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Exploring QSAR Models for the Selection of Candidate Inhibitors in Drug Development

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Abstract: *A Quantitative Structure–Activity Relationship (QSAR) model correlates the biological activity of a molecule with its structural characteristics using molecular descriptors that quantitatively define key structural features. In this study, novel molecular descriptors and modelling methods were developed for QSAR analysis across six target systems associated with diseases such as cancer, neurodegenerative disorders, HIV-AIDS, and malaria. The research introduced 2D image-based descriptors derived from optimized 3D molecular structures. These descriptors were constructed using Dijkstra's algorithm and multidimensional scaling to preserve interatomic shortest path distances and partial charges in two dimensions. Principal component analysis (PCA) and support vector regression (SVR) were employed to regress the descriptors against biological activity values, though these models were found to be computationally intensive. To enhance efficiency, a new 3D pseudo-molecular field (PMF) concept was developed based on intrinsic atomic properties such as electron affinity and electronegativity, rather than conventional electrostatic fields calculated from partial atomic charges. The PMF-based partial least squares (PMF-PLS) methodology, combined with Procrustes transformation, produced QSAR models with performance comparable to existing models while being computationally lighter. Additionally, a new regression approach, Varying Component Partial Least Squares (VC-PLS), utilizing the SIMPLS variant of PLS, was proposed for QSAR modelling. Both PMF-PLS and VC-PLS models were applied to screen natural compounds structurally similar to known bioactive molecules in the target systems. The screening outcomes from both models were consistent, and subsequent molecular docking studies validated the predicted interactions, supporting the reliability of the proposed QSAR methodologies for drug discovery applications.*

Keywords: QSAR , SVR , PMF , Drug Discovery

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