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一种预测药物活性的神经元计算新方法

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摘要 提出一种基于全变异算子遗传算法(MGA)的神经元计算新方法，用于辨识复杂药物构效关系。在MGA中，表达变量的各基因使用不同的变异概率，以便提高局部搜索效率。通过将随机初始化技术与局部搜索策略相结合，该算法能在有限时间内得到满意解。使用74个抑制还原酶的嘧啶类化合物所组成的数据集作为构效关系神经元计算的典型对象，用来考核MGA法在预测药效活性计算中的有效性。交叉验证及活性预测试验表明，用MGA法建立的构效关系模型的预测能力优于其他方法。

关键词 分子设计 神经元 遗传算法 药物化学 定量构效关系

分类号 0641

A neural computing method for identifying quantitatives structure activity relationships

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Abstract A novel genetic algorthm for neural computing to identify quantitative structure activity relationship (QSAR), named mutation- based genetic algorithm (MGA), ispresented. MGA only uses the mutation operator for local search. To enhance the efficiency of local search, the genes that represent the variables employ different time-varying mutation rates in MGA. Combining random restart technique with the local search strategy, the algorthm can give satisfactory solution in a limited time. As a typical object of the neural comuting for QSAR, a set of 74 2,4-dialmino-5-(substituted benzyl) pyrimidines that inhibit dihydrofolate reductase were used to verify the effectiveness of MGA in computings of predicting bio-activity. Cross- validation trials and the test of predicting activity demonstrated that the predictive ability of the QSAR model built with MGA is better than those provided by other methods.

Key words MOLECULAR DESIGN NEURONS PHARMACEUTICAL CHEMISTRY QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP

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