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A Mixed-Ligand Mn(II)-Coordination Polymer: Protective Activity on the Renal Calculus via Reducing the Ca^{2+} Concentration in Urine

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SUMMARY. Based on the designed tripodal linker 1,3,5-tris(2-methylimidazol-1-yl)benzene (timb), a new Mn(II) coordination polymer with the chemical formula of $\{Zn_3(timb)_2(SO_3\text{-}IPA)_2(H_2O)_2]\cdot 8H_2O\}_n$ (**1**), has been obtained by reaction of the $Zn(NO_3)_2\cdot 6H_2O$ with the timb ligand in the presenceof the $-SO_3$ group functionalized isophthalic acid (H_2IPA) ligand. For the treatment of renal calculus, serial experiments were conducted for the activity evaluation and mechanism exploration. First of all, the concentration of Ca^{2+} in urine was determined with Calcium Colorimetric Assay. In addition to this, the expression levels of the osteopontin (OPN) in the distal tubule was measured with western blotting assay. Molecular docking simulation found that the sulfonic and carboxyl functional groups have the strong activities, however, the five-membered ring containing nitrogen only has medium binding activity.

RESUMEN. Basado en el ligante trípode diseñado 1,3,5-tris(2-metilimidazol-1-il) benceno (timb), se ha obtenido un nuevo polímero de coordinación de Mn (II) con la fórmula química de $\{Zn_3(timb)_2(SO_3\text{-}IPA)_2(H_2O)_2]\cdot 8H_2O\}_n$ (**1**), por reacción del $Zn(NO_3)_2\cdot 6H_2O$ con el ligando timb en presencia del ligando ácido isoftálico funcionalizado con grupo $-SO_3$ (H_2IPA). Para el tratamiento del cálculo renal, se realizaron experimentos en serie para la evaluación de la actividad y la exploración del mecanismo. En primer lugar, se determinó la concentración de Ca^{2+} en orina con el ensayo colorimétrico de calcio. Además de esto, se midieron los niveles de expresión de la osteopontina (OPN) en el túbulo distal con un ensayo de transferencia Western. La simulación de acoplamiento molecular encontró que los grupos funcionales sulfónico y carboxilo tienen las actividades más fuertes; sin embargo, el anillo de cinco miembros que contiene nitrógeno sólo tiene una actividad de unión media.

KEY WORDS: mixed-ligand, Mn(II)-coordination polymer, molecular docking, renal calculus, Zn(II)-complex.

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