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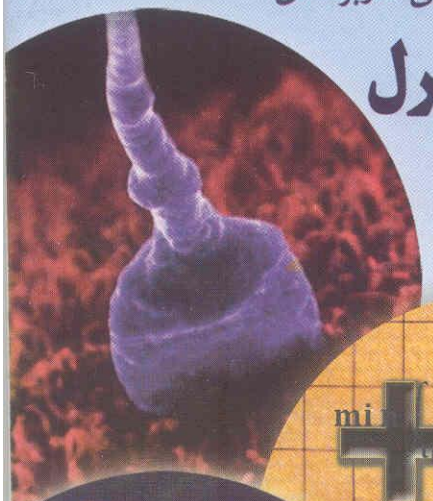
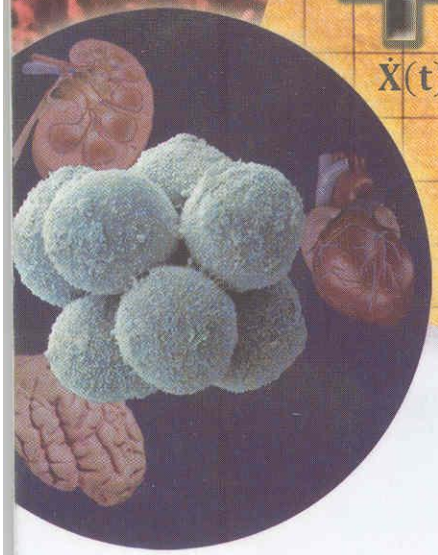
ریاضیات و نظریه کنترل در علوم پزشکی





$$\min \int_{t_i}^{t_f} f_0(X(t), U(t), t)\,dt$$

$$\dot{X}(t) = g(X(t), U(t), t)$$

$$X(t_i) = X_i$$

$$X(t_f) = X_f$$

دانشگاه علوم پزشکی خراسان شمالی

دانشگاه علوم پزشکی مشهد

Quantitative Structure Activity Relationship Studies of 4-Imidazolyl-1 ,4-dihydropyridines as Calcium Channel Blockers

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Abstract

A quantitative structure–activity relationship (QSAR) analysis was performed on a data set of 36 molecules showing L-type calcium channel blocking activity. Several types of descriptors, including electrotopological, structural, thermodynamics and ADMET, were used to derive a quantitative relationship between L-type calcium channel blocking activity and structural properties. The QSAR model developed contributed to a mechanistic understanding of the investigated biological effects. 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. A multi-parametric equation containing maximum six descriptors at AM1 method with good statistical qualities (R2train=0.860, Ftrain=28.265, Q2LOO=0.802, R2adj=0.829, Q2LGO=0.792, Q2BOOT=0.796) was obtained by Multiple Linear Regression using stepwise method. The accuracy of the proposed MLR model was illustrated using the following evaluation techniques: cross-validation, and Y-randomisation. The predictive ability of the model was found to be satisfactory and could be used for designing a similar group of 1,4- Dihydropyridines constitute a group of small organic compounds are based on a core pyridine structure which can both block and enhance calcium currents.

Key words: QSAR, Dihydropyridines, MLR, Genetic algorithm, PIC50 ratio.