SYNTHESIS AND STRUCTURE OF ETHYL 1-HYDROXY-3-OXO-5,6-DIHYDRO-3*H*-PYRROLO[3,2,1-*ij*]QUINOLINE-2-CARBOXYLATE

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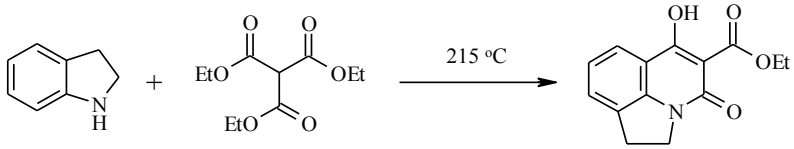
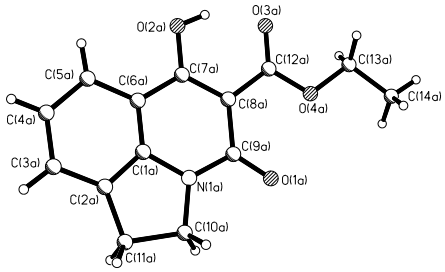
Introduction. Ethyl ester of 1-hydroxy-3-oxo-5,6-dihydro-3*H*-pyrrolo[3,2,1-*ij*]quinoline-2-carboxylate is of interest as the starting material for obtaining a potentially biologically active of tricyclic analogues of 4-hydroxyquinolone-2.

Aim. The aim of this work was to synthesis ethyl ester of 1-hydroxy-3-oxo-5,6-dihydro-3*H*-pyrrolo[3,2,1-*ij*]quinoline-2-carboxylic acid and study of the structure. **Materials and Methods.** Its quinoline synthesized by a condensation of indoline **1** with diethyl ester metantricarboxylic acid **2**:



1 **2** **3**

Results and discussions. The symmetrically independent cells of elementary ester **3,** there are two molecules (**A** и **B**), which differ by some peculiarities of structure. All non-hydrogen atoms of molecule **A**, excluding atoms $C_{(11A)}$ and $C_{(14A)}$, lay in one plane accurate within 0.02 Å. Atoms $C_{(11A)}$ and $C_{(14A)}$ deflect from a root-mean-square plane of the rest non-hydrogen atoms to -0.08 and 0.25 Å respectively. In the molecule **B** atom $C_{(11B)}$ only deflects from a root-mean-square plane of the rest non-hydrogen atoms (accuracy 0.02 Å) to - 0.11 Å.



In the molecule **A** bonding $C_{(7)}$-$C_{(8)}$ 1.414 (7) Å is extended comparing to its average value 1.326 Å, that is explained by the result of creation of quite strong intermolecular hydrogen bonds $O_{(2)}$-$H_{(2O)}$…$O_{(3)}$ (H…O 1.76 Å, O-H…O 149°). In analysis of a bond length, in a molecule **B** [bonding $O_{(1)}$-$C_{(9)}$ 1.249(7) Å and $C_{(7)}$-$C_{(8)}$ 1.404(8) Å are extended (average values 1.210 and 1.326 Å), but bonding $O_{(2)}$-$C_{(7)}$ 1.304(6) Å and $C_{(8)}$-$C_{(9)}$ 1.432(8) Å are shorten (average values 1.333 and 1.464 Å)]. This is proved by pretty weak character of intramolecular hydrogen bond in a molecule **B** $O_{(2)}$-$H_{(2O)}$…$O_{(3)}$ (H…O 1.94 Å, O-H…O 126°), that excludes a possibility of proton transferring from 4-hydroxygroup to a carboxylic atom of oxygen $O_{(3)}$. Between molecules **A** and **B** обнаружены shorten intramolecular contacts $H_{(11C)}$…$C_{(9A)'}$ (*x, y, z*) 2.78 Å, $H_{(10B)}$…$C_{(3B)'}$ (*x, y, z*) 2.84 Å have been discovered.

Conclusions. The structure of ethyl ester 1-hydroxy-3-oxo-5,6-dihydro-3*H*-pyrrolo[3,2,1-*ij*]quinoline-2-carboxylic acid was confirmed by ^{1}H NMR spectroscopy and was proved by X-ray structural analysis.