

Product Name: Deltarasin

Catalog No.: 5424

Batch No.: 1

CAS Number: 1440898-82-7

IUPAC Name: 2-[4-[(2S)-2-(2-Phenyl-1H-benzimidazol-1-yl)-2-(4-piperidinyl)ethoxy]phenyl]-1-(phenylmethyl)-1H-benzimidazole trihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₄₀H₃₇N₅O.3HCl.4H₂O

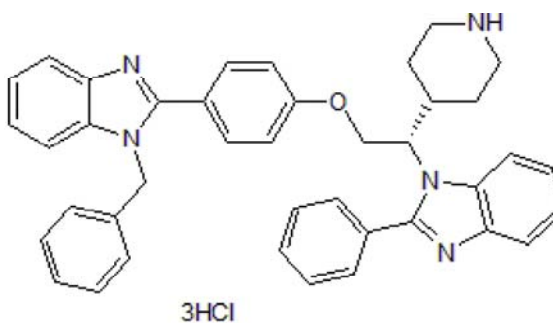
Batch Molecular Weight: 785.2

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

Chiral HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.19	6.16	8.92
Found	61.31	6.13	8.98

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

High affinity PDEδ-KRAS interaction inhibitor ($K_d = 41$ nM); binds to PDEδ. Reduces proliferation and induces cell death of KRAS-dependent Panc-Tu-1 and Capan-1 pancreatic cancer cells. Attenuates tumor growth of Panc-Tu-1 xenografts in mice.

Physical and Chemical Properties:

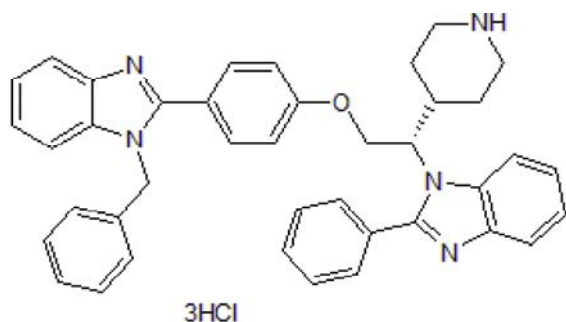
Batch Molecular Formula: $C_{40}H_{37}N_5O \cdot 3HCl \cdot 4H_2O$

Batch Molecular Weight: 785.2

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Zimmermann et al (2014) Structure guided design and kinetic analysis of highly potent benzimidazole inhibitors targeting the PDEδ prenyl binding site. *J.Med.Chem.* **57** 5435. PMID: 24884780.

Zimmermann et al (2013) Small molecule inhibition of the KRAS-PDEδ interaction impairs oncogenic KRAS signalling. *Nature* **497** 638. PMID: 23698361.

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