Quantum-Chemical Study on the Electronic Structure and Ligand–Receptor Binding Mechanisms of Some Pyridin-4(1*H*)-one and Pyran-4-one Derivatives

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Abstract—Molecular structure optimization of a series of pyridin-4-one and pyran-4-one derivatives, namely 5-hydroxy-2-hydroxymethylpyridin-4(1*H*)-one, 5-hydroxy-1-methyl-4-oxo-1*H*-pyridine-2-carboxylic acid, and 5-hydroxy-2-hydroxymethylpyran-4-one (kojic acid) as free acids, the corresponding anions, calcium salts, calcium chelates, and calcium chelate calcium salts, was performed *ab initio* in terms of the restricted Hartree–Fock method with 6-31G* basis set using GAMESS program. The effects of salt and complex formation on the geometric and electronic structure of these molecules were analyzed. The solvation effects were examined by complete geometry optimization of all substrates in terms of the polarized continuum model (PCM) with dielectric constants ε of 10 and 78.3. The energies of formation of the salts and complexes were estimated. A set of geometric parameters responsible for the possibility of ligand–receptor binding with participation of pyran-4-ones and pyridin-4(1*H*)-ones and probable mechanism of binding of the latter to opioid receptors were proposed on the basis of the calculation data.

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