Synthesis and Single Crystal X-Ray Structure of Ethyl 2-(1,3-Benzoxazol-2-yl)-5-oxo-3-(4-toluidino)-2,5-dihydro-4-isoxazolecarboxylate

Ali Souldozia, Jabbar Khalafy, Ahmad Poursattar Marjani, Katarzyna Ślepokura, Tadeusz Lis, and Ali Ramazani

a Department of Chemistry, the University of Zanjan, P.O. Box 45195-313, Zanjan, Iran
b Department of Chemistry, the University of Urmia, Urmia 57154, Urmia, Iran
c Faculty of Chemistry, University of Wrocław, 14 Joliot-Curie St., 50-383 Wrocław, Poland

Reprint requests to Dr. A. Ramazani. Fax: +98 241 5283100. E-mail: aliramazani@yahoo.com

Z. Naturforsch. 2007, 62b, 705 – 710; received October 24, 2006

Ethyl 5-oxo-3-(4-toluidino)-2,5-dihydro-4-isoxazolecarboxylate was prepared from the reaction of diethyl 2-(4-toluidinocarbothioyl)malonate with hydroxylamine. Its reaction with 2-chlorobenzoxazole gave the corresponding N-substituted isoxazolone. The structure of the final product 4 was confirmed by IR, $^1$H and $^{13}$C NMR spectroscopy and mass spectrometry, and by X-ray single crystal structure determination.

Key words: Synthesis, Hydroxylamine, 2-Chlorobenzoxazole, N-Substituted Isoxazolone, X-Ray Single Crystal Structure