Interplay of hydrogen bonding in deciding the conformers of psilocin: Computational insights

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Abstract

Conformational analysis of psilocin, a psychedelic molecule revealed two stable conformers designated as conformer-A and B which were 4.97 kcal/mol apart in energy among many other high energy conformers. AIM analysis revealed that the conformer-A (global minimum) is stable due to intramolecular H-bond formation between ethyl amine nitrogen and indolic hydroxyl group. This is in contradiction to earlier X-ray crystal studies of this molecule reported in literature. Dimers of both conformer-A and B were studied utilizing DFT method and it was observed that even in the dimer of conformer-A the intramolecular H-bond energy dominates over the intermolecular H-bond. Other calculations namely NBO, FMO, charge analysis, ESP mapping corroborated the AIM results in a significant manner. The spectroscopic study including UV, 1H-NMR and vibrational modes calculation were found to be in good agreement with the data reported in literature.

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