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X-Ray Crystallographic, Hirshfeld Surface Analysis and Docking Study of Phthalyl Sulfacetamide

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Abstract : Phthalyl Sulfacetamide belongs to well-known member of antimicrobial sulfonamide family. It is a potent antitumor drug. Structural characteristics of 4-amino-N-(2quinoxalinyl) benzene-sulfonamides (Phthalyl Sulfacetamide), C14H12N4O2S has been studied by method of X-ray crystallography. The compound crystallizes in monoclinic space group P21/n with unit cell parameters a= 7.9841 Å, b= 12.8208 Å, c= 16.6607 Å, α= 90˚, β= 93.23˚, γ= 90˚and Z=4. The X-ray based three-dimensional structure analysis has been carried out by direct methods and refined to an R-value of 0.0419. The crystal structure is stabilized by intermolecular N-H…N, N-H…O and π-π interactions. The Hirshfeld surfaces and consequently the fingerprint analysis have been performed to study the nature of interactions and their quantitative contributions towards the crystal packing. An analysis of Hirshfeld surfaces and fingerprint plots facilitates a comparison of intermolecular interactions, which are the key elements in building different supramolecular architectures. Docking is used for virtual screening for the prediction of the strongest binders based on various scoring functions. Docking studies are carried out on Phthalyl Sulfacetamide for better activity, which is important for the development of a new class of inhibitors.

Keywords : phthalyl sulfacetamide, crystal structure, hirshfeld surface analysis, docking
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