论文

优化星座聚类法和有机氟农药构效关系识别

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摘要：

关键词：

THE OPTIMIZED CLUSTERING METHOD OF THE CONSTELLATION GRAPH AND THE STRUCTURE-ACTIVITY RELATIONSHIP OF ORGANIC FLUORINATED PESTICIDES

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Abstract:

Since the study of organic fluorinated pesticides has been a noticeable field in the seaking of efficient pesticides, the research of their structure-activity relationships be-comes more and more important. If the structure features of the chemicals are consid-ered as pattern parameters, and the activities of pesticides are discretized into classes,then the quantitative structure-activity relationship (QSAR) problem can be treated by cluster analysis. Hence, the clustering method of constellation graph is employed to identify the QSAR of fluorinated organic pesticides. In order to obtain better clustering results, the weights of star-tracks are optimized by the Lagrange operator method and good results are achieved.

Keywords:

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