Molecular dynamics simulations of metal ion binding to the His-tag moti

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Abstract

In our previous study, we have observed that the chelation of various metal ions to the His-tag motifs mostly involves the i and i+2 His residues for Ni~(2+), Cu~(2+), Zn~(2+) and Co~(2+). In the present study, various 200 ps molecular dynamics simulations were further conducted to investigate the chelating pathway of various metal ions to the His-tag motif with 6 His residues (His-tag6) and the binding affinities of these metal binding pockets towards these metal ions. The results indicate that His-tag6 with the chelated metal ion located in positions His(2,4) or His(3,5) exhibits the strongest affinity for Ni~(2+) and Cu~(2+). K~+ was found to be preferred to chelate in His(1,3) and His(3,5) coordinations. However, Fe~(3+) was found to have higher affinity towards His(1,3) and His(2,4) binding pockets. Our results also suggest that Ni~(2+) exhibits the highest binding affinity towards His-tag6 over the other metal ions. Most of the structural variations of the His-tag6 motif were from the Histidyl side chains during metal ion binding. In addition, there is an inverse linear correlation between the final chelated distance and the charge/volume ratio of metal ion. There is a negative correlation between the metal binding affinity and the averaged potential energy generated from the MD simulations.