

Product Name: CRT 0066101

Catalog No.: 4975

Batch No.: 2

CAS Number: 1883545-60-5

IUPAC Name: 2-[4-[[*(2R)*-2-aminobutyl]amino]-2-pyrimidinyl]-4-(1-methyl-1*H*-pyrazol-4-yl)phenol dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₂N₆O.2HCl.H₂O

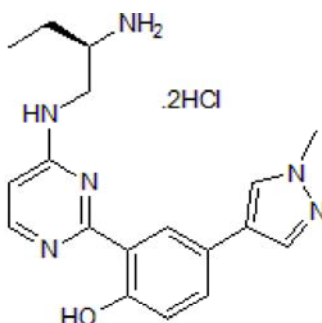
Batch Molecular Weight: 429.35

Physical Appearance: Yellow solid

Solubility: water to 100 mM
DMSO to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.35	6.1	19.57
Found	50.38	5.76	19.45

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

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Description:

Potent inhibitor of protein kinase D (PKD); inhibits all PKD isoforms (IC₅₀ values are 1, 2 and 2.5 nM for PKD1, PKD3 and PKD2 respectively). Exhibits selectivity for PKD against a panel of >90 protein kinases, including PKCα, MEK, ERK, c-Raf and c-Src. Reduces proliferation and cell viability of pancreatic cancer cells expressing moderate levels of endogenous PKD1/2. Orally bioavailable.

Physical and Chemical Properties:

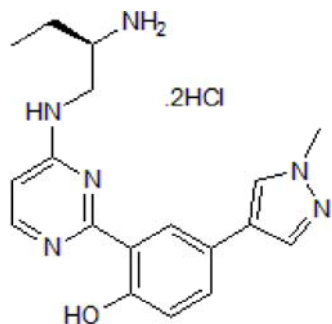
Batch Molecular Formula: C₁₈H₂₂N₆O.2HCl.H₂O

Batch Molecular Weight: 429.35

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Ni et al (2013) PKD1 mediates negative feedback of PI3K/Akt activation in response to G protein-coupled receptors. *PLoS ONE* **9** e73149. PMID: 24039875.

Harikumar et al (2010) A novel small molecule inhibitor of protein kinase D blocks pancreatic cancer growth *in vitro* and *in vivo*. *Mol.Cancer Ther.* **9** 1136. PMID: 20442301.

Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM

DMSO to 20 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.

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