



## Anti-Proliferative Activity of Heterocyclic Compounds Based on Indole: QSAR study

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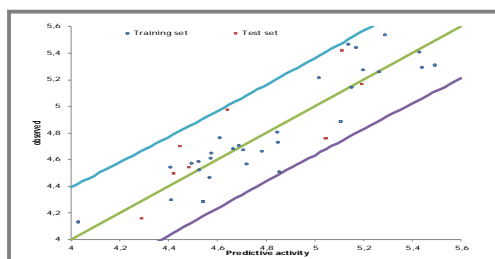
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### ABSTRACT

In work, a series of thirty-eight Indole derivatives known for their antiproliferative activity were studied by QSAR methods (Quantitative-Structure-Activity-Relationship). Multiple Linear Regression (MLR) and Multiple Non-Linear Regression (MNL) were used in model development. Refined models have been evaluated using the Leverage approach and the Inflation Factor (VIF). Some QSAR models have been subjected to numerous validation tests after their development. Given this, they gave notably encouraging outcomes upon validation ( $R=0.917$ ,  $R^2_{cv}=0.672$  for the MLR model and  $R=0.928$ ,  $R^2_{cv}=0.721$  for the MNL model). The results show that the most important descriptors affecting the antiproliferative activity which are crucial within the layout of recent set of the indole derivatives are the low-unoccupied-molecular-orbital-energy ( $E_{LUMO}$ ), the total-energy ( $E_T$ ), the dipole-moment( $\mu$ ), the partition-coefficient ( $\log P$ ) and refractive-index( $n$ ) descriptors. The influences of these descriptions on activity have been used to test and design new molecules with better activity compared to the predominant ones.

### Graphical Abstract



Observed and calculated activity obtained by MLR method.

**Keywords:** Molecular docking, Anti-cancer, Anti-depressant, Anti-bacterial, Binding affinities.