XII Международная научная конференция «Кинетика и механизм кристаллизации. Кристаллизация и материалы нового поколения» http://crystal.isc-ras.ru 18 по 22 сентября 2023 года в г. Иваново.

INTERACTION OF AQUA FORM OF VITAMIN B12 WITH THIOSEMICARBAZIDE IN AQUEOUS MEDIA

Salnikov D.S.[1], Maiorova L.A.[1,2], Koifman O.I.[13], Gromova O.A.[2], Torshin I.Yu.[2], Gromov A.N.[2]
[1]*Institute of Macroheterocyclic Compounds, Ivanovo State University of Chemistry and Technology, Ivanovo, Russia*
[2]*Federal Research Center "Computer Science and Control" of Russian Academy of Sciences, Moscow, Russia*
[3]*G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences, 153045 Ivanovo, Russia*
maiorova.larissa@gmail.com

The development of new effective pharmacological preparations based on vitamin B12, including its synthetic derivatives, and their study, including in carriers, is a promising and popular area of modern pharmacology and biomedicine [1]. At present, much attention is paid to the study of the properties and expansion of the areas of practical application of derivatives of vitamin B_{12}. Aquacobinamide can act as an antidote for poisoning with cyanide, hydrogen sulfide and methyl mercaptan. It has been hypothesized that the derivatives of vitamin B_{12} may act as antidotes for thiosemicarbazide (TH).

The interaction mechanisms between vitamin B_{12} derivatives in aqueous media and the toxicant molecules might be very complex. In addition, the activity of the derivatives can be affected by physical modifications of the molecules associated with formation of the assemblies at the interfaces [2]. Analysis of changes in the electronic absorption spectra recorded during the interaction of aquacobalamin with thiosemicarbazide showed the possibility of partial binding of thiosemicarbazide by aquacobalamin (Fig. 1). The complex between aquacobalamin and thiosemicarbazide is reversible. At the same time, the binding constant is low (K = 1000 ± 100 M^{-1}), that is, TH is able to partially bind to aquacobalamin in animal experiments.

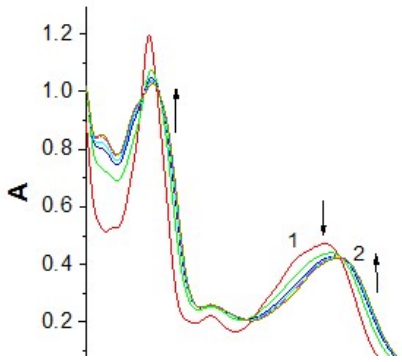

Figure 1. Changes in the electronic absorption spectrum ("A" along the ordinate at, pH = 6.86, t =15 ^{0}C) recorded upon the interaction of 50 μM aquacobalamin with 2.7 mM thiosemicarbazide. The arrows show the direction of the change in optical density during the reaction, the reaction time is 10 minutes.

The work was supported by the grant of the RSF (20-12-00175-p), ISUCT (studies) and by the Ministry of Science and Higher Education (ISUCT, FZZW-2023-0009 in part of compound synthesis).

1. Salnikov D. et al. *New J. Chem.* 2021, **45**, 535; Maiorova L. *Colloids Surf.B* 2019, **182**, 110366; Gromova O. *BioNanoScience* 2022, **12**, 74.
2. Maiorova L. et al. *Langmuir* 2023; Kharitonova N. *JPP* 2018, **22**, 509; Topchieva I.N. *DAN* 1998, **308**, 910; Maiorova L. *J Incl Phen* 2009, **35**, 243; Valkova L. *Bulletin RUS* 2007, **61**, 631; Maiorova L. *Prot Met.* 2015, **51**, 85; Maiorova L. *BioNanoScience* 2018, **8**, 81; Petrova M. *MHC* 2014, **7**, 267.