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Global Reactivity Descriptors of Norfloxacin, Sulfanilamide and Sulfadiazine †

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Abstract: Norfloxacin (NOR) is a fluoroquinolone used to treat urinary tract infections. Sulfadiazine (SDZ) and sulfanilamide (SNA) are antibacterial sulfonamides, the first has a broad spectrum of action, and the second is the lead compound of the family. In this work were calculated the excited state energies of NOR, SNA, and SDZ were in the gas phase and in different solvents: n-hexane, cyclohexane, ethanol, methanol,1-propanol, 1-butanol, 1-octanol, acetonitrile, and water. The optimization of the NOR, SDZ, and SNA molecules was performed using the density functional theory (DFT) method with the CAM-B3LYP 6-31+G(d) level of theory, and the energies were computed with TD-CAM-B3LYP 6-31+G(d). In addition, the local structural parameters HOMO, LUMO, energy gap, hardness, softness, potential, and electrophilicity were calculated. NOR, SNA and SDZ have high kinetic stability and low chemical reactivity (HOMO-LUMO energy gap of 7.03, 7.90, and 7.40 eV, respectively). The three drugs can be regarded as strong electrophiles (electrophilicity > 1.5 eV), irrespective of the solvents in which the calculations have been performed, so they are susceptible to nucleophilic attack. The global descriptors of NOR, SNA, and SDZ were calculated and characterized.

Keywords: sulfanilamide; sulfadiazine; norfloxacin; global descriptors.

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Conflicts of Interest

The authors declare no conflict of interest.