Intermolecular interactions between dopamine and promazine using computational methods

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Dopamine (3, 4-dihydroxyphenylethylamine, DAH2), an important neurotransmitter, is existing in the mammalian central nervous system [1-3]. Its improper regulation is associated with neurological diseases such as Parkinsonism, where dopamine levels are reduced and schizophrenia, which can be related to excess activity of dopamine. Promazine (PZ) is a pyschotropic drug which is used extensively in mental disorders and anticancer activities. Its interactions in metabolism with the serotonin are important in terms of its biological activity. Biologically important aromatic molecules like basic nucleotides, aromatic amino acids, some drugs have π-electron systems. In this study, intermolecular interactions between photophysically excited promazine and naturally occurring hormone (dopamine) in the human body at ground-state will be investigated using computational tools. Conformational analyses have been performed to determine the initial structures for promazine and hormone (serotonin) using Spartan 08 [4]. Ground state geometry optimizations are first performed with Gaussian 09 [5] at the ω-B97XD/6-31G(d,p) level of DFT theory without symmetry constraint in gas phase and water phase, solvation calculations were performed by Tomasi's Polarizable Continuum Model (PCM) [6,7]. The electronic transitions were calculated by the time-dependent density functional theory (TD-DFT) with CAM-B3LYP, B3LYP and ω-B97XD methods using 6-311++G(d,p) basis set in gas phase and in water. Molecular orbitals, energy differences of frontier orbitals and electrostatic potentials for studied molecules were investigated. Intermolecular charge transfer between HOMO-LUMO orbitals of DA-PZ complex was observed in both media.

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