6th International Conference on
Organic & Inorganic Chemistry
August 08-09, 2019 | Amsterdam, Netherlands

Synthesis, antitumor activity, molecular docking and DFT study of novel pyrimidiopyrazole derivatives

Asmaa M Fahim[1], **Mohamed S Elshikh**[2] and **Nora M Darwish**[3]
[1]National Research Center, Egypt
[2]King Saud University, Saudi Arabia
[3]Ain Shams University, Egypt

Facile synthesis of innovative heterocyclic compounds from the reaction of 2-cyano-N-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl) acetamide (3) with dimethyl formamide dimethyl acetal (DMF-DMA) to afford the corresponding (E)-2-cyano-3-(dimethylamino)-N-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl) acrylamide (4) utilizing microwave irradiation. The condensation reactions of (E)-2-cyano-3-(dimethylamino)-N-(2,4-dioxo-1,2,3,4-tetrahydro pyrimidin-5-yl) acrylamide (4) with hydrazine derivatives to afford the equivalent pyrazole derivatives 6a and 6b; respectively. Selected synthesized compounds demonstrated outstanding in-vitro antitumor activity against HepG2 cell line. Moreover, the evaluation of the greatest utilizing of molecular docking using Auto Dock tools for compound 1-phenyl-1H-pyrazole-5-carboxamide derivative 6b which interact with 4hdq synthase complex with interaction energy score (-4.5 Kcal/mol) which is superior with short distance (1.727 Å and 2.027 Å). Also, the optimized molecular structure of the compounds, bond length, bond angles, energy gap HOMO-LUMO, IR frequencies were observed through DFT/B3LYP/6-31G(d) which examine the equilibrium geometry of the innovative compound pyrazoles 6a and 6b and the stability of HOMO/LUMO molecular orbitals.