عنوان مقاله:

Quantitative Structure-Activity Relationship Studies of ۴-Imidazolyl- ۱,۴-dihydropyridines as Calcium Channel Blockers

محل انتشار:

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خلاصه مقاله:

Objective(s): The structure- activity relationship of a series of ۳۶ molecules, showing L-type calcium channel blocking was studied using a QSAR (quantitative structure–activity relationship) method. Materials and Methods: Structures were optimized by the semi-empirical AM۱ quantum-chemical method which was also used to find structure-calcium channel blocking activity trends. Several types of descriptors, including electrotopological, structural and thermodynamics were used to derive a quantitative relationship between L-type calcium channel blocking activity and structural properties. The developed QSAR model contributed to a mechanistic understanding of the investigated biological effects. Results:Multiple linear regressions (MLR) was employed to model the relationships between molecular descriptors and biological activities of molecules using stepwise method and genetic algorithm as variable selection tools. The accuracy of the proposed MLR model was illustrated using cross-validation, and Y-randomisation - as the evaluation techniques. Conclusion: The predictive ability of the model was found to be satisfactory and could be used for designing a similar group of ۱,۴- dihydropyridines , based on a pyridine structure core which can block .calcium channels

کلمات کلیدی:

Dihydropyridines Genetic algorithm MLR pIC۵۰ QSAR