Available online at **www.joac.info**

ISSN: 2278-1862

Journal of Applicable Chemistry

2018, 7 (3): 496-500

(International Peer Reviewed Journal)

Structural Characterization and Docking Studies of (Z)-N-Phenyl Benzo Hydrazonoyl Chloride Derivative as Promising Antimicrobial *Acinetobacter Baumannii* Penicillin-Binding Protein Target

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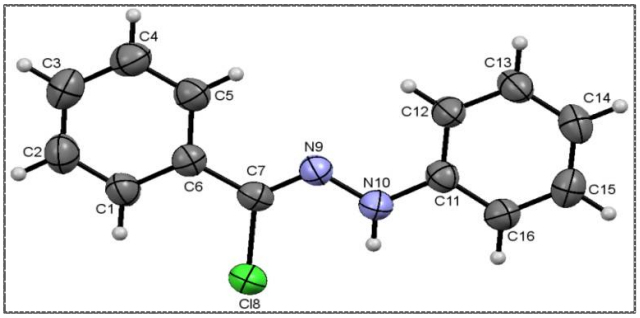
Accepted on 16th April, 2018

ABSTRACT

*Computer-aided prediction of interaction of benzohydrazonoyl chloride derivatives with protein target was carried out using open source program Auto Dock. Overall findings of the executed investigations highlight these compounds as very promising potent, broad spectrum antiviral agents. Molecular docking studies showed that the tested compound induced good fitting and forming different hydrogen bonds with the amino acid residues at the active sites of antimicrobial acinetobacter baumannii penicillin-binding target. A moderately high-yield synthesized compound (Z)-N-phenyl benzohydrazonoyl chloride (**4a**) was characterized and structure was confirmed by X-ray diffraction studies. The molecule crystallizes in orthorhombic under the space group Pcab, with cell parameters a = 7.606(1)Å, b = 11.8817(16)Å, c = 25.219(3)Å and Z=8. Crystal structure stabilized by an N10-H10...Cl8 and C1-H1...Cl8 intramolecular hydrogen bonds.*

Graphical Abstract



ORTEP of the molecule (4a) with thermal ellipsoids drawn at 50% probability

Keywords: Crystal structure, Docking study, Antimicrobial target, C-H..Cl and N-H..Cl interaction.