Knyazevich P. S.

CARBONYL DERIVATIVES OF 4-AMINE-4*H*-1,2,4-TRIAZOLE AND 7-((3-THIO-4-R-4*H*-1,2,4-TRIAZOLE-5-YL)METHYL)THEOPHYLLINE

Supervisor: Ph. D. Gotsulya A. S.
Department of Toxicology and Inorganic Chemistry
Zaporizhzhya State Medical University, Zaporizhzhya

Relevance. Derivatives of 4-amine-4*H*-1,2,4-triazole attract a lot of attention because the reaction with aldehydes creates a series of compounds showing antifungal and antimicrobial activity. Furthermore, the second nitrogen atom is featured with ketone nucleophilic addition reaction that affects electronic effects of the molecule and increases the probability of diverse biological activity in the whole.

As for theophylline derivatives, they have been proven to be relatively low-toxic and, moreover, high-reactive compounds. However, despite the extensive use of existing meds, it is always necessary to create new ones that would be able to solve current problems of medicine and pharmacy.

Goal: to obtain and study the physicochemical properties of carbonyl derivatives of 4-amine-4*H*-1,2,4-triazole and 7-((3-thio-4-R-4*H*-1,2,4-triazole-5-yl)methyl)theophylline (R = CH_3, C_2H_5, C_6H_5).

Tasks:

1 Preparation of the starting compounds and further research of α-haloketone reactions.

2 Physicochemical study of the obtained compounds by ^{1}H NMR, IR spectroscopy, elemental analysis, gas chromatography-mass spectrometry.

3 Prediction of acute toxicity and biological activity.

Materials and methods. The structure of the compound was confirmed by elemental analyzer Elemental Vario EL Cube. IR spectra have been recorded on a spectrometer Bruker ALPHA FT-IR. The prediction was made with online services PASS Online and GUSAR.

Results and discussion. Using known methods, the interacting between the starting compounds and the following α-haloketones: bromacetone, 2-bromo-1-phenylethanone, 2-bromo-1-(4-fluoro(or methoxy)phenyl)ethanone, 2-bromo-1-(thiophen-2-yl)-ethanone was carried out. 3-(5-Nitrofuran-2-yl)acrylaldehyde having been reacted with 4-amine-4*H*-1,2,4-triazole was used as aldehyde. Computer prediction data indicate that all derived ketones are low-toxic (Min LD_{50} = 345,1; Max LD_{50} = 825,8; $\bar{x}$ = 485,025). The dominant activity is a diuretic one.

Conclusions:

1 20 new carbonyl compounds.

2 Confirmed structures of obtained compounds.

3 Biological activity prediction.