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Synthesis, Characterization, Molecular Docking, and Biological Evaluation of 2-Methyl Perlolidine

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ABSTRACT An efficient new approach toward the synthesis of 2-methylperlolidine alkaloids has been illustrated, the present article describes the synthesis, in Antileukemic activities and *in-silico* molecular docking studies of compound 2-methylperlolidine **4**. The synthesis of **4** is initiated by a new, efficient, solvent-free Minisci radical reaction. The structures of the compounds are established using both spectral and analytical data. An *in-silico* prediction of activity spectra for substances, the Swiss ADME-assisted docking approach is found to be suitable to derive and synthesize effective receptor tyrosine kinase agents. Claisen ester condensation reaction resulted in the discovery of inexpensive and user-friendly solvents. Structures of the newly synthesized compounds were characterized by FT-IR, ^{1}H NMR, ^{13}C NMR, and HRMS (FTMS + PESI) analyses. Molecular docking was investigated to determine the probable binding mode. The experimental values and docking simulation exhibited that the complex had better anti-leukemic than the positive reference 2-methylperlolidine.

KEYWORDS Perlolidine, Minisci reaction, glycine, Ethyl-2-methylquinoline-3-carboxylate.

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INTRODUCTION

The 2,7-Naphthyridine small class of aromatic alkaloids occurs in a variety of (plants, sponges, tunicates, and bryozoans). The tricyclic alkaloid pyrrolidine is isolated from perennial ryegrass in New Zealand (*Lolium perenne* L.).[1,2] It was first isolated and characterized in New Zealand.[3] I. Reifer and co-workers displayed that pyrrolidine and derivatives could be prepared by oxidation of proline.[4] Although numerous synthetic methods for the preparation of naphthyridines have been reported,[5] due to their significant biological role, the literature review indicates considerable potential for improvement of the current processes, the naphthyridine derivatives have traditionally important consideration due to their exceptionally wide spectrum of genetic activity.[6-11] Recently, the characteristics of several naphthyridine derivatives, such as benzo[2,7] naphthyridine, have been patented as growth regulators, fungicides, bactericides, anticancer agents, and anti-protozoal agents.[12] Synthetic organic chemists continue to work on developing efficient strategies for the synthesis of molecules using inexpensive reagents (Figure 1).

This program of synthesis of pyrrolidine analogu has envisaged serving as a new scaffold for evaluation as Antileukemic agents by *in silico* molecular docking studies. Docking the synthesized compounds into protein receptors.[13] Molecular docking was carried out by using Auto-Dock Vina the computational approach used in this study, molecular docking was followed by the ADMET

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