Indian Journal of Chemistry
Vol. 63, February 2024, pp. 190-202
DOI: 10.56042/ijc.v63i2.6141

Quantitative structure activity relationship studies of potent Endothelin-A receptor antagonist for the treatment of pulmonary arterial hypertension

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Received 11 October 2023; accepted (revised) 25 January 2024

A traditional physicochemical descriptors-based QSAR analysis has been conducted on a data-set of Endothelin-A receptor antagonists for the treatment of pulmonary arterial hypertension. A variety of statistical techniques, including non-linear techniques like artificial neural networks and linear analytical techniques *i.e.*, 'Multiple Linear Regression' and 'Partial Least Squares' are implicated in current research. The development models have then been put through a validation process including the leave one out, which supported their high predictability and accuracy. A few statistical parameters have been used to build the model's predictive power and the resulting model has been found to have good statistical values, such as s=0.40, f=48.75, r=0.87, r^2=0.77, r^2CV=0.71 for training set. Three descriptors, including logP (whole molecule), total lipole (whole molecule), VAMP LUMO (whole molecule) are made relevant by the general model, which offers insightful information. As new results, these traits may be successfully used for the modelling and screening of new endothelin-A receptor antagonists that are active hypertensive drugs.

Keywords: Endothelin-A receptor antagonists, Quantitative structure activity relationship, Statistical analysis, Pulmonary arterial hypertension