

OH P 2

Sinteza, karakterizacija i antiproliferativna aktivnost novog tetrazolskog derivata henodeoksiholne kiseline

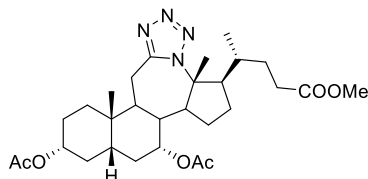
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Steroidni molekuli koji sadrže heterociklični prsten u svojoj strukturi ispoljavaju značajno antiproliferativno dejstvo. 1,5-Disupstituisani tetrazoli predstavljaju strukturne analoge *cis*-amidne grupe koji ne podležu metaboličkoj degradaciji¹. U ovom radu predstavljena je hemijska sinteza tetrazolskog derivata **1** iz holne kiseline. Jedinjenje je pored spektroskopskih tehnika karakterisano i rentgenostrukturnom analizom. U cilju boljeg uvida u osobine jedinjenja **1**, izvršena je analiza pomoću DFT metode.



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Synthesis, characterization and antiproliferative activity of chenodeoxycholic acid tetrazole derivative

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Steroidal compounds with a heterocyclic ring in their structure are exhibiting strong antiproliferative effects. 1,5-Disubstituted tetrazoles are metabolically stable structural analogs of *cis*-amide groups¹. In this work we present the chemical synthesis of tetrazole derivative **1** from cholic acid. Besides spectroscopy techniques, the structure of derivative **1** was determined by X-ray diffraction on monocrystal. In order to get a better insight into the characteristics of compound **1**, a computational study was performed using a DFT method.

1. Ostrovskii V. A., et al.; *Russ. Chem Bull.* 61. (768-780) 2012.