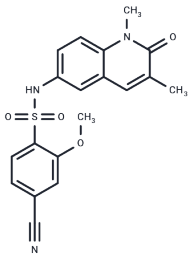
Data Sheet (Cat.No.TQ0083)

TargetMol

NI-57

Chemical Properties



CAS No. : 1883548-89-7

Formula: C19H17N3O4S

Molecular Weight: 383.42

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	NI-57 is an inhibitor of the bromodomain and plant homeodomain finger-containing (BRPF) family proteins, with IC50 values of 3.1 nM for BRPF1, 46 nM for BRPF2 (BRD1), and 140 nM for BRPF3.
Targets(IC50)	Epigenetic Reader Domain
In vitro	NI-57 binds the BRD of BRPF1 with a Kd of 31 nM, BRD1 with a Kd of 110 nM, and BRPF3 with a Kd of 410 nM, whereas binding to BRD9 is weaker (Kd 1000 nM) measured by isothermal titration calorimetry. NI-57 shows less active effect on BRD9 (IC50, 520 nM) and BRD4 (BD1) (IC50, 3700 nM), TRIM24 (IC50, 1600 nM). NI-57 also inhibits BRPF BRDs in the nucleus but shows little effect on the proliferation of many cancer cell lines with GI50s of 10.4 μM (NCI-H1703 cells), 14.7 μM (DMS114), 15.6 μM (HRA-19), and 16.6 μM (RERF-LC-Sq1). Furthermore, Inhibition on BRPF1 of NI-57 (10 μM) reduces the gene expression of CCL-22 by 27.7%.
Kinase Assay	All reagents are diluted in the recommended buffer (50 mM HEPES, 100 mM NaCl, 0.1% BSA; pH = 7.4) supplemented with 0.05% CHAPS and allowed to equilibrate to room temperature prior to addition to plates. 4 mL of HIS-tagged protein is added to low-volume 384-well plates, followed by 4 mL of either buffer, non-biotinylated peptide, solvent or compounds (NI-57, etc.). Plates are sealed and incubated at room temperature for 30 minutes, before the addition of 4 mL biotinylated peptide, resealing and incubation for a further 30 minutes. 4 mL of streptavidin-coated donor beads (25 μg/mL) and 4 μL of nickel chelate acceptor beads (25 μg/mL) are then added under low light conditions. Plates are foil-sealed to protect from light, incubated at room temperature for 60 minutes and read on a PHERAstar FS plate reader using an AlphaScreenTM 680 excitation/570 emission filter set. IC50s are calculated in GraphPad Prism 5. Results for compounds (NI-57, etc.) dissolved in DMSO are normalized against corresponding DMSO controls prior to IC50 determination, which is given as the final concentration of the compound in the 20 μL reaction volume.

Solubility Information

Solubility	DMSO: 80 mg/mL (208.65 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

In vivo Formulation	10% DMSO+90% Corn Oil: 3.3 mg/mL (8.61 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	2.6081 mL	13.0405 mL	26.0811 mL
5 mM	0.5216 mL	2.6081 mL	5.2162 mL
10 mM	0.2608 mL	1.3041 mL	2.6081 mL
50 mM	0.0522 mL	0.2608 mL	0.5216 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

Igoe N, et al. Design of a Chemical Probe for the Bromodomain and Plant Homeodomain Finger-Containing (BRPF) Family of Proteins. J Med Chem. 2017 Aug 24;60(16):6998-7011.