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Synthesis, Analysis of H-bonding Interactions, Molecular Docking Studies and Biological Activity Investigations of Molecular Salt formed between the Drug Sulfathiazole and *p*-Toluenesulfonic acid

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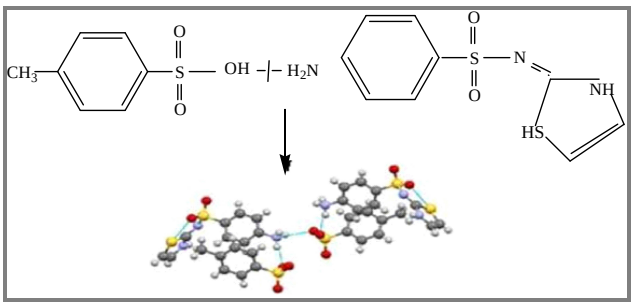
ABSTRACT

The drug sulfathiazole known to be a proton acceptor interacts with p-toluenesulfonic acid by abstracting the proton and forms a molecular salt through hydrogen bonding interactions. The molecular structure has been studied by single crystal X-ray diffraction studies and the asymmetric unit is found to contain two protonated sulfathiazole cations bonded to two p-toluene sulfonate anions. N-H···O hydrogen bonds are formed between -SO_3 group of p-toluenesulfonic acid and -NH_2 of sulfathiazole. The crystal packing is stabilized by N-H···N intramolecular hydrogen bonds in sulfathiazole and secondary H-bonds C-H···C. The new adduct is found to possess a greater antibacterial and antifungal activities compared to sulfathiazole and the activities are comparable to the standard drugs used as control. Further, the molecular docking studies compounded the bioactive nature of the molecular salt formed.

Graphical Abstract



Molecular salt formed between *p*-toluenesulfonic acid and sulfathazole

Keywords: Molecular salts, Multiple H-bonding, Molecular docking studies, Biological activity.