Characterization of a Bacillus megaterium strain with metal bioremediation potential and in silico discovery of novel cadmium binding motifs in the regulator, CadC

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Abstract

Bioremediation of toxic metal ions using bacterial strains is a promising tool. Metal binding motifs in microbial proteins are involved in the regulation and transport of such toxic metals for metal detoxification. A bacterial strain designated TWSL_4 with metal (Cu, Cd, and Pb) resistance and removal ability was isolated and identified as a Bacillus megaterium strain using 16S rRNA gene analysis. An operon with 2 open reading frames (ORFs) was identified, cloned, and sequenced. ORF1 and ORF2 were identical to the cadmium efflux system accessory protein (CadC) and cadmium-translocating P-type ATPases (CadA) of B. megaterium strain YC4-R4 respectively. A protein homology search using Swiss model retrieved no crystal structures for CadC and CadA of Bacillus sp.. CadC of TWSL_4 had a sequence identity of 53% to the CadC (121aa) protein and 51.69% to the CadC crystal structure (1U2W.1.B; GMQE=0.75) of Staphylococcus sp. pI258. Molecular dynamic simulation studies revealed the presence of three metal binding regions in CadC of TWSL_4, [ASP7-TYR9], [ASP100-HIS102], and [LYS113-ASP116]. This is the first report showing evidence for the presence of Cd^{2+} and Zn^{2+} metal binding motifs in the CadC regulator of the Bacillus megaterium cad operon. The bacterial strain TWSL_4 was also found to contain two different P type ATPases encoding genes, cadA and zosA involved in metal resistance. Furthermore, the metal bioremediation potential of strain TWSL_4 was confirmed using an industrial effluent. KEY POINTS: • Isolation of a metal-resistant bacterial strain with potential for industrial

bioremediation. • Discovery of novel Cd binding sites in CadC of the cad operon from B. megaterium. • Involvement of aspartic acid in the coordination of metal ions (Cd^{2+}).

Keywords: Bacillus megaterium; Bioremediation potential; CadA; CadC; Metal binding motifs; Molecular dynamics simulation.

Citations

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