Greener, More Efficient Synthesis of a Medicinally Applicable 1,2,3-triazole Derivative

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The 1,2,3-triazole is a stable and biologically active organic compound that can be used in a variety of applications, including pharmaceutical chemistry. The purpose of this study was to synthesize a 1,2,3-triazole derivative using synthesis protocols that maximize efficiency in terms of time, expense, reagent quantities, and use of 'greener' chemicals. By adapting protocols developed by Huisgen, regioisomerically controlled copper(I)-catalyzed azide-alkyne cycloaddition was used to synthesize the 4-alcohol-1,2,3-triazole intermediate. Because a goal of this study was to use inexpensive, readily available materials for these syntheses, copper(II) sulfate was reduced with sodium L-ascorbate (vitamin C) in situ to produce the copper(I) catalyst. Then, the 4-alcohol-1,2,3-triazole intermediate was oxidized to produce the 4-acetyl-1,2,3-triazole using Clorox® bleach (6% sodium hypochlorite) and glacial acetic acid. Since the stoichiometry of this oxidation reaction using bleach and acetic acid is not known, reaction conditions were varied to determine the combination of reagent quantities, time, and temperature that best optimized yield and reaction time. The successful synthesis, characterization, and optimization of 4-acetyl-1,2,3-triazole could lead to the medicinal application of this potentially useful molecule.