**ABSTRACT**

Novel Schiff bases derived from the treatment of mercapto-diamino pyrimidine with two different aldehydes are characterized using elemental analysis, single crystal X-ray diffraction and 1H NMR spectroscopy. The pharmacological action of the synthesized compounds *viz.*, antimicrobial, anticancer and antitubercular activities is studied. The Schiff bases show a very good activity against various test pathogens. DNA and β-CD binding interactions of the compounds are studied using UV–Visible absorption and fluorescence spectral measurements. The binding constants of the compounds towards β-CD are in the order of 103 to 104. Molecular docking is done using MOE program on the 3D structure of the enzymes, *viz.*, human thymidylate synthase complexed with dump and raltitrex, candida albicans N-myristoyltransferasepeptidic inhibitor, catalytic domain of protein kinase pKnb from mycobacterium tuberculosis in complex with mitoxantrone, pare, topoisomerase atpase inhibitor, E. coli and lactobacillus casdihydrofolatereductase. The MIC/IC50 values of the Schiff bases are compared with the glide scores from the molecular docking studies. The number of hydrogen bonding interactions between the Schiff bases and amino acid residues are also reported.