药学学报 1998, 33(10) 759-763 DOI: ISSN: CN:

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论文

紫杉烷二萜类化合物精细立体结构研究

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摘要:

抗肿瘤药物紫杉醇(taxol)是一类新型的纺锤体毒药物。已有的关于紫杉醇及其类似物的构效关系研究表明其分子结构中六元A环的C-13侧链与 C_4 - C_5 - C_{20} 四元氧环对活性有重要贡献。本文研究了紫杉烷二萜类化合物中5/7/6三环骨架C-4取代方式不同的化合物(4个)及6/8/6三环骨架C-4取代方式不同的3类化合物(10个)的晶体结构,阐述了晶态下紫杉烷二萜类化合物因C-4取代方式不同对分子立体结构的影响,从晶体学角度给出6/8/6/4骨架与抗癌活性的关系。

关键词: 紫杉烷二萜 晶体结构 构效关系

STUDIES ON THE FINE STEREOSTRUCTURE OF TAXOIDS

Wu Nan; Lu Yang; Zheng Qitai; Fang Weishuo; Gao Yongli; Fang Qicheng and Zhou Tonghui

Abstract:

The anticancer drug taxol is a new type antimicrotubular drug. The structure-activity relationship study on taxol and its analogs has indicated the importance of the $\rm C_{13}$ side chain and the $\rm C_4$ - $\rm C_5$ - $\rm C_{20}$ epoxypropane group. The crystal structures of 4 taxoids having the basic skeleton with 5/7/6 membered ring and three types of 10 taxoids having the basic skeleton with 6/8/6 membered ring have been analyzed. The effects of the induction by different substructures at $\rm C_4$ on the stereostructures of taxoids were studied, and the relationship between the 6/8/6/4 skeleton and the anticancer activity was discussed from the crystallographic point.

Keywords: Crystal structure Structure-activity relationship Taxane diterpenoids

收稿日期 1997-10-23 修回日期 网络版发布日期

DOI:

基金项目:

通讯作者:

作者简介:

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