

论文

羟甲芬太尼立体异构体的晶体结构

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摘要:

对强效镇痛剂羟甲芬太尼的两个光学异构体体 *cis*-(3*R*,4*S*,2'*R*)-羟甲芬太尼(I)和 *trans*-(3*R*,4*R*,2'*S*)-羟甲芬太尼(II)进行了X-射线衍射晶体结构分析。两个异构体均有一个sp<sup>3</sup>N(1)原子和一个sp<sup>2</sup>N(7)原子。哌啶环呈椅式构象,顺式异构体I的3-甲基处于直立键,4-*N*-苯基丙酰胺基处于平伏键;反式异构体II的3-甲基与4-*N*-苯基丙酰胺基均处于平伏键。在I分子中,C(4)原子与4-丙酰胺基组成的平面与*N*-苯环平面近似相互垂直,而在II中,两平面的二面角近似为100°。两异构体分子中均存在分子内氢键O(1)—H...N(1),反式异构体II还存在分子间氢键O(1)—H(A)...O(2)(B)。

关键词: 羟甲芬太尼 立体异构体 X-射线晶体学 晶体结构

CRYSTAL STRUCTURES OF OHMEFENTSNYL STEREOISOMERS

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Abstract:

Ohmefentanyl, *N*-[1-(2-hydroxyl-2 phenyl)-3-methyl-piperidyl]-*N*-phenylpropanamide, is a new and potent analgesic agent. Two stereoisomers : *cis*-(3*R*,4*S*,2'*R*)-ohmefentanyl ( I ) and *trans*-( 3*R*,4*R*,2'*S*)-ohmefentanyl(II), were selected for X-Ray crystallographic study. The two isomers were shown to have an sp<sup>3</sup>N(1) and an sp<sup>2</sup>N(7) and the piperidine ring has a chair conformation, The *cis*-isomer I has an axial 3-methyl with an equatorial 4-*N*-phenylpropanamide group, while the two groups of the *trans*-isomer II are all equatorial. In I molecule, the plane formed by the 4-propanamide group and atom C(4) is almost perpendicular to the 4-*N*-phenyl ring plane; in II, the dihedral angle of the two planes is about 100°. Intramolecular hydrogen bond of O(1)—H...N(1) occurs in both the two isomers and isomer II is also involved in intermolecular hydrogen bond O(1)—H(A)...O(2)(B).

Keywords: Stereoisomers X-Ray crystallography Crystal structure Ohmefentanyl

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