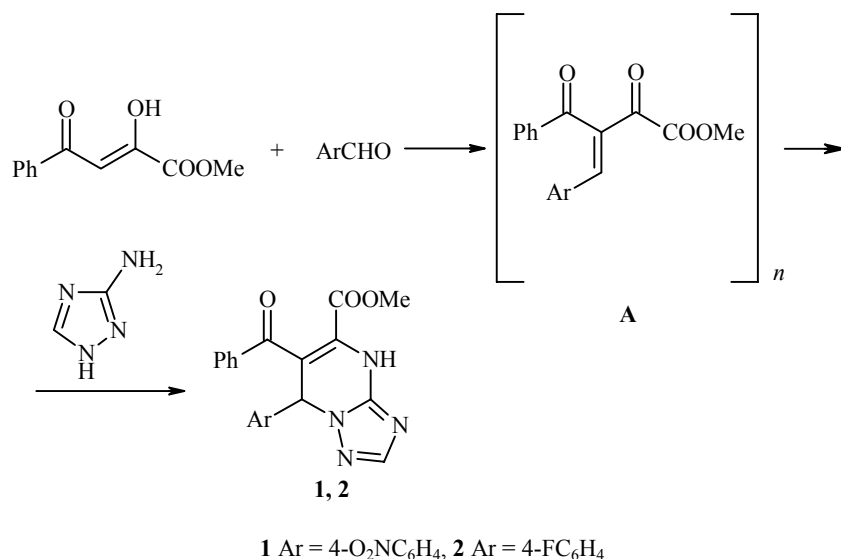


SYNTHESIS OF 4-ARYL-3-BENZOYL-2-METHOXYCARBONYL-1,4-DIHYDRO-PYRIMIDO[1,2-*b*]TRIAZOLES

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We have observed that fusion at 115-130°C of methyl esters of benzoylpyruvic acids with 3-amino-1,2,4-triazole in the presence of an aromatic aldehyde leads to 4-aryl-3-benzoyl-2-methoxycarbonyl-1,4-dihydropyrimido[1,2-*d*]triazoles (**1,2**).



Compounds **1, 2** are colorless crystalline substances that are readily soluble in DMSO and DMF and when heated are soluble in alcohol, acetic acid, and dioxane, but are insoluble in water.

Probably in the first step of the reaction the unsaturated compound **A** is formed, the reaction with which of 3-amino-1,2,4-triazole leads to compounds **1, 2**. The structure of the latter is confirmed by ¹H NMR and IR spectra and mass spectrometry.

The IR spectra were obtained on a UR-20; the ¹H NMR spectra were obtained on a Bruker DRX 500 (500 MHz) in DMSO-*d*₆. The mass spectra were taken on an MKh-1320, ionizing electron energy 70 eV.

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3-Benzoyl-2-methoxycarbonyl-4-(4-nitrophenyl)-1,4-dihydropyrimido[1,2-*b*]triazole (1). Fusion of a mixture of the methyl ester of benzoylpyruvic acid (0.01 mol), 4-nitrobenzaldehyde (0.01 mol), and 3-amino-1,2,4-triazole (0.01 mol) was carried out on a metal bath at 115-130°C until evolution of gas stopped; the mixture was cooled down and treated with ethanol; the precipitate was filtered out and recrystallized. Yield 1.55 g (38%); mp 200-202°C (EtOH). IR spectrum, ν , cm^{-1} : 1665 (CO), 1740 (COOMe), 3220 (NH). ^1H NMR spectrum, δ , ppm: 3.21 (3H, s, OMe); 6.73 (1H, s, $\text{C}_{(4)}\text{H}$); 7.40-8.16 (9H, m, arom); 7.78 (1H, s, $\text{C}_{(6)}\text{H}$); 11.35 (1H, s, NH). Mass spectrum, m/z (I_{rel} , %): $[\text{M}]^+$ 405 (33.80). Found, %: C 59.25, 59.18; H 3.73, 3.65; N 17.27, 17.32. $\text{C}_{20}\text{H}_{15}\text{N}_5\text{O}_5$. Calculated, %: C 59.30; H 3.71; N 17.40.

3-Benzoyl-4-(4-fluorophenyl)-2-methoxycarbonyl-1,4-dihydropyrimido[1,2-*b*]triazole (2) was obtained similarly. Yield 1.35 g (36%); mp 222-224°C (EtOH). IR spectrum, ν , cm^{-1} : 1645 (CO), 1730 (COOCH₃), 3200 (NH). ^1H NMR spectrum, δ , ppm: 3.23 (3H, s, OMe); 6.55 (1H, s, $\text{C}_{(4)}\text{H}$); 7.08-7.56 (9H, m, arom.); 7.75 (1H, s, $\text{C}_{(6)}\text{H}$); 11.15 (1H, s, NH). Mass spectrum, m/z (I_{rel} , %): $[\text{M}]^+$ 378 (44.48). Found, %: C 63.51, 63.48; H 3.99, 4.02; N 14.80, 14.72. $\text{C}_{20}\text{H}_{15}\text{FN}_4\text{O}_3$. Calculated, %: C 63.55; H 4.00, N 14.85.

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