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Entitled

EXCLUSIVE REGIOSELECTIVE SYNTHESIS OF POTENTIALLY BIOACTIVE 1,3,4-SELENADIAZOLE

by

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Abstract

Isoselenocyanates have a crucial role as reactants in chemical processes, facilitating the efficient synthesis of significant chemical intermediates and physiologically active chemicals. The utilization of (Z)-2-oxo-N-phenylpropanehydrazonoyl chlorides in a one-step procedure for the synthesis of the core structure of various heterocyclic compounds has been widely explored. This study focuses on the synthesis of 5-arylimino-1,3,4-selenadiazole derivatives through the reaction of isoselenocyanates with various substituted (Z)-2-oxo-N-phenylpropanehydrazonoyl chlorides. The objective is to achieve selective and accurate formation of these derivatives. The derivatives exhibit a diverse range of functional groups on both aryl rings. The synthetic procedure is conducted under ambient conditions, promoting environmental sustainability, and ensuring safe manipulation. This technique exhibits versatility in its application across several substrates, yielding outcomes of superior quality. The selenadiazoles are acquired using the process of gravity filtering, and their chemical structures are confirmed utilizing multinuclear NMR spectroscopy and precise mass spectrometry techniques. Single-crystal X-ray diffraction analysis was also used to successfully define the precise molecular structure of the reported 5-arylimino-selenadiazole regioisomer in this investigation. The substances (Z)-1-(4-(4-iodophenyl)-5-(p-tolylimino)-4,5-dihydro-1,3,4-selenadiazol-2-yl)ethan-1-one and (Z)-1-(5-(4-methoxyphenyl)imino)-4,5-dihydro-1,3,4-selenadiazol-2-yl)ethan-1-one were analyzed as-4-(4-(methylthio)phenyl)-4,5-dihydro-1,3,4-selenadiazol-2-yl)ethan-1-one. (Z)-2-oxo-N-phenylpropanehydrazonoyl chloride and (Z)-N-(3,5-bis(trifluoromethyl)phenyl)-2-oxopropanehydrazonoyl chloride are two examples of hydrazonoyl chloride reactants that have had their (Z)-geometry validated by X-ray diffraction experiments. Density functional theory (DFT) calculations were performed at the B3LYP-D4/def2-TZVP level to corroborate the experimental findings and hypothesized mechanism.

Keywords: Hydrazonoyl chloride; Isoselenocyanate; 1,3,4-Selenadiazole; Density functional theory