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THREE-COMPONENT REACTION OF 2-AMINOBENZOTHIAZOLE WITH METHYLENE-ACTIVE CARBONYL COMPOUNDS AND ALDEHYDES

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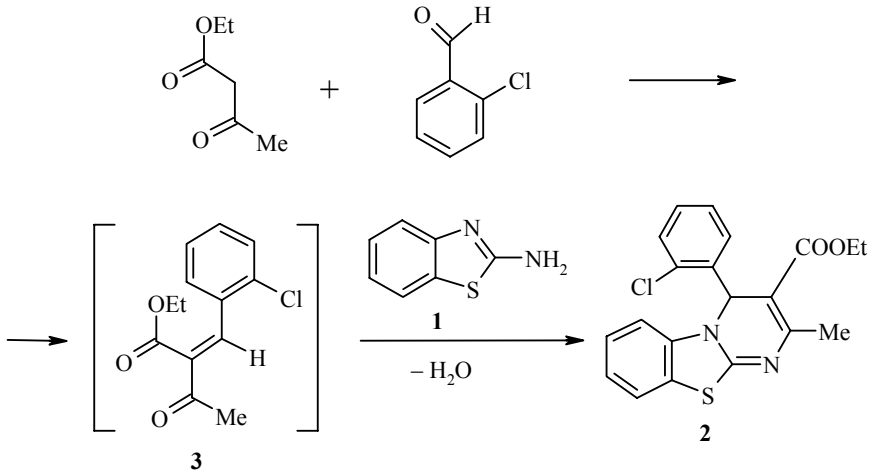
Examples are known of three-component heterocyclization of 3-aminotriazole and 2-aminobenzimidazole with aldehydes and methylene-active carbonyl compounds [1-3]. We have studied the possibility of this reaction occurring in the 2-aminobenzothiazole series.

We found that reaction of 2-aminobenzothiazole (**1**) with *o*-chlorobenzaldehyde and acetoacetic ester with prolonged boiling in butanol leads to ethyl 4-(2-chlorophenyl)-2-methyl-4H-benzo[4,5][1,3]thiazolo[3,2-*a*]-pyrimidine-3-carboxylate (**2**). Based on data in [2], we can hypothesize the following two-step scheme for the three-component condensation. In the first step, the acetoacetic ester reacts with benzaldehyde to form the corresponding arylidene derivative **3**, the condensation of which with compound **1** in the second step leads to the target product **2**.



Under analogous conditions, we were also able to carry out the reaction of aminobenzothiazole **1** with benzaldehyde and cyclohexane-1,3-dione, leading to 12-phenyl-2,3,4,12-tetrahydro-1H-benzo[4,5][1,3]-thiazolo[2,3-*b*]quinazolin-1-one (**4**).

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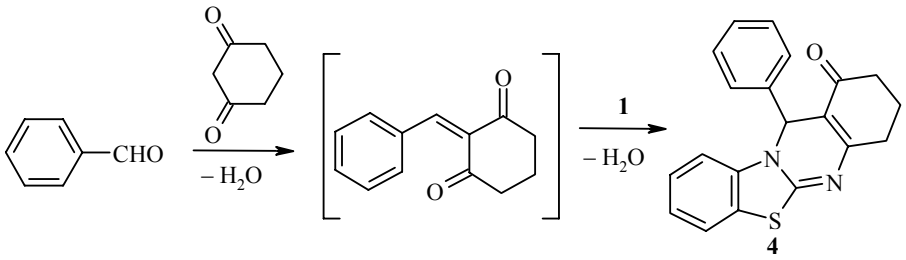

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The ^{1}H NMR spectra were recorded on a Bruker AC-300 (300 MHz) in DMSO-d_6; internal standard TMS.

Ethyl 4-(2-Chlorophenyl)-2-methyl-4H-benzo[4,5][1,3]thiazolo[3,2-*a*]pyrimidine-3-carboxylate (2). A mixture of compound **1** (0.01 mol), acetoacetic ester (0.01 mol), and benzaldehyde (0.01 mol) in *n*-butanol (30 ml) was boiled for ~50 h in a flask under reflux. At the end of the reaction (monitored by TLC), the product formed was isolated by column chromatography, using a 1:1 mixture of chloroform and ethyl acetate as the eluent. Yield 60%; mp 115-116°C. ^{1}H NMR spectrum (DMSO-d_6), δ, ppm: 0.85 (3H, t, $OCH_2\underline{CH_3}$); 2.38 (3H, s, CH_3); 4.00-4.15 (m, $O\underline{CH_2}CH_3$); 6.80 (1H, s, >$\underline{CH}$–Ar); 7.20-7.80 (8H, m, arom.). Found, %: C 62.32; H 4.33; Cl 9.05; N 7.43; S 8.45. $C_{20}H_{17}ClN_2O_2S$. Calculated, %: C 62.41; H 4.45; Cl 9.21; N 7.28; S 8.33.

12-Phenyl-2,3,4,12-tetrahydro-1H-benzo[4,5][1,3]thiazolo[2,3-*b*]quinazolin-1-one (4). A mixture of compound **1** (0.01 mol), cyclohexanedione (0.01 mol), and benzaldehyde (0.01 mol) in *n*-butanol (30 ml) was boiled in a flask under reflux for ~20 h. At the end of the reaction (monitored by TLC), the precipitate formed was filtered out and recrystallized from isopropyl alcohol. Yield 40%; mp 234-235°C. ^{1}H NMR spectrum (DMSO-d_6), δ, ppm: 1.80-2.30 (6H, m, $3CH_2$); 6.55 (1H, s, >$\underline{CH}$–Ar); 7.15-7.91 (9H, m, arom.). Found, %: C 72.12 H 4.78; N 8.59; S 9.81. $C_{20}H_{16}N_2OS$. Calculated, %: C 72.26; H 4.85; N 8.43; S 9.65.

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