Latin American Journal of Pharmacy
(formerly *Acta Farmacéutica Bonaerense)*
Lat. Am. J. Pharm. **40** (9): 2086-91 (2021)

Received: June 22, 2021
Revised: July 17, 2021
Accepted: July 18, 2021

A Mixed-Ligand Co(II) Coordination Polymer: Anti-Breast Cancer Activity Through High Intensity Focused Ultrasound

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SUMMARY. In the current study, via using the mixed-ligand synthesis approach, a new Co(II) coordination polymer (CP) with the composition of $[Co(ip)(H_2L)(H_2O)]_n$ (**1**) (H_2L = 3-(1H-pyrazol-4-yl)-5-(pyridin-2-yl)-1,2,4-triazole, H_2ip = isophthalic acid) was constructed by solvothermal reaction. The treatment activity of the new compound on breast cancer was evaluated and the related mechanism was explored at the same time. Firstly, the viability of the breast cancer cells after compound treatment was measured with Cell Counting Kit-8. In addition to this, the apoptosis levels of the breast cancer cells were measured with Annexin V-FITC/PI apoptosis assay. It has been found by molecular docking simulation that the triazole on the complex is the underlying reason for the observed anti-cancer activities.

RESUMEN. En el estudio actual, mediante el uso del enfoque de síntesis de ligandos mixtos, un nuevo polímero de coordinación (CP) de Co (II) con la composición de $[Co(ip)(H_2L)(H_2O)]_n$ (**1**) (H_2L = 3-(1H-pyrazol-4-yl)-5-(pyridin-2-yl)-1,2,4-triazole, H_2ip = ácido isoftálico) se construyó mediante reacción solvotérmica. Se evaluó la actividad de tratamiento del nuevo compuesto sobre el cáncer de mama y al mismo tiempo se exploró el mecanismo relacionado. En primer lugar, se midió la viabilidad de las células de cáncer de mama después del tratamiento con el compuesto con Cell Counting Kit-8. Además de esto, los niveles de apoptosis de las células de cáncer de mama se midieron con el ensayo de apoptosis de Anexina V-FITC/PI. Se ha descubierto mediante simulación de acoplamiento molecular que el triazol en el complejo es la razón subyacente de las actividades anticancerígenas observadas.

KEY WORDS: Coordination complex, breast cancer, molecular docking

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ISSN 0326 2383 (printed ed.)
ISSN 2362-3853 (on line ed.)