云南大学学报(自然科学版)
JOURNAL OF YUNNAN UNIVERSITY(NATURAL SCIENCES)
中文核心期刊
中国科技核心期刊

云南大学学报(自然科学版) » 2007, Vol. 29 » Issue (3): 278-282,286 DOI:

(*E*)-4-取代酰氧基-3-甲氧基苯乙烯侧链类衍生物的比较分子力场(CoMFA)研究

马玉卓[1], 陈静波[2], 刘鹰翔[1], 阎冬[3], 程卯生[3]

1. 广东药学院, 药物化学系, 广东, 广州, 510006;
2. 云南大学, 教育部自然资源药物化学重点实验室, 云南, 昆明, 650091;
3. 沈阳药科大学, 制药工程学院, 辽宁, 沈阳, 110016

Comparative molecular field analysis(CoMFA)study on(*E*)-4-subsituted cinnamoyloxy-3-methoxystyrene side line derivatives

MA Yu-zhuo[1], CHEN Jing-bo[2], LIU Ying-xiang[1], YAN Dong[3], CHEN Mao-sheng[3]

1. Department of Medicinal Chemistry, Guangdong Pharmaceutical University, Guangzhou 510006, China;
2. Key Laboratory of Medicinal Chemistry for Natural Resource(Yunnan University), Ministry of Education, School of Chemical science and technology, Kunming 650091, China

全文: PDF (330 KB) HTML (KB) 输出: BibTeX | EndNote (RIS) 背景资料

摘要 利用比较分子力场方法,建立5-脂氧合酶/环氧合酶抑制剂的三维定量构效关系,为设计新的更有效的酶抑制剂提供理论依据.在CoMFA分析中,交叉验证回归系数R^2_{CV}、非交叉验证回归系数r^2和标准偏差(SEE)分别为0.639,0.744,0.148.说明系列化合物分子周围立体场和静电场的分布与抗炎活性间有良好的相关性.利用该模型对自行合成的24个化合物进行活性预测,结果与实测值相符.所得模型支持了假设的抑制剂作用机理和作用模型.所得CoMFA模型具有一定的预测能力,可用来指导设计新的5-脂氧合酶/环氧合酶抑制剂.

关键词: 5-脂氧合酶/环氧合酶抑制剂 比较分子力场分析(CoMFA) (*E*)-4-肉桂酰氧基-3-甲氧基苯乙烯类

Abstract: Comparative molecular field analysis(CoMFA)was performed to study 3D-QSAR of(*E*)-4-cinnamoyloxy-3-methoxystyrene derivatives with biological activity in order to give a theoretical basis to design novel more effective enzyme dual inhibitor.In this analysis,the cross validated coefficient R^2_{CV} was found to be 0.639,non-cross validated coefficient r^2 and the standard deviation SEE was 0.744 and 0.148 respectively,and *F* was 198.355.The CoMFA models for twenty four of(*E*)-4-cinnamoyloxy-3-methoxystyrene derivatives showed the good relationship between steric and electrostatic properties with anti-inflammatory activity,which were very helpful for designing novel compounds as 5-lipoxygenase/cyclooxygenase inhibitor.

Key words: 5-lipoxygenase/cyclooxygenase inhibitor comparative molecular field analysis(CoMFA) (*E*)-4-cinnamoyloxy-3-methoxystyrenes

收稿日期: 2006-10-18;

基金资助:广东省自然科学基金博士启动项目(994615)

服务
把本文推荐给朋友
加入我的书架
加入引用管理器
E-mail Alert
RSS
作者相关文章
马玉卓
陈静波
刘鹰翔
阎冬
程卯生

引用本文:

马玉卓,陈静波,刘鹰翔等. (*E*)-4-取代酰氧基-3-甲氧基苯乙烯侧链类衍生物的比较分子力场(CoMFA)研究[J]. 云南大学学报(自然科学版), 2007, 29(3): 278-282,286.

MA Yu-zhuo,CHEN Jing-bo,LIU Ying-xiang et al. Comparative molecular field analysis(CoMFA)study on(*E*)-4-subsituted cinnamoyloxy-3-methoxystyrene side line derivatives[J]. , 2007, 29(3): 278-282,286.

没有本文参考文献

没有找到本文相关文献

编辑出版：云南大学学报编辑部 (昆明市翠湖北路2号, 650091)
电话：0871-5033829(传真) 5031498 5031662 E-mail: yndxxb@ynu.edu.cn yndxxb@163.com