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## 论文

烯丙胺和苄胺类抗真菌药物比较分子力场分析(CoMFA)的研究

季海涛;张万年;周有骏;吕加国;朱驹;李科;陈卫平;刘宁

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摘要:

本实验采用"活性类似物法"搜寻到烯丙胺和苄胺类抗真菌化合物的药效构象。其与药物萘替芬、特比萘芬的晶体 构象相同。以此构象构建各化合物,采用rmsfit规则叠合各分子,进行CoMFA研究,得到预测能力很强的抗6种常见致 病真菌的3D-QSAR模型。并用8个本实验室设计合成的新化合物和5个文献报道的化合物对模型预测能力进行验 证。最后结合2D-QSAR方程首次提出了烯丙胺、苄胺类抗真菌化合物与受体蛋白相互作用模式图。

关键词: 烯丙胺类抗真菌化合物 苄胺类抗真菌化合物 CoMFA 药效构象 PLS

## COMPARATIVE MOLECULAR FIELD ANALYSIS (COMFA) OF ALLYLAMINE AND BENZYLAMINE ANTIMYCOTICS

Ji Haitao; Zhang Wannian; Zhou Youjun; Lu Jiagu; Zhu Ju; Li Ke Chen Weiping and Liu Ning

#### Abstract:

"Active analog approach" has been employed to search the pharmacophoric conformation of the allylamine and benzylamine antimycotics. A local mimimum energy conformation, which is very similar to the crystallgraphically determined coordinate of naftifine or terbinafine, has been applied to build all compounds. Comparative molecular field analysis (CoMFA) has been used to examine the correlations between the activities against 6 common human pathogenic fungi and the physicochemical properties of 62 allylamine and benzylamine compounds which had been aligned by rms fit rule. The predictive abilities of the resulting 3D-QSAR models have been tested by 8 new synthetic compounds and 5 reported compounds. Finally, we propose an interaction pattern between allylamine, benzylamine antimycotics and the active site of pseudoreceptor based on the results of 2D-QSAR and 3D-QSAR.

Keywords: Benzylamine antimycotics CoMFA Pharmacophoric conformation Partial least squares Allylamine antimycotics

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