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Probing the Structure of Moxifloxacin and Norfloxacin by Density Functional Theory and Raman Spectroscopy*

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In the present work, structures of two fluoroquinolone molecules namely Moxifloxacin and Norfloxacin are investigated using density functional theory and the Raman spectroscopy. The density functional theory calculation with B3LYP-6-31+G(d,p) level of theory reveals several structures of two molecules. The low energy stable structures of Moxifloxacin show multiple intramolecular H-bonds which could be responsible for the stabilization of these structures, however, the orientation of the (4aS, 7aS)-hexahydro-1H-pyrrolo[3,4-b]pyridin (hpb) ring determines the most stable structure. In Norfloxacin, the orientation of the ethyl group in the plane perpendicular to the ring frame determines the most stable structure whereas, the orientation of piperazine ring is critical for the determination of stable structure of the Norfloxacin zwitterion. Complexes of most stable structures of Moxifloxacin and Norfloxacin with one and two water molecules were also calculated. The Raman spectra were calculated for low energy structures of Moxifloxacin and Norfloxacin and also for their complexes with one and two water molecules. The experimental Raman spectra were obtained on powder sample of two molecules utilizing our lab-built Raman spectroscopy setup. The experimental Raman spectra were analyzed in light of the calculated Raman spectra of neutral molecules and their complexes with water. It was found that, in the powder form, the Raman spectra of two molecules can be better explained if intermolecular H-bonding with water molecules is considered. The study, therefore, confirms the hygroscopic nature of two molecules under ambient environment.

Keywords: Moxifloxacin, Norfloxacin, density functional theory, Raman spectroscopy.

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