



Original Article

Synthesis, Characterisation, and Biological and Computational Studies of Novel Schiff Bases from Heterocyclic Molecules

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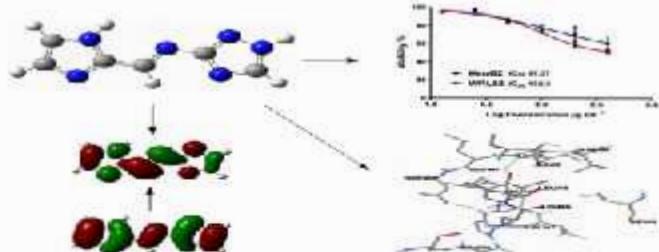
Anticancer

Molecular Docking

ABSTRACT

Four new Triazole Schiff Bases were synthesized through the green condensation and were structurally confirmed by mass spectroscopy, IR, ¹H NMR, TGA, and DSC. The chief advantages of the reported technique were its working ease, very mild reaction conditions, short reaction time, and high yield. Quantum chemical calculations were applied to investigate the optimum geometry and electronic structure of the compounds. S1-S4 DFT/B3LYP/6-31+G (d) was performed to determine the chemical quantum descriptors (CQDs). An analysis of the CQDs showed that the S2 compound had a higher molecular stability. The findings of the computational research revealed that there was a close interaction between the theoretical and experimental data. The synthesized compounds were tested for their anticancer activity against two cell lines, MCF-7 and Heptz. The results revealed that the S3 and S4 compounds had a remarkable activity, with IC₅₀ of 64.84 μ g/ml and 23.57 μ g/ml, respectively, thus, making them crucial components for anticancer medicines in future studies. Molecular docking tests were carried out on the S3 and S4 compounds with the receptors 2LKN and 3P90. The results explained that the compounds were effective in inhibiting the receptors with a good binding energy to confirm their anticancer activity.

GRAPHICAL ABSTRACT



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