Full Paper _____ *Thematic Section:* Bioactivity Research.
Reference Object Identifier – ROI: jbc-02/16-48-10-66 *Subsection:* Biochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Submitted on November 30, 2016.

The study of interrelation "structure – toxicity" in a series of benzimidazole and benzotriazole compounds

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Keywords*:* 1*H*-benzimidazole-1-ylmethanol, 1-[(2-benzyl-1*H*-benzimidazolyl-1)methyl]-1*H*-benzotriazole, 1-benzylbenzimidazole, 2-benzyl-1-(3-phenylpropyl)-1*H*-benzimidazole, toxicity, *Paramecium caudatum*.

Abstract

The genotoxic effect of 1*H*-benzimidazol-1-yl-methanol (**I**), 1-[(2-benzyl-1*H*-1-benzimidazolyl)methyl]-1*H*-benzotriazole (**II**), 1-benzyl-1*H*-benzotriazole (**III**), 2-benzyl-1-(3-phenylpropyl)-1*H*-benzimidazole (**IV**) were studied. The object of study were served ciliates *Paramecium caudatum*. We have investigated of **I-IV** in aqueous solution with different concentrations: 0.0001, 0.001, 0.01 and 0.1; 1 mg/ml. Exposure time was one and three hours. Toxicity was evaluated by number of the victims of ciliates chosen after exposure. All the testing compounds at 1 hour exposure at concentration of 0.0001 mg/ml do not influence on state of ciliates. At the concentration 1 mg/ml of the testing compounds all of them cause 100% mortality of ciliates. The substances **I-IV** at other concentration hour exposure does not statistically significant differences in the toxicity. At the three-hour exposure to the test object under study found that all the compounds at a concentration of 0.01 mg/ml caused a hundred percent mortality rate, and under the influence of substances other analyzed concentrations of most ciliates showed toxicity **III**, the smallest – **II**. A more lasting impact on *Paramecium caudatum* is more negative biological response. According to facts of the two-factor dispersive analysis the determinants for toxicity are calculated from the following contact physicochemical parameters using Gaussian 98 and ALOGPS 2.1 programs: the value of the molecular dipole moment, lipophilicity and molecular volume of the compounds **I-IV** studied. However, correlations between these parameters and the toxicity of the compounds **I-IV** are not found, which can be explained by the presence in the structures of molecular compounds considered fragments of substituents of different structures.

References

[1] J. Joule, K. Mills. Chemistry of Heterocyclic Compound. *Moscow: World.* **2004**. 728p. (russian)
[2] Yu.I. Kuznetsov, N.P. Andreeva, M.O. Agafonkina. About joint adsorption on passive iron from aqueous solutions of 1,2,3-benzotriazole and sodium phenylenedecanoate. *Electrochemistry*. **2010**. Vol.46. No.5. P.593-598. (russian)
[3] S.A. Dzhabieva, E.A. Kolosova, I.N. Karaseva, M.O. Karasev, S.V. Kurbatova. Features of water-acetonitrile solutions of some aromatic heterocycles. *Butlerov Communications.* **2016**. Vol.46. No 5. P.54-60. ROI: jbc-02/16-46-5-54
[4] I.I. Surova, E.V. Ivanova, I.V. Blokhin, I.V. Shakhkel'dyan, Yu.M. Atroshchenko, K.I. Kobrakov, D.N. Kuznetsov, I.V. Fedyanin. Synthesis of 6-thio-substituted 3,5-dinitro-1,2,3,4-tetrahydropyridines. *Butlerov Communications.* **2015**. Vol.42. No 4. P.91-95. ROI: jbc-02/15-42-4-91
[5] M.D. Mashkovskiy. Medicines. In 2 Vols. 14 Ed., *M.: Open Company Publishing house "New Wave": Publisher S.B. Divov.* **2002**. 608p. (russian)
[6] V.A. Shevyrin, M.A. Gofenberg, V.P. Melkozerov, A.S. Neverov, O.S. El'tsov, O.V. Kupriyanova, Yu.Yu. Morzherin. 3-Naphthylindazoles and 2-naphthoylbenzimidazoles are new groups of synthetic cannabinoids: chemical structure, analytical characteristics and identification of the first representatives in the composition of smoking mixtures, as well as some metabolites in the urine. *Butlerov Communications.* **2014**. Vol.37. No.1. P.156-169. ROI: jbc-02/14-37-1-156

[7] E.S. Selezneva, Z.P. Belousova. Influence of structural and physico-chemical features of *N*,*N*'-thiocarbonyl- and *N*,*N*'-sulfonyldiazoles on their antibacterial properties. *Bulletin of SamSU*. **2007**. No.8 (58). P.22-29. (russian)
[8] Quantum-chemical research was carried out as part of the Gaussian 98W program package at the Computing Center of the N.D. Zelinsky Institute of Organic Chemistry of the Russian Academy of Sciences with the participation of T.S. Pivina (IOCh RAS). (russian)
[9] http://www.vcclab.org/lab/alogps/
[10] A.A. Alekseeva. Pharmacological activity of benzimidazole derivatives containing sterically hindered phenolic substituents and their analogues exhibiting antioxidant and antiradical properties: *Abstract of diss. Cand. Farm. Sciences. Volgograd State Medical University. Pyatigorsk.* **2007**. 19p. (russian)