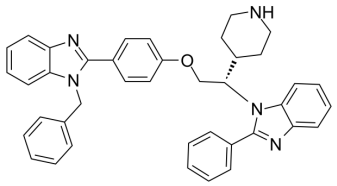
Deltarasin

Cat. No.:	HY-15747
CAS No.:	1440898-61-2
Molecular Formula:	$C_{40}H_{37}N_5O$
Molecular Weight:	603.75
Target:	Ras; Phosphodiesterase (PDE)
Pathway:	GPCR/G Protein; Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 12.5 mg/mL (20.70 mM; ultrasonic and warming and heat to 60°C)

H_2O : < 0.1 mg/mL (ultrasonic;warming;heat to 60°C) (insoluble)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
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

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 1.25 mg/mL (2.07 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 1.25 mg/mL (2.07 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.25 mg/mL (2.07 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	Deltarasin is an inhibitor of KRAS-PDEδ interaction with K_d of 38 nM for binding to purified PDEδ.
IC_{50} & Target	Kd: 38 nM (PDEδ)
In Vitro	In liver cells, deltarasin inhibits the interaction of RAS with PDEδ with K_d 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]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Deltarasin (10 mg/kg, i.p.) impairs dose-dependent tumor growth in nude mice bearing subcutaneous human Panc-Tu-I tumour cell xenografts[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Kinase Assay [1]	K_d 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 K_d 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. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Nat Commun. 2017 May 16;8:15205.
- J Med Chem. 2021 Dec 29.

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REFERENCES

[1]. Zimmermann G, et al. Small molecule inhibition of the KRAS-PDEδ interaction impairs oncogenic KRAS signalling. Nature. 2013 May 30;497(7451):638-42.

[2]. Agalioti T, et al. Mutant KRAS promotes malignant pleural effusion formation. Nat Commun. 2017 May 16;8:15205. doi: 10.1038/ncomms15205.

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