2-NITROGUANIDINE IN THE SYNTHESIS OF AZAHETEROCYCLES

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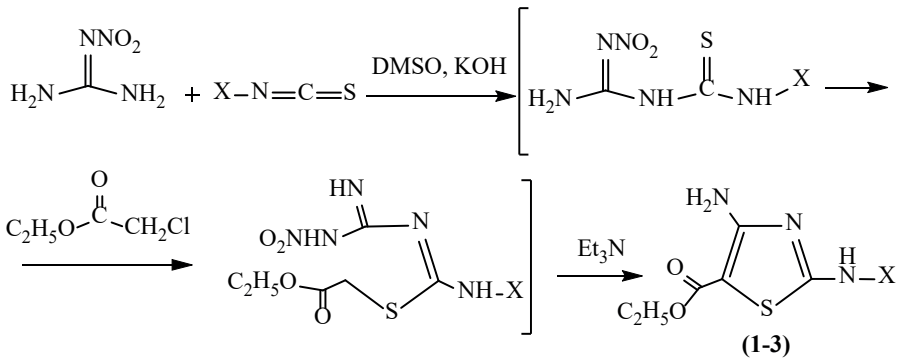
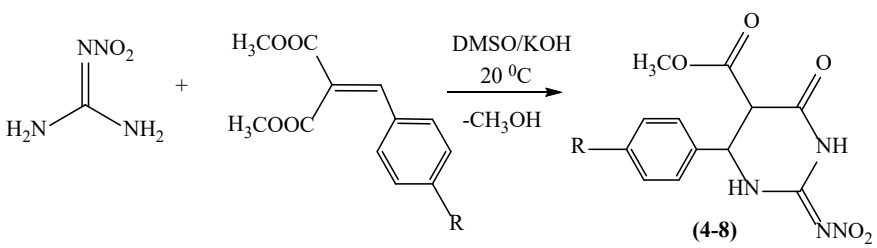
Derivatives of azoles and azines are attractive for their potential biological activity; among them are substances with analgesic, antihypoxic, antitumor, antifungal, and other beneficial properties. A convenient building block for the construction of nitrogenous heterocycles is 2-nitroguanidine. We carried out a three-component one-pot synthesis with the participation of 2-nitroguanidine, commercially available isothiocyanates and ethyl ester of chloroacetic acid, resulting in 4-amino-2-(arylamino)-5-ethoxycarbonyl-1,3-thiazolam (1-3) with yields up to 87%.



X= C_6H_4-CH_3 $^{-n}$ (1); C_6H_4-Cl^{-n} (2); C_6H_4-OCH_3 $^{-n}$ (3)

The use of preparatively available substituted dimethyl 2-benzylidene malonates in the reaction with 2-nitroguanidine as bielectrophilic reagents allowed us to obtain in yields up to 80% new representatives of methyl 6-aryl-2-nitroimino-4-oxo-5,6-dihydropyrimidin-5 carboxylates (4–8).



R= CH_3 **(4)**, OCH_3 **(5),** $N(CH_3)_2$ **(6)**, Cl **(7)**, NO_2 **(8)**

The structure of the obtained heterocyclic compounds (1-8) was established on the basis of the complex use of modern spectral methods: IR, ^1H and ^{13}C- $\{^1H\}$ NMR with the involvement of heteronuclear experiments (^1H-^{13}C HMQC, HMBC), as well as X-ray diffraction.