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# QSAR and Pharmacophore Studies on Arylbenzofuran Derivatives as Histamine $H_3$ Receptor Antagonists

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Quantitative structure activity relationship (QSAR) studies using Molecular Design Suite (VLife MDS) software and pharmacophore studies using a web based pharmacophore identification server Pharmagist were performed on 29 compounds belonging to arylbenzofuran chemical class for their histamine $H_3$ receptor antagonistic activity. 2D QSAR analysis was performed using partial least square regression (PLSR) while k-nearest neighbour molecular field analysis (kNN-MFA) methodology was applied to derive 3D QSAR models. The variable selection method applied for both strategies was stepwise forward backward. The best 2D QSAR model had squared correlation coefficient ($r^2$) = 0.8662, cross validated correlation coefficient ($q^2$) = 0.6029 and predictive correlation coefficient (pred_$r^2$) = 0.3940. The QSAR model indicated that the T_3_N_5 (count of number of triple bonded atoms separated from nitrogen atom by five bonds in a molecule), T_C_C_7 [count of number of carbon atoms (single or double bonded) separated from any carbon atom (single or double bonded) by 7 bonds in a molecule] and T_2_3_5 [count of number of double bonded atoms (i.e. any double bonded atom, T_2) separated from any other triple boded atom by 5 bonds in a molecule] were the important determinants for $H_3$-receptor antagonistic activity. The generated predictive model using kNN-MFA had internal predictivity of 70.55% ($q^2$ = 0.7055) and external predictivity 60.00% (pred_$r^2$ = 0.60). The contribution 3D plot for this model showed that steric (S_579), electrostatic (E_453) and hydrophobic (H_779) interactions play important role in determining $H_3$-receptor antagonistic activity. The identified pharmacophoric features are aromatic (2), hydrophobic (2) and hydrogen bond acceptor (2). The findings of this work can be utilized for the development of novel $H_3$-receptor antagonists.

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