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含氟新农药的构效关系研究: I. 经典QSAR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,建立有意义的构效关系模型,我们用经典QSAR(定量构效关系)方法研究了三十三个含氟化合物的两种不同的生物活性与结构的关系,其对抗黄瓜疫病活性模型有很好的解释能力和预测能力,并根据这个模型设计了一些新的活性结构。而对抑制西瓜白绢病的活性数据的处理未能获得理想模型。通过这一工作确立了先应用聚类等定性分析方法,再用多元统计分析方法作更深入研究的QSAR研究模式。

关键词 有机氟杀虫剂 农药 生物活性 结构与性能关系 构箭效关系 定量构效关系 化学结构

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SAR/QSAR study of fluorine-containing pesticides: I. Analysis by classical QSAR methods

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Abstract In order to better understand the dependence of bioactivities on the structures of the fluorine-containing new pesticidal compounds and to build up significant structure-bioactivity models, the relationships between the structures and two different kinds of bioactivities of 33 fluorine-containing compounds have been investigated by classical QSAR methods. The obtained bioactive model for cucumber disease has a good capability for the explanation and prediction. Based on this model some new active structures were designed. However, no significant model was obtained for the bioactive data of water-melon disease. This work resulted in a typical QSAR studying scheme in which the cluster analysis is applied, followed by the multivariate statistical methods for a deeper investigation.

Key words ORGANOFLUORINE INSECTICIDES PESTICIDES BIOLOGICAL ACTIVITY STRUCTURE AND PROPERTY CORRELATION QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP CHEMICAL STRUCTURE

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