

Synthesis, Crystal Structure Characterization, Hirshfeld Surface Analysis and Biological Activities of Two Schiff Base Polymorphs Derived From 2-Aminobenzonitrile

Authors : Nesrine Benarous, Hassiba Bouguerria, Nabila Moussa Slimane, Aouatef Cherouana

Abstract : Crystal polymorphism is important for the synthesis of more potent and bioactive pharmaceutical compounds, including their different properties, such as packing arrangement and conformation. In fact, polymorphism plays a vital role in drug development. Different parameters affect the crystallization and give their degree of freedom. Several properties affected polymorphism, like kinetics, thermodynamics, spectroscopy, and mechanical property. Various techniques are used for characterizing polymorphs, are crystallography, morphology, phase transitions, molecular motion, and chemical environment. In this work, crystal structures of two polymorphs (I and II) of the Schiff base (SB) title compound were prepared by condensation reaction. The crystal structures of both polymorphs were determined by single X-ray analysis. The two polymorphs crystallize in two different space groups: P21/c for I and Pbc_a for II. The dihedral angles between the two phenyl rings are 4.81° for I and 82.27° for II. Both crystal structures are built on the basis of moderate and weak hydrogen bonds, π -stacking, and halogen-halogen interactions. On the other hand, Hirshfeld surface (HS) analysis indicates that the most important contributions to the crystal packing for the two polymorphs are from Cl \cdots H/H \cdots Cl, H \cdots H, and N \cdots H/H \cdots N contacts. These are followed by C \cdots H/H \cdots C for compound I and C \cdots C and by C \cdots H/H \cdots C contacts for compound II. Afterwards, the in vitro antibacterial activity revealed that the SB have been found effective against G- bacteria *Klebsiella pneumonia* and G+ bacteria *Staphylococcus aureus* with MIC value of 14.37 μ g/mL. Moreover, the SB exhibited moderate toxicity against Brine Shrimp with LC50 value of 44.19 μ g/mL.

Keywords : polymorph, crystal structure, hirshfeld surface analysis, in vitro antibacterial activity, toxicity

Conference Title : ICCABES 2023 : International Conference on Chemical, Agricultural, Biological and Environmental Sciences

Conference Location : Istanbul, Türkiye

Conference Dates : May 04-05, 2023