



## Therapeutic Effect of a New Heterocyclic Compound on Neuropathic Pain Release and Predicted its Derivatives Based on Deep Learning Method

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**SUMMARY.** After getting the crystal structure of the new compound, its therapeutic effect and mechanism on neuropathic pain was evaluated and explored. The content of the inflammatory cytokines released into the cerebrospinal fluid was measured with ELISA assay. The real time RT-PCR was conducted and the activation of the NF- $\kappa$ B in the spinal glial cell was determined. Three drug molecules that have been selected from the deep learning framework show similar interaction mechanism as the title compound, since the compound has been used as the feed to the deep learning framework, thus, these selected drug molecules share common structural features with respect to the title compound.

**RESUMEN.** Después de obtener la estructura cristalina del nuevo compuesto, se evaluó y exploró su efecto terapéutico y mecanismo sobre el dolor neuropático. El contenido de citocinas inflamatorias liberadas en el líquido cefalorraquídeo se midió con ensayo ELISA. Se realizó la RT-PCR en tiempo real y se determinó la activación del NF- $\kappa$ B en la célula glial espinal. Tres moléculas de fármaco que se han seleccionado del marco de aprendizaje profundo muestran un mecanismo de interacción similar al del compuesto del título, ya que el compuesto se ha utilizado como alimento para el marco de aprendizaje profundo, por lo tanto, estas moléculas de fármaco seleccionadas comparten características estructurales comunes con respecto al compuesto del título.

**KEY WORDS:** deep learning, heterocyclic, neuropathic pain.

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