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NOTES

新型哒嗪酮基取代的**1**，**3**，**4**-噻二唑类化合物的**3D-QSAR**研究

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摘要 用比较分子场分析方法对5-(1-芳基-1,4-二氢-6-甲基-4-哒嗪酮-3-基)-2-芳基胺-1,3,4-噻二唑类化合物进行了三维定量构效关系研究，发现影响其抗菌活性主要为立体能和静电能，立体能与静电能分别为0.505和0.495。所得到的模型交叉验证r_{cv}^2=0.769，相关系数r^2=0.939，F=60.996，s=0.074，表明模型具有较好的预测能力。此研究结果与2D-QSAR的结果一致，对哒嗪酮基取代的1,3,4-噻二唑类化合物的改性或新类似物的合成具有指导意义。

关键词 哒嗪酮基取代的1,3,4-噻二唑, 抗菌活性, 三维定量构效关系, 比较分子场分析方法

分类号

Study on the Three-dimensional Quantitative Structure-activity Relationship of Pyridazinonyl-substituted 1,3,4-Thiadiazoles

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Abstract The three-dimensional quantitative structure-activity relationships of a series of 5-[1-aryl-1,4-dihydro-6-methyl-pyridazin-4-one-3-yl]-2-arylamino-1,3,4-thiadiazoles, related to the fungicidal activity, were studied using the comparative molecular field analysis (CoMFA). The results show that the contributions of steric and electrostatic fields to the activity are 0.505 and 0.495, respectively. The cross-validated q^2 and the correlation coefficient r^2 for the model established by the study are 0.769 and 0.938, respectively, with the F value of 60.996, and the standard deviation s of 0.074. These values indicate that the model is significant and has good predictability. The analysis results are in good agreement well with the study of 2D-QSAR, and offered important structural insights into designing highly active compounds prior to synthesis.

Key words pyridazinonylthiadiazoles fungicides 3D-QSAR comparative molecular field analysis

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