

Synthesis and Evaluation of a Novel Heterocyclic Compound against Pediatric Hepatoblastoma Cells

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SUMMARY. The new heterocyclic compound idelalisib mono-methanol and mono-hydrate (**1**), designed using 2-fluoro-6-nitro-benzonic acid as start material, was successfully obtained via multiple synthesis route and finally characterized by IR, ¹H NMR, and single crystal X-ray crystallography. In addition, the antitumor effects of the title compound **1** was studied on three pediatric hepatoblastoma cell lines (HepG2, HuH-6 and Hep-3B). The results showed that compared with the positive reference drug carboplatin, compound **1** displayed efficient anti-tumor activity.

RESUMEN. El nuevo compuesto heterocíclico idelalisib mono-metanol y monohidrato (**1**), diseñado utilizando ácido 2-fluoro-6-nitro-benzónico como material de partida, se obtuvo satisfactoriamente por vía de síntesis múltiple y finalmente se caracterizó por IR, ¹H NMR y cristalografía de rayos X de monocristal. Además, se estudiaron los efectos antitumorales del compuesto **1** en tres líneas celulares de hepatoblastoma pediátrico (HepG2, HuH-6 y Hep-3B). Los resultados mostraron que en comparación con el fármaco de referencia carboplatino, el compuesto **1** mostró una actividad antitumoral eficaz.

KEY WORDS: antitumor activity, heterocycles, single crystal.

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