A Computational Study of the Acid Dissociation in the Sulfonamide Group

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The sulfonamides constitute an important class of drugs with widely uses like antibiotic, anti-diabetic, diuretics, anticonvulsants, stimulant and others [1, 2]. Sulfa drugs were first antibiotics to be used systemically after revolution in medicine, on the other hands, nowadays your results stand out with just 3% adverse reactions when treated with antimicrobial agents [3, 4]. Biological activities are connected with chemical structure and physicochemical properties like pKa (the logarithm of negative acid dissociation constant) [5, 6]. pKa value is crucial to development of drug design mainly when a functional group is not modified [6, 7]. In this study, 19 molecules composed by sulfonamide group were optimized using M06-2X/6-311+G(d,p) and UM06-2X/6-311+G(d,p) levels to neutral and deprotonated molecules, respectively [8]. Then, we perform an investigation about the level of theory of calculations and basis set functions that can describe accurately the pKa values of these molecules. The obtained results were compared with the experimental data. From this comparison, it was possible to indicate the the best level of calculation and basis set functions to describe this class of molecules. Furthermore, this study indicate also how the radicals modify the pKa values. These features are very important to in-silico drug design.

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