Poster Presentation

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Crystal structure, DFT, docking studies of substituted pyridines

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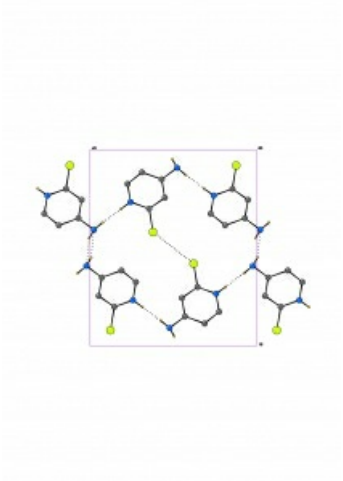
The study of substituted pyridines, mainly amino pyridines attracts pharma chemists due to their wide range of Pharmacological properties[1]. Pyridine ring systems are very widely distributed in nature, especially in plant kingdom and are used in the preparation of drugs for certain diseases such as cancer tuberculosis, neural disorders etc.,[2]. In present study reports crystal structure, DFT molecular modeling and docking studies of series of substituted of amino pyridines. The single crystals of 4-amino 2-cholro pyridine(I), diethyl 2, 6-dimethyl-4-phenylpyridine-3, 5-dicarboxylate (II), N-ethyl-6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydro pyrimidine-5-carboxamide (III) were grown by slow evaporation using methanol. The datasets were collected using Xcalibur, Eos, Nova X-ray diffractometer at 293K. Using Olex2, the structure solution with the ShelXT using Intrinsic Phasing and refined with the ShelXL refinement package using Least Squares minimization to final R-values 0.045, 0.0676 and 0.056 for (I) (II) and (III) respectively. Investigation of intermolecular interactions and crystal packing via Hirshfeld surface analysis reveals that there are more than two third inter molecular C—H•••O, N—H•••O, O—H•••O interactions. The molecular geometry was also optimized using density functional theory using (DFT/B3LYP) method with the 6-311G(d,p) basis set and compared with the experimental data. In addition to the optimized geometrical structure, molecular orbital, molecular electrostatic potential (MEP) and chemical reactivity studies of the compound have been investigated by using DFT. The docked studies was carried out for all the compounds with CDK inhibitor and which resulted a binding affinity values in the range -2.3 −6.3 kcal/mol and the results suggest that the compounds might exhibit inhibitory activity against CDK inhibitor.

[1] H. Camp, J. Derk, (2001) Handbook of Am. Chem. Soc., 31.
[2] Bombicz P, Gruber T, Fischer C, Weber E, Kalman A (2014) Cryst Eng Comm 16, 3646-3654.



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