Chemical Sciences

Crystal Structure of 1-Ethyl-2′-(furan-2-carbonyl)-1′-(furan-2-yl)-1′,2′,5′,6′,7′,7a′-hexahydrospiro[indoline-3,3′-pyrrolizin]-2-one and molecular docking studies

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Abstract

The target compound, 1-ethyl-2′-(furan-2-carbonyl)-1′-(furan-2-yl)-1′,2′,5′,6′,7′,7a′-hexahydrospiro [indoline-3,3′-pyrrolizin]-2-one (**1**), was efficiently and diastereoselectively synthesized *via* a one-pot multicomponent 1,3-dipolar cycloaddition reaction. The structure of the compound **1** was determined by IR, ^{1}H NMR, ^{13}C NMR, Mass spectrometry and single crystal X-ray diffraction method. The compound **1** crystallizes in the centrosymmetric monoclinic *P*21/*n* space group with unit cell parameters *a* = 13.9675(10) Å, *b* = 9.1490(6) Å, *c* = 16.6482(14) Å, *β* = 104.529(4)° and a cell volume of 2059.42 Å3. The crystal structure shows the formation of two-dimensional (2D) layered structure. Each 2D layer was formed by individual enantiomers of the compound **1**. In silico docking studies were carried out to evaluate anti-mycobacterial, anti-microbial and anti-cancer activities using corresponding proteins by using AutoDock Tools version 1.5.6 and AutoDock version 4.2.5.1 docking program. The compound **1** showed good activity against the proteins of mycobacterium tuberculosis (1V10 = − 8.49 kcal/mol), bacterial (4MIO = − 8.64 kcal/mol) and moderate activity against cancer protein (4L9K = − 3.63 kcal/mol).

Keywords: 1,3-Dipolar cycloaddition, Spirooxindolopyrrolizidines, *N*-Ethyl isatin, Crystal structure, Molecular docking studies.