LITERATURE CITED

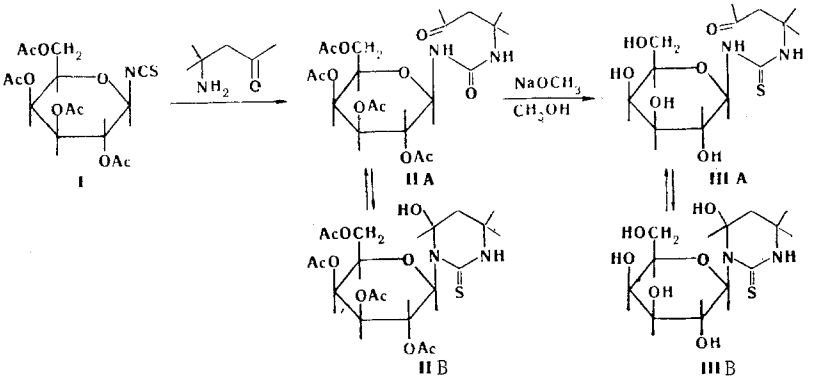
1. R. Raap and J. Howard, Can. J. Chem., 47, 813 (1969).
2. E. Einberg, J. Org. Chem., 35, 3978 (1970).

REACTION OF 2,3,4,6-TETRA-O-ACETYL-β-D-GALACTOPYRANOSYL ISOTHIOCYANATE WITH 4-AMINO-4-METHYL-2-PENTANONE

A. D. Shutalev, L. A. Ignatova, and B. V. Unkovskii

UDC 547.455.627'853.5'854.1

Hydroxyhexahydropyrimidine-2-thiones are structural analogs of the minor bases of nucleic acids, the products of their metabolism, and some medicinal preparations [1]. In order to study the structure, tautomerism, and new properties of substituted 4-hydroxyhexahydropyrimidine-2-thiones we undertook the structural modification of the latter by means of a sugar residue. As a model reaction we studied the reaction of 2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl isothiocyanate (I) [2] with 4-amino-4-methyl-2-pentanone [3] in benzene at 20°C, as a result of which we obtained N-glycoside II, with mp 89.5-91.0°C (from benzene), $[\alpha]_D^{22}$ 0.0, and $[\alpha]_{366}^{22}$ + 159.2 (c 1.1, $CHCl_3$), in 80% yield. Zemplen deacetylation of glycoside II gave III, with mp 92.0-93.5°C, $[\alpha]_D^{20}$ 0.0, and $[\alpha]_{366}^{20}$ + 4.6 (c 0.9, H_2O), in 60% yield after chromatography on silica gel in a $CHCl_3$—EtOH system (3:1).



A νC=O band at 1710 cm^{-1} is observed in the IR spectra of N-glycosides II and III recorded in mineral oil and in solution in $CHCl_3$. Signals of protons of, respectively, a CH_2C=O group at 3.16 and 3.40 ppm and of a CH_3C=O group at 2.10 and 2.12 ppm are present in the PMR spectra of II and III. The set of spectral data shows that in the crystalline state and in solution in $CDCl_3$ N-glycosides II and III have primarily the N_1-(β-D-galactopyranosyl)-N_3-(2-methyl-4-oxo-2-pentyl)thiourea structure (IIA, IIIA) with an acyclic structure of the aglycone, whereas the N_1-methylanalog, which is not bonded to a sugar residue, has a cyclic structure [4]. Thus the introduction of a sugar residue in the hydroxyhexahydropyrimidine-2-thione molecule destabilizes the cyclic structure of the heterocyclic compound.

LITERATURE CITED

1. G. L. Neil, T. E. Moxley, and R. C. Manak, Cancer Res., 30, 2166 (1970).
2. C. Gmernicka-Haftek and W. Wieniawski, Acta Pol. Pharm., 34, 23 (1977).
3. L. A. Ignatova, Yu. E. Kazantsev, and B. V. Unkovskii, Zh. Org. Khim., 5, 1792 (1969).
4. B. V. Unkovskii, L. A. Ignatova, and M. G. Zaitseva, Khim. Geterotsikl. Soedin., No. 5, 889 (1969).

M. V. Lomonosov Moscow Institute of Fine Chemical Technology, Moscow 119831. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 2, p. 269, February, 1982. Original article submitted June 11, 1981.

 0009-3122/82/1802-0214$07.50