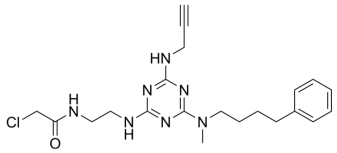
KSC-34

Cat. No.:	HY-117570
CAS No.:	2226201-97-2
Molecular Formula:	$C_{21}H_{28}ClN_7O$
Molecular Weight:	429.95
Target:	PDI
Pathway:	Cell Cycle/DNA Damage; Metabolic Enzyme/Protease
Storage:	4°C, stored under nitrogen * In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (232.59 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3259 mL	11.6293 mL	23.2585 mL
	5 mM	0.4652 mL	2.3259 mL	4.6517 mL
	10 mM	0.2326 mL	1.1629 mL	2.3259 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 (5.81 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.81 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.81 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

KSC-34, a covalent modifier of protein disulfide isomerase A1 (PDIA1), is also a selective and potent a-site inhibitor of PDIA1 with an IC_{50} of 3.5 μM. KSC-34 displays a 30-fold selectivity for a domain over a′ domain and displays high selectivity for PDIA1 in complex proteomes with minimal engagement of other members of the PDI family[1]. KSC-34 is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.

IC_{50} & Target

IC50: 3.5 μM (a active site of PDIA1), 104.5 μM (a′ active site of PDIA1)[1]

In Vitro

KSC-34 is selective for PDIA1 over other members of the PDI family, and other cellular cysteine-containing proteins. KSC-34

contains a (4-phenylbutyl)methylamine diversity element for optimized binding to the active site of the a domain of PDIA1 with a chloroacetamide electrophile for covalent modification of C53 on PDIA1[1].

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

REFERENCES

[1]. Cole KS, et al. Characterization of an A-Site Selective Protein Disulfide Isomerase A1 Inhibitor. Biochemistry. 2018;57(13):2035-2043.

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