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2D and 3D QSAR Studies and Antibacterial Activity of 4-Methyl-3-(6-{[Arylmethylene] Amino}Pyridin-3-YL)-2H-Chromen-2-One Derivatives

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SUMMARY. 4-methyl-3-(6-{[arylmethylene] amino} pyridin-3-yl)-2H-chromen-2-one derivatives containing different functional groups have been synthesized and screened for their antibacterial activity against four different strains of bacteria. 2D and 3D QSAR analysis of synthesized derivatives were performed on Vlife MDS 3.5 software. The data set for QSAR studies encompassed activities of 64 molecules divided into training and test set. The best models were selected on basis of correlation coefficient (r^2) and internal and external predictivity (Pred_r^2) of the QSAR model. QSAR models reveled that electronic, steric and liphophillic parameters have correlation with antibacterial activity. The 3D interactions and their contributions indicate multi-targeted mode of action of the compounds.

KEY WORDS: 2D QSAR, 3D QSAR, Antibacterial activity, Chromen-2-one.

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