Supplementary material

FecB, a periplasmic ferric-citrate transporter from *E. coli,* can bind different forms of ferric-citrate as well as a wide variety of metal-free and metal-loaded tricarboxylic acids

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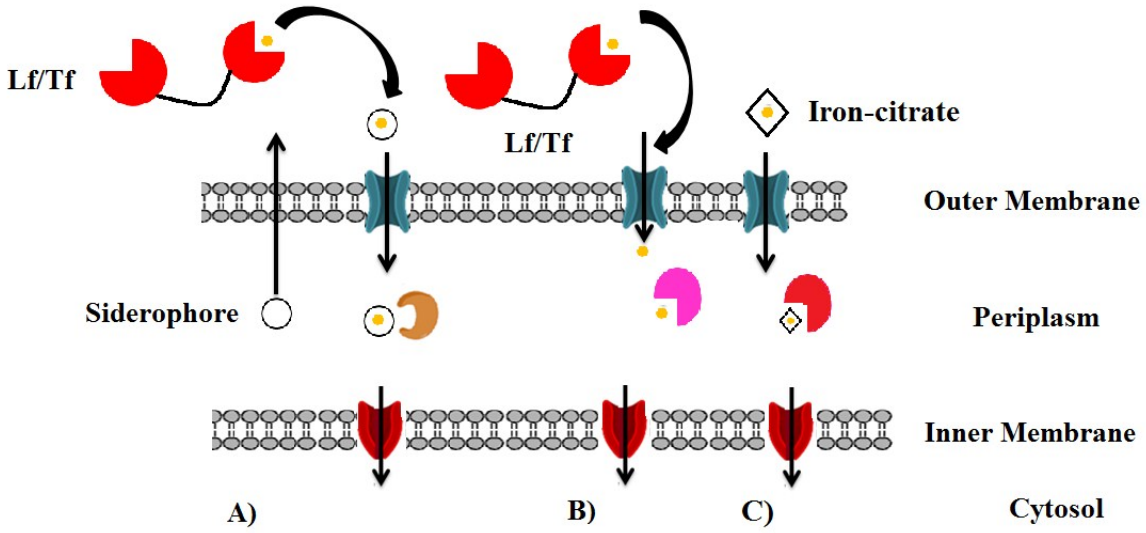
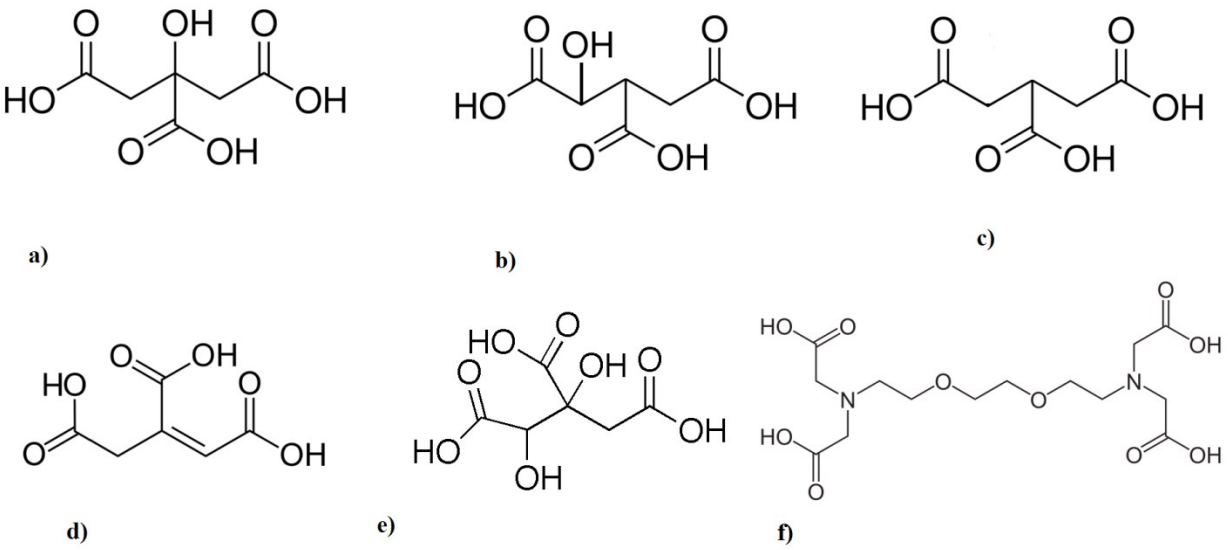
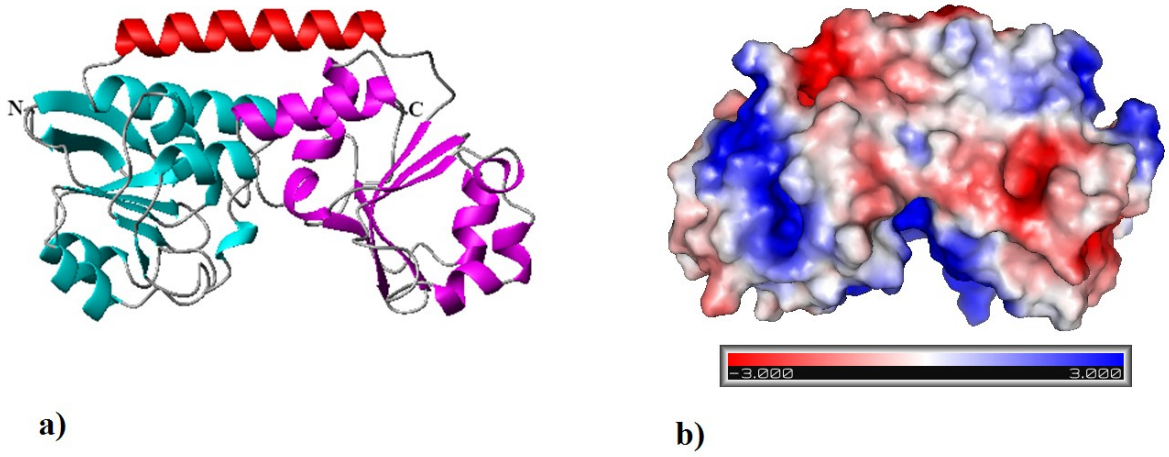


Supplementary Figure 1. Schematic representation of non-heme Fe^{3+} transport by Gram negative bacteria. The TonB complex has not been shown for clarity. A) The bacteria produces siderophore (empty black circle) and sends it out to the environment, there it competes for iron (yellow solid circle) with iron-binding proteins in the host (transferrin or lactoferrin), and then the iron-loaded siderphore is transported through a cognate OM receptor. When the iron-siderophore reaches the periplasm it is picked up by a iron-siderophore binding protein and its directed to the IM to be transported by an IM ATPase/permease complex (shown in red). B) The bacteria express cognate OM protein that will bind and steal iron from host iron-binding proteins

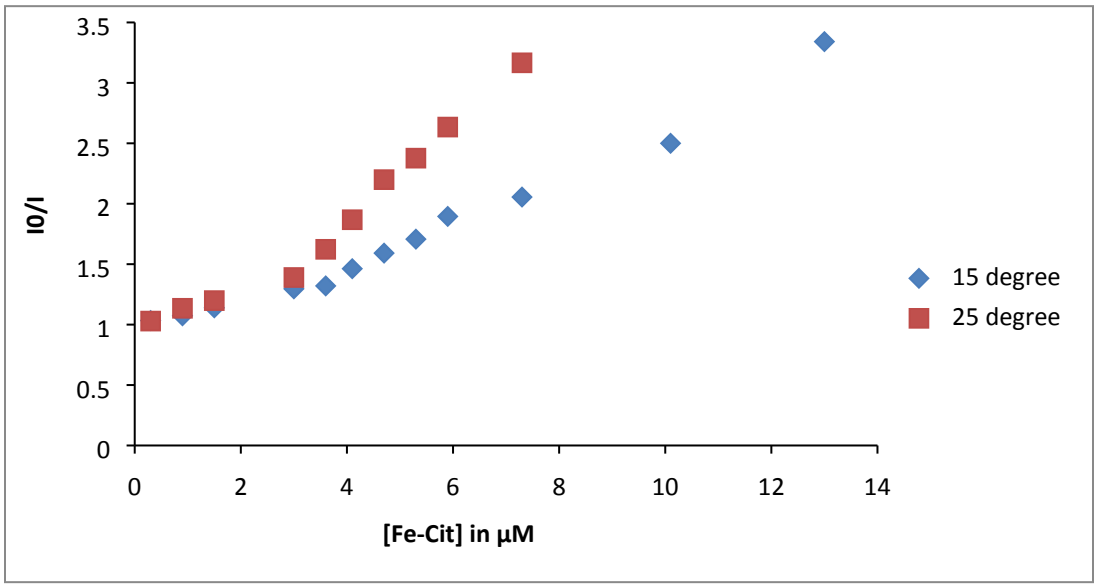
(transferrin or lactoferrin). The hijacked iron then passes through this OM receptor and upon reaching the periplasm is picked up by the ferric binding protein, FbpA (shown in pink). Finally the "free iron" is trafficked to the IM to be transported by an IM ATPase/permease complex (shown in red). C) iron-citrate (represented by black square with yellow dot at the center) is recognized and taken up by specific receptor (FecA) at the OM and once it reaches the periplasm, the iron-citrate complex is transported across with the help of periplasmic binding protein (FecB) and is finally transported into the cytosol for utilization.



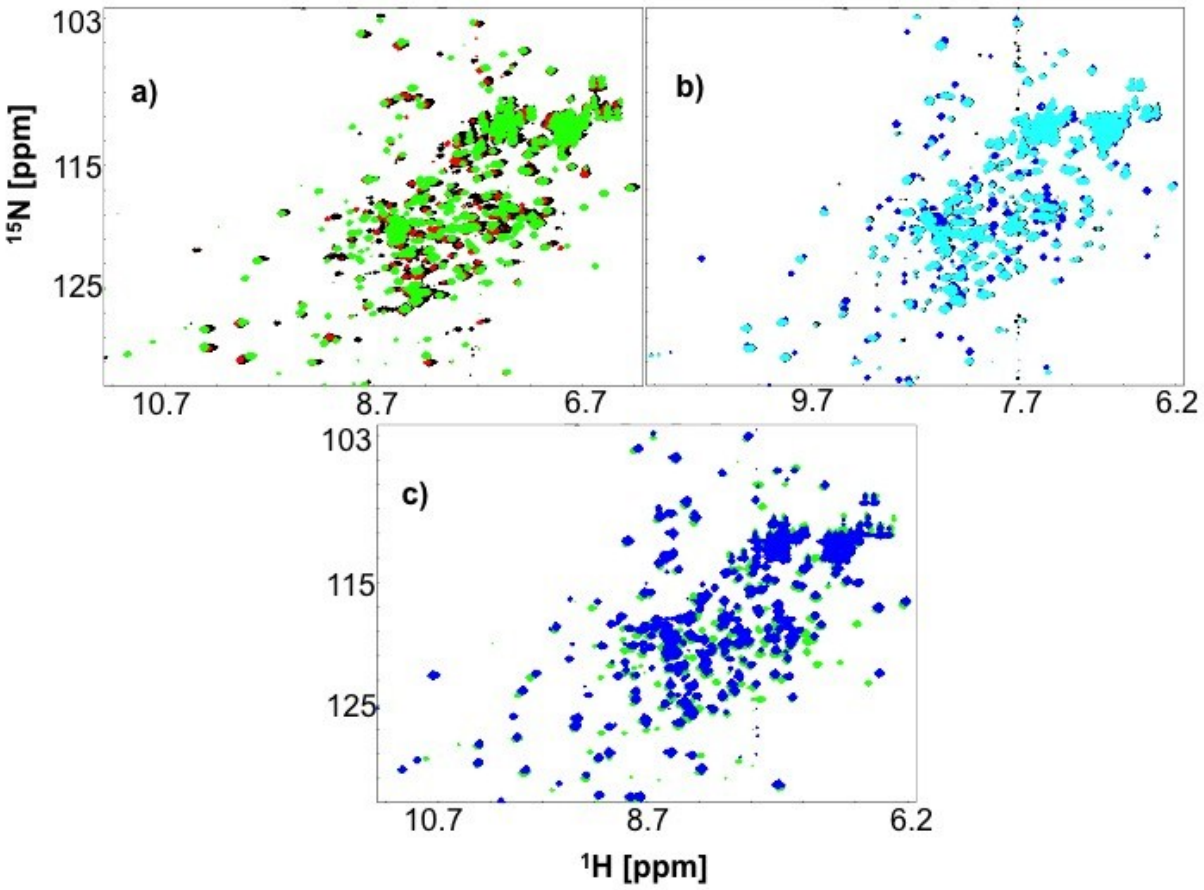
Supplementary Figure 2: Chemical formula of a) citrate, b) isocitrate, c) carballylic acid, d) cis-aconitic acid, e) hydroxycitrate and f) EGTA.



Supplementary Figure 3: The model structure of FecB a) in ribbon format as calculated by SwissModel. The N- and the C-lobes are shown in cyan and magenta colour respectively and the α-helical hinge connecting the two lobes is shown in red. The global model quality estimation value (GMQE) of the model is 0.72, which reflects higher accuracy of alignment between model and template as the value is close to one. The quality of the model is also assessed by a composite scoring function (QMEAN) to estimate the global and local model quality score where the score is -3.57 b) Model showing the surface charges as prepared using the APBS program and visualized using Pymol. See text for details.



Supplementary Figure 4: Representative plot of I_0/I vs [Fe^{3+}-citrate] for FecB emission titration. Experiments were done with 1 µM FecB in 20 mM MES, 100 mM NaCl pH 5.5 and at temperatures of 15 and 25°C. See text for details.



Supplementary Figure 5: ^{1}H, ^{15}N HSQC spectra of FecB a) Black dots for apo FecB, red dots for 5 times excess iron free citrate and green for 5 times excess Ga^{3+}-citrate pH 5.5 experiments are done in 20 mM MES. b) Black dots are for apo FecB, cyan dots are for 5 times excess iron free citrate and blue are for FecB + 5 times excess Ga^{3+}-citrate. Experiment done in 20 mM Na-phosphate pH 7.0. c) Overlay of 5 times excess Ga^{3+}-citrate at pH 5.5 (green) and pH 7.0 (blue).