

### 抗小麦赤霉病类含氟农药的3D-QSAR研究

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#### 摘要

用CoMFA方法对一组含氟农药分子的抗小麦赤霉病活性进行了定量构效关系研究。发现影响药效的立体场与静电场的贡献分别为90.3%和9.7%，立体场的影响是占主导性的。该模型非交叉验证的相关系数( $r^2$ )为0.991，F值是297.524，标准偏差(S)为0.015，表明模型具有较好的预测能力。根据该模型，设计并预测了几个新的化合物，其活性都在0.96以上。经过研究表明在预测结构的某些位置添加位阻较大的基团，活性提高比较明显。

关键词 [含氟农药](#) [小麦](#) [赤霉病](#) [构效关系](#) [三维结构](#) [比较分子力场分析](#) [计算机应用](#)

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### Study on anti-gibberella fluorine-containing pesticides by 3D-QSAR

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**Abstract** Comparative molecular field analysis (CoMFA) method was applied to a set of fluorine-containing compounds to study the relationship between their structure and the anti-gibberella activity. The results show that the contributions of steric and electrostatic fields to the activity are 90.3% and 9.7%, respectively. This means that the steric influence plays a dominant role for the investigated compounds. The relation coefficient ( $r^2$ ) of non-cross validation for the model established by the study is 0.991, its F value is 297.524 and the standard deviation (S) is 0.015. These values indicate that the model is significant and might have a good predictability. As a consequence, adding bulky groups in certain locations of the parent structure would raise their bioactivity. Accordingly, their predicted activities were found all higher than 0.96.

**Key words** [WHEAT](#) [FUSARIUM BLIGHT OR SCAB](#) [STRUCTURE ACTIVITY RELATIONSHIP](#) [THREE DIMENSIONAL STRUCTURE](#) [COMPUTER APPLICATIONS](#)

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