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A Co(II)-Coordination Polymer: Treatment Activity on Fracture by Regulating the Activation of Wnt Signaling Pathway

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SUMMARY. A phosphonic acid ligand, 4-(4H-1,2,4-triazol-4-yl)phenylphosphonic acid (H3ptz) featuring both phosphonic and triazole donor groups was used as a linker to construct a metal coordination polymer (CP), $[(CoHptz)]_n$ (**1**) in the mixed solvents of *N,N*-dimethylformamide (DMF), isopropanol, and water with the presence of a small amount of hydrofluoric acid (40% solution). The treatment activity of the compound on the fracture was evaluated, and the related mechanism was explored. Firstly, the fracture animal model was constructed and the relative expression level of cd133 was evaluated with real time RT-PCR. Next, the western blotting was performed and the activation level of the wnt signaling pathway in the mesenchymal stem cells was determined. Furthermore, molecular docking simulations indicate that the five-membered ring containing nitrogen atom to be the most relevant donators to the binding interactions.

RESUMEN. Se usó un ligando de ácido fosfónico, ácido 4-(4H-1,2,4-triazol-4-il) fenilfosfónico (H3ptz) que presenta grupos donantes tanto fosfónicos como triazólicos como un conector para construir un polímero de coordinación de metal (CP), $[(CoHptz)]_n$ (**1**) en los disolventes mixtos de *N,N*-dimetilformamida (DMF), isopropanol y agua con la presencia de una pequeña cantidad de ácido fluorhídrico (solución al 40%). Se evaluó la actividad de tratamiento del compuesto en la fractura y se exploró el mecanismo relacionado. En primer lugar, se construyó el modelo animal de fractura y se evaluó el nivel de expresión relativa de cd133 con RT-PCR en tiempo real. A continuación, se realizó la transferencia Western y se determinó el nivel de activación de la ruta de señalización de wnt en las células madre mesenquimales. Además, las simulaciones de acoplamiento molecular indican que el anillo de cinco miembros que contiene el átomo de nitrógeno es el donante más relevante para las interacciones de unión.

KEY WORDS: coordination polymer, fracture, molecular docking.

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