

## QSAR Analysis of Structurally Similar Antitubercular Isatin Analogues

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**SUMMARY.** A series of structurally similar isatin analogues with antitubercular activity have been subjected for 2D and 3D QSAR analysis using V life MDS 3.5 software. The compounds were divided into training and test set of 44 and 11 each. Best QSAR models were selected on the basis of various statistical parameters like square correlation coefficient ( $r^2$ ), cross validated square correlation coefficient ( $q^2$ ), standard error of estimation (SE) and sequential Fischer test ( $F$ ). QSAR studies reveals that new isatin analogues with less bulky substitution on nitrogen of first position and at third position electropositive side chain of optimum four atoms length whose terminal atom is substituted with aromatic system bearing polar group may be better antitubercular agents.

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**KEY WORDS:** Antitubercular activity, Isatin, QSAR.

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