Synthesis of new isoquinoline-base-oxadiazole derivatives as potent inhibitors of thymidine phosphorylase and molecular docking study

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Abstract

Here in this study regarding the over expression of TP, which causes some physical, mental and socio problems like psoriasis, chronic inflammatory disease, tumor angiogenesis and rheumatoid arthritis etc. By this consideration, the inhibition of this enzyme is vital to secure life from serious threats. In connection with this, we have synthesized twenty derivatives of isoquinoline bearing oxadiazole (1-20), characterized through different spectroscopic techniques such as HREI-MS, H-1-NMR and C-13-NMR and evaluated for thymidine phosphorylase inhibition. All analogues showed outstanding inhibitory potential ranging in between 1.10 +/- 0.05 to 54.60 +/- 1.50 mu M. 7-Deazaxanthine (IC50 = 38.68 +/- 1.12 mu M) was used as a positive control. Through limited structure activity relationships study, it has been observed that the difference in inhibitory activities of screened analogs are mainly affected by different substitutions on phenyl ring. The effective binding interactions of the most active analogs were confirmed through docking study.

Keywords

KeyWords Plus: ALPHA-GLUCOSIDASE SYNTHESIS; IN-VITRO EVALUATION; CELL GROWTH-FACTOR; BETA-GLUCURONIDASE; BIOLOGICAL EVALUATION; ANALOGS; ACETYLCHOLINESTERASE; THIOSEMICARBAZIDES

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