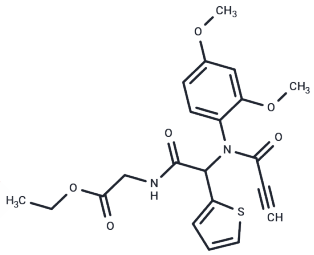
Data Sheet (Cat.No.T41277)

PACMA 31

Chemical Properties



CAS No. : 1401089-31-3

Formula: C21H22N2O6S

Molecular Weight: 430.47

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	PACMA 31 is an irreversible and covalent inhibitor of protein disulfide isomerase (PDI) with an IC50 of 10 μM. PACMA 31 significantly suppresses ovarian tumor growth and exhibits tumor targeting ability.
Targets(IC50)	Others
In vitro	In OVCAR-8 cells, PACMA 31 (0-10 μM) potently inhibits colony formation in a dose-dependent manner[1].
In vivo	In human ovarian cancer mouse xenografts, PACMA 31 (20-200 mg/kg) i.p. or per os administration of significantly inhibited tumor growth by 85% and 65% at day 62, respectively[1].

Solubility Information

Solubility	DMSO: 90.91 mg/mL (211.19 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: < 9.09 mg/mL (21.12 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 9.09 mg/mL (21.12 mM),Solution. *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	2.323 mL	11.6152 mL	23.2304 mL
5 mM	0.4646 mL	2.323 mL	4.6461 mL
10 mM	0.2323 mL	1.1615 mL	2.323 mL
50 mM	0.0465 mL	0.2323 mL	0.4646 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

Xu S, et al. Discovery of an orally active small-molecule irreversible inhibitor of protein disulfide isomerase for ovarian cancer treatment. Proc Natl Acad Sci U S A. 2012;109(40):16348-16353.