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A New Microporous Ca(II) Metal-Organic Framework for 5-Fluorouracil Loading and Inhibition of Human Osteogenic Sarcoma Cells

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SUMMARY. **A** new three-dimensional porous coordination polymer with the formula of $[Ca_3(BTATB)_2(H_2O)_2](DMF)_3$ (**1**) has been solvothermally synthesized from 4,4',4''-(benzene-1,3,5-triyltris(azanediyl))tribenzoate (H3BTATB) and $Ca(NO_3)_2.4H_2O$ under DMF media and characterized by single crystal X-ray diffraction and elemental analysis. 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 on four human osteogenic sarcoma cell lines (MG63, HOS, U2OS and 143B) have also been evaluated using MTT assay.

RESUMEN. Un nuevo polímero de coordinación poroso tridimensional con la fórmula $[Ca_3(BTATB)_2(H_2O)_2](DMF)_3$ (**1**) ha sido sintetizado solvotérmicamente a partir de 4,4',4''-(benceno-1,3,5-triiltris(azanediil)) tribenzoato (H3BTATB) y $Ca(NO_3)_2.4H_2O$ en medios DMF y caracterizados por difracción de rayos X de cristal único y análisis elemental. La encapsulación eficaz del fármaco anticancerígeno 5-fluorouracilo (5-Fu) en el **1** (**1a**) desolvatado se ha estudiado mediante la simulación de Monte Carlo Gran Canónica (GCMC). Además, también se ha evaluado la actividad anticancerosa *in vitro* de los compuestos **1** y 5-Fu **1a** cargado en cuatro lineas celulares de sarcoma osteogénico humano (MG63, HOS, U2OS y 143B) usando el ensayo de MTT.

KEY WORDS: encapsulation, osteogenic sarcoma, three-dimensional, X-ray.

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