

QSAR studies on imidazoles and sulfonamides as antidiabetic agents

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Abstract. The main objective of the present study was to establish significant and validated QSAR models for imidazoles and sulfonamides to explore the relationship between their physicochemical properties and antidiabetic activity. Two dimensional QSAR models had been developed by multiple linear regression and partial least square analysis methods, and then validated for internal and external predictions. The established 2D QSAR models were statistically significant and highly predictive. The validation methods provided significant statistical parameters with $q^2 > 0.5$ and $\text{pred}_r^2 > 0.6$, which proved the predictive power of the models. The developed 2D QSAR models revealed the significance of SlogP and T_N_O_5, and Mol.Wt and SsBrE-index properties of imidazoles and sulfonamides on their antidiabetic activity, respectively. These results should prove to be an essential guide for the further design and development of new imidazoles and sulfonamides having better antidiabetic activity.

Keywords: antidiabetic, physicochemical properties, QSAR, validation.

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