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### 论文

伊维菌素(Ivermectin)晶体结构的研究

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摘要:

用单晶X射线衍射法测定了伊维菌素Ivermectin( $H_2B_{1a}$ )的结构。Ivermectin由大于80%的 $H_2B_{1a}$ 和小于20%的 $H_2B_{1b}$ 组成。 $H_2B_{1a}$ 属单斜晶系,C2空间群,晶胞参数为a=40.763(6)A,b=9 295(3)A,c=14.966(3)A,β=106.93

(1)。 V\_5425(2) A<sup>3</sup> Z=4. DC 1 1560 cm 3, µ(MoK\_0)=0.084mm 1, R=0.0658。 H<sub>2</sub>B<sub>1</sub> 呈沿C 轴排列的链状结构,同时通过 2次轴对称,实际结构为由两条链状分子呈平符分布,相互间距离一定,但方向相反的双链,类似于生物大分子的链状结构。

关键词: 伊维菌素 阿弗菌素 单晶结构

# STUDIES ON THE CRYSTAL STRUCTURE OF IVERMECTIN (H2B1a)

Hu Xiurong; Gu Jianming; Chen Linshen and HuangPu Yonglin

#### Abstract:

The crystal structure of ivermectin  $(H_2B_{1a})$  was determined by X-ray diffraction. Ivermectin was found to be composed of more than 80%  $H_2B_{1a}$  and less than 20%  $H_2B_{1b}$ . The crystal of  $H_2B_{1a}$  belongs to the space group C 2 with a=40.736(6)A, b=9.295(3)A, c=14.966(3)A,  $\beta$ =106.93(1)°. After structure refinement using least—squares method, the final R factor of  $H_2B_{1a}$  is 0.0658. The space configuration of  $H_2B_{1a}$  is a long chain along the C—axis. The molecular aggregates are extended into pairs of long chains parallel to each other, some distance apart. The distance between chains is the same, but their direction is opposite. This structure of  $H_2B_{1a}$  is similar to some biomacromolecules.

Keywords: Avermectin Crystal structure Ivermectin

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