World Academy of Science, Engineering and Technology
International Journal of Chemical and Molecular Engineering
Vol:18, No:08, 2024

Benzene Sulfonamide Derivatives: Synthesis, Absorption, Distribution, Metabolism, and Excretion (ADME) Studies, Anti-proliferative Activity, and Docking Simulation with Theoretical Investigation

Authors : Asmaa M. Fahim

Abstract : In this elucidation, we synthesized different heterocyclic compounds attached to Benzene sulfonamide moiety via (E)-N-(4-(3-(4-bromophenyl)acryloyl)phenyl)-4-methyl benzene sulfonamide which is obtained from Nucleophilic substitution reaction between 4-methylbenzene sulfonyl chloride and 1-(4-aminophenyl)ethan-1-one in pyridine to get N-(4-acetyl phenyl)-4-methyl benzenesulfonamide which reacted 4-bromobenzal dehyde undergoes aldol condensation in NaOH to afford the corresponding chalchone 4. Moreover, the reactivity of chalchone 4 showed several active methylene derivatives utilized the pressurized microwave irradiation as a green energy resource. Chalcone 4 was allowed to react with ethyl cyanoacetate and acetylacetone, respectively, at 70 °C with pressure under microwave reaction condition to afford the 5-cyano-6-oxo-1,2,5,6-tetrahydropyridin-2-yl)-4-methylbenzenesulfonamide 6 and N-(4'-acetyl-4''-bromo-5'-oxo-2',3',4',5'-tetrahydro-[1,1':3',1''-terphenyl]-4-yl)-4-methylbenzenesulfonamide 8 derivatives. Moreover, the reactivity of this sulphonamide chalchone with NH2NH2 in EtOH and acetic acid, which gave 2,5-dihydro-1H-imidazol-4-yl)-4-methyl benzenesulfonamide, 1H-pyrazol-3-yl)-4-methyl and reactivity with NH2OH.HCl gave isoxazol-3-yl)-4-methylbenzenesulfonamide derivatives. The synthesized compounds were screened for their ADME properties and directed to antitumor activity on HepG2 hepatocellular carcinoma and MCF-7 breast cancer and exhibited excellent behavior against standard drugs; these results were confirmed through molecular simulations with different proteins. Additionally, the Density Functional Theory analysis of optimized structures investigated their physical descriptors, FMO, ESP and MEP, which correlated with biological evaluation.

Keywords : synthesis, green chemistry, antitumor activity, DFT study
Conference Title : ICGC 2024 : International Conference on Green Chemistry
Conference Location : Venice, Italy
Conference Dates : August 15-16, 2024