

Synthesis of adamantane-1,3-dicarboxylic acid derivatives and predicting the spectrum of their biological activity

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Abstract

One of the urgent problems of modern pharmaceutical science is the search for new highly effective agents, both natural and synthetic origin. Among the biologically active substances, the derivatives of adamantane carboxylic acids are very important in practice. It is known that the nitrogen-containing derivatives are more physiological in nature. Pharmacological study showed the presence among them of substances that have pronounced psychotropic, immunotropic, antiviral, antibacterial, antiallergic activity, as well as anti-HIV activity.

Thus, the preparation of new adamantane-1,3-dicarboxylic acid derivatives is important, in terms of searching for new highly effective drugs.

N,N'-Diimidazolide of adamantane-1,3-dicarboxylic acid was obtained by reaction of the reaction 1-cyanimidazole (a widely used condensing agent) and adamantane-1,3-dicarboxylic acid in 86% yield. *N,N'*-dimethyl-*N,N'*-bis(2-(pyridin-2-yl)ethyl)adamantane-1,3-dicarboxamide *via* the *N,N'*-diimidazolide of adamantane-1,3-dicarboxylic acid with a secondary amine – *N*-methyl-2-(pyridin-2-yl)ethanamine is a drug for vestibular vertigo – betahistine. The yield was 79%. The chromatographic purity of newly synthesized adamantane-1,3-dicarboxylic acid derivatives was confirmed by thin-layer chromatography and high-performance liquid chromatography. The structures of the obtained compounds were confirmed by IR and NMR ¹H spectra. Computer screening of possible biological activity in the PASS Professional 2007 program showed that the adamantane-1,3-dicarboxylic acid derivatives have enough degree of drug similarity, the *N,N'*-diimidazolide of adamantane-1,3-dicarboxylic acid can manifest antiseborrheic and anti-inflammatory activity, and *N,N'*-dimethyl-*N,N'*-bis(2-(pyridin-2-yl)ethyl)-adamantane-1,3-dicarboxamide – nootropic activity and can be used as a means against urological diseases. Thus, the results of computer screening of newly synthesized adamantane-1,3-dicarboxylic acid derivatives can be used to continue research in the field of adamantane carboxylic acid derivatives.

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