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**Record 1 of 1****Title:** Synthesis of Thymidine Phosphorylase Inhibitor Based on Quinoxaline Derivatives and Their Molecular Docking Study**Author(s):** Almandil, NB (Almandil, Noor Barak); Taha, M (Taha, Muhammad); Farooq, RK (Farooq, Rai Khalid); Alhibshi, A (Alhibshi, Amani); Ibrahim, M (Ibrahim, Mohamed); Anouar, E (Anouar, El Hassane); Gollapalli, M (Gollapalli, Mohammed); Rahim, F (Rahim, Fazal); Nawaz, M (Nawaz, Muhammad); Shah, SAA (Shah, Syed Adnan Ali); Ahmed, QU (Ahmed, Qamar Uddin); Zakaria, ZA (Zakaria, Zainul Amiruddin)**Source:** MOLECULES **Volume:** 24 **Issue:** 6 **Article Number:** 1002 **DOI:** 10.3390/molecules24061002 **Published:** MAR 2 2019**Times Cited in Web of Science Core Collection:** 0**Total Times Cited:** 0**Usage Count (Last 180 days):** 2**Usage Count (Since 2013):** 2

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 μ M). The most potent compound among the series is analog 25 with IC₅₀ value 3.20 +/- 0.10 μ 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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