**ABSTRACT**

The quantum mechanics/molecular mechanics ONIOM calculations have been performed to study the structure and metal-ion binding properties of all-trans cyclo [1R-3S-γ-Acc- Gly] 3 hexapeptide nanotube (TAG) 3 PNT. The intersubunit distances and tube angle of (TAG) 3 PNT exhibited the sturdy nature of (TAG) 3 stacks upon Li +, K +, Mg 2+, and Zn 2+ enclosure. The calculated dimer binding energies of (TAG) 3 PNT and its ionic complexes confirm that the building blocks are bound by C=O...H-N hydrogen bond interactions. The binding energy of (TAG) 3 PNT with ions interacting at the surface cavity exhibit the affinity of ions at the entrance of the channel and the many-body analysis for the ion interacting at the central region substantiates the major contribution of two-body interactions to the total binding energy. In general, the binding energies of (TAG) 3 PNT metal ion interacting complexes with well-maintained channel shows α-γ hybrid cyclic peptides as the promising peptidic nanochannels of biological interests.