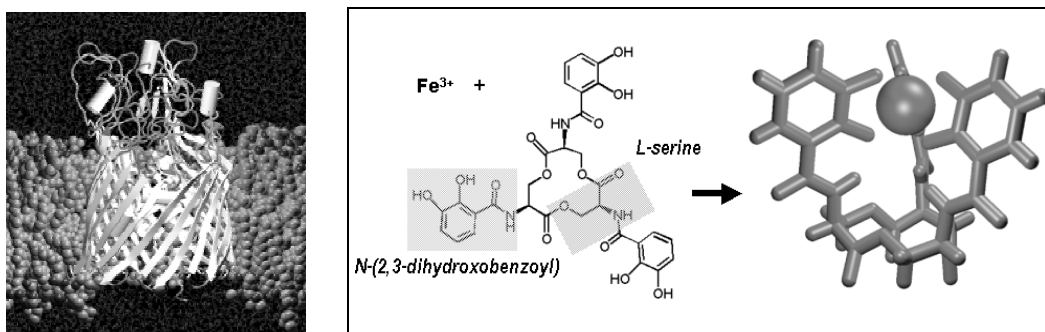
Understanding bacterial iron transport

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We present preliminary results of molecular dynamics (MD) simulations in a fully solvated lipid bilayer to probe the mechanism of bacterial iron transport.

Gram negative bacteria provide themselves with essential iron using a unique class of outer membrane proteins. The crystal structures of three members of this class of porin-like proteins, FhuA, FecA and FepA from *E. coli*, have recently been determined. [1] These bacterial transporters formed from a 22-stranded beta-barrel pose an intriguing challenge to our current understanding of the Fe^{3+} transfer mechanism as the protein barrel interior is occluded by a globular N-terminal domain, the "cork" (~150 aminoacid residues). Whether the cork "unplugs" during transport or undergoes a conformational change remains unknown.



A detailed atomic picture emerges from our MD simulations (Figure above. Left: A snapshot of the simulation system. FepA (white) embedded in a DMPC bilayer. Right : The enterobactin siderophore-iron complex, as transported by the FepA protein.), providing insights into stable *vs* mobile parts of the structure and possible pathways of transport.

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[1] S. K. Buchanan *et al.*, *Nature Struct. Biol.* **6**, 56 (1999); A. D. Ferguson *et al.*, *Science* **282**, 2215 (1998); K. P. Locher *et al.*, *Cell* **95**, 771 (1998); A. D. Ferguson *et al.*, *Science* **295**, 1715 (2002).