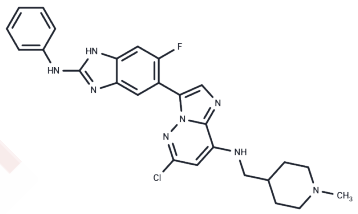
Data Sheet (Cat.No.T9564)

TargetMol

IRE1α kinase-IN-1

Chemical Properties



CAS No. : 2328097-41-0

Formula: C26H26ClFN8

Molecular Weight: 504.99

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	IRE1α kinase-IN-1 is a highly selective IRE1α (ERN1) inhibitor, with an IC50 of 77 nM, displaying 100-fold selectivity over the IRE1β isoform. It inhibits ER stress-induced IRE1α oligomerization and autophosphorylation, as well as IRE1α RNase activity (IC50=80 nM).
Targets(IC50)	IRE1
In vitro	IRE1α kinase-IN-1 (compound 31) effectively mitigates endoplasmic reticulum stress by hindering IRE1α oligomerization and phosphorylation, while also suppressing its endoribonuclease activity within human cells[1]. This compound demonstrates high specificity, showing greater than 70% inhibition for only 4 out of 455 kinases tested, indicating its select focus on IRE1α. It attenuates recombinant G547 IRE1α KEN domain pS274 autophosphorylation with an IC50 of 160 nM and disrupts ATP-site LanthaScreen tracer binding to the recombinant dephosphorylated G547 IRE1α KEN with an IC50 of 0.27 μM[1]. Additionally, it prevents tunicamycin-induced GFP-IRE1α foci formation in HEK293 cells with an IC50 of 0.74 μM and obstructs both tunicamycin- and thapsigargin-induced IRE1α-dependent XBP1 mRNA splicing, with IC50 values ranging from 0.68 to 1.63 μM in the same cell line[1]. In H929 and NCI-H929 cells, IRE1α kinase-IN-1 dose-dependently suppresses IRE1α-dependent XBP1s mRNA expression when applied at concentrations between 0 to 20 μM, demonstrating its potent inhibitory activity on tunicamycin-induced XBP1s expression[1].

Solubility Information

Solubility	DMSO: 77.5 mg/mL (153.47 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 7.75 mg/mL (15.35 mM),Solution. 10% DMSO+90% Saline: < 7.75 mg/mL (15.35 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.9802 mL	9.9012 mL	19.8024 mL
5 mM	0.396 mL	1.9802 mL	3.9605 mL
10 mM	0.198 mL	0.9901 mL	1.9802 mL
50 mM	0.0396 mL	0.198 mL	0.396 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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 Mar 14;62(5):2447-2465.