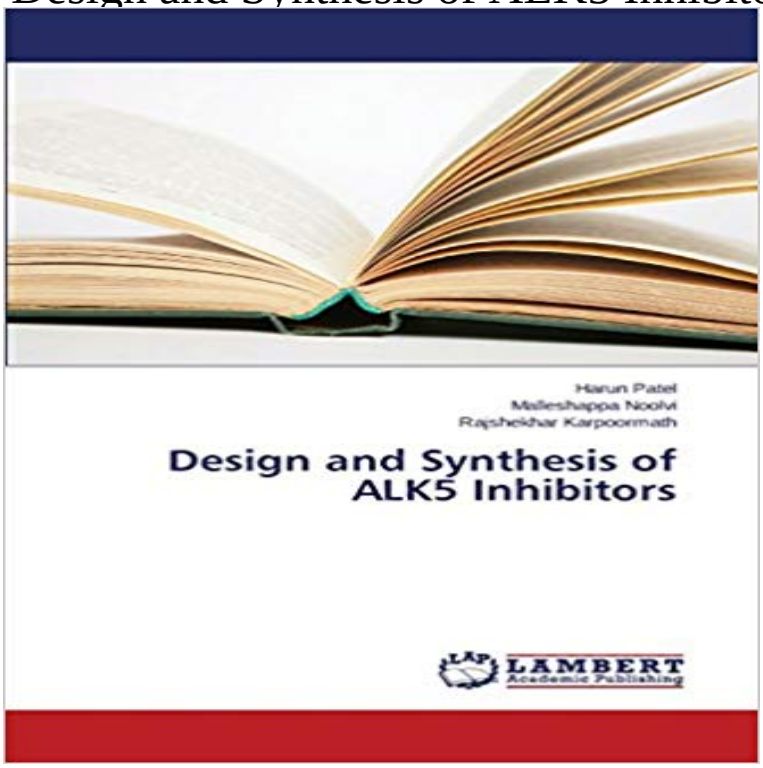
Design and Synthesis of ALK5 Inhibitors



A new series of imidazo[2,1-b][1,3,4]thiadiazoles 5(a-g), 6(a-g), 9(a-i) and 12(a-h) were synthesized. Among them, 23 compounds 5a, 5b, 5e, 5d, 5f, 5g, 6a, 6b, 6c, 6d, 6e, 9b, 9d, 9f, 9g, 9h, 9i, 12b, 12c, 12d, 12e, 12g, and 12h were evaluated at National Cancer Institute for single dose in vitro primary cytotoxicity assay. Compound 5b, 5e, 6c, 6d, 6e, 12c, 12d and 12e were further screened for 5-log dose molar range as they have shown prominent cell growth inhibition at 10-5 M concentration against variety of cell lines. Compound 5e shows significant inhibition against Leukemia HL-60 cell line with GI50 of 0.0285 M and highest selectivity towards the Leukemic Cancer cell line (selectivity ratio of 7.96) it also shows prominent ALK5 inhibition (IC50 = 0.0263 M) and elective inhibition (91%) against KDR at10 M. The binding mode of compound 5e by SP docking studies shows that it ?ts well into the active site cavity of ALK5 by forming broad and tight interactions. Lipinskis rule and in silico ADME pharmacokinetic parameters are within the acceptable range defined for human use thereby indicating their potential as a drug-like molecules.

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