

Investigation of 6-fluoroquinolones activity against *Mycobacterium tuberculosis* using theoretical molecular descriptors : a case study.

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Streszczenie

A quantitative structure-activity relationship (QSAR) study on a set of 66 structurally-similar 6-fluoroquinolones was performed using a large pool of theoretical molecular descriptors. Ab initio geometry optimizations were carried out to reproduce the geometrical and electronic structure parameters. The resulting molecular structures were confirmed to be minima via harmonic frequency calculations. Obtained atomic charges, HOMO and LUMO energies, orbital electron densities, dipole moment, energy and many other properties served as quantum-chemical descriptors. A multiple linear regression (MLR) technique was applied to generate a linear model for predicting the biological activity, Minimal Inhibitory Concentration (MIC), treated as negative decade logarithm, (pMIC). The heuristic method was used to optimize the model parameters and select the most significant descriptors. The model was tested internally using the CV LOO procedure on the training set and validated against the external validation set. The result ($Q_{2\text{ext}} = 0.7393$), which was obtained on an external, previously excluded validation data set, shows the predictive performances of this model ($R_{2\text{tr}} = 0.7416$, $Q_{2\text{tr}} = 0.6613$) in establishing (Q)SAR of 6-fluoroquinolones. This validated model could be proficiently used to design new 6-fluoroquinolones with possible higher activity.

Słowa kluczowe

Tuberculosis, Fluoroquinolones, DNA gyrase, molecular descriptors, QSAR

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