**Abstract**

This study explores the effect of N-(2-aminoethyl)-glycine peptide chain incorporated at the backbone of nucleic acid dimeric strands on the basis of reactivity descriptors. The structures of obtained PNA dimeric strands were examined through backbone (*α*, *β*, *γ*, *δ*, *ε* and *ω*) and linker (*χ*1, *χ*2 and *χ*3) torsions. The calculated torsions were found to coincide well the available experimental and theoretical data. The peptidic chain incorporated nucleic acid dimers show a drastic change in global reactivity descriptor (*gr*) values. The vertical ionisation potential (*VIP*) and polarizability (*α′*) of peptide chain incorporated Guanine constructs are found to be higher by about 0.24 eV and 98.49 *Å*3 than their natural counterparts. The obtained *gr* along with frontier molecular orbitals depict G-containing dimeric strands to have efficient donor and acceptor capability with improved sensitivity upon peptide chain inclusion. This study in general could serve as a basic tool to understand the reactivity properties of PNA modularities, which are the possible building blocks of extended nanostructures.