Conformations of 5-Hydroxytryptamine (Serotonin) in Solution

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The conformation of the neuropeptide 5-hydroxytryptamine (serotonin) was examined experimentally and computationally, with an aim to find the important conformations in solution to model physiological conditions. This was done using a combination of static quantum chemical calculations, molecular dynamics simulations, and resonance Raman spectroscopy. Vibrational frequencies were compared for explicit and implicit solvation models as well as isolated serotonin to ascertain solvation effects. Frequencies were obtained using the B3LYP/6-311+G(d,p)//B3LYP/6-31+G(d,p) model chemistries and matched to experimental data. As expected, there appear to be nine important side chain configurations. These nine conformations are mirrored in gas-phase tryptamine (T.S. Zwier; "Laser Spectroscopy of Jet-Cooled Biomolecules and Their Water-Containing Clusters: Water Bridges and Molecular Conformation," *Journal of Physical Chemistry A*; **2001**; *105*; 8827).

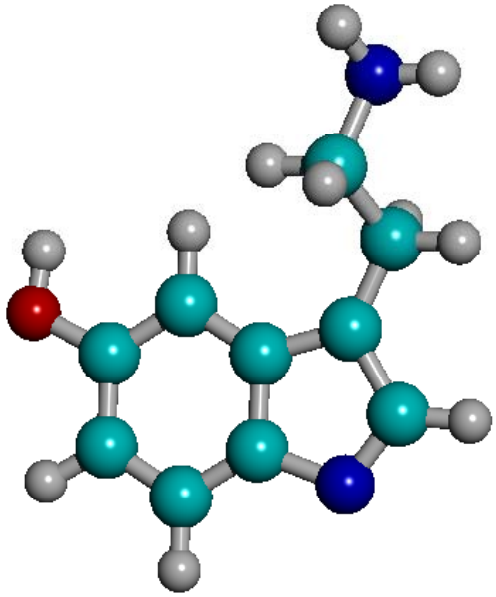

Figure 1. 5-hydroxytryptamine