

A New Microporous Er(III) Metal-Organic Framework for 5-Fu Loading and Inhibiting Human Glioma Cells

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SUMMARY. A new microporous metal-organic framework, $\{[Er(TATB)](DEF)_2(H_2O)]_n$ (1, DEF = *N,N*-Diethylformamide), was synthesized under a solvothermal condition by using the 4,4',4''-s-triazine-2,4,6-triyl-tribenzoate (H_3TATB) as the organic bridging ligand. The efficient encapsulation of an anticancer drug 5-fluorouracil (5-Fu) on the desolvated 1 (1a) has been studied by grand canonical Monte Carlo (GCMC) simulation. In addition, *in vitro* anticancer activity of compounds 1 and 5-Fu loaded 1a have also been evaluated using MTT assay.

RESUMEN. Un nuevo marco microporoso metalorgánico, $\{[Er(TATB)](DEF)_2(H_2O)]_n$ (1, DEF = *N,N*-diethylformamida), se sintetizó en condiciones solvotermales utilizando 4,4',4''-s-triazin-2,4,6-triil-tribenzoato (H_3TATB) como el ligando puente orgánico. La encapsulación eficaz de un fármaco anticancerígeno 5-fluorouracilo (5-Fu) en el 1 desolvatado (1a) se ha estudiado mediante la simulación de Grand Carlo Canonical (GCMC). Además, la actividad anticancerosa *in vitro* de los compuestos 1 y 5-Fu cargado 1a también se han evaluado usando el ensayo MTT.

KEY WORDS: glioma, *in vitro*, metal-organic framework.

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