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SYNTHESIS AND MOLECULAR STRUCTURE OF METHYL 6'-AMINO-5'-CYANO-2-OXO-3' H-SPIRO [INDOLINE-3, 4'-PYRANO [2, 3-C] PYRAZOLE]-3'-CARBOXYLATE

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The synthesis of drug-like spirocyclic oxindoles has attracted considerable attention due to their wide spread applicability in biomedical sciences as they show great potential for binding to many bioactive molecules. As a part of our plan aimed at developing new methods for the synthesis of biologically important oxindoles, we were inspired to investigate the environment friendly conditions for the synthesis of spirooxindolo pyrano pyrazole carboxylate hybrid molecule. Herein, we wish to report the selective protocol for synthesis of methyl 6'-amino-5'-cyano-2-oxo-3'*H*-spiro[indoline-3,4'-pyrano[2,3-c] pyrazole]-3'-carboxylate via Et₃N catalyzed reaction of isatin, 2-(2-hydroxy-2,5,5,8a-tetramethyldecahydronaphthalen-1-yl) acetohydrazide, malononitrile and dimethyl but-2-ynedioate in ethanol at room temperature. Colorless monocrystals of the obtained products belong to centrocymmetric monoclinic space group $P2_1/c$, a=8.8928(4), b=17.5289(5), c=11.7569(4) Å, β =90.538(4)°, v=1832.6(1) ų, thus represent a racemate. Single crystal X-ray analysis has revealed that compounds with composition $C_{16}H_{11}N_5O_4 \cdot C_2H_5OH$ crystalizes in the form of solvate. In the structure center symmetry related molecules united in dimer due to couple of N–H···O hydrogen bonds (2.945(2) Å) between amid fragments of indoline-2-one moieties. Ethanol solvent molecules form O–H···O hydrogen bonds (2.849(2) Å) with dimer, Figure 1. The ether group is coplanar with pyrazole, the torsion angle O4-C-C-N5 equal 1.91°.

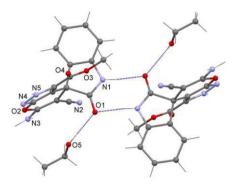


Figure 1. Fragment of crystal structure of methyl 6'-amino-5'-cyano-2-oxo-3'H-spiro [indoline-3, 4'-pyrano [2, 3-c] pyrazole]-3'-carboxylate ethanol solvate

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