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Cu(II) Coordination Polymer: Crystal Structure and Application Values on Anesthesia Pain

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SUMMARY. By employment of a NOO-type tridentate Schiff base ligand ((2-hydroxybenzylidene)amino)benzoic acid (H_2L), a new one-dimensional Cu(II) coordination polymer, $[Cu2(H_2L)_2(MeOH)]_n$, have been synthesized and characterized by CHN analysis and single crystal X-ray diffraction study. Its application values on the anesthesia pain were evaluated and the related mechanism was explored at the same time. Although from the structural point view the Cu complex is a rigid ligand, however, the polar oxygen atoms could still form multiple interactions with probe protein and exhibit excellent biological capabilities, which has been revealed from molecular docking simulations.

RESUMEN. Mediante el empleo de un ligando de base de Schiff tridentado de tipo NOO (ácido (2-hidroxibenciliden)amino)benzoico (H_2L), un nuevo polímero de coordinación de Cu(II) unidimensional, $[Cu_2(H_2L)_2(MeOH)]_n$, ha sido sintetizado y caracterizado por análisis CHN y estudio de difracción de raos X monocristalino. Se evaluaron sus valores de aplicación sobre el dolor anestésico y al mismo tiempo se exploró el mecanismo relacionado. Aunque desde el punto de vista estructural el complejo de Cu es un ligando rígido, los átomos de oxígeno polares aún podrían formar múltiples interacciones con la proteína sonda y exhibir excelentes capacidades biológicas, lo que se ha revelado a partir de simulaciones de acoplamiento molecular.

KEY WORDS: anesthesia pain, coordination polymer, Cu(II)-complex, molecular docking, Schiff base ligand.

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