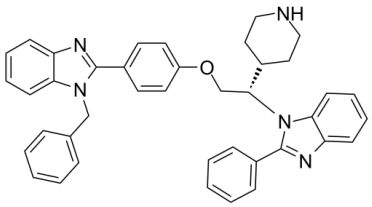
Data Sheet

Product Name:	Deltarasin
Cat. No.:	CS-1611
CAS No.:	1440898-61-2
Molecular Formula:	C40H37N5O
Molecular Weight:	603.75
Target:	Phosphodiesterase (PDE); Ras
Pathway:	GPCR/G Protein; Metabolic Enzyme/Protease
Solubility:	DMSO : ≥ 42 mg/mL (69.57 mM)



BIOLOGICAL ACTIVITY:

Deltarasin is an inhibitor of **KRAS-PDEδ** interaction with **K_d** of 38 nM for binding to purified PDEδ. IC50 & 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]. **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].

PROTOCOL (Extracted from published papers and Only for reference)

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.

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.

CAIndexNames:

1H-Benzimidazole, 2-[4-[(2S)-2-(2-phenyl-1H-benzimidazol-1-yl)-2-(4-piperidinyl)ethoxy]phenyl]-1-(phenylmethyl)-

SMILES:

C1(C2=CC=C(OC[C@@H](N3C4=CC=CC=C4N=C3C5=CC=CC=C5)C6CCNCC6)C=C2)=NC7=CC=CC=C7N1CC8=CC=CC=C8

Caution: Product has not been fully validated for medical applications. For research use only.

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