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A New 3D Ba(II)-Based Metal-Organic Framework as Anticancer Drug 5-Fu Carrier and Anti-Liver Cancer Study

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SUMMARY. The solvothermal reactions of barium nitrate and 4,4',4''-(1,3,5-triazine-2,4,6-triyl)tribenzoic acid (H_3TATB) in a mixed solvent of N,N-Dimethyl formamide (DMF) and H_2O at 120 °C leads to the formation of a new Ba(II)-based coordination polymer Ba(HTATB)(H_2O)](DMF)$_2$ (**1**) based on the ligand as a C_3 symmetric 3-connected organic node and the Ba^{2+} ion as 5-connected node. 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, the MTT assay method was assessed the ability of this drug delivery system on liver cancer HepG2 cells as well as the cytotoxicity of the carrier, which show that this drug loaded system exhibits very high biocompatibility and, hence, is promising as intracellular drug delivery carriers.

RESUMEN. Las reacciones solvotermales del nitrato de bario y el ácido 4,4',4''-(1,3,5-triazina-2,4,6-triil) tribenzoico (H_3TATB) en un disolvente mixto de N,N-dimetil formamida (DMF) y H_2O a 120 °C conduce a la formación de un nuevo polímero de coordinación basado en Ba (II) Ba (HTATB) (H_2O)] (DMF)$_2$ (**1**) basado en el ligando como un nodo orgánico C_3 simétrico conectado 3 y el ion Ba^{2+} como nodo 5-conectado. La encapsulación eficiente de un fármaco anticancerígeno 5-fluorouracilo (5-Fu) en el **1** desolvatado (**1a**) se ha estudiado mediante la simulación de Monte Carlo Grand Canonical (GCMC). Además, el método de ensayo MTT permitió evaluar la capacidad de este sistema de administración de fármacos en células HepG2 de cáncer de hígado, así como la citotoxicidad del transportador, que muestran que este sistema cargado de fármaco exhibe una biocompatibilidad muy alta y, por lo tanto, es prometedor como transportista intracelular de fármacos.

KEY WORDS: anticancer activity, coordination polymer, encapsulation, MTT assay.

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