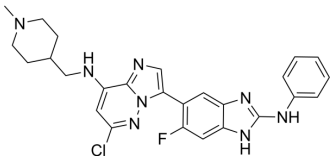
IRE1α kinase-IN-1

Cat. No.:	HY-136735
CAS No.:	2328097-41-0
Molecular Formula:	$C_{26}H_{26}ClFN_8$
Molecular Weight:	504.99
Target:	IRE1
Pathway:	Cell Cycle/DNA Damage

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 : 25 mg/mL (49.51 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9802 mL	9.9012 mL	19.8024 mL
	5 mM	0.3960 mL	1.9802 mL	3.9605 mL
	10 mM	0.1980 mL	0.9901 mL	1.9802 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (4.95 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.95 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

IRE1α kinase-IN-1 is a highly selective IRE1α (ERN1) inhibitor, with an IC_{50} of 77 nM. IRE1α kinase-IN-1 displays 100-fold selectivity for IRE1α over the IRE1β isoform. IRE1α kinase-IN-1 inhibits ER stress-induced IRE1α oligomerization and autophosphorylation, and also inhibits IRE1α RNase activity (IC_{50}=80 nM)[1].

In Vitro

IRE1α kinase-IN-1 (compound 31) prevents endoplasmic reticulum stress-induced IRE1α oligomerization and phosphorylation, and inhibits endoribonuclease activity in human cells[1].
?IRE1α kinase-IN-1 and is very high selectivity with >70% inhibition of only 4/455 kinases. IRE1α kinase-IN-1 inhibits recombinant G547 IRE1α KEN domain pS274 autophosphorylation with an IC_{50} of 160 nM. IRE1α kinase-IN-1 inhibits tunicamycin-induced GFP-IRE1α foci in HEK293 cells with an IC_{50} of 0.74 μM. IRE1α kinase-IN-1 Inhibits ATP-site LanthaScreen tracer binding to recombinant dephosphorylated G547 IRE1α KEN with an IC_{50} of 0.27 μM[1].

?IRE1α kinase-IN-1 inhibits both tunicamycin- and thapsigargin-induced IRE1α-dependent splicing of XBP1 luciferase fusion mRNA in HEK293 cells with IC_{50}s ranging 0.68-1.63 μM[1].
?IRE1α kinase-IN-1 (0-20 μM) inhibits IRE1α-dependent XBP1s mRNA expression in H929 cells.IRE1α kinase-IN-1 (0-20 μM) dose-dependently inhibits tunicamycin-induced expression of XBP1s in NCI-H929 cells[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Colombano G, et al. Binding to an Unusual Inactive Kinase Conformation by Highly Selective Inhibitors of Inositol-Requiring Enzyme 1α Kinase-Endoribonuclease. J Med Chem. 2019;62(5):2447-2465.

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

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