**Abstract**

Time dependent density functional theory (TDDFT) calculations using B3LYP/6-311++G\*\* level of theory were presented to understand the basic structural properties of peptidic chain added Watson Crick base pairs and compared to their natural counterparts. The excitation energy, oscillator strength, energy gap and wavelength of the all the base pairs were taken for the analysis. This study would pave way to understand the electronic excitation properties of all the Peptide Nucleic Acid (PNA) base pairs for the better understanding of the transitions and the luminescence properties of synthetic oligonucleotides structures.