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Crystal Structure and Treatment Activity of a New Cu(II)-Based Coordination Complex on *Candida* Vaginitis

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SUMMARY. In the present study, a new Cu(II)-based coordination complex with the chemical formula of $[Cu_4(L)_4]\cdot(H_2O)$ (**1**) has been successfully prepared by reaction of copper perchlorate hexahydrate with the Schiff base ligand of (E)-2-(((1-hydroxypropan-2-yl)imino)methyl)phenol (H_2L) under a slow evaporation reaction condition. Its application values on the *Candida* vaginitis were evaluated and the related mechanism was explored at the same time. Firstly, the ELISA detection was conducted for the measurement of the inflammatory cytokines released into the vagina. In addition to this, the real time RT-PCR was conducted and the relative expression levels of the *Candida albicans* survival genes was determined. Molecular docking simulation confirmed that only moderate activities can be observed since all polar sites on the Cu complex are intrinsically binding with the Cu ion.

RESUMEN. En el presente estudio se preparó con éxito un nuevo complejo de coordinación basado en Cu (II) con la fórmula química de $[Cu_4(L)_4]\cdot(H_2O)$ (**1**) mediante la reacción de perclorato de cobre hexahidrato con el ligando de base de Schiff de (E)-2-(((1-hidroxipropan-2-il)imino)metil) fenol (H_2L) en condiciones de reacción de evaporación lenta. Se evaluaron sus valores de aplicación en la vaginitis por *Candida* y al mismo tiempo se exploró el mecanismo relacionado. En primer lugar, se realizó la detección ELISA para medir las citocinas inflamatorias liberadas en la vagina. Además de esto, se realizó la RT-PCR en tiempo real y se determinaron los niveles de expresión relativa de los genes de supervivencia de *Candida albicans*. La simulación de acoplamiento molecular confirmó que solo se pueden observar actividades moderadas, ya que todos los sitios polares en el complejo de Cu se unen intrínsecamente al ion Cu.

KEYWORDS: Coordination complex, *Candida* vaginitis, Molecular docking

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