Poster

Investigations of the biological activity of new sulfanilamide derivative: single crystal X-ray diffraction analysis, DFT computational, *in-silico* ADME and molecular docking studies.

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Sulfanilamides were the first chemical drugs used as preventive and therapeutic agents against various infection diseases [1]. They generally act as structural analogues of *para*-aminobenzoic acid and therefore inhibit dihydropteroate synthase [2]. After the discovery of Penicillin [3], their use decreased significantly. Nevertheless, in recent years, their synergistic activity has gradually attracted the attention of researchers [4-5]. During our investigation we successfully synthesized a new compound derived from sulfanilamide, viz. (2-(2-hydroxyphenyl)quinoline-6-sulfonamide. It was prepared by two-step reaction (reflux and solvothermal) and characterized by single-crystal X-ray diffraction, which indicates that the asymmetric unit of title compound (I) contains two crystallographically independent molecules (A and B). In addition, a computer study was carried out at the theoretical level DFT-B3LYP/6-31G+(d,p) on the spectroscopic properties, including FT-IR, UV-visible and ^{1}HNMR spectroscopies and the energy gap was determined using the HOMO and LUMO energy values. Further,Drug-likeness and pharmacokinetics parameters revealed that the compound exhibited favorable ADME properties. Finally, molecular docking study was carried out to investigate the possible binding mode of the sulfanilamide derivative, using GOLD program, and revealed strong interactions. Considering the findings of the study, it has been proven that this new compound constitutes a promising therapeutic agent capable of managing bacterial infections.

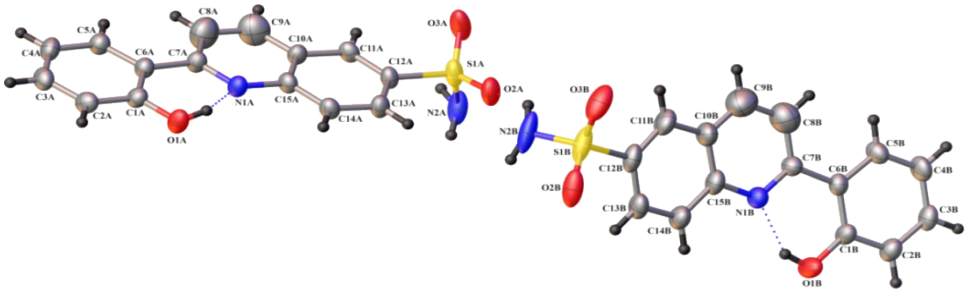

Figure 1. View of the two independent molecules of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

KEYWORDS: Sulfanilamide*; Single-crystal X-ray diffraction; DFT; Molecular Docking; Pharmacokinetics.*

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