

## Protonation of 6-aminouracile in dimethylsulphoxide

© Diana I. Kletskova,<sup>1</sup> Timur R. Nugumanov,<sup>2\*</sup> Alexander N. Lobov,<sup>2</sup>  
Leonid V. Spirikhin,<sup>2</sup> Ilshat S. Fayzrakhmanov,<sup>1+</sup> and Sergey P. Ivanov<sup>2\*+</sup>

<sup>1</sup> Bashkir State University. Z. Validi St., 32. Ufa, 450076. Republic of Bashkortostan. Russia.

Phone: +7 (347) 272-63-70. E-mail: rector@bsu.bashedu.ru

<sup>2</sup> Ufa Institute of Chemistry UFRC RAS. prosp. Oktyabrya, 69. Ufa, 450054.

Republic of Bashkortostan. Russia. Phone: + 7 (347) 235-60-96. E-mail: ivanov\_sp@anrb.ru

\*Supervising author; +Corresponding author

**Keywords:** 6-aminouracil, protonation, dimethylsulfoxide.

### Abstract

There were studied the interaction of 6-aminouracil with hydrochloric acid in a solution of dimethylsulfoxide by <sup>1</sup>H, <sup>13</sup>C, <sup>15</sup>N NMR spectroscopy. It was found that with an increase in the concentration of HCl > 0.5 mol/l, protonation of 6-aminouracil in DMSO occurs, while in weakly acidic aqueous solutions this is not observed, as previously reported. To determine mechanism of the protonation were recorded NMR spectra of the original 6-aminouracil and its solution with hydrochloric acid in deuterated DMSO. In the <sup>1</sup>H NMR spectrum of a solution of 6-aminouracil in an acid medium, maximum changes are observed in the protons N(1) of the pyrimidine ring and amine nitrogen. In the carbon spectrum in the acidic medium, the greatest displacement occurs in the fifth carbon atom (by 12 ppm into the strong field), and in the <sup>15</sup>N NMR spectra in the nitrogen of the amine group and N(1) of the pyrimidine ring (in a strong field by 44 and 37 ppm, respectively), compared with the starting 6-aminouracil spectrum. In article are given comparative data on chemical shifts of all hydrogen, carbon and nitrogen atoms of 6-aminouracil in DMSO and with the addition of HCl. On the basis of the experimental data obtained, it is possible to draw an unambiguous conclusion about the direction of protonation in the molecule of 6-aminouracil in its strongly acid solutions in a solution of dimethylsulfoxide. Thus, by <sup>1</sup>H, <sup>13</sup>C, <sup>15</sup>N NMR spectroscopy, it was shown that in the strongly acid solutions of 6-aminouracil in DMSO, its protonation takes place at the amino group of the sixth carbon atom of the pyrimidine ring, and given a scheme of protonation direction of 6-aminouracil in strongly acidic solutions in dimethylsulfoxide is proposed.

### Литература

- [1] E. Miszczak-Zaborska and K. Woźniak. The Activity of Thymidine Phosphorylase Obtained from Human Uterine Leiomyomas and Studied in the Presence of Pyrimidine Derivatives. *Z. Naturforsch.* **1997**. Vol.52. P.670-675.
- [2] F. Focher, D. Ubiali, M. Pregnolato, Zhi Ch, J. Gambino, J.E. Wright, and S. Spadar. Novel Nonsubstrate Inhibitors of Human Thymidine Phosphorylase, a Potential Target for Tumor-Dependent Angiogenesis. *J. Med. Chem.* **2000**. Vol.43. P.2601-2607.
- [3] M.D. Mashkovsky. Medicines. *Moscow: New wave.* **2010**. P.340-341. (russian)
- [4] I.V. Petrova, V.A. Kataev, S.A. Meshcheryakova, K.V. Nikolaeva, D.A. Munasipova, R.R. Farhutdinov. Antioxidant properties of pyrimidine derivatives. *Medical Bulletin of Bashkortostan.* **2013**. Vol.8. Iss.4. P.64-67. (russian)
- [5] O.V. Akchurina, V.Yu. Mishinkin, S.A. Grabovsky, N.N. Kabalnova, Yu.I. Murinov. *Russian Journal of General Chemistry.* **2016**. Vol.86. Iss.10. P.1691-1696. (russian)
- [6] B. Ionin, B.A. Ershov, A.I. Koltsov. NMR spectroscopy in organic chemistry. *Leningrad: Chemistry.* **1983**. P.187. (russian)
- [7] V.A. Semenov, D.O. Samultsev, L.B. Krivdin. Theoretical and experimental study of <sup>15</sup>N NMR protonation shift. *Magn. Reson. Chem.* **2015**. Vol.53. P.433-441.
- [8] E. Preg, F. Bulman, K. Affolter. Determination of the structure of organic compounds "Tables of spectral data". *Moscow: Mir.* **1975**. P.75. (russian)
- [9] G. Levi, G. Nelson. A Guide to Carbon Nuclear Magnetic Resonance-13 for Organic Chemists. *Moscow: Mir.* **2012**. P.84, 98. (russian)