Synthesis of bis(hydrazinecarboximidamides) by condensation of aminoguanidine with \textit{in situ} generated 1,2-diketones

Silvania Rizzi Brasil\textsuperscript{1} (PG), Adriana C. Capiotto\textsuperscript{1} (IC), Eliandro Faoro\textsuperscript{1} (PO), Davi F. Back\textsuperscript{2} (PO), Alex F. C. Flores\textsuperscript{3} (PO), Lucas Pizzuti\textsuperscript{1,*} (PO)

\textsuperscript{1}Grupo de Pesquisa em Síntese e Caracterização Molecular do MS, Universidade Federal da Grande Dourados, Dourados, MS. \textsuperscript{2}Laboratório de Materiais Inorgânicos, Universidade Federal de Santa Maria, Santa Maria, RS. \textsuperscript{3}Escola de Química e Alimentos, Universidade Federal do Rio Grande, Rio Grande, RS.

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Abstract

Chalcone epoxides generated 1,2-diketones \textit{in situ} which reacted with aminoguanidine to form bis(hydrazinecarboximidamides).

Introduction

In the last years we have investigated new methodologies for the preparation of pyrazole derivatives under mild and clean conditions.\textsuperscript{1} In this direction, we have sought to convert chalcone epoxides into aromatic pyrazoles by cyclocondensation with aminoguanidine under ultrasonic irradiation.\textsuperscript{2} However, \(\alpha,\beta\)-epoxy ketones undergo rearrangement to 1,3-diketones, 1,2-diketones and \(\alpha\)-keto aldehydes in the presence of Lewis acid catalysts, through intramolecular migration of hydrogen, aryl ring, or acyl group.\textsuperscript{3} In fact, we did not detect the desired pyrazoles from the reactions between chalcone epoxides and aminoguanidine in the presence of excess of HCl but we obtained interesting unexpected products. Then, in this work we describe the structural characterization of these products and our endeavor in order to widen the reaction scope.

Results and Discussion

The compound 3a was obtained as the main product during the screening of conditions to perform the reaction between chalcone epoxide 1a and aminoguanidine in order to obtain aromatic pyrazole 2a (Scheme 1). However, 2a was not obtained.

![Scheme 1](Image)

After adjustments in the sonication time (40 min) and amount of HCl (1 mL), the yield of 3a was improved to 78%. The molecular structure of 3a was established in view of its NMR \(^1^H\) and \(^1^3^C\) spectra and X-ray diffraction (Figure 1). The scope of the reaction was extended to chalcone epoxides containing the electron-donating groups methyl (1b) and methoxyl (1c). The corresponding bis(hydrazinecarboximidamides) 3b and 3c were obtained in 75 and 53% yields, respectively.

![Figure 1](Image)

Figure 1. Molecular structure of 3a.

Conclusion

In conclusion, we prepared three new bis(hydrazinecarboximidamides) starting from chalcone epoxides and aminoguanidine. Probably, 1,2-diketones were generated \textit{in situ} and condensed with aminoguanidine. The products present several functionalities which will be explored in the synthesis of heterocyclic compounds and metal complexes.

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