Practical Oxazole Synthesis Mediated by Iodine from α-Bromoketones and Benzylamine Derivatives

(Supplementary Information)

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General Information

The $^1$H NMR spectra were recorded at 400 MHz or 300 MHz and $^{13}$C NMR spectra were measured at 100 MHz or 75 MHz using a Bruker AV400 instrument with CDCl$_3$ or DMSO-$d_6$ as the solvent. The chemical shifts ($\delta$) were measured in ppm and with the solvents as references (For CDCl$_3$, $^1$H: $\delta$ = 7.26 ppm, $^{13}$C: $\delta$ = 77.00 ppm; for DMSO-$d_6$, $^1$H: $\delta$ = 2.50 ppm, $^{13}$C: $\delta$ = 39.43 ppm). The multiplicities of the signals are described using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, br = broad. The known compounds were identified by the comparison of their NMR spectra with reported data in the literatures. The new compounds were characterized by NMR, IR, HRMS and melting point for solid samples. IR spectra were recorded on a FT-IR Bruker EQUINOX55 spectrometer and only major peaks are reported in cm$^{-1}$. High resolution mass spectral analyses (HR-MS) were performed on a high resolution ESI-FTICR mass spectrometer (Varian 7.0 T). Melting points were recorded on a RY-1 type apparatus. Optical rotations were obtained on a Perkin-Elmer 431 Polarimeter. All solvents were obtained from commercial sources and were purified according to standard procedures. Petroleum ether (PE), where used, had the boiling point range 60-90 °C.

Control Experiments

The oxidation test of DMSO and DMF

The examination of 2,4,5-triphenyl oxazole synthesis from $\alpha$-iodo ketone generated in situ
References

NMR Spectra of Products

$^1$H NMR 400MHz CDCl$_3$

$^{13}$C NMR 100MHz CDCl$_3$