

论文

喹诺酮类抗菌剂构效关系研究:母核变化对活性的影响

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摘要:

利用量子化学半经验分子轨道AM1方法对喹啉、萘啉、吡啉[2,3-C]吡嗪环系的系列化合物进行了定量构效关系研究,建立了很好的QSAR方程。结果表明:喹诺酮3位羧基与母核的共平面性对生物活性有重要的影响;4位酮基上氧的净电荷与生物活性有一致性关系。设计了1个生物活性很高的、新母核的异噻唑啉吡啉酮类化合物。

关键词: 喹诺酮类 AM1 QSAR

STUDIES ON QSAR OF THE ANTI BACTERIAL AGENTS QUI NOLONES: CHANGING THE PARENT NUCLEUS INFLUENCED THE ACTIVITY

Li Jiangbo; Lin Ruisen; Yu Qingsen and Zhu Longguan

Abstract:

By the method of AM1, quantum chemistry indexes of 16 compounds of quinoline, 1,8 naphthyridine and pyrido(2,3-C)pyridazine analogues were calculated and 4 QSAR equations were obtained. The results showed that the net charge of 4-carbonyl oxygen is highly correlated with the antibacterial activity *in vitro*, the correlation coefficient of the regressions are high(R≥0.96). The antibacterial activity *in vitro* is strongly influenced by the coplanarity of 3-carboxylic acid and the parent nucleus. In light of this study, a new parent nucleus of isothiazoleannexed quinolizine was proposed, which is expected to have much higher activity.

Keywords: AM1 QSAR Quinolone

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