Quantum chemical study of quinolones

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Abstract

4-Oxoquinolines represent a group of heterocyclic compounds characterized with multispectral biological activity, mainly antibacterial (inhibitors of DNA gyrase, topoisomerase IV), multispectral antitumor, coccidiostatic and even antiviral activity. Nowadays, fluoro-substituted 4-oxoquinoline-3-carboxylic acids (e.g., norfloxacin, ciprofloxacin, ofloxacin, sparfloxacin, enoxacin) are applied in the medical care as broad-spectrum antibiotics. Previously it was found that upon UVA irradiation (315 nm – 400 nm) fluoroquinolones induce photosensitive reactions with phototoxic and photoallergic responses, and consequently, a great attention was focused on investigations of their photoinduced processes.
In this work, we will focus the attention on the quantum chemical calculations and spectroscopic characteristics of fluoroquinolones. The electronic structure of the molecules was calculated by Density Functional Theory (DFT) and at *ab initio* levels and their photophysics has been investigated by means on time-dependent TD-DFT. DFT calculations were based on the Becke's three parameter hybrid functional using Lee, Yang and Parr correlation functional (B3LYP). The *ab initio* Coupled Cluster (CC) approach was chosen for the reference calculations.

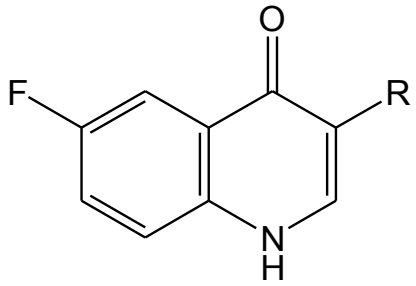

Fig. 1: Structure of studied fluoroquinolones.

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