Binding energy of metal ions to model cyclic peptides: A theoretical calculation study

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An ionophore is an ion carrier that reversibly binds ions and transports them across a cell membranes. There have been many efforts to synthesize biologically relevant ionophores. Typically, synthetic ionophores are based on podands, coronands and cryptands such as crown ethers or cyclic peptides. Among them, cyclic peptides have several amino acid residues and carbonyl oxygen atoms in their structures. They can selectively bind metal ions in aqueous solution by ion-dipole interaction between de-solvated metal ions and the oxygen atoms in the carbonyl group of amino acids. In this study, several model cyclic peptides were selected as metal ion binding agents. The stable conformers of free peptides and ion-complexes were determined by Monte Carlo conformational analysis. Then, the binding energy of de-solvated metal ions to the cyclic peptides was calculated by quantum mechanics on the basis of the selected conformers. Finally, the feasibility of selective separation of metal ions by the model cyclic peptides was studied.