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Anti-cancer Activity and Docking Studies of Pyran Derivatives

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SUMMARY. **The synthesis and characterization of two novel pyran derivatives (1 and 2) were realized by means of IR, ^{1}H NMR, HRMS and single crystal X-ray crystallography. The anticancer activity of the two compounds were investigated against four human cancer cell lines (GES-1, SGC-7901, BGC-823 and MGC-803) by MTT assay. In addition, the relationship between activity and structure of the two compounds was further investigated through molecular docking study.**

RESUMEN. La síntesis y caracterización de dos nuevos derivados de pirano (1 y 2) se realizaron mediante IR, ^{1}H NMR, HRMS y cristalografía de rayos X de cristal único. La actividad anticancerígena de los dos compuestos se investigó contra cuatro líneas celulares cancerosas humanas (GES-1, SGC-7901, BGC-823 y MGC-803) mediante ensayo de MTT. Además, la relación entre la actividad y la estructura de los dos compuestos se siguió investigando a través del estudio de acoplamiento molecular.

KEY WORDS: cancer cell, molecular docking, pyran, X-ray.

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