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ANTIOXIDANT PROPERTIES OF SOME THIAZOLO[4,5-B]PYRIDIN-2-ONES

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Development of an effective and safe antioxidant compound is still challenging in the last few decades. There has been an increasing interest in the role of reactive oxygen species (ROS) in food, drugs, and even living system. Free radical formation is associated with the normal natural metabolism of aerobic cells. They are inevitably exposed to reactive oxygen species formed as oxygen metabolites. Oxidative stress which is largely characterized by reactive oxygen and nitrogen species is implicated

in the development of a number of chronic and degenerative diseases such as atherosclerosis, cancer, cirrhosis, diabetes, wound healing and aging. Free radicals are highly reactive and therefore can attack membrane lipids, generating carbon radicals and peroxy radicals, which cause lipid peroxidation. Therefore, scientists in various disciplines have become more interested in naturally-occurring antioxidants as well as in related synthetic derivatives that could provide active components which prevent or reduce the impact of oxidative stress.

In order to study the effect of various substituents in the molecules on the nature of thepharmacological activity of thiazolo[4,5-b]pyridin-2-ones, a series of new compounds were synthesized based on the previously obtained 5,7-dimethyl-3H-thiazolo[4,5-b]pyridin-2-one. The high electrophilicity of the N3 position in 5,7-dimethyl-3H-thiazolo[4,5-b]pyridin- 2-one allows to use of its functionalization as a convenient method for obtaining various N3-substituted derivatives to expand the range of thiazolo[4,5-b]pyridines. In particular, an NH center with a mobile hydrogen atom at the N3 position in 5,7-dimethyl-3H-thiazolo[4,5-b]pyridin-2-one allows conducting a synthesis based on 3-substituted derivatives. This conversion was carried out through the stage of obtaining potassium salt. Several chloroacetamides were tested as alkylating agents, which allowed to obtain the corresponding 2-(5,7-dimethyl-2-oxo-thiazolo[4,5-b]pyridin-3-yl)-N-aryl-acetamides (1–6) – Fig.

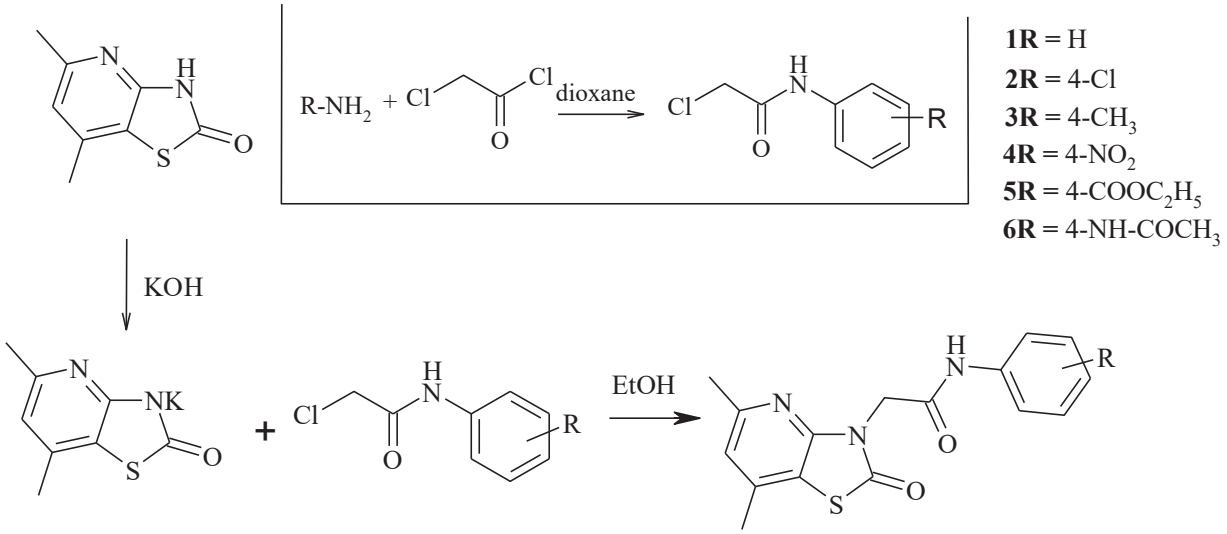

Fig. alkylating agents.

Methods of quantitative elemental analysis, mass spectrometry, and 1H NMR spectroscopy were used to confirm the structure and individuality of the synthesized substances. Interpretation of the spectra revealed that the signals for protons of all structural units were observed in their characteristic ranges.

The antioxidant activity was determined on basis of free radical scavenging activity of 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical. The DPPH method is described as a simple, rapid and convenient method for radical scavenging activity screening of many samples. These advantages make the DPPH method interesting for testing newly synthesized compounds to scavenge radicals and to find out promising

antioxidant drug candidates. The present results of antioxidant activity have shown that the synthesized compounds demonstrated considerable antioxidant effects. When compared with existing antioxidants, some our compounds were found to be more potent. Further optimization of the structure to improve biological activity is currently in progress.

COMPUTATIONAL CHEMISTRY STRATEGIES FOR ANTIOXIDANT ACTIVITY INVESTIGATION

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Mounting research has been performed in the recent decades focusing on natural and low-molecular-weight synthetic antioxidants discovering as key molecules that control oxidative damage and its pathway to disease [1, 2].

Oxidative stress is a phenomenon resulting from the imbalance between oxidation-reduction processes, in particular, the formation and accumulation reactive oxygen species (ROS) and reactive nitrogen species (RNS) in cells and tissues, and the ability of the antioxidant defence system of the organism to eliminate these by-products [3]. Oxidative stress develops under the influence of external or internal factors and leads to oxidative modification of biomolecules, in particular lipids, proteins and DNA [4]. One- and two-electron oxidation-reduction reactions, as an integral part of aerobic metabolism, often lead to free radicals' *in vivo* formation [5]. Molecular oxygen reduction processes include the stepwise single electron reduction of O_2 results in such ROS generation as superoxide anion radical ($O_2^{\bullet-}$), hydrogen peroxide (H_2O_2) and hydroxyl radical ($HO^{\bullet}$) [6]. H_2O_2 is produced as a result of two-electron O_2 reduction. Reactive nitrogen species include mainly nitric oxide ($NO^{\bullet}$), nitrogen dioxide ($NO_2^{\bullet}$) and peroxynitrite ($ONOO^-$), as well as non-radicals such as

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