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Structure and Molecular Modeling Studies of 1,3-Diphenyl-1*H*-Pyrazole Derivative as Potential Human Kinase Inhibitor

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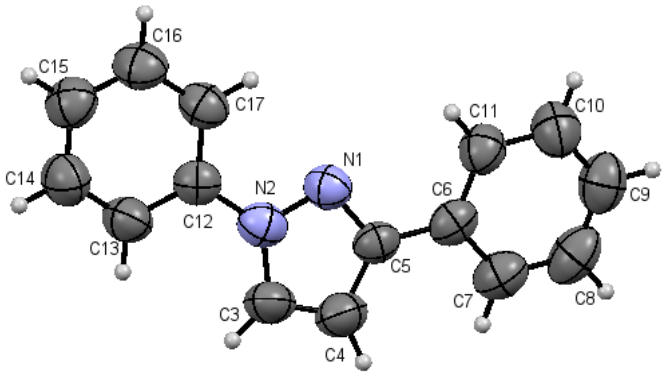
ABSTRACT

*Molecular modeling was performed for 1,3-diphenyl-1H-pyrazole (**2a**) derivative with Aurora A (3FDN) inhibitor employing flexible ligand docking method by using Auto Dock. The title molecule found to be minimum binding energy-6.31 kJmol^{-1} with ligand efficiency of -0.37. The molecular modeling results showed that pyrazole derivative (**2a**) with Aurora A inhibitor are good inhibition constant, vdW + Hbond + desolv energy with best RMSD value. The compound 1,3-diphenyl-1H-pyrazole derivative (**2a**) was characterized and structure was confirmed by X-ray diffraction studies. The molecule crystallizes in monoclinic under the space group $P2_1/c$, with cell parameters a = 5.619(2)Å, b = 9.362(4)Å, c = 22.553(10)Å, β = 95.429(7)° and Z=4. Crystal structure stabilized by anC11-H11...N1 and C17-H17...N1 intramolecular hydrogen bonds.*

Graphical Abstract:



ORTEP of the molecule-pyrazole derivative with thermal ellipsoids drawn at 50% probability

Keywords: Docking study, Aurora A inhibitor, crystal structure, C-H…N interaction.