hCYP3A4-IN-1

Cat. No.: HY-155141

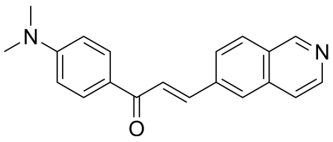
Molecular Formula: $C_{20}H_{18}N_2O$

Molecular Weight: 302.37

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

Storage: Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

hCYP3A4-IN-1 (compound C6) is a potent, orally active hCYP3A4 inhibitor. hCYP3A4-IN-1 shows the IC_{50} values of 43.93 nM and 153.00 nM against hCYP3A4 in human liver microsomes (HLMs) and CHO-3A4 stably transfected cell line, respectively. hCYP3A4-IN-1 potently inhibits CYP3A4-catalyzed N-ethyl-1,8-naphthalimide (NEN) hydroxylation in a competitive manner (Ki = 30.00 nM)[1].

IC_{50} & Target

CYP3A4
43.93 nM (IC_{50})

In Vivo

hCYP3A4-IN-1 (compound C6) exhibits suitable metabolic stability in HLMs and showed good safety profiles in mice[1].
hCYP3A4-IN-1 (100 mg/kg, orally administration, once) significantly increases the $AUC_{(0\text{-}inf)}$ of midazolam (i.e. 10 mg/kg) by 3.63-fold, and strongly prolonged its half-life by 1.66-fold compared with the vehicle group in mice[1].
Pharmacokinetic Parameters of hCYP3A4-IN-1 in mice[1].

	CMC-Na + Midazolam	C6 (25 mg/kg) + Midazolam	C6 (100 mg/kg) + Midazolam
T_{max} (min)	8.00 ± 2.74	5.83 ± 2.04	10.00 ± 0.00
C_{max} (ng/mL)	194.20 ± 138.88	312.00 ± 141.40	494.67 ± 210.22
$AUC_{0\text{-}24}$ (ng/mL*min)	7520.83 ± 2413.78	14784.92 ± 3501.33	27330.95 ± 6664.85
$t_{1/2}$ (min)	36.33 ± 14.46	54.96 ± 20.87	60.37 ± 27.67

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Lu S, et al. Design, synthesis and biological evaluation of chalcone derivatives as potent and orally active hCYP3A4 inhibitors. Bioorg Med Chem Lett. 2023 Aug 5:129435.

Caution: Product has not been fully validated for medical applications. For research use only.

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