Chemistry of Heterocyclic Compounds, Vol. 29, No. 10, 1993

SYNTHESIS OF DERIVATIVES OF A NEW THIAZOLO[2,3-i]PURINE HETEROAROMATIC SYSTEM

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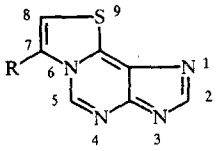
Derivatives of the thiazolo[2,3-i]purine (III) tricyclic heteroaromatic system have not yet been described. Only 7,8-dihydrothiazolo[2,3-i]purine [1] and some of its substituted derivatives are known [2-4].

In development of our work [5] we have carried out the synthesis of compounds IIIa-c by dehydration of 7-hydroxy-7,8-dihydrothiazolo[2,3-i]purine (I) and 6-acylalkylthiopurines (IIa, b) [6, 7] by the action of $POCl_3$, H_2SO_4, and polyphosphoric acid (PPA), as has previously been reported at the Conference [8].

Compound I was obtained by us by hydrolysis of the diethylacetal of 6-formyl-methylthiopurine [9].

The structure of compounds IIIa-c was confirmed by physicochemical methods. While the structure of IIIa was also confirmed by reductive desulfurization to 1-ethylpurine (IV) [1].



IIIa R = H; b R = Me; c R = Ph

7-Hydroxy-7,8-dihydrothiazolo[2,3-i]purine (I, $C_7H_6N_4OS$), mp 189-190°C (from aqueous acetone). M^+ 194. IR spectrum in mineral oil: 3200-3070 (OH), 1610, 1555 cm^{-1} (C=C, C=N), PMR spectrum (DMSO-D_6): 8.75 (1H, s, 2-H), 8.63 (1H, s, 5-H), 6.39 (1H, m, 7-H), 3.81-3.53 ppm (2H, m, CH_2). Yield, 26%.

Thiazolo[2,3-i]purine (IIIa, $C_7H_4N_4S$). Picrate, mp 268-270°C (dec., aqueous ethanol). Yield, 47%.

7-Methylthiazolo[2,3-i]purine (IIIb, $C_8H_6N_4S$), mp > 300°C (ethanol). M^+ 190, IR spectrum (mineral oil): 1600 cm^{-1} (C=C, C=N). PMR spectrum (CF_3COOH): 9.26 (1H, s, 2-H), 7.97 (1H, s, 5-H), 7.49 (1H, s, 8H), 2.92 ppm (3H, s, CH_3). Yield, 83%.

7-Phenylthiazolo[2,3-i]purine (IIIc, $C_{13}H_8N_4S$), mp > 300°C (ethanol). M^+ 252, IR spectrum (mineral oil): 1600 cm^{-1} (C=C, C=N). PMR spectrum (DMSO-D_6): 9.11 (1H, s, 2-H), 8.54 (1H, s, 5-H), 8.01 (1H, s, 8-H), 7.8-7.62 ppm (5H, m, C_6H_5). Yield, 86%.

1-Ethylpurine (IV), mp 198-199°C (isopropanol). UV spectrum (in ethanol), λ_{max} (log ε) = 221.3 (4.19), 273.4 nm (3.54). According to the data in [1], mp 198°C.

The data of the elemental analysis of the new compounds for C, H, N, S correspond to the calculated values.

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