**Abstract**

The structural and anion binding properties of all-trans cyclo[(1R,3S)-γ-Acc-Gly]3 hexapeptide[named as (TAG)3] were explored via quantum chemical studies. The (TAG)3 form complexes with F-, Cl-, and Br- ions inside the cavity exhibiting receptor like conformation. The structural arrangement of (TAG)3 upon ionic enclosure coincides well with the experimentally obtained -γ cyclic peptide anionic complexes. A good consistency is noted between geometrical parameters and electronic effects. The concentrated LUMO sites in (TAG)3 are useful in deciding the selectivity of N-H group for strong hydrogen bond interaction with anion. This study emphasize that the minimal structural distortions would have pronounced effect over anion binding affinity. The overall structure of (TAG)3 is found to be highly rigid upon Cl- and Br- ionic enclosures. The strong association of (TAG)3 towards inorganic anions with large binding energies, in general shows the hybrid α-γ cyclic peptides as promising anion receptors.