Title: Effects of osmolytes on the Protein stability: Molecular dynamics simulation

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Abstract: Introduction: The presences of osmolytes in aqueous solution have significant effects on providing essential interactions for the unique three-dimensional conformation of native proteins. Osmolytes such as trehalose or sucrose have been known to protect proteins against loss of activity and prevent the partial or even total degradation of biomolecules. Despite various experimental and theoretical works, the detailed molecular mechanism at the origin of polyols protective ability still not well understood. MD simulations can provide valuable information about the different stages of peptide–solvent interactions. Methods: All simulations were performed using the gromacs software package, version4.5.4. The Gromos96 53a6 parameter set was used as force field. The starting conformation of the peptide was obtained from the protein databank (PDB) structure 1LCI. The peptide was solvated with SPC water, a mixture of sucrose, a mixture of trehalose. Results our results showed the total number of hydrogen bonds between the protein and solvents over the course of the MD simulations is not significant. Nevertheless there is main difference in water and osmolyte direct interaction with protein. The water molecules mainly interact with protein side chains while osmolytes are more involved with protein backbone. Also, we have identified variations in the secondary structure of the protein during the simulations. In pure water some part of alpha helical conformation of protein is deteriorates with time whereas in sucrose solution protein secondary structure is maintained throughout the 100 ns duration of simulations. Conclusions: In conclusion, according to the results presented in this study it has been suggested that osmolyte with effect on special part of protein and make favorable environment, can prevent protein thermal unfolding.

Osmolytes, Protein stability, Protein –co solvents interactions, Molecular Dynamics Simulation

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