Supporting Information

Regioselective synthesis of triazoles via base-promoted oxidative cycloaddition of chalcones with azides in aqueous solution

Wenchao Yang, Tao Miao,* Pinhua Li, and Lei Wang*

a Department of Chemistry, Huaibei Normal University, Huaibei, Anhui 235000, P R China, Tel: +86-561-3802-069 Fax: +86-561-3090-518 E-mail: leiwang@chnu.edu.cn
b State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, P R China

Contents

1. Preparation of the starting materials.................................................................1
2. 1H and 13C NMR spectra of the products.........................................................2
1. Preparation of the starting materials

1.1. General procedure for the preparation of substituted-chalcones

According to the reported literature (D. Batovska, S. Parushev, A. Slavova, V. Bankova, I. Tsvetkova, M. Ninova and H. Najdenski, *Eur. J. Med. Chem.*, 2007, 42, 87), substituted acetophenone (2.0 mmol) was added to equimolar quantities of appropriate aryl aldehydes dissolved in MeOH (2.0 mL). To this solution 6 M NaOH (1.0 mL) was added and the reaction mixture was stirred for 40 min and then kept in refrigerator overnight. The product crystals were filtrated and washed carefully with ice water and cold MeOH to neutral reaction. The resulting chalcones were purified by recrystallization.

*(E)-Chalcone and (E)-4-phenylbut-3-en-2-one were purchased from Alfa Aesar.*

1.2 General procedure for the preparation of azides

To a stirred solution of the corresponding bromide (1.0 equiv) in a 50 mL water/acetone mixture (1:4) was added NaN₃ (1.5 equiv), according to the literature (L. Campbell-Verduyn, P. H. Elsinga, L. Mirfeizi, R. A. Dierckx and B. L. Feringa, *Org. Biomol. Chem.*, 2008, 6, 3461). The resulting suspension was stirred at room temperature for 24 hours. DCM was added to the mixture and the organic layer was separated. The aqueous layer was extracted with 3 x 10 mL aliquots of DCM and the combined organic layers were dried over MgSO₄. Solvent was removed under reduced pressure, and the azide was sufficiently pure to use without further work up.
2. $^1$H and $^{13}$C NMR spectra of the products