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Synthesis, Crystal Structure and Tumoricidal Activity of a Novel Pyran Annulated Heterocyclic Compound

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SUMMARY. A novel pyran annulated heterocyclic compound (**4**) was synthesized by the three-component condensation of 1,1-dimethyl-3,5-cyclohexanedione, 4-chlorobenzaldehyde, and malononitrile in the presence of catalytic amount of 4-(dimethylamino)pyridine (DMAP). Its chemical structure was determined by X-ray single-crystal diffraction. It crystallizes in monoclinic, space group $P2_1/n$ with a = 9.417(3) Å, b =16.806(5) Å, c = 10.908(4) Å, β = 112.141(4)º, V = 1599.1(9) Å^3, Z = *4*, F(000) = 688, Dc = 1.366 Mg/m^3, M_r = 328.10, μ = 0.250 mm^{-1}, λ = 0.71073 Å, the final R = 0.0380 and ωR = 0.1022 for 2599 observed reflections with $I > 2\sigma(I)$. The compound was studied subsequently for the bladder urothelial cancer cell tumoricidal activity, and it was found that the compound has LD50 value of 196 μM.

RESUMEN. Un novedoso compuesto heterocíclico pirano anulado (**4**) se sintetizó por la condensación de tres componentes de 1,1-dimetil-3,5-ciclohexanodiona, 4-clorobenzaldehído, y malononitrilo en presencia de una cantidad catalítica de 4- (dimetilamino) piridina (DMAP). Su estructura química se determinó por difracción simple de rayos X. Cristaliza en grupo espacial monoclínico $P2_1/n$ con a = 9,417 (3) Å, b = 16,806 (5) Å, c = 10,908 (4) Å, β = 112,141 (4) º, V = 1599,1 (9) A^3 , Z = 4, F (000) = 688, Dc = 1,366 Mg / m^3, M_r = 328,10, μ = 0,250 mm^{-1}, λ = 0,71073 Å, R final = 0,0380 y ωR = 0,1022 para 2599 reflexiones observadas con $I > 2\sigma(I)$. El compuesto se estudió posteriormente para la actividad tumoricida de células de cáncer urotelial de la vejiga, y se encontró que tiene un valor de DL50 de 196 μM.

KEY WORDS: Crystal structure, Pyran, Tumoricidal.

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