Cu Ion Binding of MXCXXC Peptide: A DFT Study

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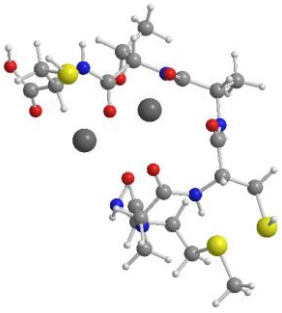
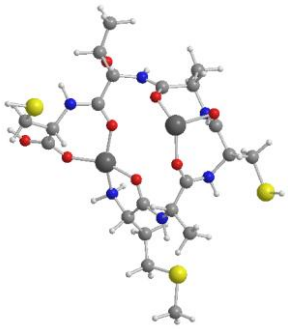
This study aims to investigate the copper binding mechanism of MXCXXC peptide by computational tools. Alanine (A), Glycine (G), Threonine (T), Valine (V), Serine (S) and Cysteine (C) are used in all possible combinations in MXCXXC for X. Most stable structures of the peptides are chosen for modeling the interactions with Cu^{+} and Cu^{2+} ions.

Conformational analysis has been carried out with molecular mechanics using the CHARMM22 force-field in HyperChem [1]. The calculations are repeated with Density Functional Theory (DFT) methods in Gaussian09 [2] at B3LYP/6-31G* level. Additionally, solvent effects will be investigated by the help of PCM models at the same level of theory.

The presence of Cu ions significantly changes the properties of the studied peptide and the stability of the formed complexes highly depends on the amino acids in the positions shown with X. Since the calculations are still in progress, we are yet unable to claim strongly that this effect is also very effective in the main protein. On the other hand, it can be concluded that the effect of the amino acids at positions X is not negligible as it is mostly believed in the literature.



MACATC-2Cu^{+}



MACATC-2Cu^{2+}

Our preliminary results indicate that the X residues are important in selective binding. Further studies and the detailed information gained in this study on the mechanism of peptide-metal interactions will provide useful data in many fields of health, biotechnology and bionanotechnology.

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[1] HyperChem 8.0, HyperCube Inc., USA.
[2] Gaussian 09 Version B01, M. Frisch et al. Gaussian Inc., Wallingford, PA, (2010).