عنوان مقاله:

A Quantitative Structure-Activity Relationship Study of ۲, ۴, ۶-s-Triazine Derivatives as Antimalarial Agents

محل انتشار:

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خلاصه مقاله:

A quantitative Structure-Activity Relationship (QSAR) model was applied to the prediction of the antimicrobial activity of ۲۲ derivatives ۲, ۴, ۶-s-triazine as anti-malarial agents. The antimicrobial activity of ۲۲ ۲, ۴, ۶-s-triazine derivatives were modeled with the descriptors of quantum-chemical calculations with density functional theory (DFT) method at B۳LYP/۶–۳۱G level and topological descriptors. This study was conducted using the multiple linear regressions (MLR), the partial least square analysis (PLS) and the principal component regression (PCR) method. Results displayed that the MLR method predicted of antimicrobial activity good enough. The best model, with six descriptors was selected. Also it indicates very good consistency towards data variations for the validation methods. The predicted values of antimicrobial activity are in suitable agreement with the experimental results. The obtained results suggested that the PLS method could be more helpful to predict the antimicrobial activity of ۲, ۴, ۶-s-triazine derivatives. This study to be usable to predict the activity of other derivatives in the same groups.

کلمات کلیدی:

Multiple linear regression, Partial Least Square, density functional theory, Principal Component Regression

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