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Synthesis of new 3-*R*-1,2,4-triazolin-5-ones and 2-amino-5-*R*-1,3,4-oxadiazoles, containing fragments of hindered phenolphenol

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Abstract

Compounds containing hindered phenol fragment are known to be effective inhibitors of oxidative processes in different materials, moreover a number of substances among compounds of this class found to show broad spectrum of biological activity. At the same time, five-membered azoles of different classes have variety, of tenunique properties. It seems reasonable to combine in the same molecule fragments screened five-membered heterocycle and phenol to obtain novel compounds having complex utilitarian properties. In this work, a number of new 1-acyl-4-*R*-semicarbazideswere obtained based on hydrazides 3-(4-hydroxy-3,5-di-*tert*-butylphenyl) propanoic, and 2-hydroxy-3,5-di-*tert*-butylbenzoic acid. The best yields are obtained by reacting of hydrazides and isocyanatesin dioxane at 85-90 °C for 2-2.5 hours, in these terms it was 60-86%. During subsequent cyclization by brief reflux 1-1-acyl-4-*R*-semicarbazides in solution of phosphorus oxychloride a number of 2-amino-5-*R*-1,3,4-oxadiazoles was obtained in a yield of 73-92%. Conducting cyclization of 1-acyl-4-*R*-semicarbazides was provided by reflux of initial reagents in aqueous sodium hydroxide solution for 1.5-2 hours and lead to the formation of 3-*R*-1,2,4-1*H*-triazolin-5-ones with 61-81% yield. Based on the ^{1}H NMR and IR-spectroscopy data it was revealed that the obtained 3-*R*-1,2,4-1*H*-triazolin-5-ones in the solid state and in solution of DMSO are in keto-form. The composition of synthesized compounds was confirmed by elemental analysis and the structure was proved by infrared spectroscopy, mass spectrometry, ^{1}H NMR spectroscopy.

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