

DI-591

Chemical Properties

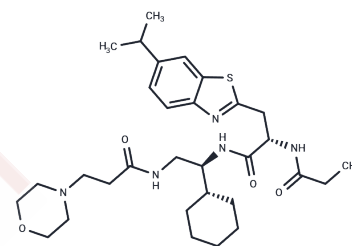
CAS No. : 2245887-38-9

Formula: C31H47N5O4S

Molecular Weight: 585.80

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	DI-591 is a potent, high-affinity, cell-penetrant inhibitor of the DCN1-UBC12 interaction. It binds to DCN1 and DCN2 with K_i values of 12 nM and 10.4 nM, respectively, while showing little to no binding to DCN3, DCN4, and DCN5. DI-591 selectively inhibits neddylation of cullin 3 without significant or only weak effects on other cullin family members.
Targets(IC50)	E1/E2/E3 Enzyme
In vitro	<p>Methods: In vitro binding assays were used to detect the binding affinity of DI-591 with DCN family proteins. Its effects on protein binding, downstream gene and protein expression were investigated in KYSE70 and THLE2 cells, respectively. The regulatory mechanism of cullin neddylation and NRF2 pathway was explored via knockdown experiments.</p> <p>Results: DI-591 bound to DCN1 and DCN2 with K values of 12 nM and 10.4 nM, respectively, and showed no obvious binding to DCN3-5. The selectivity for DCN1/2 over DCN3-5 was more than 1000-fold. DI-591 (0-10 μM, 1 h) bound to intracellular DCN1/2 in KYSE70 cells and disrupted the interaction between DCN1 and UBC12. Treatment of THLE2 cells with DI-591 (10 μM, 24 h) significantly upregulated mRNA levels of NQO1, HO1 and protein level of HO1, but had no effect on NRF2 mRNA. DI-591 selectively inhibited neddylation of Cullin 3, thereby promoting NRF2 protein accumulation and activating its transcription. Knockdown experiments revealed that DCN1 (but not DCN2) specifically regulated neddylation of Cullin 3. DI-591 can serve as a high-quality probe compound for studying the roles of Cullin 3-type CRL ubiquitin ligases in biological processes and human diseases [1].</p>

Solubility Information

Solubility	H2O: < 1 mg/mL (insoluble) DMSO: 10.00 mg/mL (17.07 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.7071 mL	8.5353 mL	17.0707 mL
5 mM	0.3414 mL	1.7071 mL	3.4141 mL
10 mM	0.1707 mL	0.8535 mL	1.7071 mL
50 mM	0.0341 mL	0.1707 mL	0.3414 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

Zhou H, et al. A potent small-molecule inhibitor of the DCN1-UBC12 interaction that selectively blocks cullin 3 neddylation. Nat Commun. 2017 Oct 27;8(1):1150.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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