

Crystal Structure and Anti-lung Cancer Activity of Novel Pyran Derivatives from Traditional Chinese Medicine

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SUMMARY. Six novel pyran derivatives (1-6) were prepared starting from 3,5-cyclohexanedione (or 1,1-dimethyl-3,5-cyclohexanedione) and aromatic aldehydes. The structures of the products were determined on the basis of IR, ¹H NMR, HRMS, and single crystal X-ray crystallography. The prepared compounds were screened for their antitumor activity against four human lung cancer cell lines, namely, Calu-3, LTEP, MSTO-211H and H1299 and compounds 4-6 showed promising activity.

RESUMEN. Se prepararon seis nuevos derivados de pirano (1-6) partiendo de 3,5-ciclohexanodiona (o de 1,1-dimetil-3,5-ciclohexanodiona) y aldehídos aromáticos. Las estructuras de los productos se determinaron sobre la base de IR, ¹H RMN, HRMS y cristalografía de rayos X de cristal único. Los compuestos preparados se ensayaron por su actividad antitumoral contra cuatro líneas celulares de cáncer de pulmón humano, a saber, Calu-3, LTEP, MSTO-211H y H1299 y los compuestos 4-6 mostraron actividad prometedora.

KEY WORDS: crystal structure, lung cancer, pyran.

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