SYNTHESIS OF INDOLYL DERIVATIVES OF TRIAZOLO[1,5-a]PYRIMIDINE

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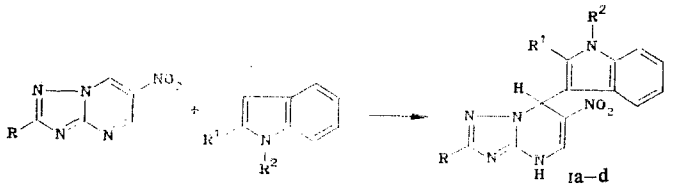
Cases are known of the direct introduction of an indole fragment into the pyrimidine nucleus of azoannelated derivatives, viz. imidazo[3,4-d]pyrimidine in [1] or 3-cyano-6,7-dicarbethoxypyrazolo[1,5-a]pyrimidine in [2], assuming activation of the substrate by formation of acyl or quaternary salts.

It was discovered by us that 6-nitro-7-(3-indolyl)-4,7-dihydro-1,2,4-triazolo[1,5-a] pyrimidines (Ia-d) were readily formed in 78-90% yield on heating indole and its 1- or 2-methyl derivatives with 2-R-6-nitro-1,2,4-triazolo[1,5-a]pyrimidines in butanol.



Ia–d

Ia $R=R^1=R^2=H$; b $R=R^1=H$, $R^2=CH_3$; c $R=R^2=H$, $R^1=CH_3$; d $R^1=R^2=H$, $R=CH_3$

The nitro group in position 6 of the pyrimidine fragment activates the triazolo[1,5-a] pyrimidine system sufficiently towards nucleophilic attack and the reaction with indoles takes place without previous transfer of substrate to the cationic form.

The molecular weight determined by mass spectrometry and the results of elemental analysis of the obtained compounds were in agreement with those calculated. Data of IR and PMR spectra of adducts (Ia-d) and X-ray structural analysis of compound (Id) confirmed the proposed structure.

The synthesized compounds were (mp°C, yield %): (Ia) 248-250, 84; (Ib) 265-266, 78; (Ic), 260-262, 80; (Id) 250-252, 90. In the IR spectra of the obtained substances the nitro group absorbed at 1550 and 1340 and the NH of the indole and pyrimidine fragment at 3300 cm^{-1}.

In typical PMR spectra (DMSO-d_6, TMS) characteristic one proton singlets were observed at 7.0 (7-H), 8.5 (5-H), 11.1 (indole NH), and 12.6 (4-H) ppm, and a multiplet at 7.0-7.5 (protons of the indole nucleus).

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