

# Usins QSAR calculations on Pyridine Derivatives as drug to treatment of cushing's syndrome

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**Abstract** Cushing's Syndrome is one of the diseases that keep increasing in human Society. Ten million people almost affected with Cushing's Syndrome in each year. This disease is caused by improper disorder of hypophysis gland or Adrenal gland resulting in more dangerous disease such as cancer. In This work, QSAR study has been done on pyridine derivatives drugs Genetic algorithm (GA), artificial neural network (ANN), stepwise multiple Linear regression (stepwise-MLR) were used to create Then on non-Linear and Linear QSAR models. For This purpose, ab initio geometry optimization performed at B3LYP Level with a known basis set (6-31G). Hyperchem chemoffice and Gaussian (05W) softwares were used for geometry optimization of the molecules and calculation of the quantum chemical descriptors. According to the obtained results, we find out GA-ANN model is the most favorable method toward the other statistical methods. General studies with GA-PCR methods and GA-PLS and Jack-Knife in different Layers and different goals following compounds have the lowest deviation the best ingredients to make the drug are advised: The best described as: More 16U, R6e , SHP2, G2V. **Keywords:** Cushing's syndrome, pyridine, Quantitative structure activity relationship (QSAR), Genetic Algorithm (GA), Artificial Neural Network (ANN)

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