

论文

5-取代苯硫基(硒基)-2,4-二氨基嘧啶对大肠杆菌(MB 1428)二氢叶酸还原酶抑制作用构效关系的研究

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摘要:

关键词: 5-取代苯硫基-2,4-二氨基嘧啶 5-取代苯硒基-2,4-二氨基嘧啶 构放关系

STRUCTURE-ACTIVITY RELATIONSHIPS OF THE INHIBITION OF *ESCHERICHIA COLI* DIHYDROFOLATE REDUCTASE (MB1428) BY 5-(SUBSTITUTED PHENYL) THIO AND 5-(SUBSTITUTED PHENYL) SELENO-2,4-DIAMINOPYRIMIDINES

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Abstract:

The inhibitory activity of 5-(X-phenyl)-thio-2,4-diaminopyrimidines (IIa), and 5-(X-phenyl)-seleno-2,4-diaminopyrimidines(IIb) on *Esekerichiacoli* (MB1428)dihydrofolate reductase were tested. The inhibitory activity of 5-(X-phenyl)-thio-2,4-diaminopyrimidines on *Escherichia coli* dihydrofolate reductase is linearly correlated with the sum of the steric parameter (MR) of 3,4,5-substitu-ents of phenyl group (n=8, r=0.871, s=0.221). Including 5-(X-phenyl)-seleno-2,4-diaminopyrimidines in the correlation analysis of 5-(X-phenyl)-thio-2,-diami-nopyrimidines with an indicator variable, the result is the same as the former (n=10,r=0.881, s=0.196). Since none of the substituents of these compounds used in the derivation of correlated equations is larger than methoxy group, whether it is neces-sary to use limited sterie parameter(MR/) to correlate as in the series of 5-(X-be-nzyl)-2,4-diaminopyrimidines should be further confirmed.

Keywords: 5-(Substitutedphenyl)-seleno-2,4-diaminopyrimidines Structure-activity relationships 5-(Substituted-phenyl)-thio-2,4-diaminopyrimidines

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