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*Abstract*

# Design of New Derivatives of Dimedone Molecules Using QSAR and Docking Molecular †

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**Abstract:** In this work, we investigated the quantitative relationship between biological activity against non-small cell lung cancer (NSCLC) and the molecular structure of a series of 38 cyclohexane-1,3-dione-dimidone derivatives. For this purpose, molecular descriptors calculated by DFT-B3LYP/6-31G, topological, and physicochemical analysis were used. The results of the evaluations of the quantitative activity structure relationship (QSAR) models developed in this work via Multiple Linear Regression and via Multiple Non-Linear Regression (MLR and MNLR) techniques indicate the high predictive power of these models, ($R^2$ = 0.913; $R^2_{CV}$ = 0.85, $R^2_{test}$ = 0.934) for the linear model and ($R^2$ = 0.991; $R^2_{CV}$ = 0.82; $R^2_{test}$ = 0.997) for the nonlinear model. Using predictions from the QSAR model, new molecular structures were designed, their activity against NSCLC was evaluated, and the most important interactions between these molecules and the human c-Met protein were predicted. The predictions from QSAR models, molecular docking, and an evaluation of the in silico ADMET properties suggested that 1 of the 16 newly designed molecules is a candidate that may be a drug for NSCLC.

**Keywords:** QSAR; ADMET; molecular docking; NSCLC; C-met



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