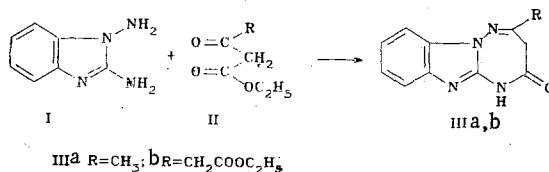


SYNTHESIS OF 3H-1,2,4-TRIAZEPINO[2,3-a]BENZIMIDAZOL-4(5H)-ONES

M. V. Povstyanoi, V. P. Kruglenko,
and V. P. Gnidets

UDC 547.89:542.953.2:543.51

Representatives of a new heterocyclic system, viz., 3H-1,2,4-triazepino[2,3-a]benzimidazol-4(5H)-ones (IIIa,b), were obtained by the reaction of 1,2-diaminobenzimidazole (I) with β -keto acid esters (II).



The reaction proceeds unambiguously in acetic acid to give 2-methyl-3H-1,2,4-triazepino[2,3-a]benzimidazol-4(5H)-one [IIIa, 72% yield, mp 281-282°C (from DMF)] and 2-(carbethoxymethyl)-3H-1,2,4-triazepino[2,3-a]benzimidazol-4(5H)-one [IIIb, 64% yield, mp 227-228°C (from methanol)].

The individuality of the compounds obtained was confirmed by thin-layer chromatography (TLC). The mass spectra confirmed the structures and empirical compositions of the molecular and fragment ions of the synthesized IIIa,b. Mass spectrum of IIIa, m/z (relative intensities, %): 214 (100), 186 (34), 173 (12), 171 (14), 145 (26), 132 (46), etc. Mass spectrum of IIIb, m/z (relative intensities, %): 286 (68), 258 (6), 240 (21), 214 (14), 213 (17), etc. Characteristic bands of vibrations at 1725-1735 (ν_{CO}) and 3420-3440 cm^{-1} (ν_{NH}) appear in the IR spectra of triazepinobenzimidazoles IIIa,b; in addition, an intense band of an ester carbonyl group at 1695 cm^{-1} (ν_{CO}) is observed for IIIb.

The results of elementary analysis confirm the empirical formulas of the compounds obtained.

Kherson Industrial Institute, Kherson 325008. Translated from *Khimiya Geterotsiklicheskikh Soedinenii*, No. 5, pp. 700-701, May, 1984. Original article submitted June 17, 1983; revision submitted October 12, 1983.