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1,8-Diazabicyclo[5.4.0]undec-7-ene Catalyzed Synthesis of Some New 7-Alkyl-6-oxo-1*H*-pyrazolo[3,4-*b*]pyridine-5-carbonitriles

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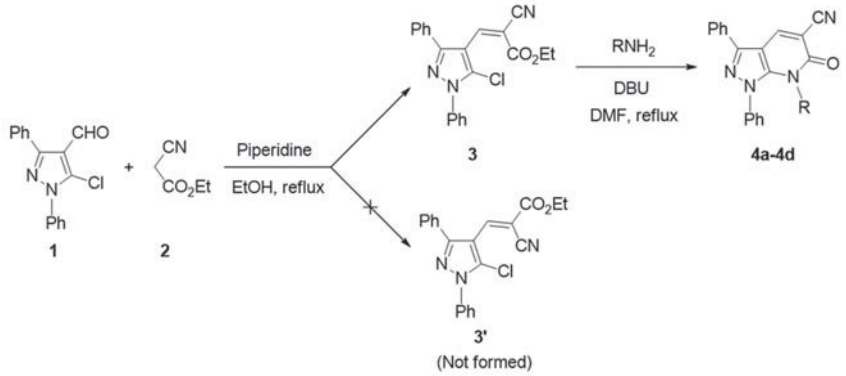
ABSTRACT Starting from 5-chloro-1,3-diphenyl-1*H*-pyrazole-4-carbaldehyde, the synthesis of some new bicyclic 7-alkyl-6-oxo-1,3-diphenyl-6,7-dihydro-1*H*-pyrazolo[3,4-*b*]pyridine-5-carbonitriles catalyzed by 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) is described. Knoevenagel condensation reaction of 5-chloro-1,3-diphenyl-1*H*-pyrazole-4-carbaldehyde with ethyl cyanoacetate in refluxing ethanol containing a few drops of piperidine afforded the (Z)-ethyl 3-(5-chloro-1,3-diphenyl-1*H*-pyrazol-4-yl)-2-cyanoacrylate. Treatment of this compound with primary alkyl amines in the presence of DBU as a catalyst in dimethylformamide at reflux temperature gave new 7-alkyl-6-oxo-1,3-diphenyl-6,7-dihydro-1*H*-pyrazolo[3,4-*b*]pyridine-5-carbonitriles in high yields. All synthetic compounds were characterized on the basis of their spectral and microanalytical data. The correct stereoisomer of the Knoevenagel product was confirmed with comparison of the experimental and calculated ^{1}H nuclear magnetic resonance (NMR) and ^{13}C NMR chemical shifts using density functional theory calculations at the B3LYP/6-31+G(d,p) level of theory.



KEY WORDS 5-Chloro-1,3-diphenyl-1*H*-pyrazole-4-carbaldehyde, Ethyl cyanoacetate, Pyrazolo[3,4-*b*]pyridine, 1,8-Diazabicyclo[5.4.0]undec-7-ene.