PP2. 2-METHYLQUINAZOLIN-4-YLIDENECYANOACETIC ACID ETHYL ESTER

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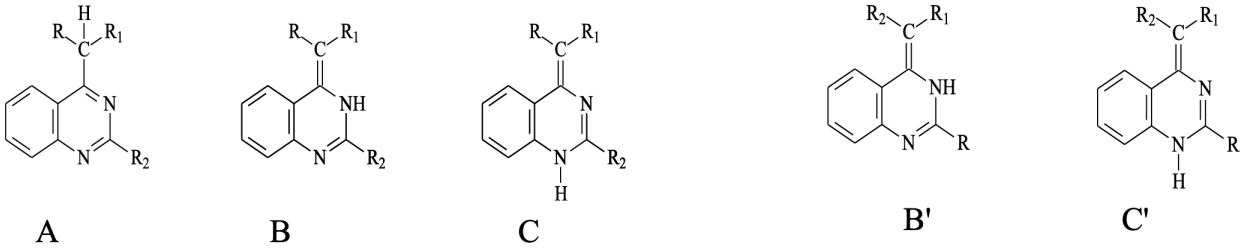
From a theoretical point of view, the 2,4-substituted quinazolines studied by us canexist in three (**A, B, C**) interconvertible tautomeric forms, and the reaction productcan be one of the most stable forms or a mixture of tautomers [1]. In addition, for the**B** and **C** forms, one can write two geometric isomers, respectively, **B'** and **C'**:



Therefore, the synthesis of these compounds and the determination of the exact structure of the final reaction products using physical methods was of great theoretical interest.

The structure of 2-methylquinazolone-4-ylidenecyanoacetic acid ethyl ester (1) synthesized by us in solution was studied by 1H NMR spectroscopy, and the crystal structure of compound 1 was determined by X-Ray (Fig. 1).

The presence of an intramolecular hydrogen bond NH---O=C between the N^3- nitrogen of the quinazoline ring and the carbonyl group of the cyanoacetic ester residue is characteristic of compound 1. The parameters of this intramolecular H- bond are as follows: N3…$O1^1$ distances 2.592 Å, H…$O1^1$ 1.78 Å and angle N3- H…$O1^1$ 141°.

Thus, based on the ^{1}H NMR spectrum of compound **1**, it was determined that they also exist in solution in the tautomeric state **B**. This is due to the presence of an intramolecular hydrogen bond NH…O=C.

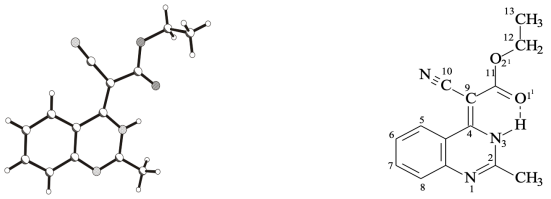


Fig. 1. Crystal structure of ethyl ester 2-methylquinazolin-4-ylidenecyanoacetic acid[1].

REFERENCE

[1] Lapachev V.V., Zagulyaeva O.A., Mamaev V.P. Tautomerism of pyrimidyl-2-cyanoacetic esters, Izv, Academy of Sciences of the USSR. Ser. Chem., Moscow, 1977; 11: 2633.