Synthesis, Molecular Docking, and Cytotoxic Activity of Novel Triazolopyridazine Derivatives

Authors : Azza T. Tahera, Eman M. Ahmeda, Nadia A. Khalila, Yassin M. Nissanb

Abstract : New 3-(pyridin-4-yl)-[1,2,4] triazolo [4,3-b] pyridazine derivatives 2a-i, 4a,b and 6a,b were designed, synthesized and evaluated as cytotoxic agents. All compounds were investigated for their in vitro cytotoxicity at a single dose 10-5M concentration towards 60 cancer cell lines according to USA NCI protocol. The preliminary screening results showed that the majority of tested compounds exhibited remarkable activity against SR (leukemia) cell panel. Molecular docking for all synthesized compounds was performed on the active site of c-Met kinase. The most active compounds, 2f and 4a were further evaluated at a seven dose level screening and their IC50 as a c-Met kinase inhibitors were determined in vitro.

Keywords : triazolopyridazines, pyridazines, cytotoxic activity, cell panel

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