

Incorporation of Anticancer Drug into a Cu(II)-based Porous Metal-organic Framework: Drug Delivery and Inhibiting Human Cervical Cancer Cells

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SUMMARY. A new robust microporous Cu(II)-based metal-organic framework with the formula of $[\text{Cu}_3(\text{TCPB})_2(\text{H}_2\text{O})_2] \cdot 8\text{DMA}$ (**1**, H_3TCPB = 1,3,5-tri(4-carboxyphenoxy)benzene) has been successfully synthesized by a one pot solvothermal reaction of a flexible tricarboxylic acid ligand with $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$. The structure of **1** has been well studied by single-crystal X-ray diffraction analysis and further characterized by elemental analysis, powder X-ray diffraction (PXRD), and thermogravimetric (TG) analyses. The efficient encapsulation of an anticancer drug 5-fluorouracil (5-Fu) on the desolvated **1** (**1a**) was studied by both of the drug delivery experiments and grand canonical Monte Carlo (GCMC) simulation. Furthermore, *in vitro* anticancer activity of compounds **1** and 5-Fu loaded **1a** were also evaluated using MTT assay.

RESUMEN. Un nuevo marco microporoso robusto a base de metal y de cobre (II) con la fórmula de $[\text{Cu}_3(\text{TCPB})_2(\text{H}_2\text{O})_2] \cdot 8\text{DMA}$ (**1**, H_3TCPB = 1,3,5-tri (4-carboxifenoxi) benceno) ha sido sintetizado con éxito mediante una reacción solvotermal de un recipiente de un ligando de ácido tricarbóxico flexible con $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$. La estructura de **1** ha sido bien estudiada por análisis de difracción de rayos X de monocristal y además caracterizada por análisis elemental, difracción de rayos X del polvo (PXRD) y análisis termogravimétrico (TG). La eficiente encapsulación de un fármaco anticancerígeno 5-fluorouracilo (5-Fu) en el **1** desolvatado (**1a**) se estudió mediante administración de fármacos y la simulación de Grand Carlo Canonical (GCMC). Además, la actividad anticancerosa *in vitro* de los compuestos **1** y **1a** 5-Fu cargado también se evaluaron usando el ensayo MTT.

KEY WORDS: anticancer activity, drug delivery, porous metal-organic framework.

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