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Short communication

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Metabolic Interference of Bruceantinol towards Cytochrome P450 (CYP) 2C9-Catalyzed Metabolism of Propofol

Cui-Yan XING [1 # *], Hong-Yan LIU [2 #], & Ming-Yi WU [3,4]

[1] *Department of Anesthesiology, Provincial Hospital Affiliated to Shandong University, No. 324, Jingwu Road, Jinan, 250021, Shandong, China*
[2] *Department of Anesthesiology, Jinan Third People's Hospital of Shandong Province, Jinan, Shandong, China*
[3] *Department of Pain, Provincial Hospital Affiliated to Shandong University, No. 324, Jingwu Road, Jinan, 250021, Shandong, China*
[4] *Department of Anesthesiology, Armed Police Corps Hospital of Shandong Province, Shandong, China*

***SUMMARY*. Propofol is a commonly used anesthetic and sedative because of its short duration of action, rapid onset, and preferable side effects and recovery profiles. Bruceantinol is an important herbal ingredient possibly used for anesthetic and sedative utilization. The present study aims to predict metabolic interference of bruceantinol towards cytochrome P450 (CYP) 2C9-catalyzed metabolism of propofol. The crystal structure of CYP2C9 was downloaded from protein data bank, and chemdraw software was employed to get the molecular structure of bruceantinol. Bruceantinol has good interaction with the binding site of CYP2C9, and the amino acids performing the interaction with bruceantinol were consisted of Val292, Gly296, and Thr301. To demonstrate the binding capability of bruceantinol towards the activity cavity of CYP2C9, bruceantinol was co-docked with the typical substrate warfarin. The results showed that bruceantinol exerted closer distance with the binding site than warfarin, indicating is a good substrate for CYP2C9. In conclusion, bioinformatics-guided molecular docking method was used to predict metabolic interference of bruceantinol towards cytochrome P450 (CYP) 2C9-catalyzed metabolism of propofol.**

RESUMEN. El propofol es un anestésico de uso común y sedante debido a su corta duración de acción, comienzo rápido, escasos efectos secundarios y buen perfil de recuperación, en tanto que el bruceantinol es un ingrediente vegetal importante utilizado como anestésico y sedante. El presente estudio tiene como objetivo predecir la interferencia metabólica del bruceantinol en el metabolismo del propofol catalizado por el citocromo P450 (CYP) 2C9. La estructura cristalina de CYP2C9 ha sido obtenida de bancos de datos de proteínas y el software ChemDraw fue empleado para obtener la estructura molecular del bruceantinol. El bruceantinol tiene buena interacción con el sitio de unión de CYP2C9 y los aminoácidos ácidos responsables de la interacción con bruceantinol son Val292, Gly296 y Thr301. Para demostrar la capacidad de unión de bruceantinol con el centro activo del CYP2C9, bruceantinol fue coacoplado con el sustrato típico warfarina. Los resultados mostraron que bruceantinol exhibe una distancia más cercana con el sitio de unión que la warfarina, indicando que bruceantinol es un buen sustrato para CYP2C9. En conclusión, se utilizó el método de acoplamiento molecular bioinformático guiado para predecir la interferencia metabólica de bruceantinol hacia citocromo P450 (CYP) 2C9, que cataliza el metabolismo del propofol.

KEY WORDS: anesthetic, bruceantinol, cytochrome P450 (CYP) 2C9, drug-drug interaction, molecular docking, propofol.

* Author to whom correspondence should be addressed. E-mail: xingcuiyanjinan@126.com
\# These authors contributed equally to the present article.

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