CYP11B1-IN-2

Cat. No.: HY-151140

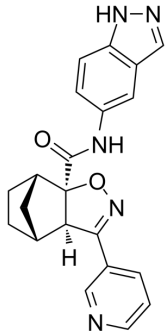
Molecular Formula: $C_{21}H_{19}N_5O_2$

Molecular Weight: 373.41

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

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



BIOLOGICAL ACTIVITY

Description

CYP11B1-IN-2 (compound 7aa) is an orally active, potent and selective CYP11B1 inhibitor, with IC_{50} values of 9 nM and 25 nM for human CYP11B1 and rat CYP11B1, respectively. CYP11B1-IN-2 can be used for the research of diseases caused by excessive cortisol[1].

IC_{50} & Target

CYP11B1 9 ± 2 nM (IC_{50}, human CYP11B1)	CYP11B1 25 nM (IC_{50}, rat CYP11B1)	CYP11B2 1121 ± 237 nM (IC_{50})	CYP1A2 >10 μM (IC_{50})
CYP2C9 >10 μM (IC_{50})	CYP2C19 >10 μM (IC_{50})	CYP2D6 >10 μM (IC_{50})	CYP2E1 >10 μM (IC_{50})
CYP3A4 >10 μM (IC_{50})			

In Vitro

CYP11B1-IN-2 (compound 7aa) exhibits good selectivity over a panel of hepatic CYP enzymes, such as CYP1A2, CYP2C9, CYP2C19, CYP3A4, CYP2D6, and CYP2E1 with IC_{50} values greater than 10 μM[1].

CYP11B1-IN-2 presents a cLog P of 3.12, indicating a good balance between lipophilicity and hydrophilicity, which was further manifested by an aqueous solubility of 196 μM[1].

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

In Vivo

CYP11B1-IN-2 (compound 7aa) (25 mg/kg, Orally, once) reduces plasma cortisol concentrations in rats[1].

CYP11B1-IN-2 (5 mg/kg (IV) or 25 mg/kg (Orally); once) has a maximum plasma concentration of 12 686 μg/L, with similar terminal half-lives of around 4.5 h[1].

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

Animal Model:	Adult Sprague-Dawley rats (male, 250-300 g)[1]
Dosage:	25 mg/kg
Administration:	Orally, once
Result:	Strongly reduced the plasma concentrations of cortisol from 376 ± 22 to 28 ± 5 ng/L after a dose of 25 mg/kg body weight per oral in rats.

Animal Model:	Adult Sprague-Dawley rats (male, 250-300 g)[1]
Dosage:	5 mg/kg (IV) or 25 mg/kg (Orally)
Administration:	IV or Orally, once
Result:	Pharmacokinetic Parameters of CYP11B1-IN-2 in male Sprague-Dawley rats[1].

	IV (5 mg/kg)	PO (25 mg/kg)
T_{max} (h)	0	4.2 ± 0.2
C_{max} (μg/L)	12 685.7 ± 421.3	7993.3 ± 478.7
$AUC_{0-\infty}$ (μg/L·h)	50 928.7 ± 982.6	54 539.2 ± 1633.9
$T_{1/2}$ (h)	4.5 ± 0.4	4.6 ± 0.2
CL (mL/h/kg)	17.2 ± 1.2	
F (%)		21.4

REFERENCES

[1]. Yin L, et al. Design, Synthesis, and Biological Evaluations of Pyridyl 4,5,6,7-Tetrahydro-4,7-Methanobenzo[d]isoxazoles as Potent and Selective Inhibitors of 11β-Hydroxylase. J Med Chem. 2022 Aug 17.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA