Reaction of 2-substituted 6-hydroxy-4-oxo-1,6-dihydropyrimidine-5-carbaldehyde with some N-nucleophiles

© Anastasia E. Potapova,⁺ Elena V. Kuvaeva, Marina V. Sopova, Galina V. Ksenofontova, and Igor P. Yakovlev*

Department of Organic Chemistry. St. Petersburg Chemical-Pharmaceutical Academy. Prof. Popov St., 14. Saint-Petersburg, 197376. Russia. Phone: +7 (812) 234-11-72. *E-mail: Anastasia.Potapova@pharminnotech.com*

*Supervising author; ⁺Corresponding author Keywords: 6-hydroxy-4-oksopirimidin-(3H)-5-carbaldehyde, nucleophilic addition reaction.

Abstract

This presentation deals with derivatives of 1,3-azine as promising structures in terms of the search for new drugs. This class of compounds includes nucleobases (uracil, thymine, cytisine) is a structural unit of DNA and RNA, orotic, uric acid, xanthine and flavins. All these compounds are included in the structure of living organisms, so a search among biologically active compounds for structural analogues seems appropriate. Currently, a lot of substances based on pyrimidine structures with anti-viral, imunostimulatory, antitumor and sedative activities are promoted on the market. The aim of our work is to obtain a new biologically active compounds belonging to the class polyhydroxypyrimidines. This article describes the synthesis and proof of the structures of new 2,5-substituted-6-hydroxypyrimidine-4(3H)-ones. The technique of preparing of 2-substituted-4-hydroxy-6-oxo-1,6-dihydropyrimidine-5-carbaldehyde is presented in the article. Products of the reactions of pyridine-5-carbaldehyde with a variety of N-nucleophiles are estimated with NMR and IR spectroscopy, elemental analysis. Rf of the reaction products and yields are described. This report also presents the results of the pre-computer screening of the biological activity of the obtained compounds. Biological activities of the substances (antiinflammatory, analgetic, antimicrobial) are predicted. This article is the first part of our research, the next one with the results of testing the biological in vivo activity of the resulting compounds will be released later.

References

- [1] L.N. Ovsyannikova, B.Yu. Lalayev, I.P. Yakovlev, T.L. Semakova. Features of reactions of 2,5substituted 4-hydroxy-6H-1,3-oxazine-6-ones with benzimidazole-2-ylhydrazine. Russian Journal of Organic Chemistry. 2016. Vol.52. No.4. P.617-618. (russian)
- [2] A.E. Potapova, E.V. Kuvaeva, I.P. Yakovlev, E.V. Fedorova, A.E. Shchegolev, Synthesis and biological activity of 2,5-substituted 6-hydroxypyrimidine-4-(3H)-ones. Butlerov Communications. 2015. Vol.44. No.11. P.65-68. ROI: jbc-02/15-44-11-65
- [3] V.M. Bryukhanov, J.F. Zverev, V.V. Lampton, A.Y. Zharikov. Lectures on pharmacology for the higher medical and pharmaceutical education. Barnaul, Publishing House "Spectrum". 2014. 95p. (russian)
- [4] A. Kolokotronis. Comparison in vivo and in vitro of the antibacterial action of the antiseptics hexetidine and povidone-iodine. ZWR. 1983. Vol.92. No.6. P.44-46.
- [5] Biological Activities of Hydrazone Derivatives. Sevim Rollas and Ş. Güniz Küçükgüzel. Molecules. 2007. Vol.12. P.1910-1939.
- [6] José Camacho, Arthur Barazarte, Neira Gamboa, Juan Rodrigue, Rosario Rojas, Abraham Vaisberg, Robert Gilman, Jaime Charris. Synthesis and biological evaluation of benzimidazole-5-carbohydrazide derivatives as antimalarial, cytotoxic and antitubercular agents. Bioorganic and Medicinal Chemistry. 2011. Vol.19. P.2023-2029.
- [7] http://www.pharmaexpert.ru/PASSOnline/