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Synthesis and characterization of new niacinamide compounds and computational and experimental investigation of their anticancer and antibacterial activity

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4-Niacinamide compounds have been synthesized and characterized. These compounds have been optimized at B3LYP-D3/6-311++G(d,p) level in water. The electronic properties of these have been investigated by employing contour plot of frontier molecular orbitals, molecular electrostatic potential map and Fukui plot. Cell viability test have been carried out against colon, breast and gastric adenocarcinoma. Of the compounds studied, only NIA1 and NIA2 are found to be effective against stomach cancer. Molecular docking calculations against epidermal growth factor receptor and thymidine kinase have also been performed by *in silico* analysis. MM-GBSA analyses have been performed and binding energies between ligand and receptor have been calculated. Finally, ADME and pharmacophore analyses of the newly synthesized molecules have been performed. After considering all the results, it is observed that both experimental and computational results of NIA1 and NIA2 are in agreement with each other, with NIA1 showing better results than NIA2.

Keywords: DFT, Synthesis, Niacinamide, Anticancer, Antibacterial