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含氟新农药的构效关系研究: II. 三维定量构效关系分析

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摘要 为了能更深入地认识含氟新化合物作为农药的生物活性和其结构间的关系,建立有意义的药物-受体作用模型,寻找同类化合物的药效团,对合成的含氟化合物在经典QSAR方法研究的基础上,又进一步运用DISCO,CoMFA和Leapfrog方法研究了它们的三维构效关系。首先根据化学结构,将分子进行了分类,然后再分别进行CoMFA计算,根据第I类分子的CoMFA结果,我们进行了含氟化合物的全新设计。根据各类中较好的构效关系模型,我们进行了分子的改造,预测了它们的活性。

关键词 有机氟杀虫剂 农药 构效关系 三维结构 化学结构

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SAR/QSAR study of fluorine containing pesticides: II. Analysis by 3D- SAR/QSAR methods

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Abstract In order to further understand the dependence of bioactivities on the structure of new fluorine-containing pesticidal compounds to build up significant ligand-receptor models, and to find out the pharmacophores of these analogues, 3D-QSAR analyses have been carried out with DISCO, CoMFA and Leapfrog approaches on the basis of our previous classical QSAR study. Firstly, the compounds were classified according to their structures. Then each class was analyzed by CoMFA. Based on the results of class I compounds some new structures were designed and the other good QSAR models were used as a basis for the optimization of structures. The bioactivities of the new designed structures were predicted.

Key words ORGANOFLUORINE INSECTICIDES PESTICIDES STRUCTURE ACTIVITY RELATIONSHIP THREE DIMENSIONAL STRUCTURE CHEMICAL STRUCTURE

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