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摘要: 本文用X射线晶体衍射法分析了抗癌药物3-吡啶氨基-5羟甲基苯胺(3-(9-acridinylamino)-5-(hydroxymethyl)aniline, AHMA)的分子结构。AHMA的化学式为C₂₀H₁₇N₃O, Mr=315.37。晶体属三斜晶系, 空间群为P-1。晶胞参数晶胞参数: $\alpha=8.043(2)$, $b=9.949(2)$, $c=11.631(3)$ Å, $\alpha=69.78(1)^\circ$, $\beta=84.02(1)^\circ$, $\gamma=65.70(1)^\circ$ 。经最小二乘修正后得到的R₁值为0.051。在晶体结构中, 吡啶环和苯胺环几乎相互垂直, 两个环平面之间的两面角为66.5°。这种结构有利于AHMA以嵌插于DNA碱基对的形式与DNA结合。

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The crystal structure of 3-(9-acridinylamino)-5-(hydroxymethyl) aniline (AHMA)
antitumor drug

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Abstract: The structure of 3-(9-acridinylamino)-5-(hydroxymethyl)aniline (AHMA)-an antitumor drug derived from the clinically used antileukemia drug m-AMSA was analyzed by x-ray crystallography. The unit cell was found to be triclinic with dimensions of $a = 8.043(2)$, $b = 9.949(2)$, $c = 11.631(3)$ Å, $\alpha = 69.78(1)^\circ$, $\beta = 84.02(1)^\circ$, $\gamma = 65.70(1)^\circ$. The space group is P-1. In the structure, the acridine and aniline plane are almost perpendicular to each other and dihedral angle between two planes is 66.5°.

Key words:

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