**ABSTRACT**

Density functional theoretical studies on hydrogen-bonded complexes of serotonin with methanol/ ethanol have been carried out in a systematic way. The conformational analysis led to ten stable conformers that can be either gauche or anti depending on the dihedral angle values taken by ethylamine side chain and the 5-hydroxyl group. Serotonin-molecules strongly bind with ethanol than methanol. Ethylamine side chain is the most reactive site in both methanol/ethanol complexes and it is responsible for the stability order. The topological parameters, electron density, and Laplacian of electron density show excellent correlation with the hydrogen bond length. Natural bond orbital analysis confirms C–H….O hydrogen bond formed between the serotonin–alcohol complexes to be red shift in nature except for Gph(out)anti complex both with methanol and ethanol to be blue shifted. The energy decomposition analysis reveals that strong interactions between serotonin and ethanol/methanol are due to the attractive contributions from the electrostatic component.