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Molecular Docking to Predict the Metabolic Site of Corynoline and the Possible Drug-Drug Interaction

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***SUMMARY*. Corynoline, an important isoquinoline alkaloid isolated from the genus *Corydalis,* has been reported to exhibit multiple biochemical and pharmacological activities, including inhibition of cell adhesion, acetylcholinesterase inhibition activity, the cytotoxic toxicity, and liver protection roles. The metabolism of corynoline by CYP3A4 and its inhibition towards CYP3A4 have been reported, however, the metabolic site and inhibition mechanism remain unclear. The present study aims to investigate the metabolic site using molecular docking. CYP3A4 was used as receptor without any constraint during the calculations. The results showed methylenedioxyphenyl (MDP) group was closer with heme than other groups in the structure of corynoline, indicating that methylenedioxyphenyl group is the most possible group undergoing CYP3A4-mediated metabolism. Furthermore, corynoline was inserted into the binding site of ketoconazole which has been widely accepted as the strong competitive inhibitor. The similar binding behaviour between corynoline and ketoconazole indicated the potential mechanism for the drug-drug interaction between corynoline and other drugs mainly undergoing CYP3A4-mediated metabolism. All these results facilitate the deep understanding of the metabolic behaviour of corynoline and its inhibitory behaviour towards CYP3A4.**

KEY WORDS: Corynoline, Cytochrome P450 (CYP) 3A4, Molecular docking.

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