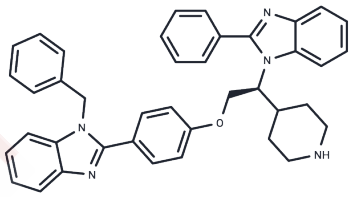
Data Sheet (Cat.No.T6462)

TargetMol

Deltarasin

Chemical Properties



CAS No. : 1440898-61-2

Formula: C40H37N5O

Molecular Weight: 603.75

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	Deltarasin is a small molecular inhibitor of KRAS-PDEδ interaction with Kd of 38 nM for binding to purified PDEδ.
Targets(IC50)	PDE,Ras
In vitro	In liver cells, Deltarasin inhibits the interaction of RAS with PDEδ with KD of 41 nM. Inhibition of PDEδ-KRAS interaction by Deltarasin suppresses proliferation of human pancreatic ductal adenocarcinoma cells that are dependent on oncogenic KRAS. [1]
In vivo	Deltarasin (10 mg/kg i.p.) impairs dose-dependent tumor growth in nude mice bearing subcutaneous human Panc-Tu-I tumor cell xenografts [1]. The finding may inspire novel drug discovery efforts aimed at the development of drugs targeting oncogenic RAS.
Kinase Assay	Kd?values are measured by fluorescence polarization measurements. For direct titrations, increasing amounts of PDEδ are added to a solution containing 50-100?nM labelled small molecule in 200?µL PBS buffer. For displacement titrations, increasing amounts of the small molecules in DMSO are directly added to fluorescein-labelled atorvastatin (24?nM) and His6-tagged PDEδ (40?nM) in 200?µL PBS-buffer (containing 0.05% CHAPS, 1% DMSO), keeping the concentration of fluorescein-labelled atorvastatin, PDEδ and DMSO constant. For Kd?measurements using isothermal titration calorimetry, PDEδ protein (280?µM) is titrated to small molecule (30?µM) in Tris/HCl buffer (temperature 25°C). In the Tm shift assays, protein melting points are detected by circular dichroism spectroscopy in the presence of small molecules.

Solubility Information

Solubility	H2O: < 1 mg/mL (insoluble or slightly soluble), Ethanol: 93 mg/mL (154.04 mM),Sonication is recommended. DMSO: 93 mg/mL (154.04 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: 2 mg/mL (3.31 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	1.6563 mL	8.2816 mL	16.5631 mL
5 mM	0.3313 mL	1.6563 mL	3.3126 mL
10 mM	0.1656 mL	0.8282 mL	1.6563 mL
50 mM	0.0331 mL	0.1656 mL	0.3313 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

Zimmermann G, et al. Nature. 2013, 497(7451), 638-642.