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DERIVATIVES OF A NEW HETEROCYCLIC SYSTEM — 4,11-DIHYDRO-10H-1,2,4-TRIAZOLO[1,5-a]PYRIMIDO[6,5-c]BENZO[b]PYRANS

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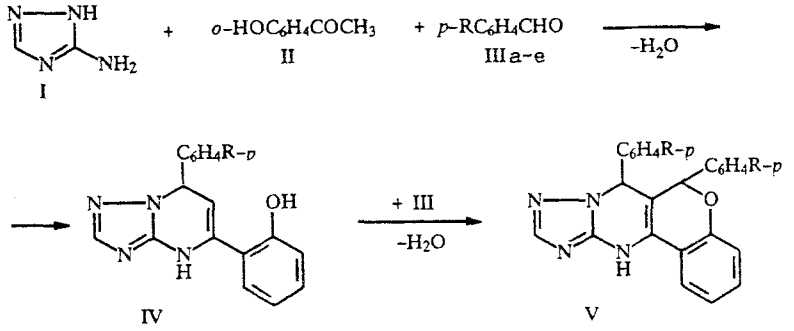
It has previously been shown that the reaction of 3-amino-1,2,4-triazole (I) with aromatic aldehydes and ketones may lead to dihydro derivatives of 1,2,4-triazolo[1,5-a]pyrimidine [1]. We found that on boiling solutions of amine I, o-hydroxyacetophenone (II) and benzaldehydes IIIa-e (molar ratio 1:1:1) in DMFA for 3 h in the presence of piperidine, together with small amounts (5-10%) of dihydrotriazolopyrimidines IVa-e, 4,11-dihydro-10H-1,2,4-triazolo[1,5-a]pyrimido[6,5-c]benzo[b]pyrans Va-e are formed. When a twofold excess of the aldehydes III is used, compounds V are the sole reaction products.



IV, Va R = H, b R = OCH_3, c R = $N(CH_3)_2$, d R = F, e R = Cl

The formation of compounds Va-e was also attained by the reaction of dihydrotriazolopyrimidines IV, obtained by an independent method, with aldehydes IIIa-e (boiling in DMFA for 1 h).

Compound Va ($C_{24}H_{18}N_4O$), mp 282°C (benzene-DMFA, 3:1). IR spectrum, $\nu_{C=C}$ (KBr) 1659 cm^{-1}. PMR spectrum (DMSO-D_6): 5.37 (1H, s, 11-H), 5.63 (1H, s, 10-H), 6.3-7.8 (14H, m, ArH), 7.66 (1H, s, 2-H), 10.5 ppm (1H, s, NH). Yield, 62%.

Compound Vb ($C_{26}H_{22}N_4O_3$), mp 267°C (benzene-DMFA, 3:1). IR spectrum, $\nu_{C=C}$ (KBr) 1658 cm^{-1}. PMR spectrum (DMSO-D_6): 3.71 (3H, s, CH_3O), 3.74 (3H, s, CH_3O), 5.33 (1H, s, 11-H), 5.55 (1H, s, 10-H), 6.2-7.8 (12H, m, ArH), 7.65 (1H, s, 2-H), 10.5 ppm (1H, s, NH). Yield, 61%.

Compound Vc ($C_{28}H_{28}N_6O$), mp 289-292°C (benzene-DMFA, 3:1). IR spectrum, $\nu_{C=C}$ (KBr) 1656 cm^{-1}. PMR spectrum (DMSO-D_6): 2.84 (6H, s, $(CH_3)_2N$), 2.87 (6H, s, $(CH_3)_2N$), 5.28 (1H, s, 11-H), 5.42 (1H, s, 10-H), 6.2-7.8 (12H, m, ArH), 7.63 (1H, s, 2-H), 10.4 ppm (1H, s, NH). Yield, 58%.

Compound Vd ($C_{24}H_{16}N_4OF_2$), mp 273-276°C (benzene–DMFA, 3:1). IR spectrum, $\nu_{C=C}$ (KBr) 1656 cm^{-1}. PMR spectrum (DMSO-D_6): 5.41 (1H, s, 11-H), 5.70 (1H, s, 10-H) 6.3-7.8 (12H, m, ArH), 7.67 (1H, s, 2-H), 10.5 ppm (1H, s, NH). Yield, 56%.

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Compound Ve ($C_{24}H_{16}N_4OCl_2$), mp 299-301°C (benzene–DMFA, 3:1). IR spectrum, $\nu_{C=C}$ (KBr) 1659 cm^{-1}. PMR spectrum (DMSO-D_6): 5.41 (1H, s, 11-H), 5.74 (1H, s, 10-H) 6.3-7.9 (12H, m, ArH), 7.67 (1H, s, 2-H), 10.5 ppm (1H, s, NH). Yield, 50%.

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