

Synthesis, spectral studies and molecular docking analysis of some aryl hydrazide derivatives

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Four series of aryl hydrazides have been synthesized using potassium hydrogen phthalate-assisted condensation by stirring aryl hydrazines with various substituted benzaldehydes and acetophenones at room temperature. The yield of this condensation is more than 85%. The influence of solvent on the yield has been studied. These hydrazides have been characterized by their physical constants, UV, IR, NMR, and mass spectral data. The characteristic spectral frequencies have been correlated with Hammett substituent constants and Swain Lupton's parameters using single and multi-regression analysis. From the statistical analysis results, the spectral quantitative structure-activity relationships have been assessed. The ligand-protein interaction ability of these hydrazines have been examined using molecular docking analysis.

Keywords: Aryl hydrazides, Potassium phthalate, Spectral correlation, Molecular docking