**Abstract**

The quantum chemical and molecular dynamics studies have been performed to infer the structural changes of all-trans and all-cis forms of cyclo[(1R,3S)-3-aminocyclohexanecarboxylicacid(γ-Acc)-α- Glycine(Gly)]3 hexapeptide. The backbone conformations of the above peptide have been analyzed using the valence and peptide deformation angles applying B3LYP/6–311G\*\* level of theory. The conformational preference of the backbone of all-trans and all-cis cyclo[(1R,3S)-γ-Acc-Gly]3 hexapeptides is found to depend on the puckering of cyclohexane rings. The non-uniform distribution of water inside the cavity is observed, where sometimes water molecules formed a chain like conformation through hydrogen bond networks while traversing the pore of all-cis cyclo[(1R,3S)-γ-Acc-Gly]3 peptide. Larger relaxation times of the order of a hundred to two hundred pico seconds for active site…water hydrogen bond interactions were noticed. The hydrophobic nature of the cavity of all-trans cyclo[(1R,3S)-γ-Acc-Gly]3 due to the presence of cyclohexane moiety has been analyzed. Further this investigation emphasized on the non-transport of molecules through the pore of all-trans cyclo[(1R,3S)-γ-Acc-Gly]3 peptide due to the obstruction produced by cyclohexane groups.