

Product Name: CRT 0066854 hydrochloride

Catalog No.: 5922

Batch No.: 1

IUPAC Name: (2S)-3-Phenyl-N¹-[5,6,7,8-tetrahydro-2-(4-pyridinyl)[1]benzothieno[2,3-d]pyrimidin-4-yl]-1,2-propanediamine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₅N₅S.2HCl.½H₂O

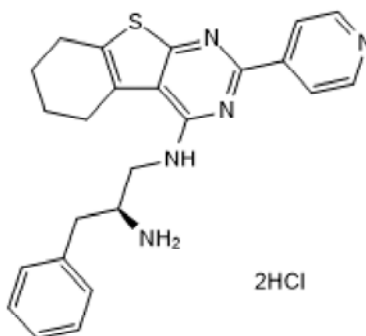
Batch Molecular Weight: 497.49

Physical Appearance: Yellow solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.48 (5% 7M ammonia in MeOH/DCM)

HPLC: Shows 99.4% purity

Chiral HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	57.94	5.67	14.08	14.25
Found	57.81	5.6	14.05	14.43

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Description:

Protein kinase C (PKC) inhibitor. Inhibits PKC_ι and PKC_ζ (IC₅₀ values are 132 and 639 nM, respectively). Restores polarized morphogenesis in oncogene expressing MDCK cells, decreases colony formation in HeLa cells and inhibits lethal giant larvae 2 (LLGL2) phosphorylation.

Physical and Chemical Properties:

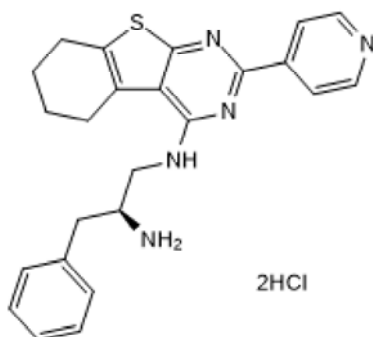
Batch Molecular Formula: C₂₄H₂₅N₅S.2HCl.½H₂O

Batch Molecular Weight: 497.49

Physical Appearance: Yellow solid

Minimum Purity: >98%

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:

Linch *et al* (2014) Regulation of polarized morphogenesis by protein kinase C iota in oncogenic epithelial spheroids. *Carcinogenesis* **35** 396. PMID: 24072773.

Kjaer *et al* (2013) Adenosine-binding motif mimicry and cellular effects of a thieno[2,3-d]pyrimidine-based chemical inhibitor of atypical protein kinase C isoenzymes. *Biochem.J.* **451** 329. PMID: 23418854.

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