عنوان مقاله:

Quantitative structure-activity relationship (QSAR) study of CCR2b receptor inhibitors using SW-MLR and GA-MLR approaches

محل انتشار:

فصلنامه ارتباطات شیمی ایران, دوره 5, شماره 1 (سال: 1395)

تعداد صفحات اصل مقاله: 20

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خلاصه مقاله:

In this paper, the quantitative structure activity-relationship (QSAR) of the CCR2b receptor inhibitors was scrutinized. Firstly, the molecular descriptors were calculated using the Dragon package. Then, the stepwise multiple linear regressions (SW-MLR) and the genetic algorithm multiple linear regressions (GA-MLR) variable selection methods were subsequently employed to select and implement the prominent descriptors having the most significant contributions to the activities of the molecules. A combined data set including numerical values of inhibition activity data (IC50) of 103 CCR2b receptor derivatives was adopted for our simulations. This study revealed that both SW-MLR and GA-MLR methods consisted of six molecular descriptors. The adopted descriptors belong to topological, charge, RDF and atom-centered fragments classes. A comparison of results by the two methodologies indicated the superiority of GA-MLR over the SW-MLR method. The authenticity of the proposed model (GA-MLR) was further confirmed using the cross-validation, validation through an external test set and Y-randomization.

کلمات کلیدی:

QSAR, CCR2b receptor inhibitors, Genetic algorithm (GA), Stepwise (SW), Multiple linear regression (MLR), Molecular descriptor