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Biological Prediction from Computational Approach, Synthesis, and Biological Evaluations of Newer Thiazolidine-2,4-dione Conjugates

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ABSTRACT Thiazolidine-2,4-dione is a toxophoric unit and its derivatives act as antimicrobial and antitubercular agents. Computational approach two-dimensional quantitative structure-activity relationship (2D-QSAR) was used to predict antitubercular activity of the thizolidine-2,4-dione derivatives. 2D-QSARS generated model using partial least squares regression method which predicted the statistically significant $r^2 = 0.3868$, $q^2 = 0.0193$, pred_$r^2 = 0.5240$, and F test = 3.7855. 2D-QSAR model equation denoted log(1/MIC) of the antitubercular activity correlated with thermodynamic descriptor SAMostHydrophobicHydrophilicDistance. Biological predicted derivatives of thiazolidine-2,4-dione (*Z*)-*N*-(2-(2,4-dichlorophenoxy)phenyl)-2-(5-substitutidene-2,4-dioxothiazolidin-3-yl)acetamide **(C_1-C_{10})** were synthesized and spectrally evicted from IR, ^{1}H NMR, ^{13}C NMR and Mass spectral data analysis as well as biologically evaluated against antitubercular and antimicrobial activities. From the biologically evaluated derivatives, compounds C_1, C_2, C_3 and C_6 were found to be active against the different antimicrobial species. Compounds C_1, C_3 and C_{10} are more progressive than others against antitubercular species.

KEYWORDS Two-dimensional structure-activity relationship, Partial least squares regression method, SAMostHydrophobicHydrophilicDistance, Thiazolidine-2,4-dione, Antimicrobial activity, Antitubercular activity.

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