

Product Name: A 419259 trihydrochloride

Catalog No.: 3914

Batch No.: 2

CAS Number: 1435934-25-0

IUPAC Name: 7-[*trans*-4-(4-Methyl-1-piperazinyl)cyclohexyl]-5-(4-phenoxyphenyl)-7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine trihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₉H₃₄N₆O.3HCl.3H₂O

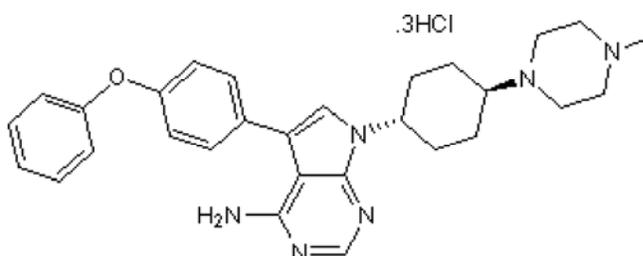
Batch Molecular Weight: 646.06

Physical Appearance: Off White solid

Solubility: water to 100 mM
DMSO to 20 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.46 (Chloroform:Methanol [75:25])

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.91	6.71	13.01
Found	53.97	6.54	12.92

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

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Description:

Potent Hck inhibitor (IC₅₀ = 0.43 nM). Also inhibits other Src family kinases (SFKs). Suppresses proliferation and induces apoptosis in CML cell lines including CD34⁺. Also inhibits acute myeloid leukemia (AML) stem cell proliferation in vitro and in vivo.

Physical and Chemical Properties:

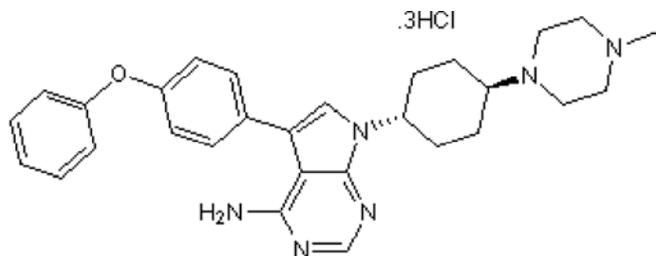
Batch Molecular Formula: C₂₉H₃₄N₆O.3HCl.3H₂O

Batch Molecular Weight: 646.06

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at RT

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.

References:

Saito *et al* (2013) A pyrrolo-pyrimidine derivative targets human primary AML stem cells *in vivo*. *Sci.Transl.Med.* **5**. PMID: 23596204.

Pene-Dumitrescu *et al* (2008) An inhibitor-resistant mutant of Hck protects CML cells against the antiproliferative and apoptotic effects of the broad spectrum Src family kinase inhibitor A-419259. *Oncogene* **27** 7055. PMID: 18794796.

Wilson *et al* (2002) Selective pyrrolo-pyrimidine inhibitors reveal a necessary role for Src family kinases in Bcr-Abl signal transduction and oncogenesis. *Oncogene* **21** 8075. PMID: 12444544.

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