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Title: Synthesis of Thymidine Phosphorylase Inhibitor Based on Quinoxaline Derivatives and Their Molecular Docking Study

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Abstract: We have synthesized quinoxaline analogs (1-25), characterized by H-1-NMR and HREI-MS and evaluated for thymidine phosphorylase inhibition. Among the series, nineteen analogs showed better inhibition when compared with the standard inhibitor 7-Deazaxanthine (IC50 = 38.68 +/- 4.42 mu M). The most potent compound among the series is analog 25 with IC50 value 3.20 +/- 0.10 mu M. Sixteen analogs 1, 2, 3, 4, 5, 6, 7, 12, 13, 14, 15, 16, 17, 18, 21 and 24 showed outstanding inhibition which is many folds better than the standard 7-Deazaxanthine. Two analogs 8 and 9 showed moderate inhibition. A structure-activity relationship has been established mainly based upon the substitution pattern on the phenyl ring. The binding interactions of the active compounds were confirmed through molecular docking studies.

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