

Novel Naphthol Derivatives: Synthesis, Docking Studies and Inhibiting Human Glioma Cells

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SUMMARY. The synthesis and characterization of four novel naphthol derivatives (1-4) were realized by means of IR, ¹H NMR, HRMS and single crystal X-ray crystallography. The anticancer activity of these compounds were investigated against four human glioma cell lines (U251, SHG-44, U87 and T98G) by MTT assay. In addition, the relationship between activity and structure of these compounds was further investigated through molecular docking study.

RESUMEN. La síntesis y caracterización de cuatro nuevos derivados de naftol (1-4) se realizó mediante IR, ¹H NMR, HRMS y cristalografía de rayos X de cristal único. La actividad anticancerígena de estos compuestos se investigó contra cuatro líneas celulares de glioma humano (U251, SHG-44, U87 y T98G) mediante ensayo de MTT. Además, la relación entre la actividad y la estructura de estos compuestos se siguió investigando a través del estudio de acoplamiento molecular.

KEY WORDS: glioma cell, molecular docking, naphthol, X-ray.

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