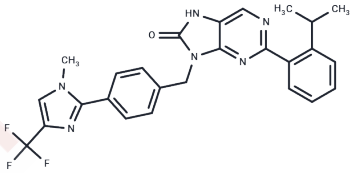
Data Sheet (Cat.No.T73560)

TargetMol

I-138

Chemical Properties



CAS No. : 2098211-50-6

Formula: C26H23F3N6O

Molecular Weight: 492.5

Storage: Store at low temperature,Keep away from direct sunlight
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	I-138 is an orally active and potent reversible inhibitor of USP1-UAF1.I-138 induces mono-ubiquitination of FANCD2 and PCNA and inhibits USP1 auto-cleavage in cells.
Targets(IC50)	DUB
In vitro	I-138 (0.5 μM; 4 hours) eliminates USP1 autodeubiquitination in HAP-1 USP1 WT and knockout cells, induces monoubiquitination of FANCD2 and PCNA in MDA-MB-436 cells, and dose-dependently (0.01-10 μM; 10 days) inhibits the viability of MDA-MB-436 cells without affecting HCC1954 cells[1].
In vivo	I-138 (50 mg/kg/day; oral administration; for 41 days) shows USP1 inhibition and moderate antitumor activity in mice with MDA-MB-436 tumors. However, combining I-138 with the PARP inhibitor Niraparib is more effective at inhibiting BRCA1/2 mutant tumors in vivo[1].

Solubility Information

Solubility	DMSO: 80 mg/mL (162.44 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: 3.3 mg/mL (6.7 mM),Sonication is recommended. *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	2.0305 mL	10.1523 mL	20.3046 mL
5 mM	0.4061 mL	2.0305 mL	4.0609 mL
10 mM	0.203 mL	1.0152 mL	2.0305 mL
50 mM	0.0406 mL	0.203 mL	0.4061 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

Simoneau A, et al. Ubiquitinated PCNA Drives USP1 Synthetic Lethality in Cancer. Mol Cancer Ther. 2023 Feb 1;22 (2):215-226.