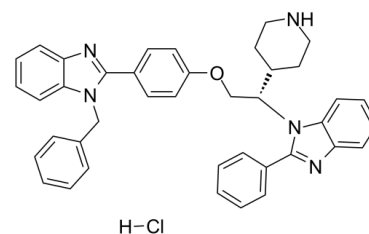


## Data Sheet

<b>Product Name:</b>	Deltarasin (hydrochloride)
<b>Cat. No.:</b>	CS-1748
<b>CAS No.:</b>	1613404-76-4
<b>Molecular Formula:</b>	C <sub>40</sub> H <sub>38</sub> ClN <sub>5</sub> O
<b>Molecular Weight:</b>	640.22
<b>Target:</b>	Phosphodiesterase (PDE); Ras
<b>Pathway:</b>	GPCR/G Protein; Metabolic Enzyme/Protease
<b>Solubility:</b>	DMSO : ≥ 52 mg/mL (81.22 mM); H <sub>2</sub> O : 50 mg/mL (78.10 mM); Need ultrasonic)



### BIOLOGICAL ACTIVITY:

Deltarasin hydrochloride is an inhibitor of **KRAS-PDEδ** interaction with  $K_D$  of 38 nM for binding to purified PDEδ. IC<sub>50</sub> & Target: K<sub>d</sub>: 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<sup>[1]</sup>. **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<sup>[1]</sup>.

### PROTOCOL (Extracted from published papers and Only for reference)

**Kinase Assay:** <sup>[1]</sup> $K_D$  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 T<sub>m</sub> 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.

### CAIndexNames:

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

### SMILES:

[H]Cl.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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