



A New Cu(II) Coordination Polymer: Crystal Structure and Treatment Activity on Non-Alcoholic Fatty Liver

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SUMMARY. In the current study, via using the mixed-ligand approach, a new Cu(II)-based coordination polymer (CP) with the chemical formula of $[\text{Cu}(\text{L})(\text{CTP})]_n$ (**1**) has been successfully hydrothermally synthesized by employing the halogenated linear ligand 2-chloroterephthalic acid (H_2CTP) and the flexible N-donor 1,2-bis(2-methylbenzimidazol-1-ylmethyl)benzene (**L**) as the co-ligands. Its treatment activity on the non-alcoholic fatty liver was determined and the related mechanism was explored at the same time. First of all, the western blotting assay was performed and the expression levels of the TAK1 in the liver cells was measured. Next, the relative expression levels of miRNA-191 were detected with real time RT-PCR. Analysis results that obtained from molecular docking simulation revealed that the detailed binding interactions between the Cu complex and the probe protein were mainly from the carboxyl groups.

RESUMEN. En el estudio actual, mediante el uso del enfoque de ligando mixto, se ha logrado hidrotérmicamente un nuevo polímero de coordinación (CP) basado en Cu(II) con la fórmula química de $[\text{Cu}(\text{L})(\text{CTP})]_n$ (**1**) sintetizado empleando el ligando lineal halogenado ácido 2-clorotereftálico (H_2CTP) y el donante N flexible 1,2-bis(2-metilbencimidazol-1-ilmetil)benceno (**L**) como co-ligandos. Se determinó su actividad de tratamiento sobre el hígado graso no alcohólico y al mismo tiempo se exploró el mecanismo relacionado. En primer lugar, se realizó el ensayo de transferencia Western y se midieron los niveles de expresión de TAK1 en las células hepáticas. A continuación, se detectaron los niveles de expresión relativa de miARN-191 con RT-PCR en tiempo real. Los resultados del análisis que se obtuvieron de la simulación de acoplamiento molecular revelaron que las interacciones de unión detalladas entre el complejo de Cu y la proteína sonda eran principalmente de los grupos carboxilo.

KEY WORDS: Coordination polymer, non-alcoholic fatty liver, molecular docking

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