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OP-07

Computational Approach Towards the Development of Novel Imidazopyridine Derivatives as Potential Antidiabetic GSK3β Inhibitors

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Abstract:

A dataset of 29 novel imidazopyridine derivatives with potential antidiabetic GSK 3β inhibitory activity was subjected to 2D and 3D Quantitative Structure-Activity Relationship (QSAR) analysis with the help of VLife Molecular Design Suite (VLife MDS) ver 4.2.1. Out of the three methods used for 2D QSAR analysis viz. Partial Least Square (PLS), multiple linear regression (MLR), and principal component regression (PCR), the MLR method led to the statistically most significant model with r^2> 0.75, F>>tabulated value, chance correlation <0.001 and q^2>0.6. The 3D QSAR analysis on the data set by k-Nearest Neighbor Molecular Field Analysis (kNN-MFA) method was performed by Step Wise (SW) forward-backward, Genetic Algorithm (GA) and Simulated Annealing (SA) methods of which the model obtained through SW was statistically most significant having q^2>0.7. Results suggested that for better pharmacological activity, a 2-methoxyethyl substitution or propan-2-one substitution on at 4- position of pyridine ring and any methyl substitution on the ring would be detrimental for the activity while an aromatic ring at R_1 and hydroxyl group separated by 4 carbon distance on pyridine ring would be beneficial for the activity. Thus, by favorable modification of the lead structure, more selective and potent antidiabetic GSK 3 β inhibitors can be synthesized.

Keywords: 2D QSAR, 3D QSAR, VLife MDS, kNN-MFA, Imidazopyridine, antidiabetic, GSK3β inhibitors