CYP1B1-IN-4

Cat. No.: HY-152118

CAS No.: 2685779-55-7

Molecular Formula: $C_{18}H_{14}N_2O_2S$

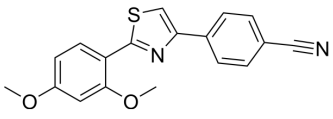
Molecular Weight: 322.38

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 62.5 mg/mL (193.87 mM; Need ultrasonic)

Preparing Stock Solutions	Concentration / Solvent / Mass	1 mg	5 mg	10 mg
	1 mM	3.1019 mL	15.5096 mL	31.0193 mL
	5 mM	0.6204 mL	3.1019 mL	6.2039 mL
	10 mM	0.3102 mL	1.5510 mL	3.1019 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

CYP1B1-IN-4 is a 2,4-diarylthiazole compound with selectively CYP1B1 inhibition (IC_{50}=0.2 nM). CYP1B1-IN-4 has little cytotoxicity and high stability in both human and rat liver microsomes[1].

IC_{50} & Target

CYP1B1	CYP1A1
0.2 nM (IC_{50})	3.98 μM (IC_{50})

In Vitro

CYP1B1-IN-4 (compound 15) (100 μM; 37 ⊠; 0-60 min) has in vitro stability in both human and rat liver microsomes, while it has low stability in mouse liver microsomes[1].

CYP1B1-IN-4 (1 nM-10 μM) also inhibits CYP1A1 with an IC_{50} value of 3.82 μM[1].

CYP1B1-IN-4 (200 μM; 72 h) parental HEK T-REx cell line , and (100 μ M; 72 h) has little cytotoxicity in HEK293 cells[1].

Stability Parameters in Human, Rat, or Mouse Liver Microsomes[1]

Parameters	$T_{1/2}$ (min)	$CL_{int(mic)}$ (μL/min/mg)	$CL_{int(liver)}$ (mL/min/kg)	% remaining$_{T=60\ min}$

Human	28.3	49.0	44.1	19.0
Rat	36.6	37.9	68.2	27.1
Mouse	2.5	545.9	2161.9	0.2

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

REFERENCES

[1]. Hachey AC, et al. Design of Cytochrome P450 1B1 Inhibitors via a Scaffold-Hopping Approach. J Med Chem. 2022 Dec 15.

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