Synthesis, crystal structure, and biological evaluation of novel 5-hydroxymethylpyrimidines.

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Streszczenie

Pyrimidine displays a wide array of bioactivities, and thence, it is still considered a potent unit of new drug research. Its derivative, 5-hydroxymethylpyrimidine, can be found as a scaffold of nontypical nitrogen bases in DNA and as a core of some natural bioactive compounds. In this study, we obtained a series of 5-hydroxymethylpyrimidines that vary in the 4-position by the reduction of proper esters. All compounds were characterized by spectroscopic analysis, and single-crystal X-ray diffraction was performed for some of them. Biological investigations estimated cytotoxic properties against normal (RPTEC) and cancer (HeLa, HepaRG, Caco-2, AGS, A172) cell lines. It was found that the derivatives with an aliphatic amino group at the 4-position are generally less toxic to normal cells than those with a benzylsulfanyl group. Moreover, compounds with bulky constituents exhibit better anticancer properties, though at a moderate level. The specific compounds were chosen due to their most promising IC50 concentration for in silico study. Furthermore, antimicrobial activity tests were performed against six strains of bacteria and one fungus. They demonstrated that only derivatives with at least three carbon chain amino groups at the 4-position have weak antibacterial properties, and only the derivative with 4-benzylsulfanyl constituent exhibits any antifungal action.

Słowa kluczowe

pyrimidines, anticancer activity, single-crystal X-ray diffraction

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