World Academy of Science, Engineering and Technology
International Journal of Chemical and Materials Engineering
Vol:17, No:05, 2023

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

**Authors :** Nesrine Benarous, Hassiba Bougueria, 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. Severalproperties 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 Pbca for II. The dihedral angles between the two phenyl rings are 4.81º for I and 82.27º for II. Both crystal structures are built on the basis of moderate and weak hydrogen bonds, □-stacking, and halogen□halogeninteractions. 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□H/H□Cl, H□H, and N□H/H□N contacts. These are followed by C□H/H□C for compound I and C□C and by C□H/H□C contacts for compound II. Afterwards, the in vitro antibacterial activity revealed that the SB have been found effective against G- bacteria Klebsiella pneumonia andG+ bacteria Staphylococcus aureuswith MIC value of14.37µg/mL. Moreover, the SBexhibited moderate toxicity against Brine Shrimp with LC50 value of 44.19µg/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