一类吡唑衍生物的**3D-QSAR**研究

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摘要   通过比较分子力场分析方法（CoMFA）和比较分子相似性指数分析方法 (CoMSIA)，系统研究了30个2-烷基（烷硫基）-5-吡唑基-1，3，4-噁二唑（噻二?
颉⑷ 颖� ⒌ 衔镄种扑 疢瓶盏【   锘钚缘娜 酆隙 抗剐Ч叵怠6 杂?
CoMFA，研究了不同移动步长对考虑静电场和立体场作用时构效关系的影响；对于 CoMSIA,
研究了移动步长、场的组合、衰减因子α等参数变化对构效关系的影响， 发现当考虑立体场、疏水场、
氢键受体场的贡献时能得到较好的结果。分别得到了 两种方法最为理想的3D-QSAR模型，
所得三维等值线图为发现更高活性化合物提供 了有力的指导作用。
关键词   吡唑 P 杀虫剂 定量构效关系 水稻害虫

分类号 O627

3D-QSAR Study of a Set of Pyrazole Derivatives

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Abstract A systematic study of three dimensional quantitative structure activity relationship (3D-QSAR) on 30 compounds of 2-alkyl (alkythio)- 5-pyrazoyl-1,3,4=oxadiazoles (thiodiazoles and triazoles) was performed with respect to their fungicidal activities against rice sheath blight through comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA). For CoMFA, the influence of different grid spaces on structure activity relationship was investigated. For CoMSIA, the influence of variations of grid space, combinations of all kinds of field types and attenuation factor α was studied. It was found that the most satisfactory 3D-QSAR models could be constructed by taking into account of the components of steric, hydrophobic and HB acceptor. The resulting 3D contour maps provided useful guidance for more potent compounds discovery.

Key words   PYRAZOLE P NSECTICIDES QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP RICE-CROP PEST-INSECTS

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